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Fundamentals of the KRAKEN Code

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Fundamentals of the KRAKEN Code

As it is presently used at Livermore, KRAKEN is an Eulerian hydrodynamics code capable of treating compressible nonviscous flow of several fluids in a two-dimensional (axially symmetric) region. In many respects it is reminiscent of the FLIC/PIC methods, though it is considerably different in detail.

Before beginning discussion of the equations themselves, it should perhaps be mentioned that for what might be called historical reasons the code is presently constructed in a somewhat cumbersome and inefficient fashion. I spent some time "re-thinking" the KRAKEN code, and Kurt Sinz is presently working on a new version starting from a set of difference equations differing considerably in some respects from those embodied in the existing code.

In other words, you are about to see some (hopefully) obsolescent equations. They are the ones that have been tried, however

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The primary variables are:

$$u, v, m_i, \epsilon_i, f_i \quad (i = 1, 2, \dots, n)$$

where u and v are the r and z components of velocity, (m_i, ϵ_i) are the mass and internal energy per unit mass of the i th material, and f_i is the fraction of the total volume of the zone occupied by the i th material. "Centering" is as shown:

At time t^n and zone with lower left corner at r_k, z_l we have:

$$u_{k, l+\frac{1}{2}}^n; v_{k+\frac{1}{2}, l}^n; m_{k+\frac{1}{2}, l+\frac{1}{2}}^n; \epsilon_{k+\frac{1}{2}, l+\frac{1}{2}}^n; f_{k+\frac{1}{2}, l+\frac{1}{2}}^n$$

Note that all variables are "centered" at the same time.

The calculation to advance the system a time Δt is performed in a series of four steps: $A(\Delta t) = L(\Delta t) R(\frac{1}{2}\Delta t) Z(\Delta t) R(\frac{1}{2}\Delta t)$.

Here $L(\Delta t)$ indicates an essentially pure Lagrangian-like two-dimensional calculation which yields u^{n+1}, v^{n+1} etc., and hence "advection velocities" $\bar{u}^{n+\frac{1}{2}} = \frac{1}{2}(u^{n+1} + u^n)$ and a similar expression for $\bar{v}^{n+\frac{1}{2}}$. Using these velocities, advection is performed in the radial direction for half a time step, then in the axial direction for a full time step, then again in the radial direction for the other half time step. In theory, this should help eliminate asymmetries dependent on which direction was done first.

Since (except for obvious minor geometrical factors) $R(\Delta t)$ and $Z(\Delta t)$ have the same structure, we need discuss only $L(\Delta t)$ and $R(\Delta t)$.

$L(\Delta t)$: The Lagrangian Phase

$$u_{k, l+\frac{1}{2}}^{n+1} = u_{k, l+\frac{1}{2}}^n - \frac{\Delta t^{n+\frac{1}{2}} g_{k, l+\frac{1}{2}}^{n+\frac{1}{2}} (p_{k+\frac{1}{2}, l+\frac{1}{2}}^{-n+1} + p_{k+\frac{1}{2}, l+\frac{1}{2}}^{-n} - p_{k-\frac{1}{2}, l+\frac{1}{2}}^{-n+1} - p_{k-\frac{1}{2}, l+\frac{1}{2}}^{-n})}{m_{k+\frac{1}{2}, l+\frac{1}{2}}^n + m_{k-\frac{1}{2}, l+\frac{1}{2}}^n}$$

$$v_{k+\frac{1}{2}, l}^{n+1} = v_{k+\frac{1}{2}, l}^n - \frac{\Delta t^{n+\frac{1}{2}} g_{k+\frac{1}{2}, l}^{n+\frac{1}{2}} (p_{k+\frac{1}{2}, l+\frac{1}{2}}^{-n+1} + p_{k+\frac{1}{2}, l+\frac{1}{2}}^{-n} - p_{k+\frac{1}{2}, l-\frac{1}{2}}^{-n+1} - p_{k+\frac{1}{2}, l-\frac{1}{2}}^{-n})}{m_{k+\frac{1}{2}, l+\frac{1}{2}}^n + m_{k+\frac{1}{2}, l-\frac{1}{2}}^n}$$

$$u_{k,l+\frac{1}{2}}^{n+1} = u_{k,l+\frac{1}{2}}^n - \frac{\Delta t^{n+\frac{1}{2}} g_{k,l+\frac{1}{2}}^{n+\frac{1}{2}} (\bar{p}_{k+\frac{1}{2},l+\frac{1}{2}}^{n+1} + \bar{p}_{k+\frac{1}{2},l+\frac{1}{2}}^n - \bar{p}_{k-\frac{1}{2},l+\frac{1}{2}}^{n+1} - \bar{p}_{k-\frac{1}{2},l+\frac{1}{2}}^n)}{m_{k+\frac{1}{2},l+\frac{1}{2}}^n + m_{k-\frac{1}{2},l+\frac{1}{2}}^n}$$

$$v_{k+\frac{1}{2},l}^{n+1} = v_{k+\frac{1}{2},l}^n - \frac{\Delta t^{n+\frac{1}{2}} g_{k+\frac{1}{2},l}^{n+\frac{1}{2}} (\bar{p}_{k+\frac{1}{2},l+\frac{1}{2}}^{n+1} + \bar{p}_{k+\frac{1}{2},l+\frac{1}{2}}^n - \bar{p}_{k+\frac{1}{2},l-\frac{1}{2}}^{n+1} - \bar{p}_{k+\frac{1}{2},l-\frac{1}{2}}^n)}{m_{k+\frac{1}{2},l+\frac{1}{2}}^n + m_{k+\frac{1}{2},l-\frac{1}{2}}^n}$$

$$r_{k,l+\frac{1}{2}}^{n+1} = r_{k,l+\frac{1}{2}}^n + \frac{1}{2} \Delta t^{n+\frac{1}{2}} (u_{k,l+\frac{1}{2}}^{n+1} + u_{k,l+\frac{1}{2}}^n)$$

$$z_{k+\frac{1}{2},l}^{n+1} = z_{k+\frac{1}{2},l}^n + \frac{1}{2} \Delta t^{n+\frac{1}{2}} (v_{k+\frac{1}{2},l}^{n+1} + v_{k+\frac{1}{2},l}^n)$$

$$\begin{aligned} \epsilon_{k+\frac{1}{2},l+\frac{1}{2},i}^{n+1} = & \epsilon_{k+\frac{1}{2},l+\frac{1}{2},i}^n - \frac{1}{4} \Delta t^{n+\frac{1}{2}} \left[g_{k+1,l+\frac{1}{2}}^{n+\frac{1}{2}} (u_{k+1,l+\frac{1}{2}}^{n+1} + u_{k+1,l+\frac{1}{2}}^n) \right. \\ & - g_{k,l+\frac{1}{2}}^{n+\frac{1}{2}} (u_{k,l+\frac{1}{2}}^{n+1} + u_{k,l+\frac{1}{2}}^n) \left. \right] + \left[g_{k+\frac{1}{2},l+1}^{n+\frac{1}{2}} (v_{k+\frac{1}{2},l+1}^{n+1} + v_{k+\frac{1}{2},l+1}^n) \right. \\ & - g_{k+\frac{1}{2},l}^{n+\frac{1}{2}} (v_{k+\frac{1}{2},l}^{n+1} + v_{k+\frac{1}{2},l}^n) \left. \right] (\bar{p}_{k+\frac{1}{2},l+\frac{1}{2},i}^{n+1} + \bar{p}_{k+\frac{1}{2},l+\frac{1}{2},i}^n) / m_{k+\frac{1}{2},l+\frac{1}{2},i}^n \end{aligned}$$

In the above equations, $m_{k+\frac{1}{2},l+\frac{1}{2},i}^n$ and $\epsilon_{k+\frac{1}{2},l+\frac{1}{2},i}^n$ are respectively the mass and energy per unit mass of the i^{th} fluid in the $k+\frac{1}{2},l+\frac{1}{2}$ zone,

$m_{k+\frac{1}{2},l+\frac{1}{2}}^n \equiv \sum_i m_{k+\frac{1}{2},l+\frac{1}{2},i}^n$ is the total mass of the zone, and $u_{k,l+\frac{1}{2}}^n$ and

$r_{k,l+\frac{1}{2}}^n$ are the velocity and position of the $k,l+\frac{1}{2}$ zone edge, with $v_{k+\frac{1}{2},l}$ and

$z_{k+\frac{1}{2},l}$ being similar quantities for the $k+\frac{1}{2},l$ edge.

$g_{k,l+\frac{1}{2}}^{n+\frac{1}{2}}$ is a geometrical factor which is essentially the surface area associated with the $k,l+\frac{1}{2}$ zone edge at time $t^{n+\frac{1}{2}}$. For plane symmetry KRAKEN uses:

$$g_{k,l+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{4} [(z_{k+\frac{1}{2},l+1}^{n+1} + z_{k-\frac{1}{2},l+1}^{n+1} + z_{k+\frac{1}{2},l+1}^n + z_{k-\frac{1}{2},l+1}^n) \\ - (z_{k+\frac{1}{2},l}^{n+1} + z_{k-\frac{1}{2},l}^{n+1} + z_{k+\frac{1}{2},l}^n + z_{k-\frac{1}{2},l}^n)]$$

Similar results obtain for $g_{k+\frac{1}{2},l}^{n+\frac{1}{2}}$; the overall accuracy of the calculation is clearly rather insensitive to the time details of the calculation of these factors.

If $p_{k+\frac{1}{2},l+\frac{1}{2},i}$ is the pressure associated with the i^{th} fluid, and we calculate an artificial viscosity $q_{k+\frac{1}{2},l+\frac{1}{2}}$ for the entire zone [KRAKEN uses a Richtmeyer-Von Neumann type "q" with mass density equal to the mass of the entire zone divided by its volume], then:

$$p_{k+\frac{1}{2},l+\frac{1}{2},i}^n \equiv p_{k+\frac{1}{2},l+\frac{1}{2},i}^n + (m_{k+\frac{1}{2},l+\frac{1}{2},i}/m_{k+\frac{1}{2},l+\frac{1}{2}}) q_{k+\frac{1}{2},l+\frac{1}{2}}^n$$

and:

$$p_{k+\frac{1}{2},l+\frac{1}{2}}^n \equiv \sum_i f_{k+\frac{1}{2},l+\frac{1}{2},i}^n p_{k+\frac{1}{2},l+\frac{1}{2},i}^n + \rho_{k+\frac{1}{2},l+\frac{1}{2}}^n$$

where $f_{k+\frac{1}{2},l+\frac{1}{2},i}$ is the fraction of the total volume of the zone $v_{k+\frac{1}{2},l+\frac{1}{2}}$ occupied by fluid i . The obvious choice (given $f_{k+\frac{1}{2},l+\frac{1}{2},i}^n$) for the density to be used in the equation of state is:

$$\rho_{k+\frac{1}{2},l+\frac{1}{2},i}^n = m_{k+\frac{1}{2},l+\frac{1}{2},i} / (f_{k+\frac{1}{2},l+\frac{1}{2},i}^n v_{k+\frac{1}{2},l+\frac{1}{2}}^n)$$

and the equation of state gives $p_{k+\frac{1}{2},l+\frac{1}{2},i}$ as a function of $\rho_{k+\frac{1}{2},l+\frac{1}{2},i}$ and $\epsilon_{k+\frac{1}{2},l+\frac{1}{2},i}$.

$v_{k+\frac{1}{2},l+\frac{1}{2}}$ is to be computed for rectangular cross sections using the appropriate values of $r_{k,l+\frac{1}{2}}$ and $z_{k+\frac{1}{2},l}$. For example, for axial symmetry we have (per radian);

$$v_{k+\frac{1}{2},l+\frac{1}{2}}^{n+1} = \frac{1}{2}[(r_{k+1,l+\frac{1}{2}}^{n+1})^2 - (r_{k,l+\frac{1}{2}}^{n+1})^2](z_{k+\frac{1}{2},l+1}^{n+1} - z_{k+\frac{1}{2},l}^{n+1})$$

Note that, in effect, corners of the zones may "overlap" at time t^{n+1} .

(This makes no difference, since this is not an ordinary Lagrange calculation anyway ...)

The above equations conserve total energy and the axial component of momentum (also the "r" component in plane symmetry). This can be seen by comparing the quantities

$$m_{k+\frac{1}{2},l+\frac{1}{2}}[\frac{1}{2}(u_{k+1,l+\frac{1}{2}}^2 + u_{k,l+\frac{1}{2}}^2 + v_{k+\frac{1}{2},l+1}^2 + v_{k+\frac{1}{2},l}^2) + \epsilon_{k+\frac{1}{2},l+\frac{1}{2}}]$$

and

$$\frac{1}{2}m_{k+\frac{1}{2},l+\frac{1}{2}}(v_{k+\frac{1}{2},l+1} + v_{k+\frac{1}{2},l})$$

at times t^n and t^{n+1} , summed over all (k,l) neglecting end point contributions and observing that they are the same.[†]

Except for the specification of $f_{k+\frac{1}{2},l+\frac{1}{2},i}^{n+1}$ the above set of equations is essentially complete. They are formally implicit, but in practice we start with $\bar{p}^{n+1} \rightarrow \bar{p}^n$, and easily obtain $\bar{p}^{n+1}$ correct to first order in Δt . A second pass through the equations using this approximation consistently everywhere is sufficient to give all necessary quantities correct to second order in Δt . This procedure is effectively explicit and can be shown to be conditionally stable with the usual Courant stability limit.

In PIC-like codes, material interface position information is carried by the particles, so that "fundamental" fractional volumes $f_{k+\frac{1}{2},l+\frac{1}{2}}^n$ are not

[†] Good Momentum and energy conservation insures satisfaction of the jump conditions across a shock front.

necessary, and it is not an unreasonable approximation to adjust the fractional volumes so that all the material pressures in a zone are equal. (This of course determines the $f_{k+\frac{1}{2}, l+\frac{1}{2}}$). This will not work in our situation, however, as can easily be seen in the case of one material and a vacuum. Here the troublesome "Eulerian mass diffusion" problem is not helped at all.

Actually, if the pressures in a zone are not in equilibrium at time t^n , they cannot possibly reach equilibrium by time t^{n+1} , since this would require at least a few passages of sound waves across the zone, which is impossible because of the Courant condition even in the zone which has the highest sound speed!

In KRAKEN, we take the simplest approximation for $f_{k+\frac{1}{2}, l+\frac{1}{2}}^{n+1}$; it is the "constant divergence approximation":

$$f_{k+\frac{1}{2}, l+\frac{1}{2}}^{n+1} = f_{k+\frac{1}{2}, l+\frac{1}{2}}^n$$

Obviously, this approximation can give completely unphysical behavior on the sub-zone level under certain conditions. For example, if all velocities on the edges of a zone vanish, equilibrium will never be achieved because nothing happens. I think there ought to be ways of correcting such pathological behavior by doing minor amounts of hydrodynamics on the sub-zone level. In the present version of KRAKEN, this had to be done only in the special case where one of the materials was a vacuum. The details are uninteresting; almost anything that insures that equilibrium is not approached too slowly or too rapidly seems to work ... The important point is that this is not a really major correction; "pathological" behavior seems to be confined to the sub-zone level.

This completes the Lagrangian phase. The velocities for advection are

$$u_{k,l+\frac{1}{2}}^{n+\frac{1}{2}} \equiv \frac{1}{2}(u_{k,l+\frac{1}{2}}^{n+1} + u_{k,l+\frac{1}{2}}^n)$$

$$v_{k+\frac{1}{2},l}^{n+\frac{1}{2}} \equiv \frac{1}{2}(v_{k+\frac{1}{2},l}^{n+1} + v_{k+\frac{1}{2},l}^n)$$

R(ΔT). The Advection (Transport) Phase

In computing advection in a given direction, all contributions due to advection in the other direction are suppressed.

For advection in the r -direction, then, we consider only mass flow across the zone edges at $k, l+\frac{1}{2}$ and $k+1, l+\frac{1}{2}$.

Let us consider a multifluid zone and fix our attention on (say) the i^{th} fluid at time t^n where no fluid motion has yet been taken into account. KRAKEN uses the approximation that the interface between fluid i and all other fluids is given by a single straight line which divides the zone into fractional areas f_i and $1-f_i$. The slope of the line is determined by fitting single straight lines to give the correct fractional areas f_i in the zone in question together with selected neighbor* zones. Either one or two neighbor zones are used to determine the slope; if two zones are used, the appropriate slope angles are averaged. If only one neighbor zone is used, the slope and the line itself are determined simultaneously. A very simple case is shown below:

* "Neighbor" zones are zones having a side in common with the zone of interest.

The exact details of these calculations are mostly rather tedious but straightforward plane geometry, except for the essentially heuristic techniques of determining which neighbor zones to consider and distinguishing cases like the one above from ones with f_i and f_i' at the top of the drawing. These parts of the code are also being completely revised, and will not be given here.

It should be noted also that for axial symmetry we often substitute the known fractional volume f_i for the "correct" but actually unknown fractional area. Except for the one or two zones immediately adjacent to the axis, this does not entail significant error. (It is also a miserable mess if you don't do it.)

Once the appropriate straight line interface has been obtained at time t^n , volume advection is effected by moving the zone edges distances given by $\tilde{u}^{n+1/2} \Delta t$, treating the interface as if it were drawn on an elastic sheet which is stretched just as the zone stretches.

This sketch shows a situation where all the $\tilde{u}$ are positive. By comparing the overlap of the new configuration with the old, we see that the fractional area of fluid i moved across the k^{th} grid line is given by the shaded area divided by $[\tilde{u}_k^{n+1/2} \Delta t]$. That is, this effective aperture $h_{n,i}$ is given by $\Delta A_{k,i} / [\tilde{u}_k^{n+1/2} \Delta t] \cdot \Delta z$ where $\Delta A_{k,i}$ is the overlap area.

Let δV_k be the total volume advected across the k^{th} grid line, and let $V'_{k+1/2}$ be the original ("Eulerian") volume of the zone. Then the "r-Lagrangian"

* Zone-edge motion with velocity $\tilde{u}$ in the r-direction only; z-direction motion suppressed.

volume of the ("stretched") zone is related to $V'_{k+\frac{1}{2}}$ by:

$$V'_{k+\frac{1}{2}} = V_{k+\frac{1}{2}} - (\delta V_{k+1} - \delta V_k)$$

[Note that both ℓ and n (time) indexes are suppressed. The time index does not contribute much to clarity here ...].

Then the post-advection fractional volume $f'_{k+\frac{1}{2},i}$ is given by:

$$f'_{k+\frac{1}{2},i} = [f_{k+\frac{1}{2},i} V_{k+\frac{1}{2}} - (h_{k+1,i} \delta V_{k+1} - h_{k,i} \delta V_k)] / V'_{k+\frac{1}{2}}$$

It is important that we have $\sum_i f'_{k+\frac{1}{2},i} = 1$; this will be maintained if $\sum_i h_{k,i} = 1$, which constitutes a constraint on the $h_{k,i}$ that must be forced by some means or other. Another constraint is that every $h_{k,i}$ must not be so large as to remove more volume of fluid i from a zone than was there to begin with. Both these constraints are taken into account in KRAKEN.

The next step is mass advection. The mass of material i moved from the $k-\frac{1}{2}$ zone to the $k+\frac{1}{2}$ zone across zone boundary k is given by:

$$\delta m_{k,i} = \frac{1}{2} h_{k,i} \delta V_k [(\rho_{k+\frac{1}{2},i} + \rho_{k-\frac{1}{2},i}) - w_{k,i} (\rho_{k+\frac{1}{2},i} - \rho_{k-\frac{1}{2},i})]$$

and of course the post-advection mass $m'_{k+\frac{1}{2},i}$ is related to the pre-advection mass $m_{k+\frac{1}{2},i}$ by:

$$m'_{k+\frac{1}{2},i} = m_{k+\frac{1}{2},i} - (\delta m_{k+1,i} - \delta m_{k,i})$$

which gives automatic mass conservation.

In the above equation for $\delta m_{k,i}$, $\rho_{k+\frac{1}{2},i}$ is the "r-Lagrangian" density:

$$\rho_{k+\frac{1}{2},i} = m_{k+\frac{1}{2},i} / (f_{k+\frac{1}{2},i} V_{k+\frac{1}{2}})$$

$w_{k,i}$ is an "interpolation factor" which governs the degree to which the effective density of the material to be transported is to be taken from "ahead" or "behind". In KRAKEN, $w_{k,i}$ is always given at present by the sign of the velocity $u_k^{n+\frac{1}{2}}$ for multifluid zones, corresponding to backward differencing in the density.

$$w_{k,i} = \text{sgn}(\delta V_k) \text{ for multifluid zones.}$$

This corresponds to "first order" accuracy in advection.

For single fluid zones, on the other hand, $w_{k,i}$ may be chosen to be of order $u_k^{n+\frac{1}{2}} \Delta t / \Delta r$, which gives formal second order accuracy. The exact form of $w_{k,i}$ is not uniquely determined; I am presently using:

$$w_{k,i} = \min(1, |h_{k,i} \delta V_i / \min(f'_{k+\frac{1}{2},i} V'_{k+\frac{1}{2}}, f'_{k-\frac{1}{2},i} V'_{k-\frac{1}{2}})|) \text{sgn}(\delta V_i) .$$

This expression is written in a form applicable to multi-fluid zones, as it is intended to be used in future versions of KRAKEN.

The advection of internal energy uses, naturally, the energy per unit mass at the end of the preceding phase; we denote this quantity by $\epsilon_{k+\frac{1}{2},i}$. We use, just as in the mass advection phase:

$$\delta E_{k,i} = \frac{1}{2} \delta m_{k,i} [(\epsilon_{k+\frac{1}{2},i} + \epsilon_{k-\frac{1}{2},i}) - \bar{w}_{k,i} (\epsilon_{k+\frac{1}{2},i} - \epsilon_{k-\frac{1}{2},i})]$$

$$\epsilon'_{k+\frac{1}{2},i} = [m_{k+\frac{1}{2},i} \epsilon_{k+\frac{1}{2},i} - (\delta E_{k+1,i} - \delta E_{k,i})] / m'_{k+\frac{1}{2},i}$$

where now: $\bar{w}_{k,i} = \text{sgn}(\delta m_{k,i})$ for first order or multifluid zones, and

$$w_{k,i} \sim \min(1, |\delta m_{k,i} / \min(m'_{k+1/2,i}, m'_{k-1/2,i})|) \text{sgn}(\delta m_{k,i})$$

for second order.

Rather than the $\delta m_{k,i}$ themselves, the velocity advection phase makes use of the total mass fluxes:

$$\delta m_k = \delta m_{k,l+1/2} \equiv \sum_i \delta m_{k,i}$$

For advection of the r component of velocity, which we denote by u_k , we define a mass flux centered at $k+1/2$:

$$\delta m_{k+1/2} \equiv \frac{1}{2}(\delta m_{k+1} + \delta m_k).$$

Then the flux of the r component of momentum is given by:

$$\delta M_{k+1/2} = \frac{1}{2} \delta m_{k+1/2} [(u_{k+1} + u_k) - w_{k+1/2}(u_{k+1} - u_k)]$$

and, defining:

$$\begin{cases} m_k \equiv \frac{1}{2}(m_{k+1/2} + m_{k-1/2}) \\ m'_k \equiv \frac{1}{2}(m'_{k+1/2} + m'_{k-1/2}) \end{cases}$$

we have:

$$u'_k = [m_k u_k - (\delta M_{k+1/2} - \delta M_{k-1/2})] / m'_k$$

Again, we could use for second order accuracy:

$$w_{k+\frac{1}{2}} = \min[1, |\delta m_{k+\frac{1}{2}} / \min(m'_{k+1}, m'_k)|] \operatorname{sgn}(\delta m_{k+\frac{1}{2}})$$

or just $w_{k+\frac{1}{2}} = \operatorname{sgn}(\delta m_{k+\frac{1}{2}})$ for first order accuracy. Momentum is conserved assuming material cannot flow out of boundary zones with fixed outer edges.

It should perhaps be noted that if the above expression for u'_k is to give $u'_k = u_k \equiv u_0$ for a (spatially) constant velocity field (as it clearly ought to), then the form of $\delta m_{k+\frac{1}{2}}$ is uniquely determined. To see this, we put $u'_k = u_k = u_0$ and get:

$$\delta M_{k+\frac{1}{2}} = \delta m_{k+\frac{1}{2}} u_0$$

and:

$$m'_k u_0 = m_k u_0 - (\delta M_{k+\frac{1}{2}} - \delta M_{k-\frac{1}{2}})$$

or:

$$[m_k - \frac{1}{2}(\delta m_{k+1} - \delta m_{k-1})] u_0 = m_k u_0 - (\delta m_{k+\frac{1}{2}} - \delta m_{k-\frac{1}{2}}) u_0$$

so:

$$\delta m_{k+\frac{1}{2}} - \delta m_{k-\frac{1}{2}} = \frac{1}{2}(\delta m_{k+1} - \delta m_{k-1})$$

The appropriate solution of this difference equation is precisely:

$$\delta m_{k+\frac{1}{2}} = \frac{1}{2}(\delta m_{k+1} + \delta m_k)$$

Note that momentum is conserved by the preceding equations as matter having different velocities is merged; this is much like an inelastic collision. It is, in fact, exactly the same kind of thing you get in PIC; kinetic energy disappears in the momentum advection process, and must be compensated for in the internal energy if total energy conservation is to be maintained. In PIC, velocity advection is first order since all the particles in a zone are given a common velocity, and velocities are zone centered. This makes the energy correction formula very simple.

Here, however, we are using an interpolated velocity formula and a staggered grid, so the energy formula is not nearly as nice; it is also quite tedious to derive. It is, for the contribution of the r component:

$$\epsilon_{k+\frac{1}{2}}'' = \epsilon_{k+\frac{1}{2}}' + a_{k+1} + a_k + b_{k+\frac{1}{2}}$$

where we write $p_{k+\frac{1}{2}} \equiv \delta m_{k+\frac{1}{2}}(u_{k+1} - u_k)$ and

$$a_k \equiv \frac{[(p_{k+\frac{1}{2}} - p_{k-\frac{1}{2}})^2 + 2(w_{k+\frac{1}{2}} - w_{k-\frac{1}{2}}) p_{k+\frac{1}{2}} p_{k-\frac{1}{2}} - (w_{k+\frac{1}{2}} p_{k+\frac{1}{2}} - w_{k-\frac{1}{2}} p_{k-\frac{1}{2}})^2]}{(4m_k')^2}$$

$$b_{k+\frac{1}{2}} \equiv [w_{k+\frac{1}{2}}(2m_{k+1}'m_k' + (m_{k+1}' - m_k') \delta m_{k+\frac{1}{2}}) - (m_{k+1}' + m_k') \delta m_{k+\frac{1}{2}}] \\ \cdot [\delta m_{k+\frac{1}{2}}(u_{k+1} - u_k)^2] / (4m_{k+1}'m_k'm_{k+\frac{1}{2}}')$$

Notice that a_k is always of order Δt^2 , and will usually be quite small, thought not negligible. Evidently $w_{k+\frac{1}{2}}$ can be chosen to make $b_{k+\frac{1}{2}}$ identically zero; this gives an expression for $w_{k+\frac{1}{2}}$ which was used in KRAKEN for awhile but was found to be somewhat marginal with respect to stability, so a slightly more conservative form was introduced.

Note that if we have $u_k \geq 0$ everywhere and first order so that $w_{k+\frac{1}{2}} = 1$, we get

$$a_k = 0 \\ b_k = \left[1 - \frac{\delta m_{k+\frac{1}{2}}}{m_{k+1}'} \right] \cdot \left[\frac{1}{2} \delta m_{k+\frac{1}{2}} (u_{k+1} - u_k)^2 \right] / m_{k+\frac{1}{2}}'$$

For small $\delta m_{k+\frac{1}{2}}$, this resembles an inelastic collision energy change expression, it also looks like the contribution to the internal energy of a velocity-dependent linear viscosity. The primary effect of second order velocity advection is the removal of such undesirable hidden damping terms in the momentum equation.

Similarly, for advection of the z component of velocity due to motion in the r direction, we restore the l index and write:

$$\delta m_k \equiv \delta m_{k,l} = \frac{1}{2}(\delta m_{k,l+\frac{1}{2}} + \delta m_{k,l-\frac{1}{2}})$$

Then, for the z component (and l index suppressed again):

$$\delta M_k = \frac{1}{2} \delta m_k [(v_{k+\frac{1}{2}} + v_{k-\frac{1}{2}}) - w_k^* (v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}})]$$

and:

$$v'_{k+\frac{1}{2}} = [m_{k+\frac{1}{2}} v_{k+\frac{1}{2}} - (\delta M_{k+1} - \delta M_k)] / m'_{k+\frac{1}{2}}$$

where:

$$\begin{cases} m_{k+\frac{1}{2}} \equiv \frac{1}{2}(m_{k+\frac{1}{2},l+\frac{1}{2}} + m_{k+\frac{1}{2},l-\frac{1}{2}}) \\ m'_{k+\frac{1}{2}} \equiv \frac{1}{2}(m'_{k+\frac{1}{2},l+\frac{1}{2}} + m'_{k+\frac{1}{2},l-\frac{1}{2}}) \end{cases}$$

and w_k^* is obtained in the same way as for the r component.

Energy change due to r-direction advection of z component of velocity.

$$\epsilon_{k+\frac{1}{2},l+\frac{1}{2}}''' = \epsilon_{k+\frac{1}{2},l+\frac{1}{2}}'' + c_{k+\frac{1}{2},l} + c_{k+\frac{1}{2},l+1}$$

$$c_{k+\frac{1}{2},l} \equiv a_{k+\frac{1}{2}} + b_{k+1} + b_k$$

where, with all l indexes equal to l but suppressed:

$$p_k \equiv \delta m_k (v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}})$$

$$a_{k+\frac{1}{2}} = [(p_{k+1} - p_k)^2 + 2(w_{k+1}^* - w_k^*) p_{k+1} p_k$$

$$- (w_{k+1}^* p_{k+1} - w_k^* p_k)^2] / (4m_{k+\frac{1}{2}}')^2$$

$$b_k = [w_k^* \left\{ 2m_{k+\frac{1}{2}}' m_{k-\frac{1}{2}}' + (m_{k+\frac{1}{2}}' - m_{k-\frac{1}{2}}') \delta m_k \right\} - (m_{k+\frac{1}{2}}' + m_{k-\frac{1}{2}}') \delta m_k]$$

$$\cdot [\delta m_k (v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}})^2] / [4m_{k+\frac{1}{2}}' m_{k-\frac{1}{2}}' (m_{k+\frac{1}{2}}' + m_{k-\frac{1}{2}}')]$$

This completes $R(\Delta t)$. The results of $R(\frac{1}{2}\Delta t)$ are the input to $Z(\Delta t)$ etc.

One of the "nice" things about KRAKEN is its rather straightforward approach to differencing. Despite certain points of fuzziness in this development of the code, the overall structure is fairly well determined and, I hope, comprehensible. It seems to work reasonably well, too. There is, of course, considerable room for improvement, and I hope I have pointed out some of the places in the equations such improvements can be introduced without seriously altering the "skeleton" of the code itself.

One last interesting point is that one can actually advect shells less than a zone thick, though the rest of the hydrodynamics will be inaccurate. This can be done by letting the material index of the shell be (say) j and obtaining $h_{k,j}$ from the expression:

$$h_{k,j} = 1 - \sum_{i \neq j} h_{k,i}$$

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