Advanced Solvers and Challenges for Nuclear Innovation

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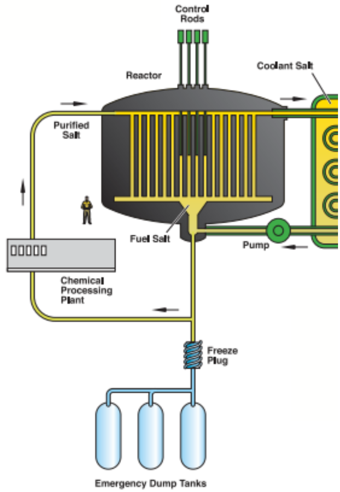
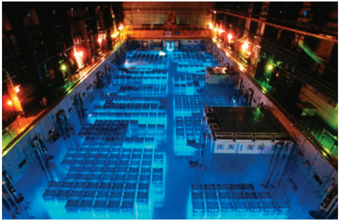
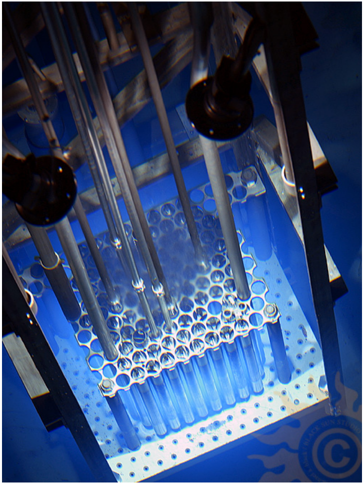
NUCLEAR INNOVATION IS NEEDED





Outline

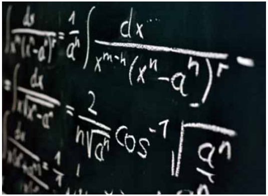
- Motivation & Background
- Hybrid Methods and Strong Anisotropies
  - Research Objectives
  - CADIS-Ω Method
  - LDO Method
- Spectrum Shaping for Strategic Research
  - Research Objectives
  - Gnowee: Metaheuristic Optimization Algorithm
  - Coeus: ETA Design Software

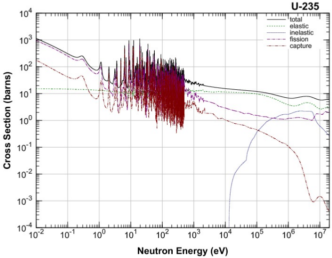


NUMERICAL METHODS FOR RADIATION TRANSPORT

To facilitate nuclear innovation, we need predictive simulation

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





SOLVING THE TE

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

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 MC

- 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

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

Project 1 motivation

- Many important nuclear applications have strong anisotropies
  - **Used fuel casks**
  - **Reprocessing facilities**
  - Reactor facilities
  - Active interrogation

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  - Including angle explicitly is too costly

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  - Including angle explicitly is too costly
- Goal: new methods that are easy to use

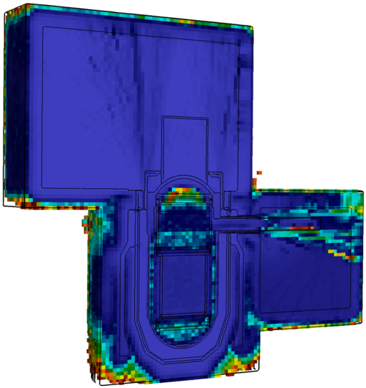

Figure: PWR relative error [1]

ADJOINT AS AN IMPORTANCE MAP

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

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

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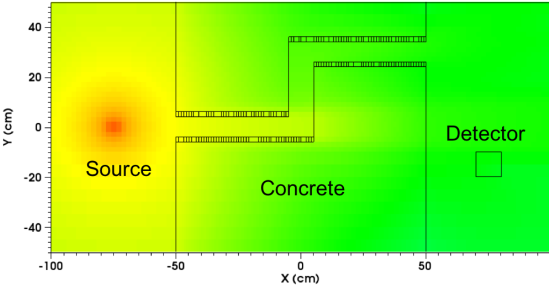
- Forward (ϕ or ψ): neutrons flow from the source (q) to the detector
- Adjoint($\phi^\dagger$ or $\psi^\dagger$): particles represent how each part of phase space contributes to the “source” ($q^\dagger$)
- $\phi^\dagger$ represents the expected contribution of a source particle to the response given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

UNDERSTANDING FORWARD FLUX

10 MeV isotropic point source; NaI detector



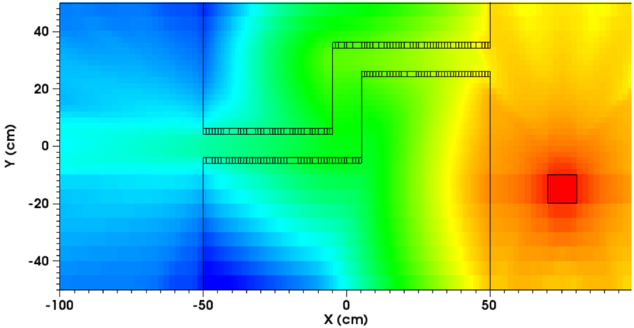
Neutrons in the forward problem will flow from the source to the detector

UNDERSTANDING ADJOINT FLUX

10 MeV isotropic point source; NaI detector

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

importance map



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 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

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

- MC VR parameters created from adjoint deterministic scalar flux that is a function of *space and energy only*

CURRENT HYBRID METHODS ARE INSUFFICIENT

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- 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

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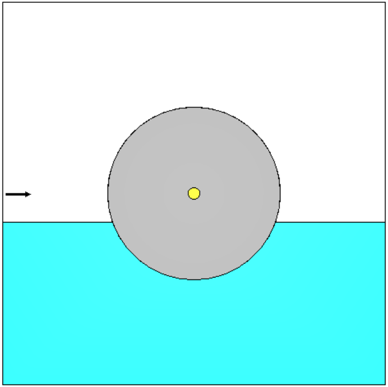

Figure: Spherical boat model with source on left and fissionable material at center

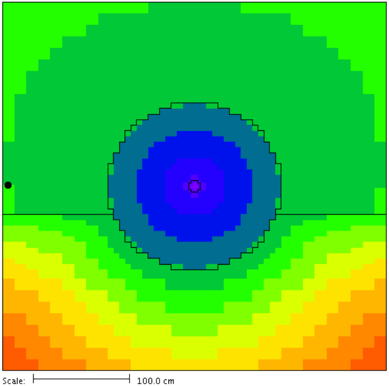

Figure: Target weight window values for 14.1 MeV neutrons

Integration weighting

Different integration plan captures angles in scalar flux creation

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

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

INTEGRATION WEIGHTING

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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 ADVANTG [3]

The New Method Captures Anisotropy

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

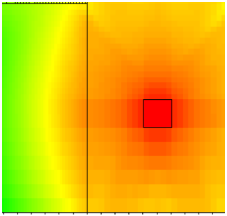

Figure: original adjoint

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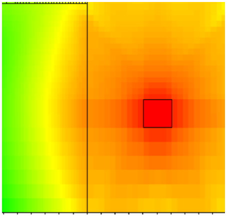

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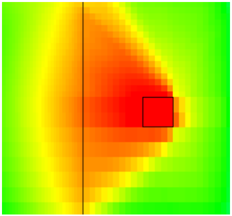


Figure: new adjoint

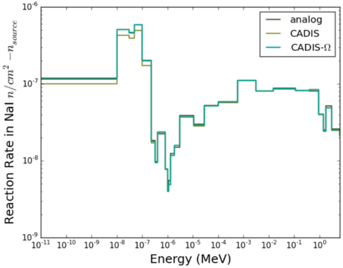
...shows that the method does incorporate problem physics differently

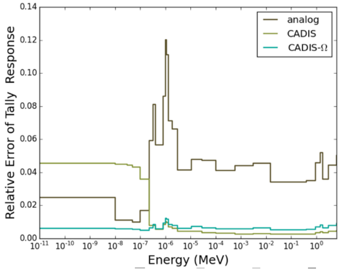
RESPONSE IN MAZE DETECTOR

CADIS-Ω has:

- Relatively uniform uncertainty distribution
- Faster runtimes than CADIS

Run Type	Time (m)	FOM
CADIS	524.9	5.1
CADIS-Ω	491.9	145



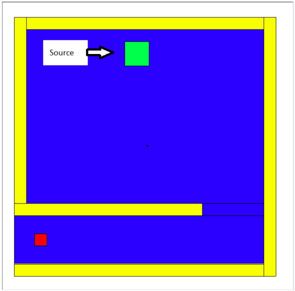


QUANTIFYING ANISOTROPY

To measure how the method performs based on the degree of problem anisotropy, we've defined several metrics

- $M_1 = \dfrac{\phi^\dagger(\vec{r},E)\phi(\vec{r},E)}{\int_{\hat{\Omega}} \psi^\dagger(\vec{r},\hat{\Omega},E)\psi(\vec{r},\hat{\Omega},E)}$
- $M_2 = \dfrac{\phi^\dagger_{\hat{\Omega}}(\vec{r},E)}{\phi^\dagger(\vec{r},E)}$
- $M_3 = \dfrac{\max(\int_{\hat{\Omega}} \psi^\dagger(\vec{r},\hat{\Omega},E)\psi(\vec{r},\hat{\Omega},E))}{\mathrm{avg}(\int_{\hat{\Omega}} \psi^\dagger(\vec{r},\hat{\Omega},E)\psi(\vec{r},\hat{\Omega},E))}$
- $M_4 = \dfrac{\max(\int_{\hat{\Omega}} \psi^\dagger(\vec{r},\hat{\Omega},E)\psi(\vec{r},\hat{\Omega},E))}{\min(\int_{\hat{\Omega}} \psi^\dagger(\vec{r},\hat{\Omega},E)\psi(\vec{r},\hat{\Omega},E))}$

Example: source in a room

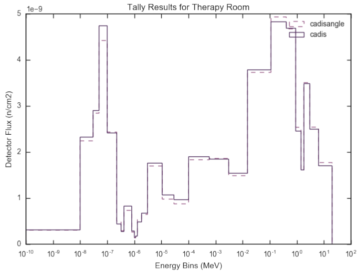


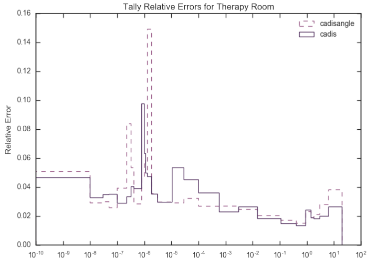
RESPONSE IN ROOM DETECTOR

CADIS-Ω again has:

- Relatively uniform uncertainty distribution
- Faster runtimes than CADIS

Run Type	Time (m)	FOM
CADIS	69.05	287
CADIS-Ω	50.4	373

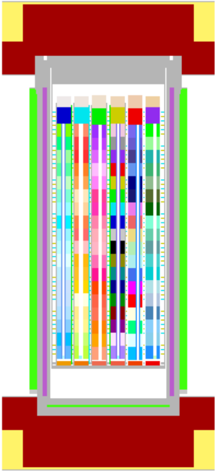




IMPACT TESTS

Real system tests will show the ability of the method to improve MC for applications of interest

We are starting with a full storage cask with highly-detailed information



LAGRANGE DISCRETE ORDINATES (LDO) [4]

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- **LDO equations naturally allow angular flux to be evaluated in directions other than those found in the quadrature set**
  - Solution of the LDO equations has interpolatory structure in angle
  - Opens the door to using angular biasing schemes for hybrid Monte Carlo calculations

Derivation of the LDO Equations

Start with the TE:

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, E, \hat{\Omega}) = S(\vec{r}, E, \hat{\Omega}) + \int_0^\infty \int_{\mathbb{S}^2} \Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \cdot \hat{\Omega})\psi(\vec{r}, E', \hat{\Omega}')d\hat{\Omega}'dE' \quad (2)$$

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- Define approximation $\psi_N(\vec{r}, E, \hat{\Omega}) = \sum_{i=1}^{d_N} \psi_i(\vec{r}, E)L_i(\hat{\Omega})$ and substitute it into the TE

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- $d_N \equiv \dim \mathcal{H}_N=(N+1)^2$;
  $\mathcal{H}_N=\text{span}\{Y_n^m : |m|\le n, 0\le n\le N\}$

Lagrange Functions (cont'd.)

The $L_i(\hat{\Omega})$ satisfy:

$$L_i(\hat{\Omega}_j) = \delta_{i,j}; \quad i,j = 1,2,\ldots,P; \quad P = d_N \tag{3}$$

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$$\int_{\mathbb{S}^2} f(\hat{\Omega}) d\hat{\Omega} = \int_{\mathbb{S}^2} \sum_{i=1}^{d_N} f_i L_i(\hat{\Omega}) d\hat{\Omega} = \sum_{i=1}^{d_N} \int_{\mathbb{S}^2} L_i(\hat{\Omega}) d\hat{\Omega} f_i = \sum_{i=1}^{d_N} w_i f_i \tag{4}$$

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Quadrature weights:

$$w_i = \int_{\mathbb{S}^2} L_i(\hat{\Omega})d\hat{\Omega} = \sum_{j=1}^{d_N} \langle L_i, L_j \rangle \tag{5}$$

Derivation of the LDO Equations (cont'd.)

- Discretize the energy variable with a standard multigroup approach

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DERIVATION OF THE LDO EQUATIONS (CONT'D.)

- Discretize the energy variable with a standard multigroup approach
- Analytically evaluate the scattering cross section and substitute it in

We invoke a collocation procedure that requires the residual to be zero at the points $\{\hat{\Omega}_i\}_{i=1}^{d_N}$, leading to the $G \times d_N$ equations:

$$\hat{\Omega}_i \cdot \nabla \psi_i^g(\vec{r}) + \Sigma_t^g(\vec{r}) \psi_i^g(\vec{r}) = \sum_{g'=1}^{G} \sum_{j=1}^{d_N} \sum_{i'=1}^{d_N} \langle L_{i'}, L_j \rangle \Sigma_{s,N}^{g' \to g}(\vec{r}, \hat{\Omega}_i \cdot \hat{\Omega}_j) \psi_{i'}^{g'}(\vec{r}) + S^g(\vec{r}, \hat{\Omega}_i) \quad (6)$$

These are the new multigroup LDO equations.

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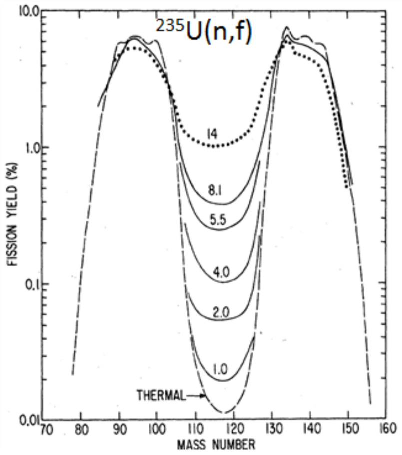
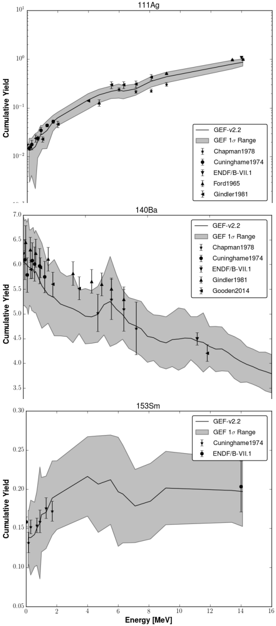
PROJECT 1 SUMMARY

- There are many situations of interest where neutron fluxes have strong anisotropies
- Current VR methods do not enhance performance sufficiently
- CADIS-$\hat{\Omega}$ is one way to capture angular information and shows strong initial promise
- Strategically using the LDO equations may provide another effective path
- We're looking at many types of problems and are scaling up to real applications

Project 2 Motivation

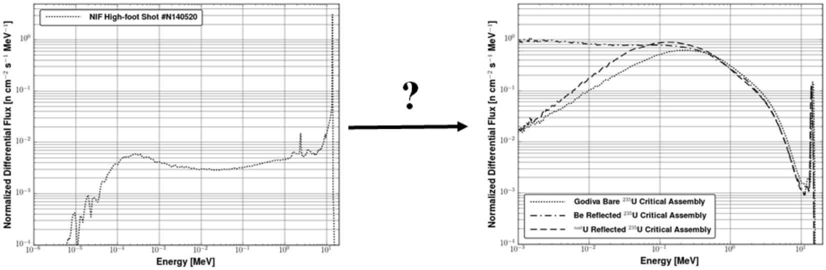




Research objectives

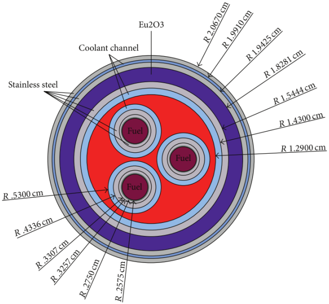
Develop a capability to design and test custom neutron energy spectra for technical nuclear forensics (TNF)

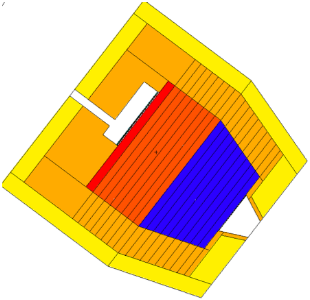
1. Design energy tuning assembly (ETA) to generate TNF relevant spectrum at NIF
2. Piece-wise application specific validation of ETA design at LBNL 88-Inch Cyclotron
3. Integral test and creation of synthetic debris at NIF



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]:

$$\underset{\vec{x}\in\mathbb{R}^d}{\text{Minimize}} \quad f_i(\vec{x}), \qquad (i = 1,\ 2,\ \ldots,\ I) \tag{7}$$

$$\text{Subject to:} \quad h_j(\vec{x}) = 0, \qquad (j = 1,\ 2,\ \ldots,\ J) \tag{8}$$

$$g_k(\vec{x}) \leq 0, \qquad (k = 1,\ 2,\ \ldots,\ K) \tag{9}$$

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, (7) and (9) are given by [9]:

$$f_1(\overrightarrow{x_p}) = \sum_{g=1}^{G} \left(\frac{\phi_g^O - \phi_g^D(\overrightarrow{x_p})}{\phi_g^O} \right)^2 * \frac{\phi_g^O}{\phi^O} \tag{10}$$

$$g_1(\overrightarrow{x_p}) = \sum_{n=1}^{N} \rho_n V_n - W \leq 0 \tag{11}$$

$$g_2(\overrightarrow{x_p}) = N_f^{min} - n\phi V(\sigma_f^{235} + \sigma_f^{238}) \leq 0 \tag{12}$$

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):

$$\begin{aligned} \overrightarrow{x_p} = \{&Cell_1[M_1, \rho_1, IR_1, OR_1, Z1_1, Z2_1],\ Cell_2[\ldots],\ \ldots, \\ &Cell_N[M_N, \rho_N, IR_N, OR_N, Z1_N, Z2_N],\ R_{foil},\ Z_{foil}\} \end{aligned} \tag{13}$$

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

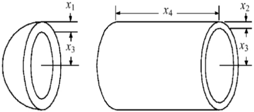
- Handles continuous and discrete variables
- Robust, complete set of search heuristics
- Nearly-global convergence
- Outperforms most other algorithms we tested on all nearly all problems of interest

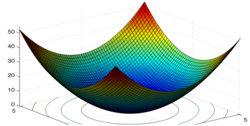
Algorithm 1: Gnowee Algorithm

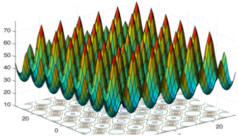
Input : User defined objective function, f; constraints, g and h; and population size, n

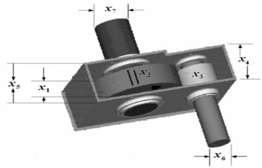
```
begin
    P.x⃗ ← Initialization(n)   // P is the parent population and x⃗ is the design variables
    P.fit ← FitCalc(P.x⃗)       // fit is the assessed fitness
    C.x⃗_d ← Inversion(P.x⃗_d)
    P.fit ← FitCalc(P.x⃗) while convergence criterion is not met do
        C.x⃗_d ← DiscLévyFlight(P.x⃗_d)   // 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)
```

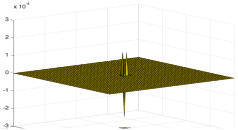
Gnowee: Benchmarking [11, 6, 12]

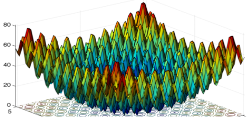


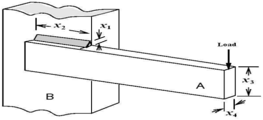


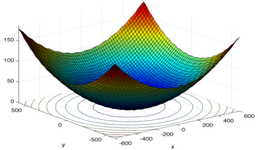


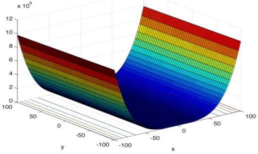












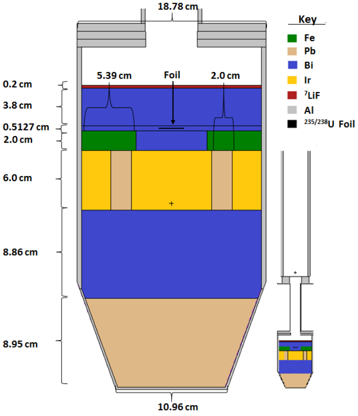
COEUS: NE OPTIMIZATION SOFTWARE

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

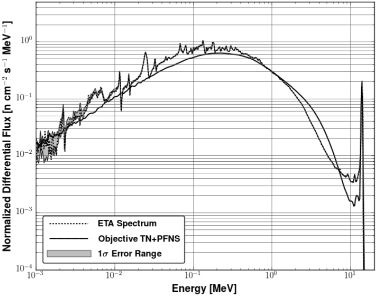
- MCNP-Denovo hybrid radiation transport engine [13, 14, 15]
- ETA designs generated with Gnowee optimization framework
- Fully operational on Savio – neutronics design in days
- Expanding capabilities by adding more objective functions, constraints, and geometric options

DEVELOPMENT APPROACH

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



ETA Design



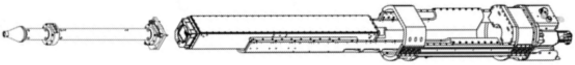
Energy Range	Target Normalized Differential Fluence	% Fluence Achieved
0-3 keV	6.24×10^{-5}	$103.4 \pm 2.0\%$
3-100 keV	3.41×10^{-2}	$140.7 \pm 0.1\%$
0.1-6 MeV	8.46×10^{-1}	$96.0 \pm 0.0\%$
6-10 MeV	1.65×10^{-2}	$117.3 \pm 0.2\%$
10-16 MeV	1.01×10^{-1}	$119.4 \pm 0.0\%$

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

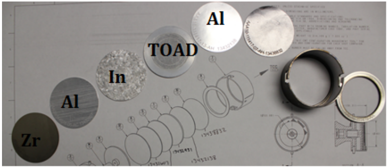


- No on-line DIM diagnostics required
- Radio-chemistry and gamma spectroscopy facilities required post-shot
- NTOF, FNADS, and MRS required to measure the source term

NIF EXPERIMENT: TNF VALIDATION

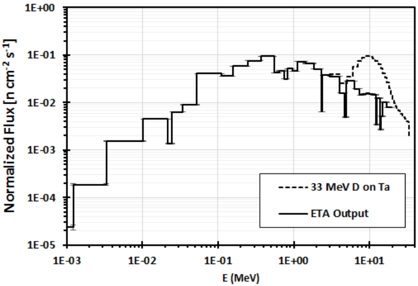
Expected Experimental Outcomes:

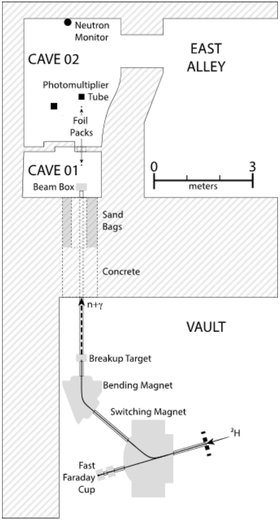
- Generation of realistic FP distribution
- Quantification of spectrum through fission splits
- Unfolding of spectrum using activation analysis



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

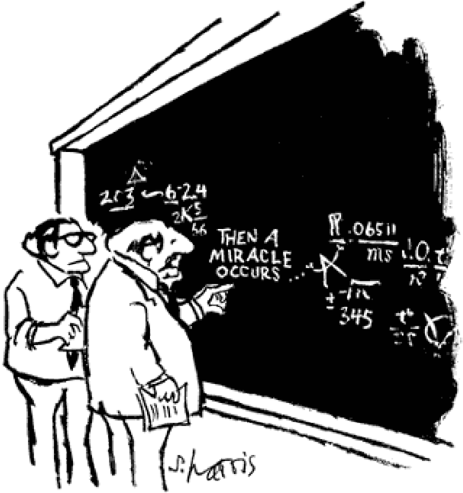
We would accomplish many more things if we did not think of them as impossible.

- 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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