COUPLED ELECTRON-PHOTON RADIATION TRANSPORT

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ABSTRACT

Massively-parallel computers allow detailed 3D radiation transport simulations to be performed to analyze the response of complex systems to radiation. This has been recently been demonstrated with the coupled electron-photon Monte Carlo code, ITS. To enable such calculations, the combinatorial geometry capability of ITS was improved. For greater geometrical flexibility, a version of ITS is under development that can track particles in CAD geometries. Deterministic radiation transport codes that utilize an unstructured spatial mesh are also being devised. For electron transport, we are investigating second-order forms of the transport equations which, when discretized, yield symmetric positive definite matrices. A novel parallelization strategy, simultaneously solving for spatial and angular unknowns, has been applied to the even- and odd-parity forms of the transport equation on a 2D unstructured spatial mesh. Another second-order form, the self-adjoint angular flux transport equation, also shows promise for electron transport.

1. INTRODUCTION

The transport of X-ray and electron radiation is the necessary first step in predicting the response of complex systems such as satellites to natural and man-made radiation environments. At Sandia National Laboratories, multi-dimensional coupled electron-photon transport codes have been, and continue to be, developed for this purpose. Both Monte Carlo and deterministic radiation transport codes are needed to calculate a wide variety of radiation effects. Under the Department of Energy's Accelerated Strategic Computing Initiative (ASCI), these coupled electron-photon transport codes are being designed to operate on massively-parallel computers capable of a performing a trillion floating point operations per second (TeraOp speed). To better model complex systems, the radiation transport codes need to utilize CAD geometries. New Monte Carlo codes are required to track particles in such geometries. New deterministic transport codes are also

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needed to utilize the unstructured spatial mesh produced from a CAD model by meshing software.

2. MONTE CARLO TRANSPORT DEVELOPMENT

The Integrated-Tiger-Series (ITS) Monte Carlo radiation transport code[1] has recently been used to assess the radiation hardness of a complex system. The goal of this effort was to predict the mechanical shock induced by radiation. ITS was used to predict the energy deposition throughout a device from radiation. This information served as the initial condition for a shock-physics code that determined the mechanical response.

For these calculations, the device itself plus the surrounding structures must be included in the model. These detailed models were created by the combinatorial geometry (CG) method already present in ITS. In CG, structures are built using Boolean operations on a set of simple body types (sphere, box, cylinder, etc.) For a reliable description of the device geometry, the CG option in Version 3.0 of ITS was extended to include the torus body type.

Calculations were also performed with a multigroup version of ITS with adjoint transport capability[2,3]. In adjoint transport mode, a single calculation can predict the radiation response at a location (point or volume) from all possible exposure angles. Typically a set of such points and volumes are examined. For visual display of the response, the phase space of exposure angles is represented as the surface of a unit sphere. The polar and azimuthal tally boundaries are generated so that the tally bins represent equally-sized solid angles (typically, over 8000 such bins were employed.) The result of each tally is the dose to the specified locality for a plane-wave source (actually, an average due to plane wave sources within the solid angle.)

Without TeraOp computers, the response of complex systems to radiation could not be predicted. The adjoint Monte Carlo calculations, requiring ~ 1000 processor-hours, could not be routinely performed without a parallelized code. The forward Monte Carlo calculations, in which the detailed dose distribution throughout the device is determined, required ~ 50,000 processor-hours, and would have been completely impossible. These calculations were performed on the massively-parallel distributed-memory computer at Sandia called ASCI-Red. At the time these calculations were performed, the machine consisted of 4500 computational processors capable of 1.3 TeraOps. Originally, each processor of ASCI-Red had 128 Mbytes of RAM, which has since been expanded to 256 MB. The message latency on ASCI-Red has been established to be 30 microseconds.

Provided the problem description can be stored on each processor, Monte Carlo calculations can be parallelized with high efficiency on a distributed-memory parallel computer.[4,5] On such machines, we now prefer Message-Passing Interface (MPI) instead of NX or PVM. Since the portable random number generator of ITS 3.0 has too short a period[6], the RANMAR algorithm[7] was implemented for the massively-parallel calculations. It appears to be well behaved for our recent ASCI application. For example,

adjoint and forward calculations are in good agreement. However, we will continue to implement more robust random number generators in our Monte Carlo codes for future applications.

To obtain dose profiles in 3D geometries, the body-based subzoning option in ITS 3.0 can be used. The user specifies the number of equal bins in each of three natural body-based coordinates for a particular zone. That zone is then divided into separate subzones (smaller volumes) for tally purposes only. However, the subzoning capability of ITS 3.0 is very restrictive, existing only for zones which are described by a single simple body. Modifications to ITS 3.0 had been developed for simple cylindrical shells[8]. For our recent ASCI application, shell sub-zoning has been made more general (e.g., toroidal shell, sphere with a cylindrical hole, etc.). For visualization, we have also added a capability to ITS to map the output into a finite-element hexahedral format (some curved surfaces of sub-zones must be squared off in this technique). Expressing the data in this form also allows the information to be used by a finite-element shock-physics code. For complete generality, the user can now specify any of the above-mentioned subzone structures as an overlay on an arbitrarily-shaped zone for tallying purposes.

A considerable effort went into the creation and refinement of the CG models utilized by ITS. Although CG is highly computationally efficient, it suffers from two limitations. First, CG models can only represent certain surface types. Second, a separate CG model must be constructed independently of CAD models created for shock-physics analysis. The necessity of creating and maintaining two separate models of the device can insert significant delays into the radiation hardness analysis process, especially if the CAD model is repeatedly altered during design and production.

A developmental effort is underway to directly utilize CAD geometries within ITS. ACIS[9] was chosen as the CAD format since it is already in use as part of the input to meshing software employed at Sandia National Laboratories. In the current implementation within ITS, the pre-existing Fortran 77 code handles transport physics and radiation sources. A C++ main() wraps the Fortran functionality, and all geometry queries for tracking purposes are performed in C++ through ACIS modeler operations. Fortran-callable C++ functions allow the results of these queries to be passed to the legacy code. Additionally, all assemblies, subassemblies, and parts are organized into Sandia-proprietary C++ class hierarchies.

Major issues encountered in developing a CAD version of ITS are:
(1) Efficiency – Surface-intersection algorithms are computationally more expensive with boundary representation models than with CG, for which analytical solutions are possible. Some techniques that have been developed to make the code more efficient include part/assembly bounding volumes, heterogeneous grids that encompass the model space, and "learning" technology.
(2) Accuracy – Boundary representation modelers define relative and absolute numerical tolerances for model entities so that the modelers can determine when surface edges coincide, when coordinate points lie on a part surface, etc. Therefore, since part surfaces

have a finite thickness, each particle propagating through an ACIS model has a small statistical probability of landing on the boundary of a part. Presently, this state is considered indeterminant, and the particle history is rejected. If modeler tolerances are too loose, particle rejections occur too often, affecting the accuracy of the simulation results.

3. DETERMINISTIC TRANSPORT DEVELOPMENT

In order to assess the radiation hardness of electronics, deterministic radiation transport codes are needed to calculate multi-dimensional charge deposition profiles and photon-induced electron emission to high-precision. For this purpose, the deterministic CEPTRE code (Coupled Electron-Photon Transport for Radiation Effects) is being created. The code is being designed to solve, on massively-parallel platforms, the Boltzmann transport equation on an unstructured spatial mesh (which can be generated by other software from CAD models.) Although the emphasis is on electron transport, the solution methods that are being developed can also be applied to neutral-particle transport.

Algorithms are being investigated with 1D and 2D prototypes. The goal is to create a 3D version of CEPTRE using features developed and studied in the prototypes. These codes solve second-order forms of the Boltzmann transport equation. The 2D prototype employs the traditional even- and odd- parity equations[10] while the 1D prototype solves the self-adjoint angular flux (SAAF) equation[11]. Either approach yields a symmetric, positive definite matrix equation that is ideally suited for parallel computing architectures. In both prototypes, the multigroup-Legendre expansion and discrete-ordinates approximations are used to treat the energy and directional dependencies, respectively.

The 2D CEPTRE prototype has these additional characteristics[12-13]:

(1) The spatial dependence is discretized on an unstructured mesh using the Galerkin finite-element method. The elements can be either triangles or quadrilateral. Both continuous and quadratic linear finite elements are employed.
(2) The standard outer iteration strategy is applied for solving the energy dependence of the discretized system. However, the space-direction dependence for each energy group is solved simultaneously using a parallel conjugate gradient solver. This eliminates the need for the conventional within-group source iteration (inner iteration) and is well suited for massively-parallel computers.
(3) Spatial-domain decomposition strategy is used to achieve high parallel efficiency. To reduce both memory and computational cost, we employ a simple strategy. We divide the spatial nodes evenly among all the processors and then partition the global matrix system accordingly. Construction and storage of the partitioned system are done locally on each processor (each processor has sufficient information to construct the distributed global matrix system independently). In the future, for very large multi-dimensional problems, we intend to incorporate more advanced software to produce a balanced partition between the finite-element nodes and the processors to reduce communication overhead.

(4) A neutral-particle form of the transport equation is used. That is, the continuous slowing down (CSD) term that is unique to charged-particle transport does not appear in the equation. Such neutral-particle forms of the transport equation can be employed for electron transport if special electron cross sections are used. For this prototype, the Goudsmit-Saunderson (G-S) modified electron cross sections are used.[14]

The aforementioned solution method provides good parallel efficiency[15]. The 2D prototype was tested on an unstructured triangular spatial mesh consisting of 10,201 nodes. The test problem was mono-energetic. Solutions were obtained with three different quadrature orders, S_8, S_{12}, and S_{16}, with 20, 42, and 72 discrete directions, respectively. For a given number of processors (512 processors on ASCI-Red), the larger the problem size the better the parallel efficiency. The speed-ups correspond to a parallel efficiency of 50% for the S_8 calculation and 90% for the S_{16} calculation. Since the conjugate gradient iterations can converge slowly, preconditioners are used to accelerate the iterations. However, the efficiency of the conjugate gradient iteration is excellent for electron transport, as these problems typically include a large removal term on the matrix diagonal. We have also investigated the convergence rate of the error due to the spatial discretization for selected test problems where the analytical solutions are available. As expected, the linear and quadratic elements provide nearly quadratic and cubic convergence, respectively.

The 1D prototype under development is based on the SAAF form of the second-order Boltzmann transport equation. The efficacy of the SAAF formulation for neutral particle transport has been recently demonstrated by Morel.[11] This equation offers a number of advantages over the even- and odd-parity approach: the angular flux is directly calculated and construction of reflective boundary conditions is straightforward. Our work has focused on extending the SAAF formulation to include the CSD operator in the solution algorithm for coupled electron-photon calculations. This will enable us to perform more accurate electron transport calculations than is possible with G-S modified electron cross sections.

The SAAF formulation is derived starting with the first-order form of the transport equation for coupled electron-photon transport that includes CSD:

$$\Omega \cdot \nabla \Psi_\alpha(\vec{r},E,\Omega) - \frac{\partial}{\partial E}\{S_\alpha(\vec{r},E)\Psi_\alpha(\vec{r},E,\Omega)\} + \sigma_{t,\alpha}\Psi_\alpha(\vec{r},E,\Omega) = Q_\alpha(\vec{r},E,\Omega) \quad (1)$$

where α indicates the primary particle type (electron or photon), S_α is the electronic stopping power (the stopping power appears in the CSD term in Eq. 1), $\sigma_{t,\alpha}$ is the total cross-section and Q_α represents the scattering and secondary production source. To derive a continuous form of the SAAF equation, we formally solve equation (1) for Ψ_α and then substitute this expression back into the first-order equation to get the second-order, self-adjoint equation given below.

$$-\Omega\cdot\nabla\left\{\frac{1}{\sigma_{t,\alpha}}\Omega\cdot\nabla\Psi_\alpha\right\}+\sigma_{t,\alpha}\Psi_\alpha=Q_\alpha-\Omega\cdot\nabla\left\{\frac{1}{\sigma_{t,\alpha}}Q_\alpha\right\}$$
$$+\frac{\partial}{\partial E}\{S_\alpha\Psi_\alpha\}-\Omega\cdot\nabla\left\{\frac{1}{\sigma_{t,\alpha}}\frac{\partial}{\partial E}\{S_\alpha\Psi_\alpha\}\right\} \quad (2)$$

A discretized version of the SAAF equation is formulated by first discretizing the energy variable in Eq. 1 and then formally solving it for the group angular flux. The expression for the group angular flux is substituted into the first-order energy discretized equation to yield the energy discretized SAAF equation. We have investigated both linear continuous and linear discontinuous finite element approximations in energy and a linear continuous finite element approximation in space.

Standard source iteration is employed and convergence acceleration is effected using a P_1 diffusion acceleration scheme consistently derived from the discretized SAAF equations using the four-step method. The linear discontinuous energy treatment of the CSD operator can require an additional set of iterations. This approach requires twice as much memory as the linear continuous treatment since two angular fluxes must be solved for each energy group: an energy-slope angular flux and a group-average angular flux. Within each energy group, the two angular fluxes are mutually dependent on one another. This results in an effective "upscatter" which can be treated by iteration or a direct solution of a block system. Under the iterative approach, an additional acceleration within each energy group between the slope and the average angular fluxes is necessary.

Our one-dimensional results[16] indicate that the SAAF approach can be used for coupled electron-photon transport problems. In the near future, we will extend the method to 2D unstructured spatial mesh.

The 3D version of CEPTRE that we propose to create will incorporate aspects of both our 1D and 2D prototypes. Since electron calculations can be readily accelerated using the spatial-angular solution strategy of our 2D prototype, we intend to use this method in our 3D code (at least for electrons). Since the SAAF form of the Boltzmann transport equation with the CSD operator offers a number of advantages, it will be incorporated into the 3D code that we intend to build.

CONCLUSIONS

Massively-parallel computers capable of TeraOp speed have enabled much more detailed Monte Carlo simulations of radiation transport on complex 3D systems than has been previously possible. To fully exploit this new computational power, higher fidelity geometrical descriptions of these systems is needed. Greater fidelity can be achieved by improvement of the combinatorial geometry models employed in coupled electron-photon transport codes like ITS. For the greatest flexibility, a version of ITS is being developed that can track particles across CAD geometric models.

Using second order forms of the transport equation (even- and odd-parity), we are able to achieve high levels of parallel efficiency for 2D unstructured mesh problems. In particular, simultaneous space/direction solution represents a viable alternative to the traditional source iteration procedure, especially for charged particles, and warrants additional investigation. Another second-order form of the transport equation, the self-adjoint angular flux formulation, also appears promising for further investigation.

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