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GAS-COOLED REACTOR
ADVANCED REACTOR TECHNOLOGIES PROGRAM

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Advanced Cross Section Library Generation using Reduced Order Models

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Hybrid Meeting at INL
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Cross-section (XS) is fundamental input to the NTE

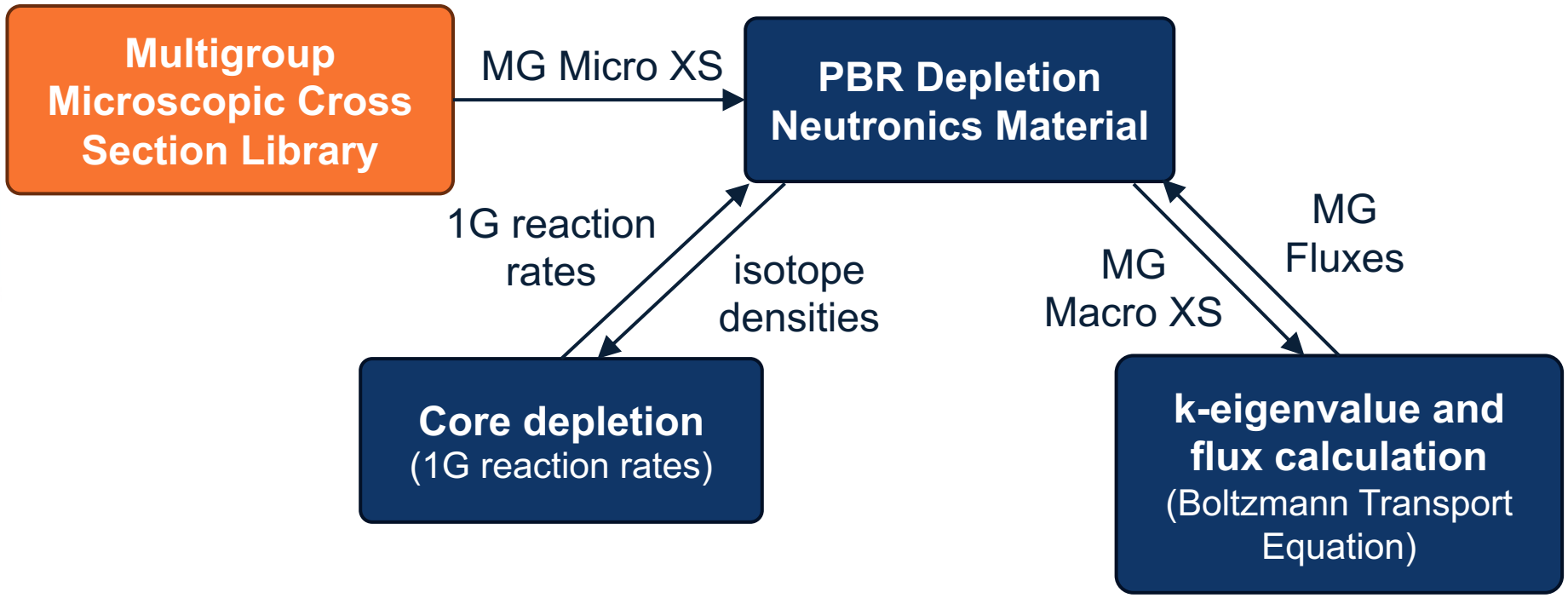
Neutron transport equation (NTE):

$$\underbrace{\frac{1}{v}\frac{\partial \psi}{\partial t}}_{\text{Time derivative}} + \underbrace{\Omega \cdot \nabla \psi}_{\text{Streaming}} + \underbrace{\Sigma_t \psi}_{\text{Collision}} = \underbrace{\int_0^\infty \int_{4\pi} \Sigma_s(\Omega' \cdot \Omega, E' \to E)\psi(\Omega', E')d\Omega' dE'}_{\text{Scattering}} +$$

$$\underbrace{\frac{\chi_p}{k_{\text{eff}} 4\pi} \int_0^\infty \nu \Sigma_f(E')\phi(E')dE'}_{\text{Fission}} + \underbrace{\frac{\chi_d}{4\pi} \sum_{i=1}^{I} \lambda_i C_i}_{\text{Delayed Neutron}}$$

Griffin core depletion calculation for PBRs

PBR data flow for core depletion calculation



Two-step XS generation

① Generation of multigroup microscopic XS Library

1. Identify neutronically important variables
(encompass relevant feed-back mechanisms and reactivity control mechanisms)

2. Select tabulation points for each variable
(cover all possible states of the reactor)

3. Generate multigroup microscopic XS
(perform reference eigenvalue calculation, typically Monte Carlo)

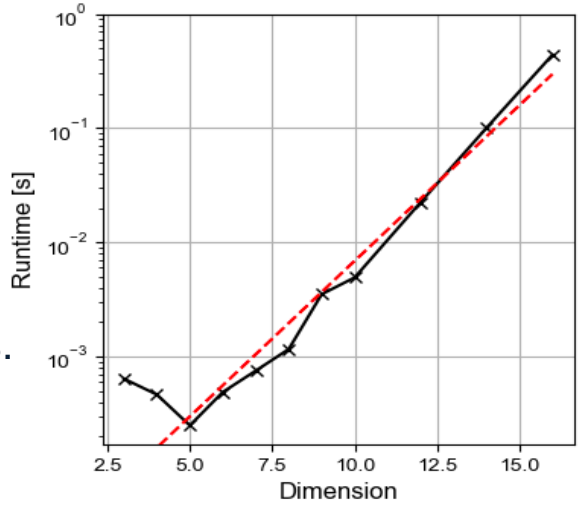
* Spatial dependency of XS represented by material IDs.

Issue: large XS files (tens of GBs or larger).

② Evaluation of multigroup XS

4. Multilinear interpolation of the XS library
(evaluate at each quadrature point)

5. Obtain macroscopic XS for NTE
(use microscopic XS and local isotope densities)

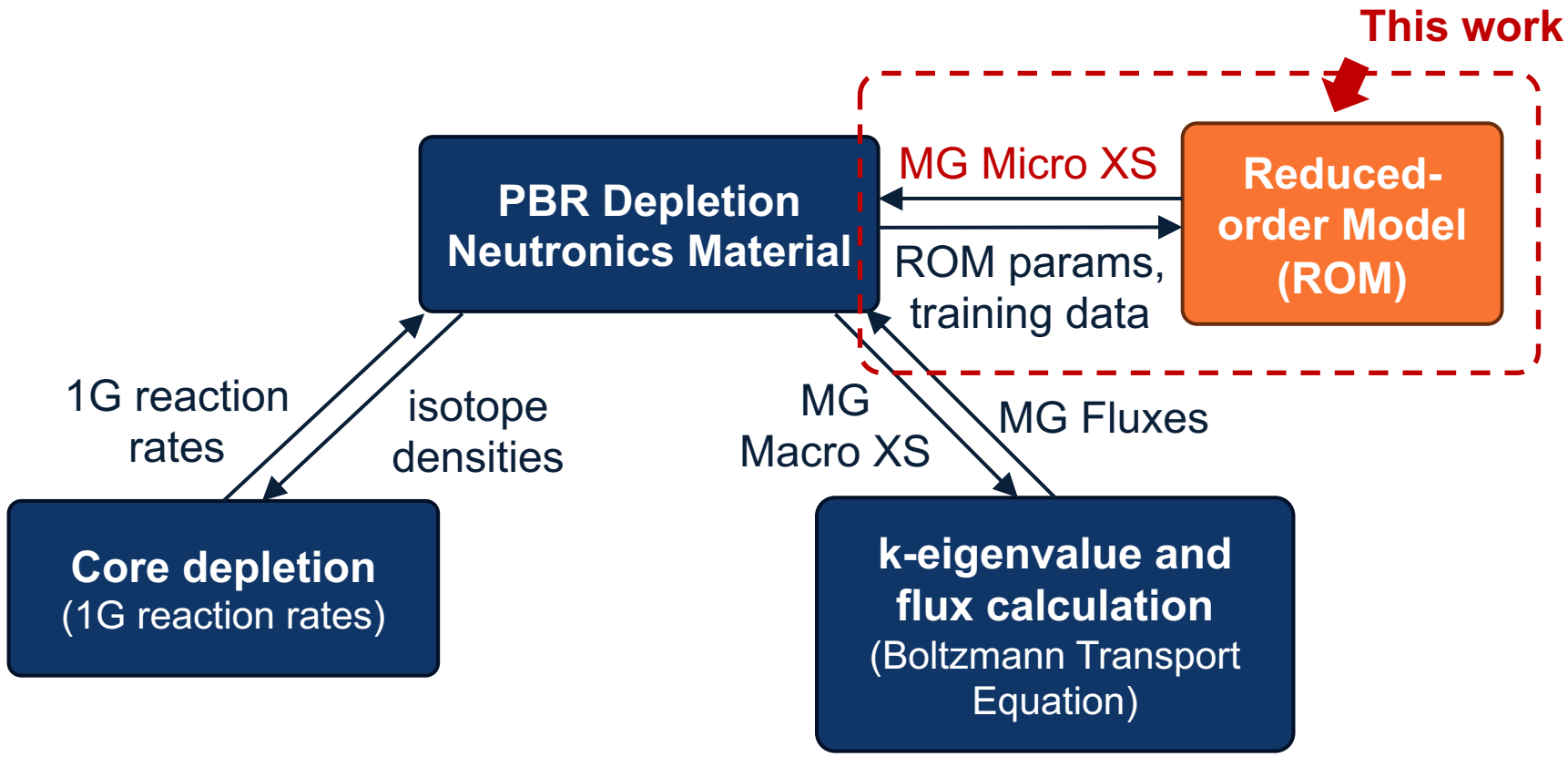


Exponential growth of the interpolation cost and number of reference calculations as the number of state variables increase.

Issue: Exponential growth of interpolation cost.

Reduced-order model (ROM) for generation of micro XS

Data flow in PBR core depletion calculation with ROM.



Goal: construct ROMs to accelerate the multigroup XS evaluation

Challenges in ROM construction for multigroup XS

① Microscopic cross-sections needed.

- For depletion analysis
- When deviating from conditions used to generate cross-sections, due to geometry changes, fuel loading, etc.

→ Large number of isotopes

② Isotopic properties vary

- Reaction types vary for different isotopes, e.g., fissionable vs. non-fissionable
- Scattering matrices have different entries
- Threshold reactions

Outline

1. DRAGON dataset of microscopic multigroup cross sections
   - Data visualization
   - Correlation analysis
2. Machine learning-assisted ROM construction
   - Down-selection of ROM techniques
   - DNNs as the selected ROM technique
3. Preliminary Griffin testing
   - 0D test case on infinite homogeneous region

DRAGON dataset of microscopic multigroup cross sections

Table 1. Reaction types considered in this work.

Reaction	DRAGON Name	Definition
σ_f	NFTOT	Fission
$\nu\sigma_f$	NUSIGF	Neutron production from fission
$\kappa\sigma_f$	H-FACTOR	Energy production from fission
σ_s	SCATRD	Neutron scattering
$\sigma_{n,\gamma}$	NG	Radiative capture
σ_a	ABS	Absorption
σ_r	REM	Removal
σ_t	STRD	Total
$\sigma_{n,2n}$	N2N	$2n$ production
$\sigma_{n,3n}$	N3N	$3n$ production
$\sigma_{n,4n}$	N4N	$4n$ production
$\sigma_{n,p}$	NP	Proton production
$\sigma_{n,d}$	ND	Deuteron production
$\sigma_{n,t}$	NT	Triton production
$\sigma_{n,np}$	NNP	$n+p$ production
$\sigma_{n,\alpha}$	NA	α production
$\sigma_{n,2\alpha}$	N2A	2α production

- 295 isotopes, 4 energy groups;
- 5,184 data in training set; 1,367 data in test set

Figure 1. Visualization of self-shielded cross sections for representative isotopes.

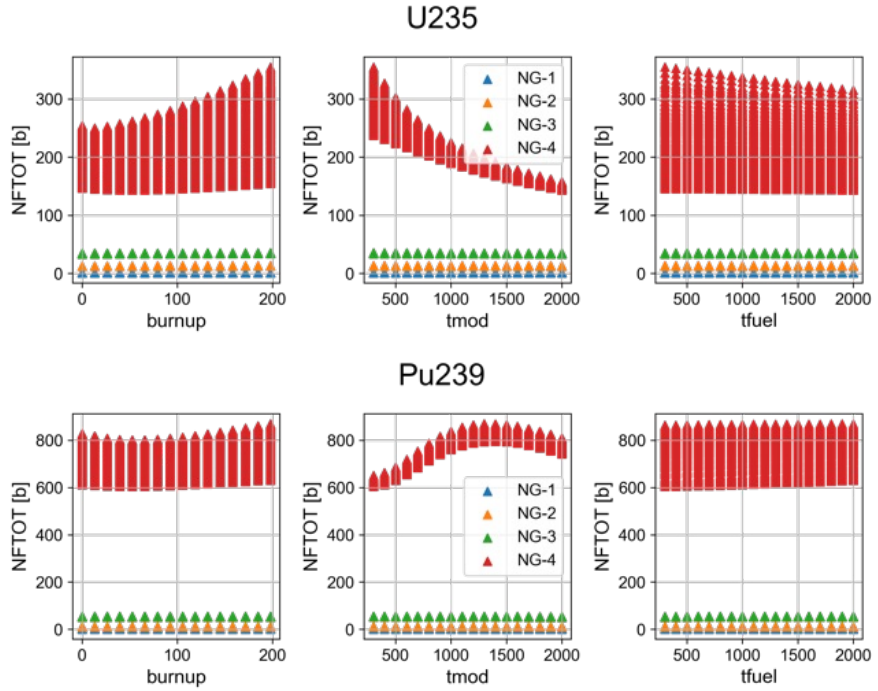


Table 2. Description of the control variables.

Control Variables	Unit	Physical Range	Number of Tabulations Points
burnup	GWd/tHM	[0, 198]	31
tmod	K	[300, 2000]	35
tfuel	K	[300, 2000]	35

Correlation analysis of the DRAGON dataset

Goal: Identify linearity in cross-section data across all isotopes, reaction types and energy groups.

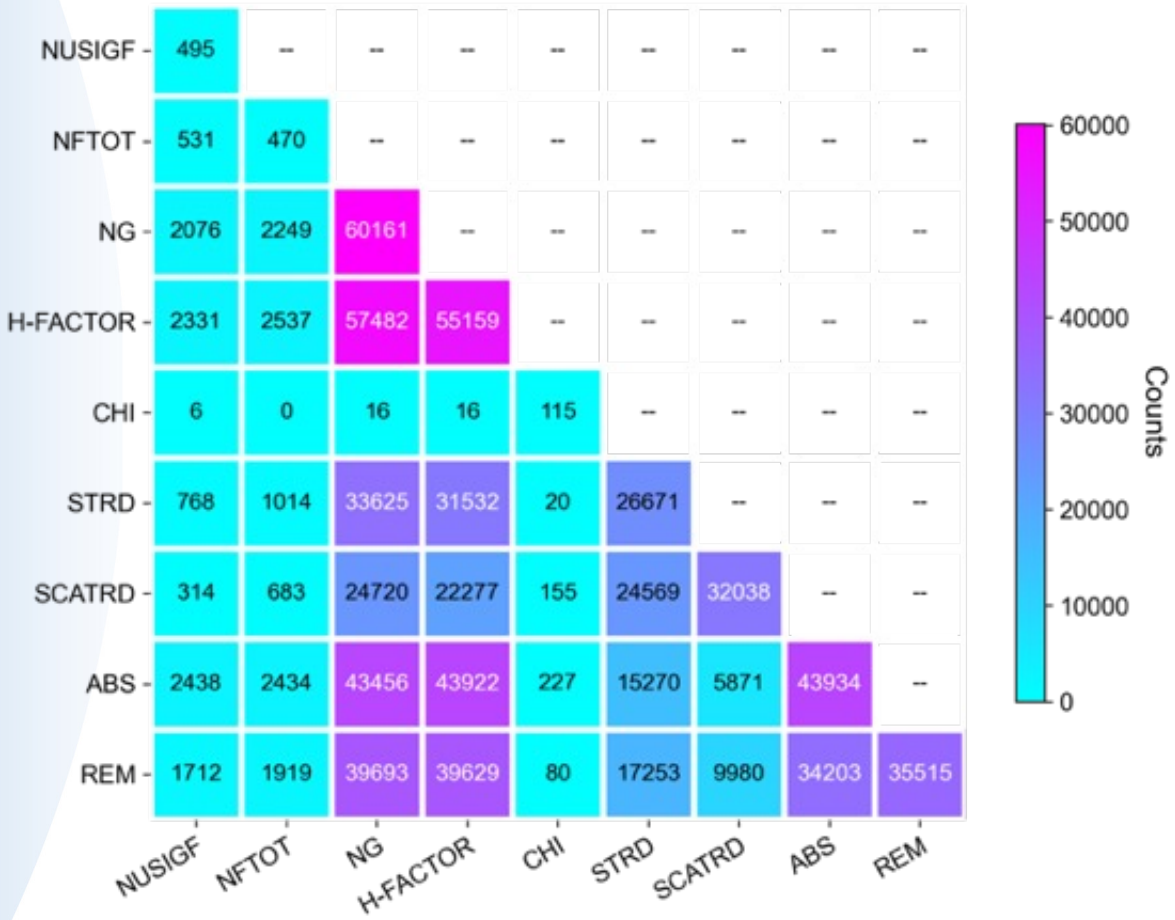


Figure 2. Total number of pairwise relationships with strong linearity ($|\rho|>0.999$) across all isotopes and all energy groups.

Pearson Correlation Coefficient ρ

$$\rho = \frac{\mathrm{Cov}(X,Y)}{\sigma_X \sigma_Y} = \frac{\mathbb{E}[XY]-\mathbb{E}[X]\mathbb{E}[Y]}{\sqrt{\mathbb{E}[X^2]-(\mathbb{E}[X])^2}\sqrt{\mathbb{E}[Y^2]-(\mathbb{E}[Y])^2}}$$

Similarity is shown:

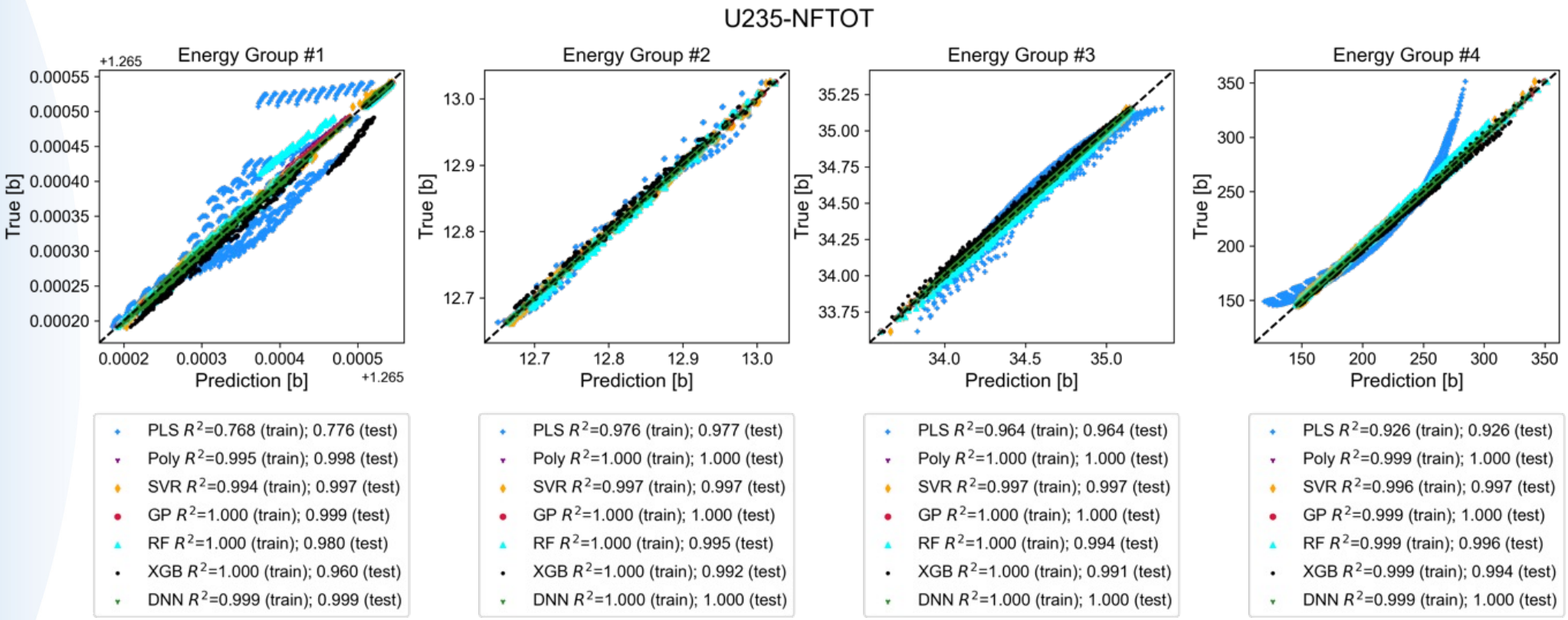
- within the same reaction (diagonal)
- among derived reactions (off-diagonal)
  - NFTOT, NUSIGF, H-FACTOR
  - REM derived from STRD and SCATRD
  - ABS is related to non-scattering interactions (NG)
- across reactions
  - STRD and NG
  - STRD and H-FACTOR
  - SCATRD and NG
  - SCATRD and H-FACTOR
  - NG and H-FACTOR

Machine learning (ML)-assisted ROM construction

Table 3. Machine learning algorithms considered

Category	Notation	Name
Linear Regression	PLS	Partial Least Squares Regression
	OLS-Poly	Ordinary Least Squares (with polynomial features)
Kernel-based Methods	SVR	Support Vector Regression
	GP	Gaussian Process
Tree-based Algorithms	RF	Random Forest
	XGB	eXtreme Gradient Boosting
Neural Networks	DNN	Deep Neural Networks

Down-selection of ML algorithms (accuracy)



Down-selection of ML algorithms (full consideration)

Table 3. Comprehensive performance comparison and down-selection of ROM techniques (based on a single isotope, a single reaction).

Algorithm	Storage Size	Training Speed (sec)	Prediction Speed (sec)	Accuracy (R^2) Train/Test	Scalability	Desirability
PLS	$\mathcal{O}(10^2)$ KB	$\mathcal{O}(10^{-2})$	$\mathcal{O}(10^{-4})$	0.909 / 0.911	✓	×
OLS-Poly	$\mathcal{O}(10^0)$ KB*	$\mathcal{O}(10^{-2})$	$\mathcal{O}(10^{-3})$	0.999 / 0.999	××	×
SVR	$\mathcal{O}(10^1)$ KB	$\mathcal{O}(10^{-1})$	$\mathcal{O}(10^{-4})$	0.996 / 0.997	×	×
GP	$\mathcal{O}(10^2)$ MB	$\mathcal{O}(10^2)$	$\mathcal{O}(10^{-2})$	1.000 / 1.000	××	×
RF	$\mathcal{O}(10^2)$ MB	$\mathcal{O}(10^0)$	$\mathcal{O}(10^{-1})$	1.000 / 0.991	✓	×
XGB	$\mathcal{O}(10^0)$ MB	$\mathcal{O}(10^0)$	$\mathcal{O}(10^{-3})$	1.000 / 0.984	✓	×
DNN	$\mathcal{O}(10^0)$ KB**	$\mathcal{O}(10^1 \sim 10^2)$**	$\mathcal{O}(10^{-4})$	1.000 / 1.000	✓	✓
Interpolation	$\mathcal{O}(10^2)$ GB	N/A	Exponential Growth	N/A	×××	×

* Size of the OLS-poly model significantly depends on the polynomial order (5 in this work).
** Size and training cost of DNNs depends on the detailed NN structure.

DNN as the selected ROM technique

Predicting all reactions at once for each isotope.

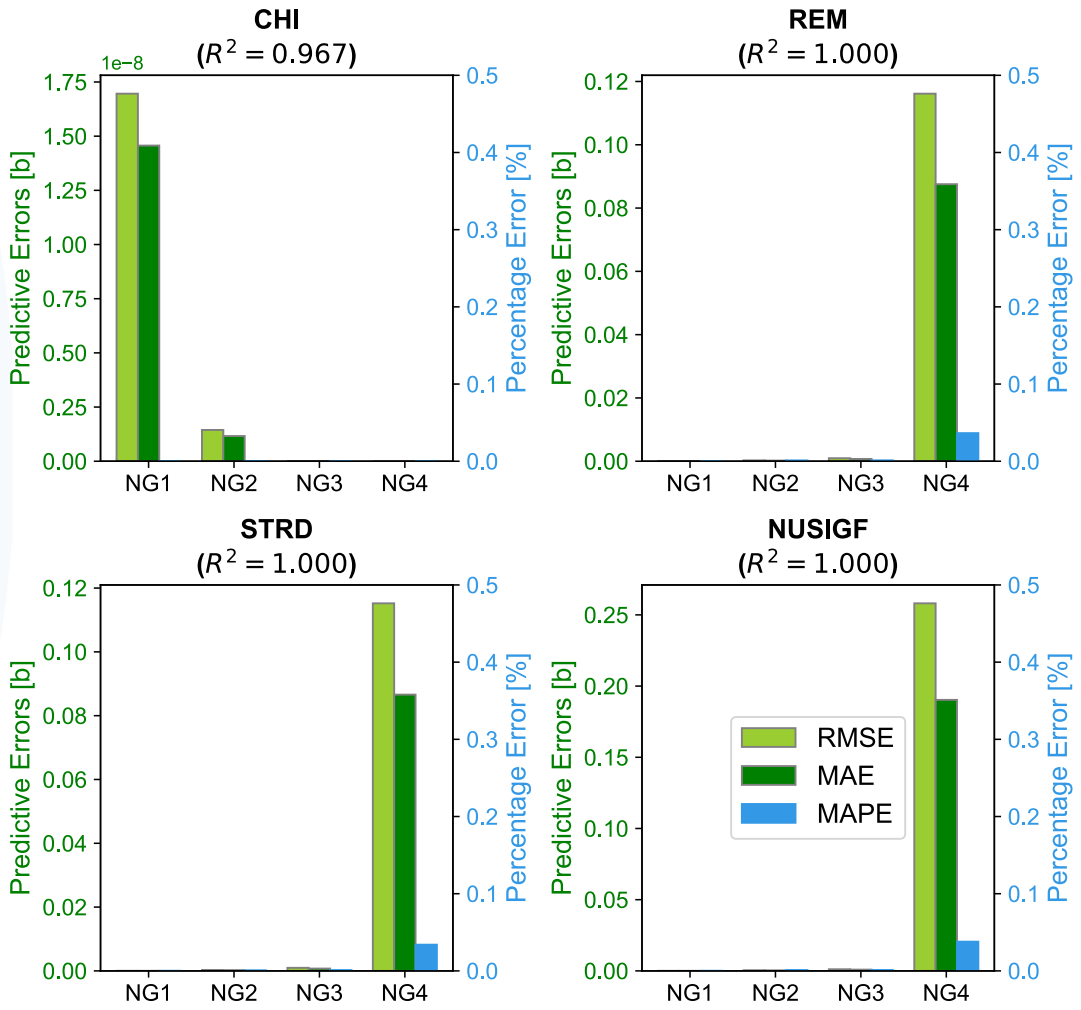


Figure 4. DNN predictive errors for essential reactions in ^{235}U.

DNN as the selected ROM technique

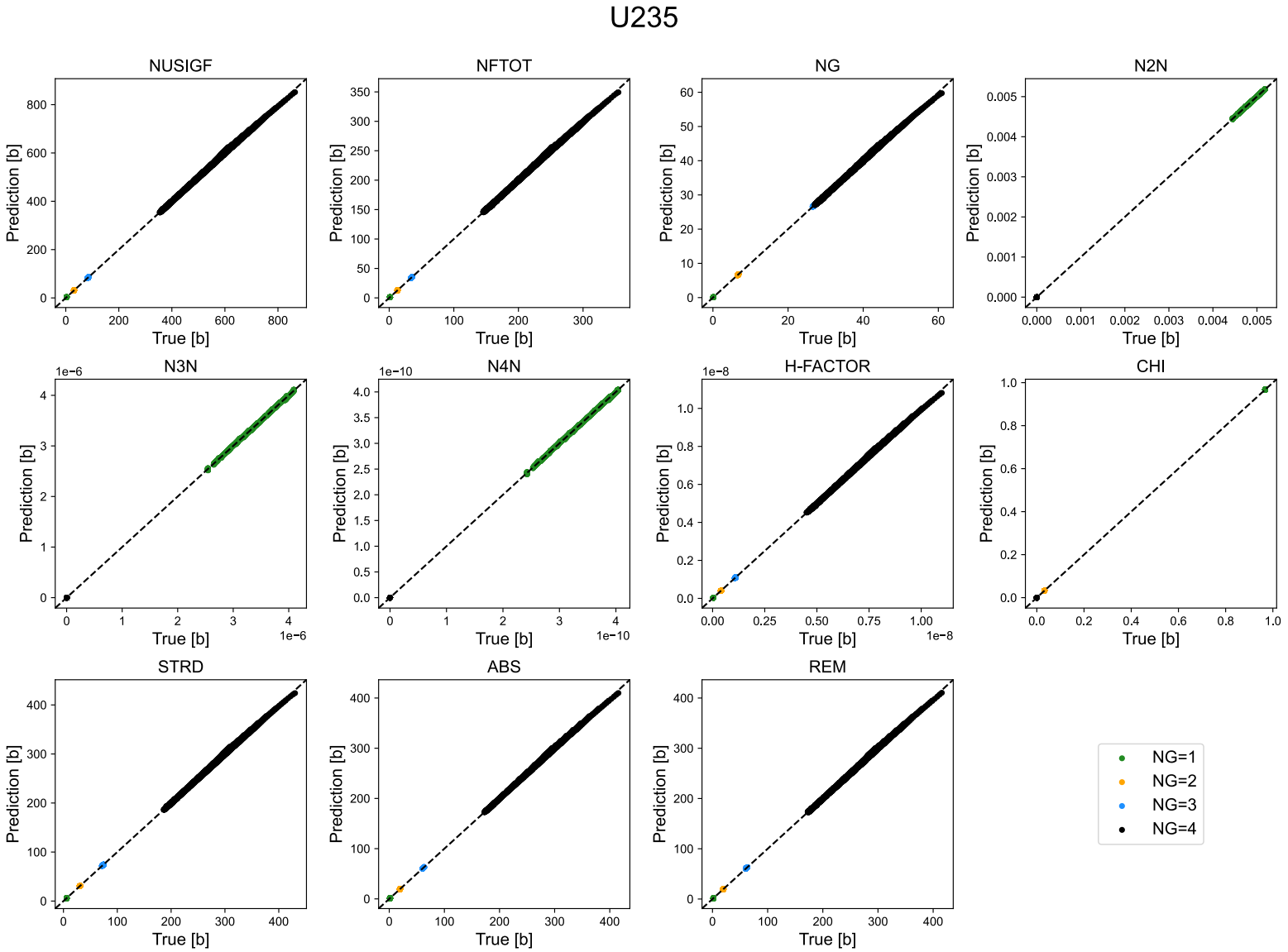


Figure 5. Predicted versus true values for all reactions except the scattering matrix in ^{235}U

Predicting the scattering matrix

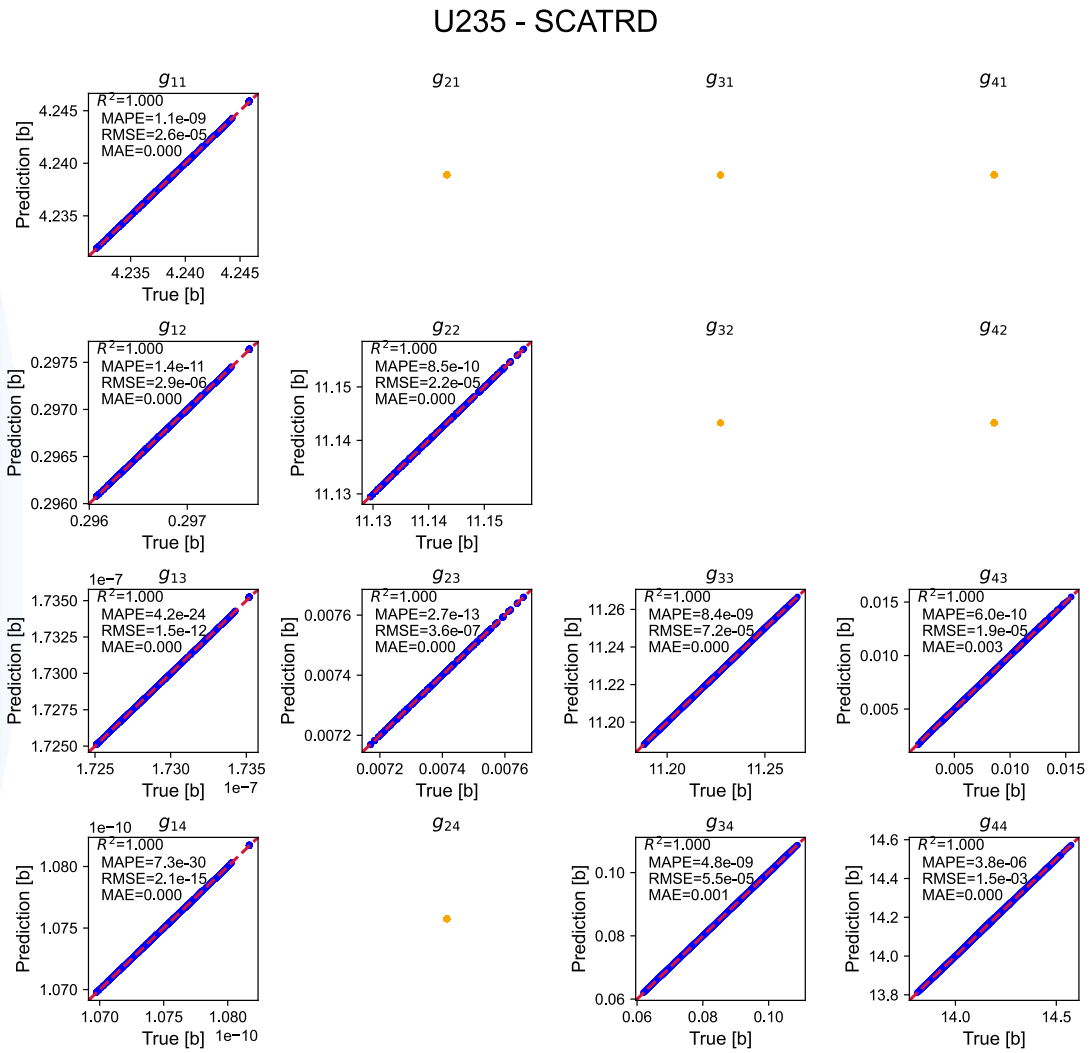


Figure 6. Predicted versus true values for non-zero entries in the scattering matrix of ^{235}U.

- Only predicts non-zero entries in the scattering matrix
- Scattering matrix predicted together with other reactions

Evaluation Metrics
Mean absolute percentage error (MAPE)
Root mean-squared error (RMSE)
Mean absolute error (MAE)

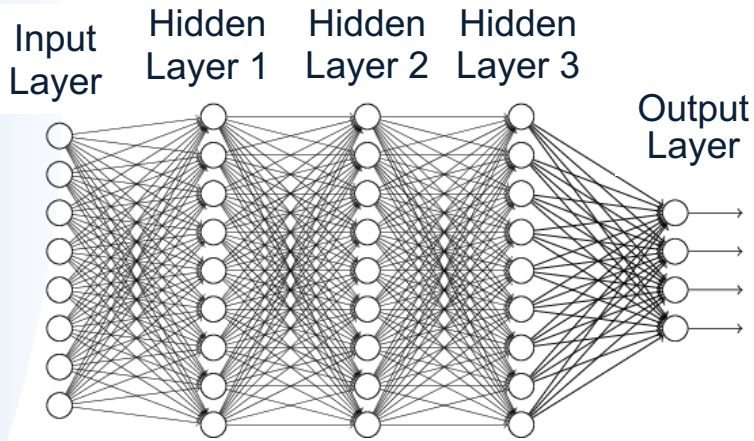
Interfacing with MOOSE

DRAGON

Microscopic multigroup cross section generation

PyTorch

DNN training



LibTorch

Griffin

ISOXML/LibTorch

- TorchXS
- MixingTable
- MultigroupLibrary

Materials

- TorchNeutronicsMaterial
- PebbleBedNeutronicsMaterial

UserObjects

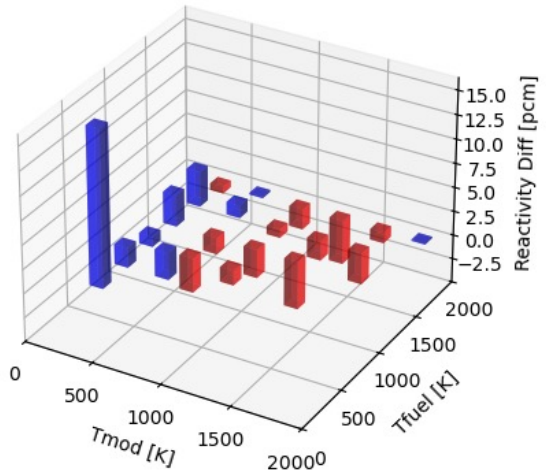
- ISOXMLMacroXS
- PebbleUserObject
- ISOXMLMultigroupLibrary
- PebbleBedXSUserObject

Actions

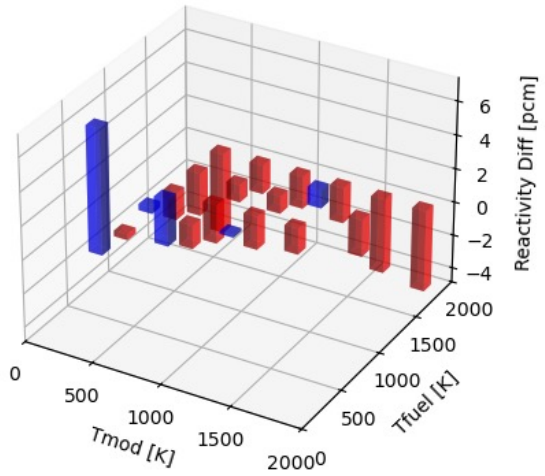
- PebbleDepletionAction

Reactivity difference w.r.t multilinear interpolation

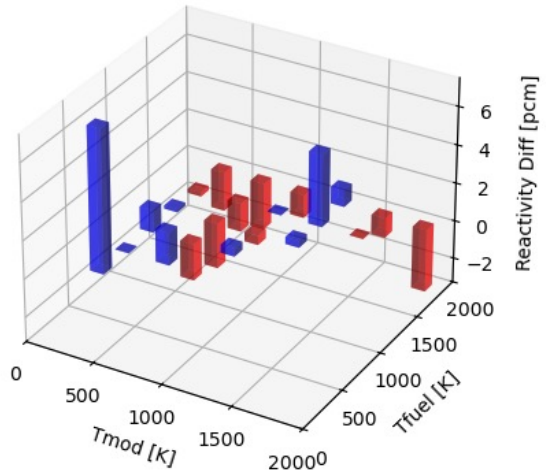
Burnup = 0.0 GWd/tHM



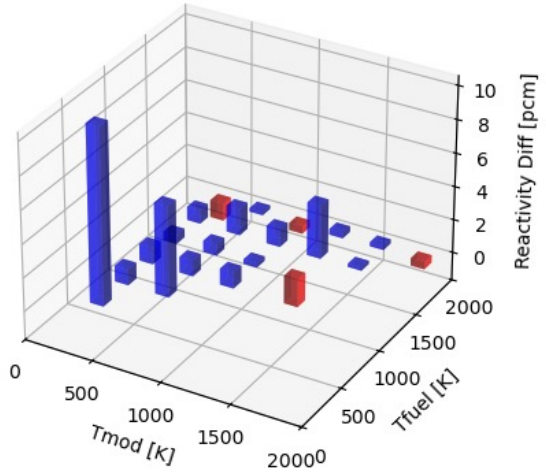
Burnup = 39.6 GWd/tHM



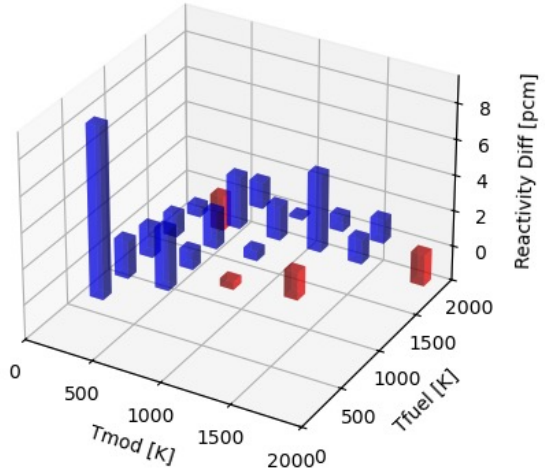
Burnup = 79.2 GWd/tHM



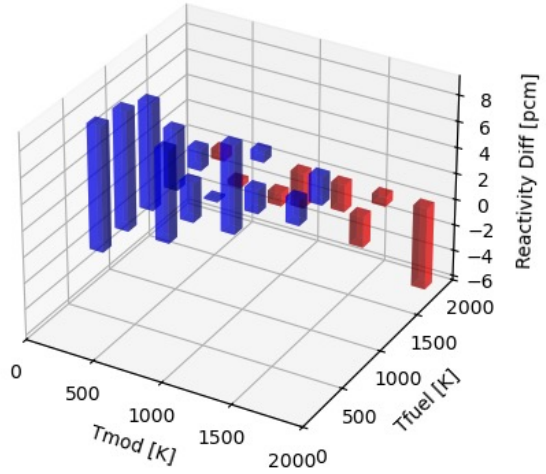
Burnup = 118.8 GWd/tHM



Burnup = 158.4 GWd/tHM



Burnup = 198.0 GWd/tHM



Conclusion and future work

- DNNs provides high memory efficiency, excellent predictive accuracy, great scalability, easy integration into MOOSE, and superior flexibility in re-training.
- More rigorous Griffin testing will be conducted to systematically test the performance of ROM in comparison to the multivariate interpolation method.
- Current work focused on solving the transport equations, and future work will also include the depletion simulations.
- In the longer term, developed ROMs will be integrated with the online XS generation capability in Griffin to enable on-the-fly update of the ROM upon generation of additional XS data.

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