CERT

Center for Exascale Radiation Transport

Uncertainty Quantification and Predictive Science for High-Energy Density Radiative Transfer using Neutron Experiments

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TEXAS A&M ENGINEERING EXPERIMENT STATION | University of Colorado Boulder | SFU SIMON FRASER UNIVERSITY ENGAGING THE WORLD | NUCLEAR ENGINEERING TEXAS A&M UNIVERSITY

Our Team

- Center for Exascale Radiation Transport (CERT) is an Single Disciplinary Center funded by the US Dept. of Energy / NNSA's Predictive Science Academic Alliance Program (PSAAP).

- Texas A&M
  - NUEN: Morel (PI), Adams, Ragusa, Braby, McClarren
  - CS: Amato, Rauchwerger
- Colorado
  - Applied Math: Manteuffel, Mccormick
- Simon Fraser
  - Bingham

CERT's Goals

- The central goal of CERT is

To maximally improve predictive science for thermal radiation transport.

- Scientific and engineering research will be required to achieve our goal:
  - Iterative solution methods.
  - Space-angle AMR methods.
  - Parallel transport algorithms and models.
  - Exascale computer science research and infrastructure development.
  - Solution verification.
  - Hierarchical VVUQ.
  - Subgrid models.

Where we hope to have an impact.

- CERT research will contribute to general radiation transport (thermal radiation, neutrons, gamma-rays, charged-particles, etc.)
- General radiation transport plays a major role in national security programs.
  - Stockpile stewardship.
  - Nuclear non-proliferation.
  - Homeland security.
- General radiation transport also plays a major role in non-defense applications.
  - Medical diagnostics and treatment planning.
  - Climate modeling.
  - Semiconductor design (electron-hole transport).
  - Astrophysics.

Our target application is thermal radiation transport

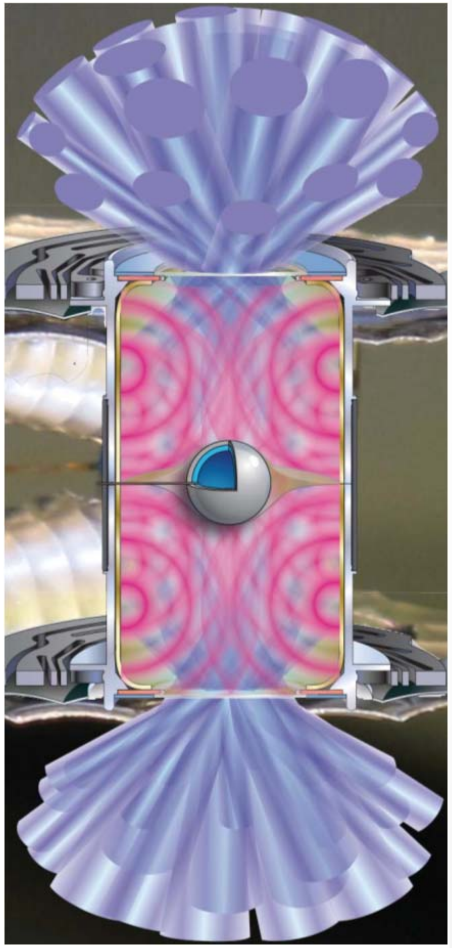
- Thermal radiation transport in the high-energy density laboratory physics (HEDLP) regime

$$\frac{1}{c}\frac{\partial I}{\partial \tau} + \hat{\Omega}\cdot\nabla I + \kappa_{\mathrm{t}} I(\vec{r},\hat{\Omega},\nu,\tau) = Q^{\mathrm{Planck}}(\vec{r},\nu,\tau) + q^{\mathrm{RScat}}(\vec{r},\hat{\Omega},\nu,\tau)$$

$$C_{\mathrm{v}}\frac{\partial T}{\partial \tau} = \int_{0}^{\infty} d\nu \int_{4\pi} d\Omega \left(\kappa_a I(\vec{r},\hat{\Omega},\nu,\tau) - Q^{\mathrm{Planck}}(\vec{r},\nu,\tau)\right)$$

Our Problem is multiscale

- HEDLP thermal radiation transport is multiscale in time, space, and direction.
  - Solutions evolve over vastly different time scales in streaming and diffusive regimes.
  - Mean-free-paths vary in energy over many orders of magnitude, resulting in subgrid phenomena.
  - Spatial boundary layers exist at the interface between streaming and diffusive regions.
  - Small streaming paths can require microsteradian resolution.



Why Exascale Radiation Transport?

- Predictive capability for HEDLP thermal radiation transport can be greatly improved by exascale computing.
    - The transport equation is seven dimensional, yielding the “curse of dimensionality”.
    - 10^{15} unknowns easily required.
    - Multiple time scales requires implicit iterative solution techniques.
    - High resolution 3D calculations will not be possible in many cases even with exascale computers.
- Thermal radiation physics essential for HEDLP.
- NNSA has significant investment in HEDLP.
    - National Ignition Facility, Omega Laser, Z-Machine .....
- In HEDLP simulations, transport usually dominates resource requirements, so efficient solution important.

Radiation Transport vs. Radiation Hydrodynamics

- Realistic HEDLP radiation transport modeling requires rad-hydro.
- Rad-hydro simulation of HEDLP experiments is problematic:
  - Sources of errors are difficult to experimentally infer.
  - UCNI code.
  - Fewer resources for transport.
- Thus we chose to avoid HEDLP experiments and do transport experiments outside the HEDLP regime.
  - This is the tricky part.

Neutrons as surrogates

- We have chosen neutron experiments as a surrogate for thermal radiation experiments after considering other options.
- Neutrons share many properties with thermal radiation transport.
  - The transport equations for both essentially exact.
  - Concept of cross sections same.
  - Radiation and neutron streaming same.
  - Radiation and neutrons have diffusion limit.
  - Radiation and neutrons multiscale in time, space, and direction.
- There are differences too.
  - Temperature coupling through Planck function.
  - Neutron scattering always important.
  - Neutron scattering more complicated than absorption/re- emission.

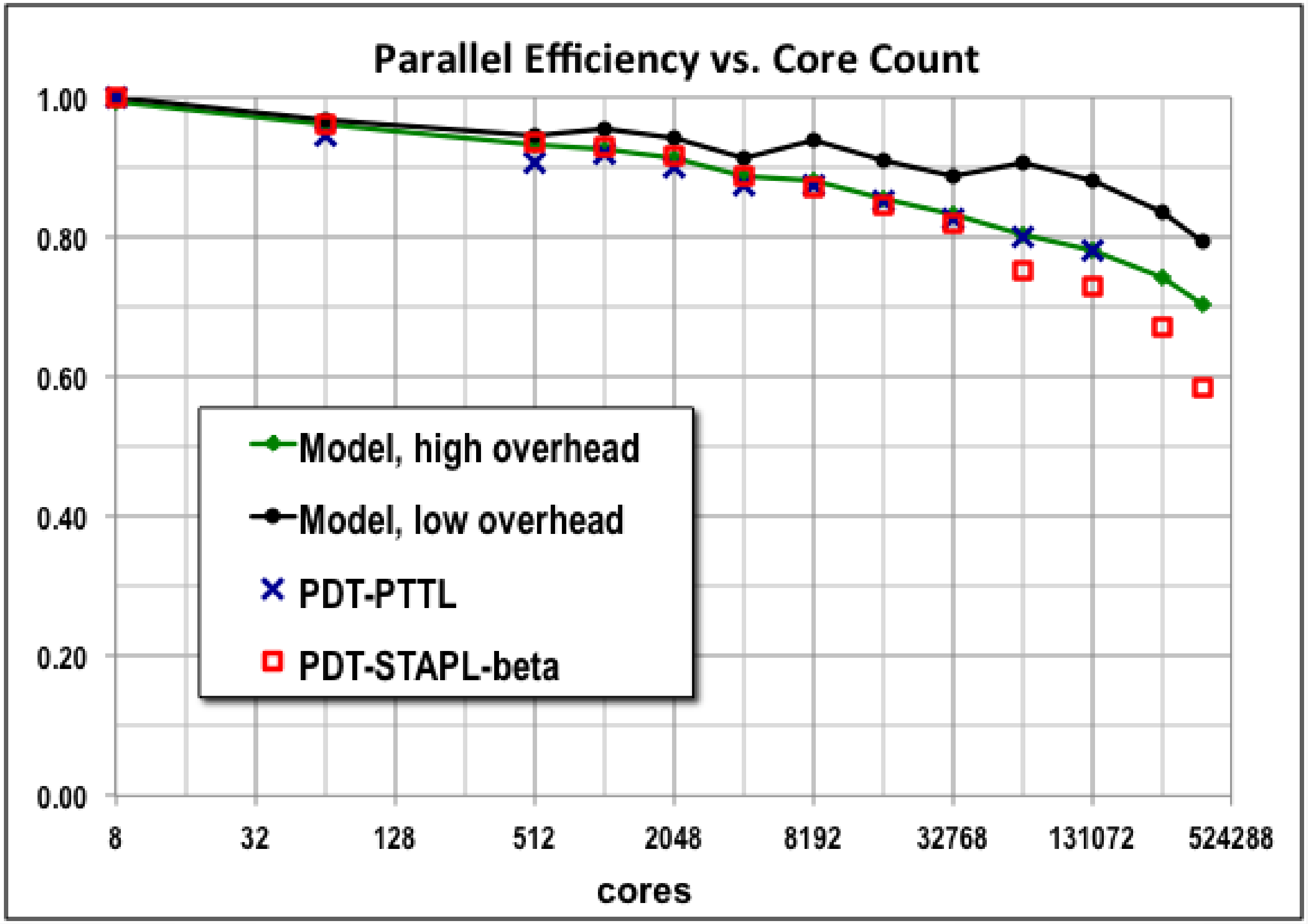
Predictive science gains higher with neutron experiments than with HEDLP experiments.

- Negligible physics model error.
- Neutron mean-free paths long enough for resolved measurements, but short enough for diffusion limit.
- Can perform experiments requiring or not requiring subgrid models.
- Enables powerful hierarchical VVUQ approach.
- We have a new VVUQ technique in which we define nonlinear thermal radiation problems that have solutions equal to experimentally determined neutron solutions.

Making Sweeps Parallel

- The discretized equations have a block lower-triangular system.
- The "sweep“ solves this system by marching through the spatial domain in the direction of particle flow, for all directions in the quadrature set.
- High parallel efficiency is difficult to achieve because of the sequential marching.
- Thus, achieving high parallel efficiency is difficult, but our performance models (which have so far worked well) indicate that with nested parallelism we can maintain excellent weak scaling of sweeps beyond 10M cores.
- Details depend on grid type and numbers of energy groups and directions.

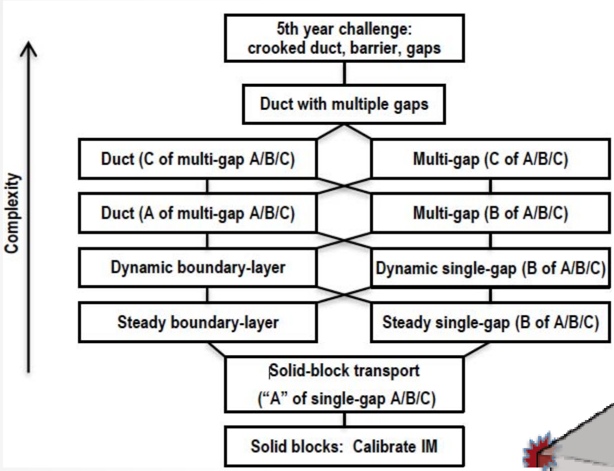
Sweeps can scale better than conventional wisdom suggests.

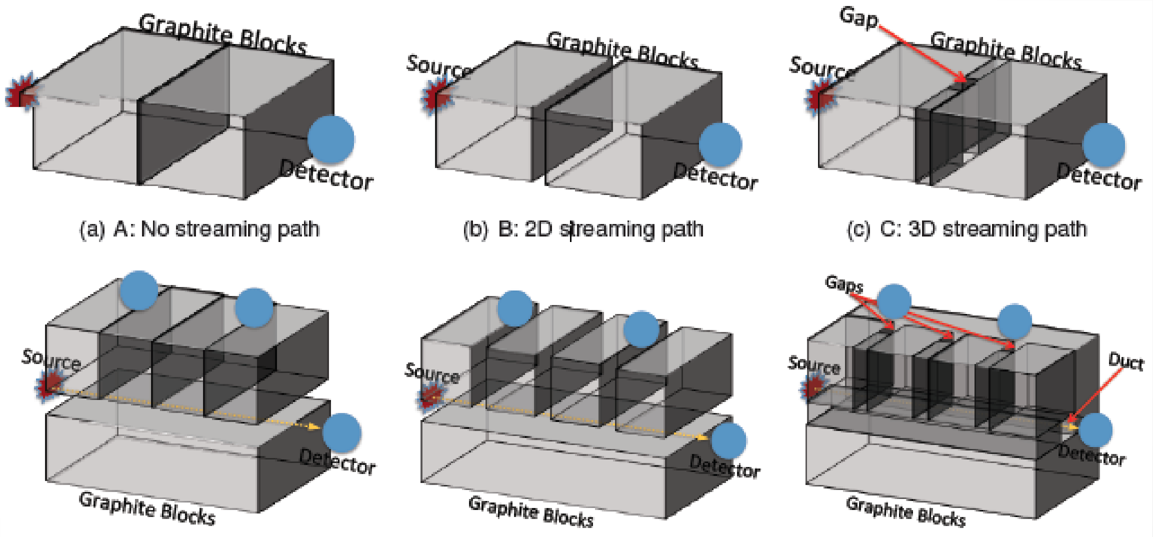


Neutron Experiments

- We will perform experiments using an accelerator- driven fusion source of neutrons which transport through graphite.
- Our experiments will follow a hierarchical VVUQ approach that enables us to infer specific numerical errors in our simulations.
- Our experiments start out with individual graphite bricks for the purpose of calibrating an impurity model.
- Then they become increasingly complicated with streaming paths, diffusive regions, and barriers.

We consider a hierarchy of studies with increasing problem complexity

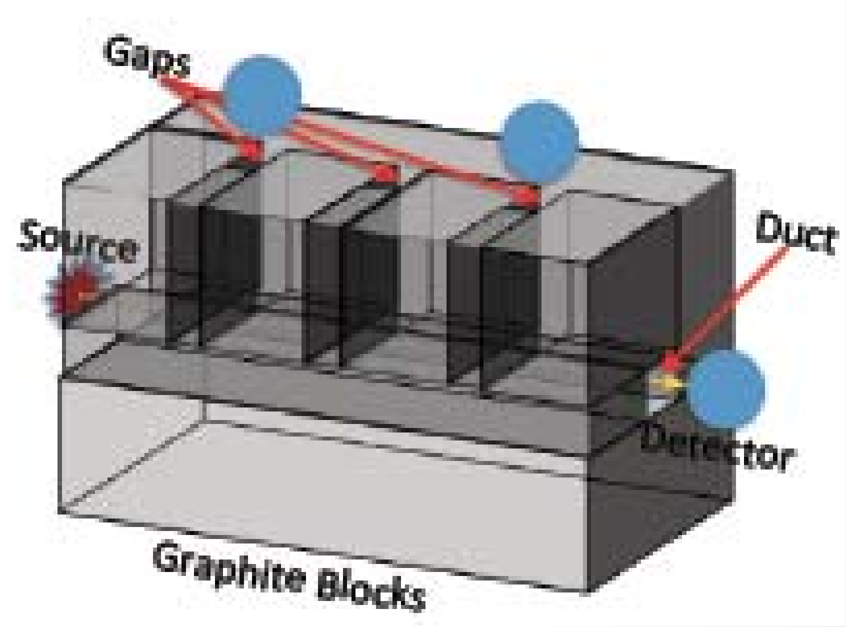




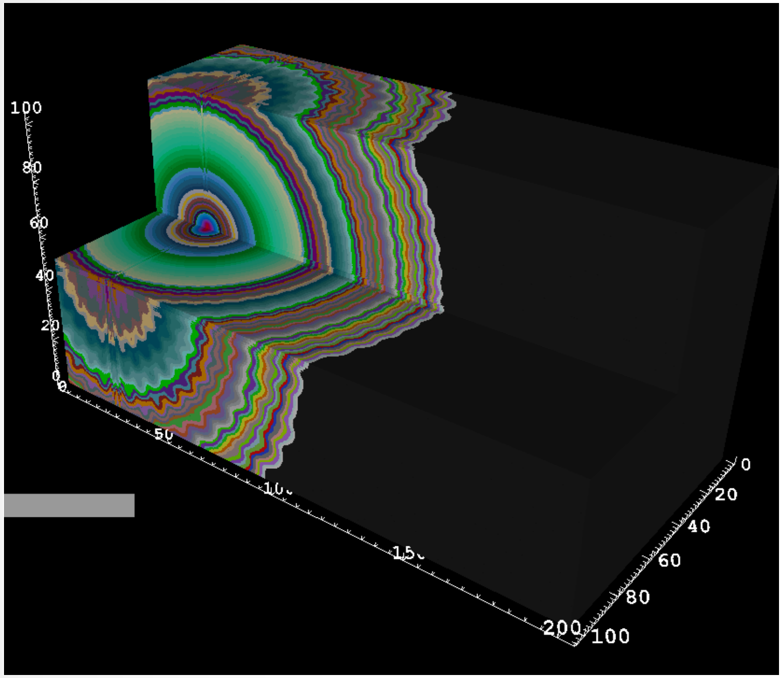
(a) A: No streaming path
(b) B: 2D streaming path
(c) C: 3D streaming path
(d) A': No streaming path
(e) B': 2D streaming path
(f) C': 3D streaming path

Challenge Experiment

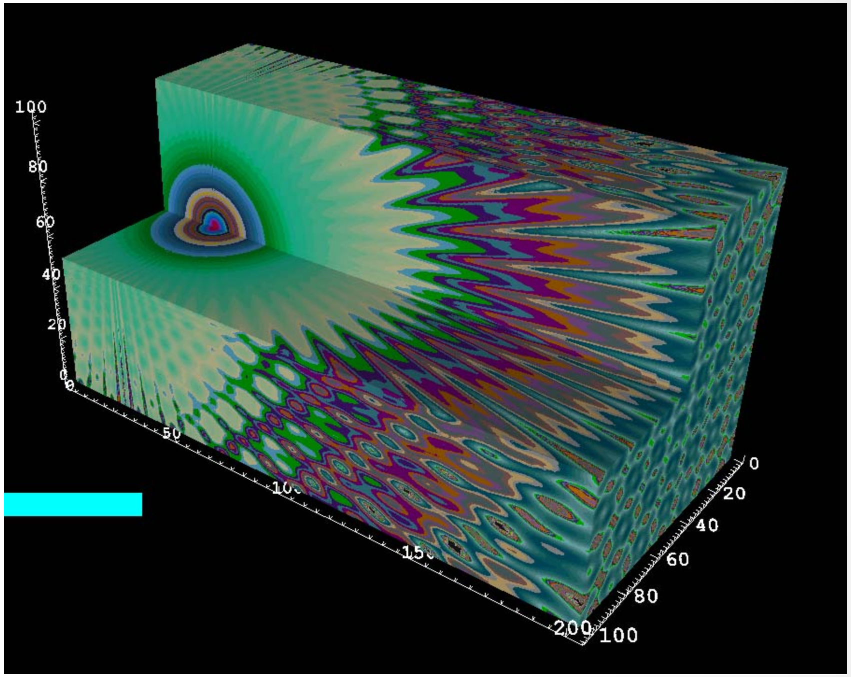
- The Year 5 experiments combine large and extremely small streaming paths, diffusive regions, and barriers:
- Our measurements will be made both in time-dependent and steady-state mode.
- Our QOI’s will take the form of detector responses and foil responses.



14 MeV Solution

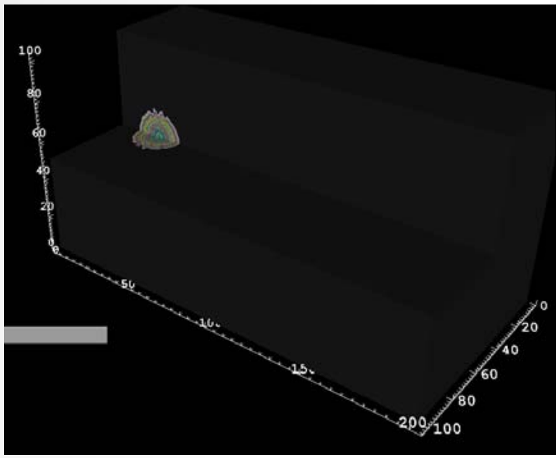


10 ns after pulse
8192 directions

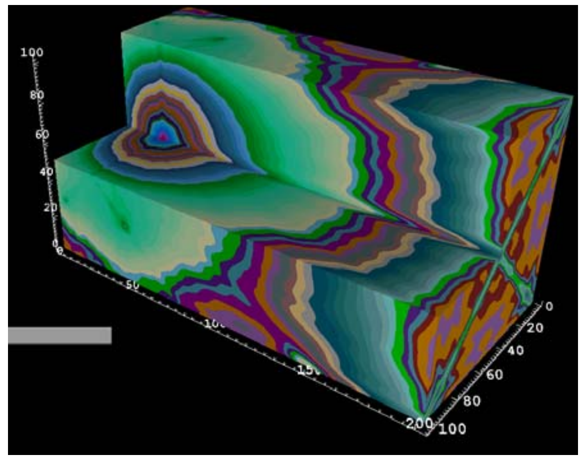


50 ns after pulse
8192 directions
¡still have ray effects!

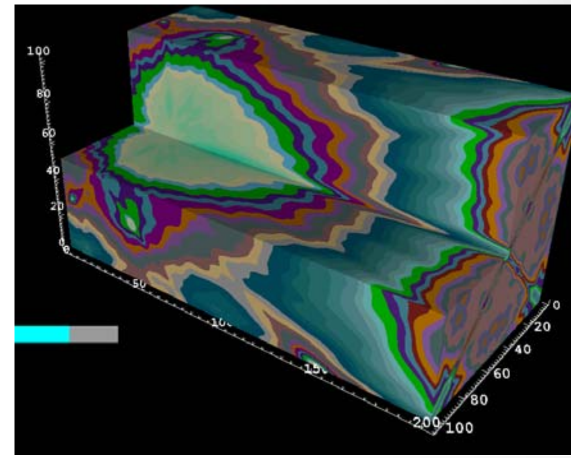
Thermal Neutrons



500 ns after pulse
8192 directions



10^5 ns after pulse
8192 directions



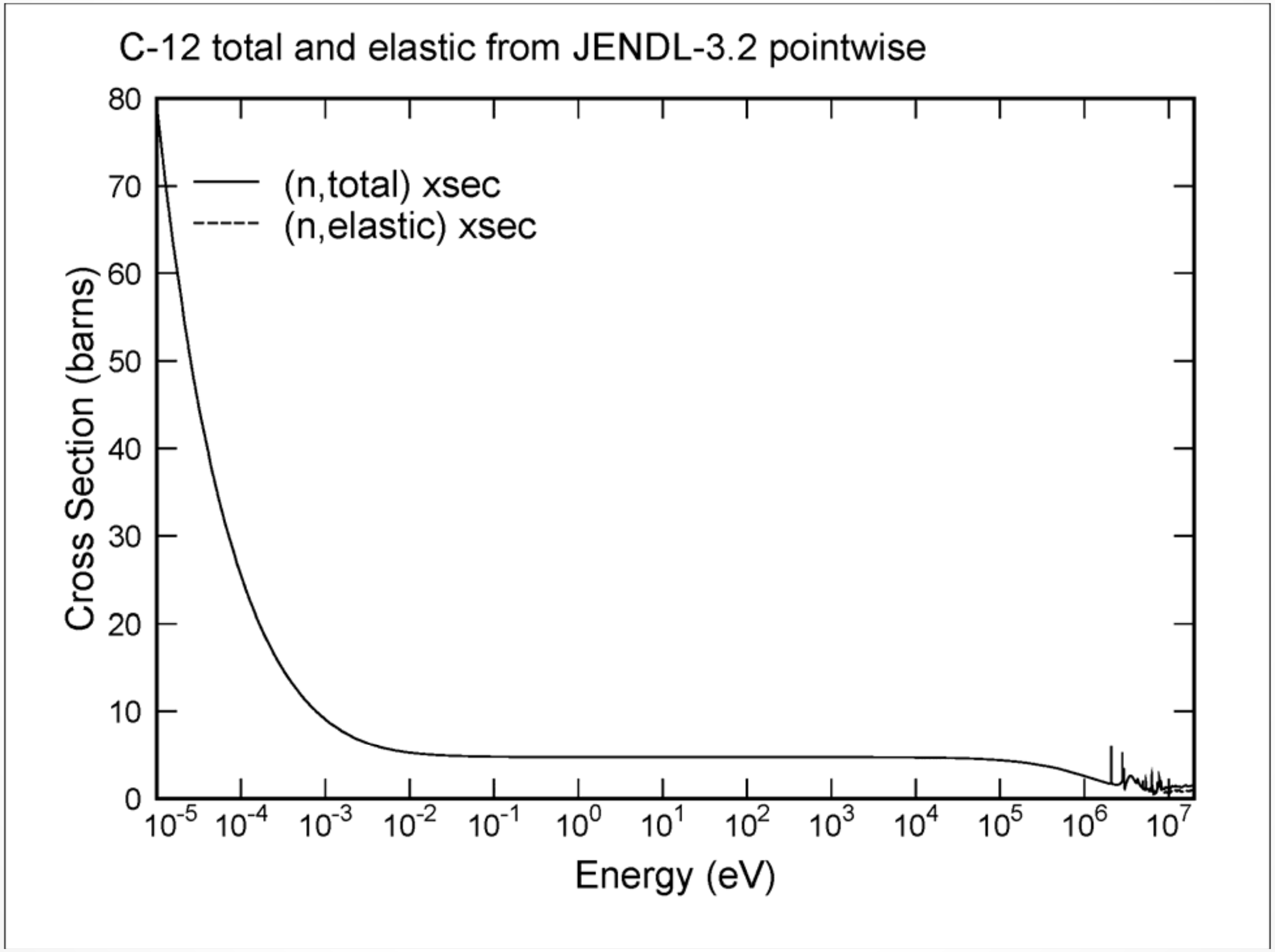
2 x 10^5 ns after pulse
8192 directions

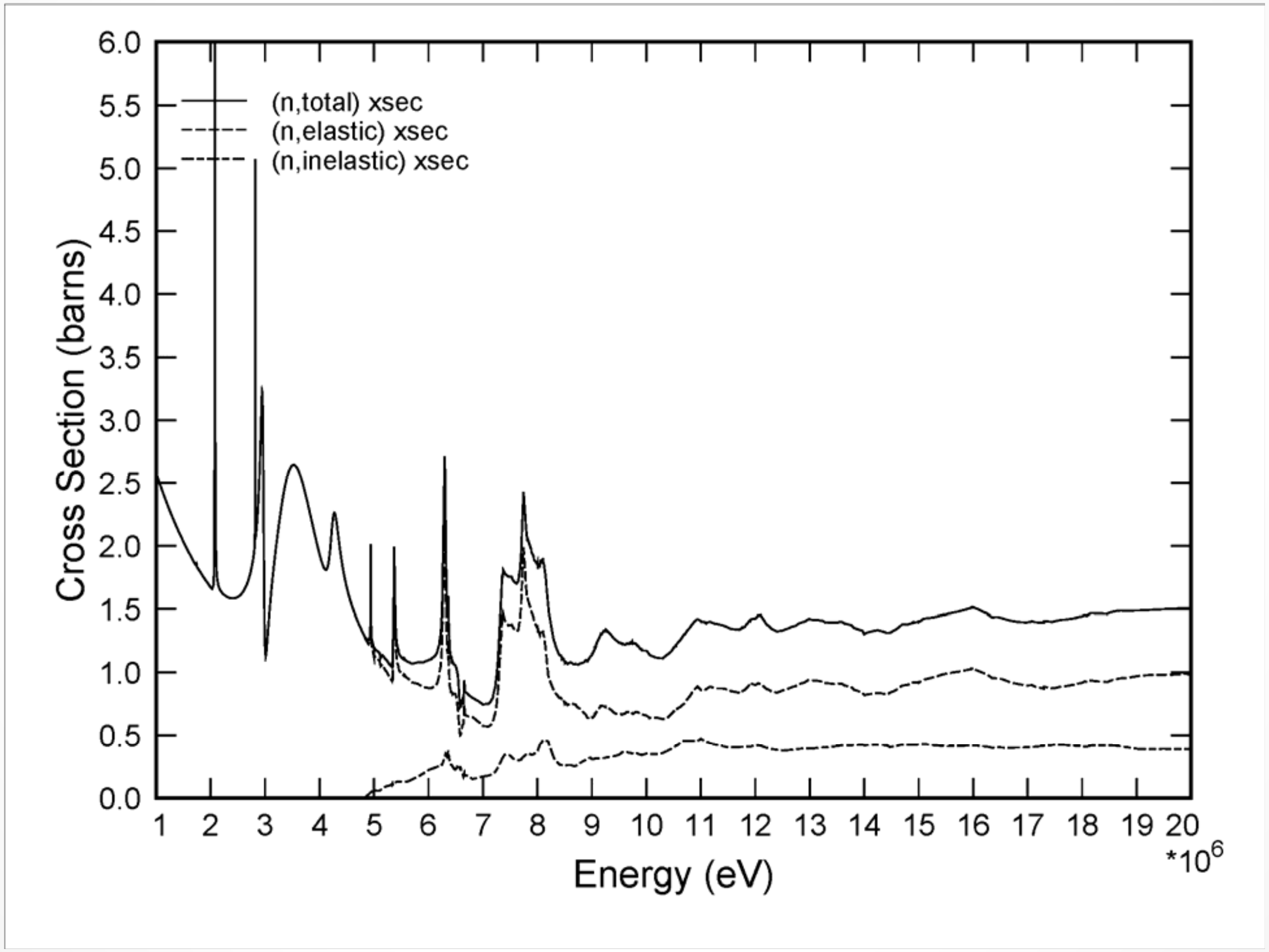
Step 1: Calibration Experiments

- The graphite we will be using is not pure ^{12}C.
  - We need to know the amount of impurities in the graphite
- The two most likely contaminants (in terms of neutron interactions)
  - Water (it's hot and humid in Texas).
  - Boron (likely small amounts, but neutronically important).
- We would like to use at most two parameters to describe the impurities in the bricks.
  - Parts per million of boron (or some equivalent measure).
  - Parts per million of a generic 1/v absorber
- From simple experiments involving a neutron source (Pu-Be) and a graphite brick.
  - From simulations we can find the likely distribution of the two parameters for a given brick.
- The experiments will give us
  - A distribution of the parameters to sample from for the large experiments
  - The most-likely value of the parameters for each brick.

Simulations of Calibration Experiments should be "easy"

- Simple geometry (source – brick – detector)
  - First and last collision sources in PDT should be enough
- We can run a lot of simulations for each experiment.
- Resonances are not much of a problem for carbon.
- We can even do some analytic study of these experiments using Fermi-age theory.
- These experiments are planned for this summer.


C-12 total and elastic from JENDL-3.2 pointwise
(n,total) xsec
(n,elastic) xsec
Cross Section (barns)
0
10
20
30
40
50
60
70
80
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7}
Energy (eV)


(n,total) xsec
(n,elastic) xsec
(n,inelastic) xsec
Cross Section (barns)
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
*10^6
Energy (eV)

We are making nonlinear thermal-radiation problems with neutron-equivalent solutions

- Our experiments define a thermal radiation problem whose solution can be **measured**.
- This is done
  - Without any knowledge of the neutronics solution
  - With minimal modification of the radiation transport code.
- **Not** a manufactured solution!
- For the first time we will have field experiments that can be used as verification tests for radiation transport codes.
  - Without all that messy hydrodynamic motion.
- Our procedure will open the door to many other possible benchmark problems.

We can do this because of an equivalence between the angular flux and specific intensity

- Equivalence means

$$I_g(\vec{r},\hat{\Omega},\tau) = \mathbf{A}\psi_g(\vec{r},\hat{\Omega},t)_{t=\tau}$$

- Where

$$\begin{aligned} I_g &= \text{radiation intensity in energy group } g \\ \psi_g &= \text{neutron angular flux in group } g \\ \mathbf{A} &= \text{constant we can choose} \\ \tau &= \text{radiation time variable } = \frac{tv_0}{c} \end{aligned}$$

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The neutron and radiation equations have similarities and differences

- Neutrons in graphite:

$$\frac{1}{v_g}\frac{\partial \psi_g}{\partial t} + \hat{\Omega}\cdot\nabla\psi_g + \sigma_{\mathrm{t},g}\psi_g(\vec{r},\hat{\Omega},t) = q_g^{\mathrm{NScat}}(\vec{r},\hat{\Omega},t) + q_g^{\mathrm{NFixed}}(\vec{r},\hat{\Omega},t).$$

- Thermal radiative transfer:

$$\frac{1}{c}\frac{\partial I_g}{\partial \tau} + \hat{\Omega}\cdot\nabla I_g + \kappa_{\mathrm{t},g} I_g(\vec{r},\hat{\Omega},\tau) = Q_g^{\mathrm{Planck}}(\vec{r},\tau) + q_g^{\mathrm{RScat}}(\vec{r},\hat{\Omega},\tau)$$

$$C_{\mathrm{v}}\frac{\partial T}{\partial \tau} = \sum_g \left(\kappa_{\mathrm{a},g}\int_{4\pi} d\Omega\, I_g - Q_g^{\mathrm{Planck}}\right) + H.$$

- The group dependent speed and sources are the differences.

Minimal Code enhancements needed to make equivalence transform

- Need
  - Fixed source
    - Required for almost any manufactured solution
  - Group-dependent speeds
    - Unusual, but not onerous.

$$\frac{v_0}{cv_g}\frac{\partial I_g}{\partial \tau} + \hat{\Omega}\cdot\nabla I_g + \kappa_{\mathrm{t},g} I_g = Q_g^{\mathrm{Planck}}(\vec{r},\tau) + q_g^{\mathrm{RScat}}(\vec{r},\hat{\Omega},\tau) + q_g^{\mathrm{RFix}}(\vec{r},\hat{\Omega},\tau)$$

With these definitions the rad-transfer equations will reproduce the neutron solution

$$\frac{1}{v_g}\frac{\partial I_g}{\partial(\tau c/v_0)} + \hat{\Omega}\cdot\nabla I_g + \kappa_{\mathrm{t},g} I_g = Q_g^{\mathrm{Planck}}(\vec{r},\tau) + q_g^{\mathrm{RFix}}(\vec{r},\hat{\Omega},\tau)$$

t

$\sigma_{\mathrm{s},g} + \sigma_{\mathrm{a},g}$

$\mathbf{A} Q_{0,g}^{\mathrm{NScat}}$

$$\mathbf{A}\left(q_g^{\mathrm{NFix}} + q_g^{\mathrm{NScat}} - \frac{Q_{0,g}^{\mathrm{NScat}}}{4\pi}\right)$$

- Recall, **A** is a constant that we can pick.
- We've set the radiation scattering to zero.

Reformulate Neutron Scattering

- We rewrite the scattering source as the sum of an isotropic and anisotropic part:

$$q_g^{\mathrm{NScat}}(\vec{r}, \hat{\Omega}, t) = \sum_{g'} \sum_{n=0}^{L} \frac{2n+1}{4\pi} \sigma_{\mathrm{s},l,g' \to g} \sum_{k=-n}^{n} \phi_{g'}^{kn} Y_{kn}(\hat{\Omega})$$

$$= \frac{\chi_g}{4\pi} \sum_{g'} \sigma_{\mathrm{s},g'} \phi_{g'} + \frac{\beta_g(\hat{\Omega}) \chi_g}{4\pi} \sum_{g'} \sigma_{\mathrm{s},g'}$$

$$\chi_g = \frac{\sum_{g'} \sigma_{\mathrm{s},0,g' \to g} \phi_{g'}}{\sum_{g'} \sigma_{\mathrm{s},g'} \phi_{g'}} \qquad \beta_g(\hat{\Omega}) = \frac{\sum_{g'} \sum_{n=1}^{L} (2n+1) \sigma_{\mathrm{s},n,g' \to g} \sum_{k=-1}^{n} \phi_{g'}^{kn} Y_{kn}(\hat{\Omega})}{\chi_g \sum_{g'} \sigma_{\mathrm{s},g'} \phi_{g'}}$$

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We define emission opacity and fixed rad source so the total sources match

$$Q_g^{\text{Planck}}(\vec{r},\tau) = \kappa_g^{\text{Emit}} B_g(T)$$

$$\kappa_g^{\text{Emit}} = \frac{\chi_g \mathbf{A} \sum_{g'} \sigma_{\text{s},g'} \phi_g'(t)_{t=\tau}}{B_g(T)}$$

$$q_g^{\text{RScat}}(\vec{r},\hat{\Omega},\tau) = 0$$

$$q_g^{\text{RFix}}(\vec{r},\hat{\Omega},\tau) = \mathbf{A}\left[q_g^{\text{NFixed}} + \beta_g \chi_g \sum_{g'} \sigma_{\text{s},g'} \phi_{g'}(\vec{r},t)\right]_{t=\tau}$$

We define absorption and emission opacities in terms of neutron cross sections

$$\kappa_{\mathrm{a},g} = \sigma_{\mathrm{s},g}$$

$$\kappa_{\mathrm{t},g} = \sigma_{\mathrm{s},g} + \sigma_{\mathrm{a},g}$$

$$C_{\mathrm{v}} = H = 0$$

- The radiation code will think there is no scattering.
- Its emission will mimic the isotropic component of neutron scattering.
- Its fixed source will mimic the anisotropic component of neutron scattering as well as the true neutron source (e.g., DT).

Big step: replace neutron solution with rad solution in definitions

- With the preceding definitions, the rad solution will be a constant times the neutron solution.
- We can therefore replace the neutron solution with the rad solution in all of the definitions:

$$\kappa_g^{\text{Emit}} = \frac{\chi_g \mathbf{A} \sum_{g'} \sigma_{\text{s},g'} \varphi'_g(\tau)}{B_g(T)}$$

$$q_g^{\text{RFix}}(\vec{r}, \hat{\Omega}, \tau) = \mathbf{A}\left[q_g^{\text{NFixed}} + \beta_g \chi_g \sum_{g'} \sigma_{\text{s},g'} \varphi_{g'}(\vec{r}, \tau) \right]$$

$$\varphi_g(\vec{r}, \tau) = \int_{4\pi} d\Omega \, I_g(\vec{r}, \Omega, \tau)$$

Result: A rad-transfer benchmark problem whose solution can be *measured*

- With infinite time, space, angle, and energy resolution, the radiation solution should match our neutron experimental results
  - within experimental uncertainty,
  - if cross sections are correct.
- The problem is entirely self-contained.

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Variations

- In our definition, neutron absorption causes energy to not be conserved in the sense commonly used in radiative transfer codes.
  - The way we've defined things $\left(\kappa_{\mathrm{a},g}\varphi_g - Q_g^{\mathrm{Planck}}\right) = 0$
  - The "absorption term" is just the total scattering rate density because $\kappa_{\mathrm{a},g} = \sigma_{\mathrm{s},g}$
- This could be problematic in some radiative transfer codes.
- One benefit of our definition is that the material temperature will stay at whatever it it initialized to.
  - That is if the nonlinearities are converged; making a good verification test.
- We could have this term include absorption.

There is a lot going on at CERT

- Methods, UQ, algorithms, experiments, etc.
- A key piece of the work is demonstrating that neutron experiments can be used to verify thermal radiation transport codes.
  - Our experiments have the flavor of a thermal radiation transport simulation
  - High energy particles transport without interacting
  - Thermal wave come much later
- We can mathematically make the equations equivalent, we have yet to do this with our codes though.

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Thank you for listening

Software

- PDT (Adams/Rauchwerger)
  - a 3-D linearized Boltzmann solver (thermal radiation, neutrons, gammas, charged particles).
  - Sn approximation in direction.
  - Multigroup approximation in energy
  - General polyhedral spatial mesh.
- Finmcool (McClarren)
  - Implicit Monte Carlo for thermal radiation transport
  - Multigroup in energy
  - Domain replicated over MPI and domain decomposed over threads

A sample of research topics needed.

- Algorithms for radiation transport combining sweeps with block-Jacobi iteration.
- Alternative algorithms based upon second-order forms of the transport equation and new multigrid methods.
- Algorithms that are non-deterministic and less precise, but fault tolerant and more scalable.
- New space-angle AMR methods.
- Subgrid models for boundary layers, small streaming
- paths, and multiple time scales.
- Parallel algorithms compatible with AMR and subgrid models.