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The Jayenne Implicit Monte Carlo Project

Where We Are, r; Where We're Heading, Ω ; and the Issues We Face, σ (r,Ω)

(LA-UR-04-6162)

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LLNL Computational Methods in Transport
Granlibakken, Lake Tahoe, California
September 11-16, 2004

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NNSA

1943 - 2003
Los Alamos
NATIONAL LABORATORY
Ideas that change the world

Outline

- Jayenne IMC Code
  - Description and Capabilities
  - Applications
  - Design and Development
- Issues
- Research
  - Hybrid Discrete Diffusion/Monte Carlo
  - Residual Monte Carlo Methods
  - Analysis of IMC Methods
  - Parallelism
  - Low-memory, time-dependent particle tracking

Code Description and Capabilities

- Fleck and Cummings IMC method
- C++, Object-Oriented, Levelized Design
- Well-Tested
- Jayenne Project has multiple products
  - Milagro: stand-alone IMC
  - Wedgehog: RZWedge/Sphyramid IMC package
  - Uncle McFlux: linear ray-tracing package
- Uses Draco for low-level components
  - ds++: memory mgmt; assertion macros
  - c4: parallel communication
  - rng: random number generator wrapper
  - cdi: common data interface

Code Description and Capabilities

- Independent Variables as Template Parameters
  - Multiple Meshes
    - Orthogonal, structured nonuniform, 1D-3D Cartesian
    - RZ-Wedge, AMR
    - Sphyramid
  - Gray or Multigroup Frequency
- Random Walk (Fleck and Canfield)
- Parallel
  - Domain replication
  - Domain decomposition
- Reproducible

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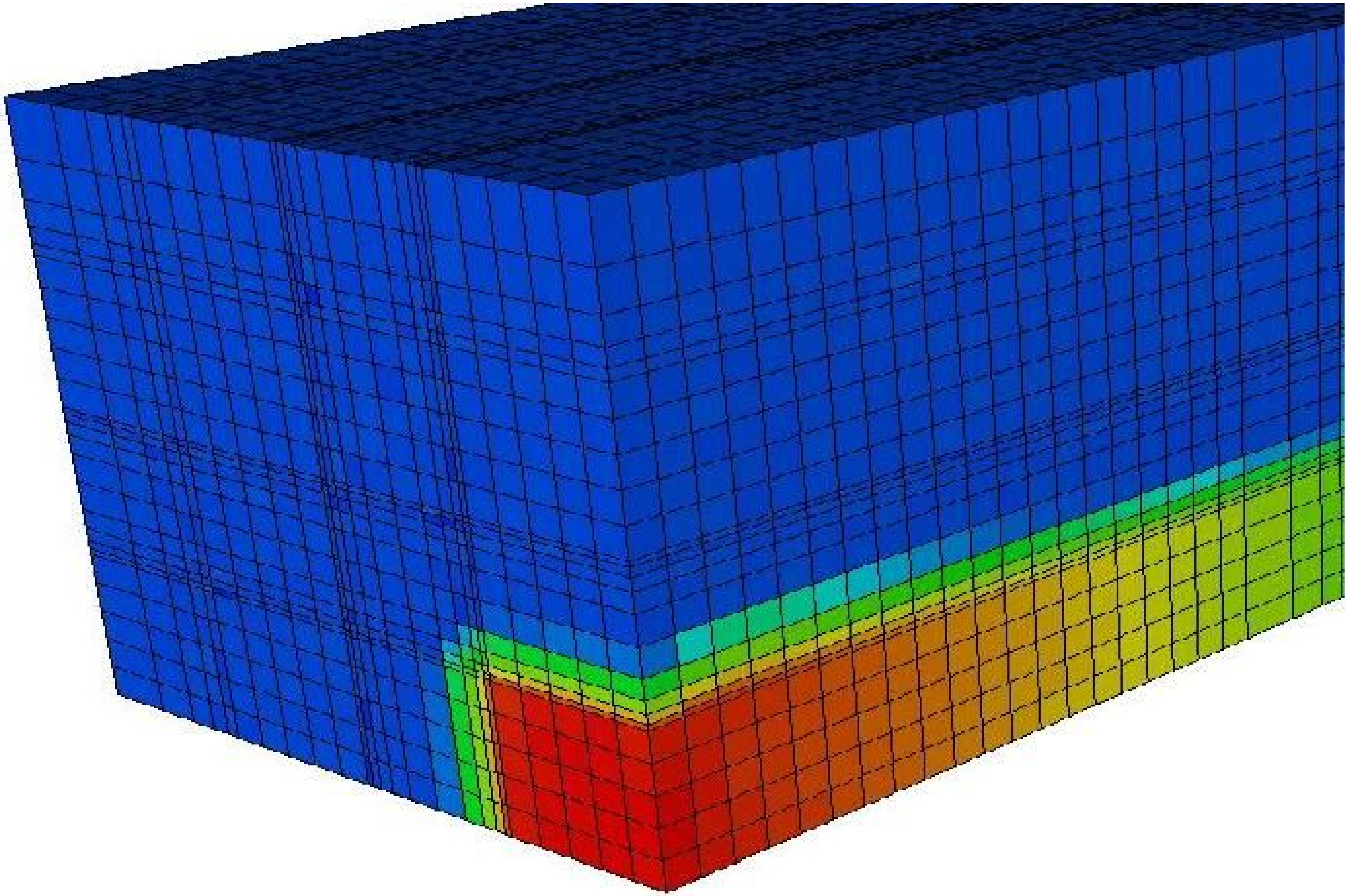
3-D Ratio-Zoned Cartesian Mesh



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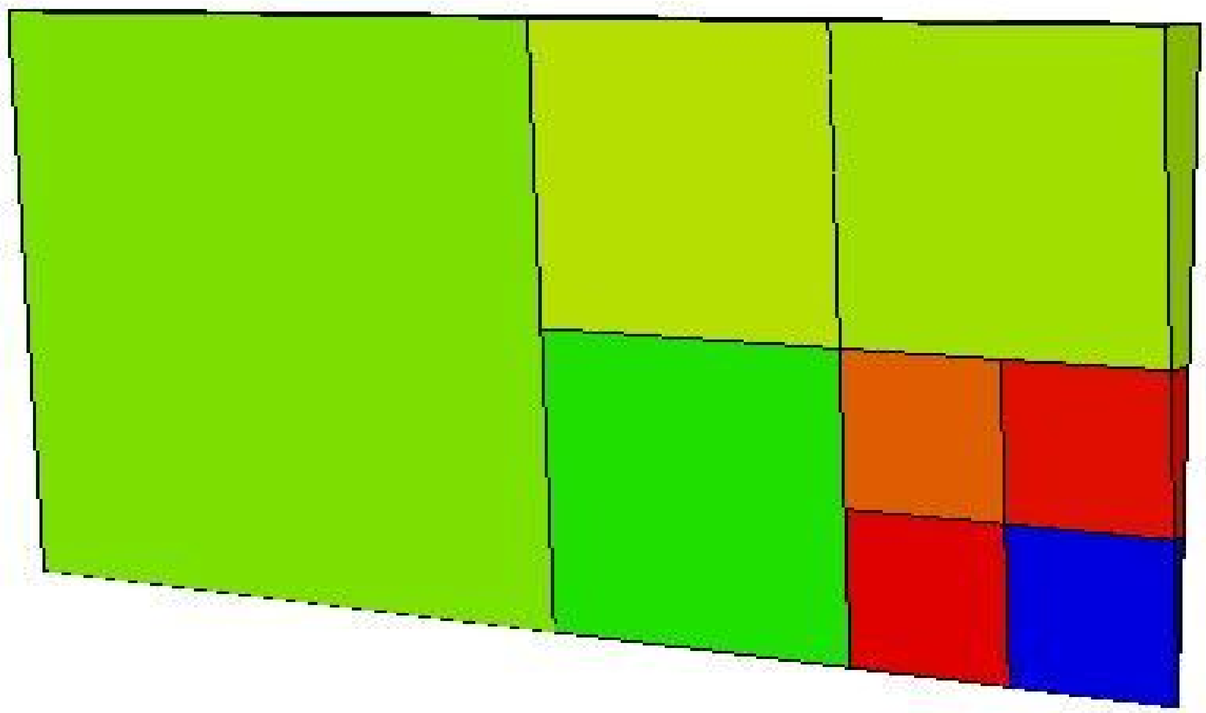
RZWedge AMR Mesh



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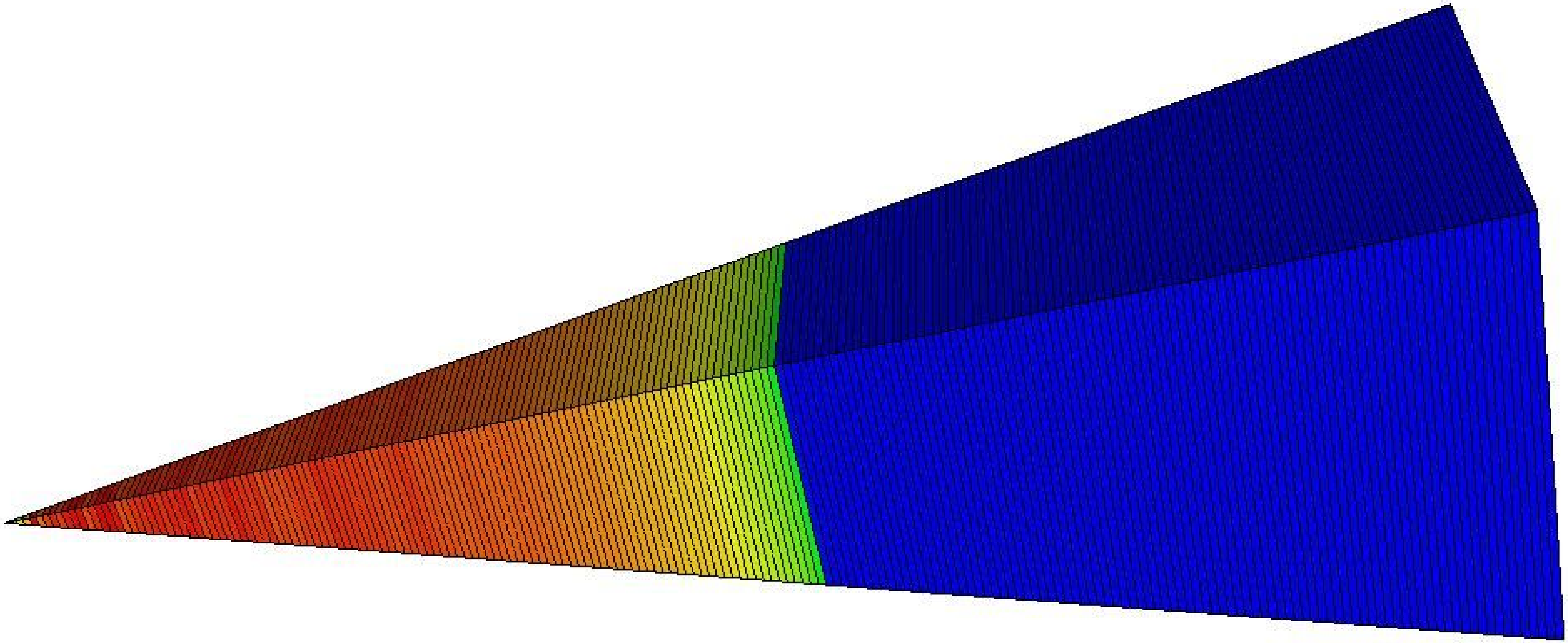
Sphyramid Mesh



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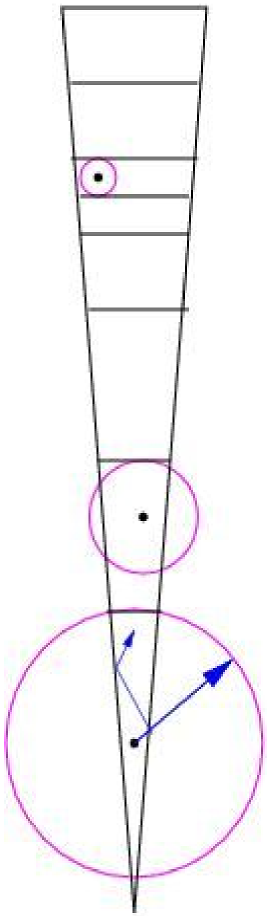
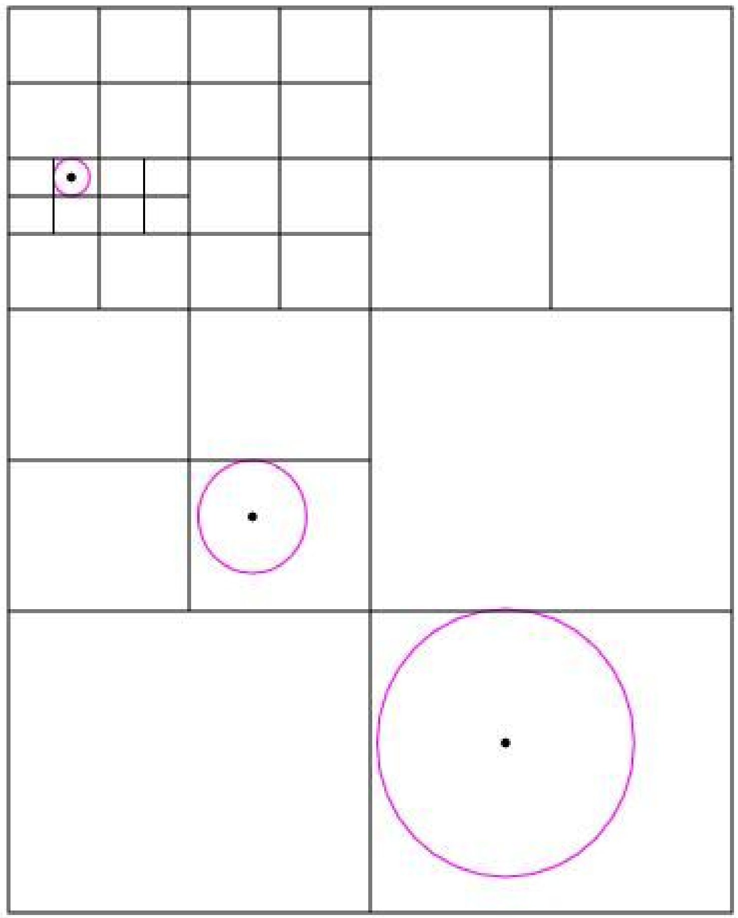
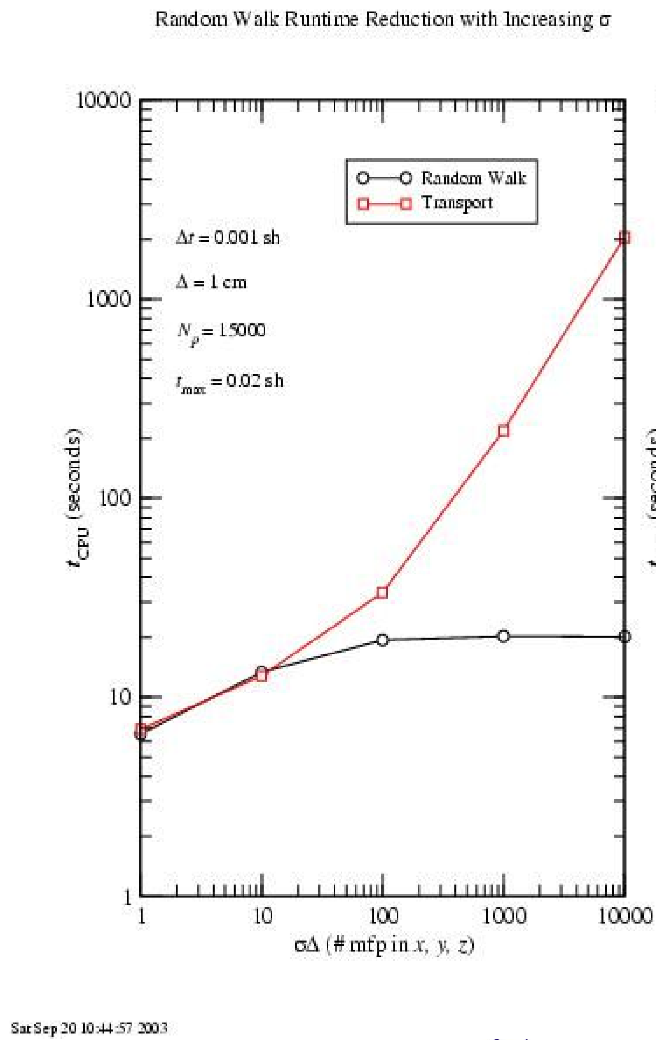
Random Walk on RZWedge Mesh



XY View



XZ View



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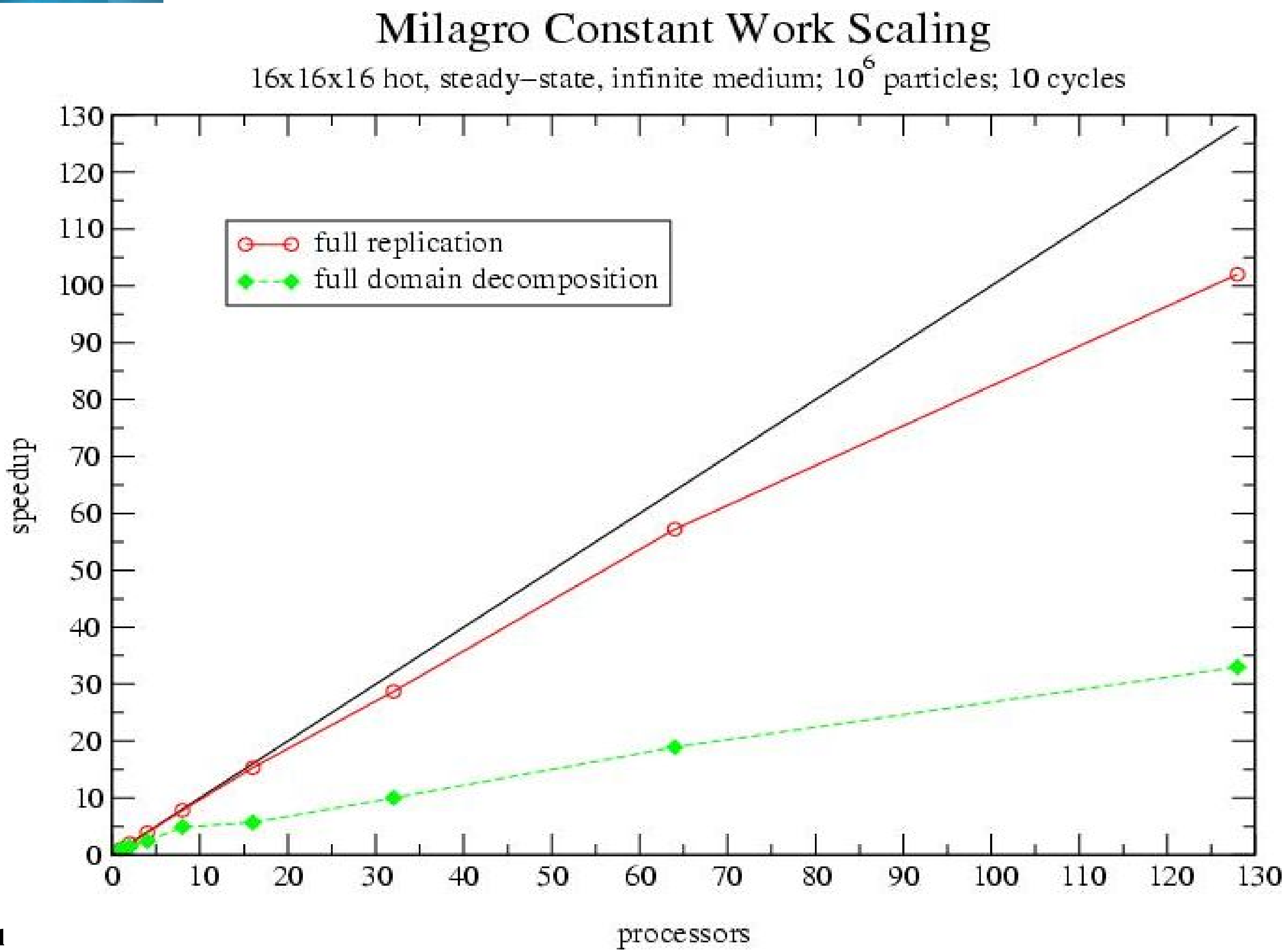
Parallel Speedups



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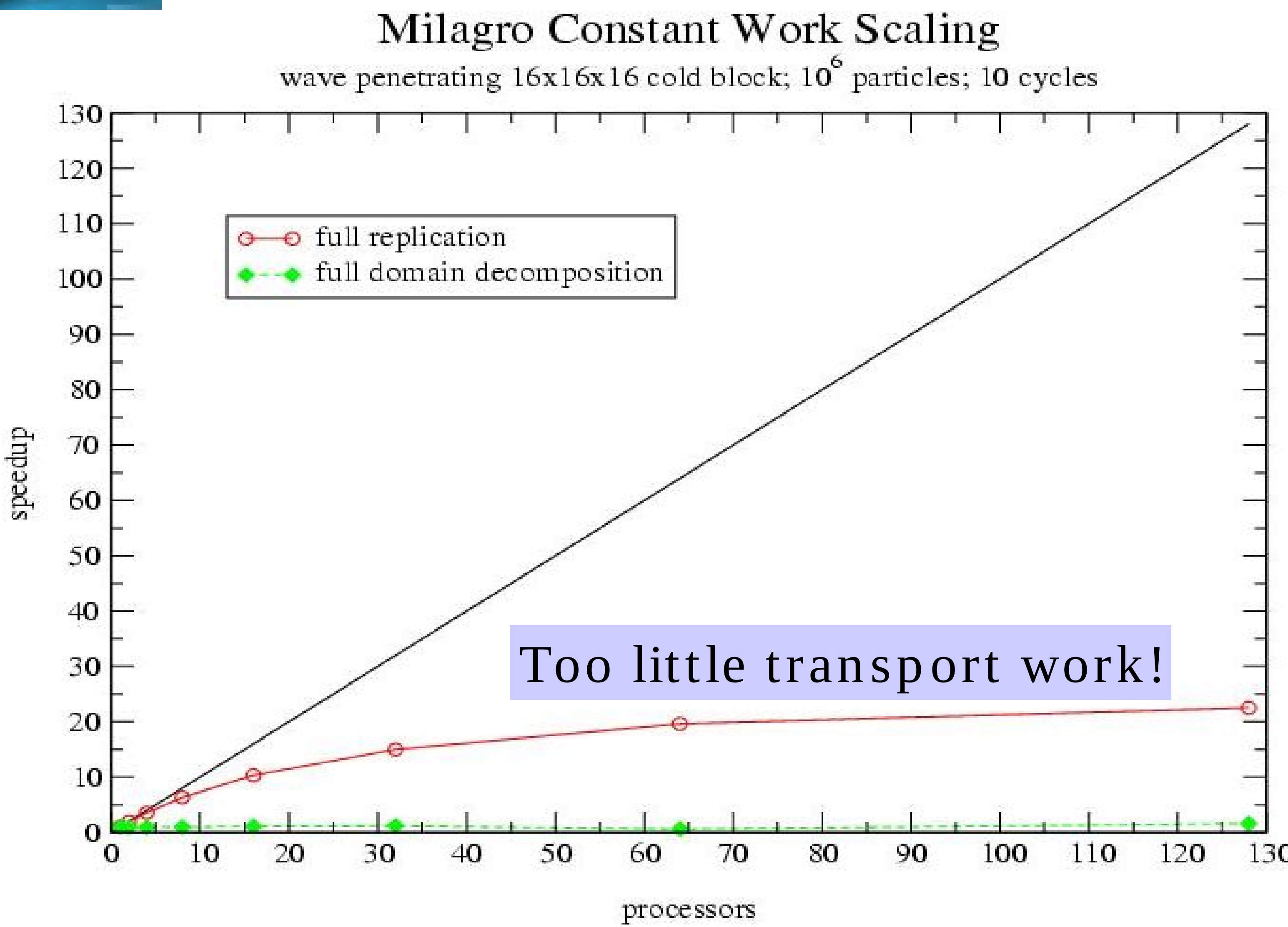

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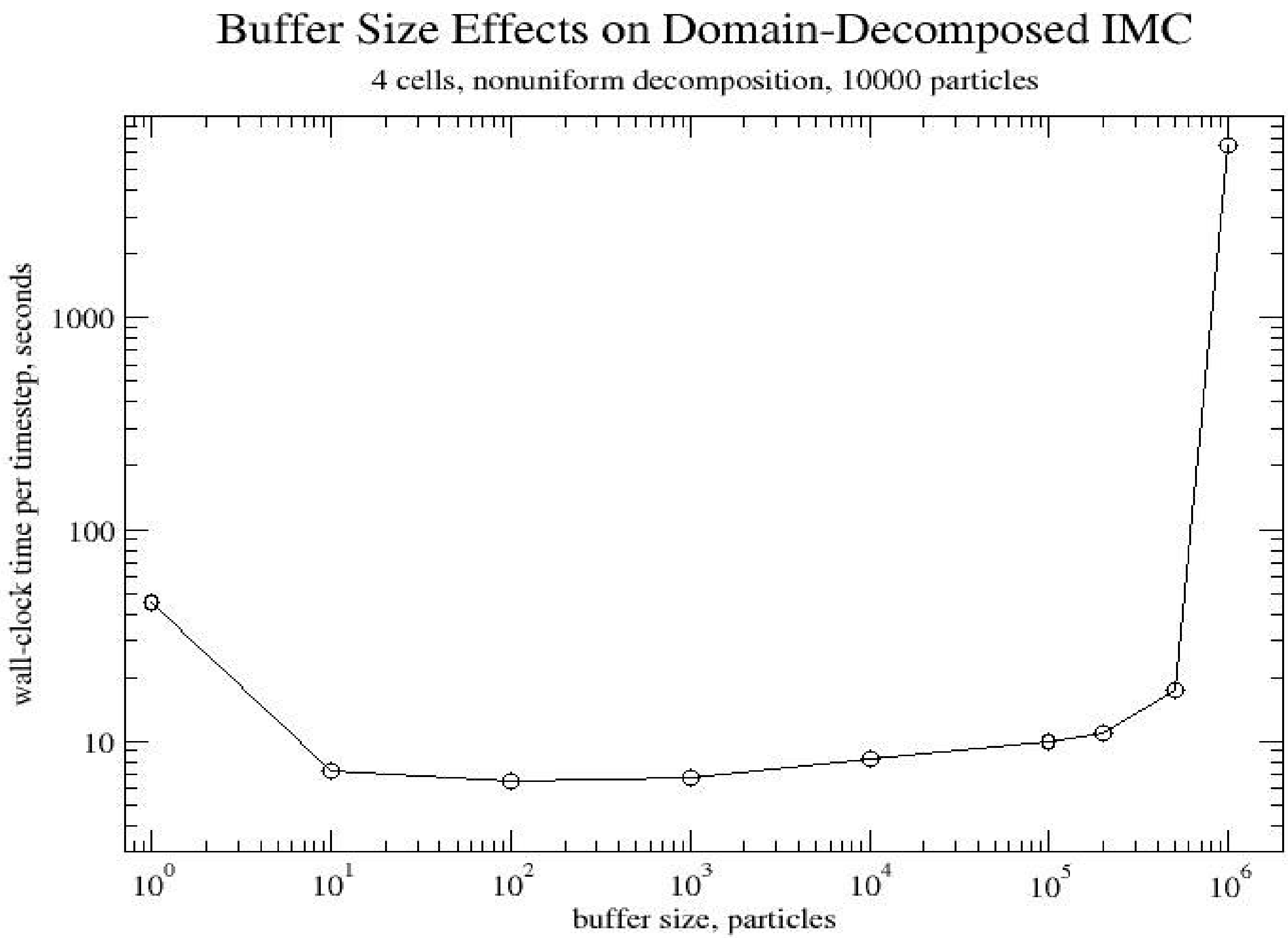
Buffer Size and DD Parallelism



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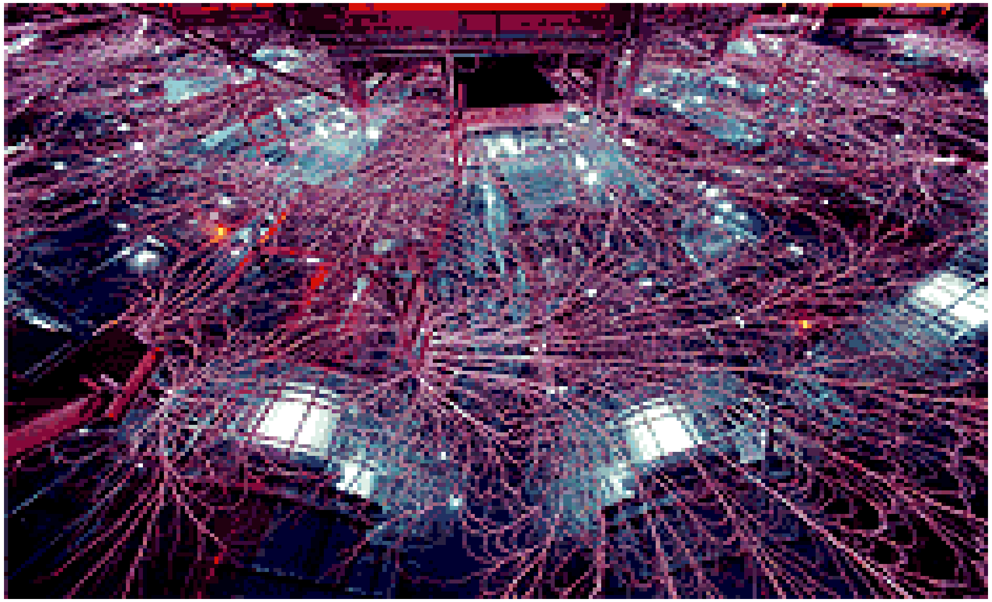
Z-Machine Applications

- Z-Pinch Experiments – Sandia Nat'l Lab
  - Radiation flow
  - Astrophysics
  - Inertial Confinement Fusion



Electrical discharges illuminate the surface of the Z -machine (Photo by Randy Montoya)

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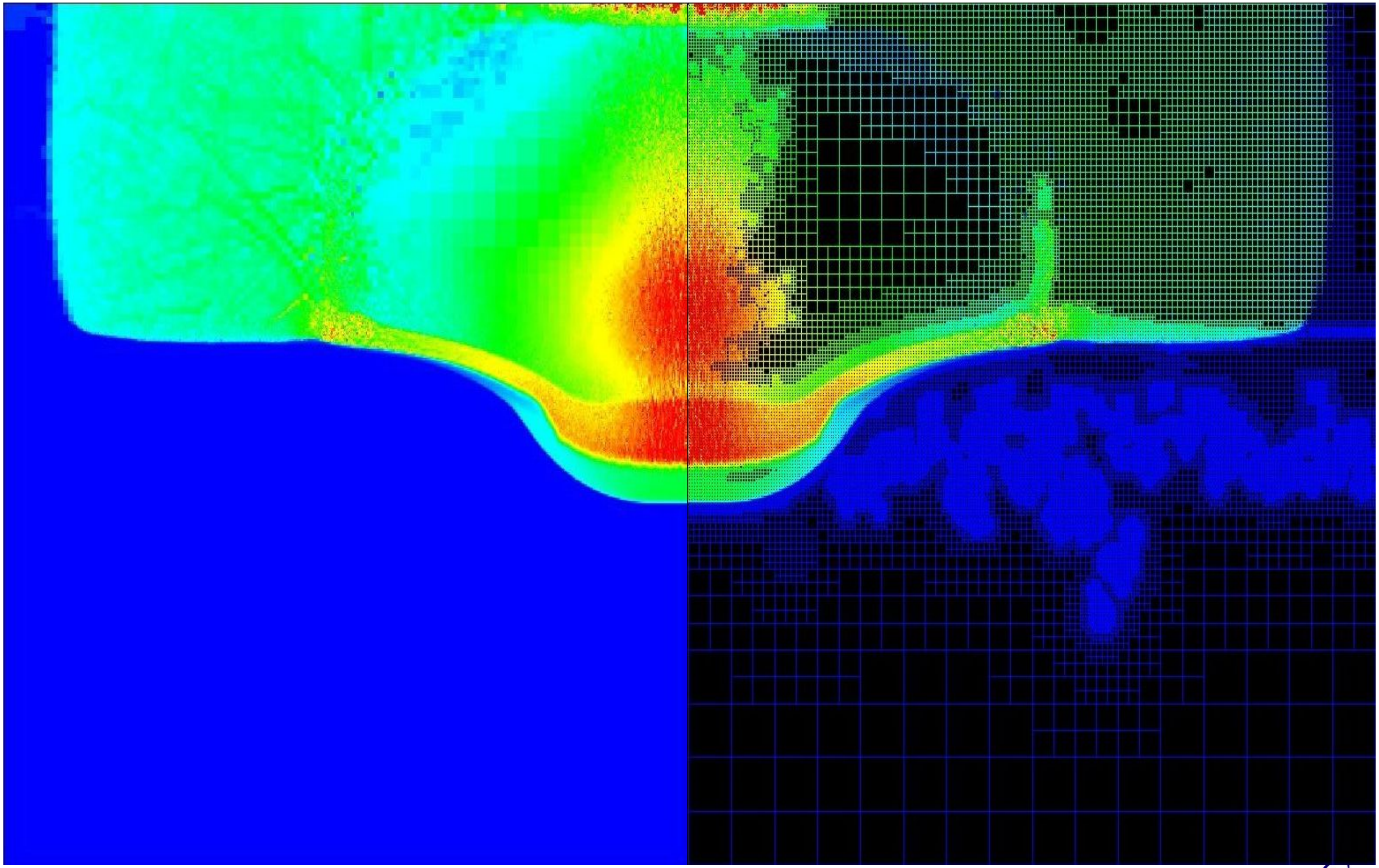
Astrophysics Applications

Hot comet impacting a granite planet



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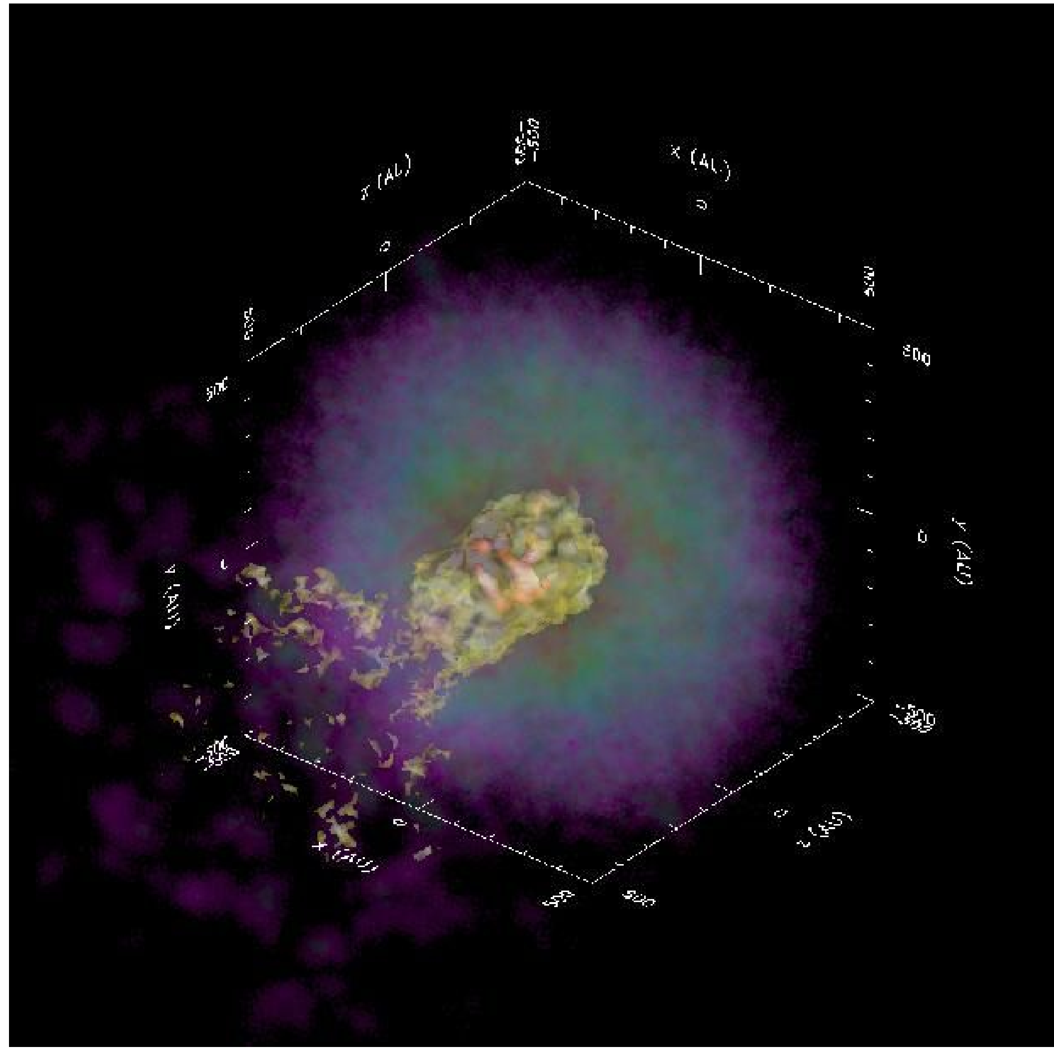
Supernova Applications

- Artificially asymmetric explosion; 3-to-1 velocity
- 1 year after explosion
- Background colors: density
- Isosurface: cobalt number density
- Linear, post-process MC transport to get light-curves
- Asymmetry produces brighter radioactive decay lines than spherical explosion
- Future work: nonlinear transport



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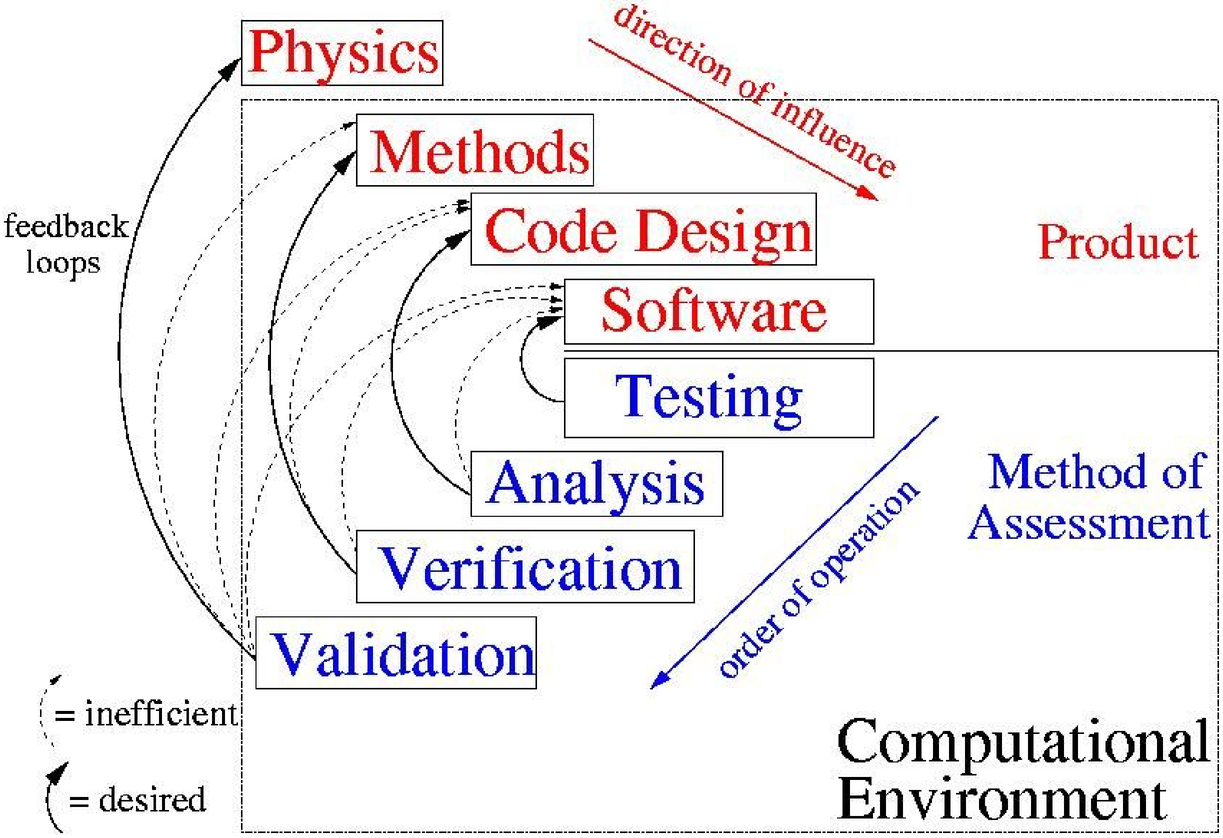
SQE Principles

- Staged Delivery via Unified Process: inception, elaboration, construction, transition (Ref: Larman)



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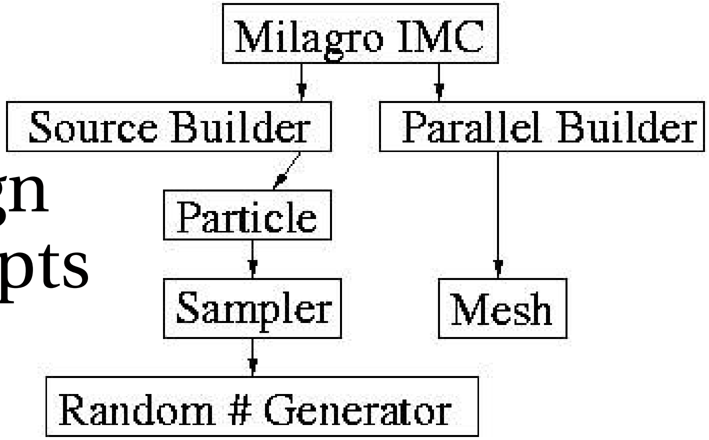
SQE Practices

- **Design and Implementation**
  - Components, levelized design
  - Template models and concepts
  - Design-by-Contract™ (DBC)



- **Development**
  - Configuration management: version control, build system, software releases
  - Reviews (accelerate the iterative process): design, post-mortem, code, code walk-through, pair-programming
  - Testing: (repeatable: on-demand and automatic) unit, integral, verification, shunt, regression
- **Buggy Pageant**

Design-by-Contract Example
During design, development, and runtime

```
//! Find a frequency group, in [1,G], given a frequency [eV]
int find_group_given_a_freq(const double hnu) const
{
    // Require a valid frequency
    Require (hnu >= 0);

    // Make sure it's multigroup
    Check (group_boundaries.size() > 1);

    ......do binary search, with embedded Checks, to find group......

    // check that the group actually contains the frequency
    Ensure (hnu >= get_group_boundaries(group).first);
    Ensure (hnu <= get_group_boundaries(group).second);

    // return the group number in [1,G]
    return group;
}
```

Turn on during development, testing, and debugging

Turn off for production
--compile time switch
--no cpu time cost

Buggy Pageant

- Todd deliberately plants bugs in the code.
- How many can Tom find during a 30-min talk?
- Simulates inadvertent "insider-produced" bug.
  - Tom utilized our integral, unit, regression, and verification tests, e.g. "gmake check"
  - No cheating: "diff", "ls –lart", "cvs diff"
- Tom found 3 bugs in 30 min.; all 5 in 60 min.
- Involve multiple code teams in the future.

The Same Old Issues

- Memory
  - Mesh and Census Particles
  - Random Number State
- Speed
  - IMC has both mesh- and particle-based work
- Error Estimation
  - Replicates
  - Expert judgement
- Methods Research vs. Software Development

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Research

- Hybrid Discrete Diffusion/Monte Carlo
- Residual Monte Carlo Methods
- Analysis of IMC Methods
- Parallelism
- Low-memory, time-dependent particle tracking

Hybrid Discrete Diffusion Monte Carlo

Introduction and Background

- Particles travel discrete space according to a discrete diffusion equation.
- Couples with Monte Carlo transport
- Speeds up particles in diffuse regimes.
- Cell-based, unlike Random Walk Spheres
- Past DDMC efforts
  - Linear diffusion/transport, static, 1-D; DDMC/S_∞
  - Equilibrium nonlinear diffusion, time-implicit, 1-D (EqDDMC)
  - Nick Gentile's Monte Carlo Diffusion (LLNL)

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Hybrid Discrete Diffusion Monte Carlo

Current status of 1-D research

- Continuous in time
  - More accurate than time-implicit
  - Other methods have to sample a time when a particle goes from DDMC to MC
  - Straightforward coupling to transport
- Improved transport-diffusion interface
  - Based on asymptotic diffusion-limit boundary condition
  - Accuracy independent of angular distribution
- New scheme for tallying momentum deposition, based on net flow into cell, suitable for MC, too.

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Hybrid Discrete Diffusion Monte Carlo

Future Work

- Automating switch between DDMC and MC
- Multigroup
- AMR and unstructured meshes

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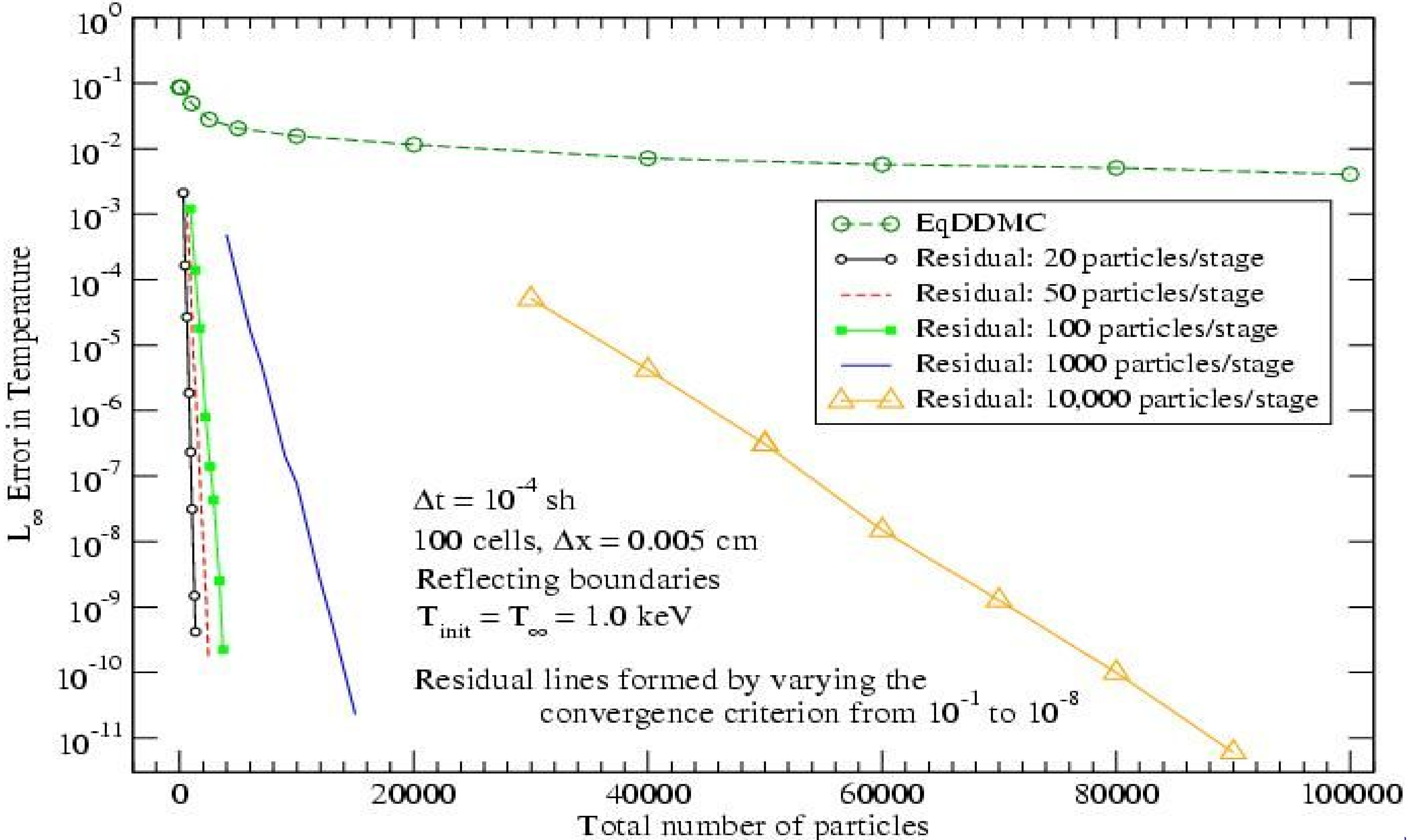
Residual Monte Carlo (ala Halton)

Introduction

- The method for solving $Ax=b$ is the same as for solving $A\delta x=r$, where $\delta x=x-x'$, x' is an approximation to x, and the residual $r=b-Ax'$.
- Only limited success applying to global, high-order polynomial expansion of continuum transport
- Instead, apply to EqDDMC (Evans, et al., JCP 189 (2003) 539-556.):
  - Start with solution estimate, x'
  - Perform stages until convergence
    - Use conventional MC to solve residual equation
    - $x' \leftarrow x' + \delta x$
  - Picard iterations on nonlinear coefficients possible

Residual Monte Carlo

Exponential Convergence with REqDDMC



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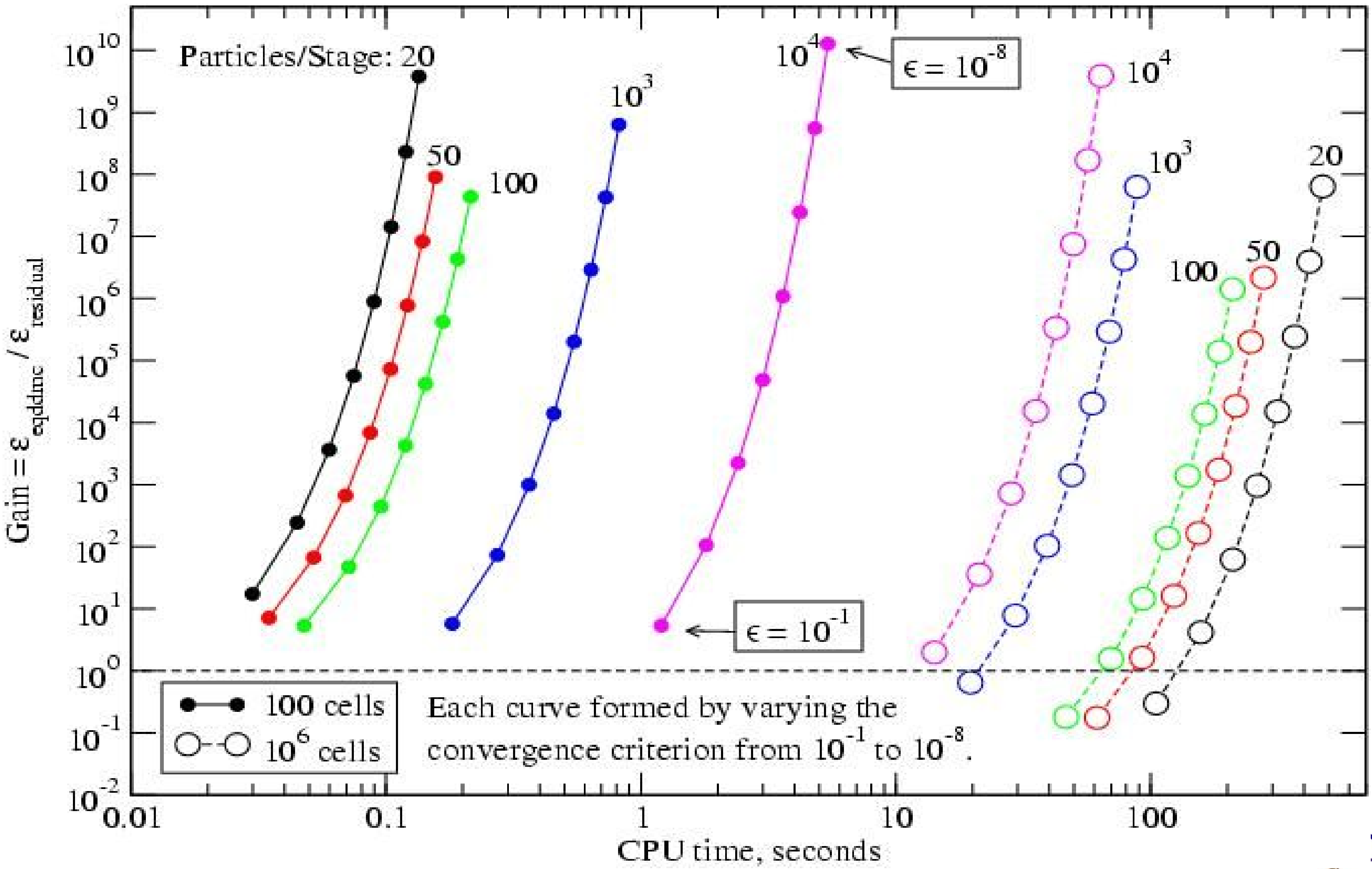
Residual Monte Carlo

Gain of REqDDMC over EqDDMC



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Residual Monte Carlo

Current and Future Work

- 3-D REqDDMC
  - Explore reduced-dimension residual
  - Hope to compete with deterministic solvers
- Newton Iteration
- Extension to Transport

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Analysis of IMC Methods

- Densmore & Larsen, *Proc. M&C*, (2003).
- Densmore & Larsen, *JCP*, 199, 175 (2004).
- Analyzed three methods
  - Fleck and Cummings
  - Carter and Forest
  - N'kaoua
- Maximum principle analysis
- Asymptotic analysis

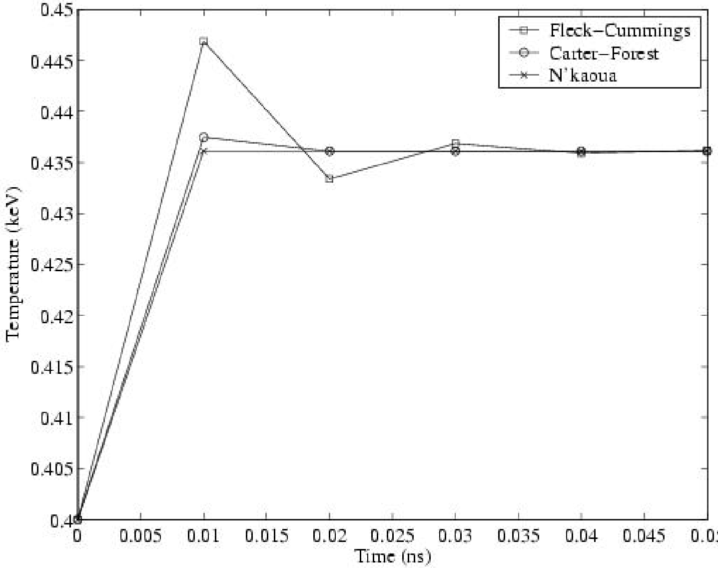
Analysis of IMC Methods

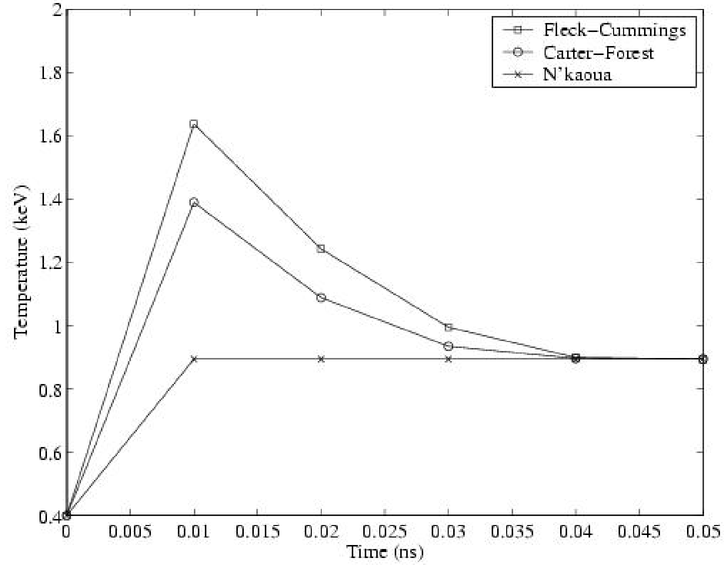
- Maximum Principle analysis
  - Analytic, FC, CF, N'k satisfy maximum principle
  - Carter-Forest reqs smaller Δt to satisfy max principle
  - Fleck-Cummings more robust than Carter-Forest
- Asymptotic analysis
  - Analytic eqns limit to equilibrium diffusion as mean-free-time and -path become small.
  - N'k always has the equilibrium diffusion limit
  - Carter-Forest does if ΔT_{mat} small enough during Δt
  - Fleck-Cummings never has the eq diffusion limit

Analysis of IMC Methods

Numerical Results

- Fleck-Cummings produces
  - Nonphysical results for extremely large Δt
  - Accurate solutions for even moderate Δt
- Both Fleck-Cummings and Carter-Forest produce nonphysical results in cold materials quickly heated by intense radiation.





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Future Work on Parallelism

- OpenMP/OpenMPI
  - C++ compilers were not ready back in 2001-2002
  - Deep objects were problematic
  - Have not returned to the issue
- General Domain Decomposition/Replication

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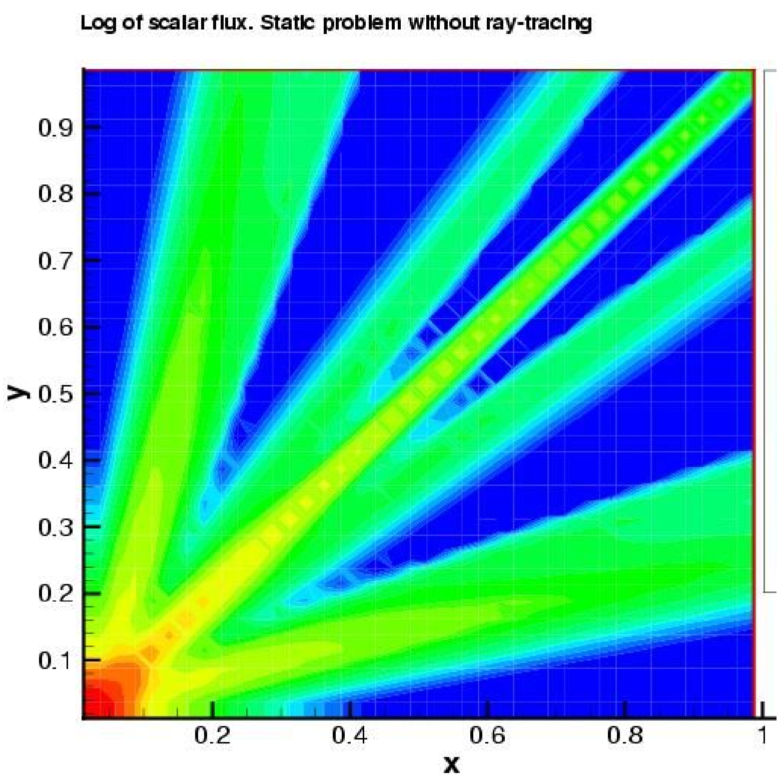
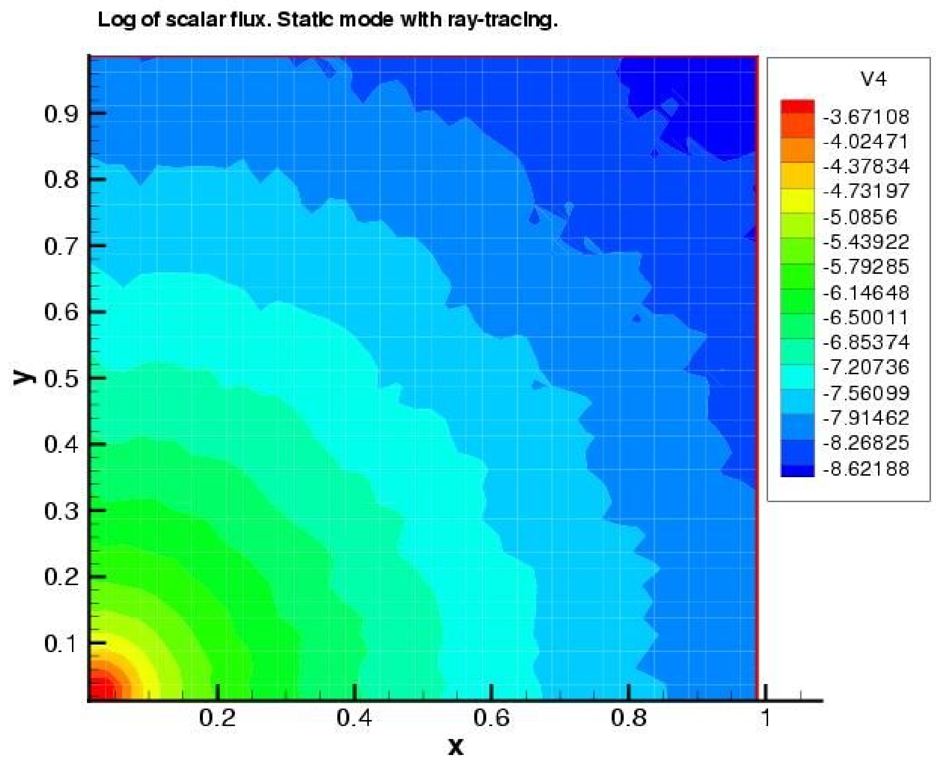
Static Uncle McFlux

Uncollided Monte Carlo flux package

- Used with S_N to mitigate ray effects
- Provides uncollided flux for 1st-collision source





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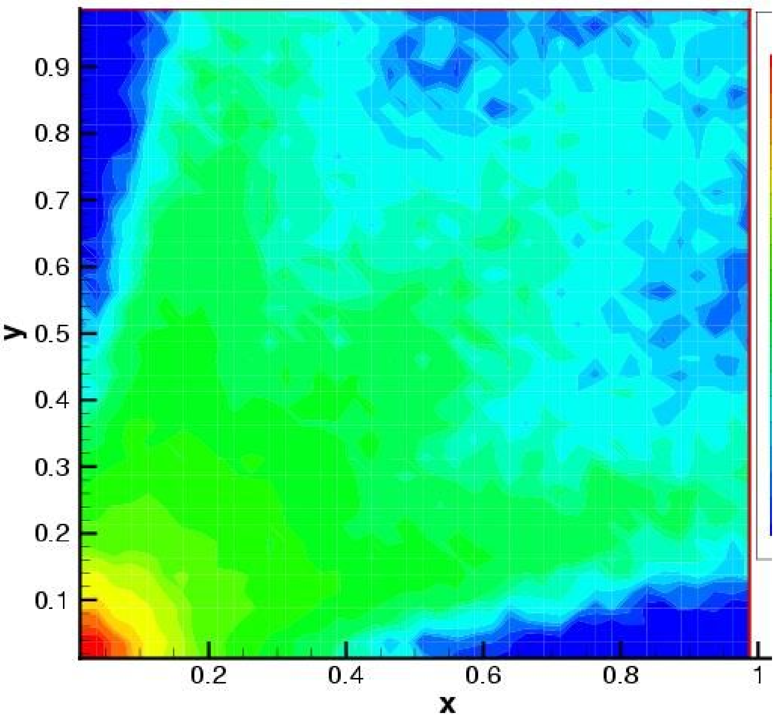
Uncle McFlux

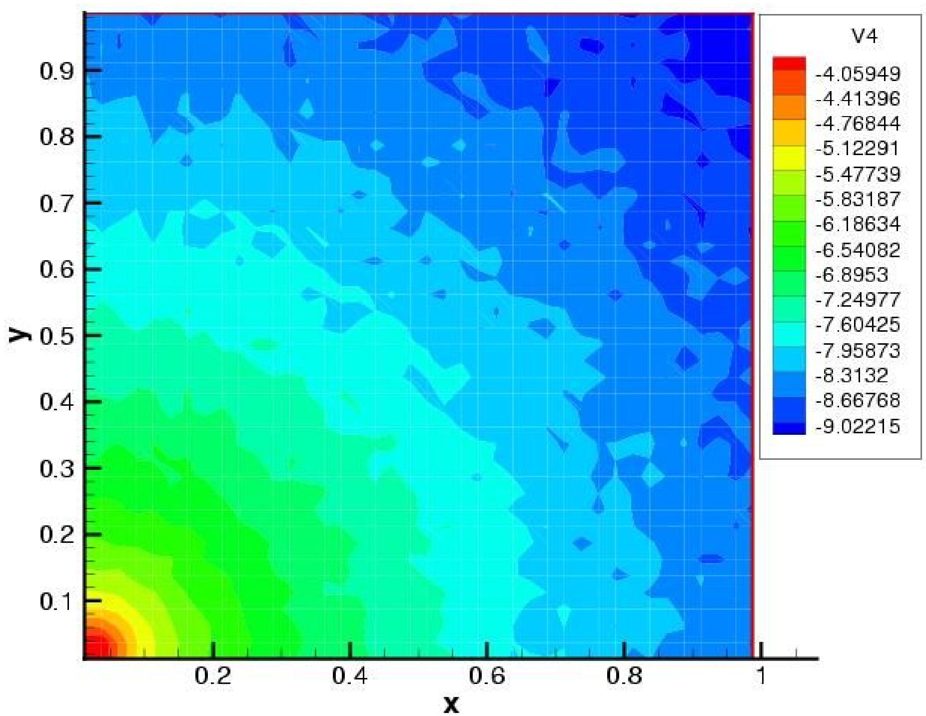
Time-Dependent

- Zombie ray-effects due to resampling
- Maintaining a census kills zombie ray-effects

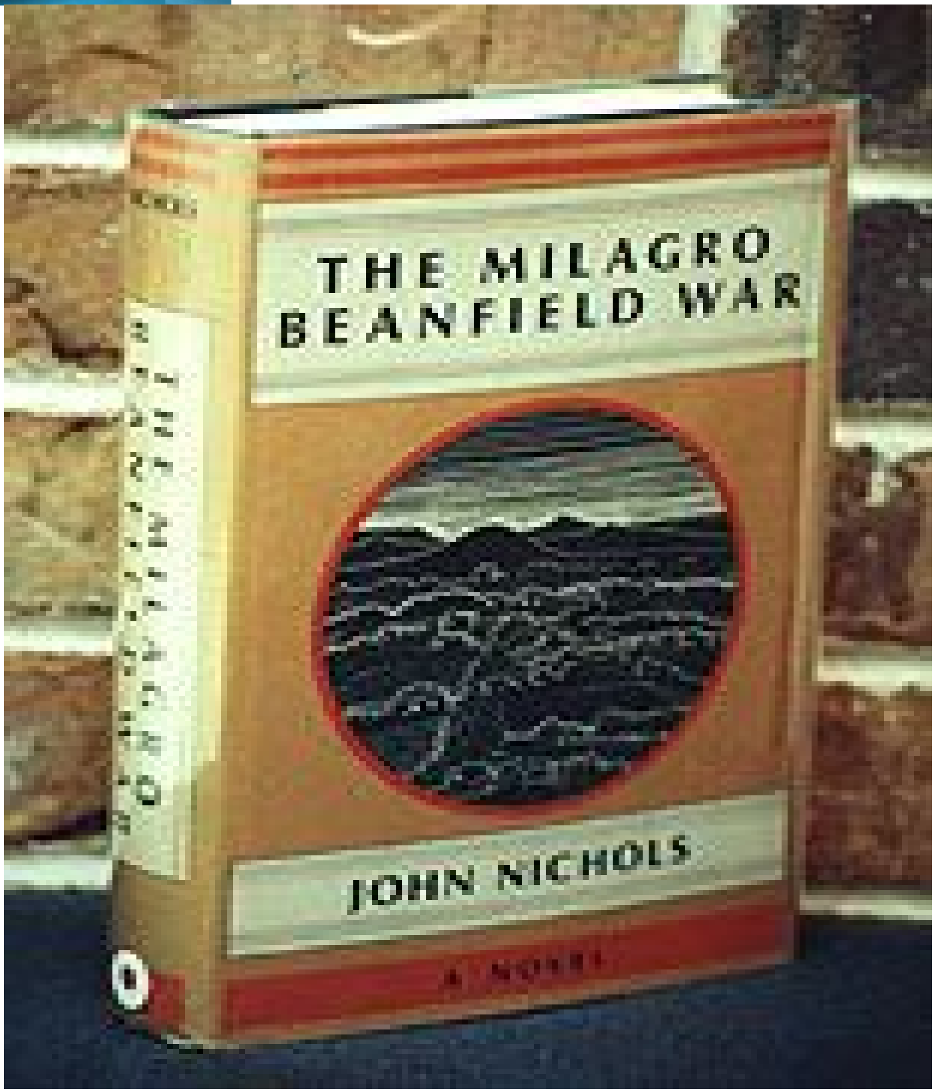
Log of scalar flux. Time dependent mode with raytracing.

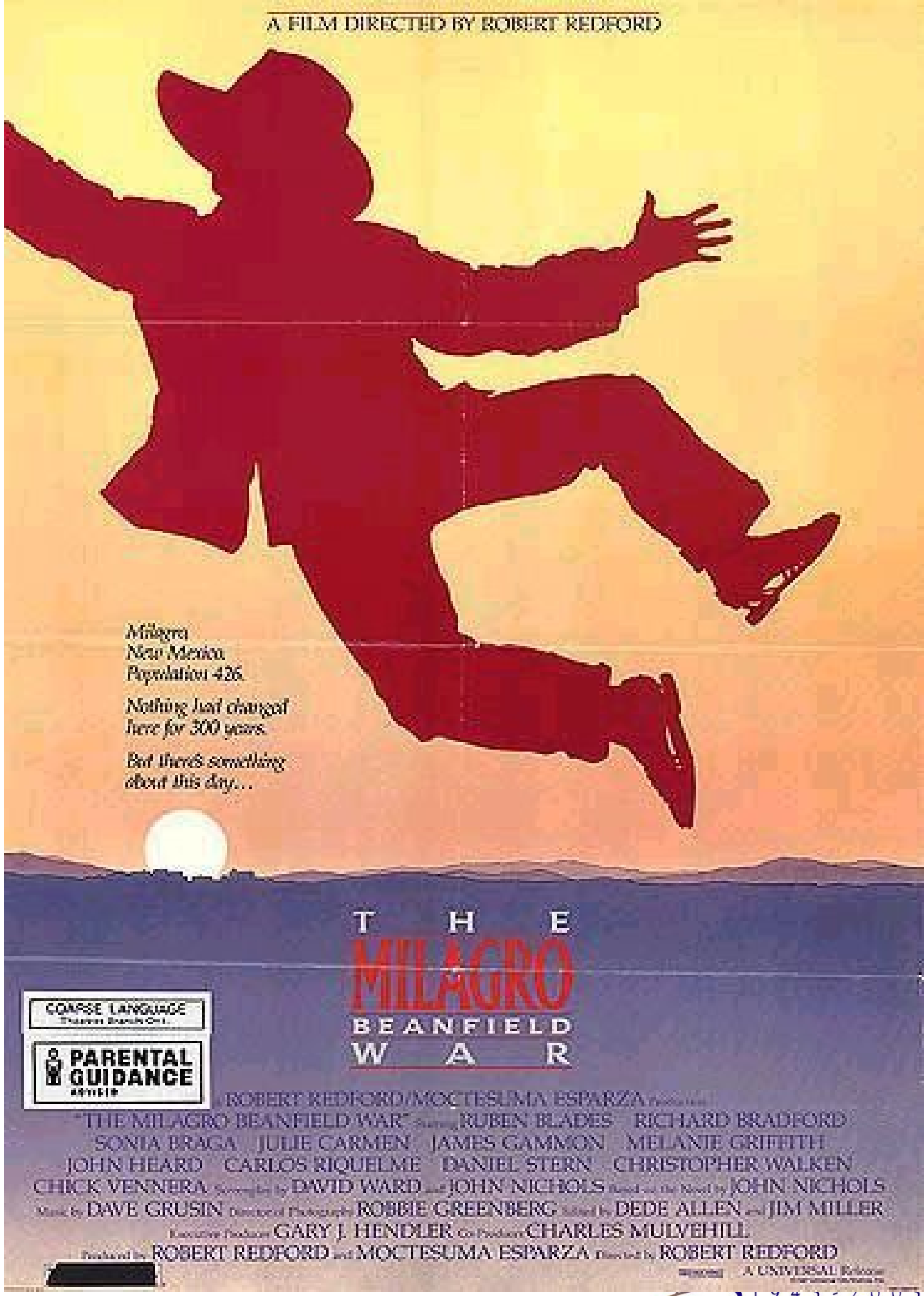


Log of scalar flux. Time-dependent mode with census



The End





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