Final Report

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The results of this project include the development of fast algorithms for solving the steady-state, monoenergetic, linear Boltzman equation in slab geometry. The physical domain is a semi-infinite slab of width $b - a$ in the x dimension. Although three dimensional, the flux of particles is assumed to be independent of the y and z coordinates. Thus, the linear Boltzman equation reduces to

$$\mu \frac{\partial \psi}{\partial x} + \sigma_t \psi - \frac{\sigma_s}{2} \int_{-1}^1 \psi(x, \mu') d\mu' = Q(x, \mu),$$

for $x \in (a, b)$, $\mu \in [-1, 1]$, where $\psi(x, \mu)$ represents the flux of particles at position x traveling at an angle θ from the x -axis ($\mu = \cos(\theta)$). The solution is well defined if the flux of particles entering the slab is given as boundary conditions:

$$\psi(a, \mu) = g_a(\mu), \quad \psi(b, -\mu) = g_b(\mu) \quad \mu \in (0, 1).$$

This project has developed a multigrid in space algorithm for the solution of the S_N equations with isotropic scattering in slab geometry [2] [5]. The algorithm was developed for the Modified Linear Discontinuous (MLD) discretization in space which is accurate in the thick diffusion limit [?]. It uses a red/black two-cell μ -line relaxation. This relaxation solves for all angles on

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two adjacent spatial cells simultaneously. It takes advantage of the rank-one property of the coupling between angles and can perform this inversion in $O(N)$ operations where N is the number of discrete angles.

The MLD scheme approximates the solution by linear elements across each spatial cell. In the thick limit the red/black two-cell μ -line relaxation leaves an error that is independent of angle and continuous up to $O(\frac{1}{\sigma_t h})$. The error is also sublinear across each two-cell pair, that is, the error at the boundary between cells of a two-cell pair is less than the average of the errors at the outer boundaries of the two-cell pair. The size of the kink can be determined analytically [6], but it is more practical to let the relaxation yield the information. In this sense, it is an operator induced interpolation.

The resulting interpolation is a kinked linear interpolation. The restriction used is a full weighting, that is, the transpose of linear interpolation. This restriction and interpolation yields coarse grid equations that are not MLD on the coarse grid. However, the new coarse grid operator can be solved by a recursion of the same relaxation and further grid coarsening. It has the same structure as the MLD operator and is amenable to the same efficient red/black two-cell μ -line relaxation. Each subsequent coarsening is accomplished by a kinked linear interpolation and a full weighting restriction. The product of all of the interpolations from the coarsest grid, which contains only two cells, up to the finest grid can be viewed as kinks on kinks. It resembles the exact solution of a homogeneous equation with isotropic boundary conditions.

The multigrid algorithm is very effective. For $\sigma_t h \gg 1$, the convergence factor is $\rho = O(\frac{1}{\sigma_t h})$. With no absorption the convergence factor is $\rho = O(\frac{1}{(\sigma_t h)^2})$. In the thin limit, that is, $\sigma_t h \ll 1$ the convergence factor is $\rho = O((\sigma_t h)^3)$. The slowest convergence occurs when $\sigma_t h \simeq .01$ on the finest grid and yields $\rho \simeq .01$. We compare this to the DSA algorithm in slab geometry, which has a convergence factor bounded by .23 independent of the size of σ_t . In general, the convergence factor for DSA is between .1 and .23 for $\sigma_t \gg 1$ and all ranges of $\sigma_t h$. Depending on the particular computer architecture, the multigrid algorithm takes 2-4 times as long per iteration, but the extremely fast convergence rates of the multigrid algorithm yield an algorithm that is faster in all regimes. The multigrid algorithm has turned the problem inside out. It is now easier to solve the problem in the thick limit and easiest with no absorption.

A version of the multigrid in space algorithm was programmed on the Thinking Machines Inc. CM-200 located at Los Alamos National Laboratories [3] [4]. The two-cell μ -line relaxation is inherently parallel. It was discovered that on the CM-200 a block Jacobi type iteration was more efficient than the block red/black iteration. Given sufficient processors all two-cell block inversions can be carried out simultaneously with a small number of parallel steps. The bottleneck is the need for sums of N values, where N is the number of discrete angles, each from a different processor. These are carried out by machine intrinsic functions and are well optimized. The overall algorithm has computational complexity $O(\log(M))$, where M is the number of spatial cells. The algorithm is very efficient and represents the state-of-the-art for isotropic problems in slab geometry.

For anisotropic scattering in slab geometry, a multilevel in angle algorithm was developed [7]. This algorithm uses a shifted transport sweep as a relaxation. It has the form,

$$\mu \frac{\partial \psi^{j+1}}{\partial x} + (\sigma_t - \alpha) \psi^{j+1} = (\sigma_s - \alpha) \int_{-1}^1 K(x, \mu' \rightarrow \mu) \psi^j d\mu' + Q,$$

where j is the iteration number. The shift α is chosen to reduce the error in the high Legendre moments. The residual is then projected onto the first $N/2$ Legendre moments. The coarse level correction is the result of solving an $S_{N/2}$ problem with the projected residual as the source. This coarse level problem is solved in the same manner, with a shifted transport sweep followed by a correction from an $S_{N/4}$ problem. The shift parameter changes from level to level and is dependent on material properties. It is chosen to reduce the error in the highest half of the moments at each level. The coarsest level is an S_2 problem. The proper shift yields an isotropic problem that can be solved by the multigrid in space algorithm described above. In this context, one v(1,1)-cycle yields an exact solution of the S_2 problem. The algorithm has a v(1,1)-cycle convergence factor of .36 for highly forward-peaked Fokker-Plank scattering. This is the first algorithm to have a convergence factor bounded away from 1 in the thick Fokker-Plank limit.

A parallel version of the multilevel in angle algorithm has also been developed. Upon first glance, the shifted transport sweep has limited parallelism. Once the right-hand-side has been computed, the sweep is completely parallel in angle, becoming N uncoupled initial value ODE's. It appears that the integration of these ODE's is sequential. However, we have developed a cyclic

reduction algorithm that renders it parallel with complexity $O(\log(M))$. The multilevel in angle algorithm visits $\log(N)$ levels, where shifted transport sweeps are performed. The overall complexity is $O(\log(N)\log(M))$. The algorithm has been coded on the CM-200 and is in the debugging stage.

C. Current Research Plan

Our current focus is on three areas. First, we are extending the multilevel in angle algorithm to two and three dimensional spatial geometries. Since the direction variable is represented by the surface of the unit sphere, these geometries represent 4 and 5 dimensional problems respectively. We believe that the algorithm can be used for both S_N and P_N approximations. The basic algorithm remains unchanged. Shifted transport sweeps will be used to reduce the error in the direction of the higher spherical harmonics. The sweeps are naturally parallel in angle, appearing as uncoupled ODE's. If the discretization is logically rectangular in space, they can again be solved by a cyclic reduction algorithm. The complexity of the sweeps will be $O(\log(M_x)\log(M_y)\log(M_z))$ where M_i represents the number of cells in each spatial coordinate. After the error becomes smooth in the angle variables the residual will be projected onto lower degree spherical harmonics. The number of spherical harmonics will be reduced by approximately 1/4 at each level. This will leave an S_2 or P_1 problem at the coarsest level. The S_2 scattering operator will be rank 4 while the P_1 scattering operator will be rank 3 in two dimensions and rank 4 in three dimensions. Thus, the scattering operator of the S_2 or P_1 problem will have either 3 or 4 eigenvalues, one with value σ_s , and the rest with values less than σ_s . A sequence of shifted transport sweeps with properly chosen shift parameters will leave the error nearly isotropic. This final error can be eliminated through either a multigrid in space algorithm or a diffusion approximation. The overall complexity should be $O(\log(N)\log(M_x)\log(M_y)\log(M_z))$.

Secondly, we are developing a multigrid in space algorithm for isotropic problems in two and three space dimensions discretized with S_N in angle and bilinear or trilinear discontinuous elements on logically rectangular grids in space. Our first approach is an application of the same ideas as in the slab geometry. Now, however, the relaxation will involve solving for all angles on a two-by-two cell patch in two dimensions and a two-by-two-by-two cell cube in three dimensions. The scattering operator remains rank-one, and thus,

the block inversions can be carried out very efficiently. The major issue will be determining the interpolation and restriction operators that define the coarse grid operator. In one dimension, the kinked elements are relatively easy to determine. In two dimensions, for example, visualize a piecewise bilinear function across a two-by-two cell square. In the thick limit, the error after relaxation will be nearly continuous, independent of angle and sublinear. Determining the proper interpolation to match this shape is an area of current research.

The third focus of our project is the construction of difference schemes for isotropic or mildly anisotropic scattering that maintain accuracy in the thick diffusion limit. As mentioned above, the usual approach to singularly perturbed problems is to look at the null space of the limit operator. Let L_{σ_t} represent the Boltzman operator parameterized by σ_t . Let $P = \int d\Omega$ be the projection onto the space of functions independent of Ω , the null space of L_∞ . In the thick limit we have

$$\begin{pmatrix} PL_{\sigma_t}P & PL_{\sigma_t}(I-P) \\ (I-P)L_{\sigma_t}P & (I-P)L_{\sigma_t}(I-P) \end{pmatrix} = \begin{pmatrix} O(\frac{1}{\sigma_t}) & O(1) \\ O(1) & O(\sigma_t) \end{pmatrix}.$$

Here the block structure of the operator corresponds to the subspace of functions independent of Ω and its orthogonal complement. The dominant term in the inverse is the Schur compliment of the dominant term in the array above:

$$[PL_{\sigma_t}P - PL_{\sigma_t}(I-P)[(I-P)L_{\sigma_t}(I-P)]^{-1}(I-P)L_{\sigma_t}P]^{-1} = O(\frac{1}{\sigma_t}).$$

The difficulty begins when L_{σ_t} is discretized. The truncation errors of the discrete analogues of the above terms must balance in a precise way in order to preserve the correct behavior in the limit.

Consider the scaling $P + \frac{1}{\sigma_t}(I-P)$. It is easily applied and easily inverted. The scaled operator

$$\hat{L}_{\sigma_t} = (P + \frac{1}{\sigma_t}(I-P))L_{\sigma_t}(P + \frac{1}{\sigma_t}(I-P))$$

is not singular in the thick limit. It is somewhat more complicated than L_{σ_t} , but not excessively. In homogeneous material, that is, for smooth σ_t , many

difference schemes will yield an accurate solution, which can be unscaled to yield an accurate solution to the unscaled problem.

This approach has been analyzed for isotropic scattering in homogeneous material in slab geometry and the results are very promising. Simple schemes like upwind differencing and piecewise linear continuous finite elements applied to the scaled problem yield unscaled solutions with accurate solutions independent of σ_t . A potential hurdle is the possibility of discontinuous σ_t , which may result from nonhomogeneous material. We believe that this difficulty can be overcome by prescribing jump conditions in the scaled solution across material interfaces. We hope this approach will lead to a formalism for constructing discretization schemes that are accurate in the thick limit.

D. Software Development Plan

A major thrust of this project is the implementation of the resulting algorithms in software, both on advanced architecture computers and in production codes. This will require continued close cooperation with Jim Morel at LANL and Milo Dorr at LLNL. Our development plans include the following:

1. Complete the parallel implementation of the multilevel in angle and multigrid in space algorithms for slab geometry on the CM-200 at Los Alamos. Vectorize the serial versions for the Cray Y/MP and perform a study of the relative efficiencies of the parallel and serial versions.
2. Implement the multilevel in angle code in the 2-dimensional anisotropic production code NIKE that is under development at Los Alamos. This code will use either S_N or P_N in angle and bilinear discontinuous finite elements in space. On the coarsest level the isotropic problem will be solved by either a multigrid in space or a diffusion approximation.
3. Implement the 2-dimensional multilevel in angle algorithm on the CM-200. The shifted transport sweeps will be performed by parallel cyclic reduction.
4. Develop a code for coupled electron-photon transport in slab geometry. The code will use S_N in angle and Linear Discontinuous (LD)

discretization in space. The serial versions of the slab geometry codes described above will be an integral part. We will use scattering cross-section files from the production code ADEPT (formerly CEPXS/1LD) developed at Sandia National Laboratories. This will allow our code to do actual production calculations. We hope to demonstrate marked superiority in performance over existing production codes. We will target the resulting code for workstations and mainframes like the Cray Y/MP.

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