Fast Algorithms for Transport Models
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The focus of this project is the study of multigrid and multilevel algorithms for the numerical solution of Boltzmann models of the transport of neutral and charged particles. In previous work a fast multigrid algorithm was developed for the numerical solution of the Boltzmann model of neutral particle transport in slab geometry assuming isotropic scattering [1], [2]. The new algorithm is extremely fast in the thick diffusion limit; the multigrid v-cycle convergence factor approaches zero as the mean-free-path between collisions approaches zero, independent of the mesh. Also, a fast multilevel method was developed for the numerical solution of the Boltzmann model of charged particle transport in the thick Fokker-Planck limit for slab geometry [4]. Parallel implementations were developed for both algorithms [3].

In the one year of this project, a reformulation of the numerical solution of the Boltzmann model was developed. In order to avoid ray effects that usually accompany S_n angular discretizations, P_n angular discretizations were considered, that is, the angular dependence was assumed to be described by the first n levels of spherical harmonics. A semi-discrete system of equations is established by enforcing a Galerkin condition on the residual equation; the residual is required to be orthogonal to the first n levels of spherical harmonics.

In the past spatial discretization was usually achieved through finite difference approximation or finite element approximation by enforcing a Galerkin condition. Much difficulty was encountered in developing discrete approximations that behave properly in the thick limits, that is, when the mean-free-path between collisions becomes small compared to the physical dimensions of the problem.

This project has developed a scaled least-squares functional approach that avoids this difficulty. In brief, the stationary, mono-energetic Boltzmann

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equation with isotropic scattering can be written as

$$\underline{\Omega} \cdot \nabla \psi + \sigma_t \psi - \sigma_s P \psi = q$$

where ψ represents the flux of particles at a position $\underline{x}$ in the direction $\underline{\Omega}$, σ_t and σ_s are the total collision cross section and scattering cross section respectively and

$$P \psi = \frac{1}{4\pi} \int \psi d\underline{\Omega}$$

is the projection onto the subspace of functions independent of direction.

Consider the scaling operator and its inverse

$$\begin{aligned} S &= P + \epsilon(I - P) \\ S^{-1} &= P + \frac{1}{\epsilon}(I - P). \end{aligned}$$

In the presence of absorption, that is, $\sigma_a \equiv \sigma_t - \sigma_s > 0$, the parameter $\epsilon = \sqrt{\sigma_a/\sigma_t}$. With no absorption, the slightly modified value, $\epsilon = \sqrt{\sigma_a/\sigma_t + 1/\sigma_t^2}$ is used.

Next, define the operator

$$Q = \frac{1}{\epsilon} S \underline{\Omega} \cdot S$$

and the scalars

$$a = \frac{\sigma_t - \sigma_s}{\epsilon}, \quad b = \sigma_s \epsilon.$$

Let $\hat{\psi} = S^{-1} \psi$ be a scaled flux, $\hat{q} = S q$ be the scaled source and define the functional

$$G(\hat{\psi}; \hat{q}) = \int \int (Q \nabla \hat{\psi} + a P \hat{\psi} + b(I - P) \hat{\psi} - \hat{q})^2 d\underline{x} d\underline{\Omega}.$$

The major result of this project has been to prove that the functional G is V -elliptic with respect to the norm

$$\|\hat{\psi}\|_V \equiv (\|Q \nabla \hat{\psi}\|_0^2 + \|\hat{\psi}\|_0^2)^{1/2},$$

independent of σ_t .

This result has several important implications. The solution of the Boltzmann equation can be found as the minimum of the functional G over the

space V defined by the closure of C^∞ , with proper boundary conditions, in the V -norm. Consider finite element subspaces of V consisting of the spherical harmonics tensored with simple spatial finite elements. The following results have been established:

1. Simple finite element approximations to the minimum of G yield optimally accurate approximations to $\hat{\psi}$ in the V -norm, independent of σ_t .
2. Accurate approximations of $\hat{\psi}$ in the V -norm yield accurate approximations to ψ in a modified H^1 norm, independent of σ_t .
3. Minimization of the functional G on simple finite element subspaces is especially amenable to multilevel techniques. In particular, a full multigrid algorithm can be used to achieve an approximate discrete solution to the level of truncation error in an amount of work equal to half a dozen sweeps of the finest grid.
4. Adaptive refinement is especially easy to implement in this context and equally amenable to solution by the full multigrid algorithm.

Thus, a new problem formulation has been developed that yields optimally accurate discrete approximate solutions independent of σ_t that are easily calculated numerically. Numerical results demonstrating the efficacy of this approach as well as the theoretical details have been published in [5].

References

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