PDT: A Deterministic Transport Code for High-Performance and High-Fidelity Calculations

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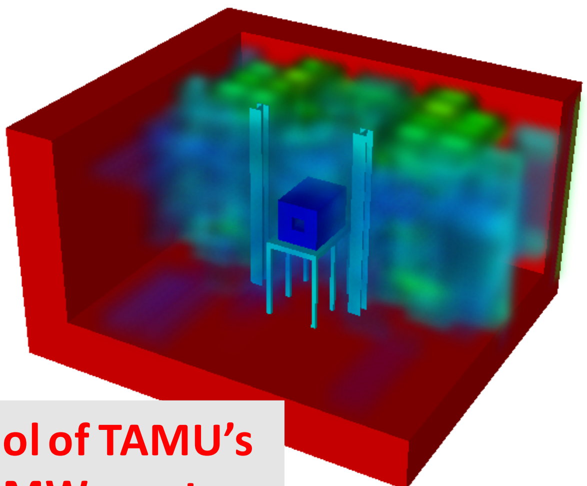
First a remark on the big picture: We do a lot of R&D in support of national security. Some recent examples:

- Center for Exascale Radiation Transport
  - NNSA ASC Center (one of 6 nationally)
  - $2M/yr in support of stockpile stewardship
- Collaborations with LLNL
  - Stockpile stewardship (circa $1M/yr; multi-disc)
  - Other (~$0.5M/yr; variety; example MeGa-Rays)
- Numerous smaller projects with LANL and LLNL
- A host of NSSPI projects
- Classified contracts in place; more in progress

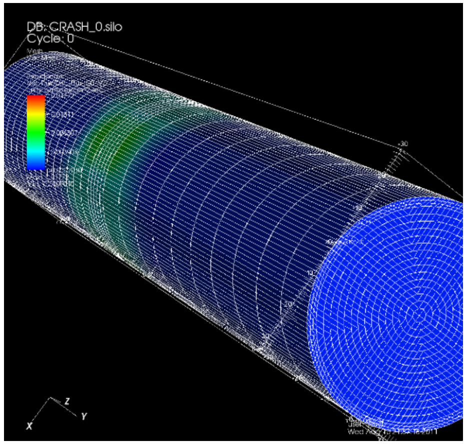
TAMU has outstanding radiation transport capabilities

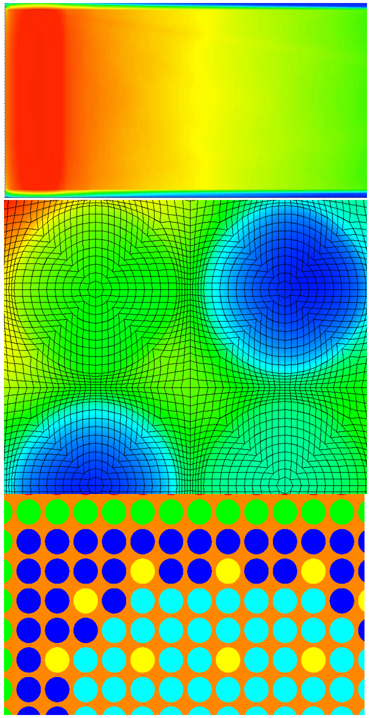
- We have outstanding Monte Carlo expertise (including MCNP)
- We have developed world-leading deterministic capabilities (PDT)
- We are developing hybrid MC/Deterministic methods and tools
- PDT is massively parallel and portable
  - Runs efficiently on > 1 million processors !!!
  - Runs on variety of platforms (clusters, BlueGene, others; working toward GPUs)
- Time-dependent, steady-state, or eigenvalue capability
- 2D/3D fully unstructured mesh for geometric fidelity
  - Arbitrary polyhedral grids, polygonal-prism grids, brick grids, morphed brick …
  - MCNP-to-Mesh capability, coupled to parallel mesh generation
- Accurate, efficient discretizations (spatial, directional, energy, time)
- Rapidly convergent iterative methods being implemented
- Adjoint-based UQ capability

Examples of PDT's geometric fidelity (unusual for deterministic codes)



Core + Pool of TAMU's TRIGA 1 MW reactor



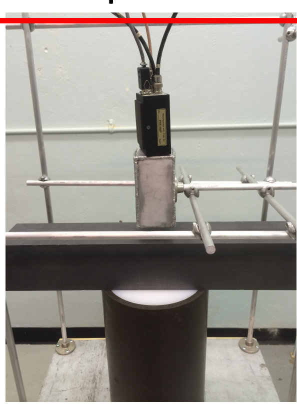


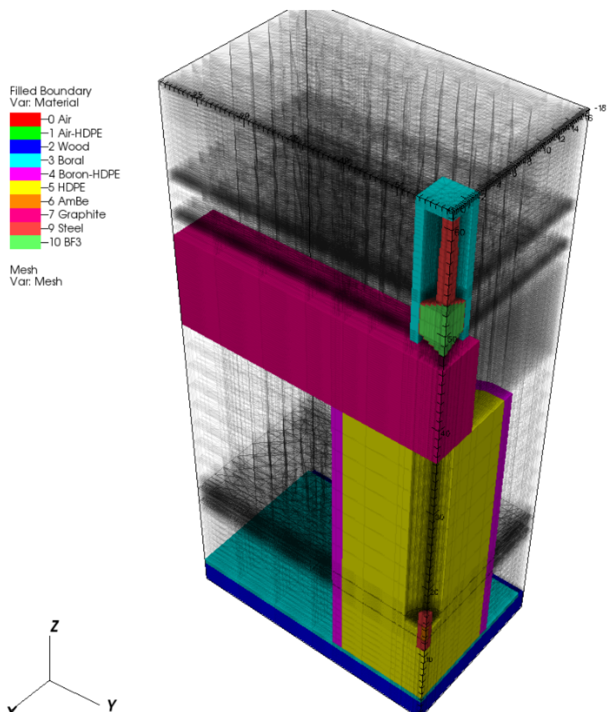
MCNP to Mesh to Solution

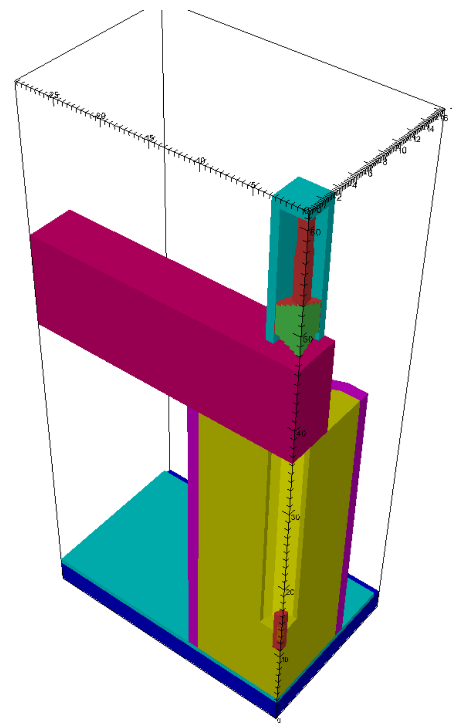
CAD SWORD User → MCNP → MCNP-To-Geom Converter → Arbitrary Parallel Mesh → Radiation Transport in PDT

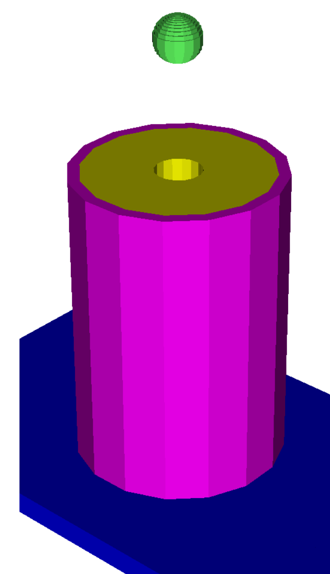
CAD → Arbitrary Parallel Mesh

PSAAP-2 neutron experiment

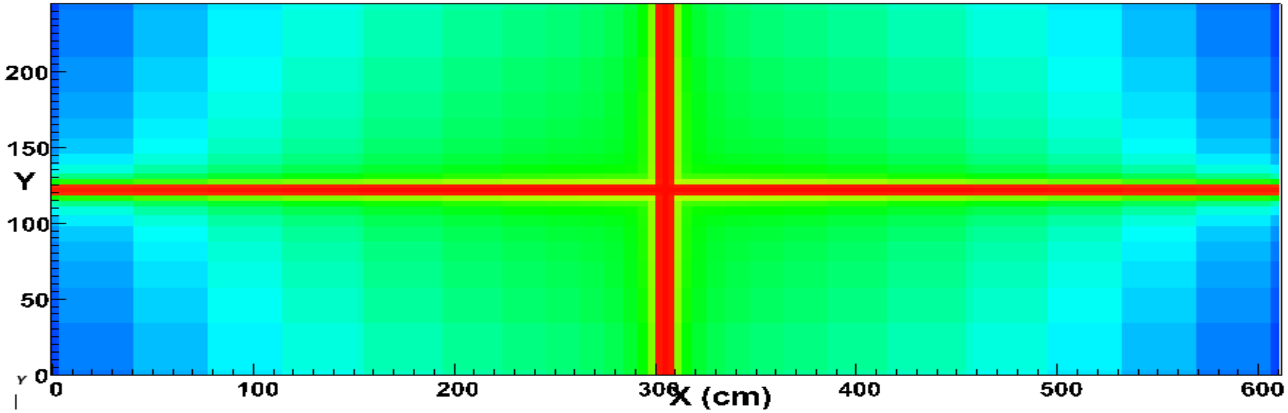








Uncollided-flux treatment resolves streaming gaps & small sources

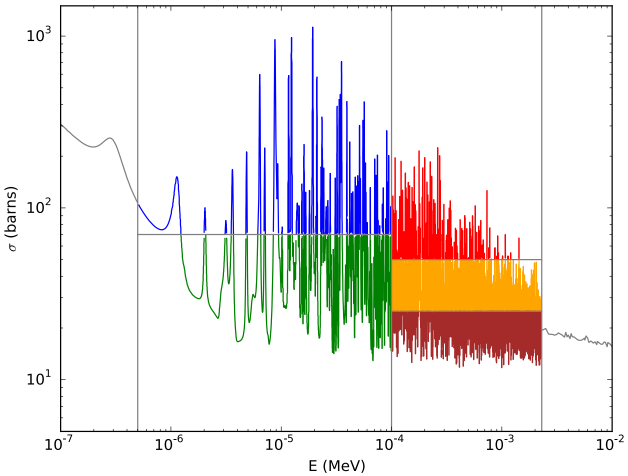


Uncollided treatment.
17-order of magnitude attenuation is captured. Color represents solution on log scale.

- 3x3x3 cm^3 HEU source on floor of cargo container. 3-cm gaps between cargo boxes.
- 1.001 MeV gamma line calculated
- PDT agrees with MCNP within 1%.

High-Fidelity Energy Treatment is comparable to Continuous Energy Monte Carlo

- Newly-developed Finite Elements with Discontinuous Support (FEDS) gives PDT a convergent energy discretization.
  - Hybrid of multigroup and multiband methods
  - Find the best discretization for a given number of degrees of freedom
  - Iteratively weight spectrum to account for leakage
- Has been tested for light-water reactor problems
- Currently extending to non-moderated systems
  - Project with LLNL
- Standard Uncertainty Quantification techniques can be adapted for this method.



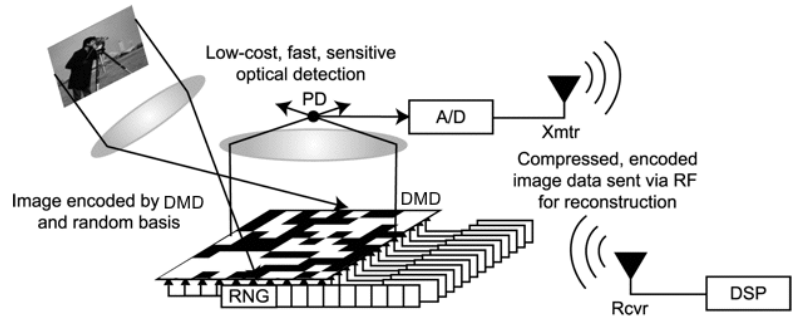
We have unique capabilities that may be of value to you

- We have many examples of accurate solutions of difficult problems
- We solve problems with PDT that most people think *require* Monte Carlo
- Unique collection of features:
  - Accurate treatment of complex geometry
  - Deterministic code that gives Monte-Carlo accuracy without statistical errors
  - Efficient on any computer
  - Validated against many experiments and benchmarks
  - State-of-art efficient uncertainty quantification (adjoints, e.g.)
- Suggestion:

Pose test problems that are of interest to you.
We will see what we can do with them.

Compressed Sensing Applied to Nuclear Problems

- Concept — Single Pixel Camera
  - Take one sample of the image and project onto a random linear combination of basis functions resulting in a single scalar value
  - Two values: the single value result and an identifier for the random linear combination are the only data that needs to be transferred
  - As the number of samples increase, the image can be reconstructed with an increasing amount of accuracy



http://dsp.rice.edu/cscamera

Disjoint Tallies – Single Pixel Tallies

- We can apply the idea of the single pixel camera and apply it to MC simulations.
- Instead of having a grid of, for example, 1024 x 1024 flux tallies,
- We can have a several random linear combinations of the tallies and then reconstruct the solution.
- We expect (and observe) the memory footprint for these calculations to be much lower.
- For example, 4x4 grid

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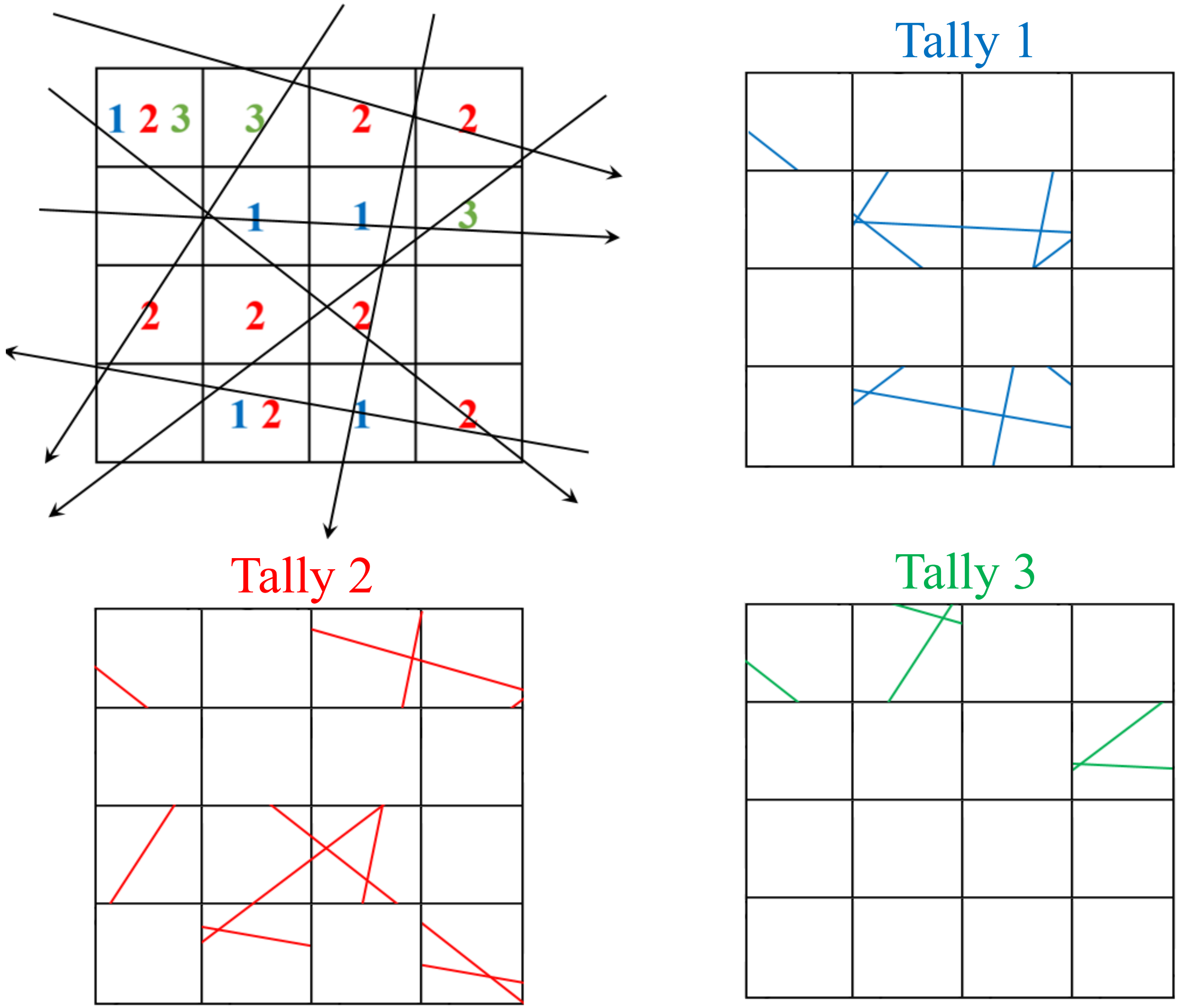
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1 2
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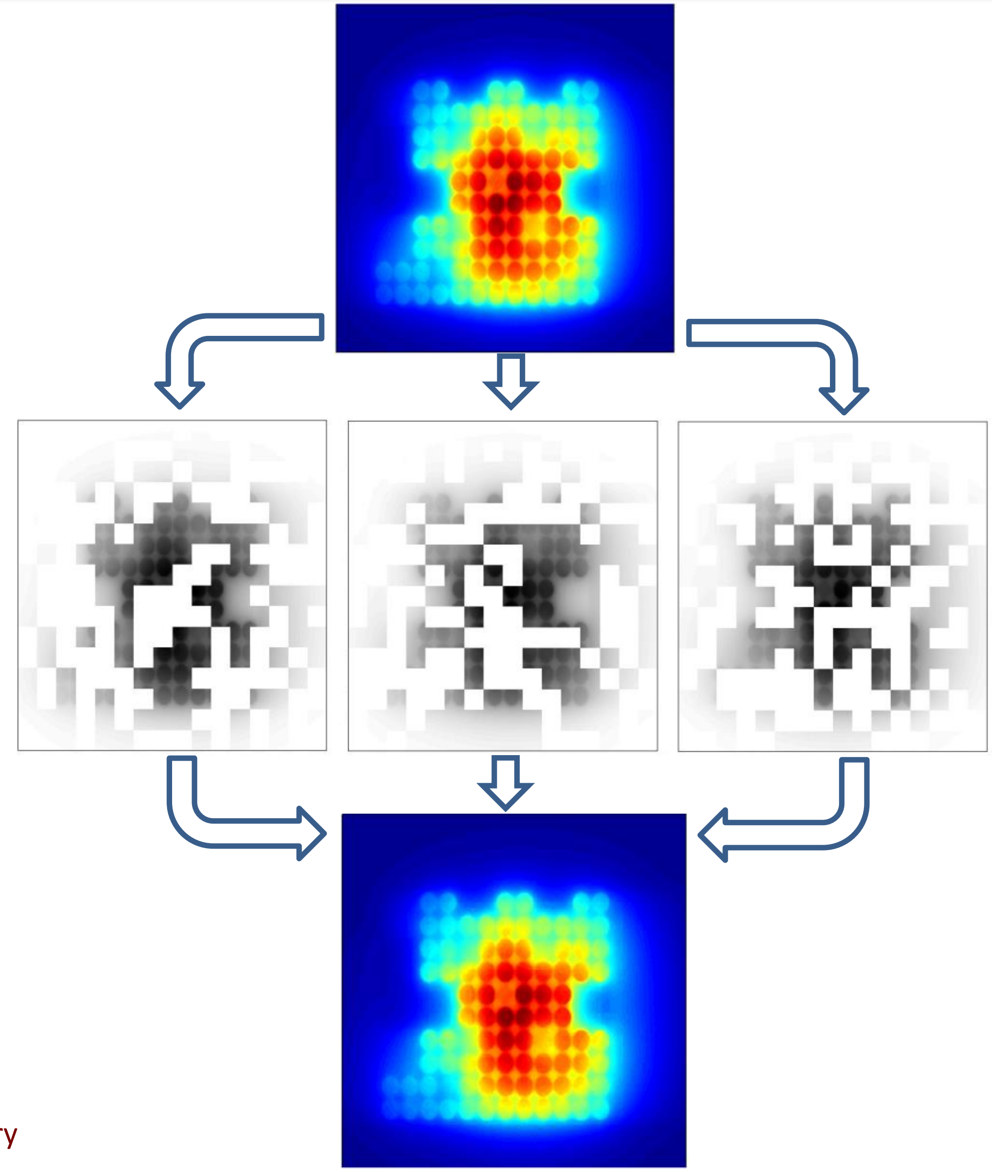
Tally 1
Tally 2
Tally 3

1. Run MC simulation

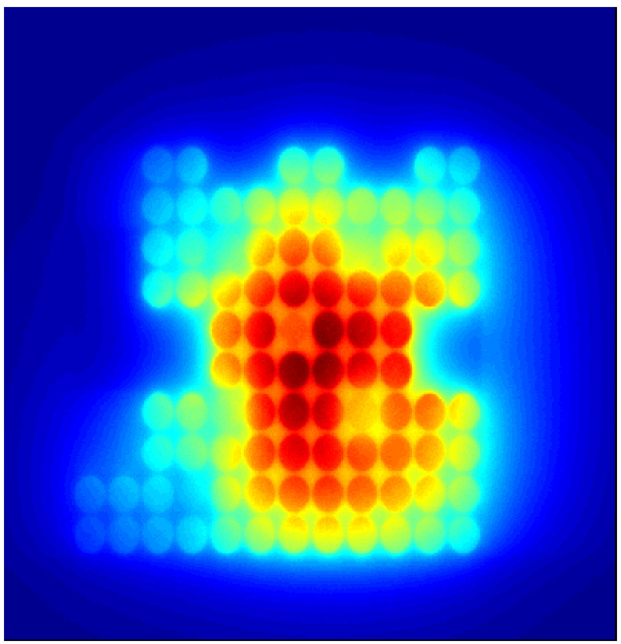
2. Tally the neutron flux using disjoint tallies
   - Store each tally as a single number!

3. Reconstruct a 2D map of the neutron flux

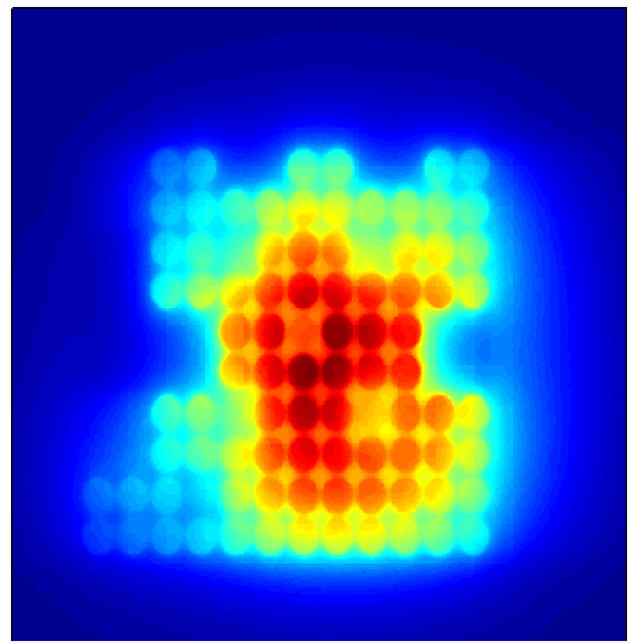


Statistically Converged Solution

Original

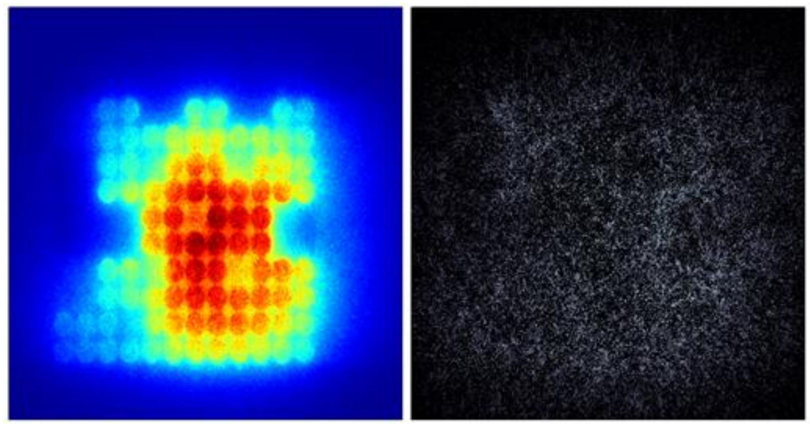


10% of Memory



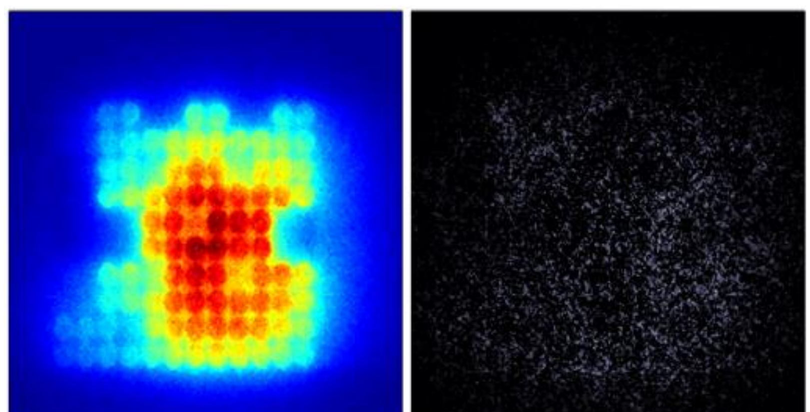
Noisy Solution – Disjoint Tallies More Accurate

Original 2D mesh tally of flux in NSCR (left) and statistical error (right)



$\|e\|_1 = 0.0078$
$\|e\|_2 = 0.0014$
$\|e\|_\infty = 0.0071$

Compressed to 10% of computer memory (left) and statistical error (right)



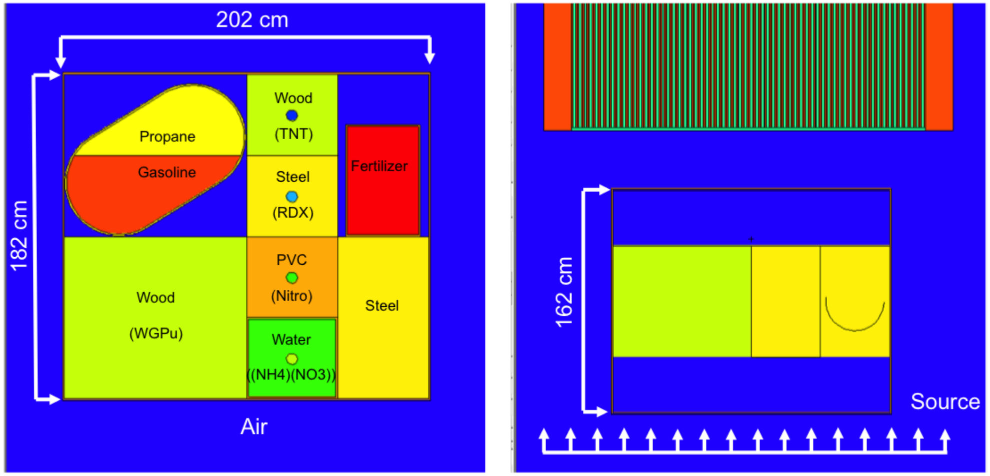
$\|e\|_1 = 0.0069$
$\|e\|_2 = 0.0012$
$\|e\|_\infty = 0.0063$

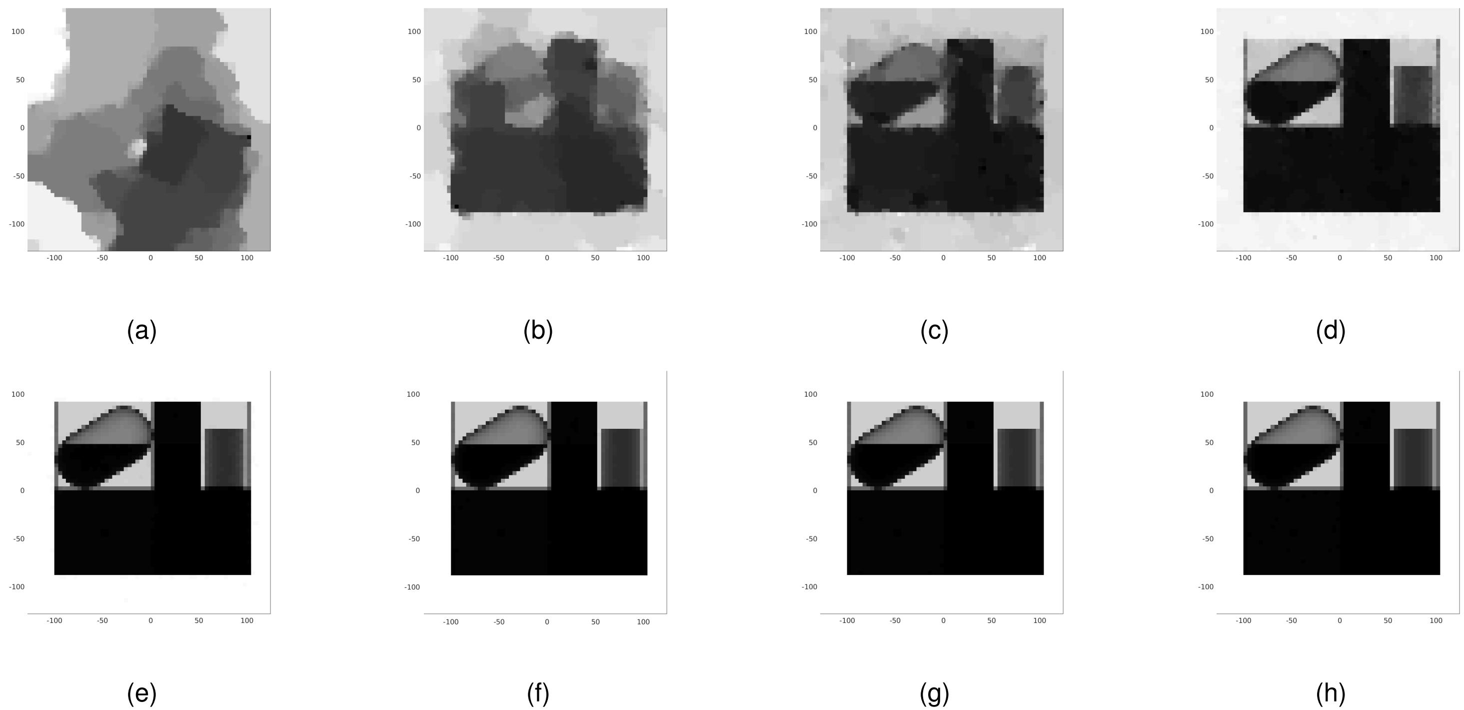
Single Pixel Neutron Camera

- Can apply the same idea to a detector:
  - Using a collimator we could randomly block some of the channels with an absorber and measure the neutrons that pass collimator.
  - Doing this repeatedly with different numbers of channels being blocked, allows us to reconstruct a neutron image.
- With this technology we can image with fast neutrons because the detector volume can be arbitrarily large.
- Possible applications to
  - Passive and active interrogation
  - Flux maps of reactors using simple fission chambers

Example: 14.1 MeV neutrons on cargo container

- Collimator with 64 x 64 grid of openings.
- Several interesting materials in cargo container.
- Full image has 64^2 (4096) pieces of data.
- We can reconstruct contents using many fewer measurements.





The reconstructions for the ULD problem using (a) 1%, (b) 5%, (c) 10%, (d) 20%, (e) 30%, (f) 40%, (g) 50%, and (h) 70% of the pixel count.

Compressed Sensing could lead to many new capabilities

- We are actively researching ways to apply these technologies to a variety of problems.
- We are keen to hear of any problems that you think these new ideas could be useful for.