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A 3D Lattice Boltzmann Code for Modeling Flow and Multi-Component Dispersion

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A 3D Lattice Boltzmann Code for Modeling Flow and Multi-Component Dispersion

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Abstract

This report documents the JB_PH lattice Boltzmann code, a program for modeling multi-component flow and dispersion. The lattice Boltzmann method is reviewed and methods are compared for increasing the efficiency of the algorithms. Accuracy of the code is tested with four benchmark problems: (1) permeability of a simple cubic array of spheres; (2) Taylor-Aris dispersion between infinite plates; (3) dispersion in a duct; and (4) dispersion in a simple cubic array of spheres. The memory and speed requirements of the method are assessed in the context of the benchmarks. The code structure and purpose of each major function are described, and instructions are given for compilation.

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1. Introduction

1.1 Motivation and Purpose

In the geosciences and biological sciences, and in chemical and thermal engineering, it is often desirable to perform accurate calculations of flow and dispersion in complex geometries. Most groundwater contaminants are dilute tracers, and dispersion describes the spreading of these tracers as aqueous and gaseous solutions move through porous and fractured rocks and soils. There is much interest in developing numerical methods that allow one to scale from microscopic flow at the scale of a pore or fracture, through the scale used in lab experiments, to flow on the scale of kilometers.^{1,2,3} Medical engineers attempt to model the dispersion of contaminants in the human lung,⁴ where nature imposes an inherent compromise on the Peclet number ($Pe \sim 100$); flow must be fast enough to ensure an adequate oxygen supply to the lungs, but not so fast that there is little time to exchange oxygen and carbon dioxide. In chemical engineering, solid catalysts are often in the form of porous beds, and the reaction of chemicals on the surfaces of the particles is influenced by the dispersion of solutes. To achieve the greatest efficiency, flows through the packed beds are often at modest to high Reynolds number (Re), a realm that is difficult to model by traditional methods. In thermal engineering, the forced cooling of a microprocessor on a circuit board typically involves flow through extremely complex geometries, and the removal of heat by diffusion and advective spreading, at Re and Pe numbers ~ 1000 . Current approaches to modeling these phenomena⁵ typically involve hybrid methods, grafting constant temperature flow fields onto simplified thermal models for the fluid solid interface. For such convoluted geometries with simultaneous flow and transport, direct, whole-system application of traditional methods, such as finite elements, is simply too costly or cumbersome.

This report describes the development of a 3D lattice Boltzmann (LB) method for modeling flow and dispersion through complex geometries at Re and Pe from 0 to ~ 1000 . The code is stable with arbitrarily complex solid-fluid interfaces, and in special cases, reaches site update rates of 2.6 million per second on a single-processor Pentium II computer. The accuracy and speed of the code have been tested for several geometries of increasing complexity. While these geometries are not as complex as catalytic beds, they are amenable to analytic solutions or comparisons with more conventional numerical methods and experiments.

1.2 The Lattice Boltzmann Method

The LB method breaks physical space into a large number of nodes or sites ($\approx 10^6$ in the simulations described in this report); at each node is a set of mass probability distributions. In each time step, the distributions translate from node to node along fixed velocity vectors, then undergo simple collisions that conserve physical properties such as momentum. The collision operator is designed so that the particle velocity distributions at each node obey the Navier Stokes equations and the advection-dispersion equations.

The LB method, and the BGK simplification, are well-described by Qian *et al.*⁶ The evolution of the particle distribution function f_i satisfies

$$f_i(\mathbf{x} + \mathbf{e}_i, t + 1) = f_i(\mathbf{x}, t) - (f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)) / \tau \quad (1)$$

where $\mathbf{x}$ is a node position in the lattice, $\mathbf{e}_i$ is one of i allowed velocities (e.g. $i=0,1,\dots,18$ in D3Q19 model⁶), t is the time step, f_i^{eq} is the equilibrium distribution, and τ is the BGK relaxation parameter, which determines the viscosity and diffusion coefficients. In typical LB computer programs, a translation or streaming function performs the left side Eq. (1), and a collision function performs the right side.

2. Computational Efficiency

For the dispersion of dilute tracers, the standard BGK method can be simplified, and programs can be substantially optimized. A single lattice can be used for a carrier fluid, which determines a velocity field $\mathbf{u}$ obeying the Navier-Stokes equations; typically we use the 19-vector D3Q19 lattice (figure 1) with the 2nd-order equilibrium distribution given by Martys and Chen:⁷

$$f_0^{eq} = \frac{\rho}{3} [1 - \frac{3}{2} u^2] \quad (2)$$

$$f_i^{eq} = t_i \rho [1 + 3\mathbf{e}_i \cdot \mathbf{u} + \frac{3}{2} (3\mathbf{e}_i \mathbf{e}_i : \mathbf{u}\mathbf{u} - u^2)] \quad \text{for } i \neq 0; \quad (3)$$

where $\rho = \sum_i f_i$, and $t_i = 1/18$ for the 6 vectors along the Cartesian axes, and $t_i = 1/36$ for the remaining vectors. The $\mathbf{u}$ determined from the carrier fluid is then used for each tracer. Flekkøy *et al.*⁸ and Noble⁹ noted the advection-dispersion equation is linear in $\mathbf{u}$, so the tracer equilibrium distributions need only be linear in $\mathbf{u}$ as well. For a tracer s , the equilibrium distribution is of the form:

$$f_{s,i}^{eq} = A + B(\mathbf{e}_{s,i} \cdot \mathbf{u}) \quad (4)$$

and the A and B are fixed by the requirement that solute be conserved ($\rho_s = \sum f_{s,i}^{eq}$), and the requirement that the solute flux at equilibrium is due entirely to advection ($\sum f_{s,i}^{eq} \mathbf{e}_{s,i} = \rho_s \cdot \mathbf{u}$). Compared to Eq. (3), Eq. (4) requires far fewer floating point operations.

Figure 1. The 19 vectors of the D3Q19 model. There is a “rest” particle at $(0,0,0)$, there are 6 vectors with weight $1/18^{\text{th}}$ along the cartesian axes, and 12 vectors with weight $1/36^{\text{th}}$ in the x - y , y - z and x - z planes.

Further savings are realized by using lattices with fewer vectors for the tracers; in 2D, 4 Cartesian vectors are adequate, and in 3D, the six Cartesian vectors will suffice. Wolf-Gladrow¹⁰ and others have suggested low-vector lattices for modeling diffusion, but Noble⁹ appears to have first performed a Chapman-Enskog expansion for Cartesian lattices, recovering the advection-dispersion equation and estimating the error term. (We emphasize that low-vector lattices, and Eq. (4), are used *only* for the dilute tracers, not the carrier.)

In many dispersion problems, $\mathbf{u}$ is at steady state, and need not be recalculated at each timestep. Furthermore, periodic boundary conditions on $\mathbf{u}$ are often appropriate, even when tracer dispersion is not periodic, as in the SC dispersion problem described in section 3. A strategy for such problems is to use a 19-vector carrier fluid in a single repeat unit, N_x by N_y by N_z lattice units on a side, then save the equilibrium $\mathbf{u}(x,y,z)$. The memory used for the 19-vector carrier fluid is then reclaimed, and reallocated for additional repeat units of the tracer lattices in the x direction. The velocity field at x,y,z is then $\mathbf{u}((x \text{ MOD } N_x), y, z)$.

The efficiency of the overall algorithm depends a great deal on the storage of the 3D lattice in memory. For systems that contain a high proportion of solids, it is often practical to store only those sites that represent open fluid or solids bounding fluid; a 3D pointer table obtains the location of the vectors in a linear array. Such an approach often leads to high locality, and can speed up the overall algorithm, by reducing the number of loads to the cache. For simplicity, we

focus here on data structures that allocate the same amount of memory to all sites, be they solid or fluid. We next consider the tradeoffs inherent in data structures that optimize for the translation vs. collision step.

Let indices s , i , z , y , and x represent, respectively, the chemical component, vector number (e.g. $i = 0$ through 18 in D3Q19), and the Cartesian directions. Two obvious alternative schemes (for coding in C) are:

```
float *****ff; /*arrays ff[s][i][z][y][x] */, and

typedef float site[NVELOC]; /* NVELOC = 19 or 6 for 3D */
site *****ff; /*arrays ff[s][z][y][x][i] */
```

The latter holds all the vectors (for a given x,y,z) close in memory, and might seem much more efficient. However, the first method can make the translation step very fast, principally because much of the translation is accomplished by pointer swaps. The efficiency is most significant for 3D, 6-vector tracers; only two of the six vectors are actually moved in memory, and those moves (in the $+$ and $-x$ directions) involve just one index and are easily optimized. The second method generates much cache traffic, and the translation step requires substantial effort to decompose and redistribute the vectors from each site. With all x86 compilers tested, the first method proved to be ~ 1.05 to 1.3 faster times than the second, and the discrepancy increased as the fraction of solids in the system increased.

Figure 2 gives simplified source code for a collision function involving just one 3D, 6-vector tracer and a predefined, static flow field uu . To lessen the burden of dereferencing 5-dimensional arrays, the pointers are dereferenced manually in steps, at the beginning of the inner loops. To ease the alias problem that plagues the C computer language, the 6 vectors for each site are copied into local $f0, f1, \dots, f5$ for most manipulations. The MOD operation is not performed explicitly, as the latter would involve a floating point division, which would consume $\sim 20\%$ of the CPU cycles. Finally, by factoring the f^{eq} equations, the number of arithmetic operations is greatly reduced. With judicious use of register declarations, the most important pointers and local variables can be kept in registers throughout the calculation, even on an Intel x86 chip.

```

/* f0=(1,0,0);f1=(0,1,0);f2=(-1,0,0);f3=(0,-1,0);f4=(0,0,1);f5=(0,0,-1) */
typedef float ff_t; typedef float u_t;
struct veloc_t { u_t x; u_t y; u_t z; u_t usqrd; } ***UU; [...]
/*****
/* Disperse ff[1] only as a 6-vector tracer; ff[0] is carrier fluid. */
void JustDisperse_1st_Tracer(ff_t ***** ff, double *const tau,
    struct veloc_t ***uu, char ***solid,
    int nz, int ny, int nx, int nx_rep)
{
    int z,y,x,xx;
    double ux, uy, uz, f0,f1,f2,f3,f4,f5; /* f's = 6-vector distribution */
    double rho, omega, beta, mux,muy,muz, mul, halfOmega, sixthOmega;
    ff_t *pf0,*pf1,*pf2,*pf3,*pf4,*pf5;
    ff_t **pf0z,**pf1z,**pf2z,**pf3z,**pf4z,**pf5z;

    struct veloc_t **uuzp, *uup;
    int solidcode;
    char **solidzp, *solidp;

    omega = 1.0/tau[1]; beta = 1.0 - omega;
    halfOmega=ONE_HALF*omega; sixthOmega=ONE_6TH*omega;

    for(z=0; z<nz; z++){
        uuzp = uu[z]; solidzp = solid[z]; /* deref outer pointers */
        pf0z = ff[1][0][z]; pf1z = ff[1][1][z]; pf2z = ff[1][2][z];
        pf3z = ff[1][3][z]; pf4z = ff[1][4][z]; pf5z = ff[1][5][z];
        for(y=0; y<ny; y++){
            solidp = solidzp[y];
            uup = uuzp[y]; /* deref inner pointers */
            pf0 = pf0z[y]; pf1 = pf1z[y]; pf2 = pf2z[y];
            pf3 = pf3z[y]; pf4 = pf4z[y]; pf5 = pf5z[y];
            for(x=xx=0; x<nx; x++,xx++,++pf0, ++pf1, ++pf2,
                ++pf3, ++pf4, ++pf5){
                if(xx==nx_rep) xx = 0; /* xx = x MOD nx_rep */
                solidcode = solidp[x];
                if(solidcode== -2) continue; /* completely surrounded */
                ux = uup[xx].x; uy = uup[xx].y; uz = uup[xx].z;
                rho = f0 = *pf0; rho += f1 = *pf1; rho += f2 = *pf2;
                rho += f3 = *pf3; rho += f4 = *pf4; rho += f5 = *pf5;
                if(solidcode){ /*bounce-back */
                    *pf0 = f2; *pf1 = f3; *pf2 = f0;
                    *pf3 = f1; *pf4 = f5; *pf5 = f4;
                    continue; /* on to next x */
                }
                mul = rho*halfOmega; /* implicit feq calc */
                mux = ux*mul; muy = uy*mul; muz = mul*uz;
                rho *= sixthOmega;
                /* put back the new f[] values */
                *pf0 = f0*beta + rho + mux;
                *pf1 = f1*beta + rho + muy;
                *pf2 = f2*beta + rho - mux;
                *pf3 = f3*beta + rho - muy;
                *pf4 = f4*beta + rho + muz;
                *pf5 = f5*beta + rho - muz;
            }
        }
    }
}
/* END JustDisperse_1st_Tracer() */

```

Figure 2. Simplified collision function for one 3D 6-vector tracer, $\partial u/\partial t = 0$.

Table 1 shows performance achievable on single-processor CPUs for several applications, given in units of MUPs (millions of site updates per second). For comparison, rates of 0.14 to 2 MUPs have been reported^{9,11} for 2- and 3-D calculations on a 64-node partition of the CM-5, containing 256 vector processors. This comparison is not intended to denigrate parallel computers. We estimate the 6-vector dispersion algorithms (2nd test problem, table 1) are nearing the RAM streaming limit, with speed controlled by the rate that site data can be fetched from and returned

to memory. In such conditions, it makes more sense to split the workload among many processors, rather than seek a faster CPU.

Table 1. Performance for LB algorithms (MUPs = Millions site Updates Per Second).

Processor	MUPs
<i>Test problem: 19-vector flow (no tracers), 50% solids</i>	
200 MHz Pentium Pro	0.29
400 MHz Pentium II	0.70
500 MHz alpha 21164a	1.10
<i>Test problem: 3D 6-vector tracer dispersion, steady flow field, 10% solids</i>	
200 MHz Pentium Pro	1.55
400 MHz Pentium II	2.55
<i>Test problem: 3D, 3-component double-diffusive fingering with buoyancy</i>	
200 MHz Pentium Pro	0.15
400 MHz Pentium II	0.30

The generation of “denormal” numbers can greatly degrade performance in LB dispersion calculations. Denormals are part of the IEEE 754 standard, and are used to provide gradual underflow, allowing one to represent numbers smaller than $\sim 10^{-37}$, the traditional lower limit of IEEE single precision.¹² Most microprocessors do not handle denormals in hardware; instead, they provide the option of either ignoring the IEEE standard, and rounding the denormal to 0, or they pass the value to a software routine for handling. Since the latter process can be excruciatingly slow, the compiler default is generally to round to 0. However the Intel x86 processors, such as the Pentium Pro, not only handle denormals in hardware, but provide no option to round these values to 0. Manipulations of denormals in x86 processors are slow, flushing the processor pipeline with each load. The problem can be delayed by using double precision, with a factor ~ 1.6 loss in initial speed and factor 2 loss of memory efficiency, and no gain in true accuracy for dispersion coefficients.

Slug dispersion problems have a strong tendency to generate denormal numbers. As a slug of solute travels downstream, very low concentrations are produced on the leading and trailing edges of the slug. In short order, the system contains many concentrations less than 10^{-37} . Benchmarks with dispersion around cylinder and sphere arrays showed up to a factor 6 performance loss within $\sim 10^4$ steps. This weakness of denormal processing was recognized by William Kahan, the principal architect of the IEEE standard, and a simple solution is given in his Berkeley lecture series (available on the world-wide-web as [ieee754.ps](#)): all initial and boundary conditions that are formally at 0 concentration, are set instead to a small number, say 10^{-32} . This artifice eliminates the slowdown, and has no effect on the calculated dispersion coefficients.

3. Accuracy

3.1 Permeability of a Simple Cubic Array of Spheres

The permeability of a simple cubic (SC) array of spheres, at low Re , is well known¹³ and provides a basic benchmark for testing pixelation effects and the applicability of LB to porous flow in single-component systems (i.e. systems that do *not* involve dispersion). The SC spheres are centered at the eight corners of a cube, as shown in figure 3; however, with wrap boundary conditions on opposing faces, a single sphere in a unit cube is adequate to model an infinite array. *Pixelation* refers to the representation of the sphere surface with a finite number of solid sites, so that the channels between the spheres appear somewhat jagged (figure 3). For non-overlapped spheres, the permeability k (units of length²) is related to the drag coefficient C_d via:

$$k = V / (6 \cdot \pi \cdot R \cdot C_d) \quad (5)$$

where V is the unit cell volume, and R is the sphere radius (e.g., Saeger et al.¹⁴). For Darcy flow,

$$k = -U \cdot \mu / (dP/dx) \quad (6)$$

where U is the superficial (or Darcy) fluid speed, averaged across an inlet or outlet face of the unit cell (including solids), μ is the dynamic viscosity, and dP/dx is the pressure gradient along the x -direction. Formally, the LB used in the present study is a constant-pressure model, so the pressure gradient must be related to the body force. To relate the permeability to units measured in the LB simulation, we apply a force balance:

$$xBody \cdot \rho \cdot X^3 = (P_{in} - P_{out}) \cdot X^2 = -(dP/dx) \cdot X^3 \quad (7)$$

or $(dP/dx) = -xBody \cdot \rho$, where X is the side of the simulation cell (in lattice units), $xBody$ is the body force, applied in the x -direction, per unit volume in the LB simulation, and ρ is the particle density per site specified in the LB simulation. Thus

$$k = U \cdot \nu / xBody, \quad (8)$$

where $\nu = \mu / \rho = (\tau - 1/2) / 3$ is the kinematic viscosity specified in the LB simulation. Customarily one reports k/X^2 rather than k , to achieve scale-independence.

Figure 3. Simple Cubic (SC) geometry. At left is a small section of an array. Right, a face of the unit cube, showing the entrance to a channel; the “ideal” spherical sections are shown in red, and the pixelation for $X=12$ ($R=6$) are shown by the black outline.

Figure 4 plots the apparent k/X^2 , measured in the LB simulation at $Re=0.25$, as a function of $X=2R$. The error in the measured permeability drops from $\sim 15\%$ at $X=12$, to $\sim 1\%$ at $X=36$. Most of the error at low X can be attributed to pixelation effects; figure 3 compares the ideal geometry of the outlet channel, vs. the actual configuration for $X=12$. In the latter case, a greater fraction of the flow is in the center of the channel, lowering the apparent permeability. The oscillations in the LB permeability are probably a function of the algorithm used to “draw” spheres with integer radii within the unit cube. Figure 5 shows the normalized permeability for the case of non-touching spheres ($R = X/3$), along with the ratio of ideal (or target) sphere radius to the true, average radius used in the simulation. It is clear that the oscillations in LB-measured permeability correlate with the deviations of the sphere geometry from the ideal.

Figure 4. LB estimate of permeability of SC array of spheres, as function cell edge $X=2R$. The deviation from the Zick and Homsy¹³ value is due mainly to the pixelation effect shown in figure 3.

Figure 5. LB normalized permeability and sphere radii for the non-touching spheres, $R=X/3$.

3.2 Wall Conditions: Taylor-Aris Dispersion between Infinite Planar Sheets

The Taylor-Aris problem for parallel plates is perhaps the simplest dispersion benchmark. The test geometry is shown on the left side of figure 6. A slug of solute is injected into an established, left-to-right Poiseuille flow between two parallel plates. Aris¹⁵ showed that after some characteristic time $t_c \sim hy^2/D_m$ (where hy is the channel width and D_m is the molecular diffusion coefficient), the projection of the solute distribution onto the x -axis is nearly Gaussian, and the dispersion coefficient D^* follows the simple rule:

$$D^*/D_m = 1 + Pe^2/210 \quad (9)$$

where the Péclet number $Pe \equiv (hy \cdot U)/D_m$ (U is the cross-channel averaged speed). Equation (9) is taken as the *predicted* D^*/D_m . We can also “measure” D^* for our numerical experiment by the method of moments:¹⁵

$$D^*/D_m = \frac{1}{2} dm_2 / dt / D_m \quad (10)$$

where m_2 is the second moment, or variance (σ^2) of the solute distribution, projected onto the x -axis. The difference between equations (9) and (10) is our estimate of error in figure 6 (calculated for a fixed $Pe = 20$). The figure compares results for two different wall collision methods. The distinction between these two methods is described below.

In recent years, much was written on the choice of wall conditions for LB calculations. The basic problem is that after the streaming step, there are f_i (equation 1) pointing into the solids, but none pointing out from the solids; these missing particle distributions must be created in a consistent manner. For pure flow calculations, the simple bounce-back condition, which fills in the missing f_i by inverting particle distributions at the solid wall, can yield acceptable accuracy. To achieve such accuracy with bounce-back, the collision parameter τ is kept reasonably low, and the wall solid wall is taken to be $\frac{1}{2}$ lattice unit out from the solid nodes.¹⁶ The subterfuge of using the $\frac{1}{2}$ location is commonly referred to as “reinterpreted” bounce-back. However, when applied to tracer particles, the justification for re-interpreted bounce-back is less clear, since the tracers have some residence time “behind” the $\frac{1}{2}$ wall.

Figure 6. Taylor-Aris dispersion between infinite parallel plates. The test geometry is at left; a slug of solute is injected into an established, left-to-right Poiseuille flow. As the slug spreads, the projection of concentration onto the x -axis eventually becomes Gaussian. At right is the error for two types of wall conditions; traditional bounce-back and a no-flux condition (error is difference between equations 9 and 10).

An alternative wall condition for tracer dispersion was suggested by Noble.⁹ In brief, one places the zero-flow position on the wall, by one of the many methods suggested in the literature.^{16,17} Both carrier fluid and tracer particles are allowed to stream along the walls. For tracer particles, the missing part of the distribution is obtained by reflecting across a plane tangent to the wall; in

effect, this is a slip condition. The tracer distributions then are sent through the relaxation step, in which they inherit the diffusion coefficients typical of the free fluid. For all but the narrowest channels, the method suggested by Noble (figure 6) proves more accurate than the simple bounce-back. The bounce-back method reaches a peak error of about 3.8%, before slowly decreasing. The causes of this non-monotone behavior are not clear, but there are probably several competing effects.

Despite the modest accuracy, there are several good reasons to retain bounce-back for dispersion problems. The first is that the method leads to extremely simple and efficient code. Second, with bounce-back, there is a simple relationship between the number of solid nodes in the system and the volume of solids modeled; the benefits of this simple relationship become more obvious when one attempts to implement dissolution and precipitation, which can create very complicated patterns of dendritic growth. If growth occurs by a transition state rule,¹⁸ the surface area and volume of each point in the automaton must be consistently known. Third, the use of bounce-back can be justified on a simpler basis: dispersion data in experiments are rarely measured to an accuracy of better than 10%, and theories for predicting dispersion in complex, 3D geometries rarely come within a factor of 2 of experimental measurements. Consequently, bounce-back walls were used in the following two benchmark exercises.

3.3 Taylor Dispersion in a Duct with Rectangular Cross-Section

Consider the 3D duct shown in figure 7, which extends infinitely along the x-axis, but is closed on the other four walls. It is commonly assumed that if $hy/hz \ll 1$, dispersion in the duct will follow the Taylor-Aris solution (Eq. 5). Surprisingly, as long as the duct has vertical sidewalls, dispersion never approaches the Taylor-Aris solution, regardless of the aspect ratio. As $hy/hz \rightarrow 0$, the solution approaches:

$$D^*/D_m = 1 + 7.95 Pe^2 / 210 \quad (\#7)$$

so for high Pe , the close-walled duct approaches a dispersion coefficient nearly 8 times the Taylor-Aris value. Figure 7 gives a hint about the origin of this enhanced dispersion; the edges of the solute slug are swept back by the vertical duct walls, since the flow speed must vanish at the walls.

Figure 7. Geometry for dispersion in a rectangular duct.

The time required to reach a dispersive steady state in the duct is $t_D = c \cdot hz^2 / D_m$, where the proportionality constant c is $\leq \frac{1}{2}$. Thus the duct must be of length $hx \sim c \cdot U_x \cdot hz^2 / D_m$, where U_x is the average flow speed in the x -direction, to contain the slug on its path toward the outlet. We define the Péclet number relative to the narrow dimension, hy , as $Pe_y = U_x \cdot hy / D_m$, and the aspect ratio $n = hz / hy$. In general, the DDG problem is studied for a variety of $n \rightarrow \infty$, for as high a Pe_y as is possible. The total number of sites required for the simulation is $hx \cdot hy \cdot hz \sim c \cdot Pe_y \cdot n^3 \cdot hy^3$; the total clock time required for a run $\propto t_D \cdot (\text{number of sites}) / (\text{MUPs} \cdot 10^6) = c^2 \cdot Pe_y \cdot n^5 \cdot hy^5 / D_m / (\text{MUPs} \cdot 10^6)$. Thus, for $hy=7$ and $n=7$ and $Pe_y=14$ achieved by $U_x = 0.03$ and $D_m = 0.015$, we require ~ 0.83 million sites, and at 2.55 MUPs, the calculation takes ~ 7 hours. While this amount of time is entirely feasible on a desktop computer, it provides motivation for more efficient methods that do not grid the lattice uniformly.¹⁹

Figure 8 compares our measurements of the DDG effect with the calculations of Chatwin and Sullivan.²⁰ The agreement is reasonably good, given that Chatwin and Sullivan used two methods that sometimes disagreed by 5%.

Figure 8. Comparison of LB calculations for dispersion in a rectangular duct, against the predictions of Chatwin and Sullivan.²⁰

3.4 Dispersion in an Infinite Array of SC Spheres

Dispersion of tracers in porous media is of great interest in chemical engineering, where packed beds are used to effect chromatographic separations, or the solids act as catalysts for chemical reaction. In environmental chemistry and hydrology, there is a great interest in measuring the sorption of tracers in flowing experiments, with eventual application to field conditions. However, in laboratory-scale tests, it is often extremely difficult to distinguish sorption from dispersion, since both phenomena create similar tail effects.^{3,21,22} It is thus useful to have accurate benchmarks for dispersion in porous media analogous to packed beds, so dispersive

effects can be quantified with reasonable accuracy. Since regular arrays provide the most reproducible and well-defined geometries, they are ideal candidates for benchmark exercises.

Surprisingly, there is little agreement among experimental results, and analytical or numerical solutions, for dispersion in regular arrays. Gunn and Pryce²³ measured the dispersivity for argon gas in simple cubic (SC) and rhombohedral packings, using frequency response techniques. Subsequently, Eidsath *et al.*,²⁴ Koch *et al.*,²⁵ Salles *et al.*,²⁶ and Lee *et al.*²⁷ modeled these experiments, with limited success. Typically the experimental and modeled coefficients differ by factors of 2 to 7, at particle Péclet numbers (Pe) from 1 to 300. However, some assumptions made in the models are not wholly consistent with the experiments. For example, the Gunn and Pryce²³ study achieved a Schmidt number Sc of 0.88, ($Sc \equiv Pe/Re$) and Reynolds numbers (Re) up to ~ 400 ; in contrast, the Koch *et al.*²⁵ and Lee *et al.*²⁷ models implicitly assumed Stokesian flow, with $Sc \rightarrow \infty$, and the Eidsath *et al.*²⁴ models used Re of 0.006 and 56. Kaviany²⁸ and Salles *et al.*²⁶ identified the Re difference as a potential cause of disagreement, but Kaviany also speculated the Re effect might be masked. The calculations by Eidsath *et al.*²⁴ approximated the spheres with 2-dimensional cylinder arrays with porosity $\varepsilon \sim 0.37$, compared to the actual SC value of $\varepsilon \sim 0.48$. The Koch *et al.*²⁵ theory is strictly valid for $\varepsilon \sim 1$ only, assumes the solute is conducted through the solids, and does not completely satisfy the boundary conditions on the particle surfaces; Koch *et al.* speculated that the latter problem caused their model to underestimate dispersion.

For the present study, dispersion in an SC array was modeled with the LB method. The main goals of the simulation were (1) to determine if inertial effects (i.e. non-Stokesian flow) could be the source of disagreement between experiments and prior analyses, and (2) to provide a dispersion benchmark more complex than simple flow in a rectangular duct, particularly a benchmark capable of capturing tailing effects. Most of the calculations employed a 19-vector Navier-Stokes carrier fluid (as described in section 2), and a single 6-vector tracer. However, a single run was made with a 19-vector tracer for comparison purposes, at $Re \sim 150$. The 19-vector and 6-vector simulations produced dispersion coefficients that agreed within 0.2%, so the 6-vector tracers (which run 3 times faster) were used for the bulk of the calculations.

As in sections 3.2 and 3.3, dispersion coefficients were measured by the method of moments. A slug of solute was placed at the upstream end of the array of spheres. The slug deforms and broadens as it travels down the column, and at steady state, the dispersion coefficient $D^* = \frac{1}{2} dm_2/dt$, where the second moment $m_2 = \sigma^2$, and σ is the standard deviation of the solute distribution along the flow direction. The characteristic time to achieve steady state is $t_c = \alpha R^2/D_m$, where R is the sphere radius. At steady state, m_2 increases linearly with time, at which point D^* is truly constant and well-defined. The magnitude of α is not well established; Eidsath *et al.*²⁴ report $0.36 \leq \alpha \leq 0.8$. In the present study, $m_2(t)$ was linear (e.g. correlation coefficient $r^2 \approx 0.99999$ for a first-order fit) for $t \geq \frac{1}{4} R^2/D_m$; for the cylindrical geometry, a longer t was required, because this geometry has inherently lower communication between the stagnant pockets and central channel.

Because of the wrap condition, the steady-state flow field (u_x, u_y, u_z) need be calculated in only one cubic unit cell, containing a single sphere. Based on the results of section 3.1, a sphere of diameter $d = 36$ in a cubic cell with edge $X = 36$ was chosen, since this configuration yields a permeability accurate to $\sim 1\%$. For the dispersive part of the problem, a column of spheres is necessary. As with the duct dispersion problem, the length of the column is set by the

requirement that the slug stay within the column for $t \sim \frac{1}{4} r^2/D_m$; for the highest Pe studied, this requirement translates to a column of ~ 60 spheres.

Figure 9 illustrates the flow fields for the $Sc=0.88$ and $Sc=32$ cases (u_x, u_y components alone are shown; the z axis points into the page). At the lower Sc (higher Reynolds number), there are clear recirculation zones in the lee of the sphere. Compared to the $Sc=32$ case, the $Sc=0.88$ case has a higher flow rate in the top and bottom regions, given the same Darcy velocity.

Figure 9. LB flow fields for $Re = 150$ (top) and $Re = 4.1$ (bottom), for the plane at fractional depth $z = 0.0694$ (2.5 lattice units). For $Pe = 132$, the corresponding Sc are 0.88 (top) and 32 (bottom). Vector lengths are 4th-root scaled to emphasize regions of low-speed flow. The true distribution of solids is indicated by the cross-hatch pattern; the dashed circle is the ideal spherical section for this z position.

The patterns of solute are shown, for early time ($t/t_c < 0.3$) and $Pe = 132$, in figure 10. For the $Sc=0.88$ case (top 4 frames), the solute is more effectively dispersed than in the $Sc=32$ case (lower 4 frames). The enhanced dispersion appears to be caused by two effects: (1) greater average fluid speed in the channels between the spheres, at the same Darcy speed; and (2) residence and mixing of solute in the recirculation zones behind the spheres.

Figure 10. Solute patterns in the early stages ($t/t_c < 0.3$) of the LB calculations, for $Sc = 0.88$ (top) and $Sc = 32$ (bottom); both are at $Pe = 132$. The step number is indicated on the upper right of each frame. Each frame shows cuts at fractional depths $z = 0$ and $z = \frac{1}{2}$ (0 and 18 lattice units, respectively). The solute is indicated in black; intensities are square-root scaled to emphasize lower concentrations. The low-concentration ripples in the $t=48$ frames are numerical artifacts that are quickly damped.

Figure 11 plots the LB-calculated dispersion coefficients against the $Pe = U d / (D_m (1-\varepsilon))$, and compares our results against available experimental data,²³ the Koch *et al.*²⁵ theory for Stokesian flow past SC spheres, and the Eidsath *et al.* theory²⁴ for flow past 2D cylinders. For the cylindrical geometry, the “effective” particle diameter $d_p = 1.5d$ is used, to allow direct comparison with the Eidsath *et al.* results. Note that the LB cylinder calculations match, within ~10%, the Eidsath *et al.* finite element results for this geometry. Thus there is some confidence that any differences, between the LB SC sphere results and the Eidsath *et al.* cylinder study, are not merely due to differences in numerical methods. For the SC sphere array, the LB $Sc = 0.88$ runs are quite close to the trend of the experimental data. In contrast, the LB $Sc = 32$ runs are between the Eidsath *et al.* and Koch *et al.* numerical results. From these comparisons, it seems reasonable to suggest: (1) the difference in Sc (and Re), including the presence of recirculation zones, accounts for some of the discrepancy between the Koch *et al.* theory and the gas dispersion experiments; and (2) the cylindrical geometry and Sc assumed by Eidsath *et al.* account for much of their disagreement with the experimental results. Note that with $\varepsilon = 0.373$ in the cylindrical geometry, small variations in ε can cause quite large changes in the measured transport coefficients (e.g. at $\varepsilon = 0.215$, there are no gaps between the cylinders). Indeed, Eidsath *et al.* do not give a clear motivation for choosing $\varepsilon = 0.373$, and they also show that rather small variations in the cylindrical geometry affect the measured dispersion coefficient by a factor of two or more. Overall, the LB results suggest the Gunn and Pryce experiments were reasonably accurate and representative for $Sc = 0.88$.

Figure 11. Comparison of LB results with experiments and theory. Gunn and Pryce²³ points (open circles) represent gas dispersion experiments.

4. Code Architecture and Function Descriptions

This section describes the basic JB_PH.C source for multi-component, 3D LB. Many variations on the basic code exist, better suited for problems involving fracture flow and double-diffusive convection. However, the streaming, collision, gravity-control and I/O algorithms are the same in most versions of the LB codes.

Throughout the listings, **ncol**, **nrow** and **nlay** (or the uppercase versions of these) refer to the sizes of the automaton in the *x*, *y* and *z* directions, respectively; that is, to the numbers of columns, rows and layers. The **nveloc[s]** refers to the number of velocity vectors for the LB lattice of component *s* (19 for the D3Q19 carrier, and 6 or 19 for the tracers), and **ncomponent** refers to the number of components in the system (always at least 1, including the carrier).

4.1 Compiling the Codes

The codes described herein were all compiled with the Intel Reference Compiler Version 2.4, P97176, hosted from the Microsoft MS C++ 4.0 integrated development environment. Benchmarks, run as part of this project, showed that the Intel compiler produced LB executables that were at least 30% faster than those produced by the Microsoft compiler, 3 times faster than the executables produced by Symantec C++ version 6.0, and 4 times faster than those produced by Watcom C++ 9.5, using all recommended switches for code optimization. The switches used for the Intel compiler were **-G6 -Qmem -Qip**. The first switch optimizes for the Pentium Pro (and above) processors; the second optimizes memory loads and stores; and the third performs interprocedural optimizations, particularly in-line function expansions. It is notable that the Microsoft compiler produced fast executables only when anti-aliasing pragmas were used to encapsulate the collision functions, but the Intel compiler did not require such non-standard directives.

4.2 JB_PH Command-Line Switches

Many aspects of an LB calculation can be passed to JB_PH via command-line switches, which eliminate the need to recompile the code, between runs, simply to make minor adjustments to program size. The available switches can be determined by running the program with only the **-h** or **-?** switches; this invocation will list the available switches on the console, and will then terminate the program. The listing will appear as:

FLAG	ARGUMENT	WHAT IT SETS	IMPLEMENTED?
----	-----	-----	-----
-x	float	xBody, x BODY force	Y
-y	float	yBody, y BODY force	Y
-u	float	uxLimit, x speed limit	Y
-v	float	uyLimit, y speed limit	Y
-n	float	viscosity component 0 (carrier)	Y
-d	float	diffusion coeff. component 1	Y
-D	float	Diffusion coeff. component 2	Y
-s	integer	MAXSTEPS, maximum number of steps	Y
-j	integer	JUST_DISPERSE_STEP (flow frozen in)	Y
-c	integer	NCOL, number of columns (max x)	Y
-r	integer	NROW, number of rows (max y)	Y
-l	integer	NLAY, number of layers (max z)	Y
-i	integer	NVELOC, # velocity vectors for solutes	Y
-b	integer	Boundary: 0=bounceback, 1=Ziegler	n
-g	integer	stepStartSlug (step tracer slug)	Y
-f	string	filename containing solids geometry	N
-o	integer	Sphere Radius (for JO.C, JO_SPH.C)	Y
-t	integer	Times (NTIMES) to multiply geometry	Y
-#	integer	x and z size alveoli grid (fin to fin)	Y
-^	integer	y height alveoli grid (inside measure)	Y
-h -?	<none>	display this list	Y

For example, if the program were invoked as:

```
JB_PH -c11 -r23 -l22 -x0.0010 -u0.03 -n.16 -d.03 -s100000 -j2000 -t10 -g1999
```

memory would be allocated, initially, for 11 columns (**-c11**), 23 rows (**-r23**), and 22 layers (**-l22**), corresponding to *x-y-z* dimensions of 11×23×22. A body force of 0.0010 would be applied initially in the *x*-direction (**-x0.0010**), until the *x*-direction speed across the outlet measuring plane reached 0.03 lattice units per timestep (**-u0.03**), at which point the **AdjustGrav()** function would monitor and adjust the body force to maintain a constant fluid flow speed of 0.03 in the *x*-direction. The viscosity of the system would be set to 0.16 (lattice units)²/timestep (**-n.16**), and the diffusion coefficient of the one tracer component would be set to 0.03 (lattice units)²/timestep (**-d.03**) (if we had specified **-D.06** as well, the program would have automatically allocated space for another component with diffusion coefficient of 0.06). The program would run for a maximum of 100000 timesteps (**-s100000**); at step 1999, a slug of solute would be injected at the upstream end (**-g1999**). At step 2000 (**-j2000**), the program would enter **JustDisperse** mode, freezing in the velocity distribution, and running the much faster (fixed flow field) tracer translation and collision functions. Since the **-t10** switch is also specified, at the time given by the **-j** switch, the automaton would replicate the solids geometry 10 times in the *x*-direction, allowing a much longer dispersion simulation (this was the method used to run the rectangular duct and SC sphere dispersion benchmarks, described in sections 3.3 and 3.4). To allow the maximum size calculation, JB_PH would first deallocate the memory used for the 19-vector carrier fluid, and reallocate this memory to new tracer arrays spanning the entire length of the automaton. The

velocity field would not be replicated explicitly, but would use the MOD approach to pick local velocities, as described in section 2.

By default, JB_PH uses the 19-vector D3Q19 lattice for the carrier, and 6-vector lattices for tracers. However, by specifying `-i19`, the program will force use of 19-vector lattices for the tracers.

4.3 Character-Mode Display

After JB_PH is invoked in a console (e.g., a DOS-box under Win95/NT, or an xterm under Unix/X-Windows), it provides a simple, character-mode graphics representation of the LB update process. The following discussion will focus on the Win95/NT version of the display. Currently, the display is set to refresh every 32 steps. The character-mode display is intended to provide a minimal capability, easily ported to diverse systems. The two sections below describe the development of a more sophisticated display capability.

The display has two basic modes: a normal 24×80 site “window” into the automaton, which can be panned over the automaton with the cursor keys; and a “Zoom” mode that zooms out to display the entire automaton, scaled to fit in the 24×80 view port. The modes are toggled with the “Z” key. The display shows an x - y plane at a fixed depth z (layer); the displayed layer is changed with the PageUp and PageDown keys. The component displayed can be changed by pressing the “S” key; component 0 (the carrier fluid) displays the average fluid speed, whereas all other components display tracer concentrations. The “Esc” (escape) key or “Q” keys terminate the program.

4.5 Passing Data to Asynchronous Graphics Programs: `plotfile.bin`

In addition to the simple character-based display, JB_PH “silently” generate a binary file that allows more flexible and colorful, “real-time” displays of automaton calculations. The `plotfile.bin` file is generated by the function `MakePlot()` (Appendix, listing 1) every n steps (n is currently set to 32, but it would be trivial to alter the source for variable intervals). In the next sub-section, an example will be given for a program that launches JB_PH, then operates asynchronously, displaying real-time images of the automaton progress.

The formats of `plotfile.bin` are specified in the “include” file `plothead.h` (Appendix, listing 2). The file is designed so its creation will impose a minimum performance penalty. As an test of the CPU burden, `plotfile.bin` was written every 32 steps when running the fastest LB tracer modes (`JustDisperse()`, ~2.55 MUPs on a PII-400); the effect on performance was < 1%. The first 4 bytes of the file contain the array `PH_MACHINE[4]`, which specifies whether the machine that produced the file is big-endian or little-endian, and specifies the size (in bytes) of integers and floats on the creator. Thus, it is possible to read and interpret a `plotfile.bin` produced on a completely different architecture. The file then contains the LB step number, the size of the `PLOTHEAD` structure, and the `PLOTHEAD` structure itself. The latter structure specifies the type of data “slice” contained by the file: an x - y slice; an x - z slice; a y - z slice; or a full x - y - z “snapshot” of the time step. The structure contains some information on average speeds and fluxes in the system, along with scaling information useful for producing

color images. After the structure, the tracer concentration or speed data are written in a manner consistent with the slice type.

4.6 Example of `plotfile.bin` Usage: a Win95/NT Interface

Listing 3 (in the Appendix) gives a short Win95/NT program that launches `JB_PH` asynchronously, awaits the creation of `plotfile.bin`, and displays the plotfile any time it changes. The program, `pix_test.c`, passes any command-line switches on to `JB_PH`. To prevent `pix_test` from using too many system resources, the program uses timers, and checks for a new plotfile every 3 seconds. To ensure a speedy update of the display, `pix_test` writes its pixels to a Windows `DIBSection`, then flashes the `DIBSection` into the video buffer. The function `GetNewPlot()` (Appendix, listing 4) reads the plotfile into the `PBUF` buffer, and `StretchPBUF2DIB()` maps the data into the display buffer.

4.7 `JB_PH` Data Structures

To understand the algorithms used in `JB_PH` (Appendix, listing 5), it is necessary to review the storage of the particle distributions, flow speeds, and other quantities used in the calculations. The precision of the particle distribution arrays (`FF` or `ff`) and the velocity components (`U` or `uu`) is controlled through the type specifications at the top of the program:

```
typedef float ff_t; typedef float u_t;
ff_t *****FF;
struct veloc_t { u_t x; u_t y; u_t z; u_t usqrdr; } ***U;
```

Thus by typing `ff_t` and `u_t` as `double`, one can propagate increased precision throughout the program.

Like most arrays in `JB_PH`, `FF` and `U` are allocated dynamically. Thus there is no need to recompile the program to handle a larger problem size; however, dynamic allocation requires some special consideration for achieving efficiency, especially in light of C's well-known alias problems. As described in section 2, the `FF` array is allocated as `FF[s][i][z][y][x]`, where `s` is the component index, `i` is the vector number (`i = 0,1,...18` in D3Q19), and the remaining indices are the Cartesian coordinates of each spatial point in the LB lattice. The `U` is allocated as an array of `veloc_t`, so the `x,y` and `z` components at a spatial point x_1,y_1,z_1 are accessed as `U[z1][y1][x1].x`, `U[z1][y1][x1].y` and `U[z1][y1][x1].z`.

Anyone attempting to modify `JB_PH` should be aware of a peculiarity in the handedness of the `x,y,z` spatial grid, vs. the handedness of the velocity components. For historical reasons, the positive *spatial* `y`-axis points down in `JB_PH`, making a left-handed coordinate system; this is an artifact of the derivation of much of the code structure from earlier lattice gas codes, where the `y` spatial axis was mapped directly into the rows of the video buffer. However, the velocity components are right-handed, with the positive u_y pointing "up", and all force and buoyancy components follow a right-handed system.

Two other important structures are **flags_struct** and **gravity**. The former holds the flags that are parsed from the command line by **SetFlags()**. For each flag, the structure holds two components: an integer with a name like **use_XXX**, which specifies if the flag will be used; and the variable **XXX**, the value of the quantity. The **use_XXX** is set to 1 by **SetFlags()** if the quantity is found on the command line, and its value falls within accepted limits; however, **use_XXX** may be reset to 0 by subsequent logic, since the main flags structure is global. The **gravity** structure begins with **do_x**, **do_y** and **do_z**; these are flags (0 or 1) that determine if the body forces in the Cartesian directions will be adjusted to maintain the speed limits specified in **uxLimit**, **uyLimit** and **uzLimit**. Currently, only **uxLimit** and **uyLimit** can be set by the command line (via the **-u** and **-v** switches). The **xBody**, **yBody** and **zBody** specify the *initial* components of the body force; if the **do_x**, **do_y** or **do_z** are set, these are target values, i.e. once the speed limit in a particular Cartesian direction is reached, the body force may be reduced. The *true* body force at a given time step is given by **txBody**, **tyBody** and **tzBody**; these values are set by the **AdjustGrav()** function. At each timestep, **AdjustGrav()** checks the average flow speeds on 1 to 3 control planes; if the average flow speeds on those planes differ from the speed limits, the corresponding **t?Body** are incremented up or down to approach the target speed. Each of the control planes has five coordinates to specify its position and extent; e.g., the control plane perpendicular to the x-axis (associated with the x-component of body force and the u_x speed limit) has coordinates **xUx**, **y1Ux**, **y2Ux**, **z1Ux** and **z2Ux**.

In a complex geometry, it is very difficult to adjust the body forces to maintain a pre-specified flow speed. The problem is most difficult when there are large variations in the effective channel width (as in the SC flow problems described in sections 3.1 and 3.4), and when more than one velocity component is controlled. In such circumstances, there may be small oscillations in the flow speed, as **AdjustGrav()** tries to alternately increase and decrease the body forces, against an out-of-sync response in the flow speed. In such circumstances, it is useful to have means to “clamp” the body forces to fixed values, then “turn off” the **AdjustGrav()** algorithm. The **gravity** structure contains two parameters, **stepStartClamp** and **stepStopClamp**, that specify an interval to measure the average body forces and flow speeds before imposing the clamp. Optimal use of the clamping capability requires some foreknowledge of the flow problem; by default, JB_PH first checks the step specified by the **-j** flag (if used), then checks the specified maximum step to determine clamping limits.

The **xBuoy**, **yBuoy** and **zBuoy** in **gravity** give the part of the information needed to calculate a position- and concentration-dependent buoyancy force. For example, the x-direction buoyancy force is $xBuoy \cdot (\rho_{REF} + \sum_{s=1} \alpha_s \cdot (\rho_s - \rho_{REF}))$ where the α_s is the molar expansivity of the s th component, and ρ_{REF} is a reference density. The α_s are stored in the **alpha[MAXCOMPONENTS]** member of **gravity**.

4.8 JB_PH Program Structure

In this section, the basic structure of JB_PH is presented in a pseudocode outline. The actual source (Appendix, listing 5) contains many commented blocks that reflect experimental

capabilities and functions. At the core of the program is the loop over update steps; each update is further divided into translation and collision functions, and forcing adjustments and imposition of boundary conditions.

JB_PH Pseudocode

```

defines
structure and type definitions;
function declarations;
Main {
  Open lb_log.txt to log errors and unusual conditions;
  Call SetFlags() to parse command line and set FLAGS structure values;
  Adjust # components, viscosities and diffusion coefficients for
    components, automaton size, disperse step,
    slug step, maximum steps, number of replications from flags;
  Set default slug size, set Character display defaults;
  Allocate and initialize FF (particle distributions), SOLID, U (array
    of velocity structures);
  Initialize SOLID by reading from file or by internal algorithm, and
    call SetSolidType() to determine if solids are internal
    or bounding;
  Initialize the gravity structure G;
  Convert special flags (e.g. viscosity or diffusion) to  $\tau$ , and initialize
    TAU and RHO;
  Perform initializations of fluids for special geometries;
  Select a dispersion mode, and point to the Collision function;
  Open the lb_data.txt file, to monitor program performance;
  LOOP over STEP to MAXSTEP {
    Look for keyboard input, and change display if required;
    if(STEP==JUST_DISPERSE_STEP){
      Recycle() memory if required, allocate new tracer units;
    }
    if(STEP<JUST_DISPERSE_STEP) Translate() all components,
      including carrier;
    else just Translate() tracers;
    if(STEP==stepStartSlug){
      Either use SetSlug(), or read slug geometry from bitmap;
      Save graphics of flow field (SaveVect(), SaveUPpm());
    }
    if(STEP<JUST_DISPERSE_STEP)
      Use the normal Collide() function;
    else Use the function JustDisp_ptr points to;
    if(STEP<JUST_DISPERSE_STEP){
      Use normal concentration boundaries (e.g. XsetConc());
      Apply AdjustGrav() to control fluid speed to limits;
    }
    else Use "JB" versions of concentration boundaries;
    if((STEP & PLOT_ANDER)==0){ /* PLOT_ANDER==31 currently */
      Calculate and display ux average (UxAvg());
      MakePlot() for plotfile.bin for asynch graph program;
      if(other special conditions) Write ppm files;
    }
  } /* END LOOP */
  Write a ux_uy.txt speed summary for debugging;
  close log files, lb_data.txt file, any ppm list pointer files;
} /* END Main */

```

Functions;

4.9 Translation (Streaming) Algorithm

As described in the section on efficiency, this version of JB_PH uses particle distribution arrays of the form `ff[s][i][z][y][x]`, with `s` selecting the component, `i` selecting the vector (`i=0,...,18` in D3Q19, or `i=0,...,5` in the Cartesian 6-vector tracer lattice), and the `z,y,x` selecting the spatial position in the lattice. While this format may seem peculiar, it allows great simplification of the translation function, so the translation can be done “in-place” with minimal buffering. It also allows the tracers to mix 6-vector and 19-vector lattices with little effect on alignment and efficiency. After the program enters JustDisperse mode, only the tracers are translated.

The vector numbering scheme is given at the top of the JB_PH source, and is reprised below. The positive u_x axis points to the right, and the positive u_y axis points toward the top of the page, with the positive u_z axis pointing out of the page (“above”).

```

/*****
/* In D3Q19, will keep old 2D numbering system for 1st 9 vectors, */
/* as indicated below: */
/*
/*      4  3  2      |      11      |      15      */
/*      \  |  /      |      |      |      */
/*      5 -- 0 -- 1   |      12 -- 9 -- 10   |      16 -- 18 -- 14   */
/*      /  |  \      |      |      |      */
/*      6  7  8      |      13      |      17      */
/*
/*      MIDDLE      |      TOP      |      BOTTOM      */
/*****
/***** below is key for velocity notations, 6 VECTOR model (D2Q6)*****/
/*      1      |      and the up (positive z) vector is 4,      */
/*      |      |      and the down (negative z) vector is 5      */
/*      2 -- * -- 0   |      */
/*      |      |      */
/*      3      |      */
/*****

```

The function:

```

int Translate(ff_t ***** const ff, int ncomponent,
             int nveloc[], int nlay, int nrow, int ncol, int sstart),

```

has an outer loop over `s`, the component index; withing this loop, the translation block for 19-vector or 6-vector lattices is determined from the contents of `nveloc[s]`. For both lattice types, the boundaries wrap left-to-right, top-to-bottom, and side-to-side; e.g., a “particle” leaving the right side of the automaton at `x=ncol-1` will be reinjected at `ncol=0` with the same velocity.

The basic strategy of `Translate()` is to decompose each vector translation into a pointer swap and a physical movement in memory that references only one index. Some translations

require only pointer swaps, and some require only physical movements in memory. Typically, at most only one pointer and one particle distribution need be buffered to effect a translation.

The character-mode function:

```
int Plot9Vec(ff_t ***** const ff, float * const rho,
             int ncomponent, int nveloc[], int nlay,
             int nrow, int ncol, int step),
```

is useful for debugging the translation step. This simple routine prints the vectors in an 8×8 set of sites to the display, broken down into vectors in the x - y plane, and vectors pointing below and above the plane. The `Plot9Vec()` function is typically used in isolation, with the collision and concentration functions commented out, so one may track that the translations and boundary wraps are properly executed.

4.10 Collision Algorithms

The JB_PH source contains several collision functions (other specialized versions of the collision function are available from the author). The most general is `Collide()`, which can operate on an arbitrary number of components, with a non-steady $\mathbf{u}$ field, and with buoyancy. The code contains “hooks” for the imposition of complex wall collisions (in the form of the `Ziegler()`, `NoFlux()` and `NoFlux6()` calls). However, `Collide()` has several features that reduce its efficiency: for example, the function applies buoyancy to an arbitrary number of components, requiring pre-calculation of densities, and the function requires a large number of indirections to fetch data from 5-dimensional arrays.

Much faster collision functions can be created for special conditions. Such conditions include: when there are only one or two tracers; when the tracers are 6-vector; or when the flow-field is steady state. For the last condition, JB_PH recognizes a special mode called `JustDisperse`. In this mode, only the tracer components are translated, and the function pointer `JustDisp_ptr` is used to select the dispersion function. In this version of JB_PH, two such functions are available: `JustDisperse3D()` and `JustDisperse3D_A()`. The former will disperse an arbitrary number of tracers, and per tracer, is up to 12 times faster than `Collide()` (when `Collide()` is running both the carrier and a single tracer). The `JustDisperse3D_A()` version is specially optimized for just one tracer. Because of memory limits, these two dispersion functions have nearly the same speed on the Intel x86 chips; that is, the routines are both so efficient, that their speed is controlled by the RAM streaming limit of main memory.

4.11 Controlling Fluid Speed and Gravity Adjustments

As described above, the function `AdjustGrav()` allows one to keep the automaton at a specified average flow speed in a given direction, to simplify the attainment of pre-selected Pe or Re . The function operates on a given Cartesian speed component (e.g. u_x) only if the flag for that component is set (e.g. `do_x > 0`), and only before reaching the value of the `stepStopClamp` member of the gravity structure. The following discussion is restricted to the x -component; the treatment of the other directions is analogous. The average speed ($\mathbf{ux}$) is measured on the

specified control plane, and if this speed is greater or less than the **uxLimit** member, the **txBody** member is correspondingly adjusted. There is some logic to adjust the body force by small or large increments, to avoid generating undamped oscillations. After performing the adjustments, the function checks to see if the step is between the clamping limits, and if it is, the **ux** and **txBody** are added to a running average. At the end of the clamping period, if the average **ux** (over the clamping period) is significantly different from the **uxLimit**, the average value of **txBody** is multiplied by **uxLimit**/(average **ux** over clamp period).

As with most discrete lattice methods, it is generally desirable to keep the maximum flow speed substantially below the numerical speed of sound in the automaton. We typically keep U less than 0.01 to 0.05 for the D3Q19 carrier fluid.

4.12 Concentration Boundaries

Several functions are capable of imposing concentration boundaries on the system. The most common use of these boundaries is to inject a slug of solute, or to impose a particle sink, to prevent particles from leaving the outlet of a long channel, with subsequent reinjection at the inlet. The desired concentrations are passed to the functions by the array of **double concList[MAX_COMP]**, where **MAX_COMP** is defined as the maximum number of components allowed in the system (currently 10). If a **concList[i] < 0**, the *i*th entry is skipped by the called function.

The function:

```
int SetSlug(ff_t *****ff, char ***solid, int ncomponent,
            int nveloc[], int nlay, int nrow, int ncol,
            int x1, int x2, int y1, int y2,
            int z1, int z2, double *concList),
```

sets the **ncomponent** components of **ff[s][i][z][y][x]** to the values specified in **concList**, over the spatial domain within **x1** to **x2**, **y1** to **y2**, and **z1** to **z2**. Typically, **SetSlug()** is called once, at the step specified by the **-g** flag, to set up a Taylor-Aris dispersion problem. There are variants of this function, such as:

```
int ReadBmp4Slug(ff_t ***** const ff, char *** const solid,
                 float rho, int nvel, int nlay, int nrow, int ncol,
                 int sstart, int x, int z, char *filename),
```

that read the slug geometry from a Windows bitmap (specified in **filename**), allowing one to inject slugs of nearly any geometry (figure 12).

Figure 12. A slug of solute injected between walls of a rough fracture. Each frame shows a single timestep (indicated in black in the upper right corner), and two cuts through the fracture. The solids are in white; the initial carrier fluid is red; and the initial slug is blue fluid. At the top of the frame is a sub-horizontal cut, midway between the bounding surfaces, at $y=nrow/2$; at the bottom of each frame is an orthogonal cut, at $z=nlay/2$. The slug was read from a bitmap via the `ReadBmp4Slug()` function, and the walls of the fracture were read with the `FractalSurface()` function.

The function:

```
int XSetConc(ff_t ***** const ff, char *** const solid,
            int ncomponent, int nveloc[], int nlay, int nrow,
            int ncol, int x, int y1, int y2, int z1, int z2,
            double * const concList),
```

sets the concentrations on the 2D rectangular section (perpendicular to the x -axis) specified by x , $y1$ to $y2$, and $z1$ to $z2$; there are analogous functions for the y - and z -axis. The `XSetConcJB()` versions are used when the program is in **JustDisperse** mode (as determined by the `-j` switch).

4.13 Measuring Velocities and Fluxes

The function:

```
double UxAvg(struct veloc_t *const*const* uu,
             char *const*const* solid,
             int nlay, int nrow, int ncol,
             int x, int y1, int y2, int z1, int z2),
```

measures the *x*-direction component of the velocity field *u* over the rectangular region, perpendicular to and intersecting the *x*-axis at *x*, and bounded by *y1* to *y2*, and *z1* to *z2*. The function returns the average value of the fluid speed *for open spaces only*. That is, the function does *not* return the superficial (Darcy) velocity, though it could be modified easily to do so. The functions *UyAvg()* and *UzAvg()* perform similar services for the *y*- and *z*-components of velocity.

Similarly, the function:

```
double XGetFlux(ff_t ***** const ff, char *** const solid,
               int ncomponent, int nveloc[], int nlay, int nrow,
               int ncol, int x, int y1, int y2, int z1, int z2,
               int s, double * const ftotPtr),
```

returns the *fluence* of the component *s* through the specified rectangular region, inclusive of the endpoints. Specifying *s==0* effectively returns a net velocity. The total amount of the component in the rectangle is returned in *ftotPtr*. To obtain true flux, the returned fluence must be divided by $(|y2 - y1| + 1) \cdot (|z2 - z1| + 1)$. There are *y*- and *z*-analogues for this function as well.

4.14 Generating PPM, Vector, and Movie Files

Several functions in the JB_PH source can generate graphics files for subsequent display or incorporation into MPEG movies. Any function whose name contains “Ppm” generates portable pixel maps, as defined in the Unix utilities “*pbmplus*”. These files have an extremely simple format, and are easily converted to Windows bitmap files by programs such as *Lview Pro*. The beginning of each ppm is written by a statement similar to:

```
fprintf(fp, "P6\012%d %d\012255\012", columns, rows);
```

where *fp* points to the open *binary* ppm graphics file. This statement writes the magic string “P6”, followed by a Unix newline, then the number of columns and rows in the map, separated by a space and followed by a newline, then the maximum color per byte (255 in this case), followed by a newline. Immediately following, the RGB data are written (3 bytes to an RGB pixel), row by row, for a total of $3 \cdot \text{columns} \cdot \text{rows}$ bytes of pixel map data.

Each ppm file has a name *Cddhhnnn.ppm*, where *C* is a character denoting the ppm file type (currently *B*, *U* or *T*, corresponding to B=bitmap, U=flow speed, or T=three-dimensional),

dd is the day of the month, **hh** is the hour the list file was created, and **nnn** is a number from 000 to 999. With the exception of **SaveUPpm()**, each ppm function returns a pointer with a name like **(FILE *)b_list_ptr**; this pointer denotes a file that contains a list of all ppm files generated during the run. The list file helps one sew the ppm files together into an MPEG movie, via utilities like the freeware program **cmpeg**. The name of the list file will be **Cddhh.1st**. If more than 1000 ppm files are created in a run, a new list file is created with the new current day and hour.

Currently, the following ppm-producing functions are available in the JB_PH source:

```
FILE *SavePpm(ff_t *****ff, char ***solid, int ncomponent,
              int nveloc[], int nlay, int nrow, int ncol,
              int sstart, int step),

*Save3DPpm(ff_t *****ff, char ***solid, int ncomponent,
            int nveloc[], int nlay, int nrow, int ncol, int sstart,
            int step),

*SavePpmXY_XZ(ff_t *****ff, char ***solid, int ncomponent,
              int nveloc[], int nlay, int nrow, int ncol, int sstart,
              int step, int colorCode);

int SaveUPpm(struct veloc_t *** const uu, char ***solid,
             int nlay, int nrow, int ncol, int zz[], int nz,
             int step);
```

The differences among the first three are in the manner of portraying “cuts” through the x - y - z space, and in the options for color schemes; all plot the concentration of the tracer with index **sstart**. The first function takes cuts at planes $z \sim nlay/2$ and $x \sim ncol/2$, and arranges them side-by-side on the page; the second plots the concentrations on the $x=0$, $y=0$ and $z=0$ faces, for a semi-3D appearance arranged in an isometric perspective (figure 13). The third makes cuts at planes $z \sim nlay/2$ and $y \sim nrow/2$, arranging the latter above the former on the page. The **SavePpmXY_XZ()** function is most useful for portraying dispersion and reaction in long, flat channels, with dimensions like figure 12.

Figure 13. Images of the Rayleigh-Taylor instability, plotted with the function `Save3DPpm()`. A denser blue fluid initially overlies a red fluid; the two overturn in mushroom-shaped patterns. The timestep is shown at the bottom of each frame.

The function `SaveUPpm()` does not return a file pointer, and is designed to give a velocity snapshot at each of the `NZ` planes specified as `z`-indices in the `ZZ[]` array. The snapshot is typically performed once, just before freezing in a flow pattern for the **JustDisperse** modes. The `NZ` images are arranged vertically on the page, with higher `z` values successively farther down-page.

The function:

```
int SaveVect(struct veloc_t *** const uu, char ***solid,
             int nlay, int nrow, int ncol, int zz[], int nz, int step,
             int nxavg, int nyavg, int useLog, int useColor,
             float maxVectFrac);
```

is analogous to `SaveUPpm()`, except it produces vector plots (like those in figure 9) instead of ppm bitmaps. The vector plots are written in the Hewlett-Packard graphics language (HPGL), and the file names have the form `Vddhhnnn.zzz`, where `V` denotes vector (and does not change), `dd` is the day of the month, `hh` is the hour, `nnn` is the number of the file in the sequence, and `zzz` is the `z` position of the cut in the lattice. Unlike `SaveUPpm()`,

SaveVect() creates a separate file for each cut, since the vector plots are each sufficiently complicated as to swamp many conversion or import utilities in word processors. Current versions of Microsoft Office (after ~1997) do not have built-in HPGL import utilities. However, the files can be converted to PostScript with the free **hp2xx** package, or with commercial conversion utilities. In principal, it should be simple to change the source code to write Windows metafiles instead of HPGL. The **nxavg** and **nyavg** tell the routine how many pixels to average (in *x*- and *y*-directions), and the **useLog** chooses linear (**useLog**=0) or pseudo-logarithmic scaling (**useLog**>0) for vector lengths (the latter is actually a fourth-root scaling, and is useful to emphasize flow in small recirculation zones at modest *Re*). The **useColor** parameter determines if the function will color the vectors to correspond to their lengths (with shortest vectors black, and longest red), and **maxVectFrac()** gives the fraction of the largest LB array dimension (e.g. **ncol**, number of columns) that will be allowed for the longest vector in the plot.

A current limit of the Ppm functions is that they typically allot a maximum **RGB_MAX_SIZE** of 8192 pixels to represent a row. For creating larger plots, this size may simply be increased, or logic added to not plot beyond the end of the array. Alternatively, the arrays could be allocated dynamically and deallocated with each call.

4.15 Measuring Dispersion: The Mean_std.txt File

To measure dispersion by the method of moments¹⁵ [EQ], it is necessary to calculate the moments of the solute distribution as functions of time. The function **MeanStd()** calculates the total solute in the automaton, and the 1st moment and standard deviation of the solute distributions in the *x*- *y*- and *z*-directions at the specified time increments, and writes them to an ASCII file called **Mean_std.txt**. The latter file is opened and closed with every call, so one can make and edit complete copies of the file while JB_PH is running in another window. The file is always opened in “append” mode, and should be pruned periodically. With each JB_PH run, a header is written to **Mean_std.txt**, containing the date, executable name and path, the component used for the moment calculations, and the size of the automaton. Then a tabbed header is written with the column titles, and each subsequent line of the file contains the parameters: **step**, **fSum**, **xMean**, **xStd**, **yMean**, **yStd**, **zMean**, and **zStd**, which correspond to the step number, total sum of solute for the component selected in the call, mean position (1st moment) in the *x*-direction, standard deviation in the *x*-direction, etc. It must be emphasized that **xStd**, **yStd** and **zStd** are standard deviations, *not* variances, and must be squared to obtain the second moments necessary for equation (10). The **fSum** is useful for determining if a slug of solute has begun to “fall off the ends” of the automaton at the end of the run, or if there is something amiss with the boundary conditions. Typically this quantity stays constant to the 5th decimal place for the bulk of a Taylor-Aris dispersion run.

4.16 Reading Solids Geometries from Miscellaneous Files

It is quite simple to read a solid geometry into JB_PH, particularly if the input file is a bitmap or is otherwise organized in *x*-*y*-*z* voxels. In general, the process involves initializing the **SOLID[z][y][x]** array to 0, then reading in the geometry file, and placing a -1 in the **SOLID** array wherever a solid occurs in the geometry file. Then the **SOLID** array is passed to the

function **SetSolidType()**, which determines if solids are at solid-fluid interfaces, or are completely internal.

In some cases, the solid geometry is specified as bounding surfaces, or surfaces that need to be scaled before the mapping into the **SOLID** array. An example is given in the function:

```
int FractalSurface(char *** const solid, int nlay, int nrow,
    int ncol, int hpix, char *fname, int topOrBottom,
    int offs),
```

which takes fractal surface files created by Stephen Brown's **fractal.for** program,^{29,30} and draws the surface into the **SOLID** array. The parameter **hpix** is the number of pixels (rows) that correspond to the maximum relief in the fractal file; **hpix** should generally be less than (**nrow** - **offs**). The solids are drawn from **offs** into the site volume, parallel to the y-direction. If **topOrBottom** is 0, the surface is taken as the "bottom" of the fracture, and solids are filled from the fracture surface down to **offs**; if **topOrBottom** > 0, the surface is taken as the top face of a fracture, and solids are filled from **offs** down to the surface. Thus by pairing the calls to **FractalSurface()**, one can create complicated and asymmetric fractures. The last call should be followed by a call to **SetSolidType()**.

4.17 Generating Pseudo-Random Spherical Packings

The function:

```
int SetFCCSolids(char ***solid, int nlay, int nrow, int ncol,
    int zrep, int yrep, int xrep, float rslop, float cslop,
    float rbias, int seed),
```

fills the **solid** array with a set of slightly randomized, quasi-FCC (face centered-cubic) spheres. The **zrep**, **yrep** and **xrep** are the number of FCC cell reps per **nlay**, **nrow** and **ncol**, respectively; there are 4 complete points per FCC cell. **rslop** is the fractional, random slop applied to the grain radius; **cslop** is the slop applied to the x,y,z position of a grain center. Both **rslop** and **cslop** should be between 0.0 and 0.5. The **rbias** is the bias applied toward smaller grain diameters, vs. larger diameters; it is a float from 0.5 to 1.0, such that 0.5 provides even distribution of radii above and below mean, and 1.0 biases all radii to be below the ideal radius. The **seed** argument is an integer seed used to initiate the random number generator. If **Mrand()** is used, **seed** is a positive integer from 1 to $2^{31}-1$ (seed CANNOT be 0). Note this function call must be followed by a call to **SetSolidType()**. **SetFCCSolids()** was used to generate the solids pattern in figure 14.

Figure 14. A pseudo-randomized solids pattern created by the `SetFCCSolids()` function. The solids are in white, and the colors show an equilibrium flow field, with the lowest flow speeds corresponding to the “coolest” colors (e.g. black), and the warmest colors (red) corresponding to highest flow speeds.

5. History of LB Code Development

The JB_PH code draws on numerous sources. Under the Department of Energy’s Basic Energy Sciences (BES) program, the author developed lattice gas codes from 1991-1995. Several algorithms in JB_PH, such as the Ppm functions and `AdjustGrav()`, are modifications of older LGA routines. Under a BES program to study double-diffusive convection (1996-1998),

the author wrote several 2D LB codes, then the program 3D.c, which included most of the functionality of JB_PH, including the 3D **Collide()** and **Translate()** functions. However, the design of 3D.c benefited from the authors' experience working on 2D codes under a Sandia National Laboratories LDRD program (principally from March 1997 to March 1998). In particular, the LDRD program allowed the author to test accuracy and boundary conditions with rigor, and to optimize and fine-tune the routines. Interactions with David Noble, under the LDRD program, allowed development of the reduced-vector methods for efficient modeling of tracer dispersion and reaction. Finally, the concept of recycling memory and cloning the tracer geometries was developed under BES, in support of the double-diffusive convection program, but was fine-tuned and tested in part under the LDRD.

6. Conclusions

With simple optimizations, the BGK LB method is fast enough, on a single-CPU computer, for modeling complex solids geometries containing millions of nodes. However, care is required to prevent numerical anomalies (such as denormal generation) from reducing overall performance. Good agreement was obtained with four benchmark problems. Simple bounce-back wall conditions are less accurate than other methods,⁹ but yield acceptable errors ($\leq 4\%$), given the inherent uncertainty of dispersion experiments in complex geometries.

7. References

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Appendix: Code Listings

Listing 1. Makeplot().

```
/* mkplot.c -- for JB*.c and 3D*.c programs. */
/* Produces a plotfile of format specified in (*ph) structure */
/* and plothead.h; a fairly compact binary file that can be */
/* intercepted and plotted by a Win32 program like current */
/* pix_test.c... */

#include "plothead.h"
#include <stdio.h>
#include <conio.h>
#include <stdlib.h>
#include <ctype.h>
#include <time.h>
#include <string.h>
#include <io.h>
#include <math.h>

/* Could put the following typedefs in a single header file */
/* used by 3D*.c and JB*.c programs... */
typedef float ff_t;
typedef float u_t;
struct veloc_t {
    u_t x;
    u_t y;
    u_t z;
    u_t usqrd; /* 7-5-97 total speed squared */
} ***U;

/*-----*/
/* NOTE a significant philosophical point: We pass sizeofDatum and */
/* sliceType explicitly, to avoid me forgetting those need to be set; */
/* BEFORE THIS CALL, SHOULD set following ph members: */
/* ux,uy,uz, fx,fy,fz, and any reserved[] members. */
/* THIS CALL WILL SET the ph members: sliceType, sizeofDatum, iComponent, */
/* iCol, iRow, iLay, minDatum, maxDatum, cOfMin, and cOfMax */
/* NOT currently designed for multithreading (multi-threading), because: */
/* buffers are internal and static (as are their lengths), */
/* but I can't imagine any reason one */
/* would want to multi-thread this write within an application, and the */
/* static buffers are safer from unintentional tampering and failed */
/* initialization logic outside this function... The buffers are */
/* reallocated if they are NULL, or if the old lengths are not adequate */
/* for the current calculations and writing... */
/* NOTE when ph->iComponent==0, we use the velocity squared, from */
/* uu[].usqrd; the program utilizing the data is responsible for sqrt(). */
/* NOTE index is the x,y,or z index of the slice (correspondence to */
/* spatial dimension is determined by sliceType), and iComponent is the */
/* component used for the slice... */
/*****/
int MakePlot(ff_t ***** const ff, struct veloc_t *** const uu,
    char *** const solid, int nveloc[], int ncomponent,
```



```

        int nlay, int nrow, int ncol, int ncol_old, int step,
        struct PLOTHEAD *ph, int sliceType, int sizeOfDatum,
        int iComponent, int index)
{
static float *pfBuf=NULL; /* holds a complete slice, densities or speeds */
static unsigned char *puBuf=NULL; /* holds one "line" of data to write,used */
/* only if this is an unsigned char type file (ph->sizeOfDatum==1) */

static int nfBuf=0, nuBuf=0; /* size of buffers above IN BYTES */
static char *fname = "plotfile.bin";

int i,k,x,y,z,s, xb,yb,zb, bCol,bRow,bLay; /* latter are into buffer */
int nfBufOld, nuBufOld;
int nvel;
ff_t ****ffs;
int iOffs, iiOffs; /* used to speed indexing into pfBuf */
float rho, rhoMin, rhoMax, fMul, fDiv;
/* rho must be same type as PH_FSOLID !! */
float fVal; /* 12-21-97 */
FILE *fp;
int istatus;
int xx, iindex; /* xx, iindex for ncol_old stuff */
int sizeOfPlotHead;

/* invalid slice type */
if(sliceType > 3 || sliceType < 0) return(0);
ph->sliceType = sliceType;
if(sizeOfDatum>4 || sizeOfDatum<1) return(0);
ph->sizeOfDatum = sizeOfDatum;

/* preserve previous buffer sizes */
nfBufOld = nfBuf;
nuBufOld = nuBuf;

if(iComponent>=0 && iComponent<ncomponent){
    ph->iComponent = s = iComponent;
    ffs = ff[s]; nvel = nveloc[s];
}
else return(0);

for(k=0; k<PH_MAXTRY; k++){
    fp = fopen(fname, "wb");
    if(fp) break;
    printf("couldn't WRITE, try=%d\n",k);
    _sleep(10);
}
if(!fp) return(0);

bLay = 0;
/* 1st get mapping from ff axes into plot axes, and calculate sizes of buffers */
switch(ph->sliceType){
    case 0: /* x-y, y downscreen, x left-right */
        bRow = ph->iRow = nrow;
        bCol = ph->iCol = ncol;
        ph->iLay = index;
        nuBuf = bCol; /* ONLY used when data size is 1 byte */
        nfBuf = bRow*bCol*sizeof(float);

```


Listing 2. plothead.h

```
/* plothead.h -- add PH_ below to cut down possible conflicts in future, and */
/* set a value to denote the solid */
#define PH_MAXTRY 10
#define PH_NRESERVED 16
#define PH_USOLID 255 /* for unsigned char plotfile, sizeofDatum = 1 */
#define PH_FSOLID -999999.0f /* for float plotfile, sizeofDatum = 4 */
/* for the 1-byte unsigned char data type: */
#define PH_MAX1BYTE 235.0f /* allow 256 minus 20 system colors... */
#define PH_MIN1BYTE 0.0f
/*****
the plot files have following format:
char PH_MACHINE[4]; 4 byte-sized integers:
... 1st is 0 if little-endian like x86, 1 if big-endian like most RISC;
... 2nd is sizeof(int) on the system that wrote file;
... 3rd is sizeof(float) on the system that wrote file;
... 4th is 0 (for now);
int step; ...normally 4-byte
int sizeofPlothead = sizeof(PLOTHEAD); ...normally 4-byte
struct plothead; ...the structure below
[...data...] ...then the data, according to sliceType type
*****/

/* note for x86 every datum is 4-byte */
struct PLOTHEAD {
int sliceType; /* xy=0, xz=1, yz=2, xyz=3 */
int iComponent; /* component number */
int iCol; /* if sliceType == 0,1,3 this is ncol; if sliceType==2, this is x of slice */
int iRow; /* if sliceType == 0,2,3 this is nrow; if sliceType==1, this is y of slice */
int iLay; /* if sliceType == 1,2,3 this is nlay; if sliceType==0, this is z of slice */
float ux; /* ...then the ux,uy,uz speed averages at the speed control slices */
float uy;
float uz;
/*****/
float fx; /* ...then the x,y,z fluxes through the flux measurement slices */
float fy;
float fz;
/*****/
float minDatum; /* minimum datum written to file, converted to float */
float maxDatum; /* maximum datum written to file, converted to float */
float cOfMin; /* the ff[] value corresponding to minimum datum (useful if 1-byte ints
written) */
float cOfMax; /* the ff[] value corresponding to maximum datum (*****) */
float reserved[PH_NRESERVED]; /* for future values; currently garbage */
int sizeofDatum; /* size of each item (bytes) in data to follow */
};

/* add: for x86 */
static char PH_MACHINE[4] = {0, 4, 4, 0};
```

Listing 3. *pix_test.c*

```
/* pix_test.c */
#define SYS_COLOR_WHITE 7
#define MAXARGS 100 //hws 12-9-97
#define HWS_TIMER 1 //hws 12-21-97
#include <windows.h>
#include "hws_rgb.h"
#include "plothead.h"
#include <stdlib.h>
#include <stdio.h>
#include <process.h>
#include <time.h>
char *CMDPTR;
char *EXE_NAME = "JB_PH.exe";
char *PLOTFILE_NAME = "plotfile.bin";
char BUFF[128]; //12-16-97 for test
time_t NEWTIME=0, LASTTIME=-1;

int FIRSTTIME=1;
struct PLOTHEAD PH; /* typed in plothead.h */
unsigned char *PBUF=NULL;
int LASTSTEP=-1, STEP=0, CTR=0;
int GetNewPlot(char *filename, struct PLOTHEAD *ph, int oldStep,
    unsigned char **ppBuf);
int StretchPBUF2DIB(unsigned char *pBuf, struct PLOTHEAD *ph, RECT *rect,
    LPBYTE pDibBits, int iStartColor, int nColorsUsable, int rowBytes);

LRESULT CALLBACK WndProc(HWND, UINT, WPARAM, LPARAM);
int WINAPI WinMain(HINSTANCE hInstance, HINSTANCE hPrevInstance,
    PSTR szCmdLine, int iCmdShow)
{
    static char szAppName[] = "Pix";
    HWND          hwnd;
    MSG           msg;
    WNDCLASSEX    wndclass;
    char *myArgv[MAXARGS];
    int iA, iLastMyArg;
    RECT rect;

    CMDPTR = szCmdLine; //hws for test 12-9-97
    for(iA=1, iLastMyArg = MAXARGS-1; iA<iLastMyArg && iA<__argc; iA++)
    {
        myArgv[iA] = __argv[iA];
    }
    if(iA<MAXARGS) myArgv[iA] = NULL;
    else myArgv[MAXARGS-1] = NULL;
    myArgv[0] = EXE_NAME;

    wndclass.cbSize        = sizeof(wndclass);
    wndclass.style         = CS_HREDRAW | CS_VREDRAW;
    wndclass.lpfnWndProc   = WndProc;
    wndclass.cbClsExtra    = 0;
    wndclass.cbWndExtra    = 0;
```

```

wndclass.hInstance      = hInstance;
wndclass.hIcon          = LoadIcon(NULL, IDI_APPLICATION);
wndclass.hCursor        = LoadCursor(NULL, IDC_ARROW);
wndclass.hbrBackground  = (HBRUSH) GetStockObject(WHITE_BRUSH);
wndclass.lpszMenuName    = NULL;
wndclass.lpszClassName  = szAppName;
wndclass.hIconSm        = LoadIcon(NULL, IDI_APPLICATION);

RegisterClassEx(&wndclass);

hwnd = CreateWindow(szAppName,          // window class name
                   "Pix",              // window caption
                   WS_OVERLAPPEDWINDOW, // window style
                   CW_USEDEFAULT,       // initial x position
                   CW_USEDEFAULT,       // initial y position
                   CW_USEDEFAULT,       // initial x size
                   CW_USEDEFAULT,       // initial y size
                   NULL,                // parent window handle
                   NULL,                // window menu handle
                   hInstance,           // program instance handle
                   NULL);              // creation parameters

ShowWindow(hwnd, iCmdShow);
UpdateWindow(hwnd);

remove(PLOTFILE_NAME);
spawnv(_P_NOWAIT, EXE_NAME, myArgv);

while(!SetTimer(hwnd, HWS_TIMER, 3000, NULL)){
    if(IDCANCEL==MessageBox(hwnd, "Can't grab timer!", szAppName,
                           MB_ICONEXCLAMATION | MB_RETRYCANCEL)) return FALSE;
} // barring exceptional circumstances, timer is set for 3 seconds

while(GetMessage(&msg, NULL, 0, 0)){
    TranslateMessage(&msg);
    DispatchMessage(&msg);
}
return msg.wParam;
} /* END WinMain() */
/*=====FUNCTIONS=====*/
LRESULT CALLBACK WndProc(HWND hwnd, UINT iMsg, WPARAM wParam, LPARAM lParam)
{
    HDC          hdc, hdcMem;
    PAINTSTRUCT  ps;
    RECT         rect;
    int i,x,x3,y,iColor, yHalf;

    /* add 12-4-97 for bitmap creation */

    struct {
        BITMAPINFOHEADER bmih;
        RGBQUAD bmiColors[1];
    } bmi;

    LPBYTE *pBits; // for CreateDIBSection; will DeleteObject deallocate?
    HBITMAP hBitmap; // return from CreateDIBSection; must delete!
    HBITMAP hBitmapNew; // for CreateDIBitmap

```



```

int iOffs,ii; // account for 3 bytes/row and dword boundary
int iLines;
static int rowBytes;

int xPixPerMeter, yPixPerMeter;
LPBITMAPINFOHEADER pDib;
LPBYTE pDibBits;
HDC hdcRef;
HBITMAP hBitmapDIB,hbmOld;
HDC hdcBitmap;
RGBQUAD *rgbPtr;
int nColors; //hws
int iStartColor = 10, nColorsUsable; //hws 12-17-97

switch(iMsg){
    case WM_CREATE:
        return(0);
    case WM_TIMER:
        STEP = GetNewPlot(PLOTFILE_NAME, &PH, LASTSTEP, &PBUF);
        if(STEP>LASTSTEP && PBUF!=NULL){
            FIRSTTIME = 0;
            LASTSTEP=STEP;
            CTR++;
            InvalidateRect(hwnd, NULL, FALSE);
        }
        return(0);
    case WM_PAINT:
        hdc = BeginPaint(hwnd, &ps);
        GetClientRect(hwnd, &rect);
        if(FIRSTTIME){
            DrawText(hdc, "Waiting for LB data", -1, &rect,
                DT_SINGLELINE | DT_CENTER | DT_VCENTER);
            EndPaint(hwnd,&ps); return(0);
        }
        // hws should make the 256 more general below
        pDib = (LPBITMAPINFOHEADER)GlobalAlloc(GPTR,(sizeof(BITMAPINFOHEADER) +
            256 * sizeof(RGBQUAD)));
        pDib->biSize = sizeof(BITMAPINFOHEADER);
        pDib->biWidth = rect.right;
        pDib->biHeight = rect.bottom;
        pDib->biPlanes = 1;
        pDib->biBitCount = 8;

        // below hws presumes biBitCount = 8 !
        rowBytes = (pDib->biWidth + 3) & 0xFFFC;
        nColors = 1 << pDib->biBitCount; //hws for future
        nColorsUsable = nColors - 20; //hws 12-17-97

        hdcRef = GetDC(0);

        hBitmapDIB = CreateDIBSection(hdcRef, (BITMAPINFO *)pDib,DIB_RGB_COLORS,
            (VOID **)&pDibBits,NULL,0);
        hdcBitmap = CreateCompatibleDC(hdcRef);

        rgbPtr = (RGBQUAD *) (pDib + 1); //hws

        GetSystemPaletteEntries(hdcRef,0,10,rgbPtr);

```

```

//hws -- add in some more colors
// 12-15-97 try other palette
for(i=10,ii=0; i<nColors-10; i++,ii++){
    (rgbPtr+i)->rgbBlue = rgbHWS0[ii].rgbBlue;
    (rgbPtr+i)->rgbGreen = rgbHWS0[ii].rgbGreen;
    (rgbPtr+i)->rgbRed = rgbHWS0[ii].rgbRed;
    (rgbPtr+i)->rgbReserved = 0;
}
ReleaseDC(0,hdcRef);
hbmOld = SelectObject(hdcBitmap,hBitmapDIB);

SetDIBColorTable(hdcBitmap,0,nColors,(RGBQUAD *) (pDib + 1));

StretchPBUF2DIB(PBUF, &PH, &rect,
    pDibBits, iStartColor, nColorsUsable, rowBytes);

//hdc = GetDC(hwnd);
BitBlt(hdc,0,0,pDib->biWidth,pDib->biHeight,hdcBitmap,0,0,SRCCOPY);
//ReleaseDC(hwnd,hdc);
// 12-16-97 test
sprintf(BUFF,"STEP=%d, CTR=%d", STEP, CTR);
DrawText(hdc, BUFF, -1, &rect,
    DT_SINGLELINE | DT_CENTER | DT_VCENTER);

SelectObject(hdcBitmap,hbmOld);
DeleteObject(hBitmapDIB);
DeleteObject(hbmOld);
GlobalFree(pDib);
GlobalFree(pDibBits);
EndPaint(hwnd,&ps);
return(0);
case WM_DESTROY:
    PostQuitMessage(0);
    return(0);

} /* END big message switch */
return DefWindowProc(hwnd, iMsg, wParam, lParam);
} /* END WndProc() */
/*-----*/
/* Routines to interpret PBUF and map to pDibBits; for now */
/* we'll just handle sizeofDatum==1... */
int StretchPBUF2DIB(unsigned char *pBuf, struct PLOTHEAD *ph, RECT *rect,
    LPBYTE pDibBits, int iStartColor, int nColorsUsable, int rowBytes){

int x,y, iOffs, iColor, xp, yp; /* latter are into the pBuf */
int ipRow, ipCol, ipLay;
int ipOffs;
float xMul, yMul, cMul, cDelta;
unsigned char cVal;

if(ph->sizeofDatum > 1) return(0); /* change when we have float handler */

/* No matter what, need to know the correspondence of iRow, iCol and */
/* iLay stored in new file with logical coordinates in pBuf... */
/* From sliceType, determine the mapping of file rows into logical */
/* screen rows... first do the setup: */

```

```

switch(ph->sliceType){
    case 0: /* x-y, y downscreen, x left-right */
        ipRow = ph->iRow;
        ipCol = ph->iCol;
        break;
    case 1: /* x-z, z upscreen, x left-right */
        ipRow = ph->iLay;
        ipCol = ph->iCol;
        break;
    case 2: /* y-z, y downscreen, z left-right */
        ipRow = ph->iRow;
        ipCol = ph->iLay;
        break;
    case 3: /* x-y-z, not currently covered */
        ipLay = ph->iLay;
        ipRow = ph->iRow;
        ipCol = ph->iCol;
        break;
    default:
        /* this type not recognized, try to exit gracefully */
        return(0);
} /* END switch to get pRow, pCol and pLay of NEW plot */

/* next calculate the conversion multipliers; MUST be positive... */
if(rect->right > 1) xMul = (float)ipCol/(float)rect->right; else return(0);
if(rect->bottom > 1) yMul = (float)ipRow/(float)rect->bottom; else return(0);

/* Next find color conversion rules; typically iStartColor is 10, and */
/* nColorsUsable=236... */
cDelta = (ph->maxDatum - ph->minDatum);
if(cDelta<1.0e-10) cMul = 0.0;
else {
    cMul = (nColorsUsable-1)/cDelta;
}
/* Logic below assumes data are unsigned char type; would need conversions */
/* if ph->sliceType were 4 and float... */
/* we let the display coords be of primary importance; thus */
/* we convert the automaton values to display (DIB) coords */
/* and always set the latter to be in DIB bounds... */
for(y=0; y<rect->bottom; y++){
    yp = y*yMul; if(yp>ipRow) yp = ipRow;
    iOffs = y*rowBytes; ipOffs = yp*ipCol; /* could condense latter! */
    for(x=0; x<rect->right; x++){
        xp = x*xMul; if(xp>ipCol) xp = ipCol;
        /* in here figure out iColor */
        cVal = *(pBuf + ipOffs + xp);
        if(cVal==PH_USOLID) iColor = SYS_COLOR_WHITE;
        else {
            iColor = (int)(cMul*(cVal - ph->minDatum));
            if(iColor>=nColorsUsable) iColor = nColorsUsable-1;
            iColor += iStartColor;
        }
        *(pDibBits + iOffs + x) = iColor;
    }
}
return(1);
} /* END FillpDIB() */

```

Listing 4. GetNewPlot()

```
/* This function checks the currently available plotfile.bin and */
/* determines if it is new. If not, it returns old step. If the file */
/* is new (as determined by step number), key vars in the old */
/* ph structure are saved; then the new structure is read in, and */
/* the old and new key values read to determine if a memory reallocation */
/* is needed (would happen if the slice type changed or the data size */
/* (e.g. 1 byte unsigned char vs float) changed. Note after call, */
/* should check *sizeofDatumPtr to determine to cast pbuf as unsigned char */
/* or as float... */
/* NOTE must be careful to not deallocate pBuf, not depend on ph, if this */
/* is the first time the function is called! */
#include <string.h>
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <process.h>
#include <conio.h>
#include <windows.h> /* may be used eventually for pipes */

#include "plothead.h"
int GetNewPlot(char *filename, struct PLOTHEAD *ph, int oldStep,
               unsigned char **ppBuf)
{
    static int firstTime=1;
    int i,n,k, sizeofHeader, sizeofDatum, step;
    FILE *fp;
    char machine[4]; /* not used 12-10-97 */
    int dummy;
    int iRowOld, iColOld, iLayOld, sliceTypeOld, sizeofDatumOld;
    int pLay,pRow,pCol; /* Logical rows and cols in pBuf; mapping to */
                        /* iLay, iRow, and iCol depend on sliceType... */
    int pz,py,px;      /* Indices along logical pLay, pRow and pCol... */
    int doAlloc;
    int istatus;
    int sizeofpBuf;

    /* char buf[64]; */

    /* 1st try PH_MAXTRY (in plothead.h) times to open the file */
    for(k=0; k<PH_MAXTRY; k++){
        fp = fopen(filename, "rb");
        if(fp) break;
    /* debug */ printf("couldn't READ, try=%d\n",k);
        _sleep(10);
    }
    /* debug */ puts("AA");
    if(!fp) return(oldStep);

    /* debug */ puts("AAAAAA");
    /* we have file pointer, now start the read */
    fread(machine, sizeof(machine), 1, fp); /* not now used; in general routine */
    /* would decide sizeof(int), endianness, etc. from machine... */

    fread(&step, sizeof(step), 1, fp);
```

```

if(step <= oldStep){
    fclose(fp);
    /* debug */ puts("BB");
    return(oldStep);
}
/* save old values of iCol, iRow, iLay, sliceType, sizeOfDatum before wiping out
*/
/* NOTE if firstTime, these will be junk! */
iLayOld = ph->iLay; iRowOld = ph->iRow; iColOld = ph->iCol;
sliceTypeOld = ph->sliceType; sizeOfDatumOld = ph->sizeOfDatum;

fread(&sizeOfHeader, sizeof(sizeOfHeader), 1, fp);
/* should put in contingency to deal with old header size not equal to new! */
/* ...in case one produced on 64-bit machine... */

/* read in the plothead, wiping out old values */
fread(ph, sizeOfHeader, 1, fp);

/* Now must determine if we have to reallocate the pBuf; DON'T do this */
/* the first time through! */
doAlloc = 0;
if(firstTime){
    doAlloc = 1;
}
else if(iLayOld != ph->iLay || iRowOld != ph->iRow || iColOld != ph->iCol
    || sliceTypeOld != ph->sliceType || sizeOfDatumOld != ph->sizeOfDatum){
    if(*ppBuf && (sliceTypeOld>=0 && sliceTypeOld<=3)) free(*ppBuf);
    doAlloc = 1;
} /* END deallocation and doAlloc setting if-else */

/* No matter what, need to know the correspondence of iRow, iCol and */
/* iLay stored in new file with logical coordinates in pBuf... */
/* From sliceType, determine the mapping of file rows into logical */
/* screen rows... first do the setup: */
switch(ph->sliceType){
    case 0: /* x-y, y downscreen, x left-right */
        pRow = ph->iRow;
        pCol = ph->iCol;
        break;
    case 1: /* x-z, z upscreen, x left-right */
        pRow = ph->iLay;
        pCol = ph->iCol;
        break;
    case 2: /* y-z, y downscreen, z left-right */
        pRow = ph->iRow;
        pCol = ph->iLay;
        break;
    case 3: /* x-y-z, not currently covered */
        pLay = ph->iLay;
        pRow = ph->iRow;
        pCol = ph->iCol;
        break;
    default:
        /* this type not recognized, try to exit gracefully */
        fclose(fp);
        /* debug */ puts("CC");
        return(oldStep);
}

```

```

    }    /* END switch to get pRow, pCol and pLay of NEW plot */

/* Get total buffer size */
sizeOfpBuf = ph->sizeOfDatum * pRow * pCol;
if(ph->sliceType == 3) sizeOfpBuf *= pLay;

if(doAlloc){
    *ppBuf = malloc(sizeOfpBuf); /* assuming unsigned char is one byte! */
    if(!(*ppBuf)){ fclose(fp); /* debug */ puts("DD"); return(oldStep);}
    } /* End if on doAlloc */

/* Now read the data into the buffer... */
istatus = fread(*ppBuf, sizeOfpBuf, 1, fp);
/* Try not deallocating ppBuf; may want to reset firsttime **
if(istatus != 1){ fclose(fp); free(*ppBuf); puts("EE"); return(oldStep);}
** */
if(istatus != 1){ fclose(fp);/* free(*ppBuf);*/ /* debug */ puts("EE");
return(oldStep);}

if(fp) fclose(fp);
firstTime = 0;
/* debug */ puts("FF");
return(step);
}    /* END GetNewPlot() */

```

Listing 5. JB_PH.C

```

/***** JB_ph.c *****/
/* 3-D LB multi-component code with D3Q19 geometry */
/* (Qian et al., 1992); Martys and Chen, 1996) and Flekkoy (1993) */
/* treatment of tracers. Will allow for 6-vec tracers as extrap. */
/* from ideas in Wolf-Gladrow, RD Kingdon et al., Maier e-mail, and */
/* D. Noble thesis. */
/* REQUIRES: mkplot.c and plothead.h */
/*****
/* THIS PROGRAM IS COPYRIGHTED BY H.W. STOCKMAN (hwstock@sandia.gov) */
/* for Sandia National Laboratories. */
/*****
/* In D3Q19, will keep old 2D numbering system for 1st 9 vectors, */
/* as indicated below: */
/*
/*      4  3  2      |      11      |      15      */
/*      \  |  /      |      |      |      */
/*      5 -- 0 -- 1   |      12 -- 9 -- 10   |      16 -- 18 -- 14   */
/*      /  |  \      |      |      |      */
/*      6  7  8      |      13      |      17      */
/*
/*      MIDDLE      |      TOP      |      BOTTOM      */
/*****
/***** below is key for velocity notations, 6 VECTOR model (D2Q6) *****/
/*      1      |      and the up (positive z) vector is 4, */
/*      |      |      and the down (negative z) vector is 5 */
/*      2 -- * -- 0   |      */
/*      |      |      */
/*      3      |      */
/***** CHANGES *****/
/* Use Kahan suggestion about initializing or setting all denorms to */
/* initially small value (in ieee754.ps at his web site)... see *.030898 */
/* version for status before today... */
#define KAHAN_0 1.0e-32f
/***** INCLUDES *****/
#include <stdio.h>
#include <conio.h>
#include <stdlib.h>
#include <ctype.h>
#include <time.h>
#include <string.h>
#include <io.h>
#include <math.h>
#include <dos.h>
#include "plothead.h"
/***** DEFINES *****/
/* For sphere volume; JoSphere() */
#define PI_4_3RDS 4.188790204
#define PI_HWS 3.14159265358979
/* For fractal surface selection; FractalSurface() */
#define TOP_SURFACE 1
#define BOTTOM_SURFACE 0
/* Defines used in SetFlags() */
/* SEE flags_struct below and SetFlags() */
#define MIN_NCOL 4

```

```

#define MAX_NCOL      10000
#define MIN_NROW      4
#define MAX_NROW      10000
#define MIN_NLAY      4
#define MAX_NLAY      10000
#define MIN_NVELOC     6
#define MAX_NVELOC    19
#define MIN_MAXSTEP    0
#define MAX_MAXSTEP 10000000
#define MIN_XBODY     -1.0
#define MAX_XBODY      1.0
#define MIN_YBODY     -1.0
#define MAX_YBODY      1.0
#define FLAG_HELP     -1
#define MIN_U         -0.15
#define MAX_U          0.15
#define MIN_BOUNDARY   0
#define MAX_BOUNDARY   1
#define MIN_NTIMES    0
#define MAX_NTIMES 1000
/* MIN_COEF, MAX_COEF serve for viscosity and diffusion coeff. */
#define MIN_COEF 1.0e-4
#define MAX_COEF 10.0

#define NPEN 8 /* pens for HPGL */
#define BOX_X1 0
#define BOX_Y1 1
#define BOX_X2 2
#define BOX_Y2 3

#define MRAND_RANGE 2147483647.0
/* above is upper limit Mrand(); note Mrand returns an INTEGR value between 1 */
/* and MRAND_RANGE! If you substitute a different random number generator, */
/* you must substitute its range here... */
#define RAND_NORM (1.0/MRAND_RANGE)

#define MAX_COMP 10 /* Maximum # components */
#define ONE_HALF 0.5
#define ONE_3RD 0.3333333333333333
#define ONE_18TH 0.05555555555555556
#define ONE_36TH 0.02777777777777778
#define ONE_6TH 0.16666666666666667
#define HALF_SQRT2 0.707106781
#define DEF_NVELOC 19 /* maximum size for any array of f-dist vectors */
#define ZIEGLER_1ST_CODE 1 /* For non-bounce-back flow boundaries */
#define ZIEGLER_END_CODE 32 /* 7-5-97 completely fictional for now */
/* DOS keystroke defines below */
#define CTRL_RIGHT 29696
#define CTRL_LEFT 29440
/* 4-1-92 */
#define CTRL_PGUP 33792
#define CTRL_PGDN 30208
#define CTRL_HOME 30464
#define CTRL_END 29952

#define RIGHT 19712
#define LEFT 19200

```



```

#define UP 18432
#define DOWN 20480
/* shifted arrow keys require numlock off, numeric keypad */
#define SHIFT_RIGHT 19766
#define SHIFT_LEFT 19252
#define SHIFT_UP 18488
#define SHIFT_DOWN 20530
#define END 20224
#define HOME 18176
#define PGUP 18688
#define PGDN 20736
#define RETURN 7181
#define ESC 283
/* 3-25-92 below */
#define INSERT 20992
#define DELETE 21248
#define TAB 3849
#define SHIFT_TAB 3840
#define F1 15104
#define F2 15360
#define F3 15616
#define F4 15872
#define F5 16128
#define F6 16384
#define F7 16640
#define F8 16896
#define F9 17152
#define F10 17408

/***** BASIC TYPES AND ARRAYS, GLOBALS *****/
typedef int box_t[4]; /* for clipping in vector drawing routines */

typedef float ff_t;
typedef float u_t;
struct veloc_t {
    u_t x;
    u_t y;
    u_t z;
    u_t usqrd; /* total speed squared */
} ***U;

struct PLOTHEAD PH; /* For writing plotfile.bin; see MkPlot.c */

ff_t ****FF;
char ***SOLID;
float RHO[MAX_COMP]; /* Average particles/site; used ONLY in initialization.
*/
double TAU[MAX_COMP], OMEGA[MAX_COMP], BETA[MAX_COMP];
/* Relaxation param and 1/tau... */

/* arbitrary defaults below */
int NCOL = 128;
int NCOL_OLD = 128;
int NTIMES = 1;
int NROW = 30;
int NLAY = 128; /* layers in z direction */
int NCOMPONENT = 2;

```

```

int NVELOC[MAX_COMP]= {19,6,6,6,6,6,6,6,6,6}; /* for now, set all tracers =6 */
int STEP=0, MAXSTEP=10000;
int RADIUS=0; /* 10-29-97 sphere radius for jo.c */
int JO_AND_STEP=31; /* 10-29-97 for jo.c only */
int JO_SOLIDS=0; /* 10-29-97 for jo.c only */
int USE_ALVEOLI=0, XZALV=2,YALV=1;

int XSCR=79, YSCR=24; /* max number rows, columns in screen */

int SOLIDS_SET = 0;
int SOLIDS_ENCLOSED = 0;
int JUST_DISPERSE_STEP = MAX_MAXSTEP;

/* List of z values to pass to SaveUPpm(), SaveVect() */
#define NZ 4
int ZZ[NZ];

/*****
/* Set up an array for ideal equil distribution in a 19-vector */
/* carrier fluid... */
double TT[19] =
/*====0=====1=====2=====3=====4=====5=====6====*/
{ ONE_3RD , ONE_18TH, ONE_36TH, ONE_18TH, ONE_36TH, ONE_18TH, ONE_36TH,
/*====7=====8=====9=====10=====11=====12=====13====*/
  ONE_18TH, ONE_36TH, ONE_18TH, ONE_36TH, ONE_36TH, ONE_36TH, ONE_36TH,
/*====14=====15=====16=====17=====18====*/
  ONE_36TH, ONE_36TH, ONE_36TH, ONE_36TH, ONE_18TH};

/* Arrays for coord deltas in x,y,z directions, corresponding */
/* to the notation at top of file; should ease logic in functions */
/* and should eventually be incorporated in an */
/* include file (*.h)... Given to help other programmers; currently unused. */
int DX[19] =
/*====0=====1=====2=====3=====4=====5=====6====*/
{ 0 , 1 , 1 , 0 , -1 , -1 , -1 ,
/*====7=====8=====9=====10=====11=====12=====13====*/
  0 , 1 , 0 , 1 , 0 , -1 , 0 ,
/*====14=====15=====16=====17=====18====*/
  1 , 0 , -1 , 0 , 0 , 0 };

int DY[19] =
/*====0=====1=====2=====3=====4=====5=====6====*/
{ 0 , 0 , -1 , -1 , -1 , 0 , 1 ,
/*====7=====8=====9=====10=====11=====12=====13====*/
  1 , 1 , 0 , 0 , -1 , 0 , 1 ,
/*====14=====15=====16=====17=====18====*/
  0 , -1 , 0 , 1 , 0 , 0 };

int DZ[19] =
/*====0=====1=====2=====3=====4=====5=====6====*/
{ 0 , 0 , 0 , 0 , 0 , 0 , 0 ,
/*====7=====8=====9=====10=====11=====12=====13====*/
  0 , 0 , 1 , 1 , 1 , 1 , 1 ,
/*====14=====15=====16=====17=====18====*/
  -1 , -1 , -1 , -1 , -1 , -1 };

/*****

```

```

struct gravity {
    int do_x;          /* logicals; determine if limits are applied */
    int do_y;
    int do_z;
    /*-----body forces, acting on component 0-----*/
    double xBody;
    double yBody;
    double zBody;
    /*-----buoyancy forces, acting on components > 0-----*/
    double xBuoy;
    double yBuoy;
    double zBuoy;
    /*-----increments for adjusting body forces-----*/
    double txBody; /* temporary, adjusted values */
    double tyBody;
    double tzBody;
    double xBodyInc; /* increments for changing gravity */
    double yBodyInc;
    double zBodyInc;
    double xBodyIncSmall; /* smaller increments for changing gravity */
    double yBodyIncSmall;
    double zBodyIncSmall;
    /*-----Speeds-----*/
    double uxLimit;      /* The maximum allowed speed */
    double uyLimit;
    double uzLimit;
    double uxLast;       /* Speed measured in previous adjustment */
    double uyLast;
    double uzLast;
    /*-----endpoints of planes used to measure speeds-----*/
    int xUx; /* the vertical y-z plane (into page) for measuring ux */
    int y1Ux;
    int y2Ux;
    int z1Ux;
    int z2Ux;
    int yUy; /* the horizontal x-z plane (into page) for measuring uy */
    int x1Uy;
    int x2Uy;
    int z1Uy;
    int z2Uy;
    int zUz; /* the x-y plane (parallel to page) for measuring uz */
    int x1Uz;
    int x2Uz;
    int y1Uz;
    int y2Uz;
    /*-----reserve a pointer for alpha coefficient array-----*/
    double alpha[MAX_COMP]; /* NEEDS to be initialized! */
    /*-----steps after 1st gravity adjustment to start/stop clamping-----*/
    int stepStartClamp;
    int stepStopClamp;
} G;

/***** for command line processing *****/
/* Reserve w for z-direction speed, and z for z-dir force, but don't implement
now. */
struct flags_struct {
    int ncol; /* flag = c */
    int use_ncol;

```

```

int nrow;      /* flag = r */
int use_nrow;
int nlay;      /* flag = l (L) add 7-16-97 */
int use_nlay;
int nveloc;
int use_nveloc; /* flag = i, # of velocity vectors for solutes, 6 or 19 */
int maxstep;   /* flag = s */
int use_maxstep;
int jdispstep; /* flag = j step start JustDisperse() */
int use_jdispstep;
int boundary;  /* flag = b */
int use_boundary;
int stepSlug;  /* flag = g (changed from l in 2D) */
int use_stepSlug;
double xBody;  /* flag = x */
int use_xBody;
double yBody;  /* flag = y */
int use_yBody;
double uxMax;  /* flag = u */
int use_uxMax;
double uyMax;  /* flag = v */
int use_uyMax;
double viscosity; /* viscosity, flag = n */
int use_viscosity;
double diff1;   /* diffusion coefficient, component 1; command flag = d */
int use_diff1;
double diff2;   /* diffusion coefficient, component 2; flag = D */
int use_diff2;
char *fname;    /* geometry file name, flag = f */
int use_fname;
int radius;
int use_radius; /* sphere radius, used by Jo*() only, flag = o */
int ntimes;
int use_ntimes;
int xzGrid;     /* flag=#, alveoli grid in x and z, inside meas. */
int use_xzGrid;
int yGrid;      /* flag=^, alveoli height in y direction */
int use_yGrid;
} FLAG;

double DENSITY_REF, DEL_DENSITY_REF;

FILE *LOG_fp=NULL; /* error logging; when we split into several input */
/* files, will have to make an extern global, or pass */

/* 7-17-97 for localtime() use */
struct tm *PTM;
time_t LTIME;
int USE_ZIEGLER=0; /* use bounceback to start */

/***** FUNCTION DECLARATIONS *****/
int Translate(ff_t ***** const ff, int ncomponent,
             int nveloc[], int nlay, int nrow, int ncol, int sstart),

Collide(ff_t *const*const*const*const* ff,
        double *const tau, double *const beta,
        double *const omega, struct veloc_t *const*const* uu,

```

```

    struct gravity * const gp, char *const*const* solid,
    int ncomponent, int nveloc[], int nlay, int nrow, int ncol),

Plot9Vec(ff_t ***** const ff, float * const rho, int ncomponent,
    int nveloc[], int nlay, int nrow, int ncol, int step),

PlotConcs(ff_t *const*const*const*const* ff,
    char *const*const* solid, float * const rho,
    struct veloc_t *const*const* uu,
    int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
    int ncol_old, /* 10-30-97 add ncol_old */
    int step, int s, int xStart, int yStart, int zz, int zoomMode),

SetSlug(ff_t *****ff, char ***solid, int ncomponent, int nveloc[],
    int nlay, int nrow, int ncol, int x1, int x2, int y1, int y2,
    int z1, int z2, double *concList),

SetSolidType(char ***solid, int nlay, int nrow, int ncol),

Mrand(int z),

SetFCCSolids(char ***solid, int nlay, int nrow, int ncol,
    int zrep, int yrep, int xrep, float rslop, float cslop,
    float rbias, int seed),

AdjustGrav(struct veloc_t *const*const* uu,
    char *const*const* solid,
    int nlay, int nrow, int ncol, struct gravity * const gp),

XSetConc(ff_t ***** const ff, char *** const solid,
    int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
    int x, int y1, int y2, int z1, int z2, double * const concList),

YSetConc(ff_t ***** const ff, char *** const solid,
    int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
    int y, int x1, int x2, int z1, int z2, double * const concList),

SaveUPpm(struct veloc_t *** const uu, char ***solid,
    int nlay, int nrow, int ncol, int zz[], int nz, int step),

SaveVect(struct veloc_t *** const uu, char ***solid,
    int nlay, int nrow, int ncol, int zz[], int nz, int step,
    int nxavg, int nyavg, int useLog, int useColor, float maxVectFrac),

ClipLine(float *x1p, float *y1p, float *x2p, float *y2p,
    box_t box),

Clipt(double p, double q, double *t1p, double *t2p),

DrawBox(float x1, float x2, float y1, float y2,
    box_t clipbox, FILE *fp, int color),

SetFlags(int argc, char *argv[], struct flags_struct *fp),

FractalSurface(char *** const solid, int nlay, int nrow, int ncol,
    int hpix, char *fname, int topOrBottom, int offs),

```

```

JustDisperse3D(ff_t *const*const*const*const* ff,
double * const tau, double * const beta, double *const omega,
struct veloc_t *const*const* uu, char *const*const* solid,
int ncomponent, int nveloc[], int nlay, int nrow, int ncol, int ncol_old),

/* Next two: add capability to select simpler function */
JustDisperse3D_A(ff_t *const*const*const*const* ff,
double * const tau, double * const beta, double *const omega,
struct veloc_t *const*const* uu, char *const*const* solid,
int ncomponent, int nveloc[], int nlay, int nrow, int ncol, int ncol_old),

(*JustDisp_ptr)(ff_t *const*const*const*const* ff,
double * const tau, double * const beta, double *const omega,
struct veloc_t *const*const* uu, char *const*const* solid,
int ncomponent, int nveloc[], int nlay, int nrow, int ncol, int ncol_old),

ReadBmp4Slug(ff_t ***** const ff, char *** const solid, float rho,
int nvel, int nlay, int nrow, int ncol, int sstart,
int x, int z, char *filename),

YSetConcJB(ff_t ***** const ff, char *** const solid,
int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
int y, int x1, int x2, int z1, int z2, double * const concList),

XSetConcJB(ff_t ***** const ff, char *** const solid,
int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
int x, int y1, int y2, int z1, int z2, double * const concList),

Recycle(ff_t ***** const ff, char *** const solid, int ncomponent,
int nveloc[], int nlay, int nrow, int ncol, int ntimes, int xRight),

JoSphere(char ***solid, int nlay, int nrow, int ncol, int radius),

/* For Eidsath et al. (1983) test */
JoDisk(char ***solid, int nlay, int nrow, int ncol, int radius),

MakePlot(ff_t ***** const ff, struct veloc_t *** const uu,
char *** const solid, int nveloc[], int ncomponent,
int nlay, int nrow, int ncol, int ncol_old, int step, struct PLOTHEAD *ph,
int sliceType, int sizeOfDatum, int iComponent, int index);

/* The 1st three are dummy placeholders for non-bounce-back walls. */
double NoFlux(double f[], int solidcode, int mode),
NoFlux6(double f[], int solidcode, int mode),
Ziegler(double f[], int solidcode, int mode),

UxAvg(struct veloc_t *const*const* uu,
char *const*const* solid,
int nlay, int nrow, int ncol, int x, int y1, int y2, int z1, int z2),

UyAvg(struct veloc_t *const*const* uu,
char *const*const* solid,
int nlay, int nrow, int ncol, int y, int x1, int x2, int z1, int z2),

UzAvg(struct veloc_t *const*const* uu,
char *const*const* solid,
int nlay, int nrow, int ncol, int z, int x1, int x2, int y1, int y2),

```

```

XGetFlux(ff_t ***** const ff, char *** const solid,
         int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
         int x, int y1, int y2, int z1, int z2, int s, double * const ftotPtr),

YGetFlux(ff_t ***** const ff, char *** const solid,
         int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
         int y, int x1, int x2, int z1, int z2, int s, double * const ftotPtr),

DrawArrow(float xx1, float yy1, float xx2, float yy2,
          float factor, float mul, int color, FILE *hpgl_fp, box_t box),

MeanStd(ff_t ***** const ff, char *** const solid, int ncomponent,
        int nveloc[], int nlay, int nrow, int ncol, int sstart,
        int step, char *pathname, int use_z);

FILE *SavePpm(ff_t *****ff, char ***solid, int ncomponent, int nveloc[],
             int nlay, int nrow, int ncol, int sstart, int step),
*Save3DPpm(ff_t *****ff, char ***solid, int ncomponent, int nveloc[],
           int nlay, int nrow, int ncol, int sstart, int step),
*SavePpmXY_XZ(ff_t *****ff, char ***solid, int ncomponent, int nveloc[],
              int nlay, int nrow, int ncol, int sstart, int step, int colorCode);

/*****
/***** MAIN ** MAIN ** MAIN ** MAIN *****/
/*****
main(int argc, char *argv[])
{
int x,y,z, i,k,m,n,s, ierror=0, key, upkey;
double concList1[MAX_COMP], concList2[MAX_COMP];
/* File pointers with "list" are lists of ppm files to be used for movies. */
FILE *b_list_fp=NULL, *fp, *t_list_fp=NULL;
float ftemp; /* 7-6-97 */
double ux; /* 7-9-97 */
double fSum; /* 7-18-97 */
double volume; /* 10-29-97 */
int istatus=0; /* 12-20-97 for MakePlot() */
int yendAlv; /* 6-14-98 */
int ii, ystartAlv; /* 6-28-98 */

int xRightConc, xLeftConc; /* 9-26-97; these ought to go in structures, */
/* for now they are the Right and Left XSetConc() boundaries... */

/* Variables for character-mode panning and zooming; in 3D (3-d) */
/* we will look at a z-slice, plotting the x-y plane at zPlot, for */
/* the component selected by sPlot... */
int zoomMode=1, yStart=0, xStart=0, yStartLast=0, xStartLast=0,
    zPlotLast=0, sPlotLast=0;
int yStartMax, xStartMax, halfXscr, halfYscr;
int zPlot=0, sPlot=0; /* 7-5-97 */
double uxmax, uyavg, uxavg;
int stepStartSlug, x1Slug, x2Slug, y1Slug, y2Slug, z1Slug, z2Slug;

/** 8:30 PM 7-5-97 temporary indices to set up an R-T instability */
int x1RT, x2RT, z1RT, z2RT;
int ctr; /* 7-9-97 for testing FCC function */

```

```

/***** START DATA LOGGING *****/
LOG_fp = fopen("lb_log.txt", "a");
if(LOG_fp){
    /* 1st get time and date */
    time(&LTIME);
    PTM = localtime(&LTIME);
    fprintf(LOG_fp,"START LOG===== %s %02d/%02d/%04d %02d:%02d:%02d =====\n",
        argv[0], PTM->tm_mon+1, PTM->tm_mday, PTM->tm_year+1900,
        PTM->tm_hour, PTM->tm_min, PTM->tm_sec);
}

/***** PARSE CONTROL FILE *****/
/** 7-17-97 in here we would put any function that would read **/
/** a control file with simulation controls, geometries etc. **/

/***** READ ANY COMMAND-LINE PARAMS (FLAGS) *****/
if(SetFlags(argc, argv, &FLAG)==FLAG_HELP){
    if(LOG_fp) fclose(LOG_fp);
    exit(0); /* if we displayed help, quit */
}

/* Now that we have flags, must decide how many components we */
/* really have (if command args set d, D, will assume 2 or 3) */
n = 1;
if(FLAG.use_diff1) n = 2;
if(FLAG.use_diff2) n = 3;
if(n>NCOMPONENT) NCOMPONENT = n;

if(FLAG.use_maxstep) MAXSTEP = FLAG.maxstep;
if(FLAG.use_jdispstep) JUST_DISPERSER_STEP = FLAG.jdispstep; /* 5-29-97 */
if(FLAG.use_ncol) NCOL = FLAG.ncol;
if(FLAG.use_nrow) NROW = FLAG.nrow;
if(FLAG.use_nlay) NLAY = FLAG.nlay;
volume = NLAY*NCOL*NROW; /* 10-29-97 */
if(FLAG.use_radius) RADIUS = FLAG.radius;
if(FLAG.use_ntimes) NTIMES = FLAG.ntimes;

NCOL_OLD = NCOL;

printf("NCOL=%d, NROW=%d, NLAY=%d, NCOMPONENT=%d\n", NCOL, NROW, NLAY,
NCOMPONENT);

/* NOTE presumes default NVELOC set at top, as always want NVELOC[0] = 19
anyway... */
if(FLAG.use_nveloc){
    for(s=1; s<MAX_COMP; s++){
        NVELOC[s] = FLAG.nveloc;
    }
}

/* Set Ziegler option from flags; NOT IMPLEMENTED */
/** if(FLAG.use_boundary) USE_ZIEGLER = FLAG.boundary; **/

/* For slug starting step: */
if(FLAG.use_stepSlug) stepStartSlug = FLAG.stepSlug;
else stepStartSlug = MAXSTEP;

```



```

/* 7-18-97 test zero-speed case, so change 1st line below temporarily */
/* 12-26-97 modify x1Slug below to get after 1st sphere-- copied from */
/* \jb_sphere\jb_1.c */
/** 2-28-98 comment out sphere-slug for Eidsath et al. Disk test **/
x1Slug = (NCOL>>1);
x2Slug = x1Slug + (NCOL >> 2);
y1Slug = 0; y2Slug = NROW-1;
z1Slug = 0; z2Slug = NLAY-1;
/** 2-27-98 end comment out **/

/* 6-14-98 comment out below */
/** 2-28-98 more appropriate slug for Eidsath et al. test **
x1Slug = 2*RADIUS-1;
x2Slug = NCOL-2;
y1Slug = 0; y2Slug = NROW-1;
z1Slug = 0; z2Slug = NLAY-1;
** 2-28-98 END more appropriate slug for Eidsath et al. test **/

/* 7-11-97 for SaveUPpm(), 7-14-97 SaveVect() */
k = NLAY / NZ;
for(i=0; i<NZ; i++) ZZ[i] = k*i;

/* 2-24-98 KLUDGE for JFM article: */
ZZ[1] = 1; ZZ[2] = 2; ZZ[3] = 3;

/* Set up plotting constraints for character-mode (console) */
/* display via PlotConc()...*/
/* last xStart before abutting end of ... */
xStartMax = NCOL-1-XSCR; yStartMax = NROW-1-YSCR;
halfXscr = XSCR >> 1; halfYscr = YSCR >> 1;
sPlot = 0; /* 7-9-97 for testing */

/* primary memory allocation; start over sigmas */

FF = malloc(sizeof(ff_t ****)*NCOMPONENT);
if(!FF) goto error_primary_alloc;
for(s=0; s<NCOMPONENT; s++){ /* 5-22-97 note NVELOC now array */
    FF[s] = malloc(sizeof(ff_t ****)*NVELOC[s]);
    if(!FF[s]) goto error_comp_alloc;
    for(i=0; i<NVELOC[s]; i++){
        FF[s][i] = malloc(sizeof(ff_t **)*NLAY);
        if(!FF[s][i]) goto error_veloc_alloc;
        for(z=0; z<NLAY; z++){
            FF[s][i][z] = malloc(sizeof(ff_t *)*NROW);
            if(!FF[s][i][z]) goto error_z_alloc;
            for(y=0; y<NROW; y++){
                FF[s][i][z][y] = malloc(sizeof(ff_t)*NCOL);
                if(!FF[s][i][z][y]) goto error_row_alloc;
            }
        }
    }
}

printf("Completed allocations!\n"); /* 5-22-97 change below */

/* initialize the FF to 0.0 out of paranoia */
for(s=0; s<NCOMPONENT; s++){
    for(i=0; i<NVELOC[s]; i++){

```

```

        for(z=0; z<NLAY; z++){
            for(y=0; y<NROW; y++){
                for(x=0; x<NCOL; x++){
                    FF[s][i][z][y][x] = KAHAN_0; /* 3-8-98 */
                }
            }
        }
    }
}

printf("Completed FF initializations!\n");

/* allocate and initialize the solids */
SOLID = malloc(sizeof(char **)*NLAY);
if(!SOLID) goto error_solidprimary_alloc;
for(z=0; z<NLAY; z++){
    SOLID[z] = malloc(sizeof(char *)*NROW);
    if(!SOLID[z]) goto error_solidlay_alloc;
    for(y=0; y<NROW; y++){
        SOLID[z][y] = malloc(sizeof(char)*NCOL);
        if(!SOLID[z][y]) goto error_solidrow_alloc;
    }
}

/* 6-30-97 note new philosophy packs U's into structure */
U = malloc(sizeof(struct veloc_t **)*NLAY);
if(!U) goto error_U_alloc;
for(z=0; z<NLAY; z++){
    U[z] = malloc(sizeof(struct veloc_t *)*NROW);
    if(!U[z]) goto error_Ulay_alloc;
    for(y=0; y<NROW; y++){
        U[z][y] = malloc(sizeof(struct veloc_t)*NCOL);
        if(!U[z][y]) goto error_Urow_alloc;
    }
}

/***** VELOCITY INITIALIZATION (U[][][]) *****/
for(z=0; z<NLAY; z++){
    for(y=0; y<NROW; y++){
        for(x=0; x<NCOL; x++){
            U[z][y][x].x = 0.0;
            U[z][y][x].y = 0.0; U[z][y][x].z = 0.0;
            U[z][y][x].usgrd = 0.0;
        }
    }
}

/***** SOLIDS INITIALIZATIONS *****/
/* NOTE , MUST (in here use a SetSolid() type routine) */
/* 7-5-97 quickie start: set all to -1 at bounding y, */
/* set rest to 0... */
/* 7-11-97 changed below to make sure we init y bounds as 0 */
for(z=0; z<NLAY; z++){
    for(y=0; y<NROW; y++){
        for(x=0; x<NCOL; x++){
            SOLID[z][y][x] = 0;
        }
    }
}

```

```

    }
/* 8-1-98 bounding planes back in for T-A at other viscosities */
/* 6-21-98 back in for bounding planes */
/** 10-29-97 comment out bounding solid planes **
for(z=0; z<NLAY; z++){
    for(x=0; x<NCOL; x++){
        SOLID[z][0][x] = -1;
        SOLID[z][NROW-1][x] = -1;
    }
}
** end 10-29-97 comment out **/

/** 6-23-98 TEMPORARY front wall and top wall for DDG test **
for(y=0; y<NROW; y++){
    for(x=0; x<NCOL; x++){
        SOLID[0][y][x] = -1;
    }
}
for(z=0; z<NLAY; z++){
    for(x=0; x<NCOL; x++){
        SOLID[z][0][x] = -1;
    }
}
** END 6-23-98 TEMPORARY front wall and top wall for DDG test **/

/* 9-17-97 read in Steve Brown's fractal geometry files... */
/* for now, just hardwire the names... 9-23-97 hpix from 10 to 16... */

/** 10-29-97 comment out fractal read **
ierror = FractalSurface(SOLID, NLAY, NROW, NCOL, 20, "srb1.txt",1,1);
printf("at Fractal read, ierror=%d\n", ierror);

ierror = FractalSurface(SOLID, NLAY, NROW, NCOL, 20, "srb2.txt",0,1);
printf("at Fractal read, ierror=%d\n", ierror);
** end 10-29-97 **/

/* 7-9-97 test the FCC algorithm */
/***** 7-18-97 comment out to do Taylor-Aris *****/
ctr = SetFCCSolids(SOLID, NLAY, NROW, NCOL, 2, 2, 2, 0.20, 0.20,
    0.75, 178923);
printf("# spheres = %d\n",ctr);
/***** END 7-18-97 comment out to do Taylor-Aris *****/

/** 2-27-98 comment out sphere test: **/
if(RADIUS){
    JO_SOLIDS = JoSphere(SOLID, NLAY, NROW, NCOL, RADIUS);
    printf("*** Number of solids is %d\n", JO_SOLIDS);
    printf("**** actual      solid/volume is %f\n", JO_SOLIDS/volume);
    printf("**** predicted solid/volume is %f\n",
        (RADIUS*RADIUS*RADIUS*PI_4_3RDS)/volume);
    if(LOG_fp){
        fprintf(LOG_fp,"*** Number of solids is %d\n", JO_SOLIDS);
        fprintf(LOG_fp,"**** actual      solid/volume is %f\n",
            JO_SOLIDS/volume);
        fprintf(LOG_fp,"**** predicted solid/volume is %f\n",
            (RADIUS*RADIUS*RADIUS*PI_4_3RDS)/volume);
    }
}

```

```

    }
/** 2-27-98 end comment out **/
/** 6-13-98 comment out Eidsath et al. disk test **
if(RADIUS){
    JO_SOLIDS = JoDisk(SOLID, NLAY, NROW, NCOL, RADIUS);
    printf("*** Number of solids is %d\n", JO_SOLIDS);
    printf("**** actual      solid/volume is %f\n", JO_SOLIDS/volume);
    printf("**** predicted solid/volume is %f\n",
        (RADIUS*RADIUS*PI_HWS*NLAY)/volume);
    if(LOG_fp){
        fprintf(LOG_fp, "*** Number of solids is %d\n", JO_SOLIDS);
        fprintf(LOG_fp, "**** actual      solid/volume is %f\n",
            JO_SOLIDS/volume);
        fprintf(LOG_fp, "**** predicted solid/volume is %f\n",
            (RADIUS*RADIUS*PI_HWS*NLAY)/volume);
    }
}
}
** 6-13-98 END Eidsath et al. disk test **/

/** 6-14-98 set up grid for alveoli test, and channel flow speed **/
if(FLAG.use_xzGrid){
    XZALV = FLAG.xzGrid;
    if(XZALV>NLAY) XZALV=NLAY;
    if(XZALV>NCOL) XZALV=NCOL;
    USE_ALVEOLI = 1;
}
if(FLAG.use_yGrid){
    YALV = FLAG.yGrid;
    if(YALV>(NROW>>1)-1) YALV = (NROW>>1)-1;
    USE_ALVEOLI = 1;
}
if(FLAG.use_yGrid && !FLAG.use_xzGrid){
    XZALV = (NCOL<NLAY) ? NCOL : NLAY;
}
if(!FLAG.use_yGrid && FLAG.use_xzGrid){
    YALV = NROW >> 2;
}
/* 6-28-98 comment out to replace with for new longitudinal baffles */
/* do actual grid -- for now, no complete sidewalls */
// if(USE_ALVEOLI){
//     /* 6-20-98 unblock to recompile for 00_open.exe */
//     /** 6-15-98 for rest of tests, block off entire z=0 wall **
//     for(y=0; y<NROW; y++){
//         for(x=0; x<NCOL; x++){
//             SOLID[0][y][x] = -1;
//         }
//     }
//     ** END 6-15-98 block off wall **/
//
//     /* plates parallel to z,y */
//     for(x=0; x<NCOL; x+=XZALV){
//         for(z=0; z<NLAY; z++){
//             /* plates coming down from top; NOTE start at 1 */
//             for(y=1; y<=YALV; y++) SOLID[z][y][x] = -1;
//             /* plates coming up from bottom; NOTE start at NROW-1 */
//             for(y=NROW-1, yendAlv=y-YALV; y>yendAlv; y--) SOLID[z][y][x] = -
1;

```

```

//      }
//    }
//    /* plates parallel to x,y */
//    for(z=0; z<NLAY; z+=XZALV){
//      for(x=0; x<NCOL; x++){
//        /* plates coming down from top; NOTE start at 1 */
//        for(y=1; y<=YALV; y++) SOLID[z][y][x] = -1;
//        /* plates coming up from bottom; NOTE start at NROW-1 */
//        for(y=NROW-1,yendAlv=y-YALV; y>yendAlv; y--) SOLID[z][y][x] = -
1;
//      }
//    }
//    /* do top plate, y=0 */
//    for(z=0; z<NLAY; z++){
//      for(x=0; x<NCOL; x++){
//        SOLID[z][0][x] = -1;
//      }
//    }
//  }
/** END 6-14-98 set up grid for alveoli test... */
/* 6-21-98 add block for plain DDG test */
/** 6-21-98 8 AM comment out for TA re-test **
else {
  for(y=0; y<NROW; y++){
    for(x=0; x<NCOL; x++){
      SOLID[0][y][x] = -1;
    }
  }
  for(z=0; z<NLAY; z++){
    for(x=0; x<NCOL; x++){
      SOLID[z][0][x] = -1;
    }
  }
}
** END 8 AM TA re-test comment out */
/* 7-25-98 comment out long. baffles */
/** 6-28-98 END comment out z-x gridded alveoli, start section */
/** to use longitudinal, alternating (start top or bottom) baffles */
// if(USE_ALVEOLI){
//   /* plates parallel to x,y */
//   for(ii=z=0; z<NLAY; z+=XZALV,ii++){
//     if(ii&1){
//       ystartAlv = 1; yendAlv = YALV;
//     }
//     else {
//       ystartAlv = NROW-YALV; yendAlv = NROW-1;
//     }
//     for(y=ystartAlv; y<=yendAlv; y++){
//       for(x=0; x<NCOL; x++){
//         SOLID[z][y][x] = -1;
//       }
//     }
//   }
//   /* do top plate, y=0 */
//   for(z=0; z<NLAY; z++){
//     for(x=0; x<NCOL; x++){
//       SOLID[z][0][x] = -1;

```

```

//      }
//      }
//      /* 7-3-98 recompile with open for last check (// comment below) */
//      /* after compiling once with above code, saved as 00_open_bafl.exe, add:
*/
//      /* do vertical plate z=0 to close off */
//      for(y=0; y<NROW; y++){
//      for(x=0; x<NCOL; x++){
//      SOLID[0][y][x] = -1;
//      }
//      } /*...and save this as 00_bafl.exe 6-28-98 */
//      }
/** END 6-28-98 new alveoli block **/

/* 7-8-97 try SetSolidType() so we can get the enclosed solids */
SOLIDS_ENCLOSED = SetSolidType(SOLID, NLAY, NROW, NCOL);
printf("Number of totally enclosed solids = %d\n", SOLIDS_ENCLOSED);
/* getch(); ** DEBUG 7-8-97 */

/* 8:30 PM 7-5-97 set all Body force to 0, but set yBuoy to neg value */
/* for R-T (Rayleigh-Taylor) instability */

/***** GRAVITY INITIALIZATIONS *****/
/* 7-18-97 move some defaults up here */
/* 7-9-97 set xBody to 0.001 for permeability test */
G.xBody = 0.000; G.yBody = 0.0000; G.zBody = 0.0000;
/* 7-9-97 drop yBuoy from -0.05 to 0 for permeability test */
G.xBuoy = 0.0000; G.yBuoy = 0.0000; G.zBuoy = 0.0000;
G.alpha[0] = 0.99823; /* 12-31-96 density pure water at 20C */

/* 10-29-97 comment out below and set up better decision logic */
/* G.stepStartClamp = 1000; G.stepStopClamp = 2000; */
/* 10-29-97 make clamping tied to other time limits, if set... */
if(FLAG.use_jdispstep && FLAG.jdispstep > 4){
    G.stepStartClamp = FLAG.jdispstep >> 1; /* 2-28-98 below was jdispstep-1 */
    G.stepStopClamp = FLAG.jdispstep - (FLAG.jdispstep >> 2);
}
else {
    G.stepStartClamp = MAXSTEP >> 4;
    G.stepStopClamp = MAXSTEP >> 3;
}

if(FLAG.use_xBody){
    G.do_x = 1; G.xBody = FLAG.xBody;
}
else G.do_x=0; /* 7-17-97 may wish to set to 0; 7-18-97 was 1 */

if(FLAG.use_yBody){
    G.do_y = 1; G.yBody = FLAG.yBody;
}
else G.do_y = 0;

G.do_z = 0; /* 7-17-97 for now, no flags used here */

/* 10-18-97 move below here (was above flag inits) */
G.txBody = G.xBody; G.tyBody = G.yBody; G.tzBody = G.zBody;

```

```

/* 7-9-97 add some inits of the UxAvg() params */
/* 6-14-98 change G.xUx to 0 (from NCOL-1) to capture between-solids Ux */
G.xUx = 0;      G.y1Ux = 0; G.y2Ux = NROW-1; G.z1Ux = 0; G.z2Ux = NLAY-1;
G.yUy = NROW-1; G.x1Uy = 0; G.x2Uy = NCOL-1; G.z1Uy = 0; G.z2Uy = NLAY-1;
G.zUz = NLAY-1; G.y1Uz = 0; G.y2Uz = NROW-1; G.x1Uz = 0; G.x2Uz = NCOL-1;

/** 7-9-97 add **/
G.xBodyInc = G.xBody*0.015625;
G.yBodyInc = G.yBody*0.015625;
G.zBodyInc = G.zBody*0.015625;
G.xBodyIncSmall = G.xBody*0.00390625;
G.yBodyIncSmall = G.yBody*0.00390625;
G.zBodyIncSmall = G.zBody*0.00390625;

/* 3-15-97 */
if(FLAG.use_uxMax) G.uxLimit = FLAG.uxMax;
else G.uxLimit = 0.02;
if(FLAG.use_uyMax) G.uyLimit = FLAG.uyMax;
else G.uyLimit = 0.0;

G.uzLimit = 0.0;

/* 7-18-97 debug */
printf("ux limit=%f, xBody=%f, do_x=%d\n", G.uxLimit, G.xBody, G.do_x);

/***** Concentration Boundary Initializations *****/
/* added 9-26-97; for now, JUST set the xRightConc */
xRightConc = NCOL - 1;

/***** RHO, TAU, ETC. INITIALIZATIONS *****/
RHO[0] = 3.0;
/* 7-17-97 flag OR default viscosity */
if(FLAG.use_viscosity){
    TAU[0] = 3.0*FLAG.viscosity + 0.5; /* note visc <-> tau conversion */
}
else TAU[0] = 0.6;

/* Paranoia below; will probably supercede in a few lines */
for(s=1; s<NCOMPONENT; s++){
    RHO[s] = BETA[s] = 0.0; TAU[s] = OMEGA[s] = 1.0;
}

/*DENSITY_REF = 1.004864; ** 1-6-97 for Clay's newer system */
DENSITY_REF = 0.99823; /* 7-5-97 to get bigger diff for R-T */

DEL_DENSITY_REF = DENSITY_REF - G.alpha[0];

concList1[0] = concList2[0] = -1.0;
if(NCOMPONENT>1){
    /* 12-29-96 component 1 is NaCl */
    RHO[1] = 0.18696; /* 1-6-97 molal, density=1.00618 @ 20C */
    TAU[1] = 0.51; /* 7-10-97 was 0.501; 1-6-97, was 0.503; 12-31-96 was 0.51 */
    G.alpha[1] = 0.04227; /* CRC for 1.088% solution */
    if(FLAG.use_diff1){
        if(NVELOC[1]==19)
            TAU[1] = 3.0*FLAG.diff1 + 0.5; /* note diffusion <-> tau conversion */
    }
}

```

```

        else if (NVELOC[1]==6) /* 7-18-97 correct 2 vs 3D */
            TAU[1] = 3.0*FLAG.diff1 + 0.5; /* note diffusion <-> tau conversion */
        }
/* TEMP assign rest of concList values */
concList1[1] = RHO[1]; concList2[1] = 0.0; /* 2-5-97 */
}

/* 12-14-96 WATCH OUT, NOTE hard-wired */
if(NCOMPONENT>2){
    /* component 2 is sucrose */
    RHO[2] = 0.0404; /* 1-6-97 molal, density=1.003548 @ 20C */
    TAU[2] = 0.5003; /* 1-6-97, was 0.501; 12-31-96 was 0.503 */
    G.alpha[2] = 0.13107; /* g/cm3/mole; from CRC values for 1.381% solution */
    if(FLAG.use_diff2){
        if(NVELOC[2]==19)
            TAU[2] = 3.0*FLAG.diff2 + 0.5; /* note diffusion <-> tau conversion */
        else if (NVELOC[2]==6) /* 7-18-97 correct 2 vs 3D */
            TAU[2] = 3.0*FLAG.diff2 + 0.5; /* note diffusion <-> tau conversion */
        }
    }
}

for(s=0; s<NCOMPONENT; s++){
    /* MUST eventually deal with tau == 0.000 */
    OMEGA[s] = 1.0/TAU[s];
    BETA[s] = 1.0 - OMEGA[s]; /* add 12-5-96 */
}

/***** FLUIDS INITIALIZATION *****/
/* 7-9-97 NOTE SOLID MUST be init by here! */
/* 7-5-97 this logic used 7-2-97 to test translate; comment out */
/***** comment out the below **
x = (NCOL-1)>>1; y = (NROW-1)>>1; z = (NLAY-1)>>1; s=0;
for(i=0; i<NVELOC[0]; i++){
    FF[s][i][z][y][x] = RHO[0]*TT[i];
}
** comment out the above ****/

/* 7-9-97 alter below to allow for solids; initailly just won't init solids */
/* with carrier fluid, but will want to change for Ziegler and NoFlux, */
/* which allow wall streaming... */
/* 7-5-97 do primitive fluid init for CARRIER; NOTE set all comp. to 0 */
/* just after allocation of FF... */
for(z=0; z<NLAY; z++){
    for(y=0; y<NROW; y++){
        for(x=0; x<NCOL; x++){
            if(SOLID[z][y][x]) continue; /* 7-9-97 */
            for(i=0; i<DEF_NVELOC; i++){
                FF[0][i][z][y][x] = TT[i]*RHO[0];
            }
        }
    }
}

}

/**** 8:30 PM 7-5-97 put in temporary block to set up R-T (Rayleigh-Taylor) ****/
/**** 7-9-97 comment out R-T 2nd component block **
printf("about to init R-T lower solute block\n");

```



```

ftemp = ONE_6TH*RHO[1];
if(NCOMPONENT>1){
    for(z=0; z<NLAY; z++){
        for(y=0; y<NROW>>1; y++){
            for(x=0; x<NCOL; x++){
                if(SOLID[z][y][x]) continue;
                for(i=0; i<NVELOC[1]; i++){
                    FF[1][i][z][y][x] = ftemp;
                }
            }
        }
    }
}

** end 7-9-97 comment out R-T **/
/* also for R-T, perturb two odd points at interface */
/** 7-9-97 comment out another R-T block **
printf("about to init R-T odd points\n");
x1RT = (NCOL>>1) + (NCOL>>2);
x2RT = (NCOL>>1) - (NCOL>>3);
z1RT = (NLAY>>1) + (NLAY>>3)-1;
z2RT = (NLAY>>1) - (NLAY>>2)+1;
for(i=0; i<NVELOC[1]; i++){
    FF[1][i][z1RT][NROW>>1][x1RT] = TT[i]*RHO[1];
    FF[1][i][z2RT][NROW>>1][x2RT] = TT[i]*RHO[1];
}
** 7-9-97 END comment out R-T **/
/* END R-T init of component 1 */

/* 6-13-98 select a simple JustDisperse3D() if possible */

if(NCOMPONENT==2 && NVELOC[1]==6){
    JustDisp_ptr = JustDisperse3D_A;
    /* puts("\007\007 USE _A !!!!!!!!!!!!!!!!!!!!!!! \007"); */
}
else JustDisp_ptr = JustDisperse3D;

/***** OPEN GENERAL DATA FILE LB_DATA.TXT *****/
/* NOTE 7-17-97 we inefficiently close this file after every write... */
fp = fopen("lb_data.txt", "a");
if(fp){
    /* 1st get time and date */
    time(&LTIME);
    PTM = localtime(&LTIME);
    fprintf(fp, "START::::: %s %02d/%02d/%04d %02d:%02d:%02d ::::::START\n",
        argv[0], PTM->tm_mon+1, PTM->tm_mday, PTM->tm_year+1900,
        PTM->tm_hour, PTM->tm_min, PTM->tm_sec);
    /* 10-29-97 add */
    fprintf(fp, "maxstep=%d, clampstep=%d, radius=%d, solids=%d\n",
        MAXSTEP, G.stepStopClamp, RADIUS, JO_SOLIDS);
    fprintf(fp, "-----\nSTEP\tUx\ttxBody\n");
    fclose(fp);
}

/***** STEPS *****/
/* %%%%%%%%%%%%%% BIG LOOP OVER STEPS %%%%%%%%%%%%%% */
printf("about to start steps!\n");

```

```

for(STEP=0; STEP<MAXSTEP; STEP++){
    if(kbhit()){ /* 2-22-97 use simple 27==ESC for VC++ version */
        key = _getch(); upkey = toupper(key);
        if(key==27 || upkey=='Q') break;
        else if(upkey=='Z' || upkey=='S'){
            if(upkey=='Z') zoomMode = !zoomMode;
            else if(upkey=='S'){
                sPlot++;
                if(sPlot >= NCOMPONENT) sPlot = 0;
                if(sPlot != sPlotLast) printf("SSSSSSS!!  s now %d
\r",sPlot);

                sPlotLast = sPlot;
            } /* 10-30-97 add NCOL_OLD below */
            ierror = PlotConcs(FF, SOLID, RHO, U, NCOMPONENT,
                NVELOC, NLAY, NROW, NCOL, NCOL_OLD, STEP, sPlot, xStart,
                yStart, zPlot, zoomMode);
        }
        else if(key==0 || key==0xE0){
            key = _getch() << 8;
            if(zoomMode){
                if(key==UP){
                    yStart -= halfYscr;
                    if(yStart < 0) yStart = 0;
                }
                else if(key==DOWN){
                    yStart += halfYscr;
                    if(yStart > yStartMax) yStart = yStartMax;
                }
                if(key==LEFT){
                    xStart -= halfXscr;
                    if(xStart < 0) xStart = 0;
                }
                else if(key==RIGHT){
                    xStart += halfXscr;
                    if(xStart > xStartMax) xStart = xStartMax;
                }
                else if(key==PGUP){
                    zPlot++;
                    if(zPlot >= NLAY) zPlot = 0;
                }
                else if(key==PGDN){
                    zPlot--;
                    if(zPlot < 0) zPlot = NLAY-1;
                }

                if(yStart!=yStartLast || xStart!=xStartLast ||
                    zPlot!=zPlotLast || sPlotLast != sPlot)
                    ierror = PlotConcs(FF, SOLID, RHO, U, NCOMPONENT,
                        NVELOC , NLAY, NROW, NCOL, NCOL_OLD,
                        STEP, sPlot, xStart,
                        yStart, zPlot, zoomMode);
                if(zPlot != zPlotLast) printf("ZZZZZZZ!!  z now %d
\r",zPlot);

                xStartLast = xStart; yStartLast = yStart; zPlotLast = zPlot;
            }
        }
    }
}

```

```

/* Plot9Vec() call below typically used in isolation to test translate step; */
/* requires getch() to halt for inspection... */
/* ierror = Plot9Vec(FF, RHO, NCOMPONENT, NVELOC, NLAY, NROW, NCOL, STEP); */

/* 9-27-97 test Recycle() capability */
if(STEP==JUST_DISPERSE_STEP){
    printf("\r@ just_disp =====\r");
    ierror = Recycle(FF, SOLID, NCOMPONENT, NVELOC, NLAY, NROW, NCOL,
        NTIMES, xRightConc);
    if(ierror>xRightConc){
        NCOL_OLD= NCOL; NCOL*=NTIMES; xRightConc=ierror;
        xStartMax = NCOL-1-XSCR;
        printf("passed Recycle(), xRightConc=%d NCOL=%d\n",
            xRightConc, NCOL);
/*          getch(); ** comment out 12-26-97 */
    }
    else printf("!!!! FAILED in Recycle()\007 !!!!!\n");
}

/* 9-23-97 mods for JustDisperse3D() */
if(STEP<JUST_DISPERSE_STEP)
    ierror = Translate(FF, NCOMPONENT, NVELOC, NLAY, NROW, NCOL, 0);
else
    ierror = Translate(FF, NCOMPONENT, NVELOC, NLAY, NROW, NCOL, 1);

if(STEP==stepStartSlug){
    printf("||| about to set slug |||\n");
    SetSlug(FF, SOLID, NCOMPONENT, NVELOC, NLAY, NROW, NCOL,
        x1Slug, x2Slug, y1Slug, y2Slug, z1Slug, z2Slug, concList1);
    printf("||| SET SLUG |||\n");

    /** below in late 9-23-97; 9-27-97 changed 0 to 10 below... **/
/** comment out 10-29-97 **
    ReadBmp4Slug(FF, SOLID, RHO[NCOMPONENT-1], NVELOC[NCOMPONENT-1],
        NLAY, NROW, NCOL, NCOMPONENT-1, 10, 0, "harlan2.bmp");
**/

    /* 9-23-97 changed last arg below from 0.1 to 0.05 */
    /* 2-21-98 changed below for new function */
/* 6-14-98 comment out SaveVect() to see if it is locking up with odd ncol */
/*      SaveVect(U, SOLID, NLAY, NROW, NCOL, ZZ, NZ, STEP,2,2,1,0,0.08); */
/*      SaveUPpm(U, SOLID, NLAY, NROW, NCOL, ZZ, NZ, STEP); */
}

/* 9-23-97 for JUST_DISP */
if(STEP<JUST_DISPERSE_STEP)
    ierror = Collide(FF, TAU, BETA, OMEGA, U, &G, SOLID, NCOMPONENT,
        NVELOC, NLAY, NROW, NCOL);
else
    ierror = JustDisp_ptr(FF, TAU, BETA, OMEGA, U, SOLID, NCOMPONENT,
        NVELOC, NLAY, NROW, NCOL, NCOL_OLD);

/***** APPLYING BOUNDARIES, ADJUSTING GRAVITY *****/
/* 9-27-97 change to use XSetConcJB() after just_disp_step... */
/* 9-26-97 change NCOL-1 in XSetConc() to xRightConc... */
/* 7-18-97 put sink back to old way, for Taylor-Aris */
/* 7-12-97 put sink on opposite end, so we can make pretty pictures */

```

```

/* via Save3DPpm() (was x=NCOL-1, now 0)... */
if(STEP<JUST_DISPERSE_STEP){
    XSetConc(FF, SOLID, NCOMPONENT, NVELOC, NLAY, NROW, NCOL,
        xRightConc, 0, NROW-1, 0, NLAY-1, concList2);
    AdjustGrav(U, SOLID, NLAY, NROW, NCOL, &G);
}
else {
    XSetConcJB(FF, SOLID, NCOMPONENT, NVELOC, NLAY, NROW, NCOL,
        xRightConc, 0, NROW-1, 0, NLAY-1, concList2);
}
/***** PLOTTING *****/
if((STEP&31)==0){ /* 7-18-97 was &15; 12-20-97 back from &31 */
    /***** PLOT TO SCREEN *****/
    ierror = PlotConcs(FF, SOLID, RHO, U, NCOMPONENT,
        NVELOC, NLAY, NROW, NCOL, NCOL_OLD, STEP, sPlot, xStart,
        yStart, zPlot, zoomMode);
    /* 7-9-97 test UxAvg() */
    ux = UxAvg(U, SOLID, NLAY, NROW, NCOL, G.xUx,
        G.y1Ux, G.y2Ux, G.z1Ux, G.z2Ux);
    printf("step %d, ux=%8.4f\r", STEP, ux);
    /* 8-2-98 comment out plotfile for timing */
    /***** PLOT TO PLOTFILE *****/
    istatus = MakePlot(FF, U, SOLID, NVELOC, NCOMPONENT,
        NLAY, NROW, NCOL, NCOL_OLD, STEP, &PH, 0, 1, sPlot, zPlot);
    if(!istatus) puts("failed to write plotfile.bin");
    /***** PLOT TO PPM *****/
    /***** 7-18-97 comment out for Taylor-Aris *****/
    /* 10-31-97 increase from ppm every 32 to every 512 */
    if((STEP&511)==0 && NCOMPONENT>1){
        /* 9-23-97 change to XY_XZ version below */
        /* 2-21-98 set colorCode==1 as last arg */
        /** 2-27-98 comment out **
            b_list_fp = SavePpmXY_XZ(FF, SOLID, NCOMPONENT, NVELOC, NLAY,
                NROW, NCOL, NCOMPONENT-1, STEP, 1);
        ** END 2-27-98 comment out */
        /**9-23-97 comment out 3D**
            t_list_fp = Save3DPpm(FF, SOLID, NCOMPONENT, NVELOC, NLAY,
                NROW, NCOL, NCOMPONENT-1, STEP);
        **/
    }
    /***** END 7-18-97 comment out for Taylor-Aris *****/
    /***** WRITE TO MeanStd *****/
    fSum = MeanStd(FF, SOLID, NCOMPONENT, NVELOC, NLAY, NROW,
        NCOL, 1, STEP, argv[0], 0);
}
}
/***** END LOOP OVER STEPS *****/
/* 6-21-98 make sure we are printing at NLAY>>1 (middle) */
fp = fopen("ux_uy.txt", "w");
fprintf(fp, "uxavg\tuyavg\tuxmax\n");
for(y=0; y<NROW; y++){ /* 6-21-98 NCOL_OLD!!, not NCOL */
    for(uxmax=-1.e20, uxavg=0.0, uyavg=0.0, x=0; x<NCOL_OLD; x++){
        uxavg += U[NLAY>>1][y][x].x; uyavg += U[NLAY>>1][y][x].y;
        if(uxmax<U[NLAY>>1][y][x].x) uxmax = U[NLAY>>1][y][x].x;
    }
    uxavg /= NCOL_OLD; uyavg /= NCOL_OLD;
    fprintf(fp, "%f\t%f\t%f\n", uxavg, uyavg, uxmax);
}

```

```

    }
fclose(fp);

if(b_list_fp) fclose(b_list_fp);
if(t_list_fp) fclose(t_list_fp);
if(LOG_fp) fclose(LOG_fp); /* 7-17-97 */

exit(0);
/*===== ERROR CODES =====*/
error_primary_alloc:
printf("couldn't allocate primary FF\n");
if(LOG_fp){
    fprintf(LOG_fp,"couldn't allocate primary pointer\n");
    fclose(LOG_fp);
}
exit(1);
/*-----*/
error_comp_alloc:
printf("couldn't allocate FF[%d]\n",s);
if(LOG_fp){
    fprintf(LOG_fp,"couldn't allocate FF[%d]\n",s);
    fclose(LOG_fp);
}
exit(2);
/*-----*/
error_veloc_alloc:
printf("couldn't allocate FF[%d][%d]\n",s,i);
if(LOG_fp){
    fprintf(LOG_fp,"couldn't allocate FF[%d][%d]\n",s,i);
    fclose(LOG_fp);
}
exit(3);
/*-----*/
error_z_alloc:
printf("couldn't allocate FF[%d][%d][%d]\n",s,i,z);
if(LOG_fp){
    fprintf(LOG_fp,"couldn't allocate FF[%d][%d][%d]\n",s,i,z);
    fclose(LOG_fp);
}
exit(4);
/*-----*/
error_row_alloc:
printf("couldn't allocate FF[%d][%d][%d][%d]\n",s,i,z,y);
if(LOG_fp){
    fprintf(LOG_fp,"couldn't allocate FF[%d][%d][%d][%d]\n",s,i,z,y);
    fclose(LOG_fp);
}
exit(5);
/*-----*/
error_solidprimary_alloc:
printf("couldn't allocate primary SOLID\n");
if(LOG_fp){
    fprintf(LOG_fp,"couldn't allocate primary SOLID\n");
    fclose(LOG_fp);
}
exit(6);
/*-----*/

```



```

/***** for veloc 1 (0 degrees) *****/
for(y=0; y<nrow; y++){
    pftemp = ff[s][1][z][y];
    ftemp = pftemp[ncol-1];
    for(x=ncol-1; x>0; x--){ /* this block to memory move
eventually */
        pftemp[x] = pftemp[x-1];
    }
    pftemp[0] = ftemp;
}
/***** for veloc 5 (180 degrees) *****/
for(y=0; y<nrow; y++){
    pftemp = ff[s][5][z][y];
    ftemp = pftemp[0];
    for(x=1; x<ncol; x++){ /* this block to memory move eventually
*/
        pftemp[x-1] = pftemp[x];
    }
    pftemp[ncol-1] = ftemp;
}
/***** for veloc 3 (90 degrees) *****/
pftemp = ff[s][3][z][0];
for(y=1; y<nrow; y++){
    ff[s][3][z][y-1] = ff[s][3][z][y];
}
ff[s][3][z][nrow-1] = pftemp;
/***** for veloc 7 (270 degrees) *****/
pftemp = ff[s][7][z][nrow-1];
for(y=nrow-1; y>0; y--){
    ff[s][7][z][y] = ff[s][7][z][y-1];
}
ff[s][7][z][0] = pftemp;
/***** for veloc 2 (45 degrees) *****/
pftemp = ff[s][2][z][0]; /* shuffle pointers */
for(y=1; y<nrow; y++){
    ff[s][2][z][y-1] = ff[s][2][z][y];
}
ff[s][2][z][nrow-1] = pftemp;
for(y=0; y<nrow; y++){ /* shuffle x */
    pftemp = ff[s][2][z][y];
    ftemp = pftemp[ncol-1];
    for(x=ncol-1; x>0; x--){ /* this block to memory move
eventually */
        pftemp[x] = pftemp[x-1];
    }
    pftemp[0] = ftemp;
}
/***** for veloc 4 (135 degrees) *****/
pftemp = ff[s][4][z][0]; /* shuffle pointers */
for(y=1; y<nrow; y++){
    ff[s][4][z][y-1] = ff[s][4][z][y];
}
ff[s][4][z][nrow-1] = pftemp;
for(y=0; y<nrow; y++){
    pftemp = ff[s][4][z][y];
    ftemp = pftemp[0];

```

```

        for(x=1; x<ncol; x++){ /* this block to memory move eventually
*/
            pftemp[x-1] = pftemp[x];
        }
        pftemp[ncol-1] = ftemp;
    }
    /***** for veloc 6 (225 degrees) *****/
    pftemp = ff[s][6][z][nrow-1];
    for(y=nrow-1; y>0; y--){
        ff[s][6][z][y] = ff[s][6][z][y-1];
    }
    ff[s][6][z][0] = pftemp;
    for(y=0; y<nrow; y++){
        pftemp = ff[s][6][z][y];
        ftemp = pftemp[0];
        for(x=1; x<ncol; x++){ /* this block to memory move eventually
*/
            pftemp[x-1] = pftemp[x];
        }
        pftemp[ncol-1] = ftemp;
    }
    /***** for veloc 8 (315 degrees) *****/
    pftemp = ff[s][8][z][nrow-1];
    for(y=nrow-1; y>0; y--){
        ff[s][8][z][y] = ff[s][8][z][y-1];
    }
    ff[s][8][z][0] = pftemp;
    for(y=0; y<nrow; y++){
        pftemp = ff[s][8][z][y];
        ftemp = pftemp[ncol-1];
        for(x=ncol-1; x>0; x--){ /* this block to memory move
eventually */
            pftemp[x] = pftemp[x-1];
        }
        pftemp[0] = ftemp;
    }
}

/*zmzmzmznm END LOOP OVER Z FOR MIDDLE OF SITE (x-y plane) zmzmzmzm*/

/*== x-z plane diagonal directions: 10,12 (+z); 14,16 (-z) ==*/
/***** for velocity 10 case (x right, z up) *****/
/* 1st shuffle the z pointers UP */
ppftemp = ff[s][10][nlay-1];
for(z=nlay-1; z>0; z--){
    ff[s][10][z] = ff[s][10][z-1];
}
ff[s][10][0] = ppftemp;
/* for each row in each layer, shuffle the x's to the right, & wrap */
for(z=0; z<nlay; z++){
    for(y=0; y<nrow; y++){
        pftemp = ff[s][10][z][y];
        ftemp = pftemp[ncol-1]; /* save wrap element */
        for(x=ncol-1; x>0; x--){
            pftemp[x] = pftemp[x-1];
        }
        pftemp[0] = ftemp; /* put wrap element */
    }
}

```



```

    }
    /***** for velocity 12 case (x left, z up) *****/
    /* 1st shuffle the z pointers UP */
    ppftemp = ff[s][12][nlay-1];
    for(z=nlay-1; z>0; z--){
        ff[s][12][z] = ff[s][12][z-1];
    }
    ff[s][12][0] = ppftemp;
    /* for each row in each layer, shuffle the x's to the right, & wrap */
    for(z=0; z<nlay; z++){
        for(y=0; y<nrow; y++){
            pftemp = ff[s][12][z][y];
            ftemp = pftemp[0]; /* save wrap element */
            for(x=1; x<ncol; x++){
                pftemp[x-1] = pftemp[x];
            }
            pftemp[ncol-1] = ftemp; /* put wrap element */
        }
    }
    /***** for velocity 14 case (x right, z down) *****/
    /* 1st shuffle the z pointers DOWN */
    ppftemp = ff[s][14][0];
    for(z=1; z<nlay; z++){
        ff[s][14][z-1] = ff[s][14][z];
    }
    ff[s][14][nlay-1] = ppftemp;
    /* for each row in each layer, shuffle the x's to the right, & wrap */
    for(z=0; z<nlay; z++){
        for(y=0; y<nrow; y++){
            pftemp = ff[s][14][z][y];
            ftemp = pftemp[ncol-1]; /* save wrap element */
            for(x=ncol-1; x>0; x--){
                pftemp[x] = pftemp[x-1];
            }
            pftemp[0] = ftemp; /* put wrap element */
        }
    }
    /***** for velocity 16 case (x left, z down) *****/
    /* 1st shuffle the z pointers DOWN */
    ppftemp = ff[s][16][0];
    for(z=1; z<nlay; z++){
        ff[s][16][z-1] = ff[s][16][z];
    }
    ff[s][16][nlay-1] = ppftemp;
    /* for each row in each layer, shuffle the x's to the right, & wrap */
    for(z=0; z<nlay; z++){
        for(y=0; y<nrow; y++){
            pftemp = ff[s][16][z][y];
            ftemp = pftemp[0]; /* save wrap element */
            for(x=1; x<ncol; x++){
                pftemp[x-1] = pftemp[x];
            }
            pftemp[ncol-1] = ftemp; /* put wrap element */
        }
    }
    /== END x-z plane diagonal directions: 10,12 (+z); 14,16 (-z) ==*/

```

```

/*== y-z plane diagonal directions: 11,13 (+z); 15,17 (-z) ==*/
/*== NOTE y is just row index; "positive" scrolls down page ==*/
/***** for veloc 11 case (z up, y negative) *****/
/* 1st shuffle the z pointers UP */
ppftemp = ff[s][11][nlay-1];
for(z=nlay-1; z>0; z--){
    ff[s][11][z] = ff[s][11][z-1];
}
ff[s][11][0] = ppftemp;
/* for each layer, do a y-row pointer swap */
for(z=0; z<nlay; z++){
    /* swap the y-pointers */
    ppftemp = ff[s][11][z];
    pftemp = ppftemp[0];
    for(y=1; y<nrow; y++){
        ppftemp[y-1] = ppftemp[y];
    }
    ppftemp[nrow-1] = pftemp;
}
/***** for veloc 13 case (z up, y positive) *****/
/* 1st shuffle the z pointers UP */
ppftemp = ff[s][13][nlay-1];
for(z=nlay-1; z>0; z--){
    ff[s][13][z] = ff[s][13][z-1];
}
ff[s][13][0] = ppftemp;
/* for each layer, do a y-row pointer swap */
for(z=0; z<nlay; z++){
    /* swap the y-pointers */
    ppftemp = ff[s][13][z];
    pftemp = ppftemp[nrow-1];
    for(y=nrow-1; y>0; y--){
        ppftemp[y] = ppftemp[y-1];
    }
    ppftemp[0] = pftemp;
}
/***** for veloc 15 case (z down, y negative) *****/
/* 1st shuffle the z pointers DOWN */
ppftemp = ff[s][15][0];
for(z=1; z<nlay; z++){
    ff[s][15][z-1] = ff[s][15][z];
}
ff[s][15][nlay-1] = ppftemp;
/* for each layer, do a y-row pointer swap */
for(z=0; z<nlay; z++){
    /* swap the y-pointers */
    ppftemp = ff[s][15][z];
    pftemp = ppftemp[0];
    for(y=1; y<nrow; y++){
        ppftemp[y-1] = ppftemp[y];
    }
    ppftemp[nrow-1] = pftemp;
}
/***** for veloc 17 case (z down, y positive) *****/
/* 1st shuffle the z pointers DOWN */
ppftemp = ff[s][17][0];
for(z=1; z<nlay; z++){

```



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        pftemp = ff[s][2][z][y];
        ftemp = pftemp[0];
        for(x=1; x<ncol; x++){ /* this block to memory move eventually
*/
            pftemp[x-1] = pftemp[x];
        }
        pftemp[ncol-1] = ftemp;
    }
    /***** for veloc 3 (270 degrees) *****/
    pftemp = ff[s][3][z][nrow-1];
    for(y=nrow-1; y>0; y--){
        ff[s][3][z][y] = ff[s][3][z][y-1];
    }
    ff[s][3][z][0] = pftemp;
}
/*zmzmzmzmm END LOOP OVER Z FOR MIDDLE OF SITE (x-y plane) zmzmzmzm*/
/*== z-only directions 4, 5 ==*/
/***** velocity 4 (z up only) *****/
/* 1st shuffle the z pointers UP */
ppftemp = ff[s][4][nlay-1];
for(z=nlay-1; z>0; z--){
    ff[s][4][z] = ff[s][4][z-1];
}
ff[s][4][0] = ppftemp;
/***** velocity 5 (z down only) *****/
/* 1st shuffle the z pointers DOWN */
ppftemp = ff[s][5][0];
for(z=1; z<nlay; z++){
    ff[s][5][z-1] = ff[s][5][z];
}
ff[s][5][nlay-1] = ppftemp;

/*== END z-only directions 4, 5 ==*/

    } /* END if-else on nveloc[s] */
} /* END big loop on s (components) */
/***** END LOOP OVER COMPONENTS *****/

return(1);
} /* END Translate() */
/*-----*/
/* This function will not alter the POINTERS in ff, uu or solid, so the */
/* const declarations may help alias optimizations. */
/*****/
int Collide(ff_t *const*const*const*const*const ff,
            double *const tau, double *const beta,
            double *const omega, struct veloc_t *const*const*const uu,
            struct gravity *const gp, char *const*const*const solid,
            int ncomponent, int nveloc[], int nlay, int nrow, int ncol)
{
    int i,k,s,x,y,z;
    double ux,uy,uz, u2const, inv_rho, uSqr;
    /* u2const = 1-1.5*u*u */
    double qian; /* 7-4-97 used to have qian1, qian0 */
    double f[DEF_NVELOC];
    double feq[DEF_NVELOC];
    /* 9-25-97 test using cu1, ... instead of array */

```

```

/* double cu[DEF_NVELOC]; */
double cu1, cu2, cu3, cu4, cu5, cu6, cu7, cu8, cu9,
      cu10, cu11, cu12, cu13, cu14, cu15, cu16, cu17, cu18;
/* 9-25-97 */
double mux,muy,muz;
/* 9-25-97 */
ff_t *const*const*const* ffs, *const*const*const* ff0;

double tau0;
int solidcode;
double dux, duy, duz; /* gravity increments in ux, uy, uz */
double rho[MAX_COMP];
double del_density; /* true difference in physical density, between */
/* reference solution and local solution at x,y,z */
double omega_s, beta_s; /* 7-5-97 */

int doBounce,doZiegler;
int nvel;
int do_buoy;

/* 7-5-97 allow us to skip buoyancy calc.; presume fabs() takes double */
do_buoy = (fabs(gp->xBuoy)<1.e-30 && fabs(gp->yBuoy)<1.e-30
          && fabs(gp->zBuoy) < 1.e-30) ? 0 : 1;

tau0 = tau[0];
ff0 = ff[0];
for(z=0; z<nlay; z++){
  for(y=0; y<nrow; y++){
    for(x=0; x<ncol; x++){
      solidcode = solid[z][y][x];
      /* 7-3-97 MUST classify solids before calling Collide()! */
      /* solidcode -2 means completely surrounded by solids */
      if(solidcode==-2) continue;
      /* We calculate these only once */
      doBounce = (solidcode && !USE_ZIEGLER) ||
        (USE_ZIEGLER && (solidcode<0 || solidcode>ZIEGLER_END_CODE));
      doZiegler = USE_ZIEGLER && solidcode>=ZIEGLER_1ST_CODE
        && solidcode<=ZIEGLER_END_CODE;

      /* first do the carrier fluid (first index s=0) */
      /* make local copies of all component 0 (fluid) vectors */
      rho[0] = f[0] = ff0[0][z][y][x];
      rho[0] += f[1] = ff0[1][z][y][x];
      rho[0] += f[2] = ff0[2][z][y][x];
      rho[0] += f[3] = ff0[3][z][y][x];
      rho[0] += f[4] = ff0[4][z][y][x];
      rho[0] += f[5] = ff0[5][z][y][x];
      rho[0] += f[6] = ff0[6][z][y][x];
      rho[0] += f[7] = ff0[7][z][y][x];
      rho[0] += f[8] = ff0[8][z][y][x];
      rho[0] += f[9] = ff0[9][z][y][x];
      rho[0] += f[10] = ff0[10][z][y][x];
      rho[0] += f[11] = ff0[11][z][y][x];
      rho[0] += f[12] = ff0[12][z][y][x];
      rho[0] += f[13] = ff0[13][z][y][x];
      rho[0] += f[14] = ff0[14][z][y][x];
      rho[0] += f[15] = ff0[15][z][y][x];

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rho[0] += f[16] = ff0[16][z][y][x];
rho[0] += f[17] = ff0[17][z][y][x];
rho[0] += f[18] = ff0[18][z][y][x];

if(doZiegler) rho[0] = Ziegler(f, solidcode, 1);
if(rho[0]<1.0e-30) continue; /* denotes a problem */
/* get rho other components-- */
/* 7-3-97 NOTE we should have functions without buoyancy, and with only */
/* 2 or 3 components; without buoy, we would eliminate the double read */
/* of ff[s] (which may pre-cache, so could be OK)... */
for(s=1; s<ncomponent; s++){
    ffs = ff[s];
    rho[s] = ffs[0][z][y][x];
    rho[s] += ffs[1][z][y][x];
    rho[s] += ffs[2][z][y][x];
    rho[s] += ffs[3][z][y][x];
    rho[s] += ffs[4][z][y][x];
    rho[s] += ffs[5][z][y][x];
    if(nveloc[s]>6){ /* kludgey, 5-26-97 */
        rho[s] += ffs[6][z][y][x];
        rho[s] += ffs[7][z][y][x];
        rho[s] += ffs[8][z][y][x];
        rho[s] += ffs[9][z][y][x];
        rho[s] += ffs[10][z][y][x];
        rho[s] += ffs[11][z][y][x];
        rho[s] += ffs[12][z][y][x];
        rho[s] += ffs[13][z][y][x];
        rho[s] += ffs[14][z][y][x];
        rho[s] += ffs[15][z][y][x];
        rho[s] += ffs[16][z][y][x];
        rho[s] += ffs[17][z][y][x];
        rho[s] += ffs[18][z][y][x];
    }
}
/* simple bounceback block */
if(doBounce){
    uu[z][y][x].x = 0.0; uu[z][y][x].y = 0.0;
    uu[z][y][x].z = 0.0; uu[z][y][x].usqrd = 0.0;
    BounceBack(f);
    for(i=1; i<nveloc[0]; i++) ff0[i][z][y][x] = f[i];
}
else {
    inv_rho = 1.0/rho[0];
    ux = inv_rho*(f[1] + f[2] + f[8] + f[10] + f[14]
        - f[5] - f[4] - f[6] - f[12] - f[16]);
    uy = inv_rho*(f[2] + f[3] + f[4] + f[11] + f[15]
        - f[6] - f[7] - f[8] - f[13] - f[17]);
    uz = inv_rho*(f[9] + f[10] + f[11] + f[12] + f[13]
        - f[14] - f[15] - f[16] - f[17] - f[18]);
/* 7-4-97 SHOULD put in logic to skip buoyancy if not needed */
/****** forcing, buoyancy block *****/
dux = gp->txBody; duy = gp->tyBody; duz = gp->tzBody;
if(do_buoy){
    for(del_density=0.0,k=1; k<ncomponent; k++){
        del_density += rho[k]*(gp->alpha[k]);
    }
    /** 1-17-97 kludgey, use a global here **/

```

```

        if(rho[0]>1e-10) del_density *= RHO[0]/rho[0];
        del_density -= DEL_DENSITY_REF;
        dux += del_density*(gp->xBuoy);
        duy += del_density*(gp->yBuoy);
        duz += del_density*(gp->zBuoy);
    }
    ux += dux*tau0; uy += duy*tau0; uz += duz*tau0;
    /* store for later */
    uSqr = ux*ux + uy*uy + uz*uz;
    uu[z][y][x].x = ux; uu[z][y][x].y = uy;
    uu[z][y][x].z = uz; uu[z][y][x].usqr = uSqr;
    u2const = 1.0 - 1.5*uSqr;
    /*-----*/
    /* 9-25-97 try cutting down number of ops by */
    /* incorp 3.0 factor into mux */
    mux = ux*3.0; muy = uy*3.0; muz = uz*3.0;

    /* 9-25-97 change to use mux, muy, muz */
    cu1 = mux; cu2 = mux + muy; cu3 = muy; cu4 = muy - mux;
    cu5 = -mux; cu6 = -cu2; cu7 = -muy; cu8 = -cu4;
    cu9 = muz; cu10 = mux + muz; cu11 = muy + muz;
    cu12 = -mux + muz; cu13 = -muy + muz; cu14 = -cu12;
    cu15 = -cu13; cu16 = -cu10; cu17 = -cu11;
    cu18 = -muz;

    /* when we have debugged, factor below with simpler */
    /* expressions or consider eliminating cu array, and */
    /* calc each cu[] in place ... */
    feq[0] = ONE_3RD*rho[0]*u2const;
    qian = rho[0]*ONE_18TH;
    /* 7-4-97 old had qian0 = rho[0]*ONE_36TH; */
    /* the Cartesian directions */
    feq[1] = qian*(u2const + cu1 + 0.5*cu1*cu1);
    feq[3] = qian*(u2const + cu3 + 0.5*cu3*cu3);
    feq[5] = qian*(u2const + cu5 + 0.5*cu5*cu5);
    feq[7] = qian*(u2const + cu7 + 0.5*cu7*cu7);
    feq[9] = qian*(u2const + cu9 + 0.5*cu9*cu9);
    feq[18] = qian*(u2const + cu18 + 0.5*cu18*cu18);
    /* the off-axis, diagonal directions */
    qian *= 0.5; /* may have to go back to qian1, qian0 */

    feq[2] = qian*(u2const + cu2 + 0.5*cu2*cu2);
    feq[4] = qian*(u2const + cu4 + 0.5*cu4*cu4);
    feq[6] = qian*(u2const + cu6 + 0.5*cu6*cu6);
    feq[8] = qian*(u2const + cu8 + 0.5*cu8*cu8);
    feq[10] = qian*(u2const + cu10 + 0.5*cu10*cu10);
    feq[11] = qian*(u2const + cu11 + 0.5*cu11*cu11);
    feq[12] = qian*(u2const + cu12 + 0.5*cu12*cu12);
    feq[13] = qian*(u2const + cu13 + 0.5*cu13*cu13);
    feq[14] = qian*(u2const + cu14 + 0.5*cu14*cu14);
    feq[15] = qian*(u2const + cu15 + 0.5*cu15*cu15);
    feq[16] = qian*(u2const + cu16 + 0.5*cu16*cu16);
    feq[17] = qian*(u2const + cu17 + 0.5*cu17*cu17);

    if(doZiegler){
        Ziegler(f, solidcode, 0);
        Ziegler(feq, solidcode, 0);
    }

```

```

    }

/* now put back new ff's */
omega_s = omega[0]; beta_s = beta[0];
ff0[0][z][y][x] = f[0]*beta_s + feq[0]*omega_s;
ff0[1][z][y][x] = f[1]*beta_s + feq[1]*omega_s;
ff0[2][z][y][x] = f[2]*beta_s + feq[2]*omega_s;
ff0[3][z][y][x] = f[3]*beta_s + feq[3]*omega_s;
ff0[4][z][y][x] = f[4]*beta_s + feq[4]*omega_s;
ff0[5][z][y][x] = f[5]*beta_s + feq[5]*omega_s;
ff0[6][z][y][x] = f[6]*beta_s + feq[6]*omega_s;
ff0[7][z][y][x] = f[7]*beta_s + feq[7]*omega_s;
ff0[8][z][y][x] = f[8]*beta_s + feq[8]*omega_s;
ff0[9][z][y][x] = f[9]*beta_s + feq[9]*omega_s;
ff0[10][z][y][x] = f[10]*beta_s + feq[10]*omega_s;
ff0[11][z][y][x] = f[11]*beta_s + feq[11]*omega_s;
ff0[12][z][y][x] = f[12]*beta_s + feq[12]*omega_s;
ff0[13][z][y][x] = f[13]*beta_s + feq[13]*omega_s;
ff0[14][z][y][x] = f[14]*beta_s + feq[14]*omega_s;
ff0[15][z][y][x] = f[15]*beta_s + feq[15]*omega_s;
ff0[16][z][y][x] = f[16]*beta_s + feq[16]*omega_s;
ff0[17][z][y][x] = f[17]*beta_s + feq[17]*omega_s;
ff0[18][z][y][x] = f[18]*beta_s + feq[18]*omega_s;
}

/** 12-8-96 add code for s=1 to ncomponent-1 ***/
for(s=1; s<ncomponent; s++){
    ffs = ff[s];
    nvel = nveloc[s]; /* 5-26-97 if-else on nvel */
    if(nvel==19){
        /* make local copy; already have rho[s]... */
        f[0] = ffs[0][z][y][x];
        f[1] = ffs[1][z][y][x];
        f[2] = ffs[2][z][y][x];
        f[3] = ffs[3][z][y][x];
        f[4] = ffs[4][z][y][x];
        f[5] = ffs[5][z][y][x];
        f[6] = ffs[6][z][y][x];
        f[7] = ffs[7][z][y][x];
        f[8] = ffs[8][z][y][x];
        f[9] = ffs[9][z][y][x];
        f[10] = ffs[10][z][y][x];
        f[11] = ffs[11][z][y][x];
        f[12] = ffs[12][z][y][x];
        f[13] = ffs[13][z][y][x];
        f[14] = ffs[14][z][y][x];
        f[15] = ffs[15][z][y][x];
        f[16] = ffs[16][z][y][x];
        f[17] = ffs[17][z][y][x];
        f[18] = ffs[18][z][y][x];
        /* 3-13-97 alter for Ziegler */
        if(doZiegler) rho[s] = NoFlux(f, solidcode, 1);
        if(doBounce){
            BounceBack(f);
            for(i=1; i<nvel; i++) ffs[i][z][y][x] = f[i];
            continue; /* 12-8-96 on to next component */
        }
        /* start w/ Flekkoy philosophy that 2nd order not */

```



```

/* needed for convect-diff eqn... */
feq[0] = ONE_3RD*rho[s];

qian = rho[s]*ONE_18TH;
/* old had qian0 = rho[s]*ONE_36TH; */
/* the Cartesian axis vectors */
feq[1] = qian*(1.0 + cu1);
feq[3] = qian*(1.0 + cu3);
feq[5] = qian*(1.0 + cu5);
feq[7] = qian*(1.0 + cu7);
feq[9] = qian*(1.0 + cu9);
feq[18] = qian*(1.0 + cu18);
/* the diagonal vectors */
qian *= 0.5; /* may have to go back to qian1, qian0 */
feq[2] = qian*(1.0 + cu2);
feq[4] = qian*(1.0 + cu4);
feq[6] = qian*(1.0 + cu6);
feq[8] = qian*(1.0 + cu8);
feq[10] = qian*(1.0 + cu10);
feq[11] = qian*(1.0 + cu11);
feq[12] = qian*(1.0 + cu12);
feq[13] = qian*(1.0 + cu13);
feq[14] = qian*(1.0 + cu14);
feq[15] = qian*(1.0 + cu15);
feq[16] = qian*(1.0 + cu16);
feq[17] = qian*(1.0 + cu17);

/* now put back new ff's */
if(doZiegler){
    NoFlux(f, solidcode, 0);
    NoFlux(feq, solidcode, 0);
}
beta_s = beta[s]; omega_s = omega[s];
ffs[0][z][y][x] = f[0]*beta_s + feq[0]*omega_s;
ffs[1][z][y][x] = f[1]*beta_s + feq[1]*omega_s;
ffs[2][z][y][x] = f[2]*beta_s + feq[2]*omega_s;
ffs[3][z][y][x] = f[3]*beta_s + feq[3]*omega_s;
ffs[4][z][y][x] = f[4]*beta_s + feq[4]*omega_s;
ffs[5][z][y][x] = f[5]*beta_s + feq[5]*omega_s;
ffs[6][z][y][x] = f[6]*beta_s + feq[6]*omega_s;
ffs[7][z][y][x] = f[7]*beta_s + feq[7]*omega_s;
ffs[8][z][y][x] = f[8]*beta_s + feq[8]*omega_s;
ffs[9][z][y][x] = f[9]*beta_s + feq[9]*omega_s;
ffs[10][z][y][x] = f[10]*beta_s + feq[10]*omega_s;
ffs[11][z][y][x] = f[11]*beta_s + feq[11]*omega_s;
ffs[12][z][y][x] = f[12]*beta_s + feq[12]*omega_s;
ffs[13][z][y][x] = f[13]*beta_s + feq[13]*omega_s;
ffs[14][z][y][x] = f[14]*beta_s + feq[14]*omega_s;
ffs[15][z][y][x] = f[15]*beta_s + feq[15]*omega_s;
ffs[16][z][y][x] = f[16]*beta_s + feq[16]*omega_s;
ffs[17][z][y][x] = f[17]*beta_s + feq[17]*omega_s;
ffs[18][z][y][x] = f[18]*beta_s + feq[18]*omega_s;
} /* END if on nvel==19 */
else if(nvel==6){
    /* make local copy; already have rho[s]... */
    f[0] = ffs[0][z][y][x];
    f[1] = ffs[1][z][y][x];

```

```

f[2] = ffs[2][z][y][x];
f[3] = ffs[3][z][y][x];
f[4] = ffs[4][z][y][x];
f[5] = ffs[5][z][y][x];
/* 3-13-97 alter for Ziegler */
if(doZiegler) rho[s] = NoFlux6(f, solidcode, 1);
else if(doBounce){ /* else (was just if) 5-28-97 */
    /* 5-26-97 replace BounceBack() with inline */
    ffs[0][z][y][x] = f[2];
    ffs[1][z][y][x] = f[3];
    ffs[2][z][y][x] = f[0];
    ffs[3][z][y][x] = f[1];
    ffs[4][z][y][x] = f[5];
    ffs[5][z][y][x] = f[4];
    continue; /* on to next component */
}
/* Flekkoy (1993) showed 2nd order not */
/* required for convection-diffusion equation... */
/* compiler optimizer should see pattern below... */
/* 7-18-97 correct below!! See page 98 in LGA#8 */
feq[0] = rho[s]*(ONE_6TH + ONE_HALF*ux);
feq[1] = rho[s]*(ONE_6TH + ONE_HALF*uy);
feq[2] = rho[s]*(ONE_6TH - ONE_HALF*ux);
feq[3] = rho[s]*(ONE_6TH - ONE_HALF*uy);
feq[4] = rho[s]*(ONE_6TH + ONE_HALF*uz);
feq[5] = rho[s]*(ONE_6TH - ONE_HALF*uz);

/* now put back new ff's... */
if(doZiegler){
    NoFlux6(f, solidcode, 0);
    NoFlux6(feq, solidcode, 0);
}
beta_s = beta[s]; omega_s = omega[s];
/* 1-22-97 this pulled inside */
ffs[0][z][y][x] = f[0]*beta_s + feq[0]*omega_s;
ffs[1][z][y][x] = f[1]*beta_s + feq[1]*omega_s;
ffs[2][z][y][x] = f[2]*beta_s + feq[2]*omega_s;
ffs[3][z][y][x] = f[3]*beta_s + feq[3]*omega_s;
ffs[4][z][y][x] = f[4]*beta_s + feq[4]*omega_s;
ffs[5][z][y][x] = f[5]*beta_s + feq[5]*omega_s;
} /* END if-else on nvel */
} /* END loop over s */
/**/ END 12-8-96 code for other components ***/
} /* END loop over x */
} /* END loop over y */
} /* END loop over z */
return(1); /* dummy 7-2-97 */
} /* END Collide() */
/*-----*/
/* 7-1-97 alter to handle 3D; start with carrier-only (9-vec); */
/* mainly used for debugging the Translate() function. Unlike */
/* PlotCells() in old D2Q9 programs, this writes to a buffer to compose */
/* the map of max 8x8 cells in yx, zx and zy planes... each cell is a map */
/* of 9 vectors in a yx, zx or zy slice through the site... */
/* REMEMBER that y is really just a row index, positive points down... */
/* NOTE we have to pick some "middle" for x,y,z, so we arbitrarily take */
/* (e.g.) (nlay-1)>>1; keep this in mind when init'ing a point for */

```

```

/* debugging... */
/*****/
int Plot9Vec(ff_t ***** const ff, float * const rho, int ncomponent,
            int nveloc[], int nlay, int nrow, int ncol, int step)
{
    int i,j,k,n,x,y,z,s,max;
    float f[5];
    float ftemp;
    static unsigned char c[5] = {'ú', '°', '±', '²', 'Û'};
    unsigned char cc;
    /* allow 24 screen rows (8sites x 3 vect layers) and 24x3 + 2separators + \0 */
#define SROW 24
#define SCOL 75
#define J4YX 0
#define J4ZX 25
#define J4ZY 50
#define MMAX 8
    unsigned char scrn[SROW][SCOL];
    int jend;

    /* 3x3 arrays to fetch the vectors (i) to plot vector views */
    static int vvx[3][3] = {{4,3,2},{5,0,1},{6,7,8}};
    static int vzx[3][3] = {{12,9,10},{5,0,1},{16,18,14}};
    static int vzy[3][3] = {{11,9,13},{3,0,7},{15,18,17}};

    /* zero out the scrn array */
    for(i=0; i<SROW; i++){
        for(j=0,jend=SCOL-1; j<jend; j++){
            scrn[i][j] = ' ';
        }
        scrn[i][jend] = 0; /* so we can write strings */
    }
    /* loop over each component */
    for(s=0; s<ncomponent; s++){
        system("cls"); /* UNIX: system("clear"); */
        /* set up some good levels to discriminate */
        f[4] = rho[s]*ONE_3RD; /* 4/9 */
        f[2] = rho[s]*ONE_18TH; /* 1/9 */
        f[0] = rho[s]*ONE_36TH; /* 1/36 */
        f[1] = (f[0] + f[2]) * 0.5;
        f[3] = (f[2] + f[4]) * 0.5;
        for(n=0; n<5; n++) f[n] *= 0.9;
        /* fill the character array; */
        /* start with yx plane... somewhat arbitrary how we pick z to start, */
        /* see NOTE at preface to function... */
        for(z=(nlay-1)>>1,y=0; y<nrow && y<MMAX; y++){
            for(x=0; x<ncol && x<MMAX; x++){
                /* cycle through the vectors to plot */
                for(i=0; i<3; i++){
                    for(j=0; j<3; j++){
                        ftemp = ff[s][vyx[i][j]][z][y][x];
                        cc = '*';
                        for(k=0; k<5; k++){
                            if(ftemp<f[k]){
                                cc = c[k]; break;
                            }
                        }
                    }
                }
            }
        }
    }
}

```

```

        /* stick cc in array */
        scrn[y*3+i][x*3+j+J4YX] = cc;
    }
}
} /* END y for yx plane */
/*.....*/
/* do zx plane; fixed y arbitrary, as described above */
for(y=(nrow-1)>>1,z=0; z<MMAX && z<nlay; z++){
    for(x=0; x<ncol && x<MMAX; x++){
        /* cycle through the vectors to plot */
        for(i=0; i<3; i++){
            for(j=0; j<3; j++){
                ftemp = ff[s][vzx[i][j]][z][y][x];
                cc = '';
                for(k=0; k<5; k++){
                    if(ftemp<f[k]){
                        cc = c[k]; break;
                    }
                }
                /* stick cc in array */
                scrn[SROW-3-(z*3)+i][x*3+j+J4ZX] = cc;
            }
        }
    } /* END y for zx plane */
/*.....*/
/* do zy plane; fixed x arbitrary, as described above */
for(x=(ncol-1)>>1,z=0; z<MMAX && z<nlay; z++){
    for(y=0; y<nrow && y<MMAX; y++){
        /* cycle through the vectors to plot */
        for(i=0; i<3; i++){
            for(j=0; j<3; j++){
                ftemp = ff[s][vzy[i][j]][z][y][x];
                cc = '';
                for(k=0; k<5; k++){
                    if(ftemp<f[k]){
                        cc = c[k]; break;
                    }
                }
                /* stick cc in array */
                scrn[SROW-3-(z*3)+i][y*3+j+J4ZY] = cc;
            }
        }
    } /* END ... for zy plane */
/*.....*/
/* put the char array to the screen */
for(i=0; i<SROW; i++){
    puts(scrn[i]);
}

}

/* print the step */
printf("STEP= %d\r", step);
/*getch(); 12-8-96 comment out */
return(1); /* 12-4-96 for now, a dummy return */

```

```

#undef SROW
#undef SCOL
#undef X4YX
#undef X4ZX
#undef X4ZY
#undef MMAX
} /* END Plot9Vec() */
/*-----*/
/*****/
double NoFlux(double f[], int solidcode, int mode)
{
return(0.0);
} /* END NoFlux() */
/*-----*/
/*****/
double NoFlux6(double f[], int solidcode, int mode)
{
return(0.0);
} /* END NoFlux6() */
/*-----*/
/*****/
double Ziegler(double f[], int solidcode, int mode)
{
return(0.0);
} /* END NoFlux() */
/*-----*/
/* 7-4-97 this quickie version presumes 19 vectors, vector 0 = rest */
/*****/
int BounceBack(double f[])
{
double ftemp;

/* in xy plane */
ftemp = f[1]; f[1] = f[5]; f[5] = ftemp;
ftemp = f[3]; f[3] = f[7]; f[7] = ftemp;
ftemp = f[2]; f[2] = f[6]; f[6] = ftemp;
ftemp = f[4]; f[4] = f[8]; f[8] = ftemp;
/* z up-and down vectors */
ftemp = f[9]; f[9] = f[18]; f[18] = ftemp;
/* off-xy-plane vectors */
ftemp = f[10]; f[10] = f[16]; f[16] = ftemp;
ftemp = f[14]; f[14] = f[12]; f[12] = ftemp;
ftemp = f[11]; f[11] = f[17]; f[17] = ftemp;
ftemp = f[13]; f[13] = f[15]; f[15] = ftemp;

return(1); /* 7-4-97 dummy return */
} /* END BounceBack() */
/*-----*/
/* 10-30-97 add ncol_old for post-Recycle() speed view... */
/* NOTE late 7-4-97 need to change typing and allow z transport, */
/* put declaration at top, install Collide() ... 7-5-97 change to handle */
/* only one passed s (s=component number), plot speed differently... */
/*****/
int PlotConcs(ff_t *const*const*const*const* ff,
char *const*const* solid, float * const rho,
struct veloc_t *const*const* uu,
int ncomponent, int nveloc[], int nlay, int nrow, int ncol, int

```

```

        ncol_old, int step, int s, int xStart, int yStart, int zz, int zoomMode)
{
int i,k,n,x,y,z,xPerPix,yPerPix,x0,y0,xx,yy;
float f[5];
ff_t ****ffs;
float ftemp,umax;
static unsigned char c[5] = {'ú', '-', 'o', '±', '²'};
unsigned char cc;
int xxx; /* 10-30-97 for modding after Recycle() */

if(zz<0 || zz>=nlay) return(0);

if(!zoomMode){
    xPerPix = (XSCR<NCOL) ? (NCOL + (XSCR >> 1))/XSCR : 1;
    yPerPix = (YSCR<NROW) ? (NROW + (YSCR >> 1))/YSCR : 1;
    x0 = 0; y0 = 0;
}
else {
    xPerPix = yPerPix = 1;
    x0 = xStart; y0 = yStart;
}

ffs = ff[s];
system("cls"); /* Unix: system("clear"); Unix || Mac: printf("\f"); */
if(s>0){ /* treat solutes */
    /* Set up levels of gradation (if-else) */
    if(nveloc[s]==19){
        f[4] = rho[s]*ONE_3RD;
        f[2] = rho[s]*ONE_6TH;
        f[0] = rho[s]*ONE_36TH;
    }
    else {
        f[4] = rho[s]; f[2] = rho[s]*ONE_6TH; f[0] = rho[s]*0.05;
    }
    f[1] = (f[0] + f[2]) * 0.5;
    f[3] = (f[2] + f[4]) * 0.5;
    for(n=0; n<5; n++) f[n] *= 0.9;
    for(y=0,yy=y0; y<nrow&&y<YSCR; y++,yy+=yPerPix){
        for(x=0,xx=x0; x<ncol&&x<XSCR; x++,xx+=xPerPix){
            if(solid[zz][yy][xx]) cc = 's';
            else {
                if(nveloc[s]==19) ftemp = ffs[0][zz][yy][xx];
                else { /* 5-22-97; 5-27-97 remove 0.25* below */
                    ftemp = (ffs[0][zz][yy][xx] + ffs[1][zz][yy][xx] +
                        ffs[2][zz][yy][xx] + ffs[3][zz][yy][xx] +
                        ffs[4][zz][yy][xx] + ffs[5][zz][yy][xx]);
                }
                cc = 'û';
                for(k=0; k<5; k++){
                    if(ftemp<f[k]){
                        cc = c[k]; break;
                    }
                }
            }
            putchar(cc);
        }
        putchar('\n');
    }
}

```

```

    }
}
else { /* if s==0 (carrier), plot speed */
/* find maximum speed IN LAYER (for now) */
umax = 0.0;
for(y=0; y<nrow; y++){
    for(x=0; x<ncol; x++){
        if(uu[zz][y][x].usqrd > umax) umax = uu[zz][y][x].usqrd;
    }
}
if(umax < 1.0e-30) umax = 0.01; /* remember these are squared */
/* Set up levels of gradation (if-else) */
f[4] = umax*ONE_3RD;
f[2] = umax*ONE_6TH;
f[0] = umax*ONE_18TH;
f[1] = (f[0] + f[2]) * 0.5;
f[3] = (f[2] + f[4]) * 0.5;
for(n=0; n<5; n++) f[n] *= 0.9;
for(y=0,yy=y0; y<nrow&&y<YSCR; y++,yy+=yPerPix){
    for(x=0,xx=x0; x<ncol&&x<XSCR; x++,xx+=xPerPix){
        /* 10-30-97 add below, subs xxx in uu reads; */
        /* performance hit with %, consider other approaches */
        xxx = (xx>=ncol_old) ? xx % ncol_old : xx;
        if(solid[zz][yy][xxx]) cc = 's';
        else {
            ftemp = uu[zz][yy][xxx].usqrd;
            cc = '0';
            for(k=0; k<5; k++){
                if(ftemp<f[k]){
                    cc = c[k]; break;
                }
            }
        }
        putchar(cc);
    }
    putchar('\n');
}
} /* END else on s==0, speed */
/* print the step */
/* printf("STEP= %d\n", step);*/
/*getch(); 12-8-96 comment out */
return(1); /* 12-4-96 for now, a dummy return */
} /* END PlotConcs() */
/*-----*/
/* 7-5-97 adapt for 3D, and put y-x and y-z cuts side by side... */
/* try to create funky colors to match Clay's; use scheme in */
/* home PPro200 D:\lb\~\f2p_graf.c... */
/* Saves a portable pixel map (ppm, as in pbmplus from Unix lore), which */
/* cmpeg can then convert into an mpeg. Also creates and saves a *.lst */
/* file of ppm file names... after save_ppm() in ilga.c... */
/*-----*/
FILE *SavePpm(ff_t *****ff, char ***solid, int ncomponent, int nveloc[],
    int nlay, int nrow, int ncol, int sstart, int step)
{
#define RGB_BASE 70
#define RGB_MAX_SIZE 8192 /* allows ncol+nlay <= 2730 */
#define LOCAL_BUF_LEN 128

```

```

static unsigned char rgb_row[RGB_MAX_SIZE+4];
/* for mpeg writes, 3* max ncol */

static int filenum=0, firsttime=1, rgb_len;
static FILE *fp, *b_list_fp;
int i,ii,x,y,z;
unsigned char r,g,b;
double c, cmax=-1.0e200, cmin=1.0e200;
double slope1,slope2,delta,chalf,craw,cpt75;
struct tm *ptm;
static int day=0,hour=0; /* because localtime destroys single internal tm */
time_t lt;
char buf[LOCAL_BUF_LEN]; /* for filenames */
int xhalf, zhalf;

if(filenum>=999){
    firsttime = 1;
    filenum = 0;
    if(b_list_fp) fclose(b_list_fp);
}
if(firsttime){
    /* ppm format has thre byte rgb values for each pixel */
    time(&lt);
    ptm = localtime(&lt);
    /* 9-12-94 for list file */
    day = ptm->tm_mday, hour = ptm->tm_hour;
    sprintf(buf,"B%02d%02d.lst",day, hour);
    buf[LOCAL_BUF_LEN-1] = 0;
    b_list_fp = fopen(buf, "w");
    firsttime=0;
}
/* 9-27-97 moved out of firsttime block */
rgb_len = (ncol+nlay+1)*3;

/* 7-5-97 allow placing y-x and y-z cuts side-by-side */
xhalf = ncol >> 1;  zhalf = nlay >> 1;

/* find the maximum and minimum conc values */
/* NOTE we initialized cmax, cmin in declarations, above */
for(y=0; y<nrow; y++){
    for(x=0; x<ncol; x++){
        if(solid[zhalf][y][x]) continue; /* 7-12-97 */
        for(i=0,c=0.0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][zhalf][y][x];
        }
        if(c >= cmax) cmax = c;
        if(c <= cmin) cmin = c;
    }
    for(z=0; z<nlay; z++){
        if(solid[z][y][xhalf]) continue; /* 7-12-97 */
        for(i=0,c=0.0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][z][y][xhalf];
        }
        if(c >= cmax) cmax = c;
        if(c <= cmin) cmin = c;
    }
}

```



```

/* Prevent funny colors due to small oscillations */
if(cmin < 0.0) cmin = 0.0;

delta = 255 - RGB_BASE; /* ASSUME maximum value for r,g or b is 255 */
chalf = 0.5*(cmax - cmin);
cpt75 = 0.75*(cmax - cmin);
if(cmax-cmin > 1e-30){
    slope1 = delta/chalf;
    slope2 = slope1*2.0;
}
else return(b_list_fp); /* was return(0) */

/* make the file name; avoid lots of unclosed files if */
/* the cmax-cmin is too small... */
/* Remember localtime structure is not "re-entrant"... */
buf[LOCAL_BUF_LEN-1] = 0;
sprintf(buf,"B%02d%02d%03d.PPM", day, hour, filenum);
filenum++;
fp = fopen(buf, "wb");
if(!fp) return(b_list_fp); /* was return(0) */
if(b_list_fp) fprintf(b_list_fp,"%s\n",buf);
/* write the standard binary ppm header; \012 is linefeed... */
fprintf(fp,"P6\012%d %d\012255\012",ncol+nlay+1,nrow);

/* Loop over all values. Do by row, ii is index into rgb_row...*/
for(y=0; y<nrow; y++){
    /* 1st loop over the y-x cut */
    for(x=0,ii=0; x<ncol && ii<RGB_MAX_SIZE; x++,ii+=3){
        /* print solids in white */
        if(solid[zhalf][y][x]==0){
            for(c=0.0,i=0; i<nveloc[sstart]; i++){
                c += ff[sstart][i][zhalf][y][x];
            }
            /* prevent funny colors */
            if(c<0.0) c = 0.0;
            /* for now we will just gray scale */
            /**** comment out simple grayscale alternative *****/
            r = scale*(c-cmin);
            if(r>255) r=255;
            g = b = r;
            **** END comment out simple gray scale alternative *****/

            /***** "default" rainbow scaling below *****/
            craw = cmax - c;
            if(craw<chalf){
                r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*craw);
                if(r<RGB_BASE) r = RGB_BASE;
                g = RGB_BASE + (int)(craw*slope1); if(g>255) g = 255;
            }
            else if(craw<cpt75){
                b = RGB_BASE; g = 255;
                r = RGB_BASE + (int)((craw-chalf)*slope2); if(r>255) r = 255;
            }
            else {
                b = RGB_BASE; r = 255;
                g = RGB_BASE + (int)(delta - slope2*(craw-cpt75));
            }
        }
    }
}

```

```

    }
}
else r=g=b=255; /* if solid, print as white */
/** END default rainbow scheme */
/* place in array */
rgb_row[ii]=r, rgb_row[ii+1]=g, rgb_row[ii+2]=b;
}
/* 2nd put a black marker line between the y-x and y-z cuts */
if(ii+3<RGB_MAX_SIZE){
    rgb_row[ii]=0, rgb_row[ii+1]=0, rgb_row[ii+2]=0;
    ii+=3;
}
/* 3rd do the y-z cut; note we don't re-init ii! */
for(z=0; z<nlay && ii<RGB_MAX_SIZE; z++,ii+=3){
    /* print solids in white */
    if(solid[z][y][xhalf]==0){
        for(c=0.0,i=0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][z][y][xhalf];
        }
        /* prevent funny colors */
        if(c<0.0) c = 0.0;
        /* for now we will just gray scale */
        /**** comment out simple grayscale alternative *****/
        r = scale*(c-cmin);
        if(r>255) r=255;
        g = b = r;
        **** END comment out simple gray scale alternative *****/

        /***** "default" rainbow scaling below */
        craw = cmax - c;
        if(craw<chalf){
            r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*craw);
            if(r<RGB_BASE) r = RGB_BASE;
            g = RGB_BASE + (int)(craw*slope1); if(g>255) g = 255;
        }
        else if(craw<cpt75){
            b = RGB_BASE; g = 255;
            r = RGB_BASE + (int)((craw-chalf)*slope2); if(r>255) r = 255;
        }
        else {
            b = RGB_BASE; r = 255;
            g = RGB_BASE + (int)(delta - slope2*(craw-cpt75));
        }
    }
    else r=g=b=255; /* if solid, print as white */
    /** END default rainbow scheme */
    /* place in array */
    rgb_row[iii]=r, rgb_row[iii+1]=g, rgb_row[iii+2]=b;
}
fwrite(rgb_row, 1, rgb_len, fp);
}
fclose(fp);
return(b_list_fp);
#undef RGB_BASE
#undef RGB_MAX_SIZE
#undef LOCAL_BUF_LEN
} /* END SavePpm() */

```

```

/*-----*/
/* Inject a slug with concentration values specified in the array concList[]; */
/* a negative value for a particular component means: skip this component. */
/* The concentrations are set along the prism x1,y1,z1 to x2,y2,z2 */
/* inclusive of the endpoints... */
/*-----*/
int SetSlug(ff_t *****ff, char ***solid, int ncomponent, int nveloc[],
           int nlay, int nrow, int ncol, int x1, int x2, int y1, int y2,
           int z1, int z2, double *concList)
{
    int x,y,z,i,s,temp;
    double f[DEF_NVELOC], rho0;
    float ftemp;

    if(z1<0 || z2<0 || y1<0 || y2<0 || x1<0 || x2<0 ||
       z1>=nlay || z2>=nlay || y1>=nrow || y2>=nrow ||
       x1>=ncol || x2>=ncol) return(0);

    if(x1>x2){
        temp = x1; x1=x2; x2=temp;
    }
    if(y1>y2){
        temp = y1; y1=y2; y2=temp;
    }
    if(z1>z2){
        temp = z1; z1=z2; z2=temp;
    }
    /* now do real meat of function; distribute concList[s] proportionally */
    /* as ff[0][i][z][y][x] are distributed among velocities ... */
    for(z=z1; z<=z2; z++){
        for(y=y1; y<=y2; y++){
            for(x=x1; x<=x2; x++){
                if(solid[z][y][x]) continue; /* don't do solids */
                for(rho0=0.0,i=0; i<nveloc[0]; i++){
                    f[i] = ff[0][i][z][y][x];
                    rho0 += f[i];
                }
                if(rho0<1.0e-30) continue; /* NOTE this "error" check */
                for(i=0; i<nveloc[0]; i++){
                    f[i] /= rho0;
                }
                /* if 6 veloc, lots of recalculation of invariants, but doesn't matter here
*/
                for(s=1; s<ncomponent; s++){
                    /* a negative number is the sign to skip this component */
                    if(concList[s] < 0.0) continue;
                    if(nveloc[s]==19){
                        for(i=0; i<nveloc[s]; i++){
                            ff[s][i][z][y][x] = f[i]*concList[s];
                        }
                    }
                    else { /* just evenly distribute */
                        ftemp = concList[s]/nveloc[s];
                        for(i=0; i<nveloc[s]; i++){
                            ff[s][i][z][y][x] = ftemp;
                        }
                    }
                }
            }
        }
    }
}

```

```

    }
  }
}

return(1);
} /* END SetSlug() */

/*-----*/
/* 7-7-97 for now, only try to recognize completely internal solids (-2). */
/* A problem, compared to D2Q9: if we eventually allow wall streaming, must */
/* consider the "octant" neighbors that are not in the D3Q19 vector set, */
/* so we can't get an easy correspondence between solid neighbors and our */
/* vector numbering scheme (note this would not be a problem if we used */
/* only bounceback, with no Ziegler- or NoFlux-type tangential vectors). */
/*-----*/
int SetSolidType(char ***solid, int nlay, int nrow, int ncol)
{
#define N_ALL_NEIGHBORS 27
int x,y,z,xend,yend,zend,xnew,ynew,znew,i,stype,dx,dy,dz,ctr;
int s[N_ALL_NEIGHBORS]; /* note s[0] IS NOT same as in old...*/
xend = ncol-1; yend = nrow-1; zend = nlay-1;

ctr = 0; /* count the number of -2 solids */

for(z=0; z<nlay; z++){
  for(y=0; y<nrow; y++){
    for(x=0; x<ncol; x++){
      if(solid[z][y][x]){
        /* get the state of the sites in each direction; */
        /* watch for wrap conditions. Note we really */
        /* need to look at ALL neighbors, not just those */
        /* sanctioned in D2Q19; there are 9+8+9 = 26.. */
        i=0; /* important! */
        for(dz=-1; dz<=1; dz++){
          znew = z + dz;
          if(znew<0) znew=zend;
          else if(znew>zend) znew = 0;
          for(dy=-1; dy<=1; dy++){
            ynew = y + dy;
            if(ynew<0) ynew=yend;
            else if(ynew>yend) ynew = 0;
            for(dx=-1; dx<=1; dx++){
              xnew = x + dx;
              if(xnew<0) xnew=xend;
              else if(xnew>xend) xnew = 0;
              s[i++] = solid[znew][ynew][xnew];
            }
          }
        }

        /*----- have all s[]; -----*/
        /* look for enclosed solids FIRST (order important) */
        for(stype=-2,i=0; i<N_ALL_NEIGHBORS; i++){
          if(!s[i]){
            stype=-1; break;
          }
        }
        solid[z][y][x] = stype;
        if(stype==-2) ctr++;
      }
    }
  }
}

```

```

    }
}

/* Kludge to warn functions that depend on SetSolidType()... */
SOLIDS_SET = 1;
return(ctr);
#undef N_ALL_NEIGHBORS
} /* END SetSolidType() */
/*-----*/
/* 7-8-97 Fill the space bounded by nlay,row,ncol with array of semi-close- */
/* packed (cubic, FCC) spheres. The positions and radii of the spheres are */
/* semi-randomly perturbed. zrep, yrep and xrep are the number of FCC */
/* cell reps per nlay, nrow and ncol, respectively; there are 4 complete */
/* points per FCC cell. rslop is the fractional, random slop applied to */
/* the grain radius; cslop is the slop applied to the x,y,z position of */
/* a grain center. Both rslop and cslop should be between 0.0 and 0.5. */
/* rbias is the bias applied toward smaller grain diameters, */
/* vs. larger diameters; it is a float from 0.5 to 1.0, such that 0.5 */
/* provides even distribution of radii above and below mean, and 1.0 biases */
/* all radii to be below the ideal radius. seed is an integer seed */
/* used to initiate the Mrand() random number generator; seed is a positive */
/* integer from 1 to 2^31-1 (CANNOT be 0)... */
/* NOTE MUST be called BEFORE SetSolidType() !! */
/*****/
int SetFCCSolids(char ***solid, int nlay, int nrow, int ncol,
    int zrep, int yrep, int xrep, float rslop, float cslop,
    float rbias, int seed)
{
    int npoints, i, x,y,z, ix,iy,iz, xrep2,yrep2,zrep2, ctr, nbytes;
    int xx, yy, zz; /* corrected fro wrap */
    typedef float coord_t;
    coord_t *xc,*yc,*zc,*rc, xhalf,yhalf,zhalf, radius_ideal, rSqr;
    coord_t dx2,dy2,dz2;
    /* must distinguish between the integer args for Mrand() below... */
    int ixrand, iyrand, izrand, irr;
    int ir; /* integer radius */
    int xend,yend,zend;

    /* ...and the floating point, normalized values below */

    if(!seed) seed = 17; /* don't allow 0 seed */

    ixrand = seed; iyrand = seed+1; izrand = seed+2; irr = seed+3;

    if(rbias<0.5) rbias = 0.5; if(rbias>1.0) rbias = 1.0;
    if(rslop>0.5) rslop = 0.5; if(cslop>0.5) cslop = 0.5;
    if(rslop<0.0) rslop = 0.0; if(cslop<0.0) cslop = 0.0;

    npoints = xrep*yrep*zrep*4;
    nbytes = npoints*sizeof(coord_t);

    /* allocate the arrays */
    xc = malloc(nbytes);
    if(!xc){
        return(0);
    }
}

```

```

yc = malloc(nbytes);
if(!yc){
    if(xc) free(xc); return(0);
}
zc = malloc(nbytes);
if(!zc){
    if(xc) free(xc); if(yc) free(yc); return(0);
}
rc = malloc(nbytes);
if(!rc){
    if(xc) free(xc); if(yc) free(yc); if(zc) free(zc); return(0);
}
/** past allocations **/
xrep2 = xrep << 1; /* mul by two, because the superlattice for FCC */
yrep2 = yrep << 1; /* has repeats of 1/2 unit cell */
zrep2 = zrep << 1;

xhalf = ((coord_t) ncol)/xrep2;
yhalf = ((coord_t) nrow)/yrep2;
zhalf = ((coord_t) nlay)/zrep2;

/* calculate an ideal radius; while we allow some asymmetry through */
/* xrep, etc., we really don't want to do ellipsoids, so we'll pick */
/* the minimal calculated value... */
if(xhalf<=yhalf && xhalf<=zhalf)
    radius_ideal = xhalf*HALF_SQRT2;
else if(yhalf<=xhalf && yhalf<=zhalf)
    radius_ideal = yhalf*HALF_SQRT2;
else
    radius_ideal = zhalf*HALF_SQRT2;

/** fill the co-ord arrays with randomly perturbed values **/
/** NOTE to avoid finding random signs, we bias the random error */
/* by starting at half the range below the xc,yc,zc or rc value; e.g. */
/* xc[ctr] = ix*xhalf - 0.5*cslop*xhalf + ixrand*RAND_NORM*cslop*xhalf */
/* = xhalf*(ix - 0.5*cslop + ixrand*RAND_NORM*cslop) */
/* = xhalf*(ix + cslop*(ixrand*RAND_NORM - 0.5)); */
/* slightly different for radius -- we substitute a val between 0.5 */
/* and 1.0 for 0.5 above, based on "bias" arg passed above... */
/*****/
for(ctr=iz=0; iz<zrep2; iz++){
    for(iy=0; iy<yrep2; iy++){ /* note ctr paranoia */
        for(ix=0; ix<xrep2 && ctr<npoints; ix++){
            /* rule for FCC: sum of indices is even */
            if(((ix+iy+iz)&1)==0){
                /* get random increments */
                ixrand = Mrand(ixrand);
                iyrand = Mrand(iyrand);
                izrand = Mrand(izrand);
                irrands = Mrand(irrand);

                xc[ctr] = xhalf*(ix + cslop*(ixrand*RAND_NORM - 0.5));
                yc[ctr] = yhalf*(iy + cslop*(iyrand*RAND_NORM - 0.5));
                zc[ctr] = zhalf*(iz + cslop*(izrand*RAND_NORM - 0.5));
                rc[ctr] =
                    radius_ideal*(1.0 + rslop*(irrands*RAND_NORM - rbias));
                ctr++;
            }
        }
    }
}

```

```

    }
}

}

}

/** 7-9-97 for debug, print a list of xc, yc, etc. **
for(i=0; i<ctr; i++){
    printf("i=%d: x=%f, y=%f, z=%f, r=%f\n", i, xc[i], yc[i], zc[i], rc[i]);
    if(i==20){puts("press a key"); getch();}
}
getch();
** end debug 7-9-97 ***/

/** have list of jittered co-ords and radii, now do the fill. Basic */
/* idea is to draw a bounding box around each point, and within that */
/* bounding box, check if a point is within the sphere centered at */
/* that point... */
/* NOTE we have to correct for the wrap, but must keep x,y,z sacrosanct to */
/* judge if x,y,z is within sphere, for test against radius... we use */
/* xx,yy,zz as the wrap-corrected indices into solid[][][]... */
/* There is still a chance that if we passed some utterly bizarre values, */
/* x,y,z could fall outside allowed range -- more error checking may */
/* be called for... */
for(i=0; i<ctr; i++){ /* loop over the points */
    ir = rc[i] + 0.5; /* round */
    rSqr = rc[i]*rc[i];
    for(z=zc[i]-rc[i]-0.5, zend=zc[i]+rc[i]+0.5; z<=zend; z++){
        dz2 = (z - zc[i])*(z - zc[i]);
        if(z<0) zz = nlay + z;
        else if(z>=nlay) zz = z - nlay;
        else zz = z;
        /* ultimate failsafe test, in case radii are screwed: */
        if(zz<0) zz = 0; else if(zz>=nlay) zz = nlay - 1;
        for(y=yc[i]-rc[i]-0.5, yend=yc[i]+rc[i]+0.5; y<=yend; y++){
            dy2 = (y - yc[i])*(y - yc[i]);
            if(y<0) yy = nrow + y;
            else if(y>=nrow) yy = y - nrow;
            else yy = y;
            /* ultimate failsafe test, in case radii are screwed: */
            if(yy<0) yy = 0; else if(yy>=nrow) yy = nrow - 1;
            for(x=xc[i]-rc[i]-0.5, xend=xc[i]+rc[i]+0.5; x<=xend; x++){
                dx2 = (x - xc[i])*(x - xc[i]);
                if(rSqr > dx2 + dy2 + dz2){
                    /* point is within sphere, now check wrap */
                    if(x<0) xx = ncol + x;
                    else if(x>=ncol) xx = x - ncol;
                    else xx = x;
                    if(xx<0) xx=0; else if(xx>=ncol) xx = ncol-1;
                    solid[zz][yy][xx] = -1;
                }
            }
        }
    }
}

}

}

/** "normal" return; free any arrays ***/
free(xc); free(yc); free(zc); free(rc);
return(ctr);

```

```

}    /* END SetFCCSolids() */
/*-----*/
/* 6-13-97 adapted from home GW2K PPro200 c:\ilga\asm_lga.asm; */
/* uses GGUBS type PRNG; avoids interger division by using */
/* "simulated" division described in Knuth "Seminumerical..." */
/* NOTE unlike rand(), does not require seed -- always gives */
/* back the next arg in sequence after z. Usual procedure is */
/* to keep reusing z, so z itself should NOT be altered between */
/* calls. Lower bits are supposedly nice and random. */
/* Unix, Linux or alpha NT users: the PRNG is: */
/* new Z = (16807*Z) MOD 0x7FFFFFFF, sometimes called "GGUBS". The */
/* range is obviously 1 to 0x7FFFFFFF, so don't use Z=0. The */
/* modded value is 2^{31}-1, a Mersenne prime number. If you have */
/* fast integer division, code can be simplified; if you have 64-bit */
/* integers, code is trivial. If your system has random(), it is */
/* probably at least as good a substitute (MS VC++ is supplied with */
/* only rand(), which gives back just 15 bits). */
/* NOTE if you subs a different random number generator, you should change */
/* MRAND_RANGE to the new generator's range! */
/*****/
int Mrand(int z)
{
    __asm
    {
        mov eax, 16807
        mul z
        shld edx,eax,1
        and eax, 7FFFFFFFH
        add edx,eax
        jns replaceZ
        sub edx, 7FFFFFFFH
replaceZ: mov eax,edx        ;return in eax..
    }
} /* compiler may complain about no return value -- it is implicitly in eax */
/*-----*/
/* 5-21-97 from lb01.c, modify to use UxAvg() and UyAvg() */
/* 2-16-97 comment out Inc adjustment, just reset Body forces */
/* and return -1, so main can turn off access to this function... */
/* 2-15-97 add code to chech gotHit and do clamping */
/* 2-4-97 adjust the gravity (xbody, ybody) if required to keep */
/* below or at a constant average speed on the Ux and Uy lines... */
/*****/
int AdjustGrav(struct veloc_t *const*const* uu,
               char *const*const* solid,
               int nlay, int nrow, int ncol, struct gravity * const gp)
{
    double ux, uy, uz;
    double uxLow,uyLow,uzLow;
    static int stepCounter=0, gotHit=0, done=0;
    static double fxSum=0.0, fySum=0.0, fzSum=0.0,
        uxSum=0.0, uySum=0.0, uzSum=0.0;
    double uRatio;
    int dt;

    if(done==-1) return(-1); /* 2-16-97 failsafe */

    uxLow = 0.99*gp->uxLimit;

```



```

uyLow = 0.99*gp->uyLimit;
uzLow = 0.99*gp->uzLimit;

if(gp->do_x){
    ux = UxAvg(uu, solid, nlay, nrow, ncol,
               gp->xUx, gp->y1Ux, gp->y2Ux, gp->z1Ux, gp->z2Ux);
    if(gp->xBody > 0.0){
        if(ux > gp->uxLimit){
            if(ux > gp->uxLast) gp->txBody -= gp->xBodyInc;
            else gp->txBody -= gp->xBodyIncSmall;
            if(gp->txBody < 0.0) gp->txBody = 0.0;
            gotHit=1;
        }
        else if(gp->txBody < gp->xBody && (ux<uxLow || ux<gp->uxLast)){
            gp->txBody += gp->xBodyIncSmall;
            gotHit=1;
        }
    }
    else if(gp->xBody < 0.0){
        if(ux < gp->uxLimit){
            if(ux < gp->uxLast) gp->txBody += gp->xBodyInc;
            else gp->txBody += gp->xBodyIncSmall;
            if(gp->txBody > 0.0) gp->txBody = 0.0;
            gotHit=1;
        }
        else if(gp->txBody > gp->xBody && (ux>uxLow || ux>gp->uxLast)){
            gp->txBody -= gp->xBodyIncSmall;
            gotHit=1;
        }
    }
}

if(gp->do_y){
    uy = UyAvg(uu, solid, nlay, nrow, ncol,
               gp->yUy, gp->x1Uy, gp->x2Uy, gp->z1Uy, gp->z2Uy);
    if(gp->yBody > 0.0){
        if(uy > gp->uyLimit){
            if(uy > gp->uyLast) gp->tyBody -= gp->yBodyInc;
            else gp->tyBody -= gp->yBodyIncSmall;
            if(gp->tyBody < 0.0) gp->tyBody = 0.0;
            gotHit=1;
        }
        else if(gp->tyBody < gp->yBody && (uy<uyLow || uy<gp->uyLast)){
            gp->tyBody += gp->yBodyIncSmall;
            gotHit=1;
        }
    }
    else if(gp->yBody < 0.0){
        if(uy < gp->uyLimit){
            if(uy < gp->uyLast) gp->tyBody += gp->yBodyInc;
            else gp->tyBody += gp->yBodyIncSmall;
            if(gp->tyBody > 0.0) gp->tyBody = 0.0;
            gotHit=1;
        }
        else if(gp->tyBody > gp->yBody && (uy>uyLow || uy>gp->uyLast)){
            gp->tyBody -= gp->yBodyIncSmall;
            gotHit=1;
        }
    }
}

```

```

    }
}
if(gp->do_z){
    uz = UzAvg(uu, solid, nlay, nrow, ncol,
        gp->zUz, gp->x1Uz, gp->x2Uz, gp->y1Uz, gp->y2Uz);
    if(gp->zBody > 0.0){
        if(uz > gp->uzLimit){
            if(uz > gp->uzLast) gp->tzBody -= gp->zBodyInc;
            else gp->tzBody -= gp->zBodyIncSmall;
            if(gp->tzBody < 0.0) gp->tzBody = 0.0;
            gotHit=1;
        }
        else if(gp->tzBody < gp->zBody && (uz<uzLow || uz<gp->uzLast)){
            gp->tzBody += gp->zBodyIncSmall;
            gotHit=1;
        }
    }
    else if(gp->zBody < 0.0){
        if(uz < gp->uzLimit){
            if(uz < gp->uzLast) gp->txBody += gp->zBodyInc;
            else gp->tzBody += gp->zBodyIncSmall;
            if(gp->tzBody > 0.0) gp->tzBody = 0.0;
            gotHit=1;
        }
        else if(gp->tzBody > gp->zBody && (uz>uzLow || uz>gp->uzLast)){
            gp->tzBody -= gp->zBodyIncSmall;
            gotHit=1;
        }
    }
}

if(gotHit){
    stepCounter++; /* 2-15-97 */
    if(stepCounter >= gp->stepStartClamp && stepCounter < gp->stepStopClamp){
        fxSum += gp->txBody; fySum += gp->tyBody; fzSum += gp->tzBody;
        uxSum += ux; uySum += uy; uzSum += uz;
    }
    if(stepCounter == gp->stepStopClamp
        && (dt=gp->stepStopClamp - gp->stepStartClamp)>0){
        if(gp->do_x){
            gp->txBody = fxSum / dt;
            uxSum /= dt;
            /* 2-16-97 add speed correction if makes sense */
            if(fabs(uxSum) > 1.0e-30){
                uRatio = gp->uxLimit / uxSum;
                if(uRatio>0.8 && uRatio<1.2) gp->txBody *= uRatio;
            }
        }
        if(gp->do_y){
            gp->tyBody = fySum / dt;
            uySum /= dt;
            /* 2-16-97 add speed correction if makes sense */
            if(fabs(uySum) > 1.0e-30){
                uRatio = gp->uyLimit / uySum;

```

```

        if(uRatio>0.8 && uRatio<1.2) gp->tzBody *= uRatio;
    }

    /*****/
    }
    if(gp->do_z){
        gp->tzBody = fzSum / dt;
        uzSum /= dt;
        /* 2-16-97 add speed correction if makes sense */
    /*****/
        if(fabs(uzSum) > 1.0e-30){
            uRatio = gp->uzLimit / uzSum;
            if(uRatio>0.8 && uRatio<1.2) gp->tzBody *= uRatio;
        }
    /*****/
    }
    done = -1;
    return(done);
}

}

return(1);
} /* END AdjustGrav() */
/-----*/
/* 6-21-98 for TA retest, remove 0.5 weighting bounding solid */
/* Obtain average x-direction speed across specified */
/* y-z plane for component 0, inclusive of endpoints. */
/* NOTE very different philosophy from ilga -- we will ignore inner */
/* solids in count, and weight our count only by the fraction of */
/* fluid encountered at each site on path... sort of presumes a */
/* Ziegler-type or Noble-type correction for wall velocity, OR */
/* that one arranges endpoints to NOT include solid... */
/* NOTE 7-9-97 to start we will use very simple weighting scheme */
/* of 0 for solidcode -2, 0.5 for solidcode -1, and 1 for open fluid... */
/* MUST CHANGE when Ziegler, NoFlux introduced... */
/*****/
double UxAvg(struct veloc_t *const*const* uu, char *const*const* solid,
             int nlay, int nrow, int ncol, int x, int y1, int y2, int z1, int z2)
{
    int z,y,i,temp,solidcode;
    double uxTot, wTot, w;

    if(x<0 || y1<0 || y2<0 || x>=ncol || y1>=nrow || y2>=nrow
        || z1<0 || z2<0 || z1>=nlay || z2>=nlay){
        return(0.0);
    }

    if(y1>y2){
        temp = y1; y1=y2; y2=temp;
    }
    if(z1>z2){
        temp = z1; z1=z2; z2=temp;
    }

    /* since solidcode == -2 doesn't increment either uxAvg or wTot, ignore */
    for(z=z1;uxTot=0.0,wTot=0.0; z<=z2; z++){
        for(y=y1; y<=y2; y++){
            solidcode = solid[z][y][x];

```

```

        if(solidcode==-1){
/**          wTot += 0.5;  **/
            /* implicitly adds 0 to uxAvg */
        }
        else if(solidcode==0){ /* open fluid FOR NOW!! */
            wTot += 1.0;
            uxTot += uu[z][y][x].x;
        }
    }
}
if(wTot>1.0e-30) return(uxTot/wTot);
else return(0.0);
} /* END UxAvg() */
/*-----*/
/* Obtain average y-direction speed across specified */
/* x-z plane for component 0, inclusive of endpoints. */
/* NOTE very different philosophy from ilga -- we will ignore inner */
/* solids in count, and weight our count only by the fraction of */
/* fluid encountered at each site on path... sort of presumes a */
/* Ziegler-type or Noble-type correction for wall velocity, OR */
/* that one arranges endpoints to NOT include solid... */
/* NOTE 7-9-97 to start we will use very simple weighting scheme */
/* of 0 for solidcode -2, 0.5 for solidcode -1, and 1 for open fluid... */
/* MUST CHANGE when Ziegler, NoFlux introduced... */
/*****
double UyAvg(struct veloc_t *const*const* uu, char *const*const* solid,
             int nlay, int nrow, int ncol, int y, int x1, int x2, int z1, int z2)
{
    int z,x,i,temp,solidcode;
    double uyTot, wTot, w;

    if(y<0 || x1<0 || x2<0 || y>=nrow || x1>=ncol || x2>=ncol
        || z1<0 || z2<0 || z1>=nlay || z2>=nlay){
        return(0.0);
    }

    if(x1>x2){
        temp = x1; x1=x2; x2=temp;
    }
    if(z1>z2){
        temp = z1; z1=z2; z2=temp;
    }

    /* since solidcode == -2 doesn't increment either uyAvg or wTot, ignore */
    for(z=z1;uyTot=0.0,wTot=0.0; z<=z2; z++){
        for(x=x1; x<=x2; x++){
            solidcode = solid[z][y][x];
            if(solidcode==-1){
/**          wTot += 0.5;  **/
                /* implicitly adds 0 to uyAvg */
            }
            else if(solidcode==0){ /* open fluid FOR NOW!! */
                wTot += 1.0;
                uyTot += uu[z][y][x].y;
            }
        }
    }
}

```

```

if(wTot>1.0e-30) return(uyTot/wTot);
else return(0.0);
} /* END UyAvg() */
/*-----*/
/* Obtain average z-direction speed across specified */
/* x-y plane for component 0, inclusive of endpoints. */
/* NOTE very different philosophy from ilga -- we will ignore inner */
/* solids in count, and weight our count only by the fraction of */
/* fluid encountered at each site on path... sort of presumes a */
/* Ziegler-type or Noble-type correction for wall velocity, OR */
/* that one arranges endpoints to NOT include solid... */
/* NOTE 7-9-97 to start we will use very simple weighting scheme */
/* of 0 for solidcode -2, 0.5 for solidcode -1, and 1 for open fluid... */
/* MUST CHANGE when Ziegler, NoFlux introduced... */
/*****/
double UzAvg(struct veloc_t *const*const* uu, char *const*const* solid,
             int nlay, int nrow, int ncol, int z, int x1, int x2, int y1, int y2)
{
    int x,y,i,temp,solidcode;
    double uzTot, wTot, w;

    if(z<0 || y1<0 || y2<0 || z>=nlay || y1>=nrow || y2>=nrow
        || x1<0 || x2<0 || x1>=ncol || x2>=ncol){
        return(0.0);
    }

    if(y1>y2){
        temp = y1; y1=y2; y2=temp;
    }
    if(x1>x2){
        temp = x1; x1=x2; x2=temp;
    }

    /* since solidcode == -2 doesn't increment either uzAvg or wTot, ignore */
    for(y=y1;uzTot=0.0,wTot=0.0; y<=y2; y++){
        for(x=x1; x<=x2; x++){
            solidcode = solid[z][y][x];
            if(solidcode==-1){
/**
                wTot += 0.5; **/
                /* implicitly adds 0 to uzAvg */
            }
            else if(solidcode==0){ /* open fluid FOR NOW!! */
                wTot += 1.0;
                uzTot += uu[z][y][x].z;
            }
        }
    }

    if(wTot>1.0e-30) return(uzTot/wTot);
    else return(0.0);
} /* END UzAvg() */
/*-----*/
/* 9-26-97 NOTE for the JB code, AFTER Recycle() we use XSetConcJB(), */
/* (below) NOT these funcs! */
/* Set the concentrations to the values specified in the array concList[], */
/* along the plane of constant Y...similar to HSetConc() in 2D models... */
/* a negative value for a particular component means: skip this component. */
/* The concentrations are set along the plane with opposite corners */

```

```

/* x1,y,z1 to x2,y,z2, inclusive of the endpoints... */
/* 7-11-97 redesign to: scale */
/* 6-vector to the corresponding cartesian vectors in 19-vector carrier... */
/* this method should prevent the bleed-through on edges we possibly got */
/* with some of the fracture x (intersection) calcs done in april 97... */
/*****/
int YSetConc(ff_t ***** const ff, char *** const solid,
            int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
            int y, int x1, int x2, int z1, int z2, double * const concList)
{
int x,z,i,s,temp,is_v19, is_v6, nvel;
/* 7-11-97 the "is_" above test is any of the solutes are 19 or 6 vector */
/* types; would be more efficient done just once outside, but seems safer */
/* to do this simple test internally, since it will be dwarfed by fetching */
/* and computation time in rest of function, and we may some day reallocate */
/* a 19-vector solute among 6 vectors after equilibration.... */

double f[DEF_NVELOC], rho0, conc;
double fv6[6], rho0v6; /* 7-11-97, for 6-vector methods */
double inv_rho0, inv_rho0v6;

if(y<0 || x1<0 || x2<0 || y>=nrow || x1>=ncol || x2>=ncol
    || z1<0 || z2<0 || z1>nlay || z2>nlay) return(0);

if(x1>x2){
    temp = x1; x1=x2; x2=temp;
}
if(z1>z2){
    temp = z1; z1=z2; z2=temp;
}

/* test for need to do 19 or 6 vector scaling */
for(is_v19=is_v6=0, s=1; s<ncomponent; s++){
    if(concList[s]>=0.0){ /* recall we don't do entries with negative... */
        if(nveloc[s]==6) is_v6=1;
        else if(nveloc[s]==19) is_v19=1;
    }
}

/* now do real meat of function; distribute concList[s] proportionally */
/* as ff[0][i][z][y][x] are distributed among velocities ... */

for(z=z1; z<z2; z++){
    for(x=x1; x<=x2; x++){
        if(solid[z][y][x]==-2) continue; /* don't do internal solids */
        if(is_v19){ /* if we found ANY solute is 19-vector model: */
            for(rho0=0.0,i=0; i<nveloc[0]; i++){
                f[i] = ff[0][i][z][y][x];
                rho0 += f[i];
            }
            if(rho0<1.0e-30) continue; /* NOTE this "error" check */
            inv_rho0 = 1.0 / rho0;
            for(i=0; i<nveloc[0]; i++){
                f[i] *= inv_rho0;
            }
        }
        if(is_v6){ /* if ANY solute is a 6-vector model */

```

```

/* see top of file for key; use Cartesian axis vectors */
/* from carrier, only... */
rho0v6 = fv6[0] = ff[0][1][z][y][x]; /* 0 degr, points right */
rho0v6+= fv6[1] = ff[0][3][z][y][x]; /* 90 degr, points north */
rho0v6+= fv6[2] = ff[0][5][z][y][x]; /* 180 degr, points left */
rho0v6+= fv6[3] = ff[0][7][z][y][x]; /* 270 degr, points south */
rho0v6+= fv6[4] = ff[0][9][z][y][x]; /* points up out of page */
rho0v6+= fv6[5] = ff[0][18][z][y][x]; /* points down into page */
if(rho0v6<1.0e-30) continue;
inv_rho0v6 = 1.0 / rho0v6;
fv6[0] *= inv_rho0v6; fv6[1] *= inv_rho0v6;
fv6[2] *= inv_rho0v6; fv6[3] *= inv_rho0v6;
fv6[4] *= inv_rho0v6; fv6[5] *= inv_rho0v6;
}
for(s=1; s<ncomponent; s++){
    nvel = nveloc[s];
    /* a negative number is the sign to skip this component */
    if(concList[s] < 0.0) continue;
    if(nvel==19){
        for(i=0; i<nvel; i++){
            ff[s][i][z][y][x] = f[i]*concList[s];
        }
    }
    else if(nvel==6){ /* if-else 5-26-97 */
        for(i=0; i<nvel; i++){
            ff[s][i][z][y][x] = fv6[i]*concList[s];
        }
    }
}
}
return(1);
} /* END YSetConc() */

/*-----*/
/* 9-26-97 NOTE for the JB code, AFTER Recycle() we use XSetConcJB(), */
/* (below) NOT these funcs! */
/* Set the concentrations to the values specified in the array concList[], */
/* along the Plane with constant x...similar to VSetConc() in 2D models... */
/* a negative value for a particular component means: skip this component. */
/* The concentrations are set along the "line" is from x,y1 to x,y2, */
/* inclusive of the endpoints... */
/* NOTE even though we advance y downward (as a row index), the positive */
/* y direction for flux calculations is UP... */
/*-----*/
int XSetConc(ff_t ***** const ff, char *** const solid,
            int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
            int x, int y1, int y2, int z1, int z2, double * const concList)
{
    int z,y,i,s,temp,is_v19, is_v6, nvel;
    /* 7-11-97 the "is_" above test is any of the solutes are 19 or 6 vector */
    /* types; would be more efficient done just once outside, but seems safer */
    /* to do this simple test internally, since it will be dwarfed by fetching */
    /* and computation time in rest of function, and we may some day reallocate */
    /* a 19-vector solute among 6 vectors after equilibration.... */

    double f[DEF_NVELOC], rho0, conc;
    double fv6[6], rho0v6; /* 7-11-97, for 6-vector methods */

```

```

double inv_rho0, inv_rho0v6;

if(x<0 || y1<0 || y2<0 || x>=ncol || y1>=nrow || y2>=nrow
    || z1<0 || z2<0 || z1>=nlay || z2>=nlay) return(0);

if(y1>y2){
    temp = y1; y1=y2; y2=temp;
}
if(z1>z2){
    temp = z1; z1=z2; z2=temp;
}

/* test for need to do 19 or 6 vector scaling */
for(is_v19=is_v6=0, s=1; s<ncomponent; s++){
    if(concList[s]>=0.0){ /* recall we don't do entries with negative... */
        if(nveloc[s]==6) is_v6=1;
        else if(nveloc[s]==19) is_v19=1;
    }
}

/* now do real meat of function; distribute concList[s] proportionally */
/* as ff[0][i][z][y][x] are distributed among velocities ... */
for(z=z1; z<z2; z++){
    for(y=y1; y<=y2; y++){
        /* 7-11-97 note -- we should consider an easy way to do EDGE */
        /* solids eventually, especially for solute sinks!! Else we */
        /* will get leakage around these... */
        if(solid[z][y][x]==-2) continue; /* don't do internal solids */
        if(is_v19){ /* if we found ANY solute is 19-vector model: */
            for(rho0=0.0,i=0; i<nveloc[0]; i++){
                f[i] = ff[0][i][z][y][x];
                rho0 += f[i];
            }
            if(rho0<1.0e-30) continue; /* NOTE this "error" check */
            inv_rho0 = 1.0 / rho0;
            for(i=0; i<nveloc[0]; i++){
                f[i] *= inv_rho0;
            }
        }
        if(is_v6){ /* if ANY solute is a 6-vector model */
            /* see top of file for key; use Cartesian axis vectors */
            /* from carrier, only... */
            rho0v6 = fv6[0] = ff[0][1][z][y][x]; /* 0 degr, points right */
            rho0v6+= fv6[1] = ff[0][3][z][y][x]; /* 90 degr, points north */
            rho0v6+= fv6[2] = ff[0][5][z][y][x]; /* 180 degr, points left */
            rho0v6+= fv6[3] = ff[0][7][z][y][x]; /* 270 degr, points south */
            rho0v6+= fv6[4] = ff[0][9][z][y][x]; /* points up out of page */
            rho0v6+= fv6[5] = ff[0][18][z][y][x]; /* points down into page */
            if(rho0v6<1.0e-30) continue;
            inv_rho0v6 = 1.0 / rho0v6;
            fv6[0] *= inv_rho0v6; fv6[1] *= inv_rho0v6;
            fv6[2] *= inv_rho0v6; fv6[3] *= inv_rho0v6;
            fv6[4] *= inv_rho0v6; fv6[5] *= inv_rho0v6;
        }
        for(s=1; s<ncomponent; s++){
            nvel = nveloc[s];
            /* a negative number is the sign to skip this component */

```



```

        if(concList[s] < 0.0) continue;
        if(nvel==19){
            for(i=0; i<nvel; i++){
                ff[s][i][z][y][x] = f[i]*concList[s];
            }
        }
        else if(nvel==6){
            for(i=0; i<nvel; i++){
                ff[s][i][z][y][x] = fv6[i]*concList[s];
            }
        }
    }
}

return(1);
} /* END XSetConc() */

/*-----*/
/* 9-26-97 NOTE for the JB code, AFTER Recycle() we use XSetConcJB(), */
/* (below) NOT these funcs! */
/* Measure x-direction (left to right) flux across specified */
/* vertical plane for component s, inclusive of endpoints. */
/* NOTE icomp can be 0, which returns the velocity, effectively; */
/* NOTE this is really fluence, since we don't adjust for "area" */
/* (number of points) on line. */
/*****/
double XGetFlux(ff_t ***** const ff, char *** const solid, int ncomponent,
               int nveloc[], int nlay, int nrow, int ncol, int x, int y1, int y2,
               int z1, int z2, int s, double * const ftotPtr)
{
    int z,y,i,temp;
    double xflux, f[DEF_NVELOC], rhoTot;

    if(x<0 || y1<0 || y2<0 || z1<0 || z2<0 ||
       x>=ncol || y1>=nrow || y2>=nrow || z1>=nlay || z2>=nlay
       || s<0 || s>=ncomponent){
        *ftotPtr = 0.0;
        return(0.0);
    }

    if(y1>y2){
        temp = y1; y1=y2; y2=temp;
    }
    if(z1>z2){
        temp = z1; z1=z2; z2=temp;
    }

    if(nveloc[s]==19){
        for(z=z1; rhoTot=0.0, xflux=0.0; z<=z2; z++){
            for(y=y1; y<=y2; y++){
                rhoTot += (f[0] = ff[s][0][z][y][x]);
                rhoTot += (f[1] = ff[s][1][z][y][x]);
                rhoTot += (f[2] = ff[s][2][z][y][x]);
                rhoTot += (f[3] = ff[s][3][z][y][x]);
                rhoTot += (f[4] = ff[s][4][z][y][x]);
                rhoTot += (f[5] = ff[s][5][z][y][x]);
                rhoTot += (f[6] = ff[s][6][z][y][x]);
                rhoTot += (f[7] = ff[s][7][z][y][x]);
            }
        }
    }
}

```

```

        rhoTot += (f[8] = ff[s][8][z][y][x]);
        rhoTot += (f[9] = ff[s][9][z][y][x]);
        rhoTot += (f[10] = ff[s][10][z][y][x]);
        rhoTot += (f[11] = ff[s][11][z][y][x]);
        rhoTot += (f[12] = ff[s][12][z][y][x]);
        rhoTot += (f[13] = ff[s][13][z][y][x]);
        rhoTot += (f[14] = ff[s][14][z][y][x]);
        rhoTot += (f[15] = ff[s][15][z][y][x]);
        rhoTot += (f[16] = ff[s][16][z][y][x]);
        rhoTot += (f[17] = ff[s][17][z][y][x]);
        rhoTot += (f[18] = ff[s][18][z][y][x]);

        xflux += (f[1] + f[2] + f[8] + f[10] + f[14]
                  - f[5] - f[4] - f[6] - f[12] - f[16]);
    }
}
else if(nveloc[s]==6){
    for(z=z1,xflux=0.0,rhoTot=0.0; z<=z2; z++){
        for(y=y1; y<=y2; y++){
            rhoTot += (f[0] = ff[s][0][z][y][x]);
            rhoTot += (f[1] = ff[s][1][z][y][x]);
            rhoTot += (f[2] = ff[s][2][z][y][x]);
            rhoTot += (f[3] = ff[s][3][z][y][x]);
            rhoTot += (f[4] = ff[s][4][z][y][x]);
            rhoTot += (f[5] = ff[s][5][z][y][x]);

            xflux += f[0] - f[2];
        }
    }
}

*ftotPtr = rhoTot;
return(xflux);
} /* END XGetFlux() */
/*-----*/
/* Measure Y-direction (left to right) flux across specified */
/* horizontal (y constant) plane for component s, inclusive of endpoints. */
/* NOTE icomp can be 0, which returns the velocity, effectively; */
/* NOTE this is really fluence, since we don't adjust for "area" */
/* (number of points) on line. */
/* NOTE even though we advance y downward (as a row index), the positive */
/* y direction for flux calculations is UP... */
/*****/
double YGetFlux(ff_t ***** const ff, char *** const solid,
               int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
               int y, int x1, int x2, int z1, int z2, int s, double * const ftotPtr)
{
    int z,x,i,temp;
    double yflux,f[DEF_NVELOC],rhoTot;

    if(y<0 || x1<0 || x2<0 || z1<0 || z2<0 || x1>=ncol || x2>=ncol
       || z1>=nlay || z2>=nlay || y>=nrow || s<0 || s>=ncomponent){
        *ftotPtr = 0.0;
        return(0.0);
    }
}

```

```

if(x1>x2){
    temp = x1; x1=x2; x2=temp;
}
if(z1>z2){
    temp = z1; z1=z2; z2=temp;
}
if(nveloc[s]==19){
    for(z=z1,yflux=0.0,rhoTot=0.0; z<=z2; z++){
        for(x=x1; x<=x2; x++){
            rhoTot += (f[0] = ff[s][0][z][y][x]);
            rhoTot += (f[1] = ff[s][1][z][y][x]);
            rhoTot += (f[2] = ff[s][2][z][y][x]);
            rhoTot += (f[3] = ff[s][3][z][y][x]);
            rhoTot += (f[4] = ff[s][4][z][y][x]);
            rhoTot += (f[5] = ff[s][5][z][y][x]);
            rhoTot += (f[6] = ff[s][6][z][y][x]);
            rhoTot += (f[7] = ff[s][7][z][y][x]);
            rhoTot += (f[8] = ff[s][8][z][y][x]);
            rhoTot += (f[9] = ff[s][9][z][y][x]);
            rhoTot += (f[10] = ff[s][10][z][y][x]);
            rhoTot += (f[11] = ff[s][11][z][y][x]);
            rhoTot += (f[12] = ff[s][12][z][y][x]);
            rhoTot += (f[13] = ff[s][13][z][y][x]);
            rhoTot += (f[14] = ff[s][14][z][y][x]);
            rhoTot += (f[15] = ff[s][15][z][y][x]);
            rhoTot += (f[16] = ff[s][16][z][y][x]);
            rhoTot += (f[17] = ff[s][17][z][y][x]);
            rhoTot += (f[18] = ff[s][18][z][y][x]);

            yflux += (f[2] + f[3] + f[4] + f[11] + f[15]
                    - f[6] - f[7] - f[8] - f[13] - f[17]);
        }
    }
}
else if(nveloc[s]==6){
    for(z=z1,yflux=0.0,rhoTot=0.0; z<=z2; z++){
        for(x=x1; x<=x2; x++){
            rhoTot += (f[0] = ff[s][0][z][y][x]);
            rhoTot += (f[1] = ff[s][1][z][y][x]);
            rhoTot += (f[2] = ff[s][2][z][y][x]);
            rhoTot += (f[3] = ff[s][3][z][y][x]);
            rhoTot += (f[4] = ff[s][4][z][y][x]);
            rhoTot += (f[5] = ff[s][5][z][y][x]);

            yflux += f[1] - f[3];
        }
    }
}

*ftotPtr = rhoTot;
return(yflux);
} /* END YGetFlux() */
/*-----*/
/* 7-11-97 modify SavePpm to plot U (speed) at successive z slices in zz[], */
/* each further downscreen. Note this version isn't oriented toward */
/* making mpegs, since we usually just want a few snapshots of speed... */
/* Note nz is number of layers specified in zz[]... */

```

```

/* Saves a portable pixel map (ppm, as in pbmplus from Unix lore), but UNLIKE */
/* SavePpm(), doesn't pass back *FILE... */
/***** */
int SaveUPpm(struct veloc_t *** const uu, char ***solid,
             int nlay, int nrow, int ncol, int zz[], int nz, int step)
{
#define RGB_BASE 70
#define RGB_MAX_SIZE      8192 /* allows ncol+nlay <= 2730 */
#define LOCAL_BUF_LEN     128
static unsigned char rgb_row[RGB_MAX_SIZE+4];
/* for mpeg writes, 3* max ncol */

static int filenum=0, firsttime=1, rgb_len;
static FILE *fp;
int i,ii,x,y,z,n;
unsigned char r,g,b;
double u, umax=-1.0e200;
double slope1,slope2,delta,uhalf,uraw,upt75,scale;
struct tm *ptm;
static int day=0,hour=0; /* because localtime destroys single internal tm */
time_t lt;
char buf[LOCAL_BUF_LEN]; /* for filenames */

if(filenum>=999){
    firsttime = 1;
    filenum = 0;
}

if(firsttime){
    /* ppm format has three byte rgb values for each pixel */
    time(&lt);
    ptm = localtime(&lt);
    day = ptm->tm_mday, hour = ptm->tm_hour;
    firsttime=0;
}
/* 9-27-97 move out of firsttime block */
rgb_len = ncol*3;

/* Because we will be using inherently positive values, won't need */
/* to check for min -- it will be 0.... */
for(n=0; n<nz; n++){
    z = zz[n];
    for(y=0; y<nrow; y++){
        for(x=0; x<ncol; x++){
            u = uu[z][y][x].usqrd;
            if(u >= umax) umax = u;
        }
    }
}
umax = sqrt(umax);

delta = 255 - RGB_BASE; /* ASSUME maximum value for r,g or b is 255 */
uhalf = 0.5*umax;
upt75 = 0.75*umax;
if(umax > 1e-30){
    slope1 = delta/uhalf;
    slope2 = slope1*2.0;
}

```

```

    }
else return(0);
if(umax>1.e-20) scale = 255.0/umax;
else scale = 0.0;

/* make the file name; avoid lots of unclosed files if */
/* the umax is too small... */
/* Remember localtime structure is not "re-entrant"... */
buf[LOCAL_BUF_LEN-1] = 0;
sprintf(buf,"U%02d%02d%03d.PPM", day, hour, filenum);
filenum++;
fp = fopen(buf, "wb");
if(!fp) return(0); /* was return(0) */
/* write the standard binary ppm header; \012 is linefeed... */
/* We'll use a divider between each of the nz zz[] layers, and there will */
/* be nz such divider lines, with one at end too... */
fprintf(fp,"P6\012%d %d\012255\012",ncol,nrow*nz + nz);

for(n=0; n<nz; n++){
    z = zz[n];
    for(y=0; y<nrow; y++){
        /* 1st loop over the y-x cut */
        for(x=0,ii=0; x<ncol && ii<RGB_MAX_SIZE; x++,ii+=3){
            /* print solids in white */
            if(solid[z][y][x]==0){
                u = sqrt(uu[z][y][x].usqrd);
                /* prevent funny colors */
                if(u<0.0) u = 0.0;
                /* for now we will just gray scale */
                **** comment out simple grayscale alternative ****
                r = scale*u;
                if(r>255) r=255;
                g = b = r>>1;
                **** END comment out simple gray scale alternative ****

                /***** "default" rainbow scaling below ****/
                /** uraw = umax - u; 7-11-97 **/
                uraw = u;
                if(uraw<uhalf){
                    r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*uraw);
                    if(r<RGB_BASE) r = RGB_BASE;
                    g = RGB_BASE + (int)(uraw*slope1); if(g>255) g = 255;
                }
                else if(uraw<upt75){
                    b = RGB_BASE; g = 255;
                    r = RGB_BASE + (int)((uraw-uhalf)*slope2); if(r>255) r =
255;
                }
                else {
                    b = RGB_BASE; r = 255;
                    g = RGB_BASE + (int)(delta - slope2*(uraw-upt75));
                }
                /** END default rainbow scheme ****/
            }
            else r=g=b=255; /* if solid, print as white */
            /* place in array */
            rgb_row[ii]=r, rgb_row[ii+1]=g, rgb_row[ii+2]=b;

```

```

    }
    fwrite(rgb_row, 1, rgb_len, fp);
}
/** at end of each z slice, write a divider line */
for(i=0; i<rgb_len; i++) rgb_row[i] = 0;
fwrite(rgb_row, 1, rgb_len, fp);
}
fclose(fp);
return(1);
#undef RGB_BASE
#undef RGB_MAX_SIZE
#undef LOCAL_BUF_LEN
} /* END SaveUPpm() */
/*-----*/
/* 7-12-97 this very different version creates a pseudo-3D ppm image */
/* with the y,x plane (z=0) on left, x-z (y=0) plane on top, and the */
/* y,z (x=ncol-1) plane on right. Because the geometry is complex, */
/* we will allocate a buffer and write the values to the buffer, then */
/* write the buffer to a file at completion (then free the buffer)... */
/* ***** */
FILE *Save3DPpm(ff_t *****ff, char ***solid, int ncomponent, int nveloc[],
    int nlay, int nrow, int ncol, int sstart, int step)
{
#define RGB_BASE 70
#define LOCAL_BUF_LEN 128
/* for now, make SINT (sin(theta)), COST, SINP (sin(phi)) and COSP */
/* defines... */
#define SINT 0.5 /* 30 degrees */
#define SINP 0.5 /* 30 degrees */
#define COST 0.866025403 /* 30 degrees */
#define COSP 0.866025403 /* 30 degrees */

static int filenum=0, firsttime=1, rgb_len;
static FILE *fp, *t_list_fp;
int i,ii,x,y,z,xend;
unsigned char r,g,b;
double c, cmax=-1.0e200, cmin=1.0e200;
double slope1,slope2,delta,chalf,craw,cpt75;
struct tm *ptm;
static int day=0,hour=0; /* because localtime destroys single internal tm */
time_t lt;
char buf[LOCAL_BUF_LEN]; /* for filenames */
char *rgb_buf; /* 7-12-97 we must allocate below */
int widthPixels, widthBytes, height, totBytes, xs1, ys1, xs0, ys0, xs, ys;
/* xs,ys are "screen" coords, and have no simple tie to x,y,z for LB array; */
/* xs increases to right, but ys increases down, like video buffer. */

/** begin by allocating and calculationg total size */
/* 7-23-97 changed + 3 to + 5 */
widthPixels = ncol*COSP + nlay*COST + 5; /* +5 allows for bounding lines */
widthBytes = widthPixels*3; /* r,g,b each take a byte */
height = nrow + ncol*SINP + nlay*SINT + 3;
totBytes = widthBytes*height;
rgb_buf = malloc(totBytes);
if(!rgb_buf) return(t_list_fp);
/** "zero" out the array with a black background; */
/** we will eventually have to deal with misalignment and bleed-through; */

```

```

/** for now avoid bleed by writing each point twice, once below current */
/** line... */
for(i=0; i<totBytes; i++) rgb_buf[i] = 0;

/* find logical positions in buffer for xs0,ys0, xs1,ys1 */
/*
      *-----*
/*  xs1  /          / \          */
/*  ys1 /          /   \         */
/*      *-----*   xs0  \         */
/*      \          \   ys0 \        */
/*      \          \   \   \       */
/*      \          \   \   /       */
/*      \          \   /   /       */
/*      *-----*          */
/*
*/
/* will be oriented vertically on screen, not cocked like this */

xs1 = 1; /* skip the first as buffer for gray line */
xs0 = xs1 + 1 + ncol*COSP;
ys1 = 1 + nlay*SINT;
ys0 = ys1 + 1 + ncol*SINP;

if(filenum>=999){
    firsttime = 1;
    filenum = 0;
    if(t_list_fp) fclose(t_list_fp);
}
if(firsttime){
    /* ppm format has thre byte rgb values for each pixel */
    time(&t);
    ptm = localtime(&t);
    /* 9-12-94 for list file */
    day = ptm->tm_mday, hour = ptm->tm_hour;
    sprintf(buf, "T%02d%02d.lst", day, hour);
    buf[LOCAL_BUF_LEN-1] = 0;
    t_list_fp = fopen(buf, "w");
    firsttime=0;
}
/* 9-27-97 move out of firsttime block */
rgb_len = (ncol+nlay+1)*3;

/* find the maximum and minimum conc values */
/* NOTE we initialized cmax, cmin in declarations, above */
/* 7-12-97 must find max amd min on all three faces... */
/* LEFT x,y face (z=0): */
for(y=0; y<nrow; y++){
    for(x=0; x<ncol; x++){
        if(solid[0][y][x]) continue;
        for(i=0,c=0.0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][0][y][x];
        }
        if(c >= cmax) cmax = c;
        if(c <= cmin) cmin = c;
    }
}
/* TOP x,z (y=0) face: */
for(z=0; z<nlay; z++){

```

```

    for(x=0; x<ncol; x++){
        if(solid[z][0][x]) continue;
        for(i=0,c=0.0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][z][0][x];
        }
        if(c >= cmax) cmax = c;
        if(c <= cmin) cmin = c;
    }
}

/* RIGHT y,z (x=ncol-1) face: */
xend = ncol-1;
for(z=0; z<nlay; z++){
    for(y=0; y<nrow; y++){
        if(solid[z][y][xend]) continue;
        for(i=0,c=0.0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][z][y][xend];
        }
        if(c >= cmax) cmax = c;
        if(c <= cmin) cmin = c;
    }
}

/* Prevent funny colors due to small oscillations */
if(cmin < 0.0) cmin = 0.0;
if(cmin > 1.e20 || cmax < -1.e20){
    if(rgb_buf) free(rgb_buf); /* 2-28-98 */
    return(t_list_fp);
}

delta = 255 - RGB_BASE; /* ASSUME maximum value for r,g or b is 255 */
chalf = 0.5*(cmax - cmin);
cpt75 = 0.75*(cmax - cmin);
if(cmax-cmin > 1e-30){
    slope1 = delta/chalf;
    slope2 = slope1*2.0;
}
else {
    if(rgb_buf) free(rgb_buf); /* 2-28-98 */
    return(t_list_fp); /* was return(0) */
}

/* make the file name; avoid lots of unclosed files if */
/* the cmax-cmin is too small... */
/* Remember localtime structure is not "re-entrant"... */
buf[LOCAL_BUF_LEN-1] = 0;
sprintf(buf,"T%02d%02d%03d.PPM", day, hour, filenum);
filenum++;
fp = fopen(buf, "wb");
if(!fp){
    if(rgb_buf) free(rgb_buf); /* 2-28-98 */
    return(t_list_fp); /* was return(0) */
}
if(t_list_fp) fprintf(t_list_fp,"%s\n",buf);
/* write the standard binary ppm header; \012 is linefeed... */
fprintf(fp,"P6\012%d %d\012255\012",widthPixels,height);

```



```

/** Loop over the 3 faces */
/* 1st over left x-y plane */
for(y=0; y<nrow; y++){
    for(x=0; x<ncol; x++){
        /* print solids in white */
        if(solid[0][y][x]==0){
            for(c=0.0,i=0; i<nveloc[sstart]; i++){
                c += ff[sstart][i][0][y][x];
            }
            /* prevent funny colors */
            if(c<0.0) c = 0.0;
            /* for now we will just gray scale */
            /**** comment out simple grayscale alternative *****/
            r = scale*(c-cmin);
            if(r>255) r=255;
            g = b = r;
            **** END comment out simple gray scale alternative *****/

            /***** "default" rainbow scaling below *****/
            craw = cmax - c;
            if(craw<chalf){
                r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*craw);
                if(r<RGB_BASE) r = RGB_BASE;
                g = RGB_BASE + (int)(craw*slope1); if(g>255) g = 255;
            }
            else if(craw<cpt75){
                b = RGB_BASE; g = 255;
                r = RGB_BASE + (int)((craw-chalf)*slope2); if(r>255) r = 255;
            }
            else {
                b = RGB_BASE; r = 255;
                g = RGB_BASE + (int)(delta - slope2*(craw-cpt75));
            }
        }
        else r=g=b=255; /* if solid, print as white */
        /**** END default rainbow scheme ****/
        /** calc ys, xs */
        xs = xs1 + x*COSP + 0.5;
        ys = ys1 + y + 1.5 + x*SINP; /* +1 to allow axis line above */
        /* place in array */
        ii = xs*3 + ys*widthBytes;
        /* do range checking */
        if(ii<0 || ii+2> totBytes) continue;
        rgb_buf[ii]=r, rgb_buf[ii+1]=g, rgb_buf[ii+2]=b;
        /* to prevent bleed through, print this line again one row down */
        ii += widthBytes;
        /* do range checking */
        if(ii<0 || ii+2> totBytes) continue;
        rgb_buf[ii]=r, rgb_buf[ii+1]=g, rgb_buf[ii+2]=b;
    }
}

/* 2nd over top x-z plane (y=0) */
for(x=0; x<ncol; x++){ /* with bleed-control, loop order affects jitters */
    for(z=0; z<nlay; z++){
        /* print solids in white */
        if(solid[z][0][x]==0){

```

```

        for(c=0.0,i=0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][z][0][x];
        }
        /* prevent funny colors */
        if(c<0.0) c = 0.0;
        /* for now we will just gray scale */
        /**** comment out simple grayscale alternative *****/
        r = scale*(c-cmin);
        if(r>255) r=255;
        g = b = r;
        **** END comment out simple gray scale alternative *****/

        /**** "default" rainbow scaling below ****/
        craw = cmax - c;
        if(craw<chalf){
            r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*craw);
            if(r<RGB_BASE) r = RGB_BASE;
            g = RGB_BASE + (int)(craw*slope1); if(g>255) g = 255;
        }
        else if(craw<cpt75){
            b = RGB_BASE; g = 255;
            r = RGB_BASE + (int)((craw-chalf)*slope2); if(r>255) r = 255;
        }
        else {
            b = RGB_BASE; r = 255;
            g = RGB_BASE + (int)(delta - slope2*(craw-cpt75));
        }
    }
    else r=g=b=255; /* if solid, print as white */
    /**** END default rainbow scheme ****/
    /** calc ys, xs **/
    xs = xs1 + 1.5 + x*COSP + z*COST; /* +1 to allow axis line */
    ys = ys1 + 0.5 + x*SINP - z*SINT;
    /* place in array */
    ii = xs*3 + ys*widthBytes;
    /* do range checking */
    if(ii<0 || ii+2> totBytes) continue;
    rgb_buf[ii]=r, rgb_buf[ii+1]=g, rgb_buf[ii+2]=b;
    /* to prevent bleed through, print this line again one row down */
    ii += widthBytes;
    /* do range checking */
    if(ii<0 || ii+2> totBytes) continue;
    rgb_buf[ii]=r, rgb_buf[ii+1]=g, rgb_buf[ii+2]=b;
}

}

/* 3rd over right y-z plane (x= xend = ncol-1) */
for(y=0; y<nrow; y++){
    for(z=0; z<nlay; z++){
        /* print solids in white */
        if(solid[z][y][xend]==0){
            for(c=0.0,i=0; i<nveloc[sstart]; i++){
                c += ff[sstart][i][z][y][xend];
            }
            /* prevent funny colors */
            if(c<0.0) c = 0.0;
            /* for now we will just gray scale */

```

```

/**** comment out simple grayscale alternative *****/
    r = scale*(c-cmin);
    if(r>255) r=255;
    g = b = r;
**** END comment out simple gray scale alternative *****/

/***** "default" rainbow scaling below ****/
    craw = cmax - c;
    if(craw<chalf){
        r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*craw);
        if(r<RGB_BASE) r = RGB_BASE;
        g = RGB_BASE + (int)(craw*slope1); if(g>255) g = 255;
    }
    else if(craw<cpt75){
        b = RGB_BASE; g = 255;
        r = RGB_BASE + (int)((craw-chalf)*slope2); if(r>255) r = 255;
    }
    else {
        b = RGB_BASE; r = 255;
        g = RGB_BASE + (int)(delta - slope2*(craw-cpt75));
    }
}
else r=g=b=255; /* if solid, print as white */
/**** END default rainbow scheme ****/
/** calc ys, xs */
xs = xs0 + 1.5 + z*COST; /* +1 allow axis line to left */
ys = ys0 + 1.5 + y - z*SINT; /* +1 to allow axis line above */
/* place in array */
ii = xs*3 + ys*widthBytes;
/* do range checking */
if(ii<0 || ii+2> totBytes) continue;
rgb_buf[ii]=r, rgb_buf[ii+1]=g, rgb_buf[ii+2]=b;
/* to prevent bleed through, print this line again one row down */
ii += widthBytes;
/* do range checking */
if(ii<0 || ii+2> totBytes) continue;
rgb_buf[ii]=r, rgb_buf[ii+1]=g, rgb_buf[ii+2]=b;
}

/** draw a black line from xs1,ys1 to xs0,ys0 */
for(x=0; x<ncol; x++){
    xs = xs1 + x*COSP + 0.5; ys = ys1 + x*SINP + 0.5;
    ii = xs*3 + ys*widthBytes;
    if(ii<0 || ii+2> totBytes) continue;
    rgb_buf[ii]=0, rgb_buf[ii+1]=0, rgb_buf[ii+2]=0;
}

/** write whole mess to file */
fwrite(rgb_buf, 1, totBytes, fp);

if(rgb_buf) free(rgb_buf);
fclose(fp);
return(t_list_fp);
#undef RGB_BASE
#undef RGB_MAX_SIZE
#undef LOCAL_BUF_LEN

```

```

} /* END Save3DPpm() */
/*-----*/
/* Modify SaveUPpm() to save an HPGL vector file, of the 4 layers... */
/* navg tells how many points in a line to include in an average, */
/* nskip tells how many points to skip between plots/averages, */
/* maxVectFrac gives the fraction of the largest dimension (e.g. ncol */
/* or nlay) to make the largest vector... */
/* 2-21-98 modify to (1) allow "log" (really fourth root) scaling), and */
/* (2) put the average of two cells in between points averaged... */
/* Change to pass nxavg, nyavg and NOT use nskip, ADD useLog, useColor */
/* 7-15-97 modify to save separate files for each zz[n]... HPGL just doesn't */
/* handle the resizing well... */
/*****/
int SaveVect(struct veloc_t *** const uu, char ***solid,
            int nlay, int nrow, int ncol, int zz[], int nz, int step,
            int nxavg, int nyavg, int useLog, int useColor, float maxVectFrac)
{
#define LOCAL_BUF_LEN 256
static int filenum=0, firsttime=1;
static FILE *fp;
int i,ii,x,y,z,n, xend,yend; /* 2-21-98 xend,yend */
/* All coords below are in SCREEN coords, and the vertical (y) screen coords */
/* have opposite sense as y index into rows... */
/* x0 and y0 are offsets from page edge, for each frame; */
float x0,y0,yinc;
/* yinc is the increment in y0 from frame to frame... */
float xc,yc,dx,dy,x1,y1,x2,y2;
/* xc,yc is the center point of each arrow; the arrow shafts will be */
/* symmetrically disposed about xc,yc. */
double maxVectScreenUnits,uLengthScale,colorScale;
box_t clipBox;

/* 2-21-98 add these: */
int xx, yy; /* for incrementing in an average block */
float xAvgInc, yAvgInc; /* these are offsets form x,y for average of points */
double uLogLengthScale;
int doAvg; /* set if EITHER nxavg OR nyavg==0... */
/* pointers to save time: */
struct veloc_t ** uuz;
char ** solidz;
int nopen; /* in averaging, the number of open (non-solid) points in block */

int pageWidth, pageHeight, color;
unsigned char r,g,b;
double u, u2, u2max=-1.0e200,umax,ux,uy, mLog; /* 2-21-98 mLog */
struct tm *ptm;
static int day=0,hour=0; /* because localtime destroys single internal tm */
time_t lt;
char buf[LOCAL_BUF_LEN]; /* for filenames */
/* if we want to write directly to printer in future, should */
/* add \033%0B\n at beginning of file, and \033%0A at end */
static char *initCode="IN;RO90;IP;IW;SC%d,%d,%d,%d;FT1;PA;SP1;PW0.2;\n",
            *endCode="PU;",
            *beforeSolids="PU;PU;PU;PU;PU;PU;PU;PU;PU;PU;PW0.5;\n";
/* beforeSolids allows us to find and remove solids block, and */
/* overlay with bitmap if we want... */

```

```

doAvg = (nxavg>1 || nyavg>1); /* 2-21-98 */
xAvgInc = (nxavg-1)*0.5;
yAvgInc = (nyavg-1)*0.5;

if(filenum>=999){
    firsttime = 1;
    filenum = 0;
}
if(firsttime){
    /* ppm format has three byte rgb values for each pixel */
    time(&t);
    ptm = localtime(&t);
    day = ptm->tm_mday, hour = ptm->tm_hour;
    firsttime=0;
}

/* Because we will be using inherently positive values, won't need */
/* to check for min -- it will be 0.... */
for(n=0,u2max=-1.e200; n<nz; n++){
    z = zz[n];
    for(y=0; y<nrow; y++){
        for(x=0; x<ncol; x++){
            ux = uu[z][y][x].x;
            uy = uu[z][y][x].y;
            u2 = ux*ux + uy*uy;
            if(u2>u2max) u2max = u2;
        }
    }
}
umax = sqrt(u2max);

maxVectScreenUnits = (ncol<nrow) ? nrow*maxVectFrac : ncol*maxVectFrac;
/* above is maximum length of a vector in plotter units */

if(umax>1.e-20){
    colorScale = NPEN/umax;
    uLengthScale = 0.5*maxVectScreenUnits/umax;
    /* 2-21-98 below really 1/4th power, not log */
    uLogLengthScale = 0.5*maxVectScreenUnits/sqrt(sqrt(umax));
    /* the 0.5 is because we will be calculating a dx,dy from */
    /* the center of the arrow, with total delta x = 2*dx, etc. */
}
else {
    colorScale = 0.0;
    uLengthScale = 0.0;
    uLogLengthScale = 0.0; /* 2-21-98 */
}

/* determine starting positions of each frame */

x0 = ncol*0.05; /* 5% slop on each end */
pageWidth = ncol*1.1 + 0.5;
pageHeight = nrow *1.1 + 0.5;
y0 = pageHeight*0.95;

clipBox[BOX_X1] = 0; clipBox[BOX_X2] = pageWidth - 1;
clipBox[BOX_Y1] = 0; clipBox[BOX_Y2] = pageHeight - 1;

```

```

/* first loop over all the vectors, so we can print solids separately, and */
/* remove them later if we want to overlay a bit map */
for(n=0; n<nz; n++){
    z = zz[n];
    uuz = uu[z]; solidz = solid[z]; /* 2-21-98 */
    /* make the file name; avoid lots of unclosed files if */
    /* the umax is too small... */
    /* Remember localtime structure is not "re-entrant"... */
    buf[LOCAL_BUF_LEN-1] = 0;
    sprintf(buf, "V%02d%02d%03d.%03d", day, hour, filenum, z);
    fp = fopen(buf, "w"); /* open as ascii */
    if(!fp) return(0); /* was return(0) */
    /* write HPGL header to define page size 7-15-97 move here */
    fprintf(fp, initCode, 0, pageWidth, 0, pageHeight);

    /* draw a box around the current z slice 7-15-97 +/- 0.5 added */
    DrawBox(x0+0.5, x0+ncol-0.5, y0-nrow+0.5, y0-0.5, clipBox, fp, 1);
    for(y=0; y<nrow; y+=nyavg){
        for(x=0; x<ncol; x+=nxavg){
            if(doAvg){ /* 2-21-98 averaging block */
                for(ux=uy=0.0, yy=y, yend=y+nyavg, nopen=0; yy<yend; yy++){
                    for(xx=x, xend=x+nxavg; xx<xend; xx++){
                        if(solidz[yy][xx]) continue;
                        ux+=uuz[yy][xx].x;
                        uy+=uuz[yy][xx].y;
                        nopen++;
                    }
                }
                if(nopen){ ux/=nopen; uy/=nopen; }
                else continue; /* don't plot a pure solid vector */
                xc = x0 + x + xAvgInc + 0.5;
                yc = y0 - y - yAvgInc - 0.5;
            }
            else {
                if(solidz[y][x]) continue;
                ux = uuz[y][x].x;
                uy = uuz[y][x].y;
                xc = x0+x+0.5; yc = y0-y-0.5;
            }
            u = sqrt(ux*ux + uy*uy);
            /* calc endpoints of the line to plot */
            if(useColor) color = colorScale*u;
            else color = 0; /* 2-21-98 add if for monotone */
            if(useLog==0){
                dx = uLengthScale*ux; dy = uLengthScale*uy;
            }
            else if(u>1.0e-50){ /* log scale */
                mLog = uLogLengthScale*sqrt(sqrt(u))/u;
                dx = ux*mLog; dy = uy*mLog;
            }
            else continue; /* don't print a zero vector */

            x1 = xc-dx; x2 = xc+dx; y1 = yc-dy; y2 = yc+dy;
            DrawArrow(x1, y1, x2, y2, 0.3, 0.7, color, fp, clipBox);
        }
    }
}

```

```

/* Do solids grid; 1st write an easily recognized separator */
fprintf(fp,beforeSolids);
for(y=0; y<nrow; y++){
    for(x=0; x<ncol; x++){
        /* print solids in white */
        if(!solidz[y][x]) continue;
        xc = x0+x+0.5; yc = y0-y-0.5;
        x1 = x0+x; x2 = x1+1; y1 = y0-y; y2 = y1-1;
        DrawBox(x1,x2,y1,y2, clipBox,fp,0);
    }
}
fprintf(fp,endCode); /* 7-15-97 moved here */
fclose(fp); /* 7-15-97 moved here */
}
filenum++; /* moved here 7-15-97 */
return(1);
#undef LOCAL_BUF_LEN
} /* END SaveVect() */
/*-----*/
/* 4-12-96 in anticipation of HPGL output, pass the index of color in color */
/* array, rather than color in FG units... */
/* 4-11-96 draw an arrow with head between x1,y1 and x2,y2 screen coords. */
/* NOTE: the doubles for pixel screen coords; */
/* factor is the fraction of vector length to make head; mul */
/* is the fraction of arrow head length to make the half-width of the */
/* base of the arrow head... */
/*****/
double DrawArrow(float xx1, float yy1, float xx2, float yy2,
    float factor, float mul, int color, FILE *hpgl_fp, box_t box)
{
    float xx3, yy3, xx4, yy4, xx5, yy5;
    float rsin, rcos, r, BigR, rho, dx, dy;
    /* think of rsin, rcos as "r*sin(theta)" and "r*cos(theta)"... */
    int kolor, status1, status2, status3; /* 4-12-96 */
    /* pencolors */
    static int penColor[NPEN] = {1,6,5,7,3,4,8,2};
    int iYellow = 5;

    dx = xx2 - xx1; dy = yy2 - yy1; /* 4-11-96 fixed */
    rho = sqrt(dx*dx + dy*dy);
    if(rho < 0.1) return(0.0);

    BigR = rho*factor; r = BigR*mul;
    rsin = r*dy/rho; rcos = r*dx/rho;

    xx3 = xx2 - factor*dx; yy3 = yy2 - factor*dy;

    xx4 = xx3 - rsin; yy4 = yy3 + rcos;
    xx5 = xx3 + rsin; yy5 = yy3 - rcos;

    /* draw HPGL arrow if specified */
    /* need to clip the values; remember to pass floats to ClipLine() */
    status1 = ClipLine(&xx1, &yy1, &xx2, &yy2, box);
    status2 = ClipLine(&xx4, &yy4, &xx2, &yy2, box);
    status3 = ClipLine(&xx5, &yy5, &xx2, &yy2, box);
    if(status1 && status2 && status3){
        fprintf(hpgl_fp,

```

```

        "PUSP%dPA%.2f,%.2fPD%.2f,%.2fPU;\nPA%.2f,%.2fPD%.2f,%.2f,%.2f,%.2fPU;\n",
        penColor[color],xx1,yy1,xx2,yy2,xx4,yy4,xx2,yy2,xx5,yy5);
    }
/* kludge to make yellow more visible in Word */
if(color==iYellow && iYellow<NPEN-1){
    fprintf(hpgl_fp,"LT2,0.1,1;\n");
    if(status1 && status2 && status3){
        fprintf(hpgl_fp,

"PUSP%dPA%.2f,%.2fPD%.2f,%.2fPU;\nPA%.2f,%.2fPD%.2f,%.2f,%.2f,%.2fPU;\n",
        penColor[color+1],xx1,yy1,xx2,yy2,xx4,yy4,xx2,yy2,xx5,yy5);
        }
    fprintf(hpgl_fp,"LT;\n");
}
return(rho);
} /* END DrawArrow() */
/*-----*/
/* 3-6-93 use for hardcopy output (HPGL, PS) and x,y graphs; found that */
/* Flash Graphics routines do odd things with some clips. */
/* Adapted from NCSA telnet 2.303 \tek\vgtek.c source. */
/* Seems like x1,y1 do not need to be ordered relative to x2,y2 before call. */
/* *****/
int ClipLine(float *x1p, float *y1p, float *x2p, float *y2p,
             box_t box)
{
    /* Original authors' comment:
    Draw a vector in box from [x1,y1 to x2,y2].
    Zoom the vector to the current visible window,
    and clip it before drawing it.
    Uses Liang-Barsky algorithm from ACM Transactions on Graphics,
    Vol. 3, No. 1, January 1984, p. 7.
    */

    double t,b,l,r;
    double x1,y1,x2,y2,t1,t2,deltay,deltax;

    /* t=top, b=bottom, r=right, l=left */
    t = box[BOX_Y2];
    b = box[BOX_Y1];
    l = box[BOX_X1];
    r = box[BOX_X2];

    /* totally visible */
    if(*x1p<=r && *x2p<=r && *x1p>=l && *x2p>=l && *y1p<=t
        && *y2p<=t && *y1p>=b && *y2p>=b) return(1);

    /* trivially invisible */
    if((*x1p>r && *x2p>r) || (*x1p<l && *x2p<l) || (*y1p<b && *y2p<b) ||
        (*y1p>t&&*y2p>t)) return(0);

    /* the clipping algorithm */
    x1 = *x1p;
    y1 = *y1p;
    x2 = *x2p;
    y2 = *y2p;
    t1 = 0.0;
    t2 = 1.0;

```



```

deltax = x2 - x1;

if(Clipt(-deltax,x1-l,&t1,&t2)){
    if(Clipt(deltax,r-x1,&t1,&t2)){
        deltay=y2-y1;
        if(Clipt(-deltay,y1-b,&t1,&t2)){
            if(Clipt(deltay,t-y1,&t1,&t2)){
                if(t2<1.0){
                    x2=x1+t2*deltax;
                    y2=y1+t2*deltay;
                }
                if(t1>0.0){
                    x1+=t1*deltax;
                    y1+=t1*deltay;
                }
            }
        }
        /* draw the line, it is at least partially visible */
        *x1p = x1;
        *x2p = x2;
        *y1p = y1;
        *y2p = y2; /* 2-2-96 change to return -1 */
        return(-1); /* for partly visible */
    }
}

} /* end if */
return(1);
} /* END ClipLine() */

/*-----*/
/* Called by ClipLine() only ; modified from NCSA telnet 2.303 vgtek.c. */
/*-----*/
int Clipt(double p, double q, double *t1p, double *t2p)
{
    double r;
    int accept = 1;

    if(p < 0.0){
        r=q/p;
        if(r > *t2p) accept = 0;
        else if(r > *t1p) *t1p = r;
    }
    else if(p > 0.0){
        r=q/p;
        if(r < *t1p) accept = 0;
        else if(r < *t2p) *t2p = r;
    }
    else if(q < 0.0) accept=0;
    return(accept);
} /* END Clipt() */

/*-----*/
/* draw the specified box in pen color; note color is PEN color, not index */
int DrawBox(float x1, float x2, float y1, float y2,
            box_t clipbox, FILE *fp, int color)
{
    float ftemp;
    if(color<1 || color>NPEN) color = 1;
    if(!fp) return(0);
    if(x1>x2){

```

```

        ftemp = x1; x1 = x2; x2 = ftemp;
    }
    if(y1>y2){
        ftemp = y1; y1 = y2; y2 = ftemp;
    }
    /* don't do off-screen box */
    if(x1>clipbox[BOX_X2]) return(0);
    if(y1>clipbox[BOX_Y2]) return(0);
    if(x2<clipbox[BOX_X1]) return(0);
    if(y2<clipbox[BOX_Y1]) return(0);
    /* clipping here is pretty simple */
    if(x1<clipbox[BOX_X1]) x1=clipbox[BOX_X1];
    if(y1<clipbox[BOX_Y1]) y1=clipbox[BOX_Y1];
    if(x2>clipbox[BOX_X2]) x2=clipbox[BOX_X2];
    if(y2>clipbox[BOX_Y2]) y2=clipbox[BOX_Y2];
    fprintf(fp, "PUSP%dPA%.2f,%.2fPD%.2f,%.2fPD%.2f,%.2fPD%.2f,%.2f;\n",
        color, x1,y1,x2,y1,x2,y2,x1,y2,x1,y1);
    return(1);
} /* END DrawBox() */
/*-----*/
/* 7-16-97 modify 2D code to allow 1 (L) for nlay, and change old -l to -g */
/* for stepStartSlug, and add -i for number of vectors used for solutes. */
/* Modify old \ilga\ilga.c function set_flags() to scan command line and */
/* set some important params... */
/* NOTE here fp is NOT a file pointer! */
/* RETURNS: FLAG_HELP !=1 if finds a "help" character; 1 otherwise. */
/* The -l condition should be used to terminate the program... */
/* SEE flags_struct for other notes */
/* 6-14-98 add alveoli grid # and ^ flags */
/*****
int SetFlags(int argc, char *argv[], struct flags_struct *fp)
{
    int i,flag,uflag, len;
    char *argptr;

```

static char *str=

" FLAG	ARGUMENT	WHAT IT SETS	IMPLEMENTED?\n\
----	-----	-----	-----\n\
-x	float	xBody, x BODY force	y\n\
-y	float	yBody, y BODY force	y\n\
-u	float	uxLimit, x speed limit	y\n\
-v	float	uyLimit, y speed limit	y\n\
-n	float	viscosity component 0 (carrier)	y\n\
-d	float	diffusion coeff. component 1	y\n\
-D	float	Diffusion coeff. component 2	y\n\
-s	integer	MAXSTEPS, maximum number of steps	y\n\
-j	integer	JUST_DISPERSE_STEP (flow frozen in)	y\n\
-c	integer	NCOL, number of columns (max x)	y\n\
-r	integer	NROW, number of rows (max y)	y\n\
-l	integer	NLAY, number of layers (max z)	y\n\
-i	integer	NVELOC, # velocity vectors for solutes	y\n\
-b	integer	Boundary: 0=bounceback, 1=Ziegler	n\n\
-g	integer	stepStartSlug (step tracer slug)	y\n\
-f	string	filename containing solids geometry	N\n\
-o	integer	Sphere Radius (for JO.C, JO_SPH.C)	y\n\
-t	integer	Times (NTIMES) to multiply geometry	y\n\
-#	integer	x and z size alveoli grid (fin to fin)	y\n\

```

    ^      integer      y height alveoli grid (inside measure)      y\n\
-h | -?    <none>      display this list                          y";

```

```

fp->use_ncol=0; fp->use_nrow=0; fp->use_maxstep=0; fp->use_xBody=0;
fp->use_yBody=0; fp->use_viscosity=0; fp->use_diff1=0; fp->use_diff2=0;
fp->use_fname=0; fp->use_boundary=0; fp->use_stepSlug=0;
fp->use_uxMax=0; fp->use_uyMax=0; fp->use_jdispstep=0;
fp->use_nlay=0; fp->use_nveloc=0; fp->use_radius=0;
fp->use_xzGrid=0; fp->use_yGrid=0;
/* 6-14-98 note we don't compare grid measures against max and min in */
/* here, since intelligent comparison can be made ONLY when we have */
/* all the rows, cols, layers known... */

for(i=1; i<argc; i++){
    /* find next '-' switch */
/* NOTE i<argc MUST come first to avoid core dump at end of list */
    for(;i<argc && argv[i][0]!='-'; i++);
    if(i==argc) break;
    flag = argv[i][1];
    uflag = toupper(flag);
    len = strlen(argv[i]);
    if(len<=1) continue;
    if(len==2 && (uflag=='H' || flag=='?')){
        puts(str); /* 3-7-97 correct */
        return(FLAG_HELP);
    }
    argptr = argv[i]+2; /* normal case, e.g. -fmyfile */
    if(len==2){ /* has form -f; check if next token is argument */
        if(i<argc-1 && argv[i+1][0] != '-'){
            argptr = argv[i+1];
        }
        else continue;
    }
    else argptr = argv[i] + 2;

    /* set flags according to switch */
    switch(uflag){
        case 'F':
            fp->fname = argptr;
            fp->use_fname = 1;
            break;
        case 'X':
            sscanf(argptr,"%lf",&(fp->xBody));
            if(fp->xBody < MIN_XBODY){
                fp->xBody = MIN_XBODY;
                if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.xBody to min\n");
            }
            if(fp->xBody > MAX_XBODY){
                fp->xBody = MAX_XBODY;
                if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.xBody to max\n");
            }
            fp->use_xBody = 1;
            break;
        case 'Y':
            sscanf(argptr,"%lf",&(fp->yBody));
            if(fp->yBody < MIN_YBODY){
                fp->yBody = MIN_YBODY;

```

```

        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.yBody to min\n");
    }
    if(fp->yBody > MAX_YBODY){
        fp->yBody = MAX_YBODY;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.yBody to max\n");
    }
    fp->use_yBody = 1;
    break;
case 'U': /* 3-15-97 U, V */
    sscanf(argptr, "%lf", &(fp->uxMax));
    if(fp->uxMax < MIN_U){
        fp->uxMax = MIN_U;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.uxMax to min\n");
    }
    if(fp->uxMax > MAX_U){
        fp->uxMax = MAX_U;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.uxMax to max\n");
    }
    fp->use_uxMax = 1;
    break;
case 'V':
    sscanf(argptr, "%lf", &(fp->uyMax));
    if(fp->uyMax < MIN_U){
        fp->uyMax = MIN_U;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.uyMax to min\n");
    }
    if(fp->uyMax > MAX_U){
        fp->uyMax = MAX_U;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.uyMax to max\n");
    }
    fp->use_uyMax = 1;
    break;
case 'N':
    sscanf(argptr, "%lf", &(fp->viscosity));
    if(fp->viscosity < MIN_COEF){
        fp->viscosity = MIN_COEF;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.viscosity to
min\n");
    }
    if(fp->viscosity > MAX_COEF){
        fp->viscosity = MAX_COEF;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.viscosity to
max\n");
    }
    fp->use_viscosity = 1;
    break;
case 'D':
    if(flag=='d'){
        sscanf(argptr, "%lf", &(fp->diff1));
        if(fp->diff1 < MIN_COEF){
            fp->diff1 = MIN_COEF;
            if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.diff1 to
min\n");
        }
        if(fp->diff1 > MAX_COEF){
            fp->diff1 = MAX_COEF;

```

```

        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.diff1 to
max\n");
    }
    fp->use_diff1 = 1;
}
else {
    sscanf(argptr,"%lf",&(fp->diff2));
    if(fp->diff2 < MIN_COEF){
        fp->diff2 = MIN_COEF;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.diff2 to
min\n");
    }
    if(fp->diff2 > MAX_COEF){
        fp->diff2 = MAX_COEF;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.diff2 to
max\n");
    }
    fp->use_diff2 = 1;
}
break;
case 'C':
    sscanf(argptr,"%d",&(fp->ncol));
    if(fp->ncol < MIN_NCOL){
        fp->ncol = MIN_NCOL;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.ncol to min\n");
    }
    if(fp->ncol > MAX_NCOL){
        fp->ncol = MAX_NCOL;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.ncol to max\n");
    }
    fp->use_ncol = 1;
break;
case 'B': /* 3-14-97 add boundary for Ziegler-type */
    sscanf(argptr,"%d",&(fp->boundary));
    if(fp->boundary < MIN_BOUNDARY){
        fp->boundary = MIN_BOUNDARY;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.boundary to min\n");
    }
    if(fp->boundary > MAX_BOUNDARY){
        fp->boundary = MAX_BOUNDARY;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.boundary to max\n");
    }
    fp->use_boundary = 1;
break;
case 'R':
    sscanf(argptr,"%d",&(fp->nrow));
    if(fp->nrow < MIN_NROW){
        fp->nrow = MIN_NROW;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.nrow to min\n");
    }
    if(fp->nrow > MAX_NROW){
        fp->nrow = MAX_NROW;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.nrow to max\n");
    }
    fp->use_nrow = 1;
break;
case 'O':

```

```

    sscanf(argpstr,"%d",&(fp->radius));
    if(fp->radius < MIN_NROW){
        fp->radius = MIN_NROW;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.radius to min\n");
    }
    if(fp->radius > MAX_NROW){
        fp->radius = MAX_NROW;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.radius to max\n");
    }
    fp->use_radius = 1;
    break;
case 'T':
    sscanf(argpstr,"%d",&(fp->ntimes));
    if(fp->ntimes < MIN_NTIMES){
        fp->ntimes = MIN_NTIMES;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.ntimes to min\n");
    }
    if(fp->ntimes > MAX_NTIMES){
        fp->ntimes = MAX_NTIMES;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.ntimes to max\n");
    }
    fp->use_ntimes = 1;
    break;
case 'L':
    sscanf(argpstr,"%d",&(fp->nlay));
    if(fp->nlay < MIN_NLAY){
        fp->nlay = MIN_NLAY;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.nlay to min\n");
    }
    if(fp->nlay > MAX_NLAY){
        fp->nlay = MAX_NLAY;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.nlay to max\n");
    }
    fp->use_nlay = 1;
    break;
case 'I': /* 7-16-97 added for 3D */
    sscanf(argpstr,"%d",&(fp->nveloc));
    if(fp->nveloc < MAX_NVELOC){ /* 7-18-97 want either 6 or 19 */
        fp->nveloc = MIN_NVELOC;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.nveloc to min\n");
    }
    if(fp->nveloc > MAX_NVELOC){
        fp->nveloc = MAX_NVELOC;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.nveloc to max\n");
    }
    fp->use_nveloc = 1;
    break;
case 'S':
    sscanf(argpstr,"%d",&(fp->maxstep));
    if(fp->maxstep < MIN_MAXSTEP){
        fp->maxstep = MIN_MAXSTEP;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.maxstep to min\n");
    }
    if(fp->maxstep > MAX_MAXSTEP){
        fp->maxstep = MAX_MAXSTEP;
        if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.maxstep to max\n");
    }

```

```

        fp->use_maxstep = 1;
        break;
    case 'J':
        sscanf(argp, "%d", &(fp->jdispstep));
        if(fp->jdispstep < MIN_MAXSTEP){
            fp->jdispstep = MIN_MAXSTEP;
            if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.jdispstep to
min\n");
        }
        if(fp->jdispstep > MAX_MAXSTEP){
            fp->jdispstep = MAX_MAXSTEP;
            if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.jdispstep to
max\n");
        }
        fp->use_jdispstep = 1;
        break;
    case 'G': /* stepStartSlug, solute slug */
        sscanf(argp, "%d", &(fp->stepSlug));
        if(fp->stepSlug < MIN_MAXSTEP){
            fp->stepSlug = MIN_MAXSTEP;
            if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.stepSlug to min\n");
        }
        if(fp->stepSlug > MAX_MAXSTEP){
            fp->stepSlug = MAX_MAXSTEP;
            if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.stepSlug to max\n");
        }
        fp->use_stepSlug = 1;
        break;
    case '#': /* 6-14-98 for xz Grid for alveoli */
        sscanf(argp, "%d", &(fp->xzGrid));
        if(fp->xzGrid < 2){
            fp->xzGrid = 2;
            if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.xzGrid to min\n");
        }
        fp->use_xzGrid = 1;
        break;
    case '^': /* 6-14-98 for y Grid for alveoli */
        sscanf(argp, "%d", &(fp->yGrid));
        if(fp->yGrid < 1){
            fp->yGrid = 1;
            if(LOG_fp) fprintf(LOG_fp, "adjusted FLAG.yGrid to min\n");
        }
        fp->use_yGrid = 1;
        break;
    }
}
return(1);
} /* END SetFlags() */
/*-----*/
/* 7-16-97 make 3D (3-D) version from LB01.c 2D (2-D) version; since we */
/* dont yet have a Ziegler version, we'll ignore use_z.... */
/* 2-13-97 calculate mean of solute at specified component sstart, and */
/* write to file mean_std.txt... */
/* NOTE pathname is pointer to string, typically argv[0]... */
/* RETURNS fSum (total amount solute) to check mass balance... */
/*-----*/
double MeanStd(ff_t ***** const ff, char *** const solid, int ncomponent,

```

```

        int nveloc[], int nlay, int nrow, int ncol, int sstart, int step,
        char *pathname, int use_z)
{
    int x,y,z,i;
    static int firstTime = 0;
    FILE *fp;
    double fx2Sum, fxSum, f, fSum, fy2Sum, fySum, xtemp, ytemp, xx, yy;
    double xMean, xVar, xStd, yMean, yVar, yStd;
    /* 7-16-97 add: */
    double zz, fz2Sum, fzSum, ztemp, zMean, zVar, zStd;
    /* currently assume solids will have valid ff values */
    struct tm *ptm;      /* 2-22-97 convert to localtime() in time.h */
    time_t lt;
    char *str;

    int sc; /* solidcode */

    fp = fopen("mean_std.txt", "a");
    if(!fp) return(-1.0);
    if(firstTime==0){
        /* 3-17-97 use use_ziegler instead of flags... */
        if(use_z) str = "Ziegler";
        else str = "BounceBack";

        time(&lt);
        ptm = localtime(&lt);
        fprintf(fp, "=====%s %02d/%02d/%04d %02d:%02d:%02d =====\n",
            pathname, ptm->tm_mon+1, ptm->tm_mday, ptm->tm_year+1900,
            ptm->tm_hour, ptm->tm_min, ptm->tm_sec);
        fprintf(fp, "NCOL=%d, NROW=%d, NLAY=%d, COMPONENT %d, %s\n",
            ncol, nrow, nlay, sstart, str);
        fprintf(fp, "step\tfSum\txMean\txStd\tyMean\tyStd\tzMean\tzStd\n");
        firstTime = 1;
    }

    fx2Sum=0.0, fxSum=0.0, fSum=0.0, fy2Sum=0.0, fySum=0.0;
    fz2Sum=0.0, fzSum=0.0; /* 7-16-97 */

    for(z=0; z<nlay; z++){
        zz = z;
        for(y=0; y<nrow; y++){
            yy = y; /* make double */
            for(x=0; x<ncol; x++){
                /* 3-17-97 block: solids */
                sc = solid[z][y][x];
                if(sc) continue; /* 7-16-97 for now, just ignore solids */
                for(f=0.0, i=0; i<nveloc[sstart]; i++){
                    f+= ff[sstart][i][z][y][x];
                }
                xx = x;
                fSum += f;
                xtemp = xx*f, ytemp = yy*f, ztemp = zz*f;
                fxSum += xtemp; fySum += ytemp; fzSum += ztemp;
                fx2Sum += xx*xtemp; fy2Sum += yy*ytemp; fz2Sum += zz*ztemp;
            }
        }
    }
}

```



```

if(fSum){
    xMean = fxSum / fSum;
    xVar = fx2Sum / fSum - xMean*xMean;
    xStd = sqrt(xVar);
    yMean = fySum / fSum;
    yVar = fy2Sum / fSum - yMean*yMean;
    yStd = sqrt(yVar);
    zMean = fzSum / fSum;
    zVar = fz2Sum / fSum - zMean*zMean;
    zStd = sqrt(zVar);
}
else {
    xMean = yMean = zMean = zVar = yVar = xVar = xStd = yStd = zStd = 0. ;
}

fprintf(fp, "%d\t%.5e\t%.5e\t%.5e\t%.5e\t%.5e\t%.5e\n",
    step, fSum, xMean, xStd, yMean, yStd, zMean, zStd);

fclose(fp); /* NOTE we open and close file each time... */
return(fSum);
} /* END MeanStd() */
/*-----*/
/* 9-16-97 process the "fractals" (srb's FM2D.FOR) outputs; assume */
/* filenames parsed by SetFlags() by default. fname is the filename */
/* for the surface; topOrBottom selects, uses 0 for bottom, non-zero */
/* for top. hpix is the number of pixels (rows) that correspond to */
/* the maximum relief in the fractal file; generally should be less than */
/* (nrow - offs). The solids are draw from offs into the site volume, */
/* parallel to the y direction. */
/* NOTE we assume the solids have been initialized beforehand; i.e. we */
/* only write -1s, do not zero out any other solids. The SetSolidType() */
/* call should FOLLOW this function... */
/*****
int FractalSurface(char *** const solid, int nlay, int nrow, int ncol,
    int hpix, char *fname, int topOrBottom, int offs)
{
#define N_FR_BUF 64
static char *mess1="!!!!!! Couldn't open surface file %s !!!!!\n";
static char *mess2="?????? Surface file %s has slay=%d, scol=%d ?????\n";
static char *mess3="..... Couldn't allocate for surface file %s ..... \n";
/* NOTE to HWS: make sure %f below is OK below if 1.xe-01 */
static char *mess4="----- Odd height value h[%d]=%f in surface file %s -----\n";
static char *mess5=",,,,,, Unexpected end of file %s at line %d ,,,,,,\n";
float *h, hmin,hmax, hdiff, mul, htemp;
int x,y,z,i, layXcol, ystart, yend;
int slay,scol; /* Steve's col, layer */
FILE *fp;
char buf[N_FR_BUF], *str;
int istatus=0;
int ctr = 0;

fp = fopen(fname, "r");
if(!fp){
    if(LOG_fp) fprintf(LOG_fp,mess1,fname); /* global log file */
    printf(mess1,fname); return(0);
}
/* read the # layers, columns in Steve's grid */

```

```

str = fgets(buf, N_FR_BUF, fp);
istatus = sscanf(buf, "%d %d", &slay, &scol);
if(istatus!=2 || slay<0 || scol<0 || slay>2000 || scol>2000){
    if(LOG_fp) fprintf(LOG_fp, mess2, fname, slay, scol);
    printf(mess2, fname, slay, scol);
    fclose(fp);
    return(0);
}
printf("%d layers, %d columns in surface file\n", slay, scol);
/* allocate the scratch buffer to read the file */
layXcol = slay*scol;

h = (float *) malloc(sizeof(float)*layXcol);
if(!h){
    if(LOG_fp) fprintf(LOG_fp, mess3, fname);
    printf(mess3, fname);
    fclose(fp);
    return(0);
}
/* read in the values */
for(i=0; i<layXcol; i++){
    str = fgets(buf, N_FR_BUF, fp);
    if(str!=buf){
        if(LOG_fp) fprintf(LOG_fp, mess5, fname, i);
        printf(mess5, fname, i);
        for(; i<layXcol; i++) h[i] = 0.0;
        break;
    }
    istatus = sscanf(buf, "%f", h+i);
    if(istatus!=1 || h[i]>1000.0 || h[i]<-1000.0){
        if(LOG_fp) fprintf(LOG_fp, mess4, i, h[i], fname);
        printf(mess4, i, h[i], fname);
        for(; i<layXcol; i++) h[i] = 0.0;
        break;
    }
}
/* now have raw h[] array, must find high and low values */
for(i=0, hmin=1.0e30, hmax=-1.0e30; i<layXcol; i++){
    if(hmin>h[i]) hmin = h[i];
    if(hmax<h[i]) hmax = h[i];
}
hdiff = hmax - hmin;
if(fabs(hdiff)<1.0e-20){
    free(h);
    fclose(fp);
    printf("hdiff too small, = %f\n", hdiff);
    return(0);
}
mul = hpix/hdiff;

/**** 9-27-97 comment out *****/
printf("mul=%f, hmin=%f, hmax=%f (hit a key)\n", mul, hmin, hmax);
getch();
****/

for(z=0; z<slay && z<nlay; z++){
    for(x=0; x<scol && x<ncol; x++){

```

```

        htemp = h[scol*z + x];
        if(topOrBottom){
            yend = offs + mul*(htemp - hmin);
            for(y=offs; y<yend && y<nrow; y++) solid[z][y][x] = -1;
        }
        else {
            ystart = nrow-1-offs + mul*(htemp - hmax);
            for(y=ystart; y<nrow; y++) solid[z][y][x] = -1;
        }
    }
}

if(fp) fclose(fp);
if(h) free(h);
return(1);
#undef N_FR_BUF
} /* END FractalSurface() */
/*-----*/
/* 2-27-98 pointerize to speed up? */
/* 9-27-97 modify to pass ncol_old so we can find uu[z][y][xx] position.. */
/* 9-22-97 create 3D version of JustDisperse() (2D versions in lb01.c), */
/* a collide function that assumes velocity field is static, therefore */
/* does not do buoyancy or carrier fluid... */
/* NOTE: for now, simplify by not using lots of pointers and by keeping */
/* ONLY bounceback mode... */
/*****/
int JustDisperse3D(ff_t *const*const*const*const* ff,
    double * const tau, double * const beta, double *const omega,
    struct veloc_t *const*const* uu, char *const*const* solid,
    int ncomponent, int nveloc[], int nlay, int nrow, int ncol, int ncol_old)
{
    int s,i,z,y,x,xx; /* 9-27-97 xx is index into uu[z][y][xx]... */
    double ux, uy, uz;
    double qian;
    double f[DEF_NVELOC], feq[DEF_NVELOC];
    ff_t *const*const*const* ffs;
    ff_t *pf0,*pf1,*pf2,*pf3,*pf4,*pf5,*pf6,*pf7,
        *pf8,*pf9,*pf10,*pf11,*pf12,*pf13,*pf14,*pf15,
        *pf16,*pf17,*pf18;

    struct veloc_t *uuz;

    int solidcode,nvel;
    double rho, omega_s, beta_s;
    double mux,muy,muz, mul;
    const static double half = ONE_HALF;

    for(s=1; s<ncomponent; s++){
        nvel = nveloc[s];
        omega_s = omega[s]; beta_s = beta[s];
        ffs = ff[s];
        for(z=0; z<nlay; z++){
            for(y=0; y<nrow; y++){
                uuz = uu[z][y];
                pf0 = ffs[0][z][y];
                pf1 = ffs[1][z][y];

```

```

pf2 = ffs[2][z][y];
pf3 = ffs[3][z][y];
pf4 = ffs[4][z][y];
pf5 = ffs[5][z][y];
if(nvel==19){
    pf6 = ffs[6][z][y];
    pf7 = ffs[7][z][y];
    pf8 = ffs[8][z][y];
    pf9 = ffs[9][z][y];
    pf10 = ffs[10][z][y];
    pf11 = ffs[11][z][y];
    pf12 = ffs[12][z][y];
    pf13 = ffs[13][z][y];
    pf14 = ffs[14][z][y];
    pf15 = ffs[15][z][y];
    pf16 = ffs[16][z][y];
    pf17 = ffs[17][z][y];
    pf18 = ffs[18][z][y];
}
if(nvel==6){
    for(x=xx=0; x<ncol; x++,xx++,++pf0, ++pf1, ++pf2,
        ++pf3, ++pf4, ++pf5){
        /* MUST have next xx as top of loop */
        if(xx==ncol_old) xx = 0; /* 9-27-97 assume regular access

*/

        solidcode = solid[z][y][x];
        if(solidcode==-2) continue;
        ux = uuzy[xx].x; /* 9-27-97 was plain [x] */
        uy = uuzy[xx].y;
        uz = uuzy[xx].z;
        rho = f[0] = *pf0;
        rho += f[1] = *pf1;
        rho += f[2] = *pf2;
        rho += f[3] = *pf3;
        rho += f[4] = *pf4;
        rho += f[5] = *pf5;
        if(solidcode){
            *pf0 = f[2];
            *pf1 = f[3];
            *pf2 = f[0];
            *pf3 = f[1];
            *pf4 = f[5];
            *pf5 = f[4];
            continue; /* on to next x */
        }
        /* calculate the feqs */
        mul = rho*half;
        mux = ux*mul; muy = uy*mul; muz = mul*uz;
        rho *= ONE_6TH;
        feq[0] = rho + mux;
        feq[2] = rho - mux;
        feq[1] = rho + muy;
        feq[3] = rho - muy;
        feq[4] = rho + muz;
        feq[5] = rho - muz;
        /* put back the new f[] values */
        *pf0 = f[0]*beta_s + feq[0]*omega_s;

```

```

        *pf1 = f[1]*beta_s + feq[1]*omega_s;
        *pf2 = f[2]*beta_s + feq[2]*omega_s;
        *pf3 = f[3]*beta_s + feq[3]*omega_s;
        *pf4 = f[4]*beta_s + feq[4]*omega_s;
        *pf5 = f[5]*beta_s + feq[5]*omega_s;
    }
}
else { /* nvel==19 */
    for(x=xx=0; x<ncol; x++,xx++,++pf0, ++pf1, ++pf2, ++pf3,
++pf4,
        ++pf5, ++pf6, ++pf7, ++pf8, ++pf9, ++pf10, ++pf11, ++pf12,
++pf13, ++pf14, ++pf15, ++pf16, ++pf17, ++pf18){
        /* MUST have next xx as top of loop */
        if(xx==ncol_old) xx = 0; /* 9-27-97 assume regular access
*/
        solidcode = solid[z][y][x];
        if(solidcode==-2) continue;
        ux = uzy[xx].x; /* 9-27-97 was plain [x] */
        uy = uzy[xx].y;
        uz = uzy[xx].z;
        /* 2-27-98 rearrange order for read-buffer bug? */
        rho = f[0] = *pf0;
        rho += f[4] = *pf4;
        rho += f[8] = *pf8;
        rho += f[12] = *pf12;
        rho += f[16] = *pf16;
        rho += f[1] = *pf1;
        rho += f[2] = *pf2;
        rho += f[3] = *pf3;
        rho += f[5] = *pf5;
        rho += f[6] = *pf6;
        rho += f[7] = *pf7;
        rho += f[9] = *pf9;
        rho += f[10] = *pf10;
        rho += f[11] = *pf11;
        rho += f[13] = *pf13;
        rho += f[14] = *pf14;
        rho += f[15] = *pf15;
        rho += f[17] = *pf17;
        rho += f[18] = *pf18;
        if(solidcode){
            /* BounceBack(f); */
            /* 10-16-97 stop; inline BounceBack() */
            /* in xy plane */
            *pf5 =f[1]; *pf1 =f[5];
            *pf7 =f[3]; *pf3 =f[7];
            *pf6 =f[2]; *pf2 =f[6];
            *pf8 =f[4]; *pf4 =f[8];
            /* z up-and down vectors */
            *pf18 =f[9]; *pf9 =f[18];
            /* off-xy-plane vectors */
            *pf16 =f[10]; *pf10 =f[16];
            *pf12 =f[14]; *pf14 =f[12];
            *pf17 =f[11]; *pf11 =f[17];
            *pf15 =f[13]; *pf13 =f[15];
            continue;
        }
    }
}

```

```

/* calculate the feqs */
feq[0] = ONE_3RD*rho;

qian = rho*ONE_18TH;
mul = qian*3.0;
mux = mul*ux;
muy = mul*uy;
muz = mul*uz;

/* old had qian0 = rho[s]*ONE_36TH; */
/* the Cartesian axis vectors */
feq[1] = qian + mux;
feq[5] = qian - mux;
feq[3] = qian + muy;
feq[7] = qian - muy;
feq[9] = qian + muz;
feq[18] = qian - muz;
/* the diagonal vectors; hope compiler catches on */
qian *= half; mux *= half; muy *= half; muz *= half;
feq[2] = qian + mux + muy;
feq[6] = qian - mux - muy;

feq[4] = qian + muy - mux;
feq[8] = qian - muy + mux;

feq[10] = qian + mux + muz;
feq[16] = qian - mux - muz;

feq[12] = qian - mux + muz;
feq[14] = qian + mux - muz;

feq[13] = qian - muy + muz;
feq[15] = qian + muy - muz;

feq[11] = qian + muy + muz;
feq[17] = qian - muy - muz;
/* ... */
/* put back the new f[] values */
/* 2-27-98 rearrange order to improve caching? */
*pf0 = f[0]*beta_s + feq[0]*omega_s;
*pf4 = f[4]*beta_s + feq[4]*omega_s;
*pf8 = f[8]*beta_s + feq[8]*omega_s;
*pf12 = f[12]*beta_s + feq[12]*omega_s;
*pf16 = f[16]*beta_s + feq[16]*omega_s;
*pf1 = f[1]*beta_s + feq[1]*omega_s;
*pf2 = f[2]*beta_s + feq[2]*omega_s;
*pf3 = f[3]*beta_s + feq[3]*omega_s;
*pf5 = f[5]*beta_s + feq[5]*omega_s;
*pf6 = f[6]*beta_s + feq[6]*omega_s;
*pf7 = f[7]*beta_s + feq[7]*omega_s;
*pf9 = f[9]*beta_s + feq[9]*omega_s;
*pf10 = f[10]*beta_s + feq[10]*omega_s;
*pf11 = f[11]*beta_s + feq[11]*omega_s;
*pf13 = f[13]*beta_s + feq[13]*omega_s;
*pf14 = f[14]*beta_s + feq[14]*omega_s;
*pf15 = f[15]*beta_s + feq[15]*omega_s;
*pf17 = f[17]*beta_s + feq[17]*omega_s;

```

```

        *pf18 = f[18]*beta_s + feq[18]*omega_s;
    }
}

} /* END over s (ncomponent) */
return(1); /* 9-22-97 dumb return for now */
} /* END JustDisperse3D() */
/*-----*/
/* 2-22-98 see jb_ph.c.bak for previous; now modify colorCode 2 to have */
/* white to black for concentration... */
/* 2-21-98 modify to allow colorCode =0,1,2: 0 is rainbow; 1=white solids */
/* with light gray conc=0, and highest conc=black; 2=black solids with */
/* white conc=0, and light gray conc=max */
/* 9-23-97 modify SavePpm() to save an XZ plane cut on top of an XY plane */
/* cut, more for Steve Brown's fractal surface dispersion problem... */
/* 7-5-97 adapt for 3D, and put y-x and y-z cuts side by side... */
/* try to create funky colors to match Clay's; use scheme in */
/* home PPro200 D:\lb\~\f2p_graf.c... */
/* Saves a portable pixel map (ppm, as in pbmplus from Unix lore), which */
/* cmpeg can then convert into an mpeg. Also creates and saves a *.lst */
/* file of ppm file names... after save_ppm() in ilga.c... */
/*-----*/
FILE *SavePpmXY_XZ(ff_t ****ff, char ***solid, int ncomponent, int nveloc[],
    int nlay, int nrow, int ncol, int sstart, int step, int colorCode)
{
#define RGB_BASE 70
/* #define RGB_MAX_SIZE      8192 */ /* allows ncol+nlay <= 2730 */
#define RGB_MAX_SIZE      16384 /* 6-14-98 allows ncol+nlay <= 5460 */
#define LOCAL_BUF_LEN      128
static unsigned char rgb_row[RGB_MAX_SIZE+4];
/* for mpeg writes, 3* max ncol */

static int filenum=0, firsttime=1, rgb_len;
static FILE *fp, *b_list_fp;
int i,ii,x,y,z;
unsigned char r,g,b;
double c, cmax=-1.0e200, cmin=1.0e200;
double slope1,slope2,delta,chalf,craw,cpt75;
double scale; /* 2-21-98 */
struct tm *ptm;
static int day=0,hour=0; /* because localtime destroys single internal tm */
time_t lt;
char buf[LOCAL_BUF_LEN]; /* for filenames */
int yhalf, zhalf; /* 9-23-97 replace xhalf with yhalf */

if(filenum>=999){
    firsttime = 1;
    filenum = 0;
    if(b_list_fp) fclose(b_list_fp);
}
if(firsttime){
    /* ppm format has thre byte rgb values for each pixel */
    time(&lt);
    ptm = localtime(&lt);
    /* 9-12-94 for list file */
    day = ptm->tm_mday, hour = ptm->tm_hour;

```

```

    sprintf(buf, "B%02d%02d.lst", day, hour);
    buf[LOCAL_BUF_LEN-1] = 0;
    b_list_fp = fopen(buf, "w");
    firsttime=0;
}
/* 9-27-97 move out of firsttime block */
rgb_len = ncol*3; /* 9-23-97 change */

/* 7-5-97 allow placing y-x and y-z cuts side-by-side */
yhalf = nrow >> 1; /* zhalf = nlay >> 1; */
/* 2-21-98 set zhalf=0 for JFM paper */
zhalf = 0;

/* find the maximum and minimum conc values */
/* NOTE we initialized cmax, cmin in declarations, above */
/* 9-23-97 alter for yhalf vs. xhalf, outer loop now on x... */
for(x=0; x<ncol; x++){
    for(y=0; y<nrow; y++){
        if(solid[zhalf][y][x]) continue; /* 7-12-97 */
        for(i=0, c=0.0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][zhalf][y][x];
        }
        if(c >= cmax) cmax = c;
        if(c <= cmin) cmin = c;
    }
    for(z=0; z<nlay; z++){
        if(solid[z][yhalf][x]) continue; /* 7-12-97 */
        for(i=0, c=0.0; i<nveloc[sstart]; i++){
            c += ff[sstart][i][z][yhalf][x];
        }
        if(c >= cmax) cmax = c;
        if(c <= cmin) cmin = c;
    }
}

/* Prevent funny colors due to small oscillations */
if(cmin < 0.0) cmin = 0.0;

if(colorCode==0){
    delta = 255 - RGB_BASE; /* ASSUME maximum value for r,g or b is 255 */
    chalf = 0.5*(cmax - cmin);
    cpt75 = 0.75*(cmax - cmin);
    if(cmax-cmin > 1.0e-30){
        slope1 = delta/chalf;
        slope2 = slope1*2.0;
    }
    else return(b_list_fp); /* was return(0) */
}
else {
/* 2-21-98 block for new grayscales */
if(cmax<1.0e-30) cmax = 1.0e-30;
if(colorCode==1){ /* white solids */
    scale = 240.0/sqrt(cmax); /* 2-23-98 */
}
else {
    scale = 255.0/cmax;
}
}
}

```



```

/* make the file name; avoid lots of unclosed files if */
/* the cmax-cmin is too small... */
/* Remember localtime structure is not "re-entrant"... */
buf[LOCAL_BUF_LEN-1] = 0;
sprintf(buf,"B%02d%02d%03d.PPM", day, hour, filenum);
filenum++;
fp = fopen(buf, "wb");
if(!fp) return(b_list_fp); /* was return(0) */
if(b_list_fp) fprintf(b_list_fp,"%s\n",buf);
/* write the standard binary ppm header; \012 is linefeed... */
fprintf(fp,"P6\012%d %d\012255\012",ncol,nlay+nrow+1); /* 9-23-97 */

/* 9-23-97 do the X-Z cut first */
for(z=0; z<nlay; z++){
    for(x=0,ii=0; x<ncol && ii<RGB_MAX_SIZE; x++,ii+=3){
        /* print solids in white */
        if(solid[z][yhalf][x]==0){
            for(c=0.0,i=0; i<nveloc[sstart]; i++){
                c += ff[sstart][i][z][yhalf][x];
            }
            /* prevent funny colors */
            if(c<0.0) c = 0.0;
            if(colorCode==1){
                r = scale*sqrt(c);
                if(r>240) r=240;
                r = 240 - r;
                g = b = r;
            }
            else if(colorCode==2){
                r = scale*(cmax-c);
                if(r>255) r = 255;
                g = b = r;
            }
            else {
                /***** "default" rainbow scaling below *****/
                craw = cmax - c;
                if(craw<chalf){
                    r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*craw);
                    if(r<RGB_BASE) r = RGB_BASE;
                    g = RGB_BASE + (int)(craw*slope1); if(g>255) g = 255;
                }
                else if(craw<cpt75){
                    b = RGB_BASE; g = 255;
                    r = RGB_BASE + (int)((craw-chalf)*slope2); if(r>255) r =
255;
                }
                else {
                    b = RGB_BASE; r = 255;
                    g = RGB_BASE + (int)(delta - slope2*(craw-cpt75));
                }
            }
            /**** END default rainbow scheme ****/
        }
        else r=g=b=255; /* if solid, print as white */
        /* place in array */
        rgb_row[ii]=r, rgb_row[ii+1]=g, rgb_row[ii+2]=b;
    }
}

```

```

        fwrite(rgb_row, 1, rgb_len, fp);
    }
    /* 9-23-97 next write a black divider line */
    for(ii=0; ii<rgb_len; ii++){
        rgb_row[ii] = 0;
    }
    fwrite(rgb_row, 1, rgb_len, fp);
    /*** next loop over the XY plane ***/
    for(y=0; y<nrow; y++){
        for(x=0,ii=0; x<ncol && ii<RGB_MAX_SIZE; x++,ii+=3){
            /* print solids in white */
            if(solid[zhalf][y][x]==0){
                for(c=0.0,i=0; i<nveloc[sstart]; i++){
                    c += ff[sstart][i][zhalf][y][x];
                }
                /* prevent funny colors */
                if(c<0.0) c = 0.0;
                if(colorCode==1){
                    r = scale*sqrt(c);
                    if(r>240) r=240;
                    r = 240 - r;
                    g = b = r;
                }
                else if(colorCode==2){
                    r = scale*(cmax-c);
                    if(r>255) r = 255;
                    g = b = r;
                }
                else {
                    /**** "default" rainbow scaling below ***/
                    craw = cmax - c;
                    if(craw<chalf){
                        r = RGB_BASE; b = RGB_BASE + (int)(delta - slope1*craw);
                        if(r<RGB_BASE) r = RGB_BASE;
                        g = RGB_BASE + (int)(craw*slope1); if(g>255) g = 255;
                    }
                    else if(craw<cpt75){
                        b = RGB_BASE; g = 255;
                        r = RGB_BASE + (int)((craw-chalf)*slope2); if(r>255) r =
255;
                    }
                    else {
                        b = RGB_BASE; r = 255;
                        g = RGB_BASE + (int)(delta - slope2*(craw-cpt75));
                    }
                }
                /*** END default rainbow scheme ***/
            }
            else r=g=b=255; /* if solid, print as white */
            /* place in array */
            rgb_row[ii]=r, rgb_row[ii+1]=g, rgb_row[ii+2]=b;
        }
        fwrite(rgb_row, 1, rgb_len, fp);
    }

    fclose(fp);
    return(b_list_fp);

```

```

#undef RGB_BASE
#undef RGB_MAX_SIZE
#undef LOCAL_BUF_LEN
} /* END SavePpmXY_XZ() */
/*-----*/
/* 9-23-97 modify ~lb01\lb04.c function ReadBmp4Slug() to extrude */
/* slug along y, and since we may eventually use in situation with */
/* ff[0][i] dellocated, just distribute the concentrations equally */
/* (scaled to e.g. 1/3 or 1/18 or 1/36 for D3Q19) over vectors... */
/* 6-2-97 try reading in bmp files to use as input for lb01.c. */
/* This func reads slug file only, interprets any color darker */
/* than brightest color as solute at sstart... */
/* NOTE unlike SetSlug(), takes a single rho, not concLis... */
/* Modify from bmp.c, created under home GW2K PPro200 D:\lb for */
/* easy debugging. */
/*****/
int ReadBmp4Slug(ff_t ***** const ff, char *** const solid, float rho,
    int nvel, int nlay, int nrow, int ncol, int sstart,
    int x, int z, char *filename)
{
    int i,j,k,m,n,istatus,kend,zoffs, xx, yy, zz;
    FILE *fp;
    char buf[32];
    double ftemp, rho0;
    ff_t f[DEF_NVELOC],f6;
    int fSize,dummy,width,height,compression,sizeImage,colorsUsed,colorsImp;
    short planes,bitCount,bitsPerPix;
    unsigned char rgb[4];
    int jmax, jmin, max, min, sum, rowBytes, color;
    unsigned char *rowBuf;

    /* open the passed filename */
    fp = fopen(filename, "rb");
    if(!fp){
        printf("can't open %s\n", filename);
        return(0);
    }

    istatus = fread(buf,1,2,fp);
    if(istatus<2 || buf[0]!='B' || buf[1]!='M'){
        puts("Not a valid Windows bitmap file");
        fclose(fp);
        return(0);
    }

    puts("got here! saw BM!");
    istatus = fread(&fSize,4,1,fp); /* size of this ? file ? */
    printf("this file is %d bytes long\n", fSize);
    istatus = fread(&dummy,4,1,fp); /* reserved1, reserved2 */
    istatus = fread(&dummy,4,1,fp); /* offsetBytes */
    printf("Offset bytes to data: %d\n", dummy);
    /* read BitmapInfoHeader */
    istatus = fread(&dummy,4,1,fp); /* size of this structure */
    printf("size of InfoHeader Record: %d\n", dummy);
    istatus = fread(&width,4,1,fp); /* width in pixels */
    istatus = fread(&height,4,1,fp); /* height in pixels */
    istatus = fread(&planes,2,1,fp); /* planes (should be 1); note 2-byte */
    istatus = fread(&bitCount,2,1,fp); /* bits per pixel; note 2-byte */

```

```

bitsPerPix = bitCount;
printf("Bits / Pixel = %d\n", bitsPerPix);
istatus = fread(&compression,4,1,fp); /* Compression -- handle uncompress. only */
if(!istatus || compression){
    puts("Sorry, can't handle compressed file!");
    fclose(fp);
    return(0);
}
istatus = fread(&sizeImage,4,1,fp); /* size of pixel map */
printf("the pixel map takes up %d bytes\n",sizeImage);
istatus = fread(&dummy,4,1,fp); /* XPelsPerMeter, discard */
istatus = fread(&dummy,4,1,fp); /* YPelsPerMeter, discard */

istatus = fread(&colorsUsed,4,1,fp); /* */
istatus = fread(&colorsImp,4,1,fp); /* */

if(colorsUsed==0){ /* maximum number of colors is used */
    colorsUsed = 1 << bitsPerPix;
}
if(colorsImp==0){
    colorsImp = colorsUsed;
}
printf("The colormap has %d colors, of which %d are important.\n",
    colorsUsed,colorsImp);

/* test version will handle only 8-bit, 256 color mode */
if(bitsPerPix!=8){
    puts("this version 6-1-97 handles only 8-bit color mode");
    return(0);
}
/* read the color map and translate into black or white for now */
for(j=max=jmax=jmin=0, min=2000000000; j<colorsUsed; j++){
    istatus = fread(rgb,1,4,fp);
    if(istatus!=4 || rgb[3]){
        puts("ERROR in color map"); fclose(fp); return(0);
    }
    printf("%d: r=%d, g=%d, b=%d\n", j, rgb[0],rgb[1],rgb[2]); /*
    /* if(j%24==0) getch(); */
    sum = (int)rgb[0] + (int)rgb[1] + (int)rgb[2];
    if(sum >= max){
        max = sum; jmax = j;
    }
    if(sum <= min){
        min = sum; jmin = j;
    }
}
if(jmin==jmax){
    puts("error -- max and min colors identical!");
    fclose(fp); return(0);
}
printf("index of black=%d, index of white=%d\n", jmin, jmax);

/* determine how many bytes to read with padding -- NOTE */
/* MUST alter for non-8-bit modes... */

rowBytes = (width + 3) & 0xFFFC; /* pad to 4-byte boundary */
printf("padded row is %d, vs. width=%d\n", rowBytes, width);

```

```

/* getch(); */

/* allocate row buffer */
rowBuf = malloc(rowBytes);
if(!rowBuf){
    puts("couldn't allocate rowBuf!");
    fclose(fp); return(0);
}

/* read the bitmap */

/* NOTE need to make kend relative to ncol and x */
if(x+width > ncol) kend = ncol - x;
else kend = width;

zoffs = z + height; /* 9-24-97, more error checking below */

/* 9-23-97 add block to calc the f6 and f19 vectors */
f6 = rho*ONE_6TH;
for(n=0; n<DEF_NVELOC; n++) f[n] = TT[n]*rho;
/* END 9-23-97 block to calculate f6 and f19 vectors */

puts("about to start reading row data");
for(i=0; i<height; i++){
    istatus = fread(rowBuf, 1, rowBytes, fp);
    if(istatus != rowBytes){
        printf("stopped at row %d\n", i);
        free(rowBuf);
        fclose(fp); return(0);
    }

    /* read the pixel values in the row and plot */
    zz = zoffs-i;
    if(zz<0 || zz>=nlay) continue; /* 9-23-97,9-24-97 */
    for(k=0; k<kend; k++){
        xx = k+x;
        if(rowBuf[k] != jmax){
            for(yy=0; yy<nrow; yy++){
                if(solid[zz][yy][xx]) continue;
                if(nvel==6) for(n=0; n<nvel; n++)
                    ff[sstart][n][zz][yy][xx] = f6;
                else for(n=0; n<nvel; n++)
                    ff[sstart][n][zz][yy][xx] = f[n];
            }
        }
    }

    if(rowBuf) free(rowBuf);
    if(fp) fclose(fp);
    return(1);
} /* END ReadBmp4Slug() */

/*-----*/
/*-----*/
/* 9-26-97 recycle the ff[0] array space to produce a geometry expanded */
/* by factor ntimes in the x-direction. We will not expand uu array of */
/* structs, but will later access it by implicit mod with old ncol... */
/* NOTE return the new xRight! If return val is <=0, signals error */
/*-----*/
int Recycle(ff_t ***** const ff, char *** const solid, int ncomponent,

```

```

        int nveloc[], int nlay, int nrow, int ncol, int ntimes, int xRight)
{
    ff_t *ffbuf;
    char *solidbuf;
    int s,i,z,y,x, nvel, ncol_new, n, xstart;
    int iflag=1, aflag=1;
    static char *mess1 = "Failed to deallocate ff[0] in Recycle()\n";
    static char *mess2 = "Failed to reallocate ff[s] in Recycle()\n";
    static char *mess3 = "Failed to reallocate solid in Recycle()\n";

    ffbuf = malloc(ncol*sizeof(ff_t));
    solidbuf = malloc(ncol*sizeof(char));
    if(!solidbuf || !ffbuf) return(0);

    nvel = nveloc[0];
    /* 1st free the ff[0] data space */
    for(iflag=1,i=i; i<nvel; i++){
        for(z=0; z<nlay; z++){
            for(y=0; y<nrow; y++){
                if(ff[0][i][z][y]) free(ff[0][i][z][y]);
                else iflag = 0;
            }
            if(ff[0][i][z]) free(ff[0][i][z]);
            else iflag = 0;
        }
        if(ff[0][i]) free(ff[0][i]);
        else iflag = 0;
    }
    if(!iflag){
        if(LOG_fp) fprintf(LOG_fp, mess1);
        printf(mess1);
        free(ffbuf); free(solidbuf);
        return(0);
    }

    /* Next reallocate the ff[s>0] data space (x only), but buffer and recopy */
    /* old data and zero out right side of array... */
    /* Start by allocating a buffer for old x data... */
    ncol_new = ncol*ntimes;
    for(iflag=aflag=1,s=1; s<ncomponent; s++){
        nvel = nveloc[s];
        for(i=0; i<nvel; i++){
            for(z=0; z<nlay; z++){
                for(y=0; y<nrow; y++){
                    if(ff[s][i][z][y]){
                        /* save old data in buf */
                        for(x=0; x<ncol; x++) ffbuf[x] = ff[s][i][z][y][x];
                        free(ff[s][i][z][y]);
                        if(!(ff[s][i][z][y] = malloc(ncol_new*sizeof(ff_t)))){
                            aflag = 0; break;
                        }
                        /* set right part new line =0, copy back buffer */
                        for(x=ncol; x<ncol_new; x++) ff[s][i][z][y][x] = KAHAN_0;
                        /* 3-8-98 above kahan_0 */
                        for(x=0; x<ncol; x++) ff[s][i][z][y][x] = ffbuf[x];
                    }
                }
            }
            else iflag=0;
        }
    }
}

```

```

    }
    }
}

if(!iflag || !aflag){
    if(LOG_fp) fprintf(LOG_fp, mess2);
    printf(mess2);
    free(ffbuf); free(solidbuf);
    return(0);
}

/* reallocate the solids array, replicating the old solids */
for(iflag=aflag=1,z=0; z<nlay; z++){
    for(y=0; y<nrow; y++){
        if(solid[z][y]){
            /* save old data in buf */
            for(x=0; x<ncol; x++) solidbuf[x] = solid[z][y][x];
            free(solid[z][y]);
            if(!(solid[z][y] = malloc(ncol_new*sizeof(char)))){
                aflag = 0; break;
            }
            /* copy back buffer, ntimes */
            for(xstart=0; xstart<ncol_new; xstart+=ncol){
                for(x=0; x<ncol; x++) solid[z][y][x+xstart] = solidbuf[x];
            }
        }
        else iflag=0;
    }
}

if(!iflag || !aflag){
    if(LOG_fp) fprintf(LOG_fp, mess3);
    printf(mess3);
    free(ffbuf); free(solidbuf);
    return(0);
}

/* recalculate the xRight (probably xRightConc to outside world) */
xRight = ncol_new - (ncol-xRight) ;

/* make sure we have freed the ffbuf and solidbuf! */
if(ffbuf) free(ffbuf);
if(solidbuf) free(solidbuf);
return(xRight);
} /* END Recycle() */

/*-----*/
/* 9-26-97 for the JB code, use these functions AFTER Recycle(); */
/* use use XSetConc(), YSetConc() BEFORE Recycle() called... */
/* Set the concentrations to the values specified in the array concList[], */
/* along the plane of constant Y...similar to HSetConc() in 2D models... */
/* a negative value for a particular component means: skip this component. */
/* The concentrations are set along the plane with opposite corners */
/* x1,y,z1 to x2,y,z2, inclusive of the endpoints... */
/* 7-11-97 redesign to: scale */
/* 6-vector to the corresponding cartesian vectors in 19-vector carrier... */
/* this method should prevent the bleed-through on edges we possibly got */
/* with some of the fracture x (intersection) calcs done in april 97... */
/******/

```

```

int YSetConcJB(ff_t ***** const ff, char *** const solid,
               int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
               int y, int x1, int x2, int z1, int z2, double * const concList)
{
    int x,z,i,s,temp, nvel, solidcode;
    /* 7-11-97 the "is_" above test is any of the solutes are 19 or 6 vector */
    /* types; would be more efficient done just once outside, but seems safer */
    /* to do this simple test internally, since it will be dwarfed by fetching */
    /* and computation time in rest of function, and we may some day reallocate */
    /* a 19-vector solute among 6 vectors after equilibration.... */

    ff_t f[DEF_NVELOC];

    if(y<0 || x1<0 || x2<0 || y>=nrow || x1>=ncol || x2>=ncol
        || z1<0 || z2<0 || z1>nlay || z2>nlay) return(0);

    if(x1>x2){
        temp = x1; x1=x2; x2=temp;
    }
    if(z1>z2){
        temp = z1; z1=z2; z2=temp;
    }

    for(s=1; s<ncomponent; s++){
        /* a negative number is the sign to skip this component */
        if(concList[s] < 0.0) continue;
        if(concList[s] <1.0e-30) concList[s] = KAHAN_0; /* 3-8-98 */
        nvel = nveloc[s];
        if(nvel==6) for(i=0; i<6; i++) f[i] = concList[s]*ONE_6TH;
        else for(i=0; i<nvel; i++) f[i] = concList[s]*TT[i];
        for(z=z1; z<z2; z++){
            for(x=x1; x<=x2; x++){
                solidcode = solid[z][y][x];
                if(solidcode==-2) continue; /* don't do internal solids */
                if(solidcode && concList[s]>1.0e-30) continue;
                for(i=0; i<nvel; i++) ff[s][i][z][y][x] = f[i];
            }
        }
    }
    return(1);
} /* END YSetConcJB() */

/*-----*/
/* 9-26-97 use AFTER Recycle() called; less sophisticated than handling */
/* of solids in XSetConc()... */
/* Set the concentrations to the values specified in the array concList[], */
/* along the Plane with constant x...similar to VSetConc() in 2D models... */
/* a negative value for a particular component means: skip this component. */
/* The concentrations are set along the "line" is from x,y1 to x,y2, */
/* inclusive of the endpoints... */
/* NOTE even though we advance y downward (as a row index), the positive */
/* y direction for flux calculations is UP... */
/*-----*/
int XSetConcJB(ff_t ***** const ff, char *** const solid,
               int ncomponent, int nveloc[], int nlay, int nrow, int ncol,
               int x, int y1, int y2, int z1, int z2, double * const concList)
{
    int z,y,i,s, nvel, temp, solidcode;

```



```

double f[DEF_NVELOC];

if(x<0 || y1<0 || y2<0 || x>=ncol || y1>=nrow || y2>=nrow
    || z1<0 || z2<0 || z1>=nlay || z2>=nlay) return(0);

if(y1>y2){
    temp = y1; y1=y2; y2=temp;
}
if(z1>z2){
    temp = z1; z1=z2; z2=temp;
}

for(s=1; s<ncomponent; s++){
    /* a negative number is the sign to skip this component */
    if(concList[s] < 0.0) continue;
    if(concList[s] <1.0e-30) concList[s] = KAHAN_0; /* 3-9-98 */
    nvel = nveloc[s];
    if(nvel==6) for(i=0; i<6; i++) f[i] = concList[s]*ONE_6TH;
    else for(i=0; i<nvel; i++) f[i] = concList[s]*TT[i];
    for(z=z1; z<z2; z++){
        for(y=y1; y<=y2; y++){
            solidcode = solid[z][y][x];
            if(solidcode===-2) continue; /* don't do internal solids */
            if(solidcode && concList[s]>1.0e-30) continue;
            for(i=0; i<nvel; i++) ff[s][i][z][y][x] = f[i];
        }
    }
}

return(1);
} /* END XSetConcJB() */
/*-----*/
/* Modify SetFCCSolids() to do one, non-perturbed sphere in middle of */
/* ncol,nrow,nlay domain... ideally designed for case of nlay,nrow,ncol */
/* even, though will work for odd... */
/*-----*/
int JoSphere(char ***solid, int nlay, int nrow, int ncol,
    int radius)
{
    int x,y,z, xx, yy, zz; /* corrected for wrap */
    typedef float coord_t;
    coord_t xc,yc,zc,rc, rSqr;
    coord_t dx2,dy2,dz2;
    int xend,yend,zend, ctr;
    int xhalf, yhalf, zhalf;

    /* 10-29-97 sub 1 */
    xhalf = (ncol >> 1) - 1;
    yhalf = (nrow >> 1) - 1;
    zhalf = (nlay >> 1) - 1;

    xc = xhalf + 0.5;
    yc = yhalf + 0.5;
    zc = zhalf + 0.5;
    rc = radius;
    rSqr = rc*rc;

```

```

/** have co-ords and radii, now do the fill. Basic */
/* idea is to draw a bounding box around the point, and within that */
/* bounding box, check if a point is within the sphere centered at */
/* that point... */
/* NOTE many unnecessary remnants of complicated FCC logic; I don't care... */
for(ctr=0, z=zhalf-radius, zend=zhalf+radius+1; z<=zend; z++){
    dz2 = (z - zc)*(z - zc);
    zz = z;
    if(zz<0) zz = 0; else if(zz>=nlay) zz = nlay - 1;
    for(y=yhalf-radius, yend=yhalf+radius+1; y<=yend; y++){
        dy2 = (y - yc)*(y - yc);
        yy = y;
        if(yy<0) yy = 0; else if(yy>=nrow) yy = nrow - 1;
        for(x=xhalf-radius, xend=xhalf+radius+1; x<=xend; x++){
            dx2 = (x - xc)*(x - xc);
            if(rSqr > dx2 + dy2 + dz2){
                /* point is within sphere, now check wrap */
                xx = x;
                if(xx<0) xx=0; else if(xx>=ncol) xx = ncol-1;
                solid[zz][yy][xx] = -1; ctr++;
            }
        }
    }
}

return(ctr); /* 10-29-97 return # solids actually hit */
} /* END JoSphere() */
/*-----*/
/* Modify JoSphere() to do one, non-perturbed cylinder in middle of */
/* ncol,nrow domain... to test against Eidsath et al. (1983) results... */
/******/
int JoDisk(char ***solid, int nlay, int nrow, int ncol,
            int radius)
{
    int x,y,z, xx, yy; /* corrected for wrap */
    typedef float coord_t;
    coord_t xc,yc,rc, rSqr;
    coord_t dx2,dy2;
    int xend,yend,zend, ctr;
    int xhalf, yhalf;

    xhalf = (ncol >> 1) - 1;
    yhalf = (nrow >> 1) - 1;

    xc = xhalf + 0.5;
    yc = yhalf + 0.5;
    rc = radius;
    rSqr = rc*rc;

    /** have co-ords and radii, now do the fill. Basic */
    /* idea is to draw a bounding box around the point, and within that */
    /* bounding box, check if a point is within the sphere centered at */
    /* that point... */
    /* NOTE many unnecessary remnants of complicated FCC logic; I don't care... */
    for(ctr=0, z=0; z<nlay; z++){

```

```

    for(y=yhalf-radius, yend=yhalf+radius+1; y<=yend; y++){
        dy2 = (y - yc)*(y - yc);
        yy = y;
        if(yy<0) yy = 0; else if(yy>=nrow) yy = nrow - 1;
        for(x=xhalf-radius, xend=xhalf+radius+1; x<=xend; x++){
            dx2 = (x - xc)*(x - xc);
            if(rSqrdd > dx2 + dy2){
                /* point is within sphere, now check wrap */
                xx = x;
                if(xx<0) xx=0; else if(xx>=ncol) xx = ncol-1;
                solid[z][yy][xx] = -1; ctr++;
            }
        }
    }
}
return(ctr); /* 10-29-97 return # solids actually hit */
} /* END JoDisk() */
/*-----*/
/* 6-13-98 create a version for just one tracer */
/* 2-27-98 pointerize to speed up? */
/* 9-27-97 modify to pass ncol_old so we can find uu[z][y][xx] position.. */
/* 9-22-97 create 3D version of JustDisperse() (2D versions in lb01.c), */
/* a collide function that assumes velocity field is static, therefore */
/* does not do buoyancy or carrier fluid... */
/* NOTE: for now, simplify by not using lots of pointers and by keeping */
/* ONLY bounceback mode... */
/*****/
int JustDisperse3D_A(ff_t ***** ff,
    double * const tau, double * const beta, double *const omega,
    struct veloc_t *** uu, char *** solid,
    int ncomponent, int nveloc[], int nlay, int nrow, int ncol, int ncol_old)
{
    int z,y,x,xx; /* 9-27-97 xx is index into uu[z][y][xx]... */
    double ux, uy, uz;
    double f0,f1,f2,f3,f4,f5;
    ff_t *pf0,*pf1,*pf2,*pf3,*pf4,*pf5;
    ff_t **pf0z,**pf1z,**pf2z,**pf3z,**pf4z,**pf5z;

    struct veloc_t **uuzp, *uup;

    int solidcode;
    unsigned char **solidzp, *solidp;

    double rho, beta_s;
    double mux,muy,muz, mul;
    /* const static double half = ONE_HALF; */
    double halfOmega,sixthOmega; /* 6-13-98 */

    if(ncomponent!=2 || nveloc[1]!=6){
        puts("incorrect JustDisperse3D_A() function");
        exit(-11);
    }
    halfOmega = ONE_HALF*omega[1];
    sixthOmega = ONE_6TH*omega[1];
    beta_s = beta[1];

    for(z=0; z<nlay; z++){

```

```

uuzp = uu[z];
solidzp = solid[z];
pf0z = ff[1][0][z]; pf1z = ff[1][1][z]; pf2z = ff[1][2][z];
pf3z = ff[1][3][z]; pf4z = ff[1][4][z]; pf5z = ff[1][5][z];
for(y=0; y<nrow; y++){
    solidp = solidzp[y];
    uup = uuzp[y];
    pf0 = pf0z[y];
    pf1 = pf1z[y];
    pf2 = pf2z[y];
    pf3 = pf3z[y];
    pf4 = pf4z[y];
    pf5 = pf5z[y];
    for(x=xx=0; x<ncol; x++,xx++,++pf0, ++pf1, ++pf2,
        ++pf3, ++pf4, ++pf5){
        /* MUST have next xx as top of loop */
        if(>xx==ncol_old) xx = 0; /* 9-27-97 assume regular access */
        solidcode = solidp[x];
        if(solidcode== -2) continue;
        ux = uup[xx].x; /* 9-27-97 was plain [x] */
        uy = uup[xx].y;
        uz = uup[xx].z;
        rho = f0 = *pf0;
        rho += f1 = *pf1;
        rho += f2 = *pf2;
        rho += f3 = *pf3;
        rho += f4 = *pf4;
        rho += f5 = *pf5;
        if(solidcode){
            *pf0 = f2;
            *pf1 = f3;
            *pf2 = f0;
            *pf3 = f1;
            *pf4 = f5;
            *pf5 = f4;
            continue; /* on to next x */
        }
        /* calculate the feqs */
        mul = rho*halfOmega;
        mux = ux*mul; muy = uy*mul; muz = mul*uz;
        rho *= sixthOmega;
        /* put back the new f[] values */
        *pf0 = f0*beta_s + rho + mux;
        *pf1 = f1*beta_s + rho + muy;
        *pf2 = f2*beta_s + rho - mux;
        *pf3 = f3*beta_s + rho - muy;
        *pf4 = f4*beta_s + rho + muz;
        *pf5 = f5*beta_s + rho - muz;
    }
}
}
return(1); /* 9-22-97 dumb return for now */
} /* END JustDisperse3D_A() */
/*-----*/
/*-----*/
/*-----*/
/*-----*/

```

```
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