(Nuclear) Engineering the Future

Prof. Rachel Slaybaugh
5 October, 2016
Departmental Colloquium
University of Tennessee, Knoxville

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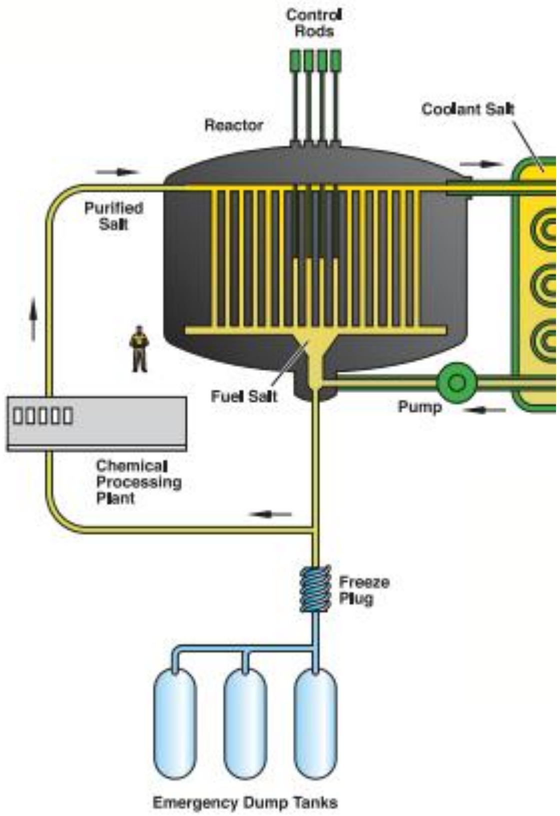
Environment, Health, Prosperity

How do we help the world develop **sustainably**?

http://www.insidesources.com/wp-content/uploads/2015/11/bigstock-Energy-4298515-300x300.jpg

Nuclear Innovation is Needed



Enable New Reactors

Enhance Nuclear Security

Develop Medical Devices

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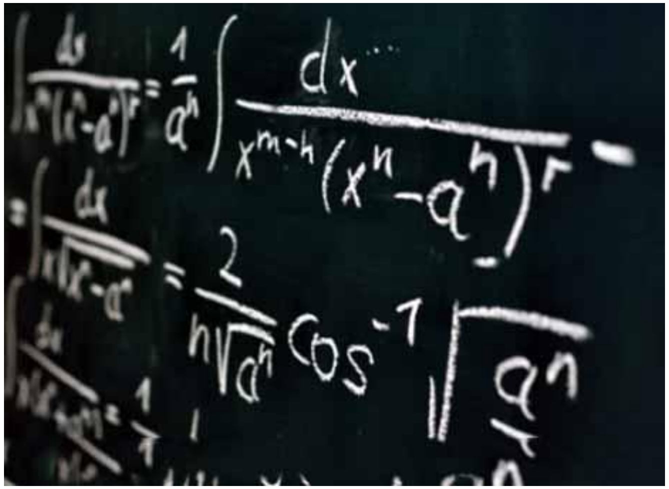
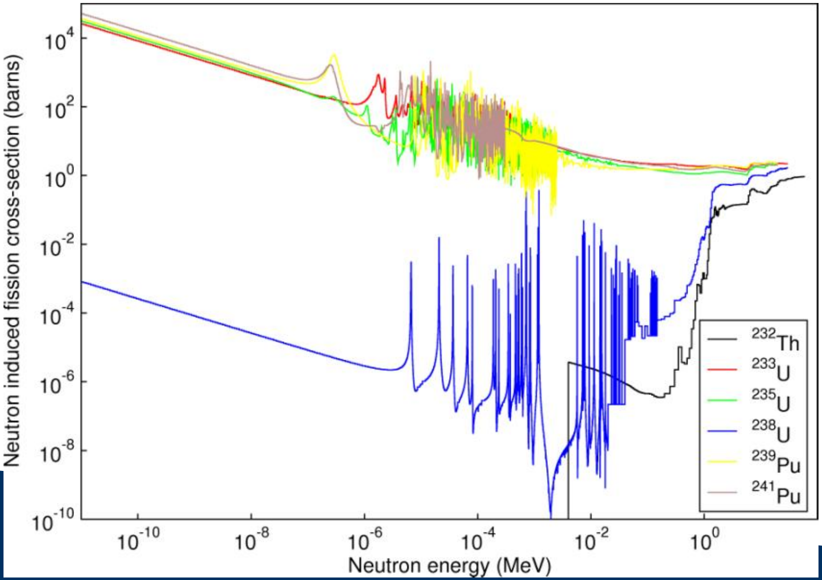
My Contribution: Numerical Methods

To facilitate innovation,
we need *predictive simulation*

- I build tools (translate applied math into code) used to design and analyze these systems
- I focus on high performance computing
- and inform algorithm development with physics of problems of interest





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Finding All of the Neutrons

$$[\hat{\Omega} \cdot \nabla + \Sigma(\vec{r}, E)]\psi(\vec{r}, \hat{\Omega}, E) =$$

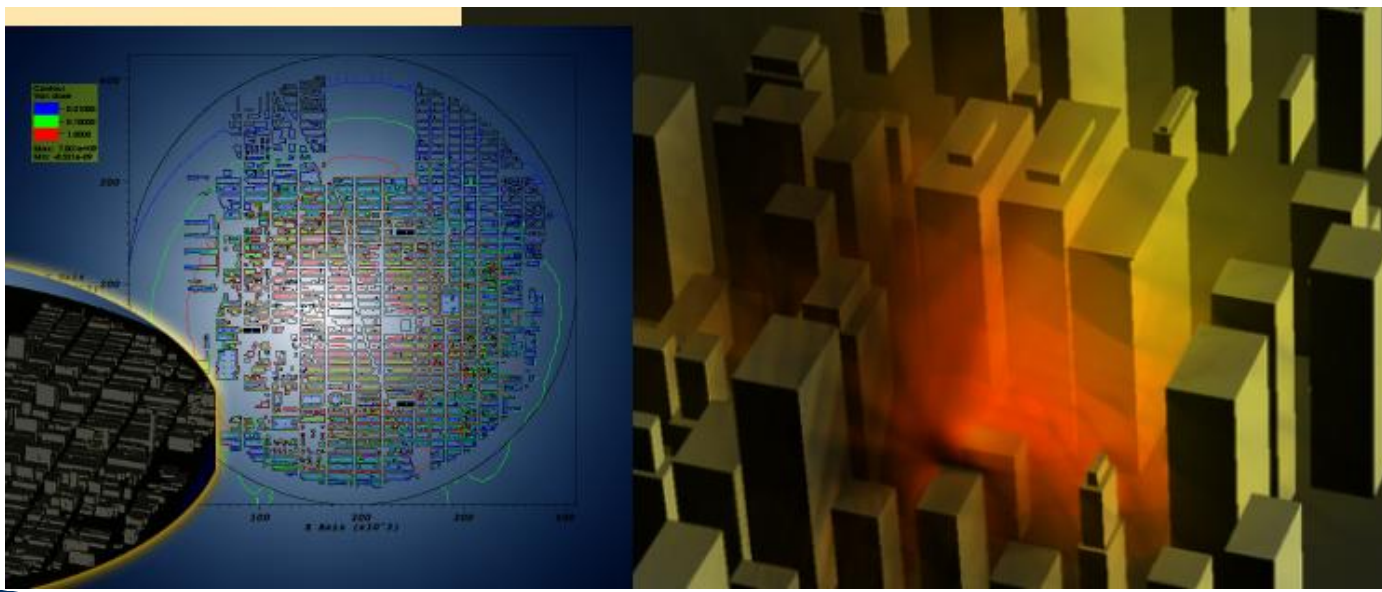
$$\int dE' \int d\hat{\Omega}' \, \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega})\psi(\vec{r}, \hat{\Omega}', E')$$

$$+ \frac{\chi(E)}{k} \int dE' \, \nu\Sigma_f(\vec{r}, E') \int d\hat{\Omega}' \, \psi(\vec{r}, \hat{\Omega}', E')$$

- $\psi(r, \Omega, E)$: eigenvector; angular neutron flux (n / cm^2-steradian)
- *k:* dominant eigenvalue; governs steady-state system behavior
- $\Sigma(r, E)$: probability of neutrons interacting with a material (cm^-1)

Accurately is Hard

- 6-D phase space: location (3), direction (2), energy (1)
- Can be geometrically large and/or physically complex and/or coupled to other physics
- The physics data is *Complicated*

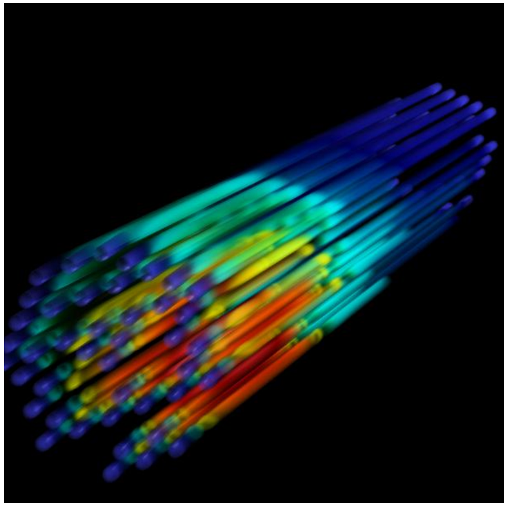


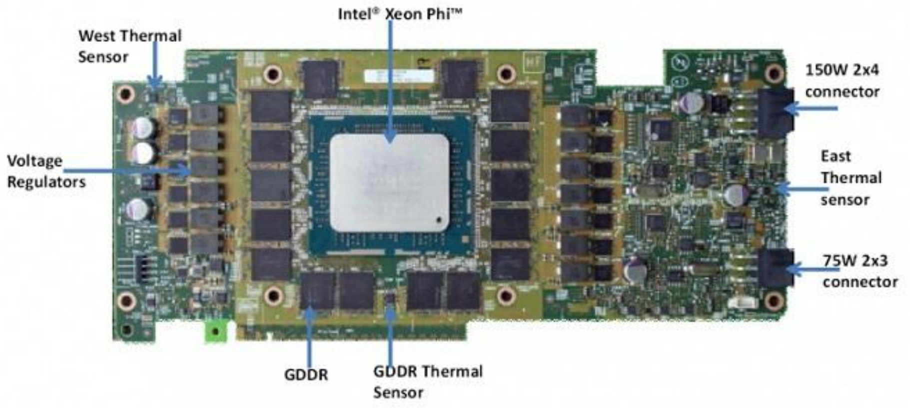
- Strategies:

Deterministic

Monte Carlo

Algorithms = Physics + Architecture





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Quick Brief: Deterministic Methods

- Discretize phase space; represent as a matrix; apply linear algebra-type solvers
  - Space: mesh (think finite difference/volume)
  - Energy: break into multiple groups
  - Angle: capture with a quadrature set or expand in polynomials
- Quality of solution is tied to
  - Quality of discretization
  - Accuracy of solution methods
- Can be memory and FLOP intensive
- Strategically-designed parallelization techniques

$$\mathbf{L}\psi = \mathbf{MS}\phi + \frac{1}{k}\mathbf{MF}\phi$$

$$\phi = \mathbf{D}\psi$$

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ex. 1: Rayleigh Quotient Iteration

- Power iteration (historical) converges as $e_{j+1} = C\left|\lambda_2/\lambda_1\right| e_j$

$$\sigma(A) \equiv \{\lambda \in \mathbb{C}: (A - \lambda I) \leq n\}$$

- Where ( ) μ $(A - \mu I)$ A
- We apply a shift, μ, and $(A - \mu I)$ has the same eigenvectors as A

$$\sigma(A - \mu I) \equiv \{\frac{1}{\lambda - \mu}; \lambda \in \sigma(A)\}$$

$$e_{j+1} \approx C\left|\frac{\lambda_1 - \mu}{\lambda_2 - \mu}\right| e_j$$

- And make the shift the Rayleigh Quotient (optimal guess)
- *However*, now looks like every group has upscattering!!
- This method only makes sense with Block Krylov and a preconditioner

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Less Time, Fewer Iterations

- RQI using a Block Krylov solver in space energy with a multigrid-in-energy preconditioner
- Applied to problem with 1.73 trillion unknown on ~140,000 cores

Solver	Precond	Krylov	Eigen	Time (m)
Original	none	5,602	149	612.2
New	w1r2v2	70	5	54.8

- 10x improvement; strong scales very well
- **New:** applying to alpha eigenvalue formulation with LLNL

R.N. Slaybaugh, T.M. Evans, G.G. Davidson, and P.P.H. Wilson, "Rayleigh Quotient Iteration with a Multigrid in Energy Preconditioner for Massively Parallel Neutron Transport," Proceedings of M&C-SNA in Nashville, TN, April 2015.

Quick Brief: Monte Carlo

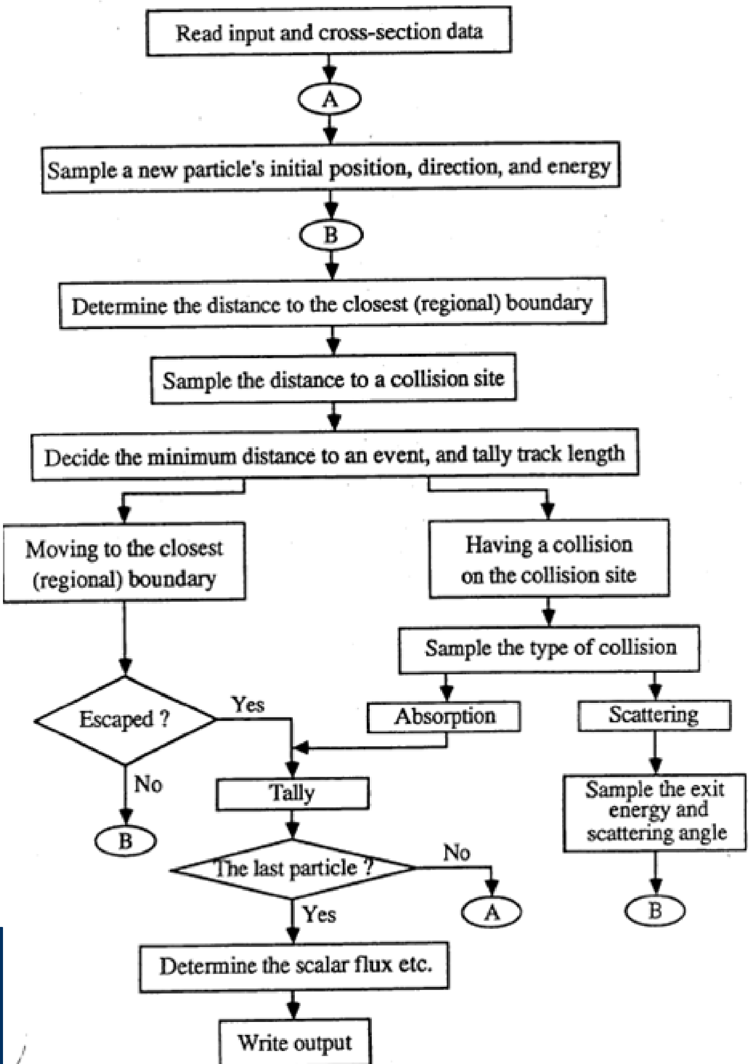
- Physics expressed continuously; sampled with random numbers
- Quality of solution is tied to
  - Number of samples in phase space
  - Adequacy of sampling phase space
- *Variance Reduction* methods can reduce variance faster while maintaining a fair game
- Can be memory and FLOP intensive
- Historically straightforward to parallelize

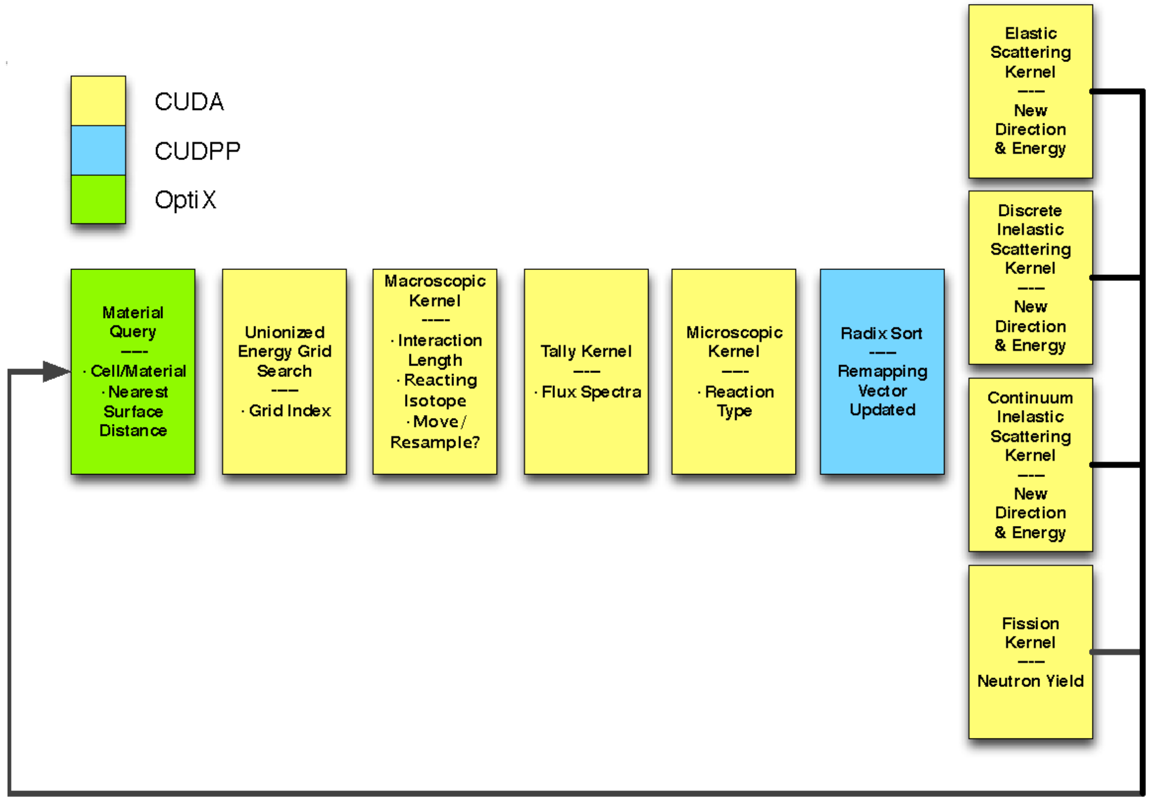
ex. 2: Monte Carlo on GPUs

- WARP: Weaving All the Random Particles
- 3D continuous-energy Monte Carlo neutron transport code developed for efficient implementation of the algorithm on GPUs
- Relative to CPUs, GPUs have higher aggregate memory bandwidth, much higher floating-point operations per second (FLOPS), lower energy consumption per FLOP
- CPU-optimized parallel algorithms not directly portable to GPUs
- Particle transport codes need to be rewritten to execute efficiently on GPUs

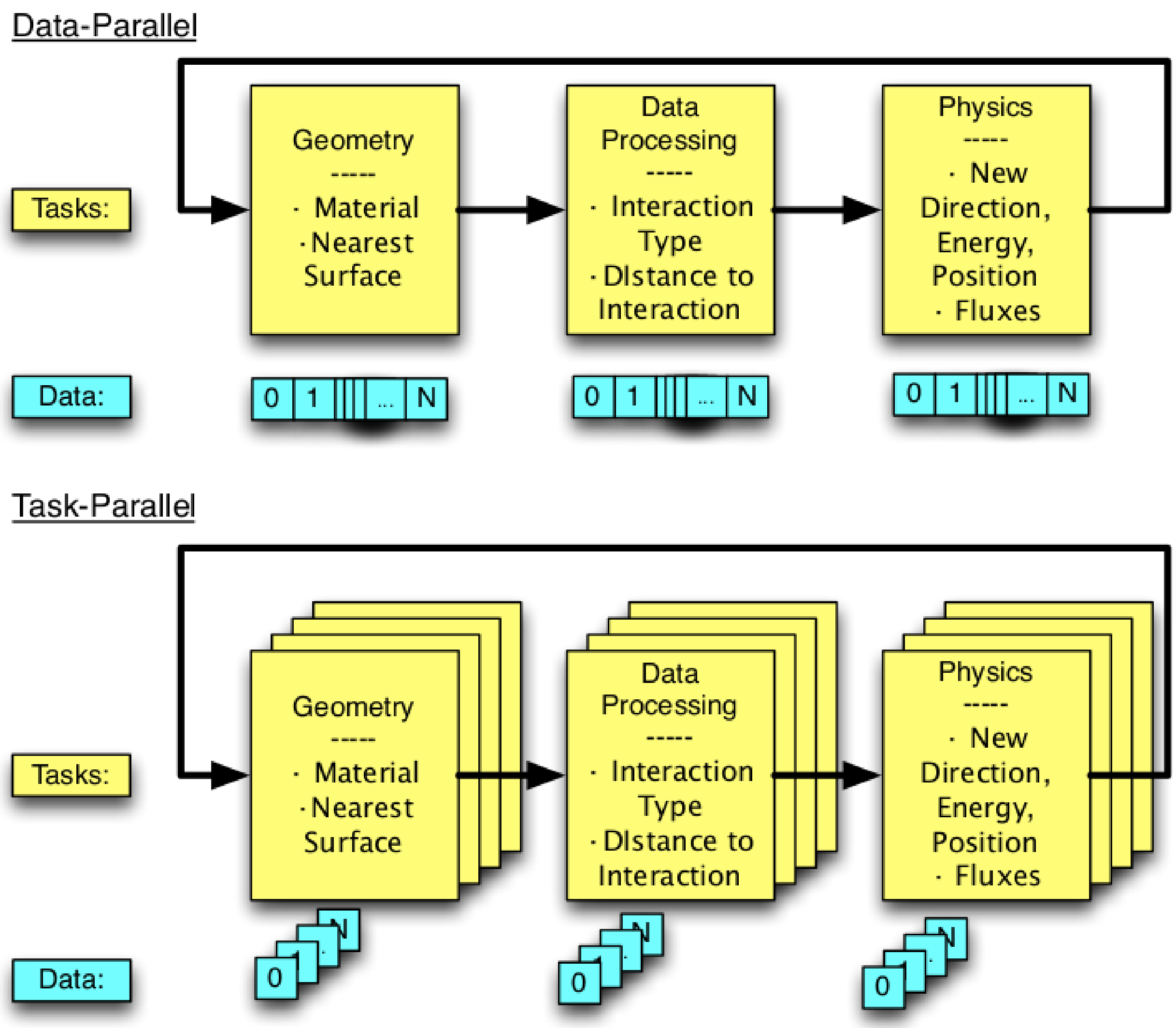
Ryan M. Bergmann, Jasima L. Vujic. "WARP – A framework for continuous energy Monte Carlo neutron transport in general 3D geometries on GPUs," *Annals of Nuclear Energy* **77** (2015) 176-193.

WARP Uses an Event-Based Algorithm





and is Data Parallel



WARP Remaps Data

After Microscopic Kernel, Before Radix Sort

Data Index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Reaction Number	2	800	2	2	51	61	1102	81	67	91	2	2	816	51	91	810	91	818	54	800

After Radix Sort

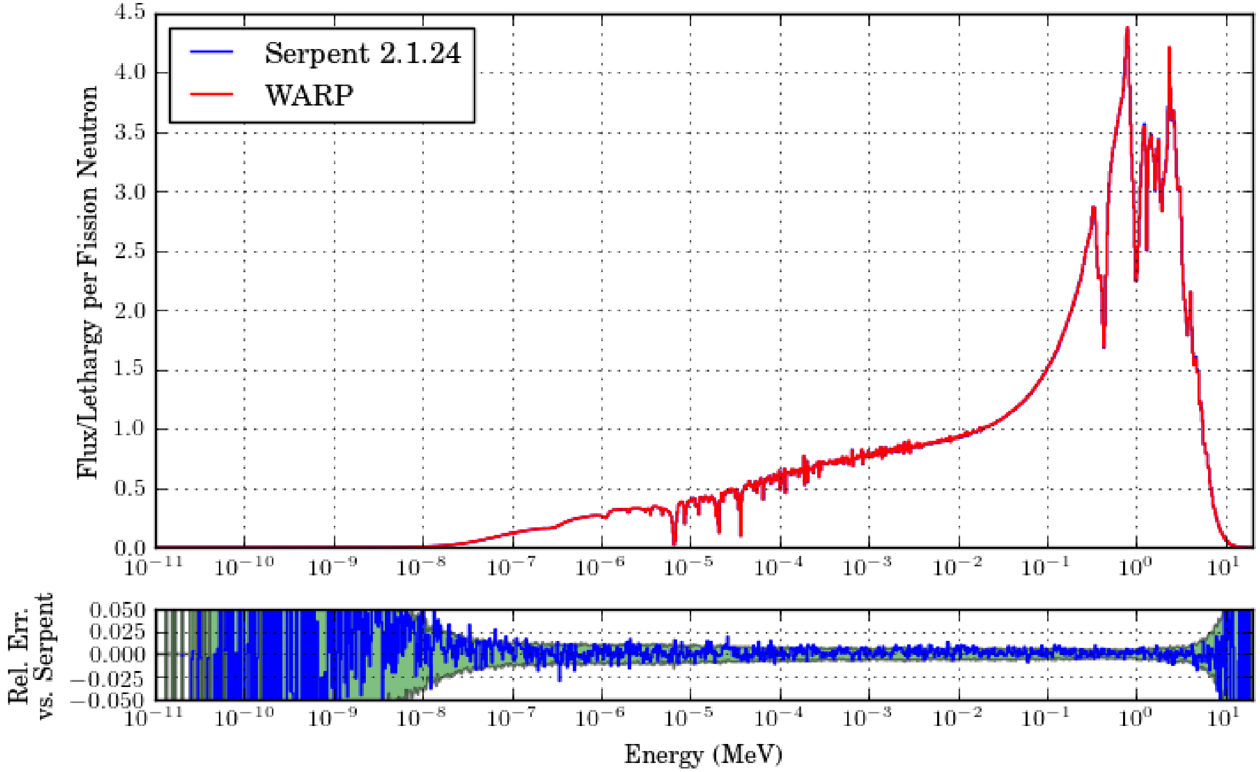
Data Index	0	2	3	10	11	4	13	18	5	8	7	9	14	16	1	19	15	12	17	6
Reaction Number	2	2	2	2	2	51	51	54	61	67	81	91	91	91	800	800	810	816	818	1102
	Elastic Scatter Kernel					Discrete Inelastic Kernel						Continuum Inelastic Kernel			Resample - Rxn kernels skipped		Fission Kernel - Terminated after processing yields			Complete - No longer referenced

A radix key-value sort is used to create a remapping vector, grouping neutrons by reaction in order to minimize thread divergence

Correct Results in Less Time

WARP took 2.062 s (k20; 32 threads)

Serpent took 137.0 s (AMD Opteron 6172; 12 cores)

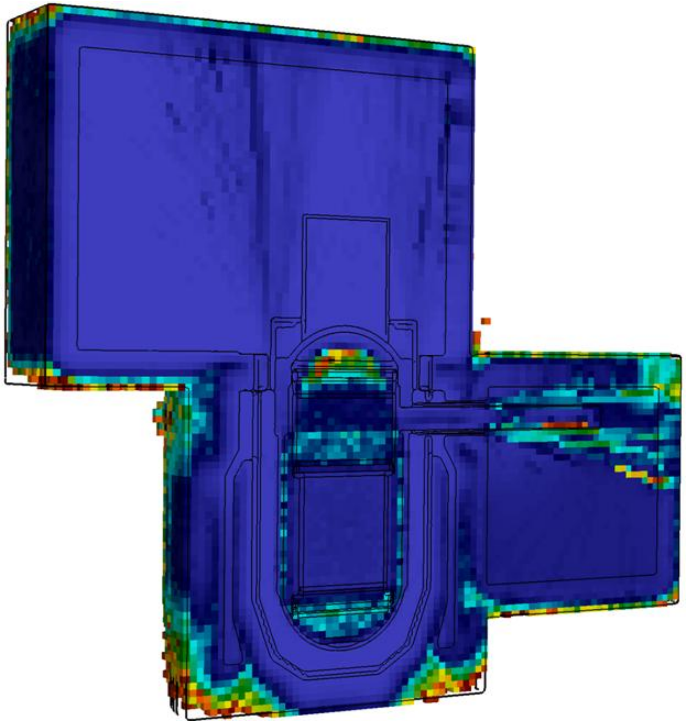


Quick Brief: Hybrid Methods

- Monte Carlo highly accurate; can be slow
- Deterministic methods usually fast; can have accuracy issues
- Hybrid methods use deterministic solutions to create variance reduction parameters for MC
  - Particles are assigned weights that map to impact
  - Set how to update weights
  - Set how to bias the source

ex. 3: Angle-Informed Methods

- Radiation shielding is a tough problem, especially when there are strong angular anisotropies
- Hybrid methods currently only include space and energy information
- Including angle explicitly is too costly
- Other attempts haven't worked well
- We're trying a new way to incorporate angle strategically



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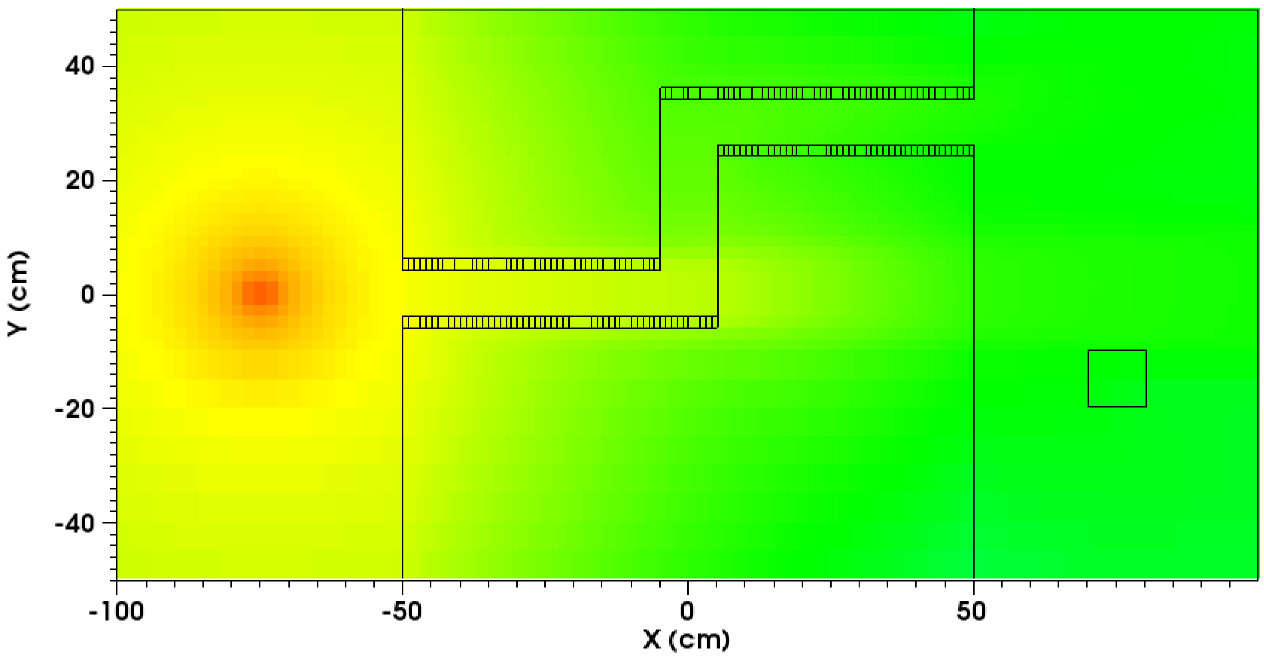
Start with Importance

- Many hybrid methods use adjoint transport information, which we think of as the importance of a source particle to the solution



Neutrons in the forward problem will flow from the source to the detector:

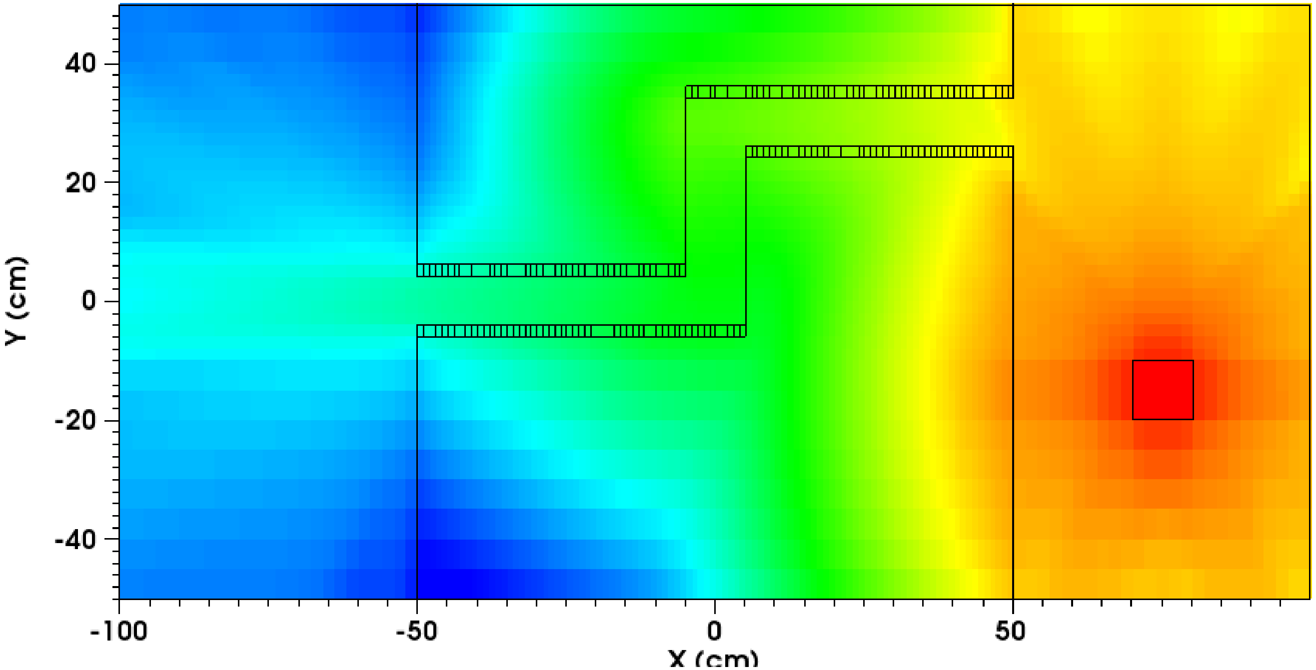
group 0 forward

Start with Importance

- Many hybrid methods use adjoint transport information, which we think of as the importance of a source particle to the solution

Adjoint particles are how each part of phase space contributes to the solution:

group 11 importance map



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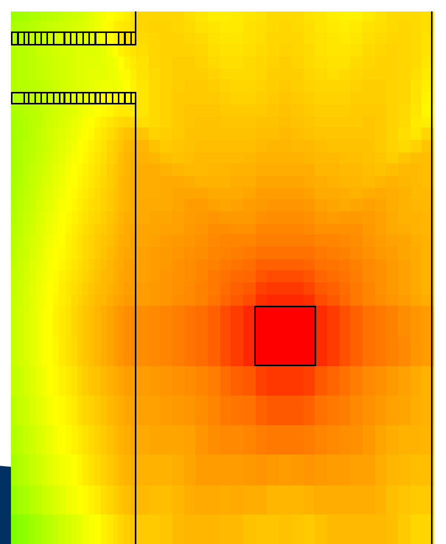
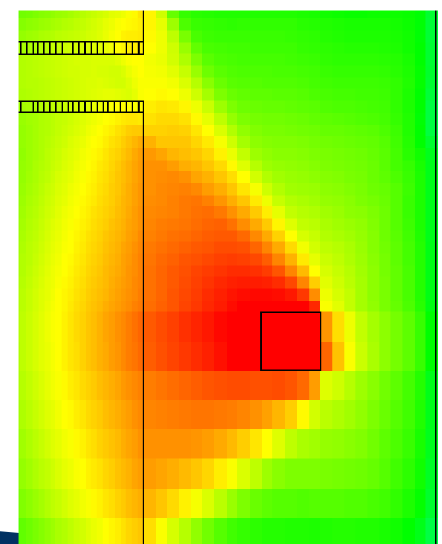
and Use Contributon Theory

- We've modified FW/CADIS to include angular information without changing the method's end use

$$\phi_+(r,E) = \frac{\int \psi_+\, r,E,\Omega \;\psi\; r,E,\Omega \; d\Omega \quad \left(\int \psi \; r,E,\Omega \; d\Omega\right) \left(\quad \right)}{\left(\quad \psi_+ \right) r,E,\Omega}$$

- Enabled by ability to write and store ( )





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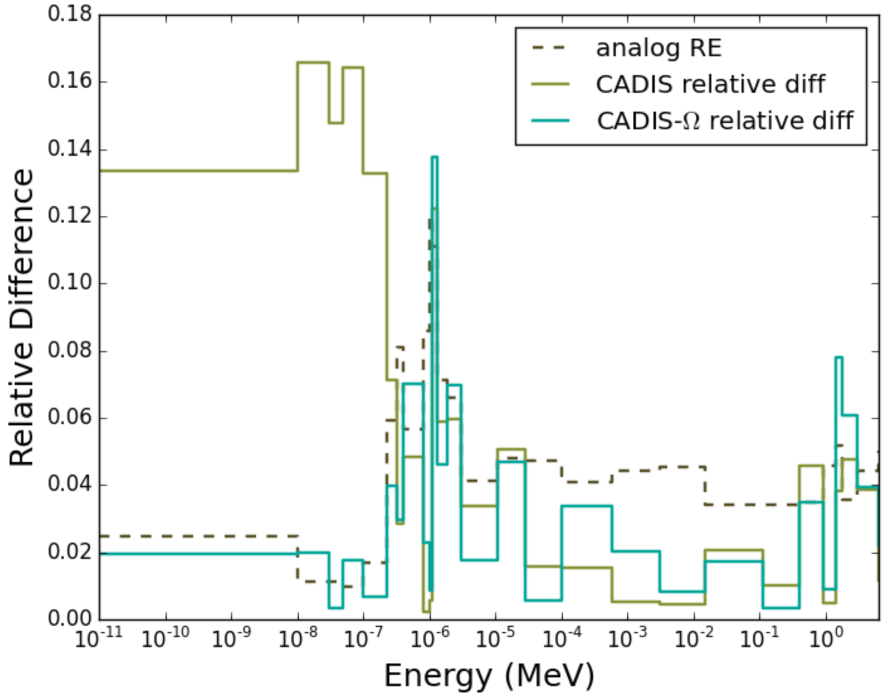
M. Munk, R.N. Slaybaugh, "An Angle-Informed Hybrid Method for CADIS and FW-CADIS." Proceedings of the PHYSOR 2016 Meeting in Sun Valley, ID, May 2016.

Good Initial Results



CADIS-Ω has:

- A relatively uniform uncertainty distribution

- Better FOM than CADIS
  - CADIS: 5.1
  - CADIS-Ω: 145.0

Further testing underway

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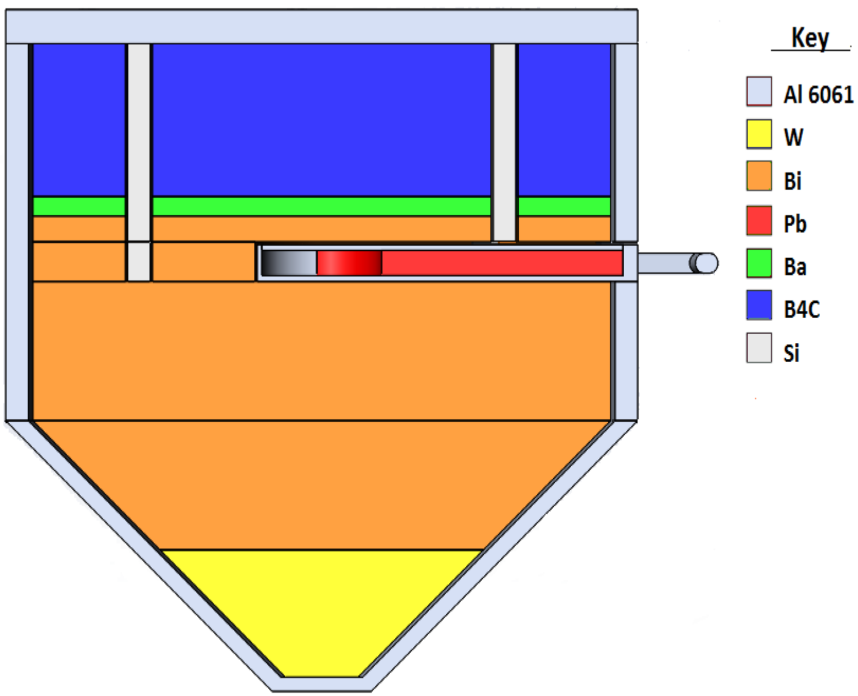
ex. 4: Optimizing Spectrum Shaping

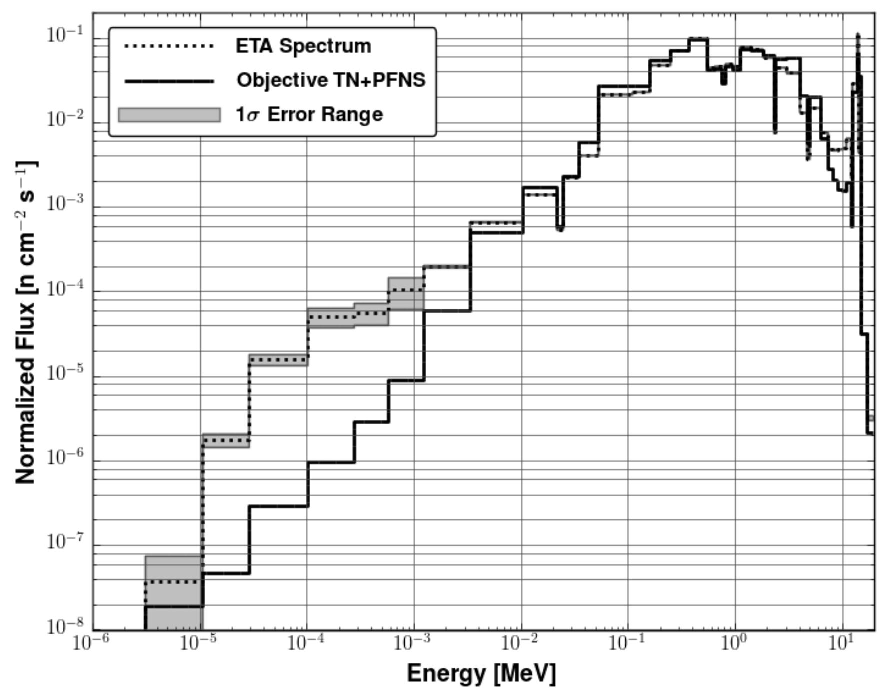
- **Challenge:** we want a neutron source with a specific spectral shape, but it doesn’t exist naturally (or easily)
- **Idea:** we can use a material stackup to modify the spectrum (Energy Tuning Assembly, ETA)
- **Goal:** general purpose metaheuristic optimization algorithm
- Gnowee (implemented in Coeus)
  - Handles continuous and discrete variables
  - Robust, complete set of search heuristics
  - Nearly-global convergence
- MCNP-Denovo hybrid radiation transport engine; parallel execution

Synthetic Debris



ETA Design

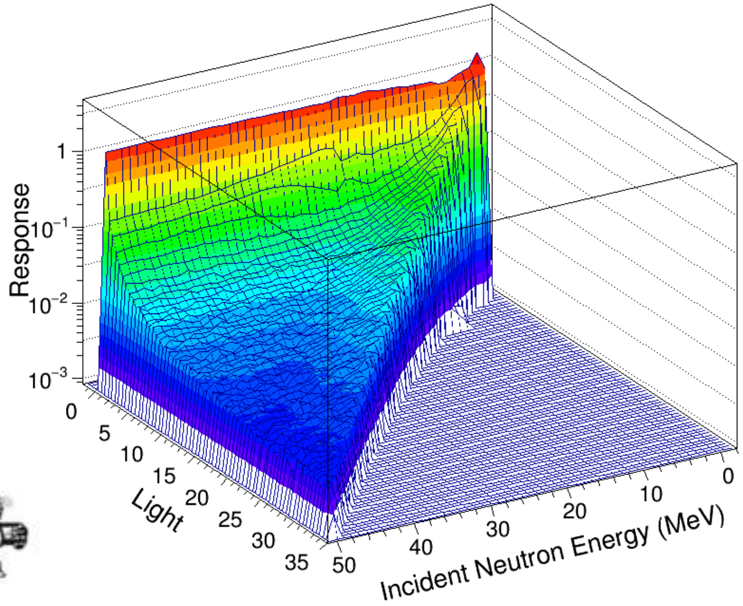
First application: nuclear forensics - create TN+PFNS from NIF

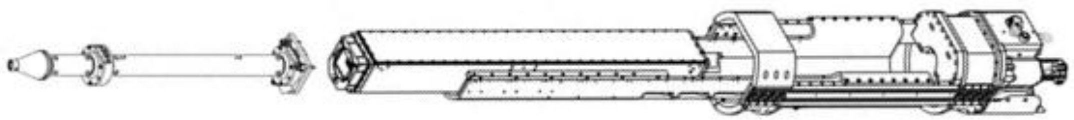


J. Bevins, R. Slaybaugh, L. Bernstein, E. Henry, W. Dunlop, "Targeted Modification of Neutron Energy Spectra for National Security Applications." Proceedings of the 2016 Hardened Electronics And Radiation Technology Technical Interchange Meeting in Monterey, CA, April 2016.

Widely Applicable and Flexible

- Spectral shaping methods can be used to expand the capabilities of existing facilities to cover new mission spaces
- Coeus provides an efficient capability to design and optimize ETAs for spectral shaping
- Experimental validation of TNF application at LBNL 88-Inch Cyclotron proceeding
- Planning underway for NIF shot





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Introducing the Advanced Nuclear Industry

~50 companies

~$1.3B of private capital

Build A Pipeline

TRAIN the current and next generations through Bootcamps

A U.S. example

SUPPORT companies through Innovation Centers

LEVERAGE public resources through GAIN

UPDATE Policy and Regulation to support innovation
TRANSFORM Communication

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GAIN: Public-Private Leverage

GAIN
Gateway for Accelerated Innovation in Nuclear

New DOE-NE Initiative within the Clean Energy Initiative

Integrated institute managing a distributed test-bed and demonstration platform, dedication to innovation in Nuclear Energy

Public-private partnership including Industry, Entrepreneurs, National Laboratories, and Academia

Headquartered at the Idaho National Laboratory

- Tens of $B in DOE and partner assets (experimental and computational)
- More than $1M in yearly investments for R&D and infrastructure
- $12.5B in loan guarantees
- $10M in SB vouchers
- Expertise and intellectual infrastructure

Innovation Centers

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

Regulators

<u>Incubator/Accelerator</u>
key physical capabilities
key intellectual capabilities
coordination
funding
support

GAIN

Technical resources

- Learn from other programs: YC, Lemnos Labs, Breakout Labs, etc.
- Leverage Cyclotron Road program
- Investigate future paths forward

cyclotronroad

2016 Nuclear Innovation Bootcamp

http://www.nuclearinnovationalliance.org/bootcamp

- Teach students *how* to innovate:
  - Entrepreneurship
  - Nuclear aspects
  - Non-traditional material
- Pilot program August 1-12, 2016 held at UC Berkeley
- Team design projects
- Large company involvement
- Experts teach and mentor
- Judged completion

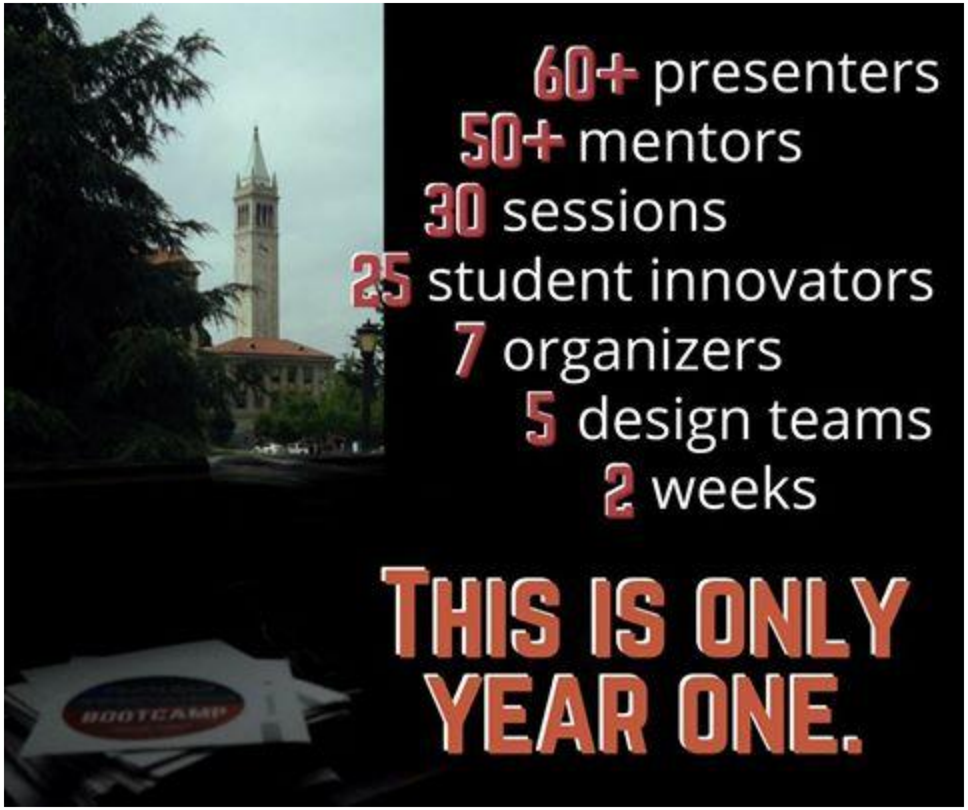
Unprecedented Success

Learning through sessions, projects, and play

Abdalla Abou Jaoude • Adam Scheider • Adriana Ureche • Advanced Reactor Concepts, LLC • Advanced Reactor Solutions • Alan Bolind • Alex Cheung • Alex Polonsky • Alphabet Energy • Alyse Scurlock • American Nuclear Society • Andrea Saltos • Andres Alvarez • Andrew Greenop • Andrew Worrall • Andy Klein • April Novak • Argonne National Laboratory • Aries Loumis • Arun Khuttan • August Fern • August Fern Consulting LLC • Bala Ramamurthy • Bart Roe • Behnam Taebi • Ben Reinke • Beth Zotter • Bipartisan Policy Center • Boris Hombourger • Breakthrough Institute • Brenden Heidrich • Brett Rampal • Canadian Nuclear Laboratories • Canon Bryan • Caroline Hughes • Center for Financial Services Innovation • Chris Comfort • Chris Poresky • Christina Castellanos • Cindy Rodriguez • Cyclotron Road • Daine L. Danielson • Dan Yurman • Darby Kimball • Dave Pointer • David Charpie • David Matthews • Delft University • Dennis Hussey • Dishcraft Robotics • Doug Crawford • Dr Atambir RAO • Duke Energy • Ed Blanford • Edward Kee • Ehud Greenspan • Electric Power Research Institute • Elizabeth McAndrew-Benavides • Emily Nichols • Eric Fettner • Exelon • Fran Bolger • Frank Rahn • Gaetan Bonhomme • Garon Morgan • GE Hitachi Nuclear Energy • GE Power & Water • General Fusion • Georgia Institute of Technology • Gigi Wang • Gil Brown • Gilbert Brown • Haas School of Business • Harvard Business School • Ian Hamilton • Idaho National Laboratory • Igor Bolotnov • Ilan Gur • Institute of Nuclear Power Operations • Irfan Ali • Ivan Maldonado • Jacob DeWitte • Jacopo Buongiorno • James Kendrick • James Lim • Jared Friedman • Jeremy Conrad • Jessica Chow • Jessica Lovering • Jing Hu • Joe Lassiter • Joey Kabel • John Jackson • John Kotek • Karl van Bibber • Kathryn Yates • Kathy Shield • Kurion Veolia • Kyle Brumback • Lara Pierpiont • Lars Jorgensen • Lawrence Berkeley National Laboratory • Lemnos Labs • Leslie Dewan • Lightbridge Corporation • Linda Pouliot • Lindsay Dempsey • Linsday Miller • Lin-wen Hu • Lucas Davis • Lydia Sohn • Marissa Zweig • Marius Stan • Mark Mawdsley • Markus Piro • Massachusetts Institute of Technology • Massimiliano Fratoni • Matt Thompson • Matthew A. Hertel • Matthew C. Thompson • Megan Casper • Michael Martin • Michael Trinh • Michael Van Loy • Mike Kurzeja • Mike Laufer • Mike Safyan • Milos Atz • Mintz Levin • Mitch Negus • Modeste Tchakoua • Morgan, Lewis & Bockius LLP • Nathan Gilliland • Nathan Gold • Nick Touran • Nikhil Bharadwaj • Nnaemeka Nnamani • North Carolina State University • Nuclear Economics Consulting Group • Nuclear Energy Consultants, Inc. • Nuclear Energy Institute • Nuclear Innovation Alliance • Nuclear Technology Innovation Laboratory • NuScale Power • Oak Ridge National Laboratory • Oklo • Ondrej Chvala • Oregon State University • Oscar Espinoza • Out Educated • Paul Lorenzini • Pavel Tsvetkov • Per Peterson • Peter Hosemann • Peter Secor • Phil Hildebrandt • Phil Russell • Planet • Positron Dynamics • Rachel Slaybaugh • Raluca Scarlat • Ray Rothrock • RedSeal, Inc. • Richard Pearson • Richard Vasques • Robert J. Budnitz • Robert Petroski • Roe Energy Consulting LLC • Ronald Horn • Ryan Falvey • Sam Brinton • Sama Bilbao y Leon • Samuel Brinton • SAP • Sara Harmon • Sarah Stevenson • SC Moatti • Sebastian Lounis • Senate Energy Committee • Seth Grae • Shane Johnson • Shannon Yee • Shrey Satpathy • Shyam Dwaraknath • Southern Company • Southern Nuclear • Stephen Clement • Stephen R. Booker • Steve Herring • Sutardja Center for Entrepreneurship & Technology • Suzy Baker • TerraPower • Terrestrial Energy • Texas A&M University • The Demo Coach • Third Way • ThorCon • ThreeBridges Ventures • Timothy Crook • Todd Allen • Tom Isaacs • Transatomic • Tri Alpha Energy • U.S. Department of Energy • UC Berkeley College of Engineering • UC Berkeley Department of Nuclear Engineering • University of California, Davis • University of Massachusetts, Lowell • University of New Mexico • University of Tennessee, Knoxville • University of Wisconsin, Madison • Virginia Commonwealth University • Walter Howes • Wendolyn Holland • Whitekoat, Inc. • Whitney Research Services • Will Boyd • Y Combinator • Yishu Qiu

2016 Nuclear Innovation Bootcamp

- https://www.youtube.com/watch?v=aicVAXorRq4
- Multiple articles,
  blog posts, and features…
  still coming
- Large social media impact
- And the narrative continues!



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2017 Nuclear Innovation Bootcamp

- Full program Summer 2017
- Deeper content, bigger projects
- Expand to include professionals
- Partner with other campus initiatives
- Intellectual collaboration with other universities

http://www.nuclear innovationalliance.org/bootcamp

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Sutardja Center for Entrepreneurship & Technology

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Nuclear Innovation Pipeline

- **Goal:** reduce the non-technical barriers while enabling technical breakthroughs

NUCLEAR INNOVATION BOOTCAMP *NUCLEAR UPENDED*

Incubator/Accelerator
key physical capabilities
key intellectual capabilities
coordination
funding
support

GAIN

- Global participation; expand model
- Beyond GAIN: need a coordinated interagency (U.S.) and international strategy for global deployment

Global Nuclear Innovation

Now is the time

Motivated by Global Health, Prosperity, and Environment, we have the opportunity to **reinvent** the way we do things

What do we want the world to look like?

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Acknowledgements

- Ex. 1: Tom Evans, Greg Davidson, Paul Wilson, Marissa Zweiger
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  Department of Energy award number DE-NE0008286
- Ex. 4 James Bevins, Lee Bernstein, Bill Dunlop, Eugene Henry, Dawn Shaughnessy, et al.

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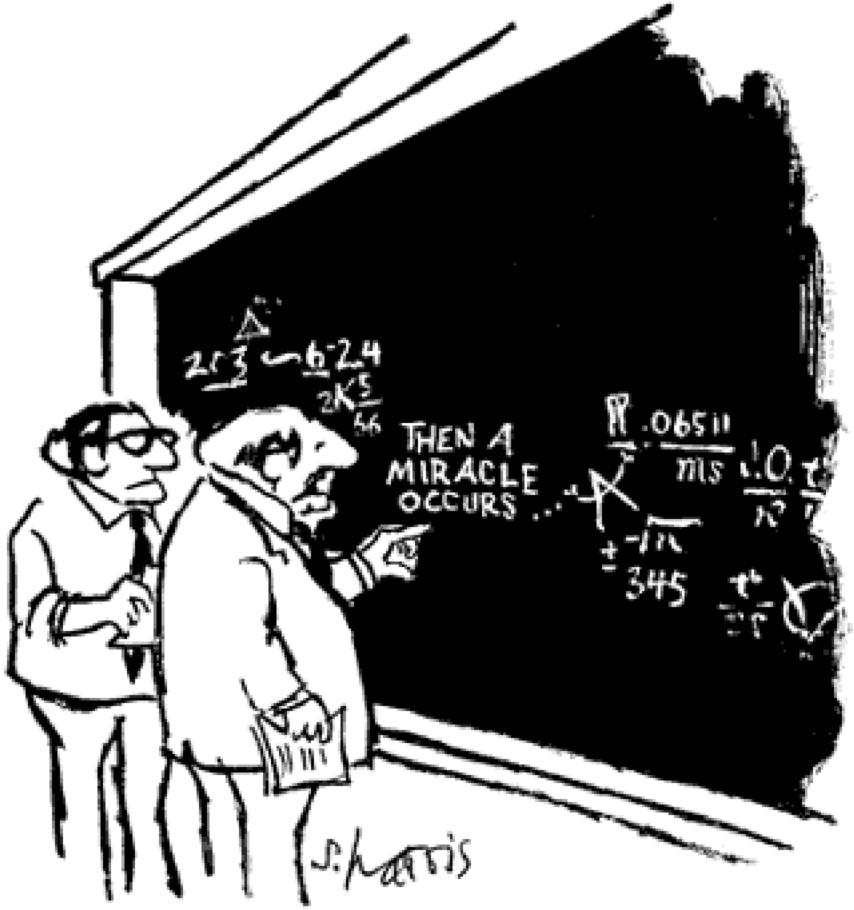
Questions?



"I think you should be more explicit here in step two."

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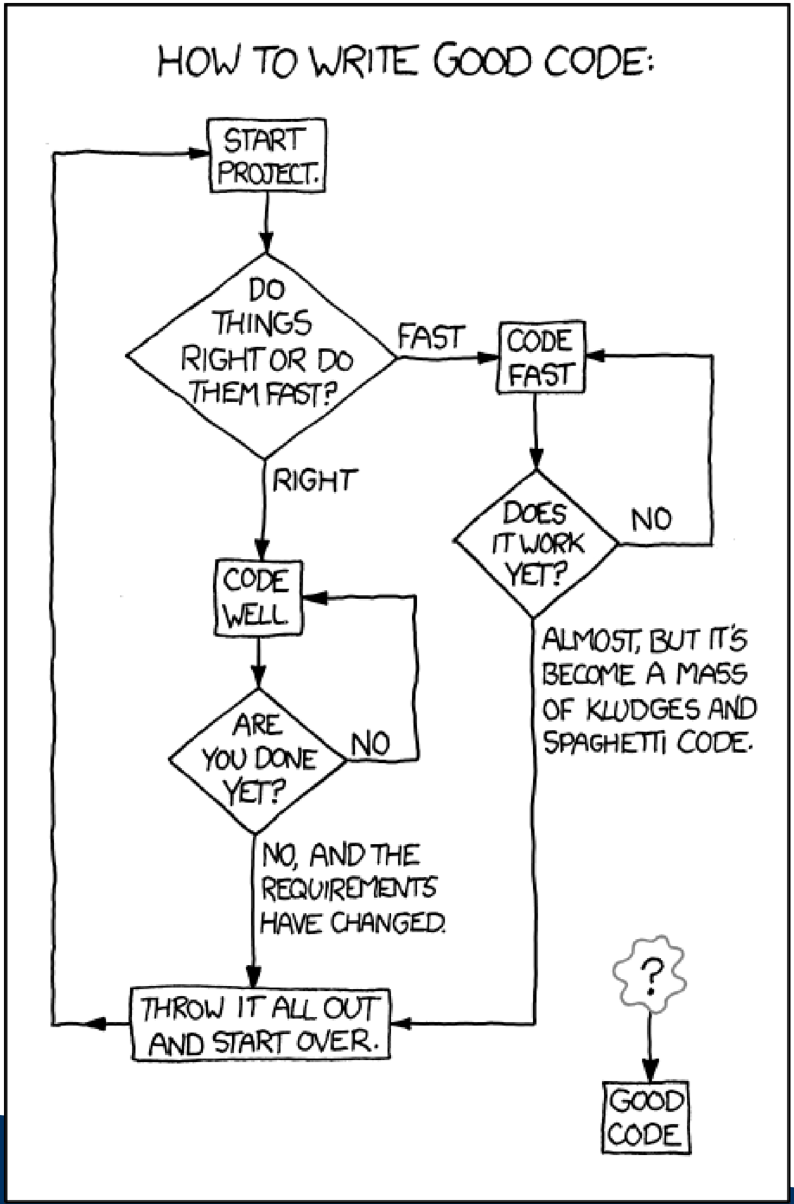
P.S. Quality Software Required



THW

software carpentry

PyNE

BERKELEY Institute for Data Science

Quick Brief: Deterministic Methods

- $\mathbf{L} = \hat{\Omega} \cdot \nabla + \Sigma$ is the transport operator,
- $\mathbf{M}$ converts harmonic moments into discrete angle sets,
- $\mathbf{D} = \mathbf{M}^T \mathbf{W} = \sum_{a=1}^{n} Y_{lm}^{e/o} w_a$ is the discrete-to-moment operator.
- f contains the fission source, $\nu \Sigma_f$;
- $\mathbf{F} = \chi f^T$,
- $\mathbf{S}$ is the scattering matrix,

$$\mathbf{L}\psi = \mathbf{MS}\phi + \frac{1}{k}\mathbf{MF}\phi$$

$$\phi = \mathbf{D}\psi$$

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