NE 155/255, Fall 2019
Spatial Discretization
October 14, 2019

So far we've dealt with

- Discretization of *energy* using the multigroup approximation, where we assume group-integrated values.
- *Expanding sources*, in particular scattering, in spherical harmonics – which we reduce to Legendre Polynomials in the case of azimuthal symmetry
- Discretization of *angle*, one of
  - S_N: get solutions along specific angle sets (quadrature points), use corresponding quadrature weights to integrate over angle
  - P_N: expand the angular flux in spherical harmonics (which we only do in 1-D, so Legendre polynomials in practice) and solve a set of coupled equations for each expansion term
  - SP_N: take the 1-D P_N equations and transform them to 3-D by replacing the 1-D diffusion operators with the 3-D diffusion operator and replacing the derivatives at the boundary with the outward normal derivatives

When we do all of this we get $g = 0, \ldots, G-1$ equations in energy, and some number of equations in angle that depends on which approach we take. However, we still have one major item to deal with: space.

Space

(Largely from Evans; some from Vujíc, Lewis and Miller)

There are *many* spatial discretization choices out there. What you choose can depend on the geometry and physical properties, as well as if you're using Cartesian or curvilinear formulations. Fundamentally, we can characterize the differencing schemes in a few ways

- Cell balance, which includes
  - Finite Difference Method (FDM) – using point value solution
  - Finite Volume Method (FVM) – using cell-averaged value solution
- Finite element (FEM) – using basis function for expansion:

  - Piecewise linear: hat functions
  - Piecewise quadratic or cubic basis functions
  - Piecewise higher order Gauss-Legendre polynomials
- Spectral and Pseudo Spectral Methods – using orthogonal global series as the basis function:
  - Fourier series
  - Bessel, Chebyshev, Legendre series

We'll talk about cell balance and finite element methods; in nuclear engineering we have specific versions of these. For example, Denovo, the 3-D Cartesian mesh deterministic code from ORNL, offers these choices:

- Simplified P_N: finite volume
- Discrete ordinates: weighted diamond difference (WDD) without flux fixup is equivalent to a Crank-Nicolson method; cell balance.
- Discrete ordinates: weighted diamond difference with flux fixup to zero (WDD-FF) is a nonlinear method; cell balance
- Discrete ordinates: theta weighted diamond difference (TWD) is a nonlinear method; cell balance
- Discrete ordinates: linear discontinuous (LD) is a Galerkin method formed from the basis set $\{1, x, y, z\}$; FEM
- Discrete ordinates: bilinear discontinuous (BLD) in 2-D; FEM
- Discrete ordinates: trilinear discontinuous (TLD) is a Galerkin method formed from the basis set $\{1, x, y, z, xy, yz, xz, xyz\}$ and maintains the asymptotic diffusion limit on the grid used in Denovo; FEM
- Discrete ordinates: step characteristics (SC) in 2- or 3-D does not produce negative fluxes and does not have oscillatory behavior; can be written as a cell balance or finite element scheme

The WDD, WDD-FF, TWD, LD, BLD, and TLD schemes are all second-order, and the SC scheme is first-order.

LANL's PARTIS$_N$ has similar choices, but their new Capsaicin code has unstructured mesh and uses Discontinuous Finite Element Method (DFEM): Linear, Bars, Triangles, Quadrilaterals, Polygons. They also have an ability to deal with non-convex meshes using Continuous FEM. Finally, they have structured meshes in 3-D with DD and LD.

INL's Rattle$S_N$ake uses finite element methods for unstructured higher-order meshes as well, and

has capabilities for both discontinuous and continuous Galerkin.

We'll use the diagram in 1 to think through our discretization schemes.

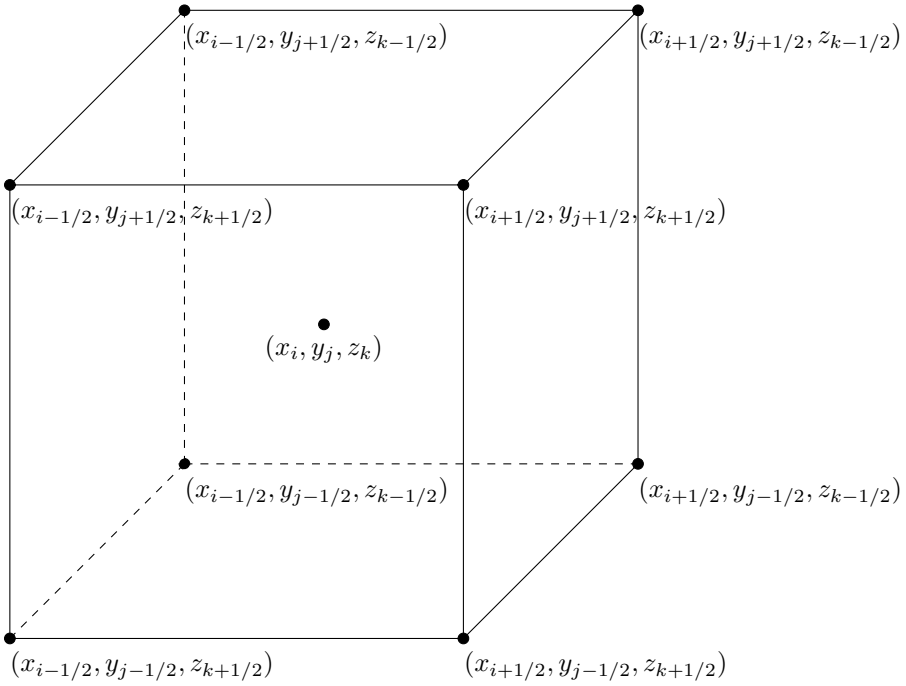

Figure 1: General three-dimensional mesh cell (from Exnihilo Methods Manual).

The mesh cell is centered at the i^{th} position along the x-axis, the j^{th} position along the y-axis, and the k^{th} position along the z-axis. Indexing is such that there are I mesh cells with $I+1$ grid points in the x-direction, J mesh cells with $J+1$ grid points in the y-direction, and K mesh cells with $K+1$ grid points in the z-direction. It is assumed that all material properties are constant within a given cell.

For any given group, angle, and source, the transport equation can be reduced to

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}) + \Sigma_t(\vec{r}) \psi(\vec{r}) = s(\vec{r}) \,, \tag{1}$$

where $s(\vec{r})$ is a total accumulated source. In operator form, this equation is

$$\mathbf{L}\psi = s \,, \tag{2}$$

where $\mathbf{L}$ is the differential transport operator ($\hat{\Omega} \cdot \nabla + \Sigma_t(\vec{r})$). We will be required to perform operations of the type

$$\psi = \mathbf{L}^{-1} s \,, \tag{3}$$

to solve discrete forms of Eq. (2).

Operators and Transport Sweeps

An *operator* is a mapping from one vector space or module to another. Operators are of critical importance to both linear algebra and functional analysis, and they find application in many other fields of pure and applied mathematics.

For all the spatial differencing schemes discussed below, $\mathbf{L}$ can be *implicitly* formed as a lower-left triangular matrix and inverted by "sweeping" through the mesh in the direction of particle flow. In effect, the discretized form of Eq. (1) is solved in each cell. The outgoing fluxes become input to the downwind cells, or in other words, each cell looks "upwind" to find its incoming fluxes. Once all the incoming fluxes are defined on the entering faces of a cell, the outgoing fluxes can be calculated, and the process is repeated until the entire mesh is solved for a given angle. For each cell, the entering and exiting faces are defined by

$$\hat{\Omega} \cdot \mathbf{n} < 0 \,, \quad \text{(entering face)} \tag{4}$$

$$\hat{\Omega} \cdot \mathbf{n} > 0 \,, \quad \text{(exiting face)} \,. \tag{5}$$

Mathematically, this is called a *wavefront* solver. The operation $\mathbf{L}^{-1}$ is regularly referred to as a *sweep* in the nuclear engineering and transport communities.

Finite Difference

Finite Difference gives pointwise values on a grid. We use points to approximate derivatives and are able to obtain a corresponding expression for the *Local Truncation Error* (LTE).

A note about *convergence*: the solution of the finite difference equations should converge to the true solution of the PDE as grid spacing (mesh size) goes to zero.

We're actually going to skip this formulation; other methods handle complex scenarios better.

Finite Volume

Finite volume methods approximate the average integral on a reference volume. This handles discontinuities much better – why might that be? If cell boundaries line up with material boundaries and we integrate half way into each cell, we capture the impact of the neighboring materials. Thus, the cell-balance equation can be derived by integrating Eq. (1) over the mesh cell in Fig. 1, which yields a statement of conservation of particles within the mesh cell.

Weighted Diamond Difference

To integrate the differential term, we will note

$$\int_{x_{i-1/2}}^{x_{i+1/2}} dx \, \frac{\partial \psi}{\partial x} = \int_{x_{i-1/2}}^{x_{i+1/2}} \partial \psi = \psi_{i+1/2} - \psi_{i-1/2} \, .$$

For the other terms we will use the *midpoint integration rule*. We won't derive that rule here, but know that the midpoint rule comes from open Newton Cotes with Lagrange polynomials (a way to make integration rules) using $n = 0$ (which uses one point only):

$$\int_a^b f(x)dx = \int_{x_{i-1/2}}^{x_{i+1/2}} f(x)dx = hf(x_i) + \frac{h^3}{3} f''(\xi_i) \, .$$

For us, $x_{i+1/2} - x_{i-1/2} = h \equiv \Delta_i$. Thus, applying $\iiint (\cdot) \, dxdydz$, dividing by differential volume, and separating flux into x, y, and z differential components gives (letting $\Sigma_{ijk} \equiv \Sigma_{t,ijk}$),

$$\frac{\mu}{\Delta_i}(\psi_{i+1/2} - \psi_{i-1/2}) + \frac{\eta}{\Delta_j}(\psi_{j+1/2} - \psi_{j-1/2}) + \frac{\xi}{\Delta_k}(\psi_{k+1/2} - \psi_{k-1/2}) + \Sigma_{ijk}\psi_{ijk} = s_{ijk} \, . \quad (6)$$

Note that we now need a way to relate the center (ψ_{ijk}) and edge ($\psi_{n\pm1/2}$) fluxes to one another! The diamond-difference method (using Lewis & Miller and Exnihilo manual) is derived by closing Eq. (6) with a weighted average of the face-edge fluxes, which is equivalent to a Crank-Nicolson method in space. (note that Lewis & Miller uses a slightly different scheme that is mathematically

equivalent)

$$
\begin{aligned}
\psi_i &= \frac{1}{2}\big((1+\alpha_i)\psi_{i+1/2} + (1-\alpha_i)\psi_{i-1/2}\big) \\
&\quad -1 \le \alpha \le 1 \\
\psi_{i+1/2} &= \frac{2}{(1+\alpha_i)}\psi_{ijk} - \frac{(1-\alpha_i)}{(1+\alpha_i)}\psi_{i-1/2}\,, \quad \mu > 0 \ (\psi_{i-1/2} \text{ is incoming}) \\
\psi_{i-1/2} &= \frac{2}{(1-\alpha_i)}\psi_{ijk} - \frac{(1+\alpha_i)}{(1-\alpha_i)}\psi_{i+1/2}\,, \quad \mu < 0 \ (\psi_{i+1/2} \text{ is incoming})
\end{aligned}
$$

The plus/minus depends on direction–going in $\mu > 0$ the $\psi_{i-1/2}$ is the flux incoming and $\psi_{i+1/2}$ is outgoing. This flips for $\mu < 0$. We will use $\bar{\psi}$ to indicate the incoming fluxes on each face to help us keep track of which direction we're going.

The α terms are weighting factors such that $\alpha = 0$ gives the classic diamond-difference equations (the central flux is the average of the incoming and outgoing). $\alpha = \pm 1$ gives the step-difference equations in which the center flux is determined entirely from the incoming flux. Setting $\alpha = \pm 1$ yields a first-order spatial differencing scheme. The default behavior of Denovo for WDD uses $\alpha = 0$, which gives the second-order diamond-difference method.

Substituting and rearranging the cell-balance equation with this closure yields the following system of equations,

$$
\mu \gtrless 0\,,\ \eta \gtrless 0\,,\ \xi \gtrless 0
$$

$$
\psi_{ijk} = \frac{s_{ijk} + \frac{2}{(1\pm\alpha_i)}\frac{|\mu|}{\Delta_i}\bar{\psi}_{i\mp 1/2} + \frac{2}{(1\pm\alpha_j)}\frac{|\eta|}{\Delta_j}\bar{\psi}_{j\mp 1/2} + \frac{2}{(1\pm\alpha_k)}\frac{|\xi|}{\Delta_k}\bar{\psi}_{k\mp 1/2}}{\Sigma_{ijk} + \frac{2}{(1\pm\alpha_i)}\frac{|\mu|}{\Delta_i} + \frac{2}{(1\pm\alpha_j)}\frac{|\eta|}{\Delta_j} + \frac{2}{(1\pm\alpha_k)}\frac{|\xi|}{\Delta_k}} \tag{7}
$$