LA-UR-24-25791
Approved for public release; distribution is unlimited.

Title: Radiation Transport: Deterministic Approach

Author(s): Hart, Nathan Henry

Intended for: Presentation at LANL CPW 2024

Issued: 2024-06-14

Radiation Transport: Deterministic Approach

Nathan Hart, Scientist
nhhart@lanl.gov // 7-3768
CCS-2, Computational Physics and Methods

CPW 2024
June 14, 2024

LA-UR-24-XXXXX

Agenda

Introduction

Basic Nuclear Physics

Modelling

Discretization, Simplification, and Parallelization – Solving the BTE

Advanced Transport Methods

Thermal Radiative Transfer

Introduction

Introduction – BLUF

- This lecture covers **deterministic particle transport**
  - **Deterministic**: non-random, reproducible, implies discretized equations
  - **Particle**: describing the behavior of (an aggregate of) free particles, not fluids or materials
  - **Transport**: rooted in Boltzmann's kinetic theory of gases, distribution of particles is not fully described by a Maxwellian or Planckian distribution

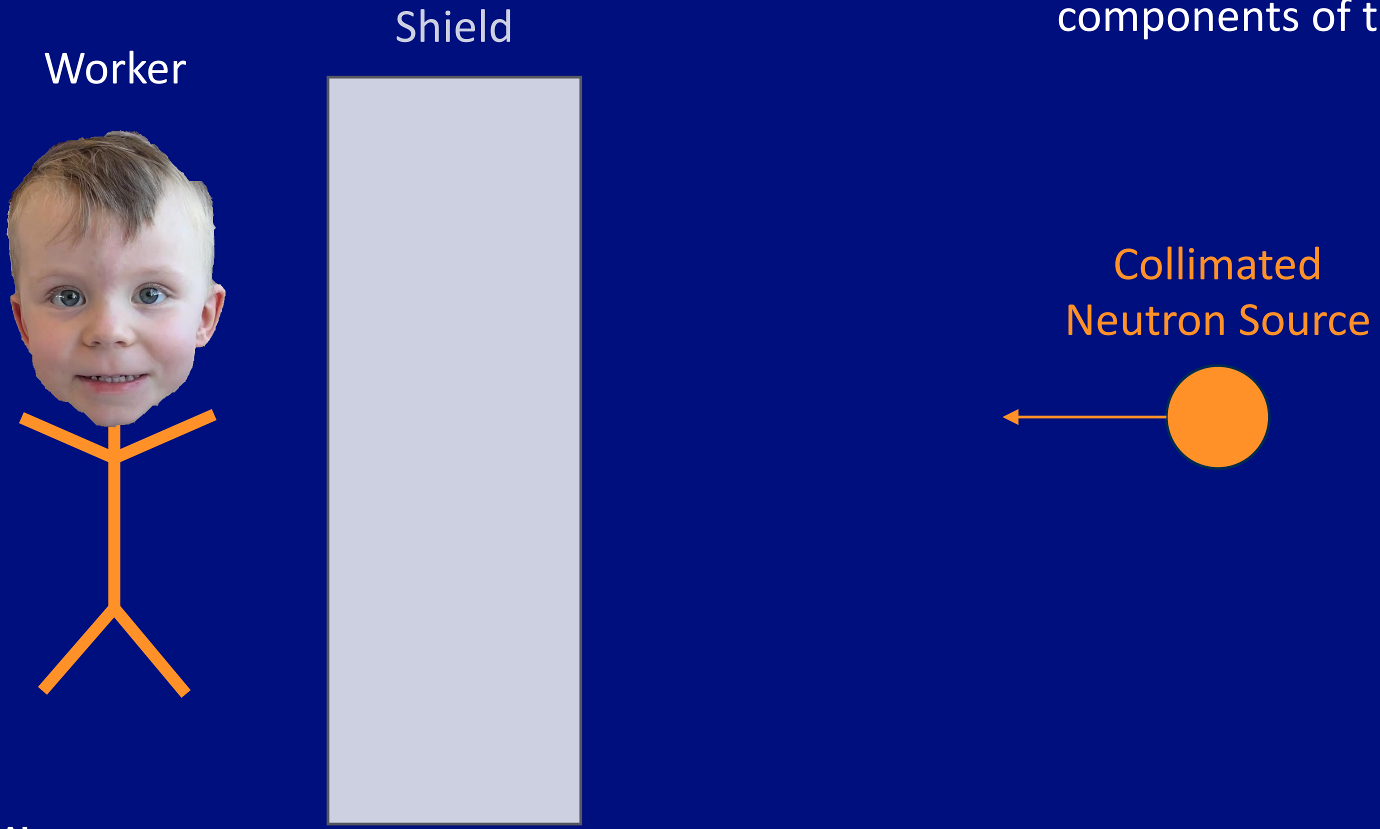
- This lecture does **not** cover:
  - Non-neutral (i.e., charged) particles – equations and methods get too complicated for an intro course
    - Neutral particle examples: neutrons, gamma rays, thermal photons via thermal radiative transfer (TRT)
    - I will primarily talk about neutron/gamma (n/γ) transport in this talk, but most is applicable to TRT as well
  - Monte Carlo methods – some information in passing, but that is another lecture

Introduction – Some Context

- Transport is a big part of the Lab's computational efforts
  - ASC-IC-Transport funds four teams that primarily focus on transport methods and code development – PARTISN, MCATK, Jayenne, and Capsaicin; >25 staff + additional support + students
  - Additional transport code teams, namely MCNP, outside(ish) of ASC Transport aegis
  - Huge user base of LANL-developed transport codes internally and externally
- Transport team members have a diverse educational background – typically nuclear engineering, astrophysics, and mathematics
- Historically, many, if not most, transport methods and discretization schemes used at LANL were developed at LANL, by scientists in academia with LANL connections, or elsewhere in the DOE complex

Introduction – Shielding Example

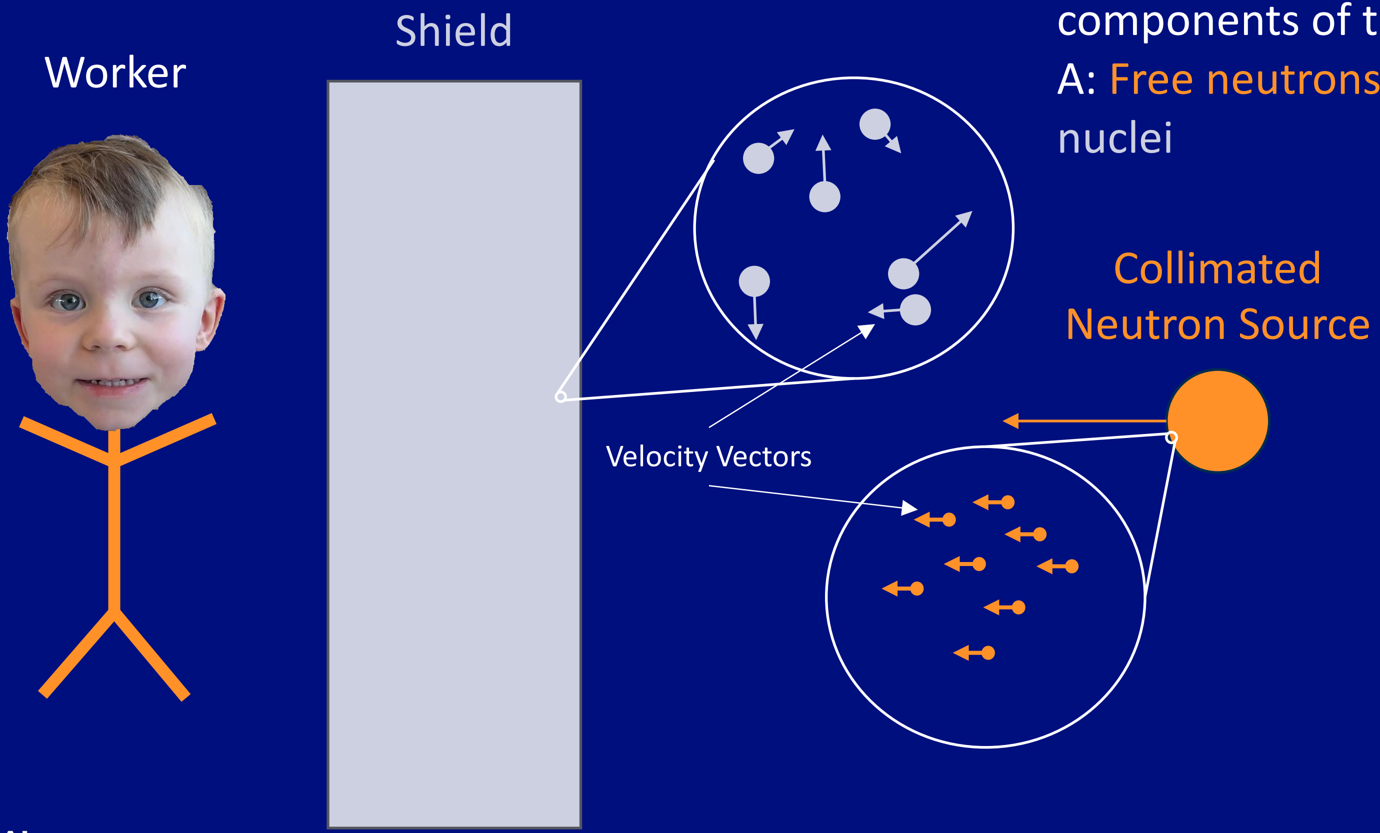
Q: What are the relevant components of this system?



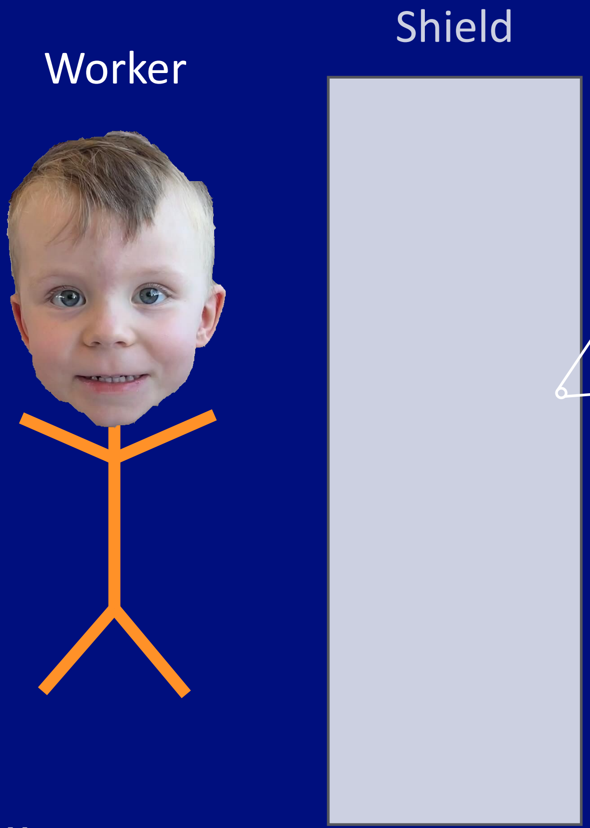
Introduction – Shielding Example

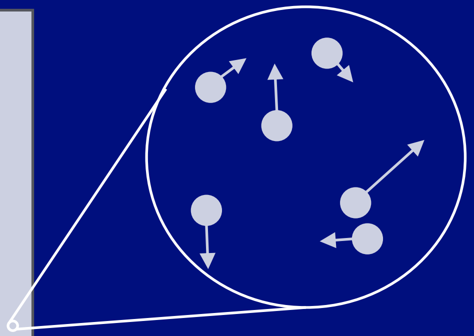
Q: What are the relevant components of this system?

A: Free neutrons and atomic nuclei



Introduction – Shielding Example

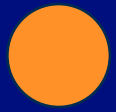




Q: What are the relevant components of this system?

A: Free neutrons and atomic nuclei

Collimated Neutron Source



Atomic nuclei are isotropic in direction of travel and Maxwellian in energy – treated as a fluid

Introduction – Shielding Example

Worker

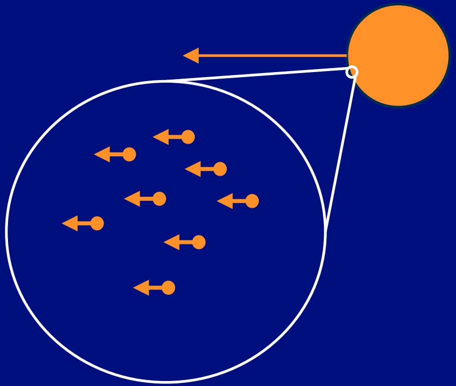
Shield

Free neutrons are monodirectional and monoenergetic – must be treated kinematically and tracked as particles

Q: What are the relevant components of this system?

A: Free neutrons and atomic nuclei

Collimated Neutron Source



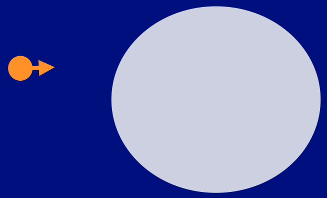
Basic Nuclear Physics

Basic Nuclear Physics – Microscopic Cross Sections

- In our example, how do we determine if a neutron interacts with a nucleus?
- We use a probabilistic quantity called the "microscopic cross-section", σ, which has units of area (1 barn = 1e-24 cm^2)
  - Units of area are merely an abstraction, but a useful one – larger the effective size of a nucleus, the higher the probability of interaction (nucleus is not physically bigger)

Small σ = Small Probability of Interaction

Big σ = Large Probability of Interaction



Microscopic cross sections are specific to a nuclide and change with the energy (i.e., temperature) of the nucleus

Basic Nuclear Physics – Macroscopic Cross Sections

- We are not really interested in whether a single neutron interacts with a single nucleus – we are interested in whether an aggregate of neutrons interact with an aggregate of nuclei
- The microscopic cross section, σ, is averaged over nuclei locally to get a ”macroscopic cross section”, Σ, which has units of inverse-distance (cm^{-1})

$$\Sigma = \sum_i \frac{\rho_i N_A}{M_i} \sigma_i$$

- i – nuclide
- ρ_i – mass density of constituent nuclide in material
- N_A – Avogadro’s number
- M_i – atomic mass of nucleus

- A “mean-free-path” (mfp) is the average distance between interactions
  - Typical neutron mfp’s are ~1 cm
- Analogous quantity called “opacities” in TRT

Notation note: σ is often used as macroscopic cross section, too, especially in TRT

Basic Nuclear Physics – Interaction Types

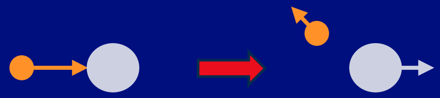
- Every interaction type has its own cross section; total cross section, Σ_t, is the summation of cross sections of all interaction types

$$\Sigma_t = \sum_x \Sigma_x$$

where x is an interaction type

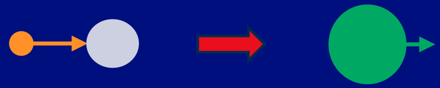
- Neutron interactions fall into two basic categories: scattering and absorption

Scattering



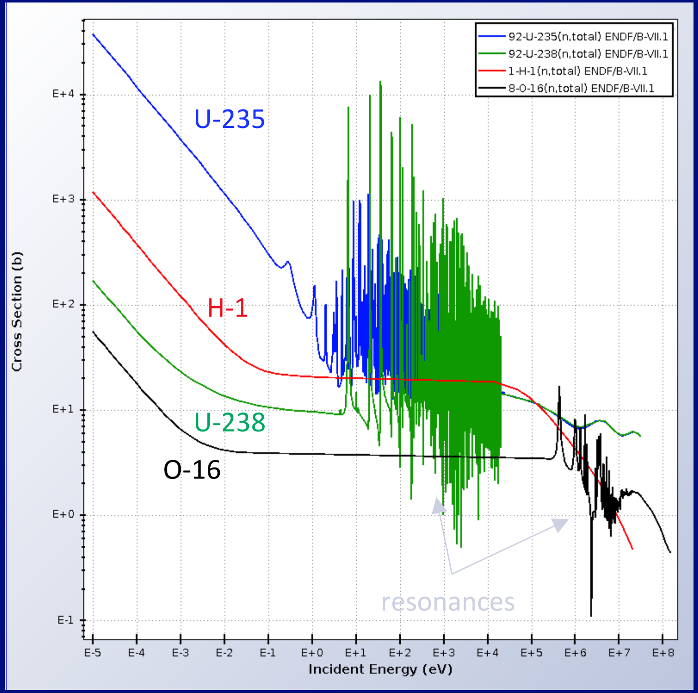
- A neutron hits a nucleus causing a change in direction and energy
- Scattering may be elastic or inelastic
- The event may liberate additional neutrons/particles

Absorption



- A neutron hits a nucleus and is captured, incrementing the neutron number of the nucleus by one
- The nucleus is left in an excited state
- The nucleus may fission or otherwise release one or more neutrons, but still considered an absorption event
- Other forms of radioactive decay or particle emission may occur, too

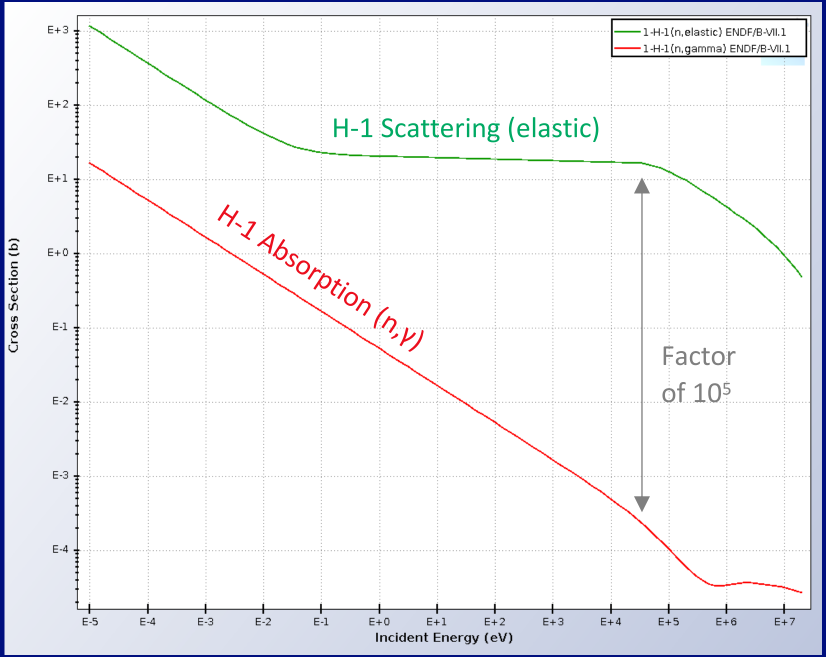
Basic Nuclear Physics – Energy Dependence



From nndc.bnl.gov/sigma

- Cross sections are a function of incoming neutron energy
- *Generally*, cross sections decrease with increasing incident energy, but it's complicated…
- "Resonances" are maxima and minima in the cross section that arise from many possible excited states of compound nuclei
  - This will become very important when we get to modelling

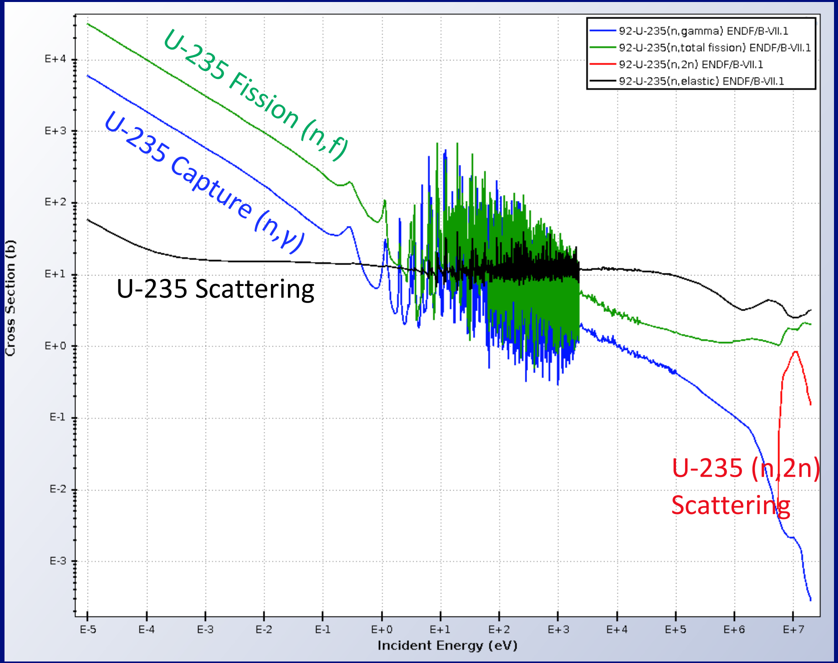
Basic Nuclear Physics – Interaction Type and Energy



From nndc.bnl.gov/sigma

- H-1 is the simplest nucleus, just 1 proton
- Scatter is up to 5 orders of magnitude more likely than absorption
- From a design perspective, different materials provide different properties that can be beneficial or detrimental
    - Neutron shielding often uses hydrogenous material (e.g., water or polyethylene) to slow down (de-energize) neutrons via scatter to make them easier to absorb
    - The same strategy is used for better neutron detection

Basic Nuclear Physics – Interaction Type and Energy



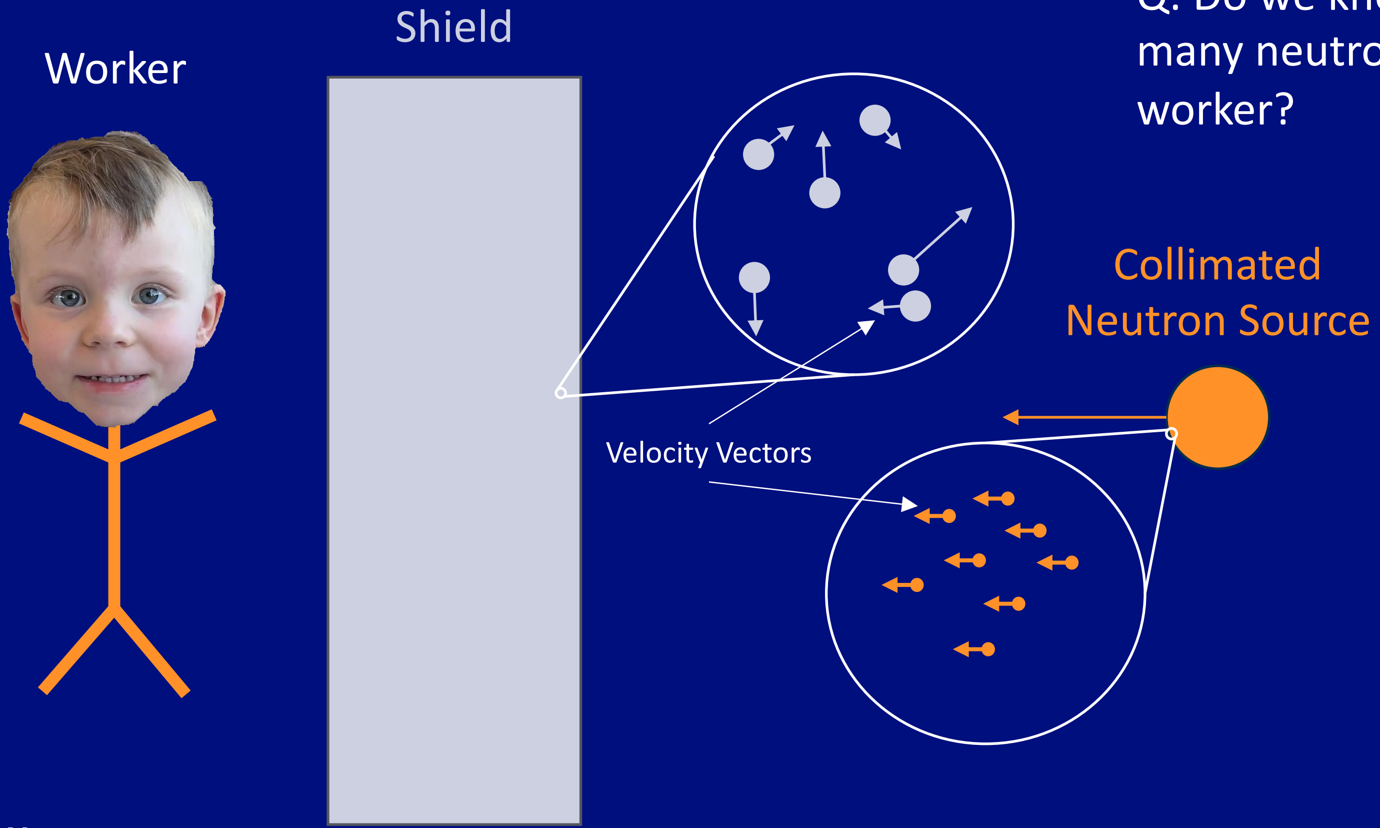
From nndc.bnl.gov/sigma

- U-235 is a complicated nucleus
  - 92 protons and 143 neutrons
  - Is fissile (no threshold for fission)
  - Has endothermic reactions like (n,2n)
- The Big Picture:
  - Cross sections are complicated – multiple interaction types, complicated dependence on energy, etc.
  - Scattering is especially complicated – dependent on incident *and* resultant neutron energies, plus anisotropy
  - “Opacities” are the analogous quantity for thermal photons
  - XCP-5 nuclear data team processes cross sections and gives us data we can use in transport codes

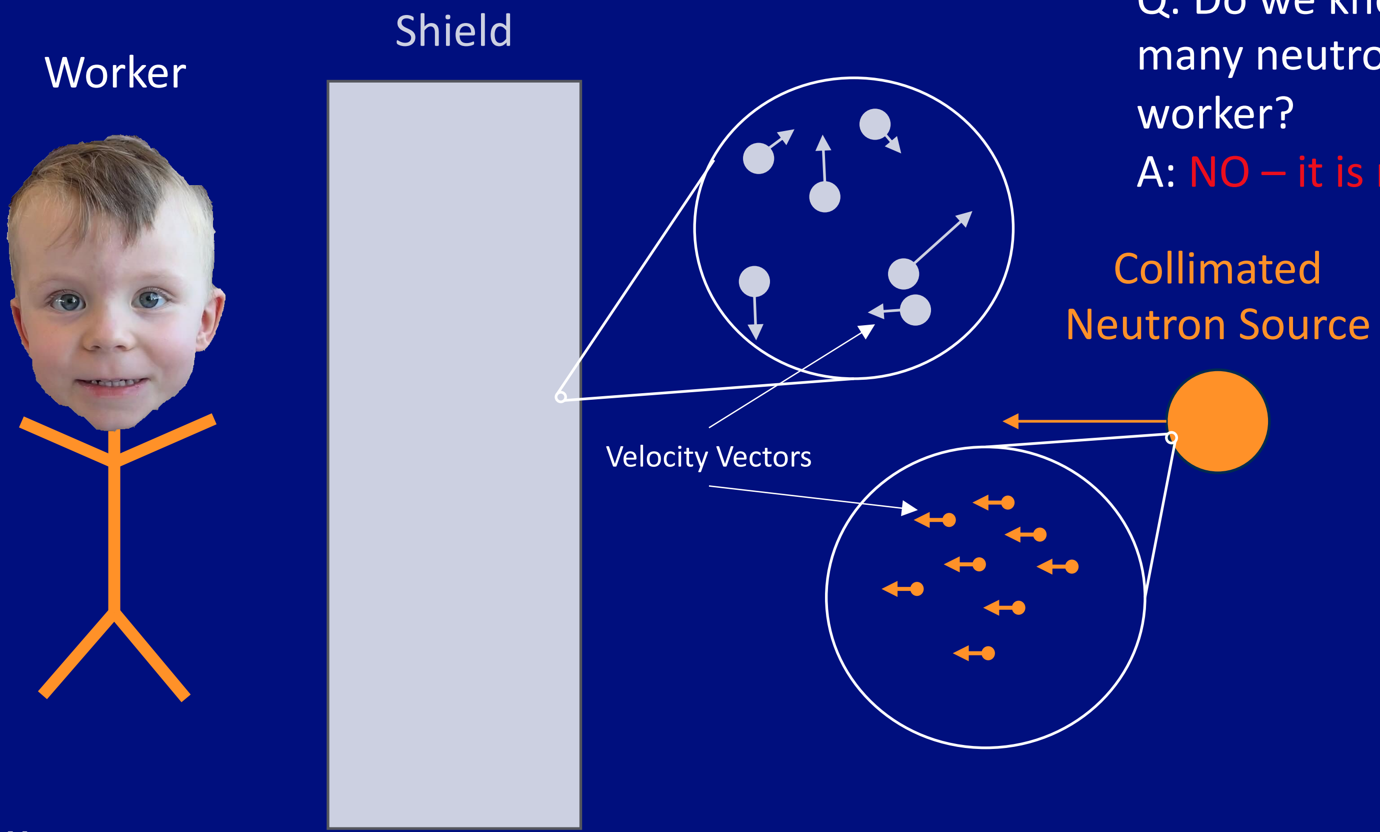
Fission – a neutron collides with a nucleus causing it to split into multiple nuclei and release additional particles like gamma rays and neutrons

Basic Nuclear Physics – Determinism

Q: Do we know exactly how many neutrons will reach our worker?



Basic Nuclear Physics – Determinism



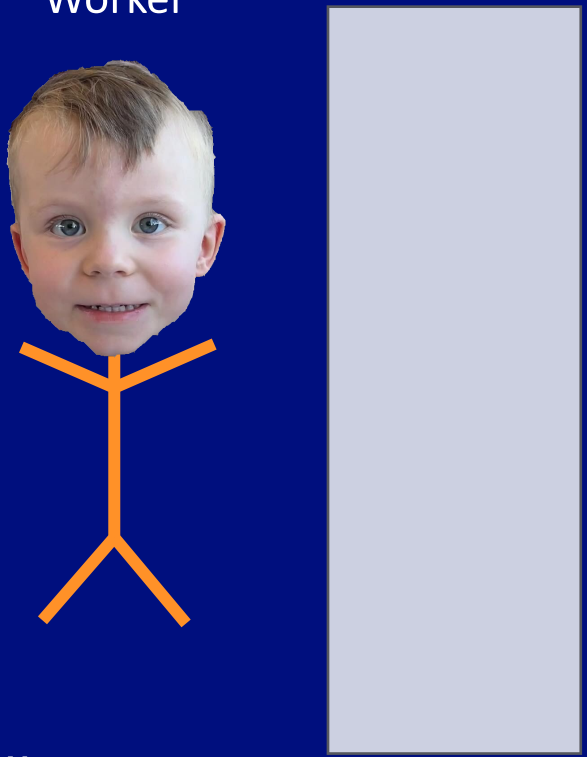
Q: Do we know exactly how many neutrons will reach our worker?

A: NO – it is random!

Basic Nuclear Physics – Determinism

Shield

Worker

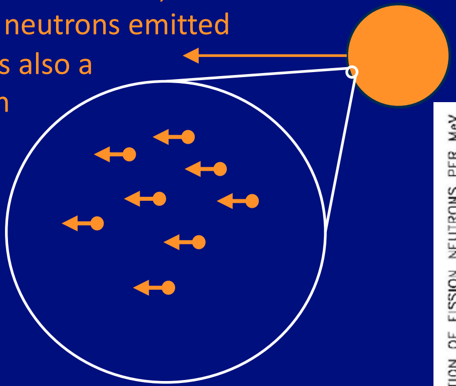


- Neutron emission is given by a *rate* – merely describes the *average* behavior
- Neutron energy and direction of travel (when not collimated) also belong to a distribution
- If source is from fission, number of neutrons emitted per event is also a distribution

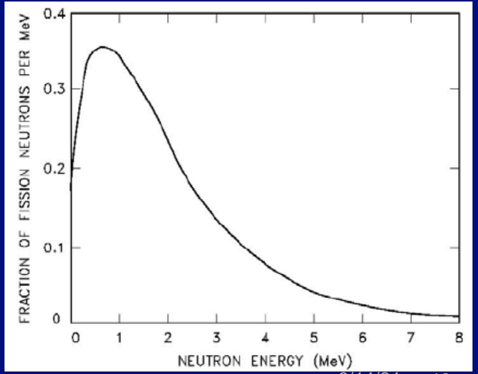
Q: Do we know exactly how many neutrons will reach our worker?

A: NO – it is random!

Collimated Neutron Source

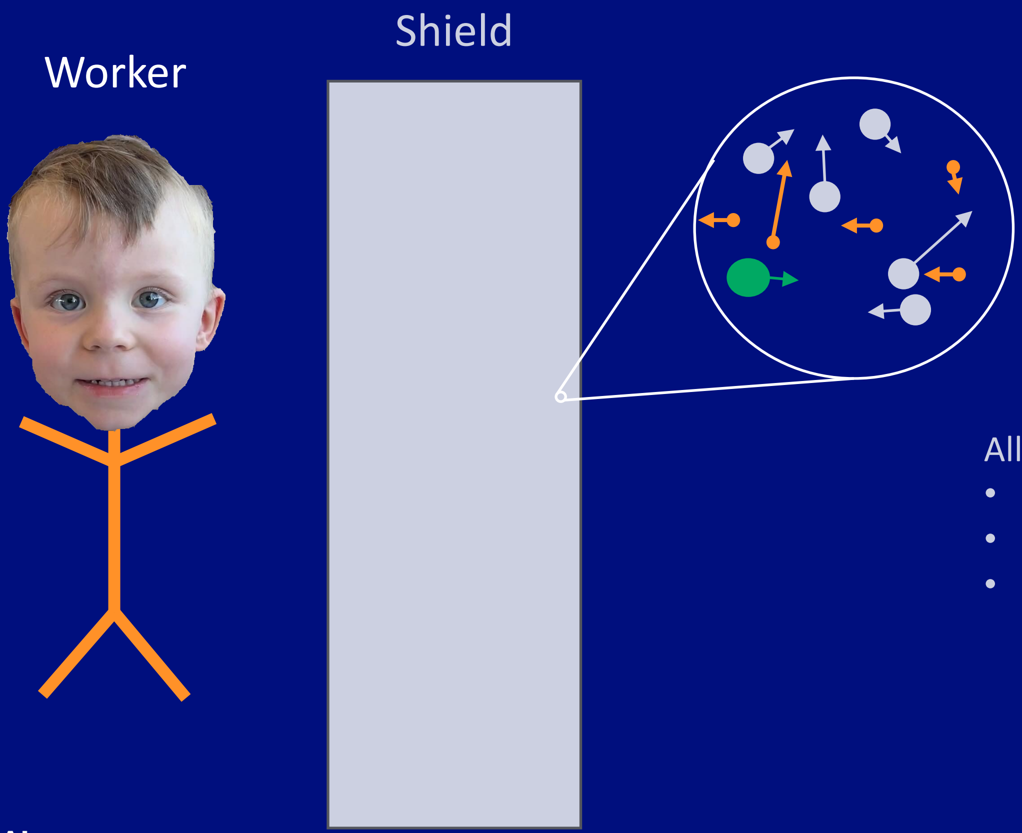


Neutron energy spectrum from thermal fission of U-235



Prelas, Mark & Weaver, Charles & Watermann, Matthew & Lukosi, Eric & Schott, Robert & Wisniewski, Denis. (2014). A review of nuclear batteries. Progress in Nuclear Energy. 75. 117–148. 10.1016/j.pnucene.2014.04.007.

Basic Nuclear Physics – Determinism



Q: Do we know exactly how many neutrons will reach our worker?

A: NO – it is random!

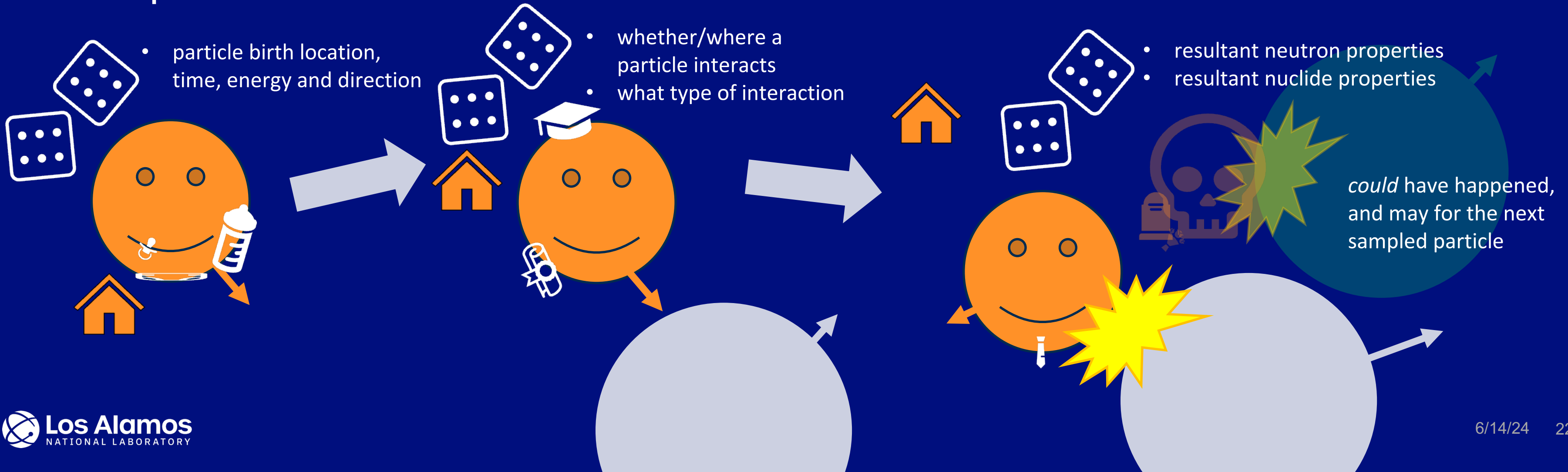
All probabilistic:

- Whether an interaction occurs
- What type of interaction occurs
- Resultant properties of the target nuclei, incident neutrons, and any production particles

Modelling

Modelling – Monte Carlo Approach

- There are two ~~competing~~ complementary ways to figure out what particles are doing – Deterministic and Monte Carlo
- Monte Carlo follows a neutron over the course of its life, using a random number generator to sample from distributions to make decisions as to what the particle will do while it is alive



Modelling – Monte Carlo Approach

- Many (10^6-10^{10}) source particles ($N_{part.}$) are modeled to obtain an average behavior of the aggregate of particles

Pros:

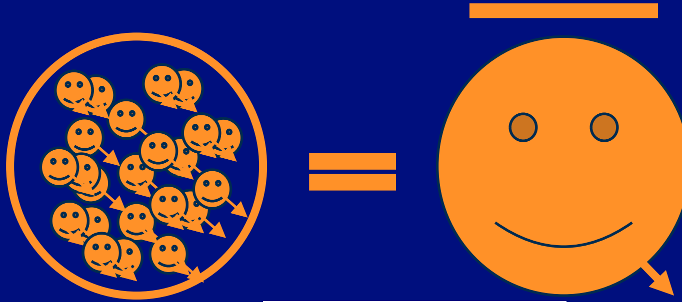
- Highly tunable to a specific quantity of interest
- No need for complicated meshing
- Can use continuous-energy cross sections
- Arguably more intuitive to understand
- User feedback on solution quality through statistical metrics
- “Embarrassingly” parallel

Cons:

- Computationally intensive – variance scales as $1/\sqrt{N_{part.}}$
- Full phase-space solution requires many particles and lots of sophisticated “tricks”

Modelling – Deterministic Approach

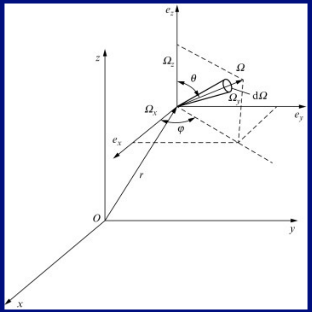
- Rather than follow around individual particles, model the average behavior of particles in a continuum of phase-space
  - In order to be accurate to real-life, the system must be adequately characterized by the mean – many particles must be present



- The neutron distribution is represented by:

$$N(\vec{r}, \vec{\Omega}, E, t)\, d\vec{r}\, d\vec{\Omega}\, dE$$

- **The total number of particles in a differential spatial element $d\vec{r}$ about $\vec{r}$, a differential energy element dE about E, and a differential solid angle element $d\vec{\Omega}$ about $\vec{\Omega}$ at time t**



Modelling – BTE: Assumptions 1/2

- Can use Kinetic Theory of Gases, statistical mechanics, and Newton's Laws to derive the **Boltzmann Transport Equation (BTE)**

NOTE: questioning these assumptions produces much of the cutting-edge research of our transport teams!

1. Particles may be described as **points**
   - On average, particles travel many interatomic distances between collisions
2. Particles travel in straight lines between **point collisions**
   - Particles are neutral
   - Atomic radius << interatomic distance
3. Collisions and absorption/reemission (fission, scattering) events occur **instantaneously**
   - Prompt fission neutrons are emitted 10^{-4}-10^{-5} ns after absorption
4. **Delayed neutrons** may be neglected
   - Not necessary, but it simplifies the equations
   - Delayed neutrons only account for 0.2-0.7% of fission neutrons, depending on target nuclide
5. **Particle-particle** interactions may be neglected

Modelling – BTE: Assumptions 2/2

6. Material properties are **isotropic**
   - Anisotropy can still exist, but only in a relative sense
7. **Neutron decay** can be neglected
   - Neutron half-lives are ~12 minutes, neutron lifetimes are much less
8. The distribution function can be adequately characterized by the **mean**
   - We have enough particles for “good” statistics
   - Also not a requirement – while we never model individual particles with deterministic methods, we can derive equations that model the broader statistical behavior of the distribution
9. Assume the **material is at rest**
   - Also not a requirement, but makes the equation and algorithm for solving it much easier
10. External forces (e.g., gravity) can be neglected

and more…

Modelling – Heuristic Derivation of BTE

- For a differential element centered about a given point in phase space, a statement of particle balance is made

change in particle number = production of neutrons – loss of neutrons

$$\frac{dN}{dt}(\vec{r},\vec{\Omega},E,t) = \dot{G}(\vec{r},\vec{\Omega},E,t) - \dot{L}(\vec{r},\vec{\Omega},E,t)$$

- Production:
  1. Fission: $\bar{\nu}$ neutrons emitted on average
  2. (n,xn) reactions: energy absorbed in neutron capture liberates x neutrons
  3. Source: boundary or volumetric source independent of processes in BTE
- Loss:
  1. Capture: particle is captured by material, regardless if one or more particles are later emitted by the excited nucleus
  2. Leakage: particles exit the domain of interest
- Redistribution (shifting between phase-space elements):
  1. Streaming: particles travel the domain in straight lines with constant momentum
  2. Scattering: collisions with material nuclei cause a change in momentum

Modelling – The BTE in "Numbers"

$$\frac{\partial N}{dt} + \vec{\Omega} \cdot \nabla v(E) N(\vec{r}, \vec{\Omega}, E, t) + \Sigma_t(\vec{r}, E, t) \cdot v(E) N(\vec{r}, \vec{\Omega}, E, t) =$$

$$\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s(\vec{r}, E' \to E, \vec{\Omega}' \cdot \vec{\Omega}, t) \cdot v(E') N(\vec{r}, \vec{\Omega}', E', t)\right] +$$

$$\int_0^\infty dE' \, \bar{\nu}\Sigma_f(\vec{r}, E', t) \chi(E' \to E, t) \cdot \left[\int_{4\pi} d\vec{\Omega}' \, v(E') N(\vec{r}, \vec{\Omega}', E', t)\right] + Q(\vec{r}, \vec{\Omega}, E, t)$$

- $E', \vec{\Omega}'$ – incoming neutron energy, angle
- $v(E)$ – neutron speed
- $\bar{\nu}\Sigma_f(\vec{r}, E', t)$ – average number of neutrons released by fission multiplied by fission cross section
- $\Sigma_s(\vec{r}, E' \to E, \vec{\Omega}' \cdot \vec{\Omega}, t)$ – scattering cross section from E' to E with scattering angle $\vec{\Omega}' \cdot \vec{\Omega}$
- $\chi(E' \to E, t)$ – probability that a fission neutron born from a fission event caused by incoming neutron with energy E' has energy E
- $Q(\vec{r}, \vec{\Omega}, E, t)$ – inhomogeneous source term

Modelling – The BTE in "Numbers"

$$\frac{\partial N}{dt} + \vec{\Omega} \cdot \nabla v(E) N\left(\vec{r}, \vec{\Omega}, E, t\right) + \Sigma_t(\vec{r}, E, t) \cdot v(E) N\left(\vec{r}, \vec{\Omega}, E, t\right) =$$

$$\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s\left(\vec{r}, E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega}, t\right) \cdot v(E') N\left(\vec{r}, \vec{\Omega}', E', t\right)\right] +$$

$$\int_0^\infty dE' \, \bar{\nu} \Sigma_f(\vec{r}, E', t) \chi(E' \rightarrow E, t) \cdot \left[\int_{4\pi} d\vec{\Omega}' \, v(E') N\left(\vec{r}, \vec{\Omega}', E', t\right)\right] + Q\left(\vec{r}, \vec{\Omega}, E, t\right)$$

Time rate of change of the neutron population in the phase space element

Straight-line "streaming" to and from spatial element

Modelling – The BTE in “Numbers”

$$\frac{\partial N}{dt} + \vec{\Omega} \cdot \nabla v(E) N\left(\vec{r}, \vec{\Omega}, E, t\right) + \Sigma_t(\vec{r}, E, t) \cdot v(E) N\left(\vec{r}, \vec{\Omega}, E, t\right) =$$

$$\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s\left(\vec{r}, E' \to E, \vec{\Omega}' \cdot \vec{\Omega}, t\right) \cdot v(E') N\left(\vec{r}, \vec{\Omega}', E', t\right)\right] +$$

$$\int_0^\infty dE' \, \bar{\nu} \Sigma_f(\vec{r}, E', t) \chi(E' \to E, t) \cdot \left[\int_{4\pi} d\vec{\Omega}' \, v(E') N\left(\vec{r}, \vec{\Omega}', E', t\right)\right] + Q\left(\vec{r}, \vec{\Omega}, E, t\right)$$

Total interaction rate, considered a “loss” from the phase-space element, even if the interaction ultimately produces a neutron in the phase-space element.

Modelling – The BTE in "Numbers"

$$\frac{\partial N}{dt} + \vec{\Omega} \cdot \nabla v(E) N(\vec{r}, \vec{\Omega}, E, t) + \Sigma_t(\vec{r}, E, t) \cdot v(E) N(\vec{r}, \vec{\Omega}, E, t) =$$

$$\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega}, t) \cdot v(E') N(\vec{r}, \vec{\Omega}', E', t)\right] +$$

$$\int_0^\infty dE' \, \bar{\nu} \Sigma_f(\vec{r}, E', t) \chi(E' \rightarrow E, t) \cdot \left[\int_{4\pi} d\vec{\Omega}' \, v(E') N(\vec{r}, \vec{\Omega}', E', t)\right] + Q(\vec{r}, \vec{\Omega}, E, t)$$

Scattering from all velocity vectors (including this one) into this one

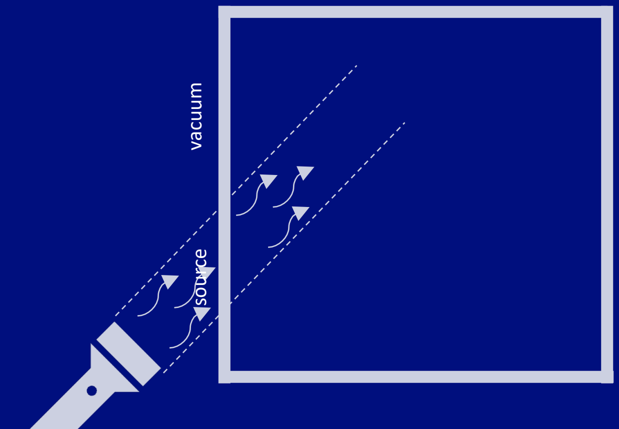
Fission neutrons caused by fissions from all velocity vectors into this one

Inhomogeneous source (all other sources of neutrons)

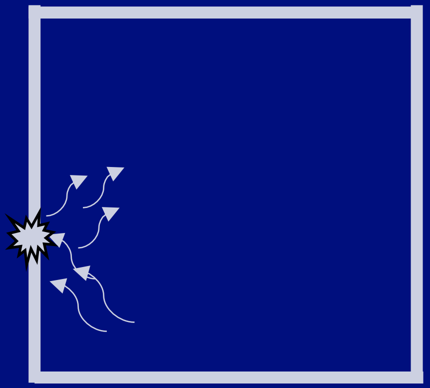
Modelling – BTE Boundary Conditions

- BTE requires boundary fluxes on one edge of the spatial and time boundaries
  - We do not know the end state of the system or the outgoing neutron state, so we make educated approximations of the beginning and inflow neutron states

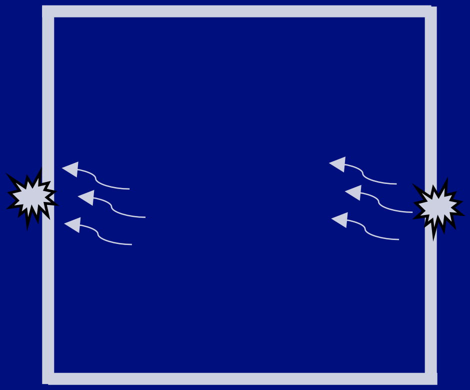
1. Vacuum/Source



2. Reflective/Albedo



3. Periodic



  - Time boundary condition is always an initial condition analogous to 1, but obtaining a suitable initial guess at the neutron distribution is a subject of much work

Modelling – The BTE in "Fluxes"

$$\frac{1}{v(E)}\frac{\partial\psi}{dt} + \vec{\Omega}\cdot\nabla\psi(\vec{r},\vec{\Omega},E,t) + \Sigma_t(\vec{r},E,t)\cdot\psi(\vec{r},\vec{\Omega},E,t) =$$
$$\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s(\vec{r},E'\to E,\vec{\Omega}'\cdot\vec{\Omega},t)\cdot\psi(\vec{r},\vec{\Omega}',E',t)\right] +$$
$$\int_0^\infty dE'\,\bar{\nu}\Sigma_f(\vec{r},E',t)\chi(E'\to E,t)\cdot\phi(\vec{r},E',t) + Q(\vec{r},\vec{\Omega},E,t)$$

- In neutron/gamma transport, we typically operate in angular and scalar "fluxes":

$$\psi(\vec{r},\vec{\Omega},E,t) = v(E)N(\vec{r},\vec{\Omega},E,t)\ \frac{\#}{cm^2\cdot MeV\cdot ster\cdot sh}$$
$$\phi(\vec{r},E,t) = \int_{4\pi} d\vec{\Omega}\,\psi(\vec{r},\vec{\Omega},E,t)\ \frac{\#}{cm^2\cdot MeV\cdot sh}$$

- Linear, time-dependent, integro-differential equation
- 6-dimensional phase-space (+time)
- This equation is the basis for all S_N/P_N/Monte Carlo/MoC transport codes

Stretch Break

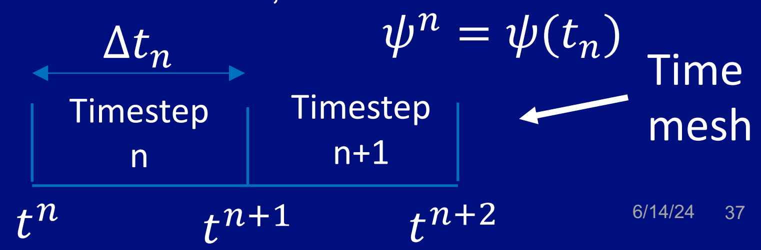
Solving the BTE

Solving the BTE – Summary

- Aside from some extremely idealized and simplified problems, the BTE cannot be solved analytically (i.e., with a pen and paper)
- Each aspect of the phase-space requires discretization
  - Time: first-order derivative
  - Space: first-order derivative
  - Direction: integral
  - Energy: integral
- Typically, many orders of magnitude are spanned by the phase-space, making discretization a difficult problem
  - Note: in the following slides there is a lot of dropping of superfluous indices and dependencies for brevity's sake

Solving the BTE – Time Discretization

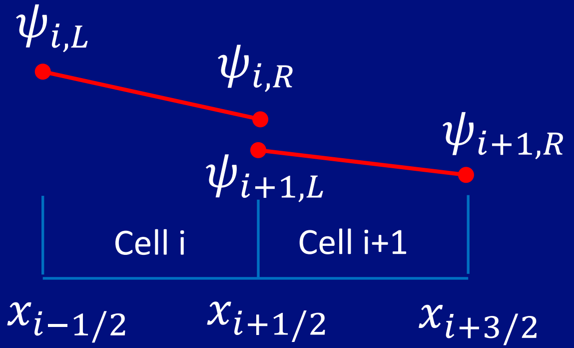
- TRT - Backward Euler: $\frac{1}{\Delta t_n}\int_{t^n}^{t^{n+1}} dt\,\psi(t) \approx \psi^{n+1}$
  - Pros: robust - no oscillation, implicit (unconditionally stable), always positive (physically correct) - good for large opacities in TRT
  - Cons: only $O(\Delta t)$, often unable to resolve absorption-emission timescales in TRT
- n/γ - Crank-Nicolson: $\frac{1}{\Delta t_n}\int_{t^n}^{t^{n+1}} dt\,\psi(t) \approx \frac{\psi^{n+1}+\psi^n}{2}$
  - Pros: semi-implicit (still unconditionally stable), $O(\Delta t^2)$, can resolve typical time-scales for n/γ transport
  - Cons: can oscillate at high Δt values, can go negative (physically incorrect)
    - requires flux fixup, which is nonlinear - can cause iterative oscillations, and can be nonconservative

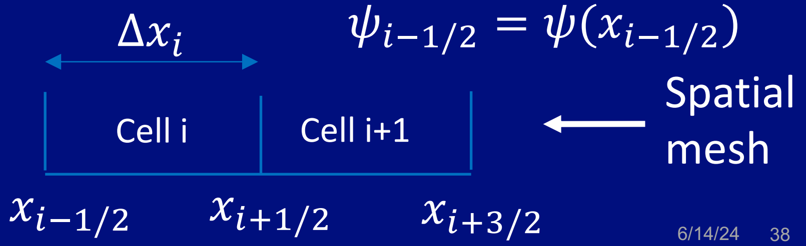


Solving the BTE – Space Discretization

$$\bar{\psi}_i = \frac{1}{\Delta x_i}\int_{x_{i-1/2}}^{x_{i+1/2}} dx\, \psi(x)$$

- n/γ – Diamond difference: $\bar{\psi}_i = \frac{\psi_{i+1/2}+\psi_{i-1/2}}{2}$
  - Analogous to Crank-Nicolson (a.k.a. "diamond difference in time") – same pros and cons
- TRT – LDFEM: $\begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix}\begin{pmatrix}\psi_{i,L}\\ \psi_{i,R}\end{pmatrix} = \begin{pmatrix}\cdot\\ \cdot\end{pmatrix}$ ← Depends on $\psi_{i-1,R}$, assuming $\Omega_x > 0$
  - Pros: $O(\Delta x^2)$, always positive, approaches the diffusion limit
  - Cons: $2^{N_{dim.}}$x more unknowns than DD → higher memory usage and longer compute times

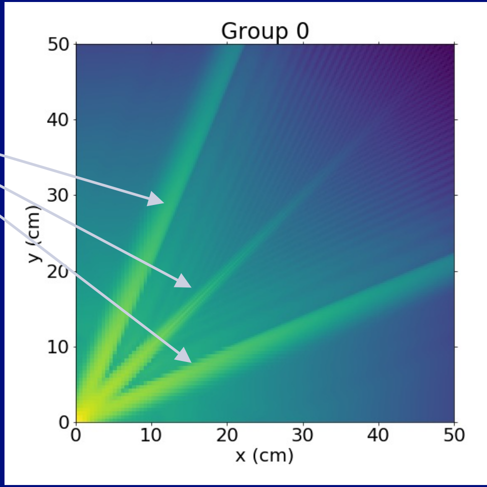




Solving the BTE – Angle Discretization: Collocation

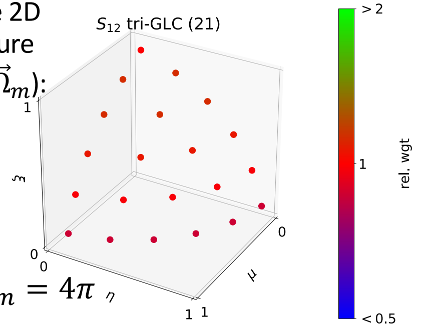
TRT/n/γ – Discrete Ordinates (S_N): $\phi = \int_{4\pi} d\vec{\Omega}\ \psi(\vec{\Omega}) \approx \sum_{m=1}^{M} w_m \psi(\vec{\Omega}_m)$

- Use quadrature rules to solve integrals by performing discrete summation
  - choice of quadrature weights (w_m) and "points" ($\vec{\Omega}_m$) on the unit-sphere is important
- Pros: highly tunable to problem of interest – can "aim" at important areas of the domain, parallelizable
- Cons: ray effects – unphysical numerical artifacts



Example 2D quadrature points ($\vec{\Omega}_m$):

$$\sum_{m=1}^{M} w_m = 4\pi$$

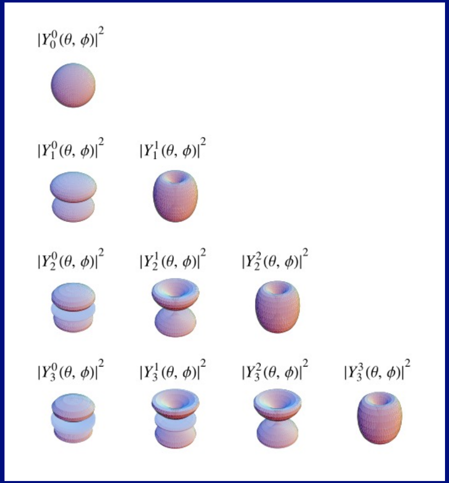


Solving the BTE – Angle Discretization: Anisotropic Scattering

n/γ – Spherical Harmonics:

$$\phi_{kl} = \sum_{m=1}^{M} Y_{kl}\,(\vec{\Omega}_m) w_m \psi(\vec{\Omega}_m)$$

$$\psi(\vec{\Omega}_m) = \sum_{k=0}^{K} \sum_{l=-k}^{k} Y_{kl}(\vec{\Omega}_m)\phi_{kl}$$



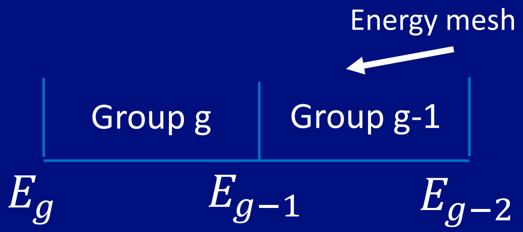
c/o – Wolfram Alpha

- Angular moments of the scattering cross section come from nuclear data team
- Able to approximate anisotropic scattering:

$$\int_{4\pi} d\vec{\Omega}' \left[\Sigma_s(\vec{\Omega}' \cdot \vec{\Omega}_m) \cdot \psi(\vec{\Omega}')\right] \approx \sum_{k=0}^{K} \sum_{l=0}^{k} (2 + \delta_{m0}) Y_{kl}(\vec{\Omega}_m) \Sigma_{s,k} \phi_{kl}$$

TRT – Isotropic scattering sufficient to describe most processes

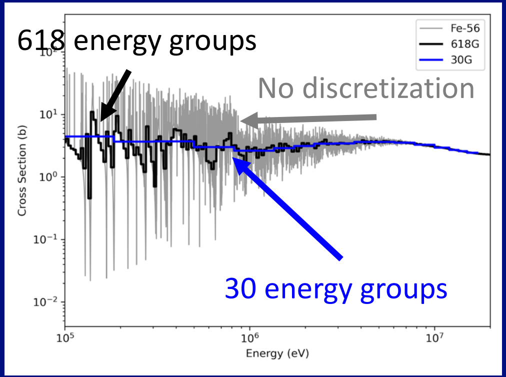
Solving the BTE – Energy Discretization



- Multigroup approximation - weighted average of cross sections over group
  - n – group 1 is highest-energy; γ/TRT – group G is highest-energy

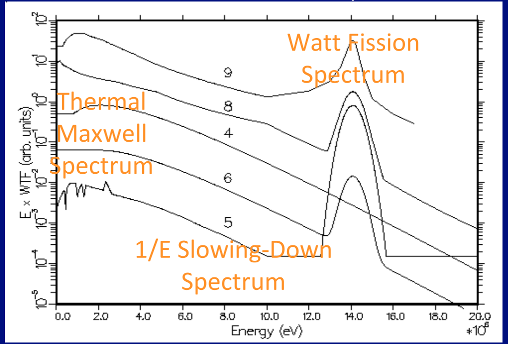
$$\Sigma_{x,g} = \frac{\int_{E_g}^{E_{g-1}} dE\, f(E) \Sigma_x(E)}{\int_{E_g}^{E_{g-1}} dE\, f(E)}$$

$$\psi_g = \int_{E_g}^{E_{g-1}} dE\, \psi(E)$$



Fe-56 cross section (full of resonances)

- Accuracy of multigroup approximation depends on $f(E)$
  - $\Sigma_{x,g}$ would be EXACT if $f(E) = \psi(E)$, but $\psi(E)$ is not known
  - In practice, ψ is a function of the full phase-space, so it will *never* be exactly right

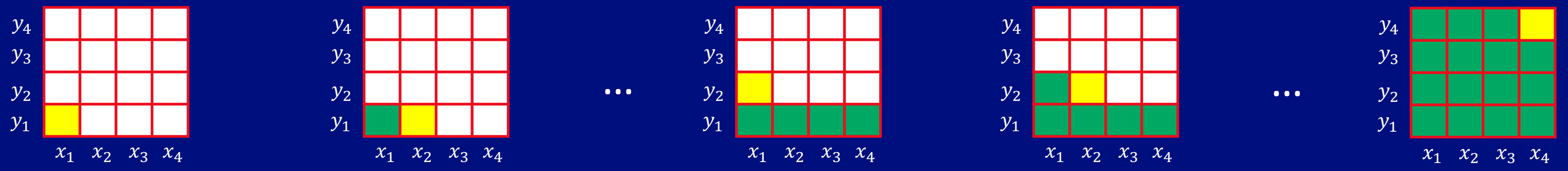


Example $f(E)$

Solving the BTE – The Transport Sweep

- The discretized BTE forms a linear system for each angle and group that can be solved by back substitution
  - We never actually form the linear system, which would be huge - we do the back substitution on the fly in what is called a "sweep"

Sweep Step 1	Sweep Step 2		Sweep Step 5	Sweep Step 6		Sweep Step 16
$\Omega_x > 0, \Omega_y > 0$	$\Omega_x > 0, \Omega_y > 0$		$\Omega_x > 0, \Omega_y > 0$	$\Omega_x > 0, \Omega_y > 0$		$\Omega_x > 0, \Omega_y > 0$



Compute $\psi_{m,1,1}$ from known inflows	Compute $\psi_{m,2,1}$ from $\psi_{m,1,1}$ and known inflow	Compute $\psi_{m,1,2}$ from $\psi_{m,1,1}$ and known inflow	Compute $\psi_{m,2,2}$ from $\psi_{m,2,1}$ and $\psi_{m,1,2}$	Compute $\psi_{m,4,4}$ from $\psi_{m,3,4}$ and $\psi_{m,4,3}$

- "But wait… isn't the right-hand side of the equation dependent on ϕ, which is dependent on ψ, which is what you're solving for?"

Solving the BTE – Inner and Outer Iterations

L - LHS of BTE
S_{in-g} - Within-group scattering source
S_{out-g} - Out-group scattering source
F - Fission source
Q - Inhomogeneous source term

- Inner iterations:
  - for a given energy group, the angular flux solution is obtained with the previous inner and outer iteration's scattering and fission source
  - after the sweeps are finished, update the in-group scattering, and do another set of sweeps
  - when the iterative error of the scalar flux solution reaches a user-defined threshold, inner iteration has converged
- Outer iterations:
  - when all energy groups have converged their inner iterations, update out-group scattering and fission, and proceed with another set of inner iterations
  - continue until outer iterations reach convergence

Inner: $L\psi^{s+1} = S_{in-g}(\phi^s) + S_{out-g}(\phi^r) + F(\phi^r) + Q; \phi^{s+1} = \sum_{m=1}^{M} w_m \psi_m^{s+1}$

if $\|\phi^{s+1}-\phi^s\| / \|\phi^s\| \le \epsilon$, continue to outer, else, $s = s+1$, do another inner

Outer: $\phi^{r+1} = \phi^{s+1}$, if $\|\phi^{r+1}-\phi^r\| / \|\phi^r\| \le \epsilon$, you are done ☺, else, $r = r+1$, go back to inner

For those keeping track, we're up to $\geq$ 10 indices now…

Solving the BTE – Source Iteration

The previous scheme is known as "Source Iteration" (SI) or "fixed-source iteration"

- Requires an initial guess of the solution
  - For time-dependent, the previous time-step's solution will do, though you can "time accelerate"
  - For static, zero everywhere or a constant value tends to be popular

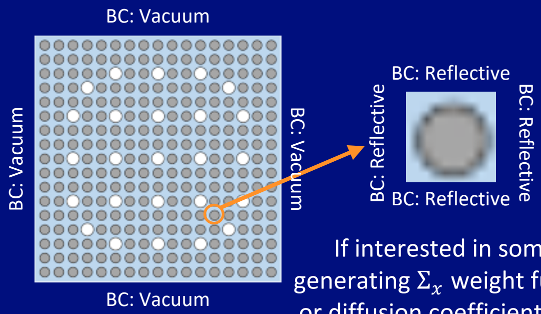
ϕ^1 - Uncollided Flux ϕ^2 - 1st-collision Flux ϕ^3 - 2nd-collision Flux ϕ^4 - 3rd-collision Flux etc.

For a zero initial guess, each SI iteration "s" corresponds with the $(s-1)$th-collision source,
i.e., the sth iteration is the solution of particles that have undergone $(s-1)$ collisions

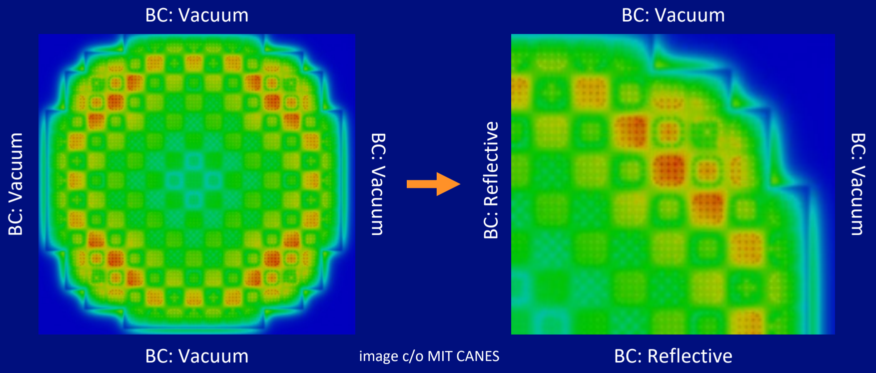
- For highly-scattering (optically-thick) media, it takes many iterations to converge
  - Other linear solvers (e.g., GMRES, Gauss-Seidel, Davidson) exist
  - Acceleration methods also exist
    - Diffusion Synthetic Acceleration (DSA)
    - Variable Eddington Factor (VEF), a.k.a., Quasi-Diffusion (QD)
    - Nonlinear Diffusion Acceleration (NDA)
    - Coarse Mesh Rebalance (CMR), Multilevel/Multigrid, High-Order-Low-Order (HOLO) schemes

Solving the BTE – Simplification

- If I haven’t convinced you already - it is a lot of work to solve the BTE deterministically
- We try not to solve a full phase-space system if we can help it
  - Represent a 3D geometry as 2D or 1D
  - Use tricks to reduce number of unknowns
  - Model with steady-state when possible



If interested in something like peak pin power, generating Σ_x weight functions, collapsing group sets, or diffusion coefficients, no need to model the entire reactor or even the entire fuel pin lattice

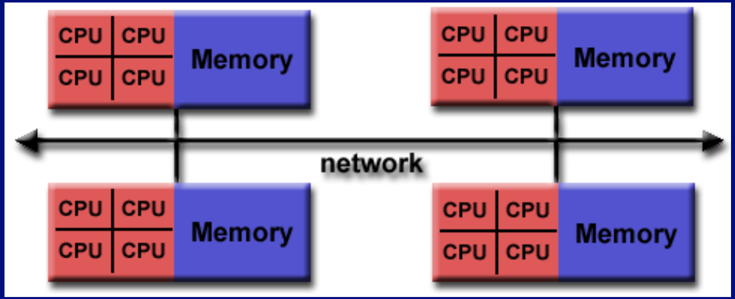


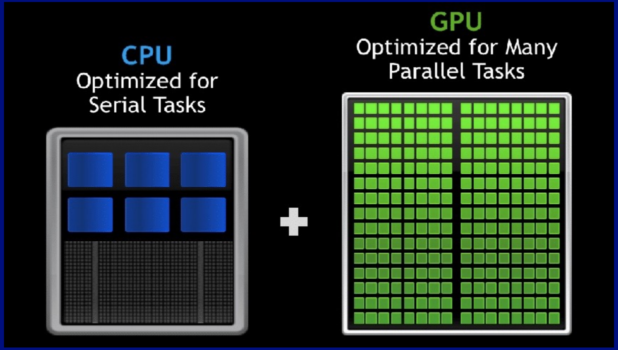
Judiciously using reflective BCs to take advantage of symmetry decreases unknowns by 4x

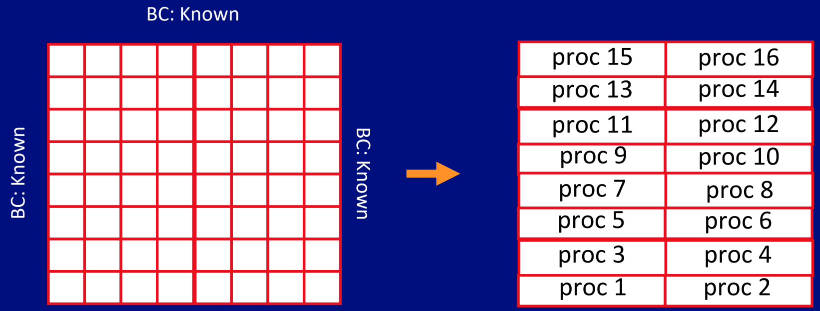
- Reactor design *needs* to take advantage of modelling tricks afforded by the BTE

Solving the BTE – Parallelism

- General 3D deterministic transport is intractable without leveraging parallel computing
- The catch: Integro-differential nature of BTE makes exposing parallelism difficult
- Some flexibility in how we parallelize – energy, angle, space







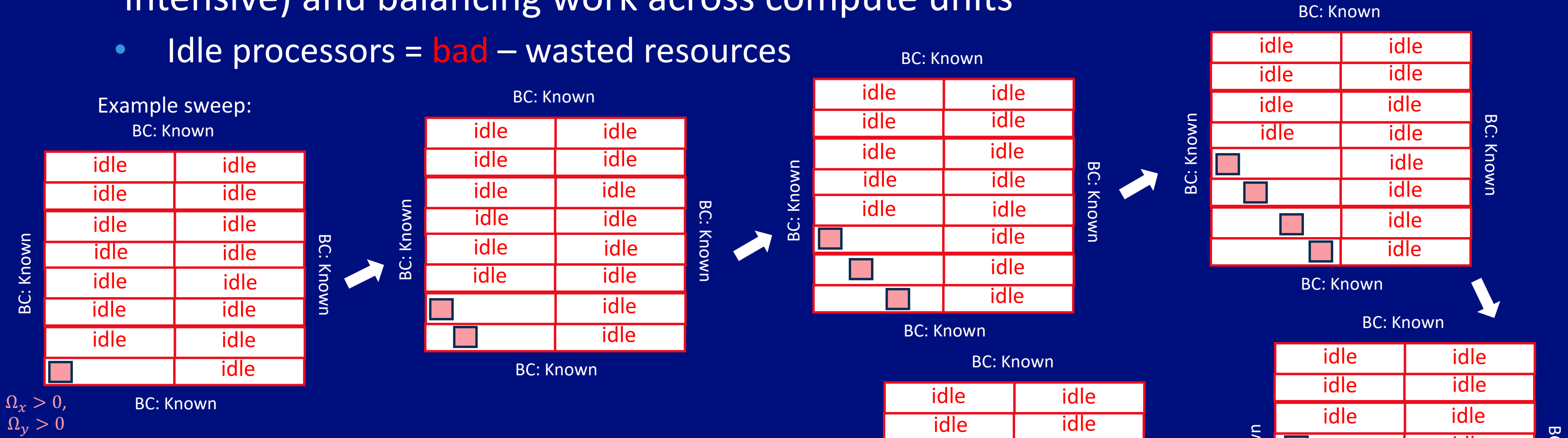
x-y Spatial Mesh

16 Proc Spatial Decomposition

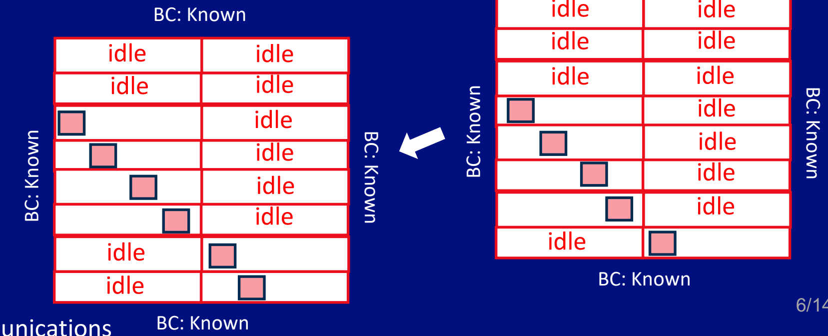
one 8x8 domain becomes 16 4x2 domains with BCs updated iteratively

Solving the BTE – Parallelism

- Parallelism is a balance between reducing communications (very computationally intensive) and balancing work across compute units
  - Idle processors = bad – wasted resources



Max of 8 procs (50%) working at any given time in this example.
16 stages/octant.

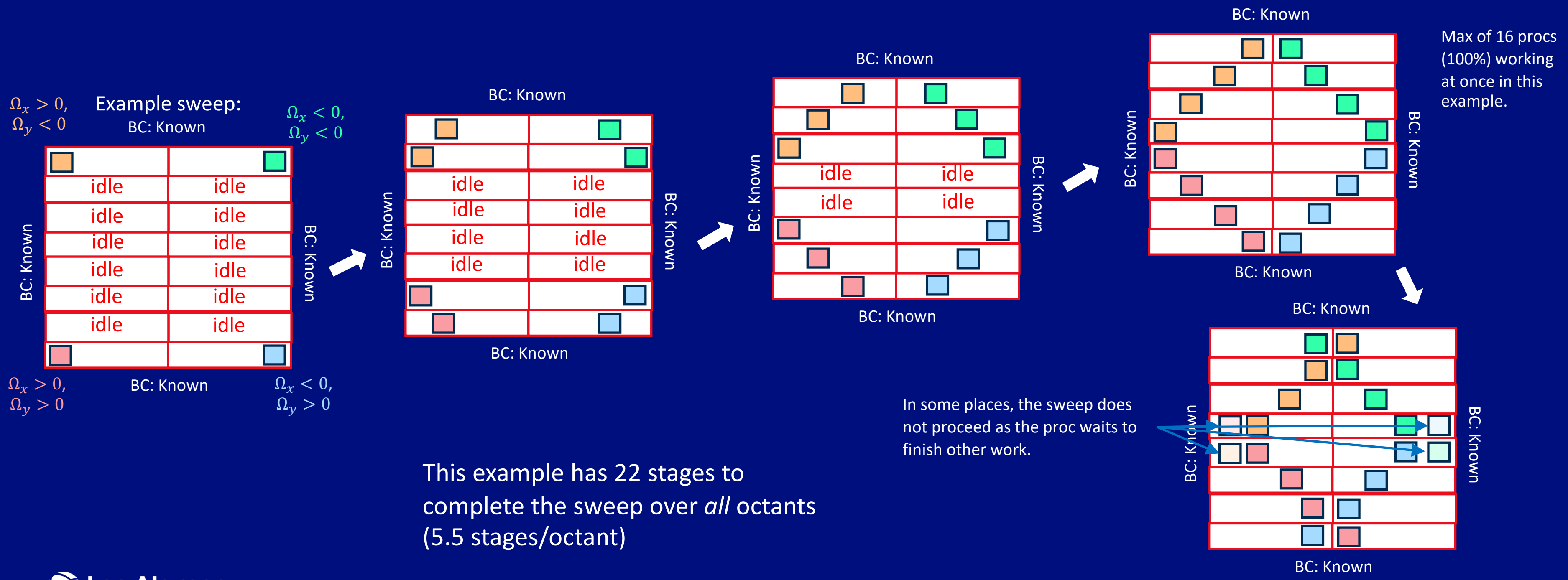


stage – a piece of work bookended by cross-processor communications

Los Alamos NATIONAL LABORATORY

Solving the BTE – Multisweep

- To minimize communications and increase work distribution, we utilize multisweep



This example has 22 stages to complete the sweep over *all* octants (5.5 stages/octant)

Solving the BTE – Summary

- To summarize, in order to make a working deterministic transport solver, you need:
  - angle discretization
    - + anisotropic scattering approximation
    - + directional derivative scheme for non-Cartesian geometries
  - space discretization
    - I have not even covered meshing; n/γ is typically structured rectangular, TRT is unstructured arbitrary polygons/polyhedral
  - energy discretization
    - + accurate nuclear data and weight functions
  - time discretization
  - iterative scheme
    - + possibly an acceleration scheme
  - probably a parallelism scheme if you want to solve anything anyone cares about with alacrity
  - a lot of money to buy after-work beers

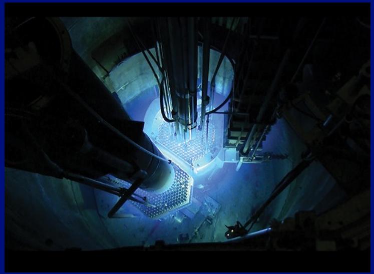
Advanced Transport Methods

Advanced Transport Methods – k_{eff}-Eigenvalue

- For a static approximation ($t \to \infty, \frac{\partial \psi}{\partial t} = 0$), it is impossible to converge the transport solution for a supercritical system
  - Fission neutron production will grow towards infinity with each successive iteration
  - We define a k_{eff}-eigenvalue problem that balances fission production with losses (dependencies dropped for brevity)

$$\vec{\Omega} \cdot \nabla \psi_k + \Sigma_t \cdot \psi_k = \int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s \cdot \psi_k\right] + \frac{1}{k_{eff}} \int_0^\infty dE' \, \bar{\nu} \Sigma_f \chi \cdot \phi_k$$

- Three states: supercritical ($k_{eff} > 1$), critical ($k_{eff} = 1$), subcritical ($k_{eff} < 1$)
- Accurate flux solution when close to critical (like a reactor), can normalize the integrated flux to a quantity like reactor power
- Also useful in criticality safety



Sandia Labs' ACRR

Advanced Transport Methods – α-Eigenvalue

- Assume material properties are static and define an ansatz: $\psi(t) \approx e^{\alpha t}\psi_\alpha$
  - We define an α-eigenvalue problem that describes the dominant time-dependent state of the system (dependencies dropped for brevity)

$$\frac{\alpha}{v}\psi_\alpha + \vec{\Omega}\cdot\nabla\psi_\alpha + \Sigma_t\cdot\psi_\alpha = \int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s\cdot\psi_\alpha\right] + \int_0^\infty dE'\, \bar{\nu}\Sigma_f\chi\cdot\phi_\alpha$$

- Three states: supercritical ($\alpha > 0$), critical ($\alpha = 0$), subcritical ($\alpha < 0$)
- Can use advanced solvers (like Davidson) to obtain higher order eigenpairs and reconstruct the time-dependent behavior of the solution
- In point kinetics (a 0-D time-dependent representation of the neutron population), the following equation relates α to k_{eff}:

$$\alpha = \frac{k_{eff} - 1}{l}$$

Neutron lifetime - the total phase-space-integrated loss rate divided by the neutron population

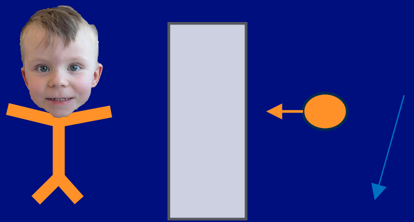
Advanced Transport Methods – Adjoint Transport

- Define an adjoint operator H^* such that $\langle \zeta^* H \zeta \rangle = \langle \zeta H^* \zeta^* \rangle$ is satisfied
- The non-multiplying adjoint transport equation is:

$$\frac{-1}{v(E)}\frac{\partial \psi^*}{dt} - \vec{\Omega} \cdot \nabla \psi^*(\vec{r}, \vec{\Omega}, E, t) + \Sigma_t(\vec{r}, E, t) \cdot \psi^*(\vec{r}, \vec{\Omega}, E, t) =$$

$$\int_0^\infty dE' \int_{4\pi} d\vec{\Omega}' \left[\Sigma_s(\vec{r}, E \to E', \vec{\Omega} \cdot \vec{\Omega}', t) \cdot \psi^*(\vec{r}, \vec{\Omega}', E', t)\right] + Q^*(\vec{r}, \vec{\Omega}, E, t)$$

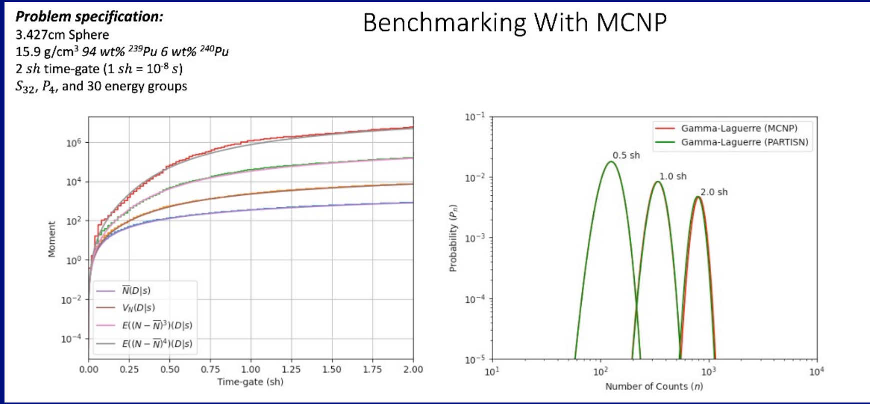
- The adjoint equation can be thought of as going ”backwards” in time and space
  - Initial and inflow boundary conditions are replaced by “final” and outflow boundary conditions
  - ψ^* is often conceptualized as an importance or sensitivity for inverse problems
  - Choice of boundary conditions and Q^* dictate the physical relevance of ψ^* - what is the quantity of interest?



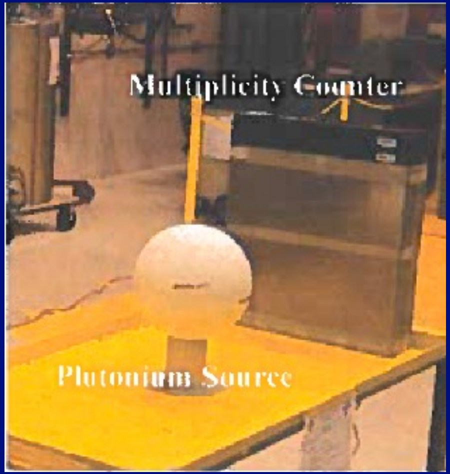
What happens *here* is not very relevant to protecting the worker. The adjoint solution, with a proper Q^*, would tell us that.

Advanced Transport Methods – Stochastic Transport

- We said previously that the deterministic transport solution is only valid as a mean
- We can derive adjoint-like equations that can be solved for either probabilities of specific numbers of neutrons in the system, or moments of the neutron distribution
  - I will spare you even a glimpse of this math, as it's quite overwhelming for an intro talk
  - New eigenvalue problems can be formulated with these equations
- Very useful for nonproliferation and SNM assay



Moussa, Prinja, Hart, Davis, 2023



Mattingly, 2012

Advanced Transport Methods – Moving Materials

- Define a general neutron transport equation in co-moving frame:

$$\frac{\partial N}{\partial t} + \vec{\nabla}_{\vec{r}} \cdot (\vec{u}N) + \vec{q} \cdot \vec{\nabla}_{\vec{r}} N + \Sigma_t q N = \dot{G} + \vec{\nabla}_{\vec{q}} \cdot (N\vec{H})$$

$\vec{q}$ - neutron velocity in co-moving frame

$\vec{u}$ - material velocity

$\dot{G}$ - combined source term

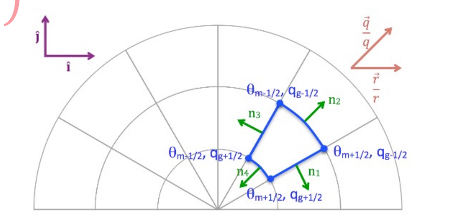


Figure 1. Velocity mesh.

Davis, 2018

- Spatial advection term – how material motion affects spatial position of neutrons
- Momentum advection term – how material motion affects energy and direction of neutrons
- Requires operator splitting - all the memory and parallelism paradigms we set up for the transport operator pretty much get nuked by the momentum advection operator

Advanced Transport Methods – Error Transport

- Cast the transport equation in operator notation as:

$$L\psi = \dot{G} + q$$

- The spatially discretized equation and solution become:

$$\tilde{L}\tilde{\psi} = \dot{\tilde{G}} + q$$

- Inserting ψ into the discretized equations gives:

$$\tilde{L}\psi = \dot{G} + q + R$$

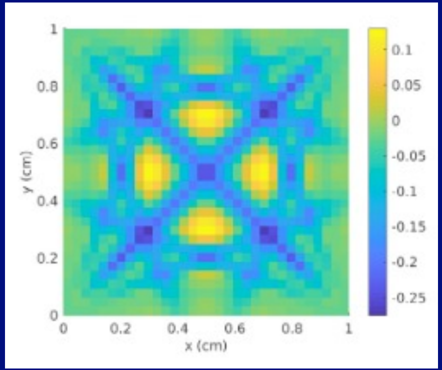
Residual term – the true solution does not satisfy the discretized equation perfectly

- Subtracting the two gives:

$$\tilde{L}e = \dot{\tilde{G}}_e + R$$

Combined error source term

- Accurately approximating R and solving the transport equation gives an estimate of the spatial discretization error



Example $\log_{10}$ Estimated/True Error
Hart, Azmy, Duo, 2020

Thermal Radiative Transfer

Thermal Radiative Transfer

- Hot materials emit photons at energies proportional to material temperature

$$B(E,T) = \frac{2}{h^3c^2}\frac{E^3}{e^{\frac{E}{kT}}-1}$$ ← Planck Function

$$4\pi\int_0^\infty dE\; B(E,T) = acT^4$$ ← Grows quickly with material temp. (T)

- Simplified TRT equations (nonlinear in T)

Radiation Intensity

$$\frac{1}{c}\frac{\partial I}{\partial t} + \vec{\Omega}\cdot\nabla I(\vec{r},E,\vec{\Omega},t) + \sigma_a(E,T(\vec{r},t))I(\vec{r},E,\vec{\Omega},t) = \sigma_a(E,T(\vec{r},t))B(E,T(\vec{r},t))$$

$$C_v(\vec{r},t)\frac{\partial T(\vec{r},t)}{\partial t} = \int_{4\pi} d\vec{\Omega}'\int_0^\infty dE'\,\sigma_a(E',T(\vec{r},t))\left[I(\vec{r},E',\vec{\Omega}',t) - B(E',T(\vec{r},t))\right]$$

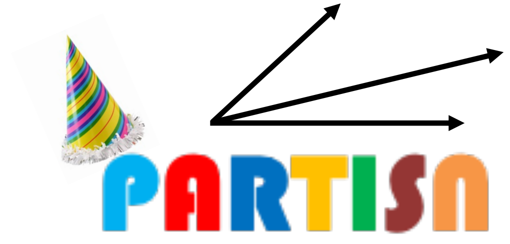
Material Temp.

- Intensity (I) and temperature are coupled, hence, nonlinear
- Radiation deposits energy non-locally (heat transfer)

Congrats! You now know everything there is to know about deterministic transport (well, not really…)

Deterministic Particle Transport at LANL

- Workhorse deterministic code for neutron/gamma transport:



- Workhorse deterministic code for thermal radiative transfer:

Acknowledgements

- Thank you to Tom Saller (CCS-2) and Andrew Till (LLNL) by extension for providing reference slides
- Thank you to all the people sitting in 03-0422 who I bothered while fact-checking this presentation

- Alex Long (XCP-3) will be giving a lecture on Monte Carlo particle transport methods