Advanced Solvers and Radiation Transport

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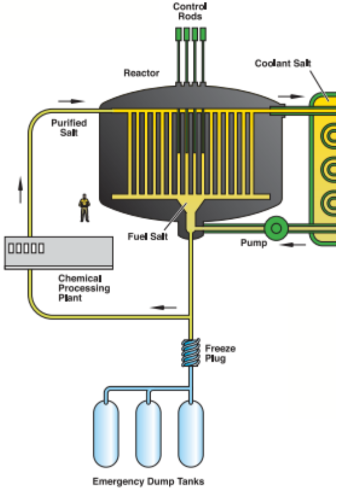
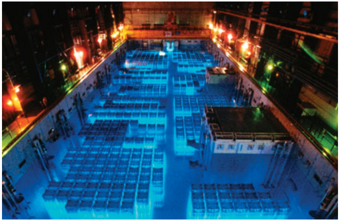
UIUC Graduate Colloquium

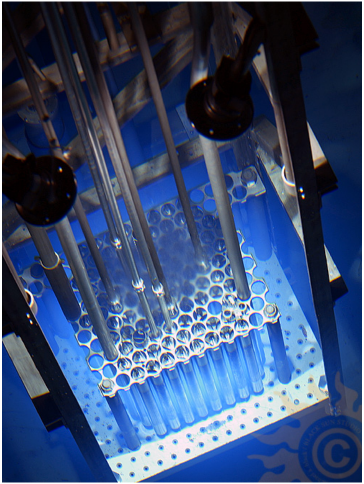
NUCLEAR INNOVATION IS NEEDED





OUTLINE

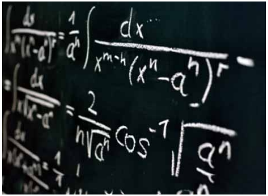
- Motivation & Background
- Hybrid Methods and Strong Anisotropies
  - Research Objectives
  - Cadis-Ω method and highlights
- Spectrum Shaping for Strategic Research
  - Research Objectives
  - Gnowee: Metaheuristic Optimization Algorithm
  - Coeus: ETA Design Software

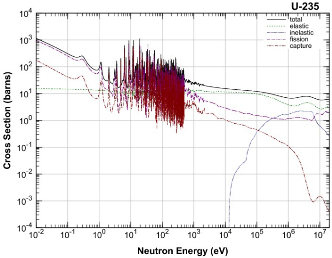


NUMERICAL METHODS FOR RADIATION TRANSPORT

To facilitate nuclear innovation, we need predictive simulation

- My group builds tools (translate applied math into code) used to design and analyze nuclear systems
- We focus on high performance computing,
- and inform algorithm development with physics of problems of interest





SOLVING THE TRANSPORT EQUATION

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}) + \Sigma_t \psi(\vec{r}, E, \hat{\Omega}) = S(\vec{r}, E, \hat{\Omega}) + \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' \, \Sigma_s(E', \hat{\Omega}' \to E, \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}')$$

Monte Carlo

- *Continuous* phase space
- Solution has statistical error
- Localized solutions
- Optically thick = *slow*

Deterministic

- *Discretized* phase space
- Solution equally valid everywhere
- Truncation errors
- Streaming = *ray effects*

SPEEDING UP MONTE CARLO

- Variance reduction (VR) used to improve Monte Carlo: reduce relative error *and* time by augmenting game
- Particles are assigned weights that map to impact
- VR can be used to
  - set weights at birth
  - update weights throughout problem
- Improvement measured as

$$\mathrm{FOM} = \frac{1}{\mathrm{R}^2\mathrm{t}} \quad \mathrm{R} = \text{relative error; t} = \text{time}$$

Hybrid Methods: we use deterministic results to make Monte Carlo VR parameters

https://github.com/SlaybaughLab

- Hybrid methods
  - Kelly Rowland: Lagrange Discrete Ordinates
  - Vanessa Goss and Emily Vu: analysis
  - Madicken Munk (alumna): Omega methods
- Deterministic methods
  - Mario Ortega: eigenvalue acceleration methods
  - Weixiong Zhang: finite element methods
  - Josh Rehak: finite element methods
  - Marissa Ramirez Zweiger: finite element methods
  - Sam Olivier: finite element methods
- Other adventures
  - April Novak: coupled neutronics and TH
  - Mitch Negus: PWR analysis
  - Ethan Boado: pelletron experiment design
  - James Bevins (alumnus): optimization methods
  - Richard Vasques (alumnus): non-classical transport

Project 1 motivation

- Many important nuclear applications have strong anisotropies
  - **Used fuel casks**
  - **Reprocessing facilities**
  - Reactor facilities
  - Active interrogation
- New ideas are needed for these problems
  - Current hybrid methods are only $f(\vec{x}, E)$
  - Including angle explicitly is too costly
- Goal: new methods that are easy to use

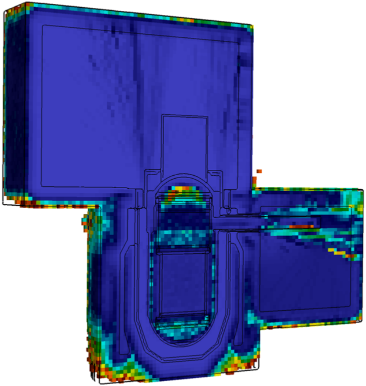


Figure: PWR relative error [1]

Adjoint as an importance map

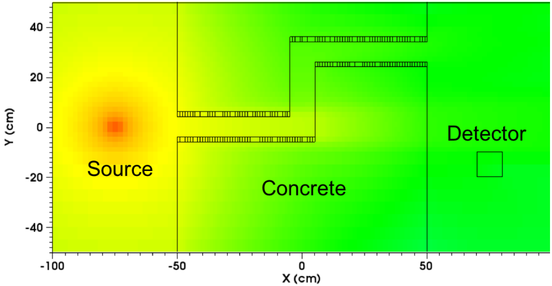
Define response with function $f(\vec{r}, E)$ in volume V_f as

$$R = \int_E \int_{V_f} f(\vec{r}, E)\phi(\vec{r}, E) dV dE \tag{1}$$

- Forward (ϕ or ψ): neutrons flow from the source (q) to the detector
- Adjoint($\phi^\dagger$ or $\psi^\dagger$): particles represent how each part of phase space contributes to the "source" ($q^\dagger$)
- $\phi^\dagger$ represents the expected contribution of a source particle to the response given the source, q.

UNDERSTANDING FORWARD FLUX, $\phi(\vec{r}, E)$

10 MeV isotropic point source; NaI detector



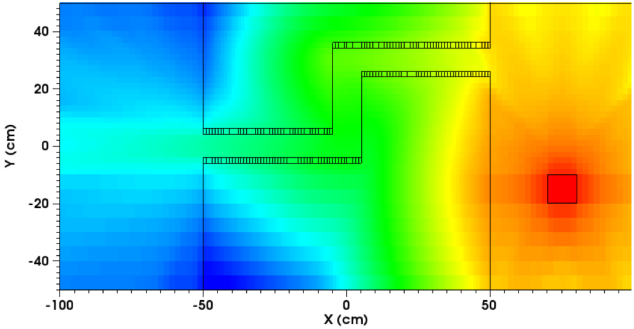
Neutrons in the forward problem will flow from the source to the detector

UNDERSTANDING ADJOINT FLUX, $\phi^{\dagger}(\vec{r}, E)$

10 MeV isotropic point source; NaI detector

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

importance map



FORWARD-ADJOINT RELATIONSHIP [2]

Define response with function $f(\vec{r}, E)$ in volume V_f as

$$R = \int_E \int_{V_f} f(\vec{r}, E)\phi(\vec{r}, E) dV dE \quad (2)$$

$$H\phi = q \quad \text{(forward)} \qquad \langle H\phi, \phi^\dagger \rangle = \langle H^\dagger \phi^\dagger, \phi \rangle \text{, and therefore}$$

$$H^\dagger \phi^\dagger = q^\dagger \quad \text{(adjoint)} \qquad \langle q, \phi^\dagger \rangle = \langle q^\dagger, \phi \rangle$$

If we let $q^\dagger = f(\vec{r}, E)$ then

$$\langle q^\dagger, \phi \rangle = \langle f, \phi \rangle = R = \langle q, \phi^\dagger \rangle \quad (3)$$

Eq. (3) expresses that $\phi^\dagger$ represents the expected contribution of a source particle to the respons.

ADJOINT AS AN IMPORTANCE MAP

Use *adjoint*: the importance of a source particle to the solution

- Define $q^\dagger$ as the response of interest
- Coarse deterministic calculation to get $\phi^\dagger$ and R
- The current state of the art for VR is FW/CADIS [2]

$$imp(\vec{r}, E) = \frac{\phi^\dagger(\vec{r}, E)}{\langle q(\vec{r}, E), \phi^\dagger(\vec{r}, E)\rangle} = \frac{\phi^\dagger(\vec{r}, E)}{R}$$

$$\hat{q}(\vec{r}, E) = \frac{\phi^\dagger(\vec{r}, E) q(\vec{r}, E)}{R}$$

$$w_0(\vec{r}, E) = \frac{q(\vec{r}, E)}{\hat{q}(\vec{r}, E)} = \frac{R}{\phi^\dagger(\vec{r}, E)}$$

Current hybrid methods are insufficient

$$\text{Note:} \qquad \phi^{\dagger}(\vec{r}, E) = \int \psi^{\dagger}(\hat{\Omega}, \vec{r}, E) d\hat{\Omega}$$

- MC VR parameters created from adjoint deterministic scalar flux that is a function of *space and energy only*
- Angular dependence of the importance function is not retained, otherwise the map would be
  - very large (tens or hundreds of GB) and
  - more costly and complex to use in the MC simulation
- Drawback: within a given space/energy cell, map provides average importance of a particle moving in *any direction* through the cell–excluding information about how particles move toward the objective

Current hybrid methods are insufficient

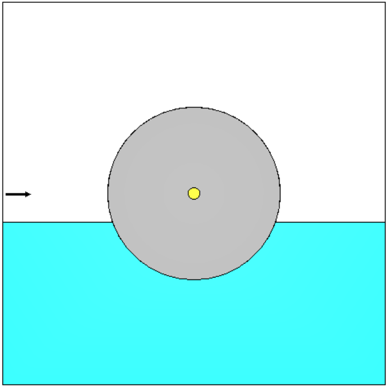


Figure: Spherical boat model with source on left and fissionable material at center

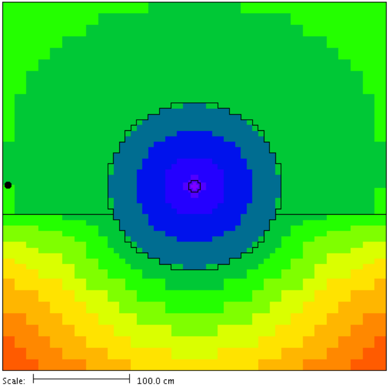


Figure: Target weight window values for 14.1 MeV neutrons

Integration weighting

Different integration plan captures angles in scalar flux creation

$$\phi^\dagger(\vec{r},E) = \int \psi^\dagger(\hat{\Omega},\vec{r},E)d\hat{\Omega} \qquad \text{original}$$

$$\phi^\dagger(\vec{r},E) = \frac{\int \psi(\hat{\Omega},\vec{r},E)\psi^\dagger(\hat{\Omega},\vec{r},E)d\hat{\Omega}}{\int \psi(\hat{\Omega},\vec{r},E)d\hat{\Omega}} \qquad \text{new}$$

Major challenges and areas of investigation:

1. Data storage and handling (many GBs)
2. More, less, or differently sensitive to
    - quality of the discrete ordinates calculation?
    - ray effects?

METHOD IMPLEMENTATION

- The space- and energy-dependent importance map is normalized and source biasing parameters are generated in the same ways as the current implementation of FW/CADIS
- Immediately useful; widely applicable
- We are studying and characterizing the impact
- Is available currently ADVANTG [3]

THE NEW METHOD CAPTURES ANISOTROPY

Comparing the original adjoint to CADIS-Ω....

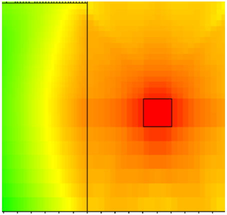


Figure: original adjoint

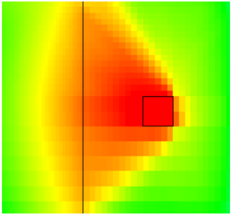


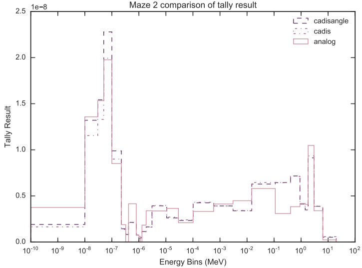
Figure: new adjoint

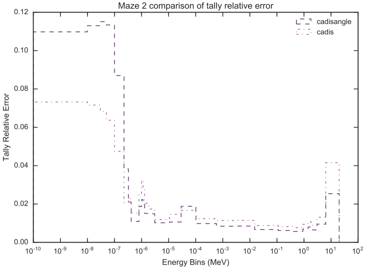
...shows that the method does incorporate problem physics differently

SINGLE-TURN MAZE RESULTS

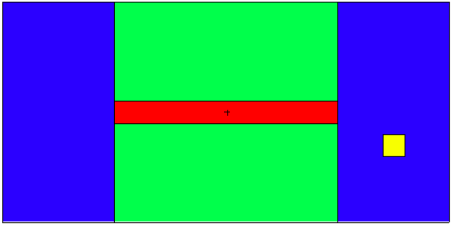
- CADIS-Ω has lower REs at higher energies
- Analog has high RE
- CADIS-Ω was in the middle for FOM using the worst RE

Run Type	Time (m)	FOM
CADIS	84.4	2.21
CADIS-Ω	237	0.318
analog	11.7	0.0857





STEEL BEAM IN CONCRETE

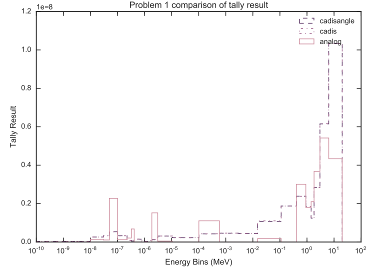


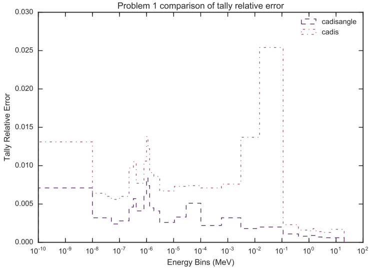
- Steel plate embedded in concrete; air on each end
- ^{235}U fission spectrum plane source
- Steel streams neutrons, concrete scatters them

STEEL BEAM IN PLATE RESULTS

- CADIS-Ω has lower REs at all energies
- Analog has high RE
- CADIS-Ω performed best for all FOMs

Run Type	Time (m)	FOM
CADIS	420	3.69
CADIS-Ω	2,110	6.71
analog	22	0.0448





Results Summary

We tested a variety of characterization problems

- Problems with air streaming did not work well for any solver
- With weight windows
  - flux changes magnitude too quickly
  - causes lots of splitting and dramatic weight change
  - causes high variance and long runtime

- CADIS-Ω was great for problems with denser streaming materials
- These have enough scattering so flux changes more slowly
- And enough streaming that anisotropy is strong
- *This is exactly the problem we want to solve*

Project 1 Summary

- There are many situations of interest where neutron fluxes have strong anisotropies
- Current VR methods do not enhance performance sufficiently
- CADIS-Ω is one way to capture angular information and shows strong initial promise
- We're looking at many types of problems and are scaling up to real applications

INTERLUDE: WHO ARE YOU, ANYWAY?

PennState College of Engineering | MECHANICAL AND NUCLEAR ENGINEERING

American Nuclear Society

software carpentry

NAVAL REACTORS

DEPARTMENT OF Engineering Physics UNIVERSITY OF WISCONSIN–MADISON

PyNE

Nuclear Engineering University of California, Berkeley

Nuclear Engineering Student Delegation

THW

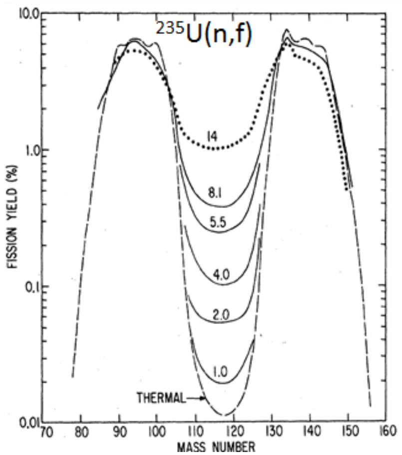
BERKELEY Institute for Data Science

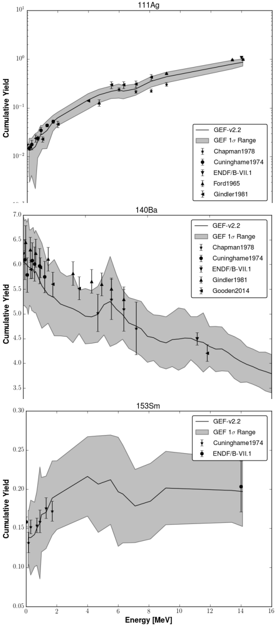
NUCLEAR INNOVATION BOOTCAMP

ENERGY HUB

arpa·e CHANGING WHAT'S POSSIBLE

PROJECT 2 MOTIVATION

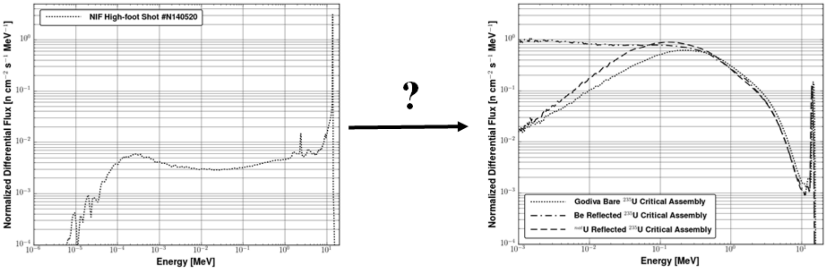




RESEARCH OBJECTIVES

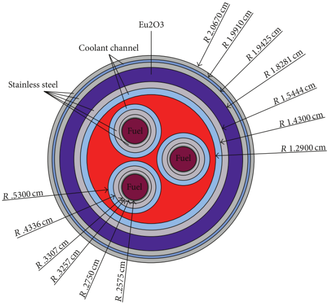
Develop a capability to design and test custom neutron energy spectra for technical nuclear forensics (TNF)

1. Design energy tuning assembly (ETA) to generate TNF relevant spectrum at NIF
2. Piece-wise application specific validation of ETA design at LBNL 88-Inch Cyclotron
3. Integral test and creation of synthetic debris at NIF

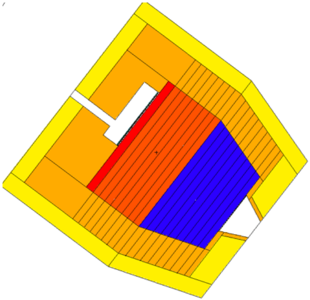


POTENTIAL APPLICATION AREAS

- Radiation shielding
- Radiation effects/damage
- Medical physics
- Radio-isotope production



- Nuclear data
- Detector calibration and development
- Fusion blanket design
- Reactor design



Optimization problem classes

Optimization problems can be formulated as [5, 6]:

$$
\begin{aligned}
&\underset{\vec{x}\in\mathbb{R}^d}{\text{Minimize}} \quad && f_i(\vec{x}), \quad && (i = 1,\ 2,\ \ldots,\ I) \quad && (4)\\
&\text{Subject to:} && h_j(\vec{x}) = 0, && (j = 1,\ 2,\ \ldots,\ J) && (5)\\
& && g_k(\vec{x}) \leq 0, && (k = 1,\ 2,\ \ldots,\ K) && (6)
\end{aligned}
$$

where $\vec{x}$ is a vector of the problem design variables

Optimization problems can be classified by [7, 8]:

- Single or multi-objective
- Linear or non-linear
- Constrained or unconstrained
- Continuous or combinatorial (discrete)
- Uni-modal or multi-modal

ETA design is a single objective, non-linear, constrained, continuous <u>and</u> discrete multi-modal optimization problem

ETA OPTIMIZATION

For the ETA optimization problem, (4) and (6) are given by [9]:

$$f_1(\overrightarrow{x_p}) = \sum_{g=1}^{G} \left(\frac{\phi_g^O - \phi_g^D(\overrightarrow{x_p})}{\phi_g^O} \right)^2 * \frac{\phi_g^O}{\phi^O} \tag{7}$$

$$g_1(\overrightarrow{x_p}) = \sum_{n=1}^{N} \rho_n V_n - W \leq 0 \tag{8}$$

$$g_2(\overrightarrow{x_p}) = N_f^{min} - n\phi V(\sigma_f^{235} + \sigma_f^{238}) \leq 0 \tag{9}$$

Where ϕ^O is the design objective neutron spectrum and $\phi^D(\overrightarrow{x_p})$ is the neutron spectra corresponding to a candidate design

$\overrightarrow{x_p}$ is a vector of the variables for a candidate design given by (in 2-D):

$$\begin{aligned} \overrightarrow{x_p} = \{&Cell_1[M_1, \rho_1, IR_1, OR_1, Z1_1, Z2_1],\ Cell_2[\ldots],\ \ldots, \\ &Cell_N[M_N, \rho_N, IR_N, OR_N, Z1_N, Z2_N],\ R_{foil},\ Z_{foil}\} \end{aligned} \tag{10}$$

OPTIMIZATION METHODS: METAHEURISTICS [10]

Hill Climbing

Intent: Follow a sequence of local improvements in order to find a locally optimal solution. A single move is performed at each step. If this leads to a better solution, the algorithm then moves on to explore a variant of this new solution, otherwise it remains at the original point and considers a different move.

Adaptive Memory Programming

Intent: Use of memory of past search experience to guide future search.

Population-Based Search

Intent: Multiple, cooperating search processes that are typically executed in parallel.

Multi-Start

Intent: Restart the search process in a different region once it has converged at a local optimum. After this has been repeated a number of times, the best local optimum seen is returned.

Variable Neighborhood Search

Intent: Search different neighborhoods around the location of a known local optimum.

Directional Search

Intent: Identify productive directions within the search space, and then carry out moves accordingly.

Search Space Mapping

Intent: Construct a map to guide search processes across search space

Intermediate Search

Intent: Explore the region between two or more previously visited search points, each of which is known to have a relatively high objective value.

Neighborhood Search

Intent: Find new solutions by exploring those that are a step change – a move – away from the current one. A move could be anything from flipping a single bit to randomly replacing the entire solution.

Accepting Negative Moves

Intent: Allow moves to worse solutions.

PSO	EA/GA	CS	ACO

GNOWEE: HYBRID METAHEURISTIC OPT.

General purpose metaheuristic optimization algorithm

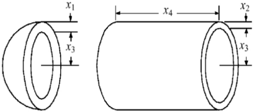
- Handles continuous and discrete variables
- Robust, complete set of search heuristics
- Nearly-global convergence
- Outperforms most other algorithms we tested on all nearly all problems of interest

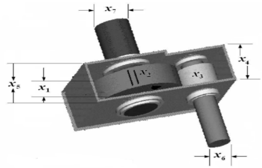
Algorithm 1: Gnowee Algorithm

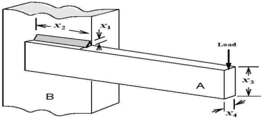
Input : User defined objective function, f; constraints, g and h; and population size, n

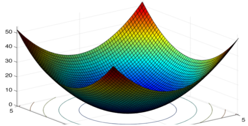
```
begin
    P.x⃗ ← Initialization(n)   // P is the parent population and x⃗ is the design variables
    P.fit ← FitCalc(P.x⃗)     // fit is the assessed fitness
    C.x⃗_d ← Inversion(P.x⃗_d)
    P.fit ← FitCalc(P.x⃗) while convergence criterion is not met do
        C.x⃗_d ← DiscLévyFlight(P.x⃗_d)   // C is the child population and x⃗_d is the subset of the design vector containing continuous variables
        for i ← 1 to n do
            if f(C_i.x⃗_d) < P_i.fit then
                P_i.x⃗_d ← C_i.x⃗_d
                P_i.fit ← f(C_i.x⃗_d)   // NOTE: This fitness calc and design update is performed after every procedure but is not repeated below for brevity
        C.x⃗_c ← ContLévyFlight(P.x⃗_c)   // x⃗ is the subset of the design vector containing discrete variables
        C.x⃗_c ← ContCrossover(P.x⃗_c)
        C.x⃗_c ← Mutation(P.x⃗_c)
        C.x⃗_d ← DiscCrossover(P.x⃗_d)
        C.x⃗_d ← 2-Opt(P.x⃗_d)
        C.x⃗_d ← 3-Opt(P.x⃗_d)
```

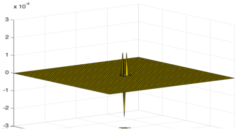
Gnowee: Benchmarking [11, 6, 12]

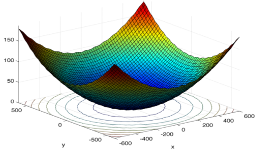


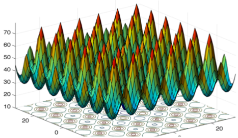


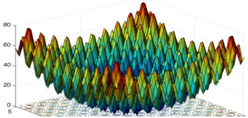


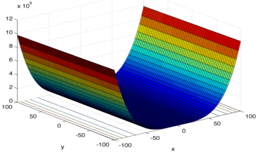












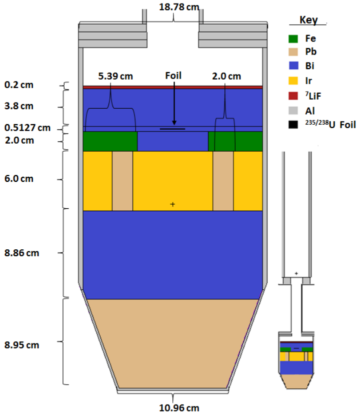
COEUS: NE OPTIMIZATION SOFTWARE

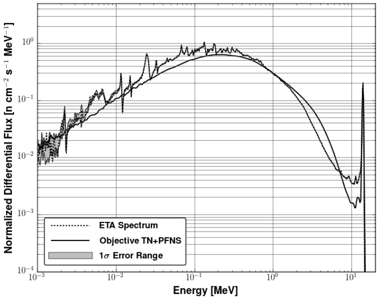
ETA design tool to build custom neutron spectra from existing facilities and sources

- MCNP-Denovo hybrid radiation transport engine [13, 14, 15]
- ETA designs generated with Gnowee optimization framework
- Fully operational on Savio – neutronics design in days
- Expanding capabilities by adding more objective functions, constraints, and geometric options

DEVELOPMENT APPROACH

- 1.2 g HEU foil
- $\sim$ 80 kg
- $1 \times 10^8 - 1 \times 10^9$ Fissions





Energy Range	Target Normalized Differential Fluence	% Fluence Achieved
0-3 keV	6.24×10^{-5}	103.4 ± 2.0%
3-100 keV	3.41×10^{-2}	140.7 ± 0.1%
0.1-6 MeV	8.46×10^{-1}	96.0 ± 0.0%
6-10 MeV	1.65×10^{-2}	117.3 ± 0.2%
10-16 MeV	1.01×10^{-1}	119.4 ± 0.0%

ETA vs Objective Spectrum

NIF EXPERIMENT: TNF VALIDATION

Experimental Overview:

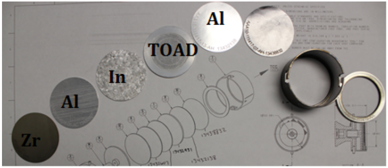
- $\sim$1.0 $\times$ 10^{15} neutrons in 4π
- Minimize ρR in direction of the ETA DIM
- ETA fielded as snout on DIM DLP located 75 mm from TCC

- No on-line DIM diagnostics required
- Radio-chemistry and gamma spectroscopy facilities required post-shot
- NTOF, FNADS, and MRS required to measure the source term

NIF EXPERIMENT: TNF VALIDATION

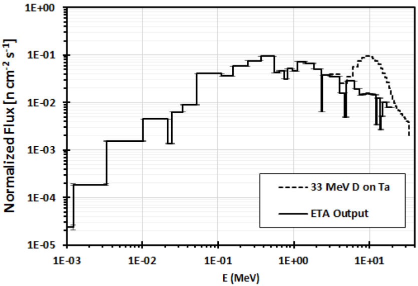
Expected Experimental Outcomes:

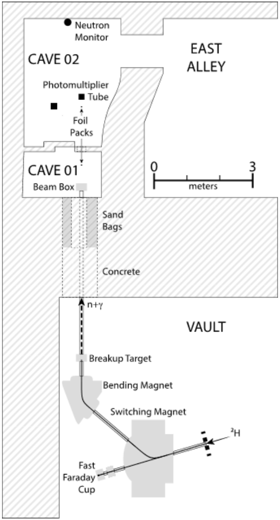
- Generation of realistic FP distribution
- Quantification of spectrum through fission splits
- Unfolding of spectrum using activation analysis



88-INCH EXPERIMENTS: TNF VALIDATION

- 29/33 MeV D-breakup on Ta
- Field NIF ETA design
- Field partial ETA stackups
- EJ-309 detectors, activation, and fission products measurements





Project 2 Summary

- 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
  - *Not* input or output specific
  - Further development to improve user flexibility underway

- Experimental validation of TNF application at LBNL 88-Inch Cyclotron executed

- Planning underway for NIF shot
  - Scoping study has shown feasibility
  - Partial funding/support from DNDO/NTNFC, DTRA, and LANL

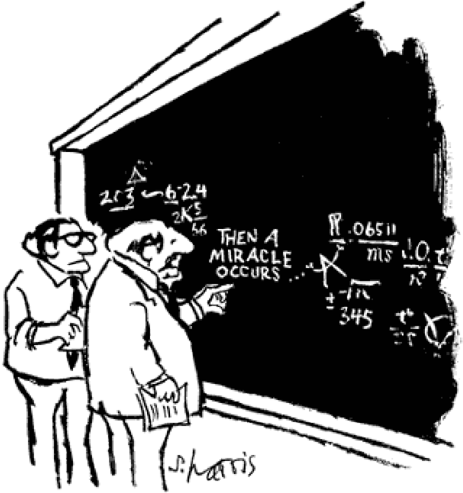
We would accomplish many more things if we did not think of them as impossible.

- Vince Lombardi

SUMMARY

- Innovation is needed for many nuclear technologies
- Predictive simulation can play a key role
- We're developing better hybrid methods
  - for problems with strong anisotropies
  - and to provide evaluative flexibility
- Energy tuning assemblies can provide strategic investigative tools
  - for technical nuclear forensics
  - as well as many other applications

Questions?



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

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DISCLAIMERS

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