Experience with Unstructured-Mesh Electron Transport with Massively Parallel Computing

Clifton R. Drumm, Wesley C. Fan, Leonard J. Lorence, Jr., and Jennifer L. Powell

Sandia National Laboratories

Jens Lorenz

University of New Mexico

(June 30, 2000)
DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.
I. INTRODUCTION

The ability to model the transport of electrons through materials is needed for such diverse applications as the radiation hardening of electronics, satellite shield design, and medical radiotherapy. Furthermore, it is desirable to faithfully model complex geometries with an arbitrary grid and to perform the computations efficiently on massively parallel computers\(^1\). Monte Carlo methods have been applied to electron transport problems for some time\(^2\). However, Monte Carlo is notoriously inefficient for computing differential quantities and for tracking unlikely events.

We are developing a prototype deterministic code called CEPTRE (Coupled Electron-Photon Transport for Radiation Effects) under the Department of Energy’s Accelerated Strategic Computing Initiative (ASCI). Due to the nature of the physical interactions, electron transport presents some interesting challenges beyond those encountered in neutral-particle transport. This summary includes an overview of the methods used in the CEPTRE code, with emphasis on those methods specific to electron transport, and a review of the experience gained using CEPTRE.

II. METHODS

Electron transport is characterized by cross sections that are enormous and extremely forward peaked, corresponding to a huge number of collisions during a particle lifetime (14,820 elastic collisions for an electron to slow down from ~1 MeV to 1 keV in aluminum\(^2\)). Analogous to what is commonly done in Monte Carlo electron transport, rather than attempting to model individual collision events, effective cross sections are defined, corresponding to a condensed random walk. These effective cross sections are based on a Goudsmit-Saunderson (GS) solution of the elastic scattering and continuous slowing down (CSD) events\(^3\). The step size for the condensed random walk corresponds to the energy group width used in the transport calculation. This greatly reduces the number of collisions (~2.5 collisions per energy
group for 1-MeV electrons on aluminum or ~100 effective collisions for an electron to slow down from 1 MeV to 1 keV for a 40-energy-group mesh).

A further difficulty is that convergence of the source iterations can be extremely slow for optically thick regions with a large scattering fraction, typical of electron transport. CEPTRE uses a different approach, which is extremely efficient for problems with optically thick regions and large scattering ratio. Rather than performing sweeps to determine the solution for each discrete direction separately, the CEPTRE approach is to solve the spatial and directional dependence simultaneously, for each energy group. CEPTRE uses a second-order form of the transport equation, which is symmetric positive definite (SPD), so that the highly-efficient preconditioned conjugate gradients (PCG) algorithm may be applied. Furthermore, PCG algorithms for massively parallel computers have reached a high level of sophistication, so that CEPTRE calculations typically result in parallel efficiencies greater than 90%. Internal void regions, which may be problematic for second-order forms of the transport equation, are handled by a penalty finite elements approach.

The spatial dependence is discretized by an unstructured mesh of triangles in 2D or tetrahedra in 3D, with either linear- or quadratic-continuous basis functions. The energy dependence is handled by a standard multigroup approach, and the directional dependence is approximated by a standard discrete ordinates scheme. Matrix construction and data layout are designed for the distributed computing architecture such that each processor has sufficient information to construct the distributed global matrix system independently. This reduces both memory and communication requirements.

III. APPLICATION

As an application of the CEPTRE code, we investigate an effect known as dose enhancement. This effect occurs within an electron range of material interfaces, such as in a device chip, where a high-Z metal such as gold forms a bond with silicon. Electron emission from the gold may result in as much as a factor of 30 increase in dose in the surrounding silicon,
compared with the equilibrium silicon dose. Figure 1 shows the CEPTRE energy deposition profile for two gold regions imbedded in silicon, resulting from a 100-keV planar photon source incident from the upper right. The 2D CEPTRE calculation used 20 photon and 90 electron groups, 10-keV cutoff energy, \( P_3 \) Legendre angular expansion, \( S_8 \) fully symmetric quadrature, and quadratic spatial basis functions. Table I compares the integrated charge and energy depositions from CEPTRE with those from the ITS Monte Carlo code, for the lower gold region. Excellent agreement is observed for energy deposition, while the CEPTRE charge deposition is about 10% lower than the charge deposition computed by ITS.

IV. CONCLUSIONS

A number of modifications to the CEPTRE code are underway, which will improve both accuracy and efficiency. The GS effective cross sections used in CEPTRE are based on a low-order energy difference scheme, which accounts for the large number of electron-energy groups needed in the preceding application. Work is in progress to determine cross sections based on a higher-order energy difference scheme, while retaining the positivity of the cross sections. Although the CG convergence for the electron groups is very fast, convergence of the photon groups could be accelerated by preconditioning the matrix, and both diffusion and low-order \( S_n \) are being investigated for use as preconditioners of the linear system. Because CEPTRE solves the space-direction dependence simultaneously, the linear system may be huge. The Aztec software is designed to take full advantage of the sparsity of the matrix, but further advantage can be gained by taking advantage of the structure of the submatrices arising from the scattering term. Work is in progress to exploit this structure by computing matrix elements on the fly from a few precomputed submatrices, substantially reducing storage. Finally, extensive benchmarking of CEPTRE against Monte Carlo and experimental measurement is underway.
ACKNOWLEDGMENTS

The authors wish to express appreciation to Professor Ed Larson of the University of Michigan for pointing out the similarity between the Goudsmit-Saunderson cross sections used in CEPTRE and the condensed history approximation used in electron Monte Carlo codes. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.
REFERENCES


Fig. 1. Energy deposition distribution in silicon from 100-keV photons on 10x20-μm gold lands embedded in silicon.
TABLE I
Comparison of CEPTRE energy and charge depositions with ITS Monte Carlo in the lower-gold region.

<table>
<thead>
<tr>
<th>Code</th>
<th>Energy Deposition (MeV)</th>
<th>Charge Deposition (electrons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ITS</td>
<td>$1.68 \times 10^{-3}$ (0)</td>
<td>$-4.18 \times 10^{-3}$ (1)</td>
</tr>
<tr>
<td>CEPTRE (even parity)</td>
<td>$1.67 \times 10^{-3}$</td>
<td>$-3.88 \times 10^{-3}$</td>
</tr>
<tr>
<td>CEPTRE (odd parity)</td>
<td>$1.67 \times 10^{-3}$</td>
<td>$-3.58 \times 10^{-3}$</td>
</tr>
</tbody>
</table>