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Adjoint Charge Deposition and CAD Transport in ITS

Charge Deposition

- Net charge deposited is the difference between the removal and absorption of charged particles in a medium
- Charge removal
  - Interactions imparting energy to secondary charged particles
  - The production of secondary charged particles above the cutoff energy due to Boltzmann interactions
- Charge deposited
  - Due to the “absorption” of charged particles slowing down in the medium
  - Interactions that leave the particle with less than the cutoff energy due to either the CSD operator or an inelastic Boltzmann interaction
- Adjoint allows for an easier calculation of localized deposition
  - When electronic equilibrium exists with a photon source the charge deposition is highly localized near material interfaces

Adjoint Particle Source for Charge Deposition

- Extend MITS to charge deposition
  - Combination of ITS and CEPXS
- Developing a proper adjoint particle source
- Modifications to the cross section form
  - low-energy groups

Adjoint Electron-Photon with ITS

- Coupled electron-photon transport to solve Boltzmann-Fokker-Planck (BFP) equation

The adjoint BFP:

$$-\vec{\Omega}\cdot\vec{\nabla}\psi^{\dagger}+\sigma_t(\vec{r},E)\,\psi^{\dagger}=Q^{\dagger}(\vec{r},E,\vec{\Omega})+\int_0^{\infty}dE'\int_0^{4\pi}d\vec{\Omega}'\,\sigma_s(\vec{r},E\rightarrow E',\vec{\Omega}\rightarrow\vec{\Omega}')\,\psi^{\dagger}(\vec{r},E',\vec{\Omega}')$$

$$+\frac{\alpha(\vec{r},E)}{2}\left(\frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial}{\partial\mu}\psi^{\dagger}\right]+\frac{1}{1-\mu^2}\frac{d^2}{d\phi^2}\psi^{\dagger}\right)-\frac{\partial}{\partial E}\left[S(\vec{r},E)\,\psi^{\dagger}\right]+\left(\frac{\partial}{\partial E}S(\vec{r},E)\right)\psi^{\dagger}$$

- The 1st line contains the Boltzmann terms
- The 2nd line contains the Fokker-Planck terms
  - Represent electron interactions with small deflections or energy loss
- α is the restrictive momentum transfer & S is the restrictive stopping power

MITS

- The Multigroup/Continuous-Energy (hybrid) Integrated TIGER Series (ITS)
- CEPXS/ONELD cross-section generator
- ITS input/output and combinational geometry routines
- Converts the multigroup-Legendre format cross sections into cumulative probability distributions for CM scattering
- A particle's group index is needed for Boltzmann scattering
- A particle's discrete energy is needed for Fokker-Planck energy loss

Boltzmann-Interaction Contributions to Charge Deposition

- Requires accurate modeling of the lowest-energy electron group
  - Most positive contributions to the electron deposition, will pass through the lowest-energy group
- Finite total cross-section required for adjoint
  - Cannot invert a non-finite cross section
  - Used in calculating higher energy adjoint particles

$$N_g = \Sigma_{g \to L} \cdot \frac{\Delta E_g}{\Delta E_L} \cdot \frac{1}{\Sigma_{tL}}$$

Lowest-Energy Cross-Section

- Introduce a Boltzmann interaction for the lowest group
  - A pseudo-group is created for the lowest-energy group to "scatter" into
- The Boltzmann-scattering cross section between adjoining groups
  - Based on the transfer of particles between adjoining groups
  - For the lowest group

$$\Sigma_{g\to g+1} = \frac{\beta_{g\to g+1}}{E_g^m - E_{g+1}^m} \longrightarrow \Sigma_{aL} = \frac{\beta_{L\to L+1}}{E_L^m - E_{L+1}^m}$$

Adjoint Particle Weight

- Adjoint particle weight at cutoff is equal to the stopping power
- When adjoint particle speeds up between groups, its weight is adjusted by the ration of stopping powers
  - Can use to determine the size of the pseudo-group
- Adjoint particle weight in the lowest group can be defined as

$$W_L = \Sigma_{aL} \Delta E_L$$

- Requires pseudo-group to have the same energy width as the lowest group

$$E_{L+1}^m = E_L^m - \Delta E_L$$

Modeling Geometries in ITS

ITS

- Uses simple geometric shapes (sphere, cylinder, etc)
- Combines geometries using Boolean operations
- Efficient for computational run-time
  - Combinational geometry makes intersection calculations for ray tracing easy
  - All spaces is defined, even void
- Enormous setup effort for complex geometries
  - Some objects just cannot be accurately modeled

Modeling Geometries

CAD

- More accurate geometric representation
- Faster setup time
  - Some models may be preexisting in CAD format
- Low geometric tolerances may result in history rejection
  - Code can no longer follow particle trajectory if it slips into the cracks
- Slower computationally
  - Additional face intersection calculations required for ray tracing
  - Not all space is well defined

Developing CAD routine for ITS

- ACIS file format was used
  - Format will be automatically updated, no maintenance required
  - Common format for several commercial CAD packages
- Routines can interrogate the geometry in the following manner:
  - Given a point and a direction, determine the closest boundary intersection.
  - Given a point, identify the region enclosing that point
  - Given a point on a surface, determine the outgoing surface normal
  - Given a point, determine the minimum distance to a boundary

Speeding up the CAD routine

- A regular grid is superposed on the entire geometry
  - A list is created of all regions that intersect each cell
  - Entering a void only requires not being in all other regions within a cell
- Create bounding volume around each part and each face
  - If the ray misses the bounding volume, it misses the object within
- Screens rays intersecting bounding volumes
  - Object interrogated only if distance is closer than the closest object found
- Code remembers which regions can be entered while exiting a given region
- Code prevents the remaining zones from being checked more than once when determining where it is headed

Questions?