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ONEBFP Development Issues

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Abstract

ONEBFP is a 1-D discrete-ordinates coupled electron-photon transport code that was recently developed to replace the ONELD code. The reasons for this replacement are explained in terms of a comparison of the programming structure and numerics of the two codes.

1 Introduction

ONELD is 1-D discrete-ordinates coupled electron-photon transport code that was developed in 1989 at LANL with funding from the Defense Nuclear Agency (DNA). The development of ONELD was part of a larger DNA project to develop a code for box-IEMP analysis. Specifically, ONELD was developed to provide the BOXIEMP-II code with charge deposition profiles resulting from photo-Compton electron generation in electronic boxes irradiated by x-rays. The BOXIEMP-II code was developed for the DNA by JAYCOR. In 1996 ONELD was replaced with an upgraded transport code called ONEBFP. The purpose of this report is to explain why this replacement was made. This is done by comparing these two codes in terms of both programming structure and numerics.

2 ONELD Background

The ONELD code is a descendent of the ONEDANT¹ neutral-particle multi-group transport code. ONEDANT has a spatial discretization scheme that

is unsuitable for electron transport calculations. ONELD essentially consists of ONEDANT with a spatial linear-discontinuous (LD) finite-element differencing scheme replacing the original diamond differencing (DD) scheme. Strictly speaking, the Boltzmann equation solved by ONELD is not adequate for electron transport. One must add a Fokker-Planck operator, known as the continuous-slowing-down (CSD) operator, to the Boltzmann equation. The resulting equation is known as a Boltzmann-Fokker-Planck (BFP) equation.² Explicitly adding this operator to ONELD would have required considerable additional modifications to ONEDANT. This was completely avoided by using a scattering cross-section representation for the CSD operator. In particular, a multigroup-Legendre moment representation was used that is equivalent to the CSD operator differenced in energy with the diamond scheme.³ The cross-section data used in ONELD is read from an input file at run time. Coupled electron-photon cross-section data (including the CSD operator data) is generated with the CEPXS code.⁴

3 ONELD Deficiencies

Over the past several years it became clear that ONELD had several significant deficiencies in terms of both programming structure and numerics. Specifically:

- ONELD uses a huge input/output module (approximately 90,000 lines of FORTRAN) that was originally written for an entire family (1-D, 2-D, and 3-D) of transport codes. This module is very complex and proved to be very difficult for JAYCOR personnel (the developers of BOXIEMP-II) to maintain as the code was ported to new computers. Furthermore, an extremely small subset of the sophisticated capabilities of the ONELD input/output module were used when the code was executed in BOXIEMP-II.
- ONELD is coded in FORTRAN-77 and stores all arrays that depend upon problem size in a single container array. The memory pointers for these arrays must be explicitly calculated, and these arrays must be passed to all subroutines through the calling sequence. This approach was common before the advent of modern memory management capabilities, but it is now quite obsolete. The presence of this programming

structure in ONELD makes it very time consuming to make even the simplest modifications to the code.

- The diamond-differenced form of the continuous-slowng-down operator used in ONELD is second-order accurate, but it can yield highly oscillatory non-physical solutions when stressed.

4 ONEBFP Properties

ONEBFP was developed to eliminate the deficiencies of ONELD. The most important properties of ONEBFP follow:

- ONEBFP was developed specifically for DNA applications. The extraneous capabilities characteristic of ONELD are not present in ONEBFP. This is why ONELD has on the order of 100,000 lines of FORTRAN while ONEBFP has fewer than 5000. This alone makes ONEBFP much easier to maintain and port to new platforms than ONELD.
- ONEBFP was written using modern FORTRAN-77 dynamic memory allocation extensions available on essentially all workstations, e.g., temporary arrays. This makes it much easier to make significant modifications to the code, and contributes to a more modular and compact code.
- ONEBFP was written to explicitly solve the Boltzmann-Fokker-Planck equation, whereas ONELD was written to solve the Boltzmann equation. Additional Fokker-Planck operators necessary for charged-particle transport had to be represented in terms of effective Boltzmann cross sections. Because the Boltzmann-Fokker-Planck equation is explicitly solved in ONEBFP, it was possible to implement an advanced nodal discretization scheme in both space and energy. The space-energy discretization scheme in ONELD is third-order accurate in space and second-order accurate in energy. Furthermore, as previously discussed, the energy scheme is prone to yield oscillatory solutions when stressed. The nodal space-energy discretization scheme in ONEBFP is fourth-order accurate in both space and energy, and is far less likely to yield oscillatory solutions than the ONELD scheme. This nodal scheme in

space and energy (x and E) represents a straightforward generalization of the nodal scheme in 2-D space (x and y).⁵ An extensive computational comparison of ONEBFP and ONELD is given in Reference 6. The results from this comparison clearly demonstrate the superiority of the numerics in ONEBFP.

5 Conclusions

Overall, ONEBFP represents a considerable improvement relative to ONELD: ONEBFP is roughly 20 times smaller than ONELD, easier to maintain and modify, and its numerics are much more accurate and robust. Furthermore, ONEBFP was built in 1995 for a total of \$100K, which is the same dollar amount needed to develop ONELD in 1989. Therefore the development of ONEBFP was highly cost-effective.

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