Center for Exascale Radiation Transport

Project Overview

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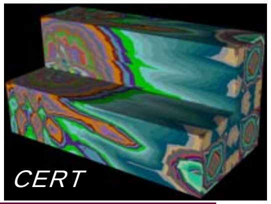
Kick-off Meeting, Albuquerque, NM, December 9-10, 2013

Outline



1. Overarching Application
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5. Software
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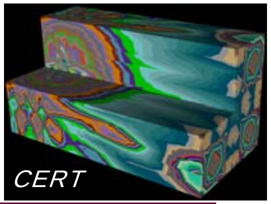
Our Overarching Application is



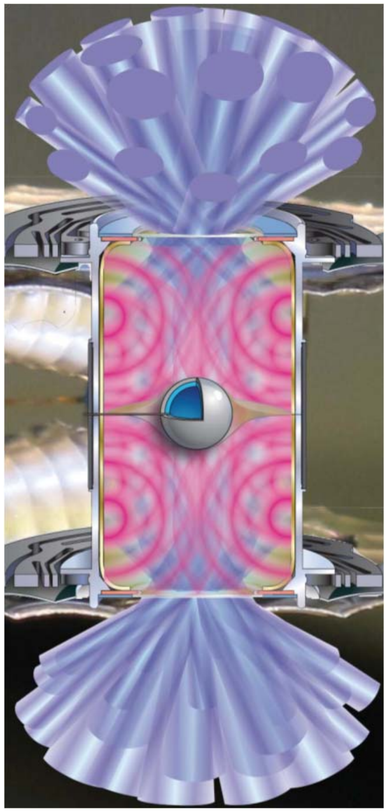
- Thermal radiation transport in the high-energy density laboratory physics (HEDLP) regime.

$$\frac{1}{c}\frac{\partial \psi}{\partial t}+\vec{\Omega}\bullet\vec{\nabla}\psi+\sigma_a\psi=\sigma_a B,$$

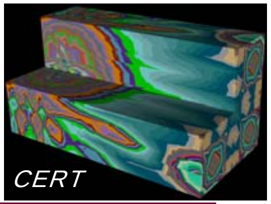
$$C_v\frac{\partial T}{\partial t}=\int_0^{\infty}\int_{4\pi}\sigma_a(\mathrm{E})\Big(\psi(\vec{\Omega},\mathrm{E})-B(T,E)\Big)\,d\Omega\,dE\,.$$

Overarching Application 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.*



Exascale Greatly Improves Predictive Science

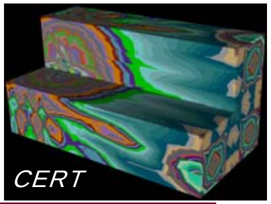


- Predictive capability for HEDLP thermal radiation transport can be greatly improved by exascale computing.
  - *The transport equation is seven dimensional, yielding the "curse of dimensionality".*
  - *10^{15} unknowns easily required.*
  - *Multiple time scales requires implicit iterative solution techniques.*
  - *High resolution 3D calculations will not be possible in many cases even with exascale computers.*

Radiation Transport Essential for HEDLP

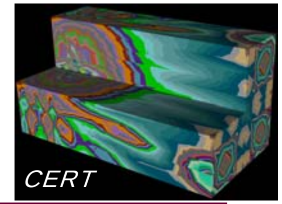
- Thermal radiation physics essential for HEDLP.
- NNSA has significant investment in HEDLP.
  - *National Ignition Facility, Omega Laser, Z-Machine …..*
- In HEDLP simulations, transport usually dominates resource requirements, so efficient solution important.

CERT Research Widely Applicable



- 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.*

Goals

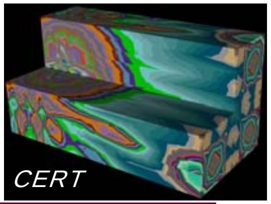


- The central goal of CERT is

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.*

HEDLP Experiments Problematic



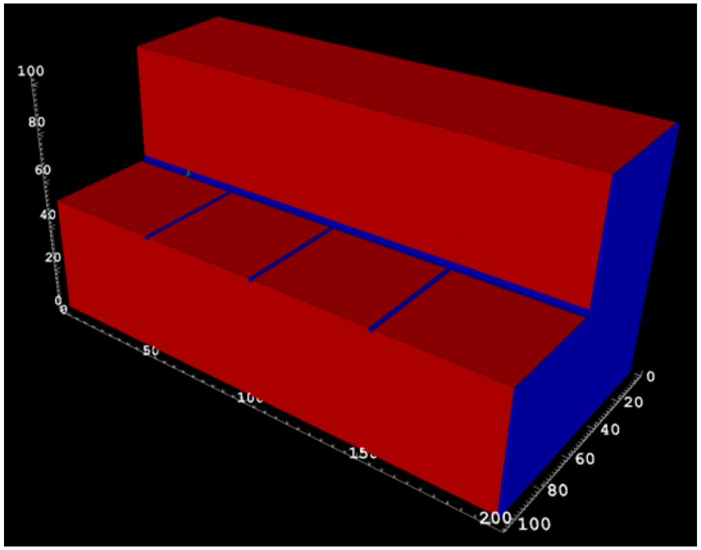
- Realistic HEDLP radiation transport modeling requires rad-hydro.
- Rad-hydro simulation of HEDLP experiments is problematic:
  - *Sources of errors are difficult to experimentally infer.*
  - *UCNI code.*
  - *Fewer resources for transport.*
- Thus we chose to avoid HEDLP experiments and do transport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

Neutrons as Surrogates

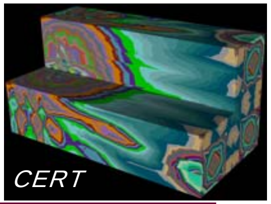
- We have chosen neutron experiments as a surrogate for thermal radiation experiments after considering other options.
- Neutrons share many properties with thermal radiation transport.
  - *The transport equations for both essentially exact.*
  - *Concept of cross sections same.*
  - *Radiation and 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.

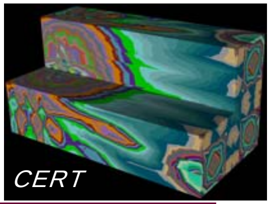


Software



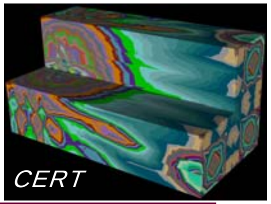
- PDT (Adams/Rauchwerger)
  - *a 3-D linearized Boltzmann solver (thermal radiation, neutrons, gammas, charged particles).*
  - *Sn approximation in direction.*
  - *Multigroup approximation in energy*
  - *General polyhedral spatial mesh.*
- STAPL (Rauchwerger/Amato) – general-purpose parallel library.
- At present, PDT is build on top of STAPL.
- We will develop TAXI – a domain-specific parallel library that will sit between PDT and STAPL.
- We have had a PDT/STAPL collaboration for over 15 years.

Research Contributions – Transport Algorithms and Methods



- 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.

The sweep is a key step in many iterative methods for transport

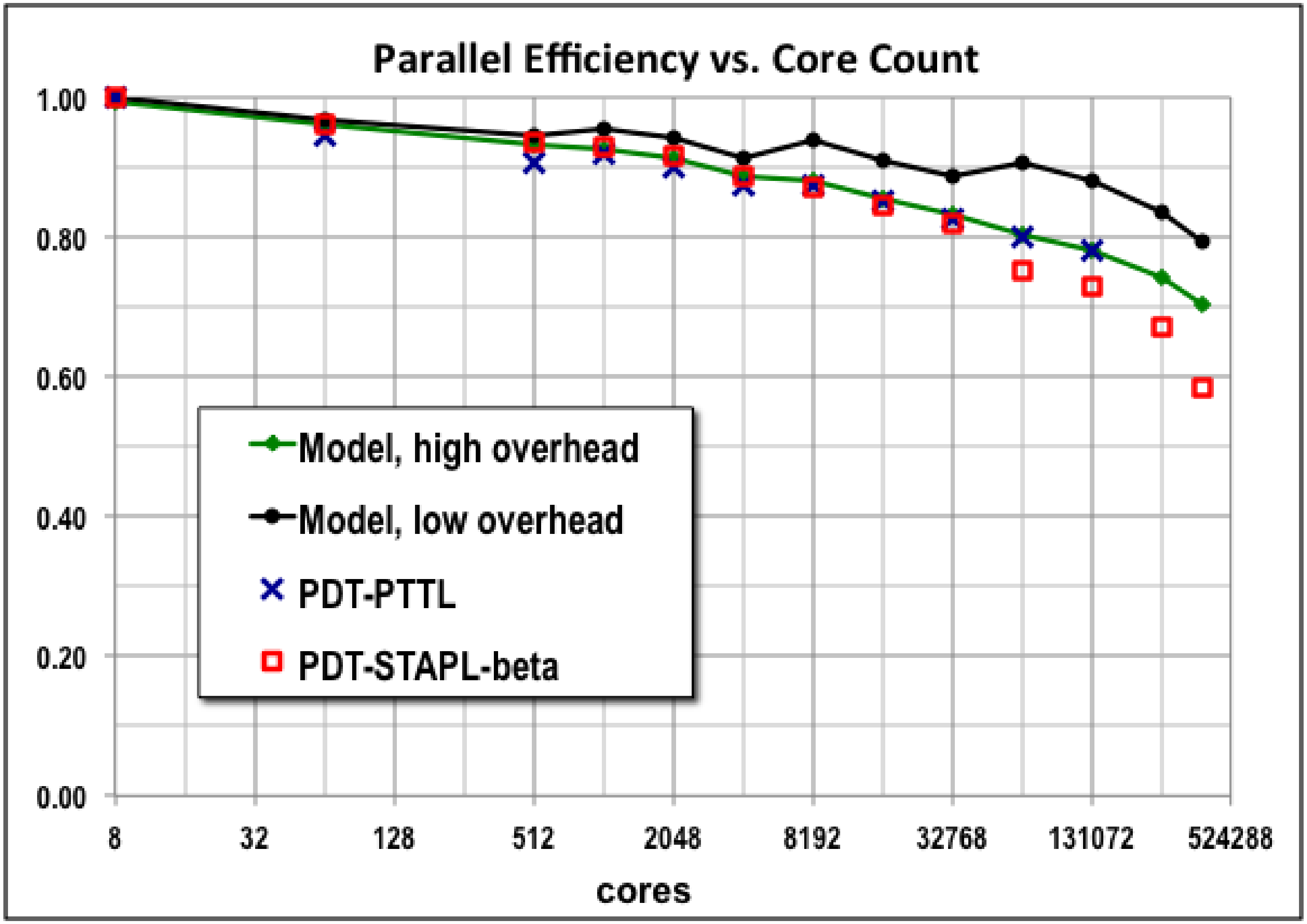


- The discretized equations have a block lower-triangular system.
- The "sweep“ solves this system by marching through the spatial domain in the direction of particle flow, for all directions in the quadrature set.
- High parallel efficiency is difficult to achieve because of the sequential marching.
- For instance, for each direction in a 3-D domain, only a 2-D subset of cells (a diagonal plane) is available for parallel solution at each stage.

The sweep is a key step in many iterative methods for transport (cont.)

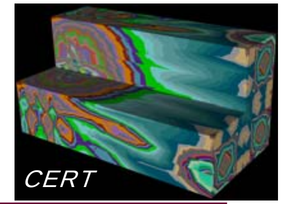
- Thus, achieving high parallel efficiency is difficult, but our performance models (which have so far worked well) indicate that with nested parallelism we can maintain excellent weak scaling of sweeps beyond 10M cores.
- Details depend on grid type and numbers of energy groups and directions.

We have developed provably optimal parallel sweep algorithms



Conventional wisdom:
Sweeps don't work well past ~4k cores!
Our results:
They do if done properly!

Research Contributions – Computer Science



- New basic computer algorithms to map the transport solution algorithms to exascale computers.
- Software-imbedded fault tolerance to enable exascale computing.
- Extension of generic software infrastructure (STAPL) to hierarchical heterogeneous exascale architectures.
- Transport-specific library built upon STAPL.
- Performance models for solution algorithms.

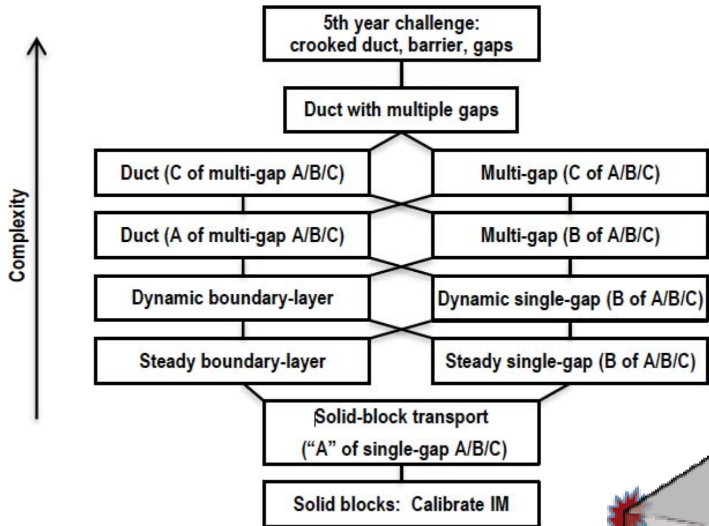
Research Contributions - VVUQ

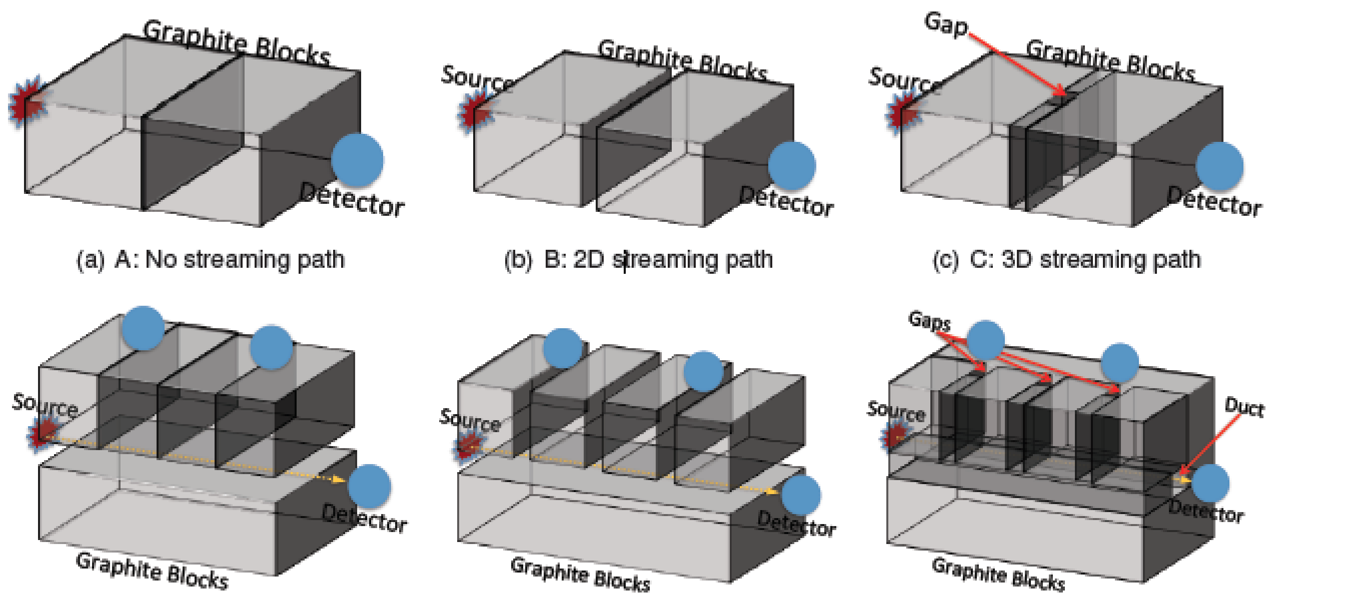
- Techniques for estimation of numerical error (solution verification), and assessment via experiment.
- Methods and experimental data for hierarchical VVUQ.
- A new VVUQ approach that produces a radiative transfer equation whose solution is an experimentally measured neutron transport solution.

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

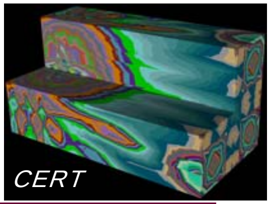




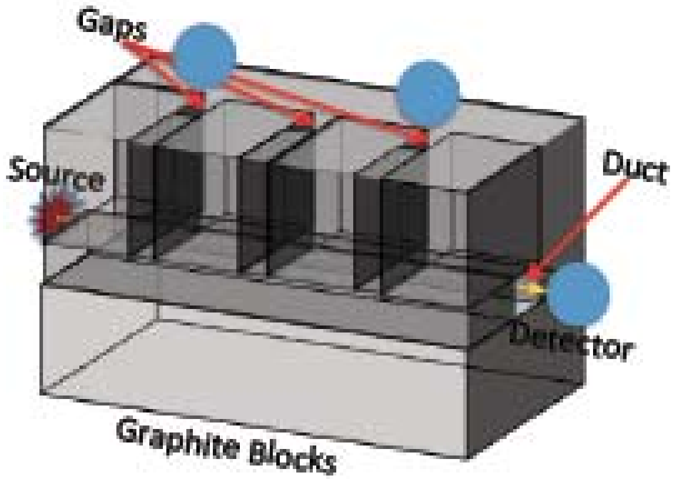
(a) A: No streaming path (b) B: 2D streaming path (c) C: 3D streaming path

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

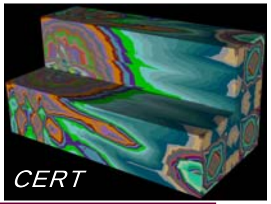
Experiments



- 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.

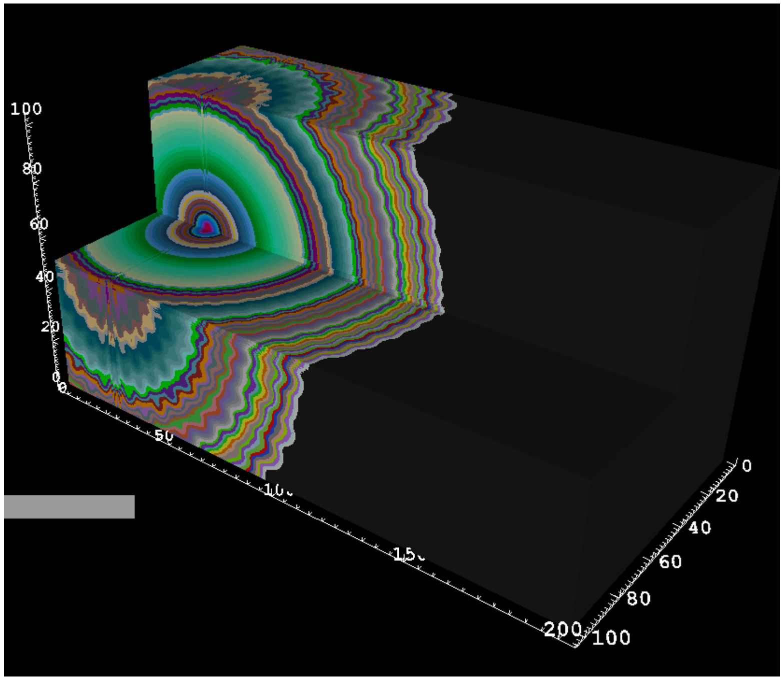


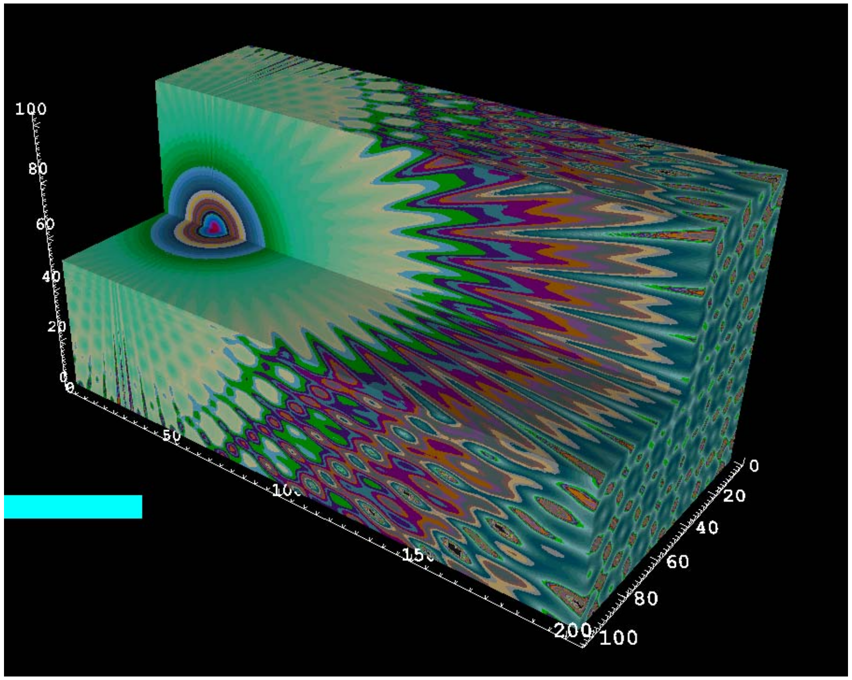
Collaborating Institutions



- We are collaborating with mathematicians from the University of Colorado and a statistician from Simon Fraser University.
- The mathematicians (Tom Manteuffel and Steve McCormick) are contributing in the area of multigrid methods for diffusion and transport.
- The statistician (Derek Bingham) is contributing in the area of VVUQ.

14 Mev Neutron Solution

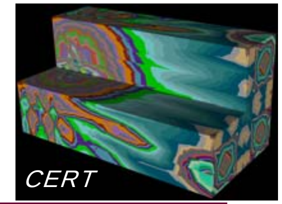


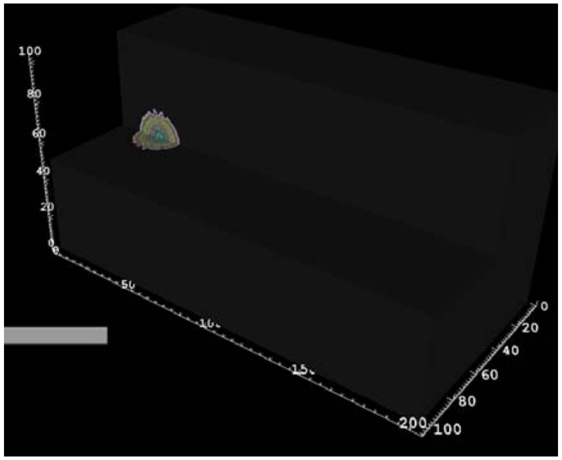


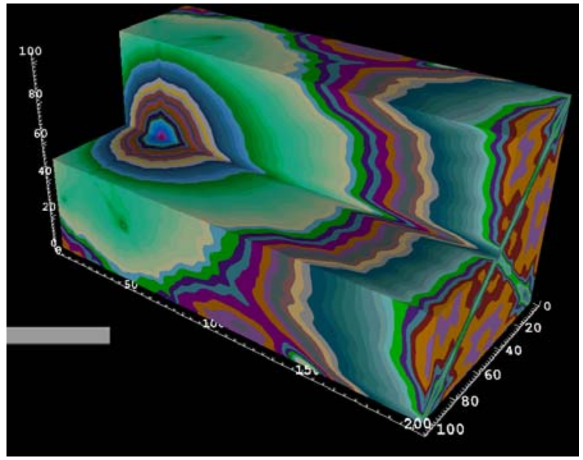
14-MeV neutrons
10 ns
8192 directions

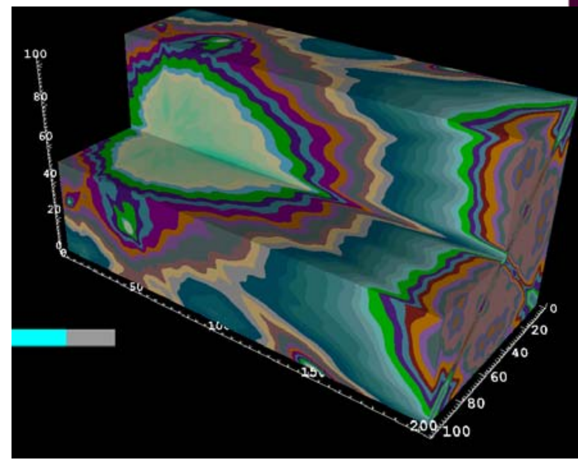
14-MeV neutrons
50 ns
8192 directions – still have "ray effects"!

Thermal Neutron Solution







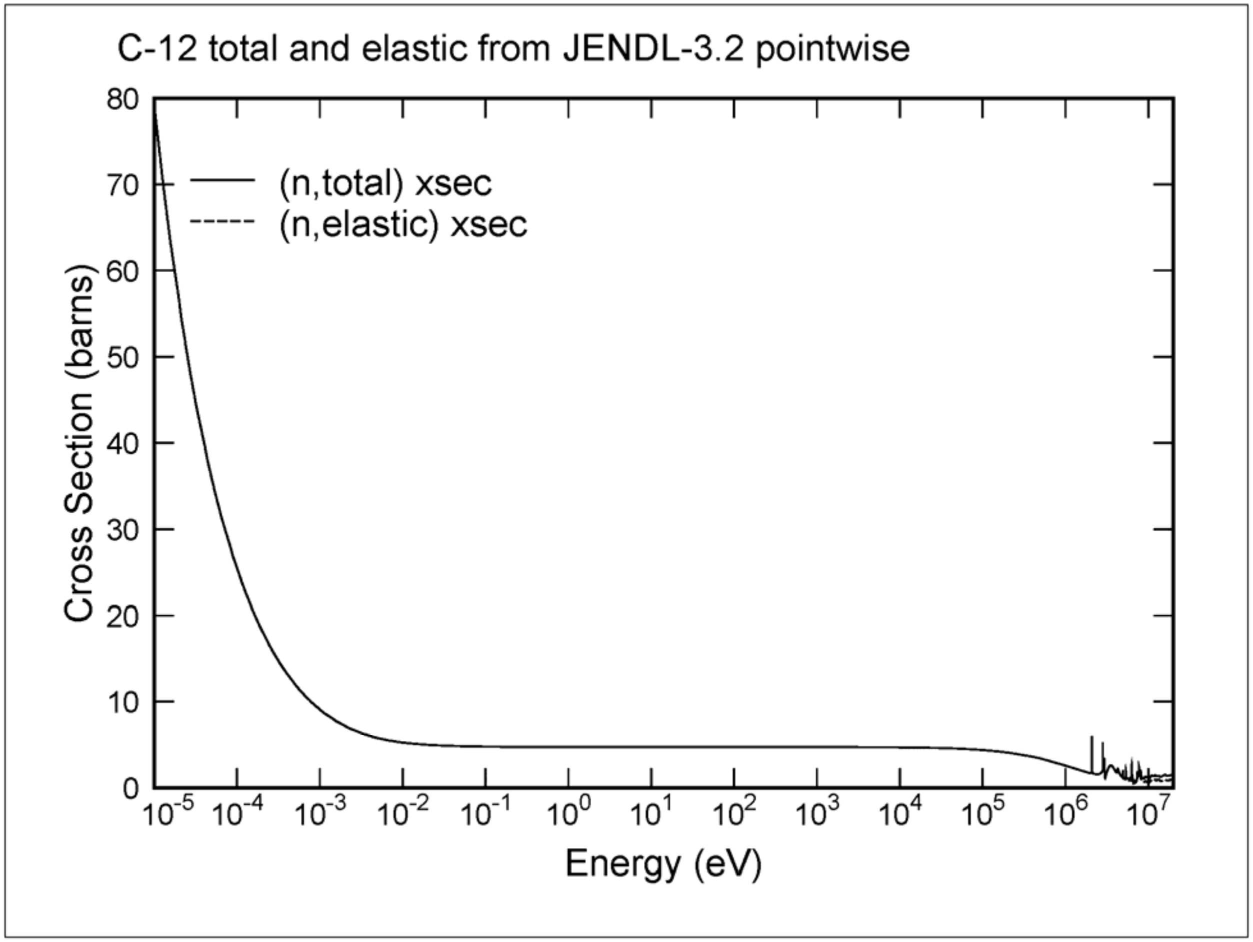


low-energy n's
500 ns

low-energy n's
10^5 ns

low-energy n's
2×10^5 ns

Carbon Cross-sections



Carbon Cross-sections