Physics-based Uncertainty Quantification for ZrH_x Thermal Scattering Law

Weixiong Zheng

Nuclear Engineering,
Texas A&M University,
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Synopsis

- Background
- Motivations
- Introduction
- Parameterized Models and Model Tests
- Calibration based on MCNP Simulations
- Conclusions and Future Work
- References

Background

- Basics for TRIGA Reactors
  - TRIGA reactors are thermal reactors using U-ZrH_x fuel
  - Thermal neutrons, which are heavily affected by thermal scattering, are important
- Scattering Complexity
  - Binding forces affect thermal neutron scattering cross sections
  - Different ZrH_x compositions (different x) result in different bindings, and then different vibration frequency distributions (also called phonon spectrum), thus different scattering cross sections
  - Different temperatures result in different bindings, thus different phonon spectra and cross sections
- Existing data
  - ENDF based on Slaggie's study on ZrH_2; IKE simplified the H phonon spectrum for ZrH_2; the evaluations use phonon spectra at RT for all temperatures
- Possible Problem
  - x=1.523 (i.e. $ZrH_{1.523}$)
  - Accurate scattering cross scattering data specific for x=1.523 at multiple temperature are needed

Motivations

- Establish valid parameterized phonon spectrum models for H and Zr in ZrH_x
- Find sensitive quantities of interest in the TRIGA simulations which could be used to calibrate the parameters in the phonon spectrum models
- Tabulate the reasonably accurate thermal scattering law table for TRIGA at TAMU for future reactor simulation uses

Introduction

- Theory

Double differential scattering cross section

$$\sigma(E' \to E, \Omega' \cdot \Omega) = \frac{\sigma_b}{4\pi kT}\sqrt{\frac{E}{E'}}S(\alpha,\beta)$$

where $\alpha \equiv \frac{E+E'-2\mu\sqrt{EE'}}{AkT}$ and $\beta \equiv \frac{E-E'}{kT}$.

The $S(\alpha,\beta)$ is the scattering law. It can be given by:

$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\beta t}e^{-\gamma(t)}dt$$

where

$$\gamma(t) = \alpha\int_{-\infty}^{\infty} P(\beta)\left[1-e^{-i\beta t}\right]e^{-\beta/2}d\beta \text{ and } P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)}$$

The $\rho(\beta)$ is the phonon spectra in terms of β.

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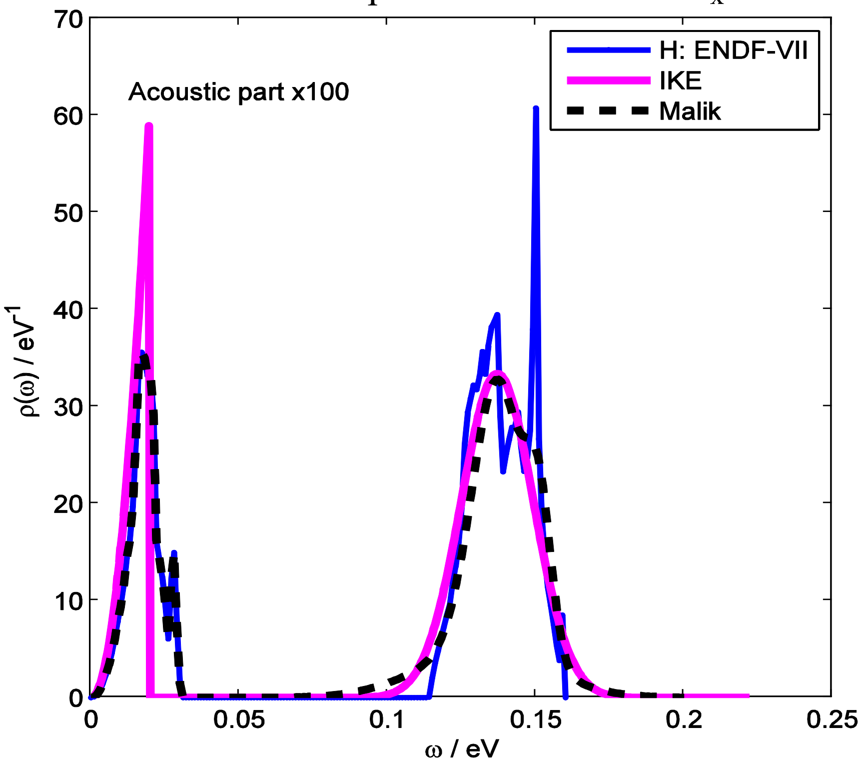
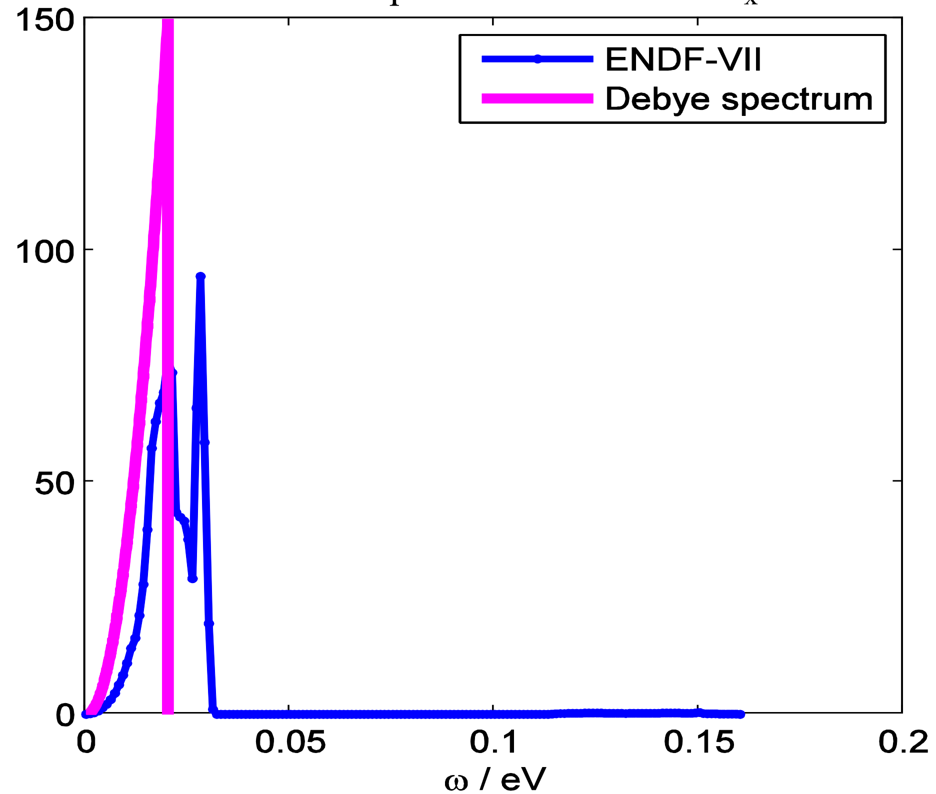
Parameterized Model and Model Tests

- Some existing spectra

Phonon spectra for H in ZrH_x



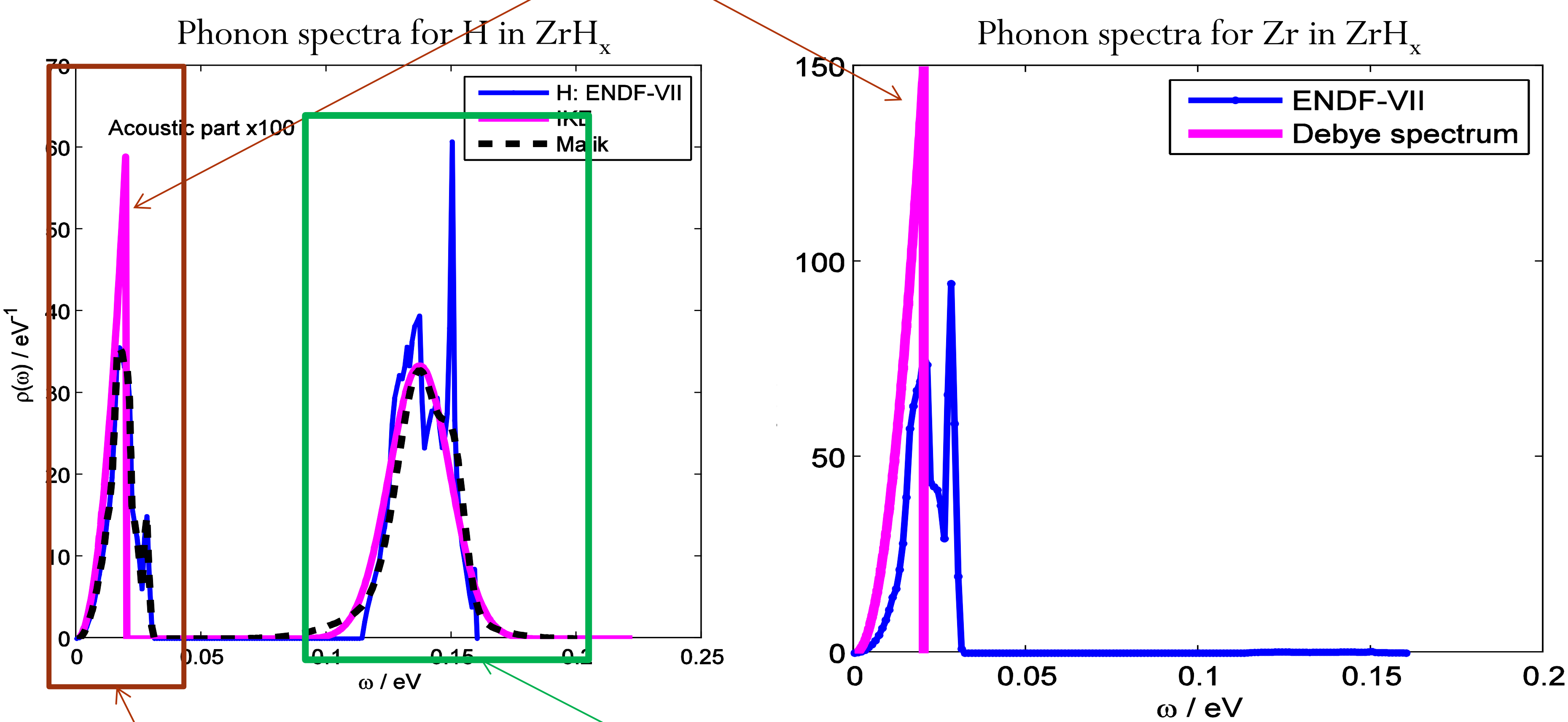
Phonon spectra for Zr in ZrH_x



Parameterized Model and Model Tests

- Some existing sp

Debye distribution



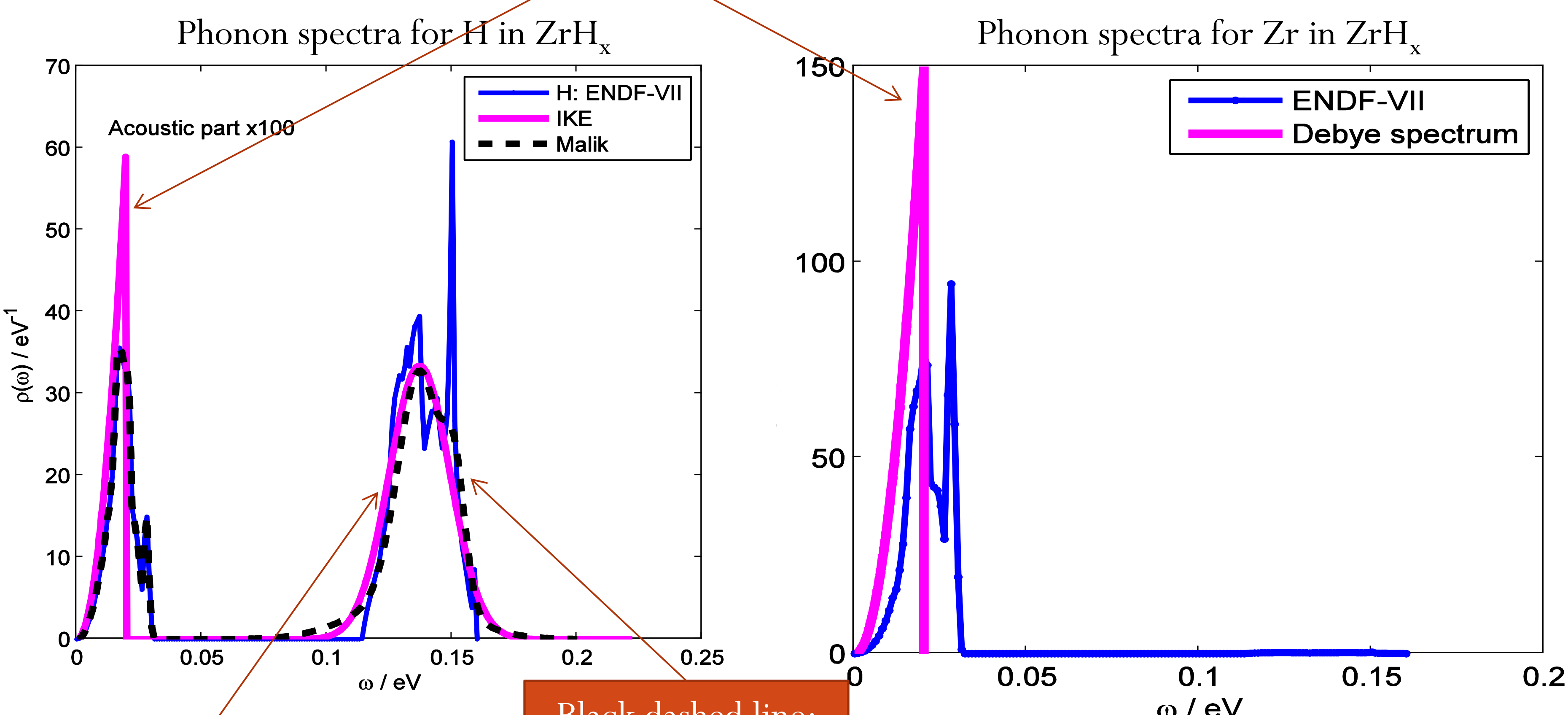
Acoustic mode

Optical mode

Parameterized Model and Model Tests

- Some existing sp

Debye distribution

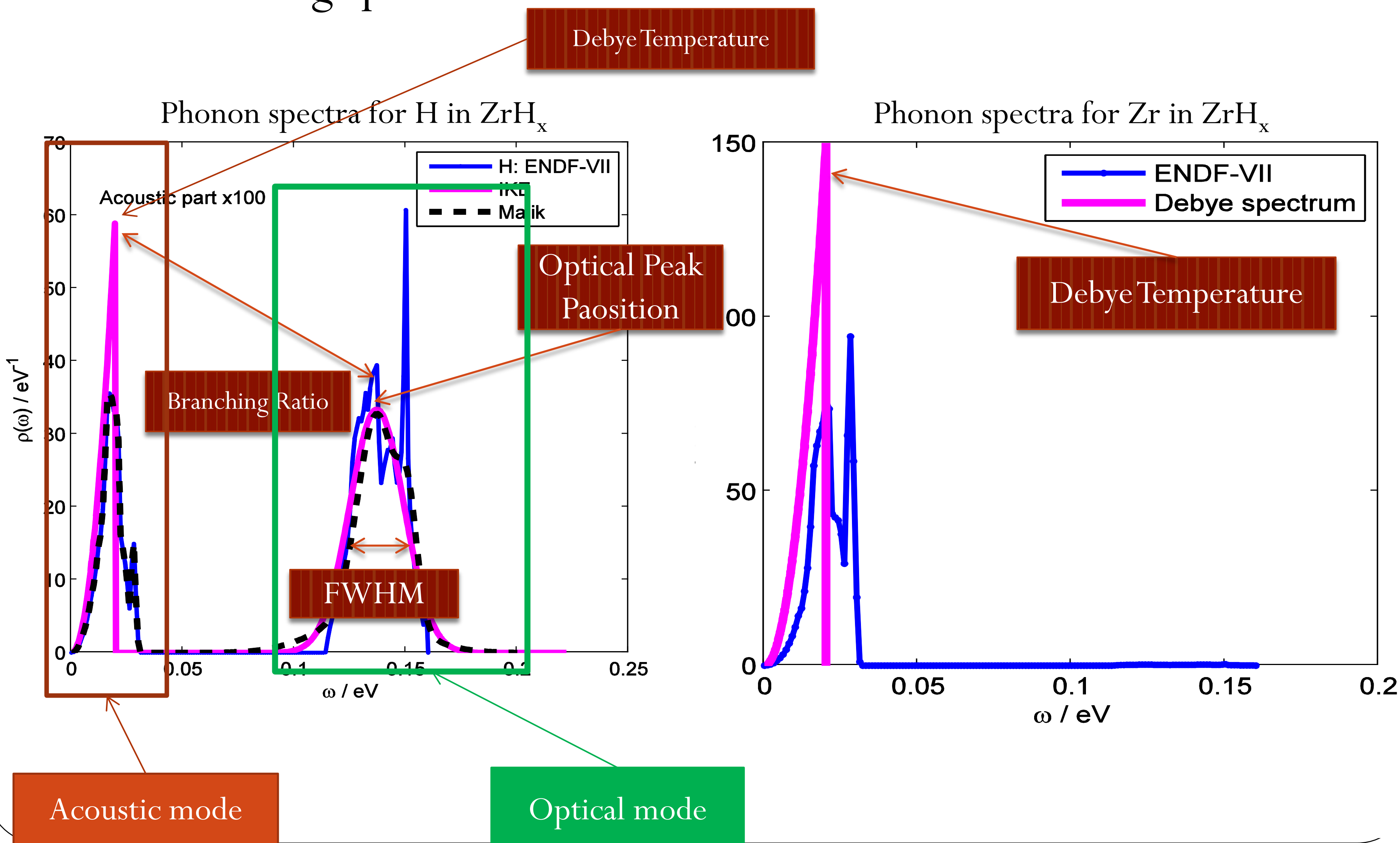


Pink: Gaussian distribution

Black dashed line: three Gaussian specific for $ZrH_{1.58}$

Parameterized Model and Model Tests

- Some existing spectra



Parameterized Model and Model Tests

- Parameterized Phonon Spectra (PPS)
  - For H:

$$\rho(\omega)_{\mathrm{H}} = \begin{cases} \dfrac{3b}{2T_{\mathrm{DH}}^3}\omega^2, \omega < T_{\mathrm{DH}} \\ \dfrac{3b}{2T_{\mathrm{DH}}^3}(\omega - 2T_{\mathrm{DH}})^2, T_{\mathrm{DH}} \le \omega \le 2T_{\mathrm{DH}} \\ \dfrac{c(b)}{\sqrt{2\pi}\sigma}\exp\left[-\dfrac{(\omega - p)^2}{2\sigma^2}\right], 2T_{\mathrm{DH}} \le \omega \le \omega_{\mathrm{max,H}} \end{cases}$$

  - For Zr:

$$\rho(\omega)_{\mathrm{Zr}} = \begin{cases} \dfrac{r(1+c)}{T_{\mathrm{DZr}}^{1+c}}\omega^c, \omega \le T_{\mathrm{DZ}r} \\ \dfrac{(1+c)r}{T_{\mathrm{DZr}}}\exp\left[\dfrac{(1+c)^r}{1-r}\left(1 - \dfrac{\omega}{T_{\mathrm{DZr}}}\right)\right], T_{\mathrm{DZ}r} \le \omega \le \omega_{\mathrm{max,Zr}} \end{cases}$$

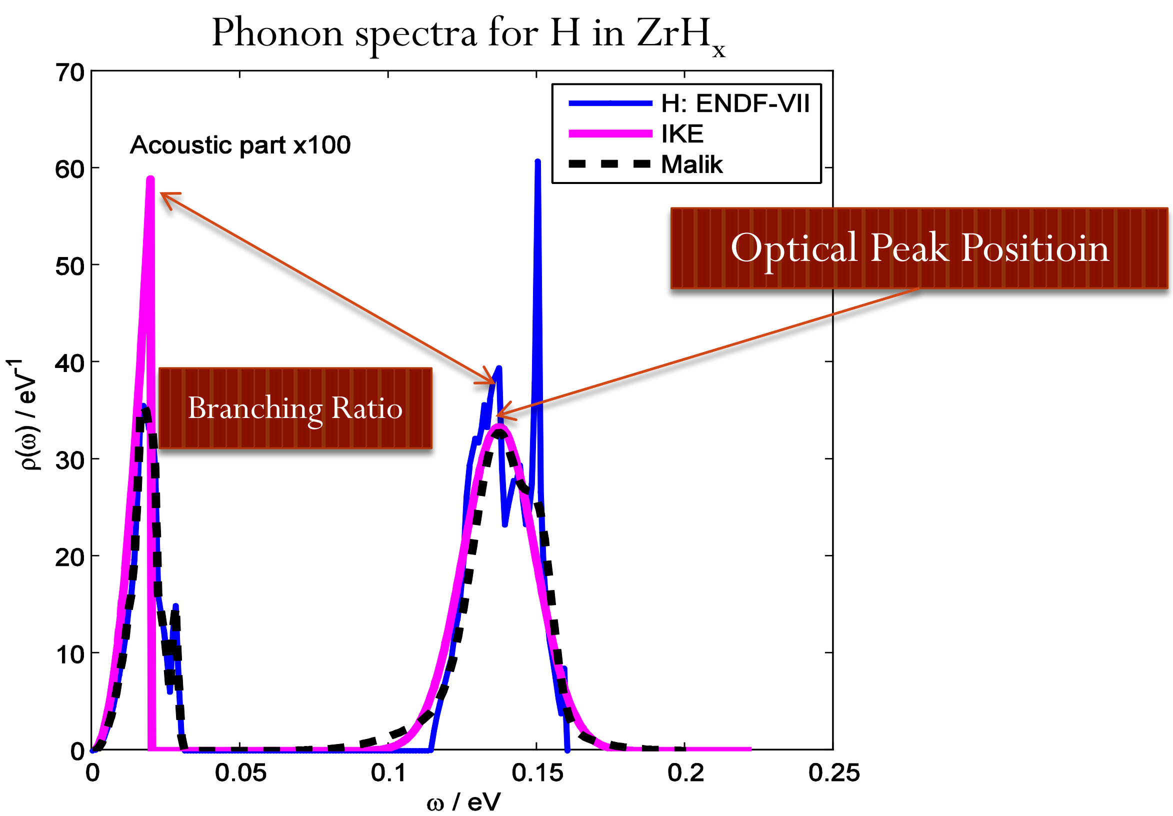
  - Parameters:

$T_{\mathrm{DH}}, b, p,$ FWHM$, r, c$ and T_{DZr}

Parameters	FWHM/meV	b	p/meV	T_{DH}/meV	T_{DZr} /meV	r	c
Ranges	[25,31]	[1/361,1/91]	[127,147]	[16,24]	[16,24]	[0.4,0.8]	[2,2.8]

Parameterized Model and Model Tests

- Some existing spectra for H in ZrH_x



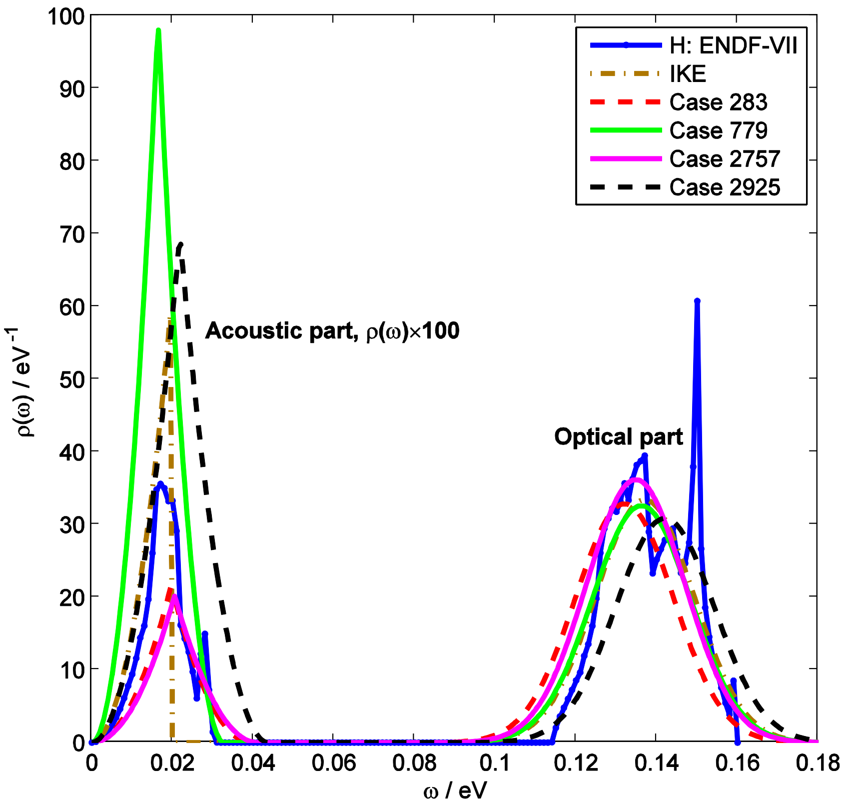
Parameterized Model and Model Tests

- Latin Hypercube sampling design (LHS)
  - Sampled 3000 sets of parameters over the seven dimensional input space
  - Generated 3000 realizations of phonon spectrum based on the LHS design
  - Each realization gives unique phonon spectra for H and Zr, respectively.

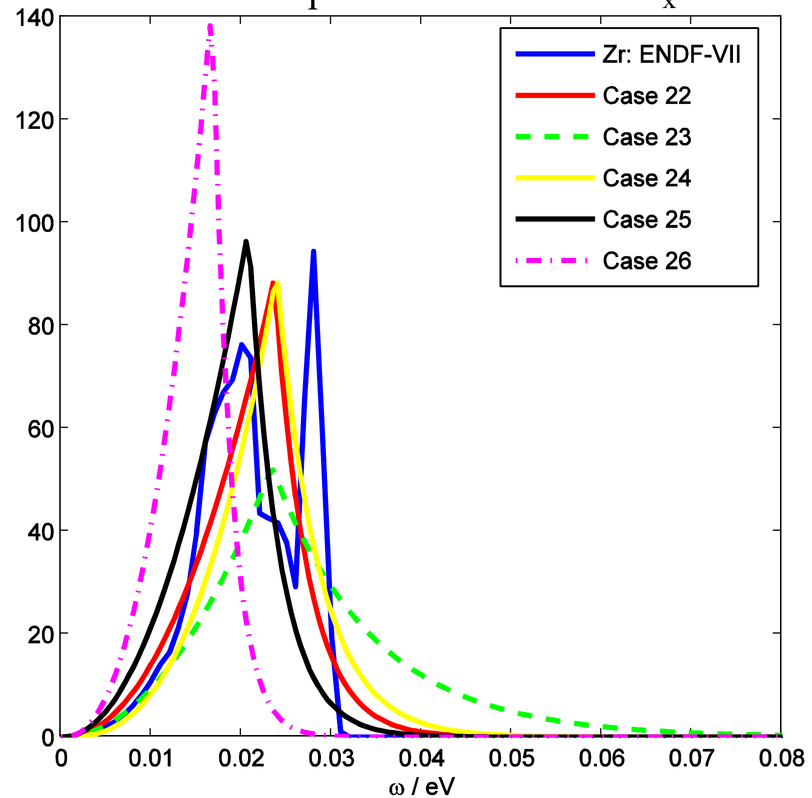
Parameterized Model and Model Tests

- For each realization, we get a unique phonon spectrum

Phonon spectra for H in ZrH_x

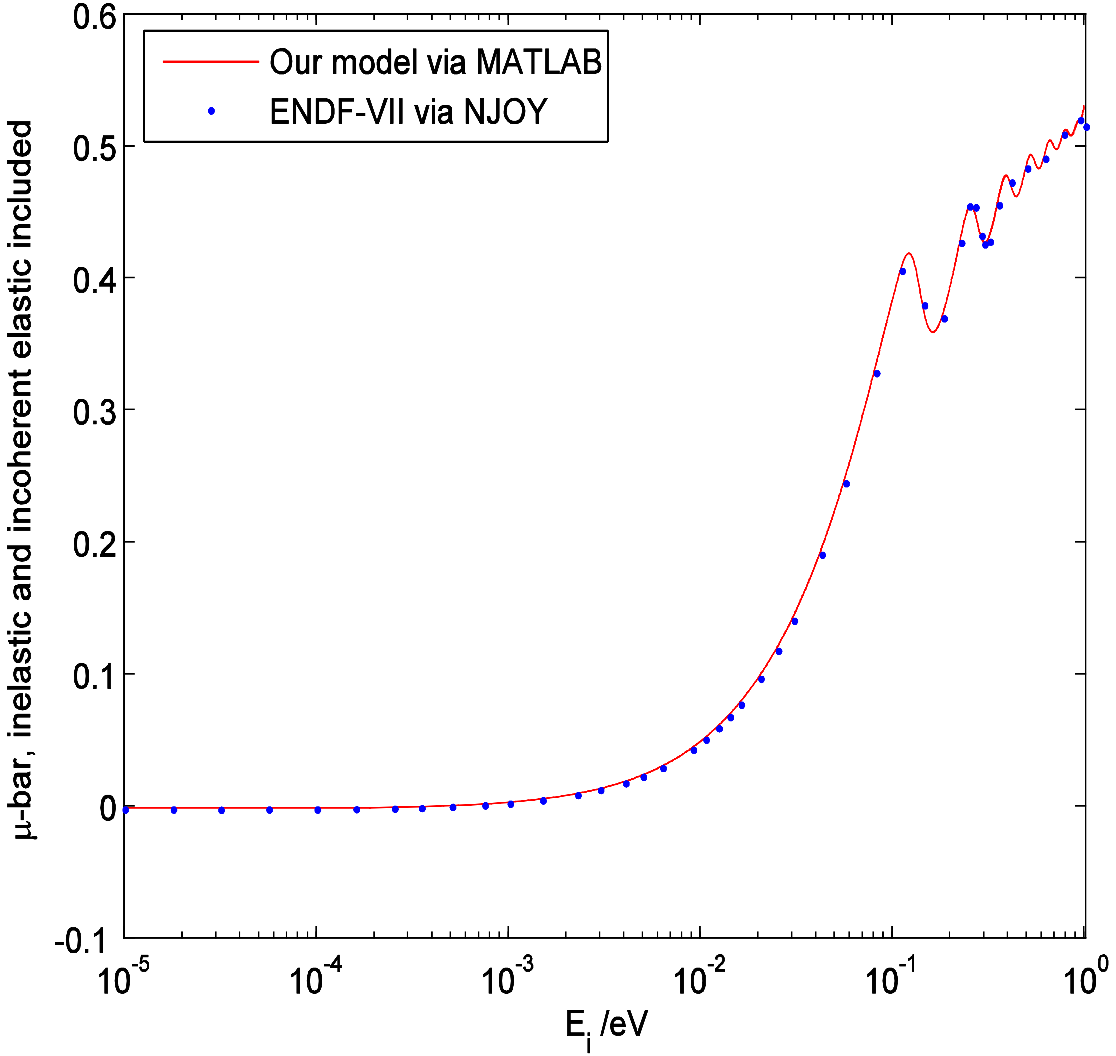


Phonon spectra for Zr in ZrH_x



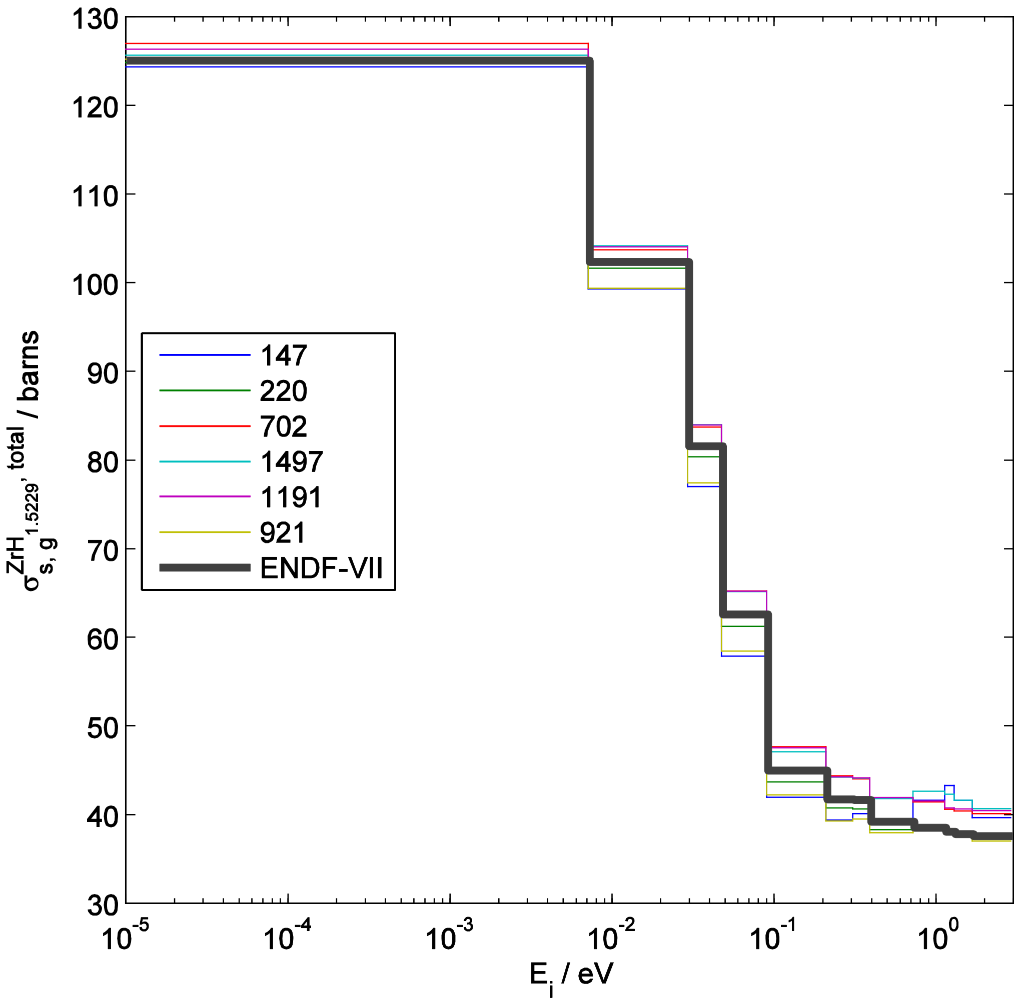
Parameterized Model and Model Tests

- Model Tests: $\bar{\mu}_{\mathrm{ZrH}_{1.84}}$



Parameterized Model and Model Tests

- Model Tests: $\sigma_{g'}^{tot,ZrH_{1.5229}}$



Calibration based on MCNP Simulations

- Calculation and Analysis Procedure

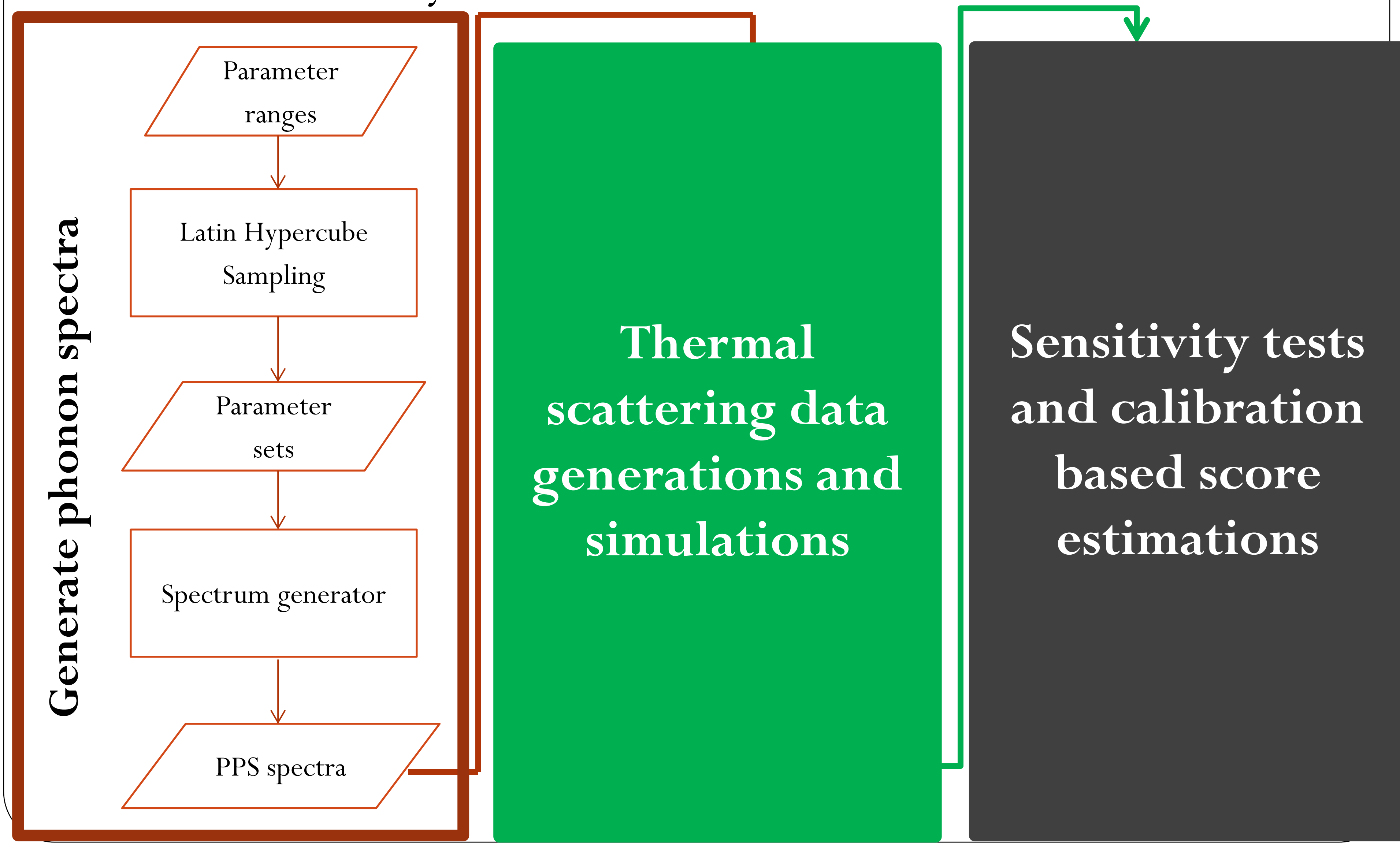
Parameterized phonon spectra generation

Thermal scattering data generations and simulations

Sensitivity tests and calibration based score estimations

Calibration based on MCNP Simulations

- Calculation and Analysis Procedure



Calibration based on MCNP Simulations

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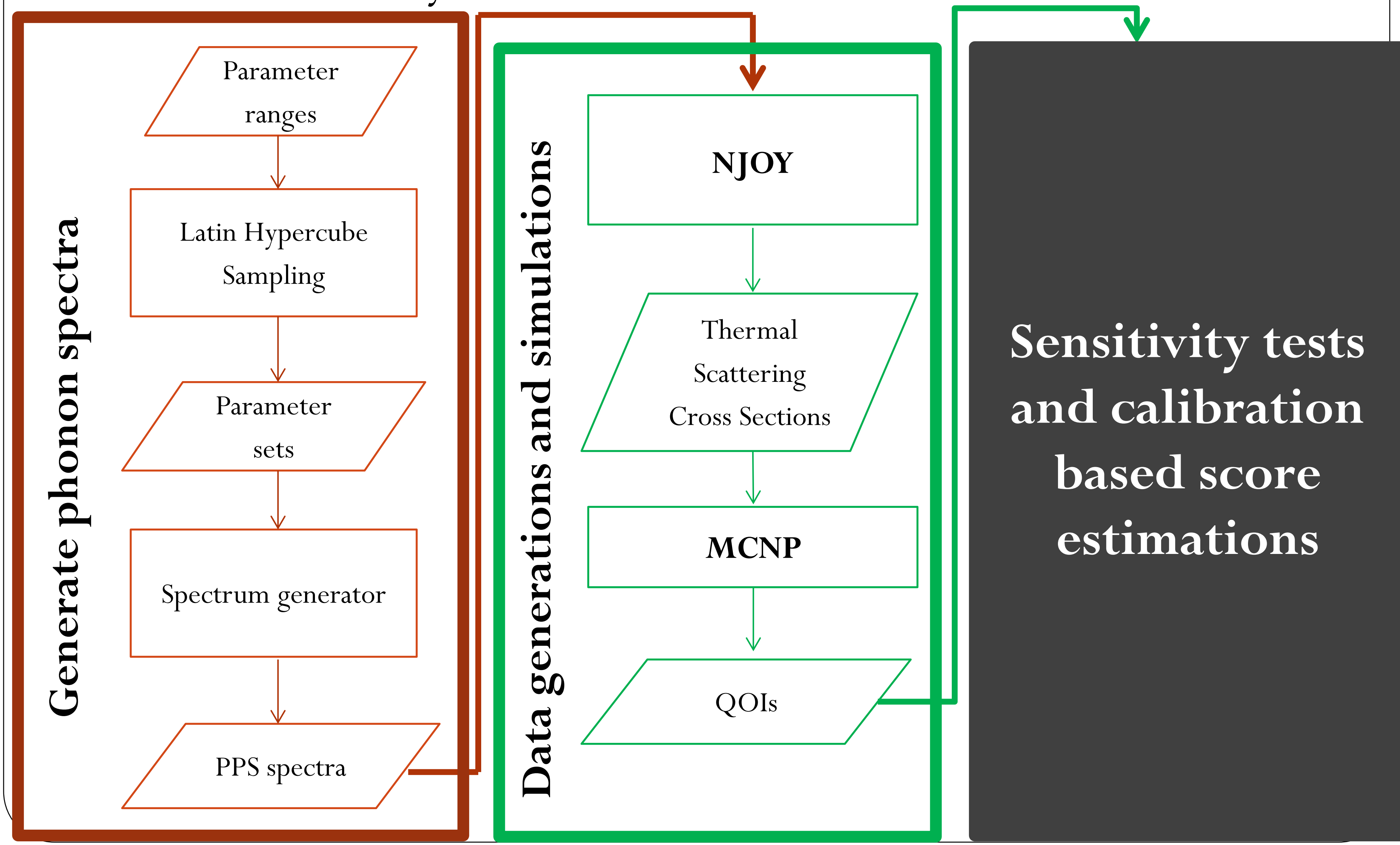

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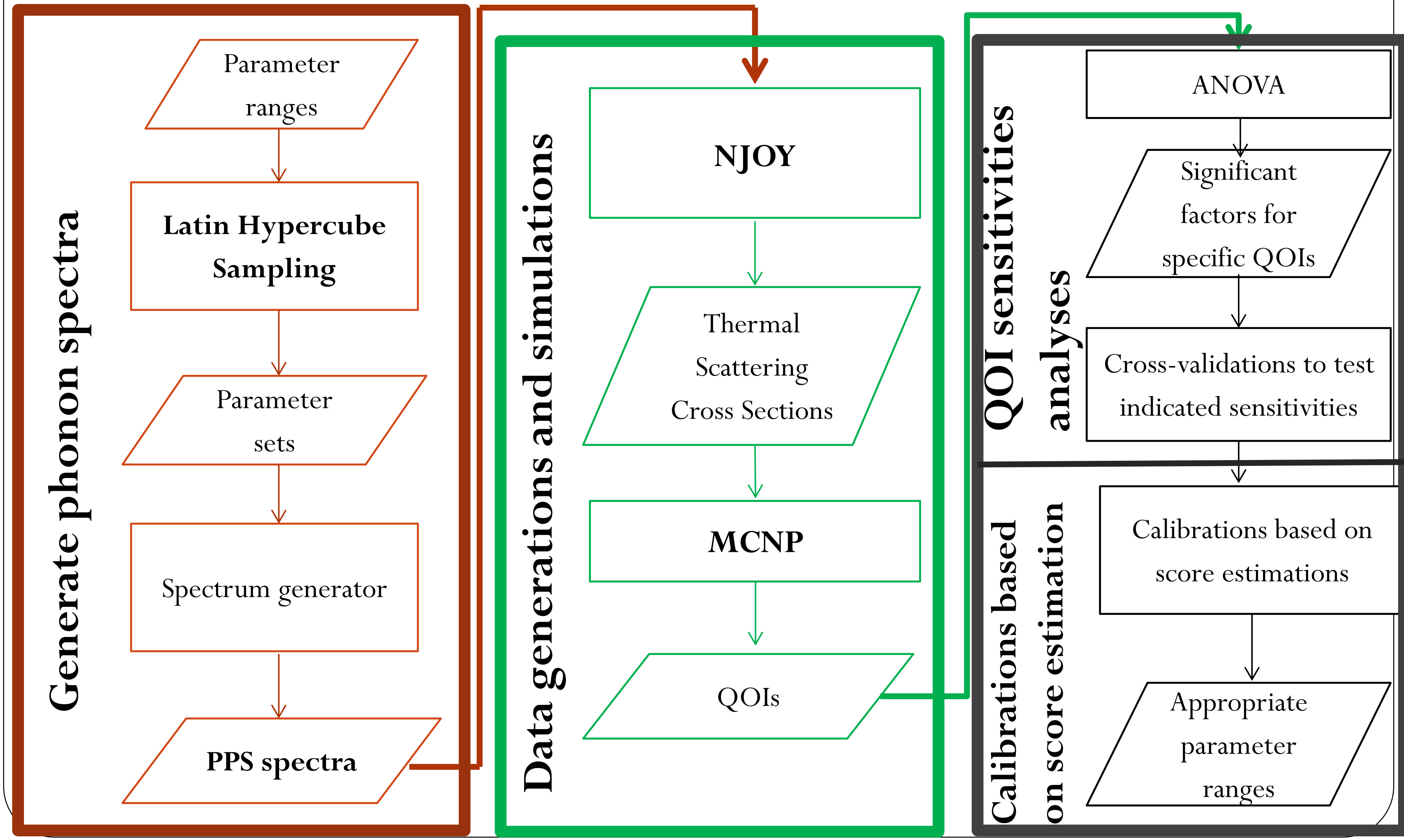
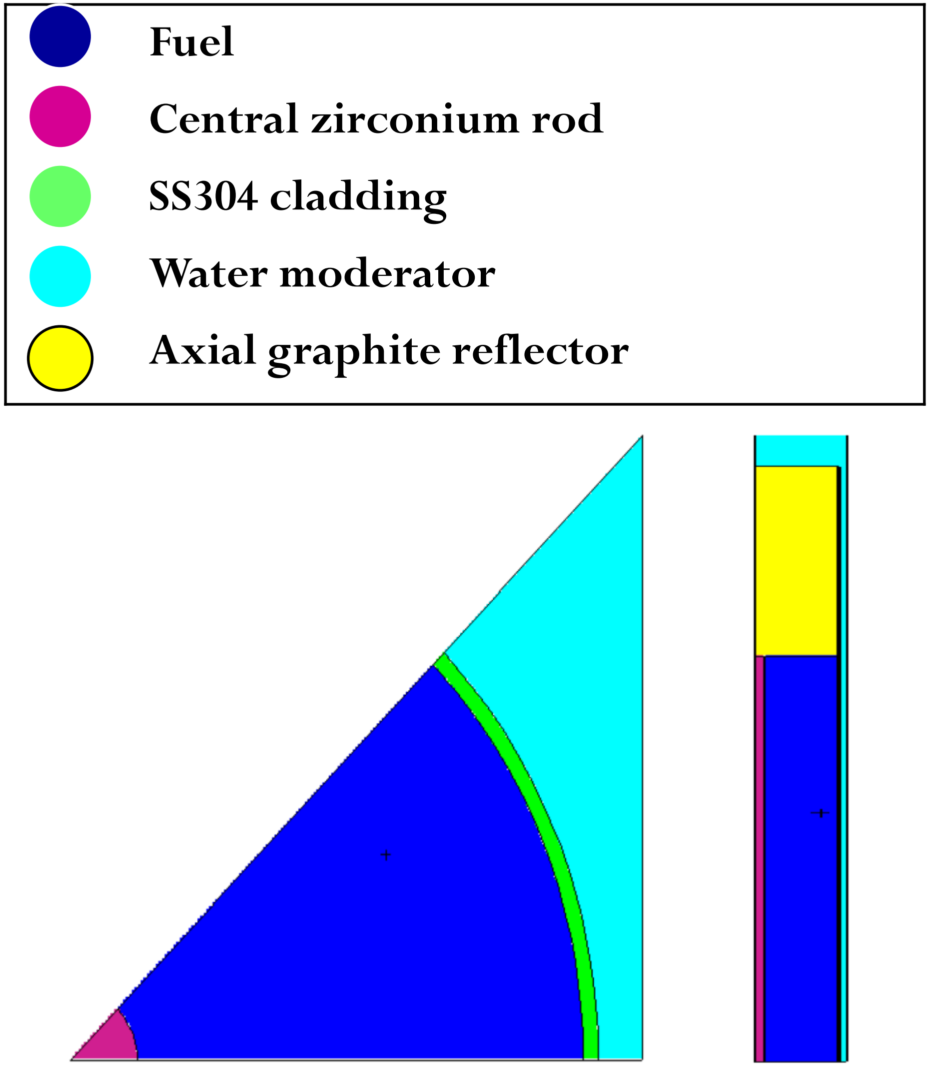


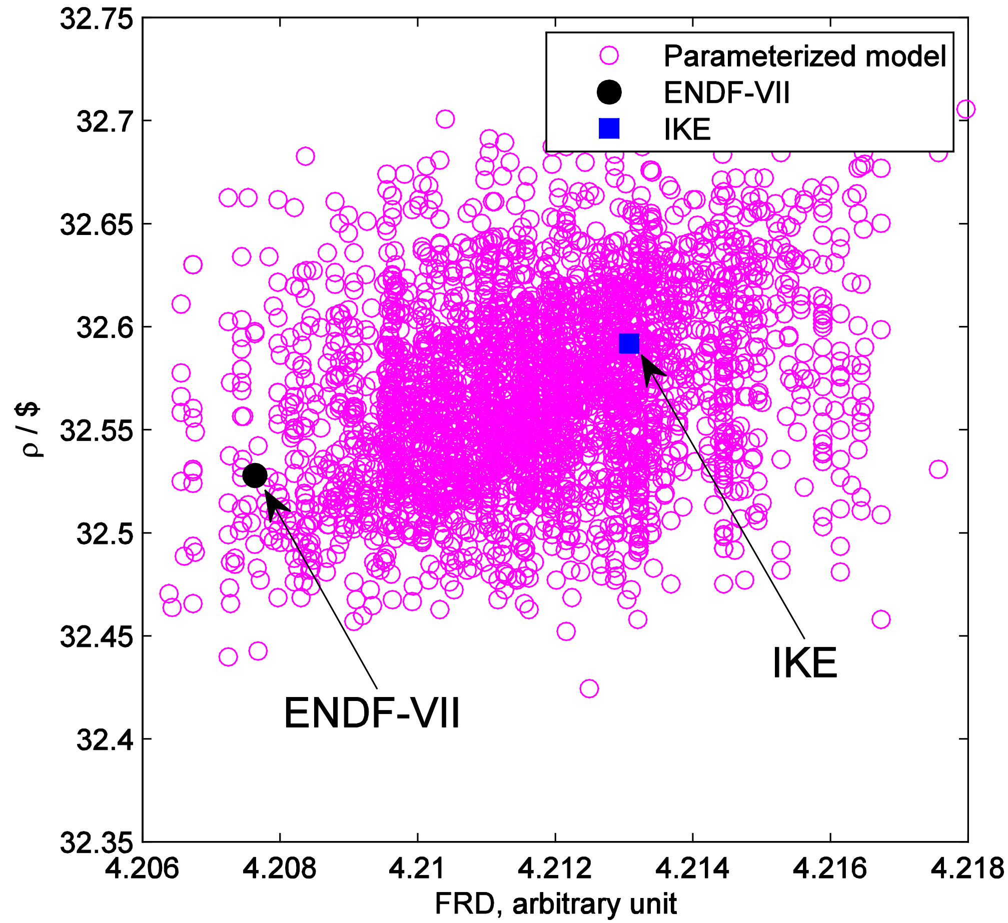
Calibration based on MCNP Simulations

- Geometry in MCNP
  - TRIGA lattice model at TAMU
  - 3000 MCNP simulations
- QOIs
  - ρ: reactivity
  - FRD: fission rate density



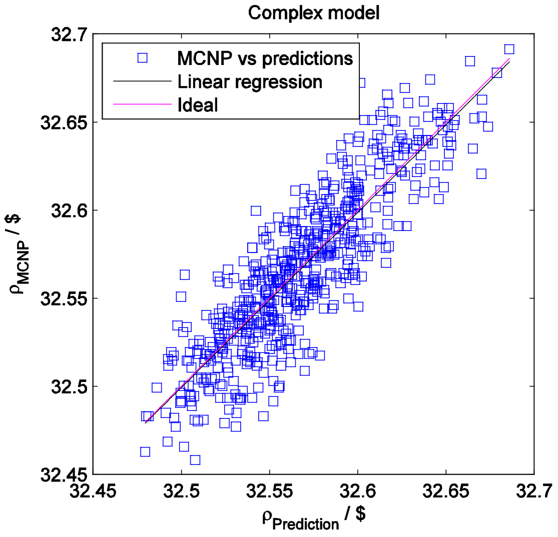
Calibration based on MCNP Simulations

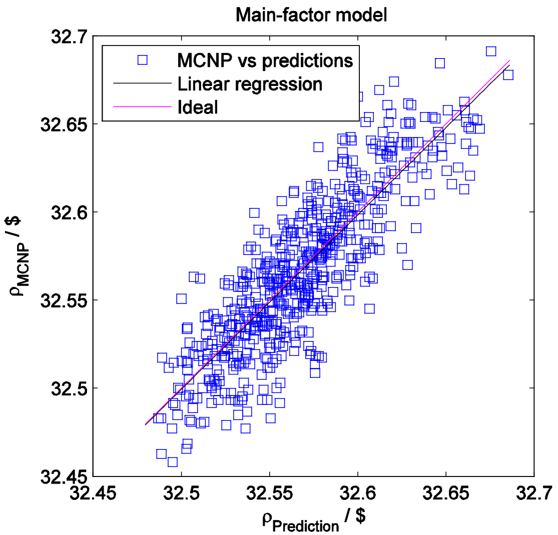
- Scatterplot on reactivity(ρ)-FRD plane
  - Reference results are surrounded by PPS model results
  - Two reference results stay in different parts of the plot



Calibration based on MCNP Simulations

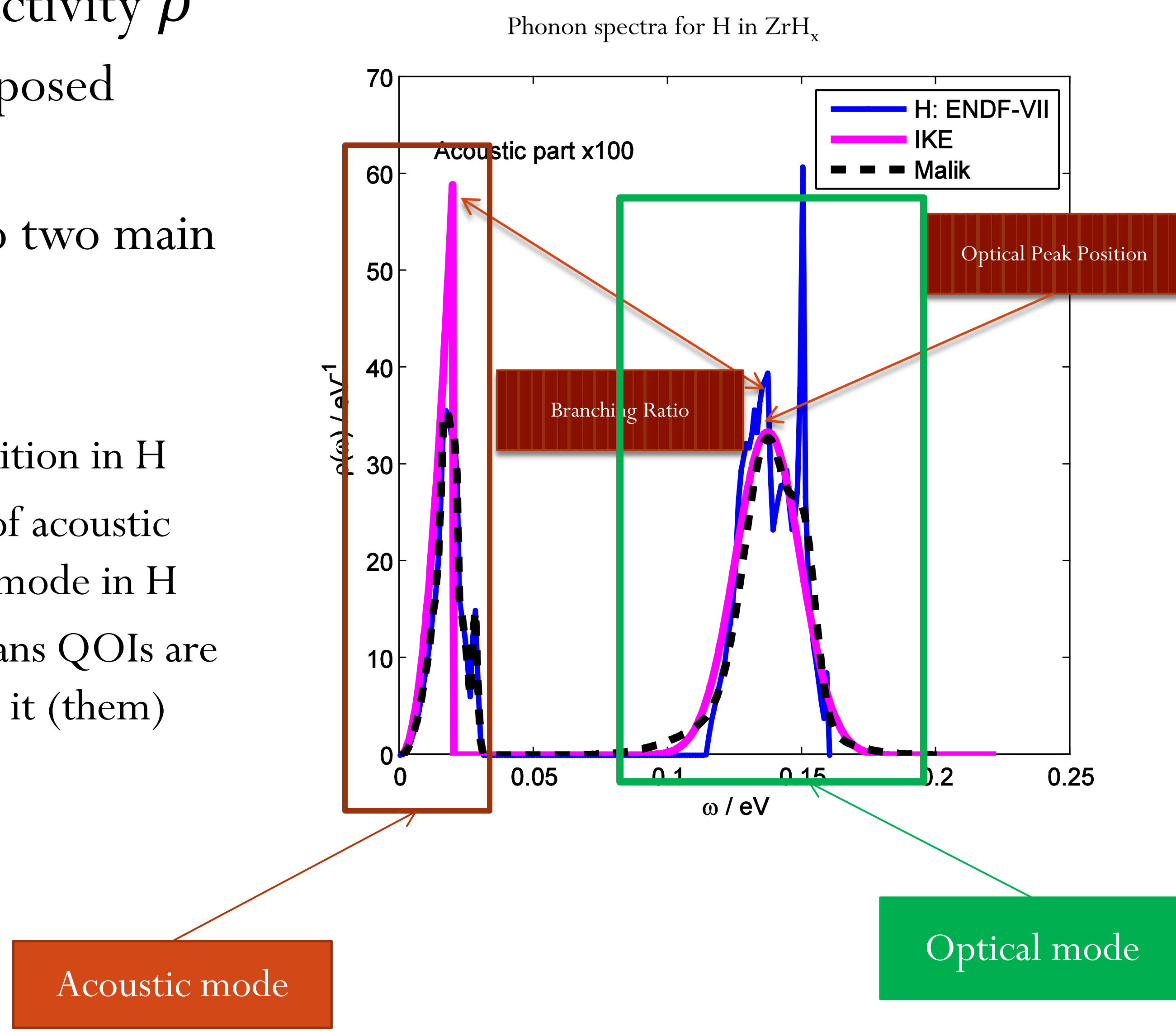
- ANOVA indicated reactivity is sensitive to the parameters
- Cross-validation for reactivity ρ
  - To test the indicated sensitivities
  - 2400 realizations were used to get the regression models based on the parameters
  - Use the regression models to predict outputs for the rest 600 realizations and compare the predictions with the simulations





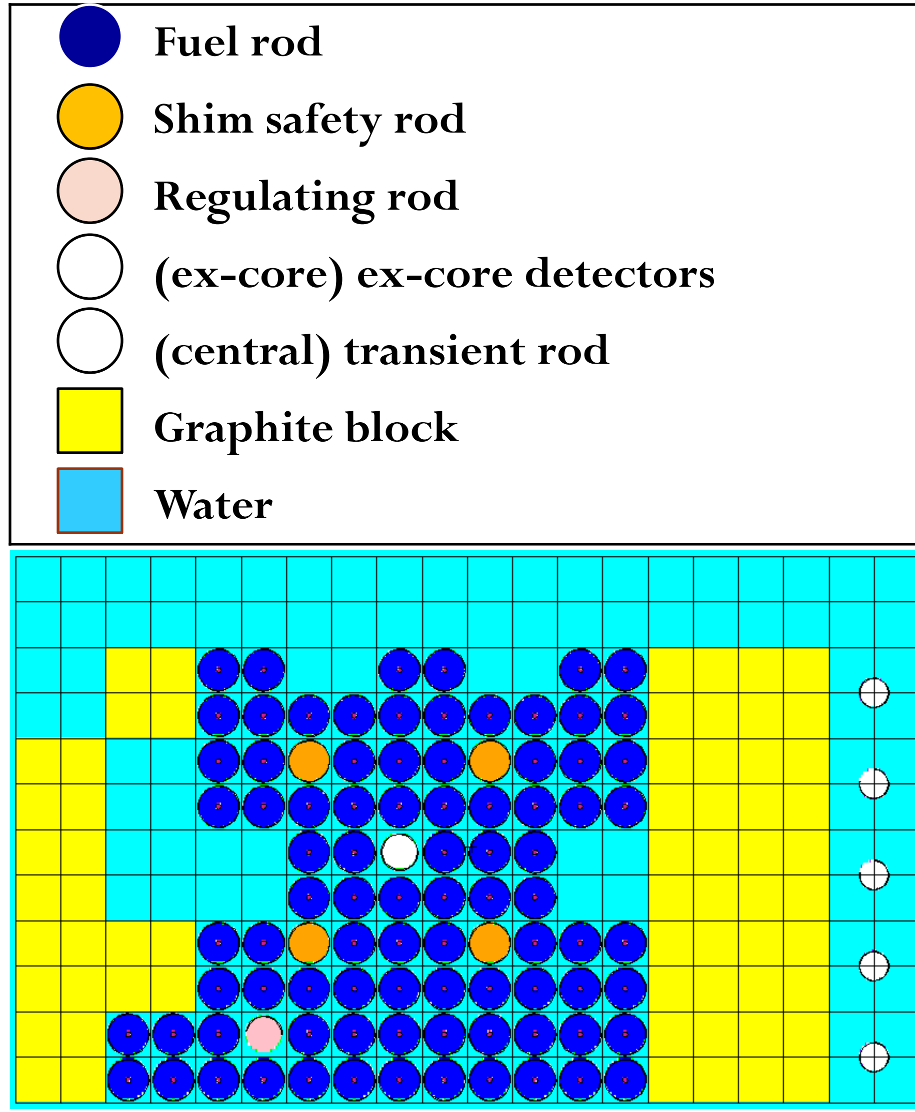
Calibration based on MCNP Simulations

- Sensitivity for reactivity ρ
  - Sensitive to proposed parameters
  - Most sensitive to two main factors
  - Main factors:
    - Optical peak position in H
    - Branching ratio of acoustic mode to optical mode in H
    - By "main", it means QOIs are most sensitive to it (them)



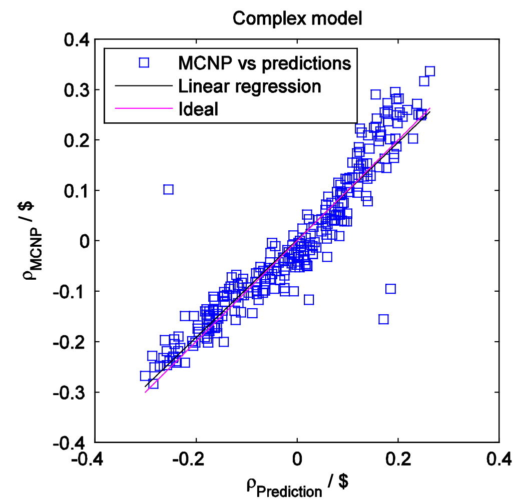
Calibration based on MCNP Simulations

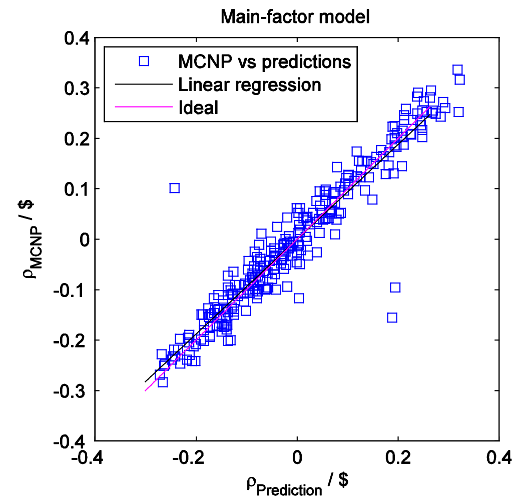
- Geometry in MCNP
  - Simplified full-core TRIGA model at TAMU
  - Configuration: to make TRIGA near critical ($k_{eff}=1.00000 \pm 0.00013$ with ENDF)
- QOIs
  - ρ: reactivity (not the phonon spectrum!)
  - Λ: neutron mean generation time
  - $\alpha_{T_{\text{fuel}}}$: fuel temperature feedback coefficient
  - β_{eff}: effective delayed neutron fraction
  - R_{abs}: ex-core detector absorption rate



Calibration based on MCNP Simulations

- Cross-validation test the significances of the factors indicated by ANOVA
  - 1331 MCNP simulation results in total
    - 1064 for forming regression models
    - 267 for comparing simulations and predictions based on regression models
  - Complex model (right upper): based on all "significant" factors from ANOVA
  - Main-factor model (right lower): based on optical peak position and branching ratio of acoustic mode to optical mode in H
- Reactivity is most sensitive to these two factors





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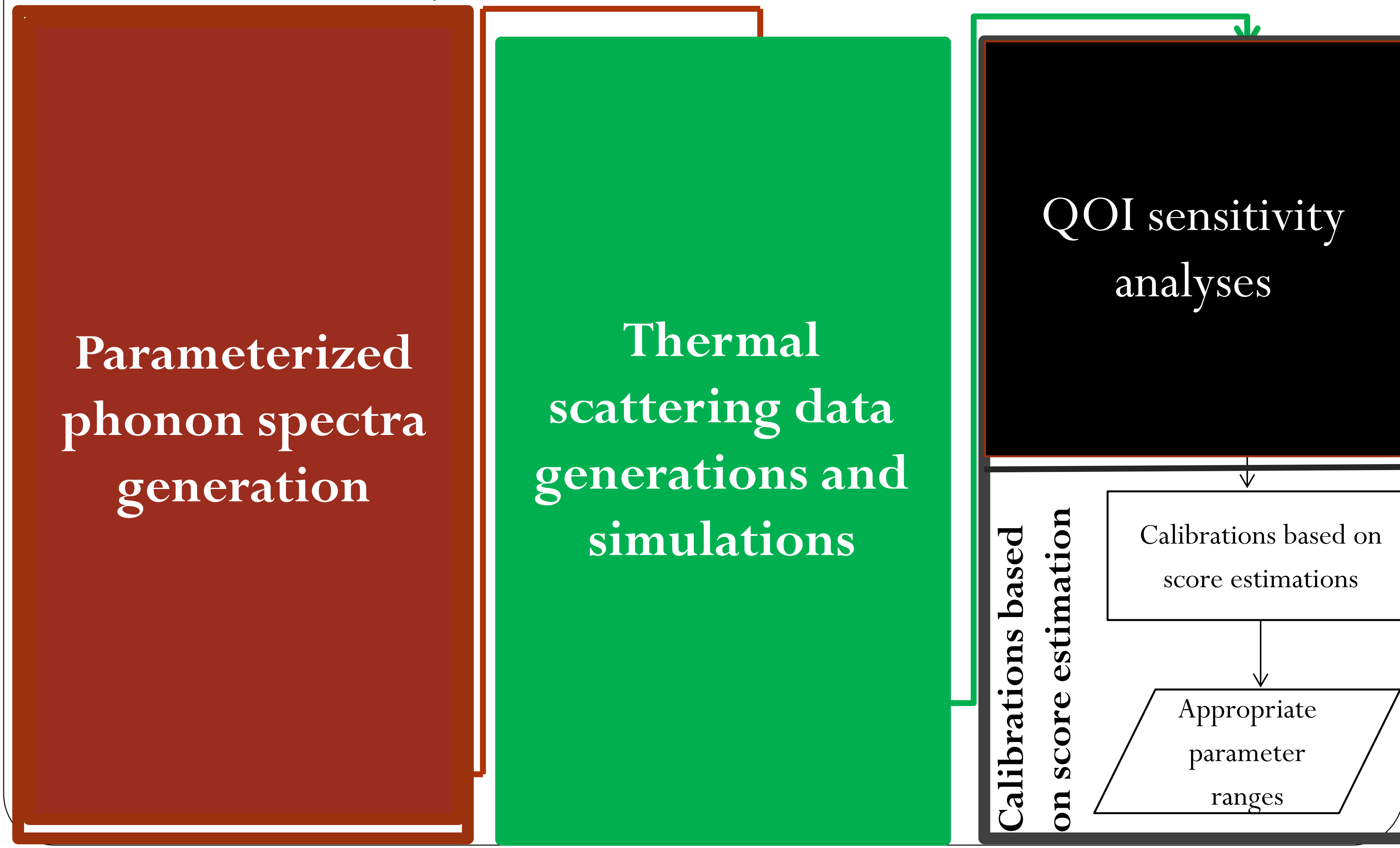
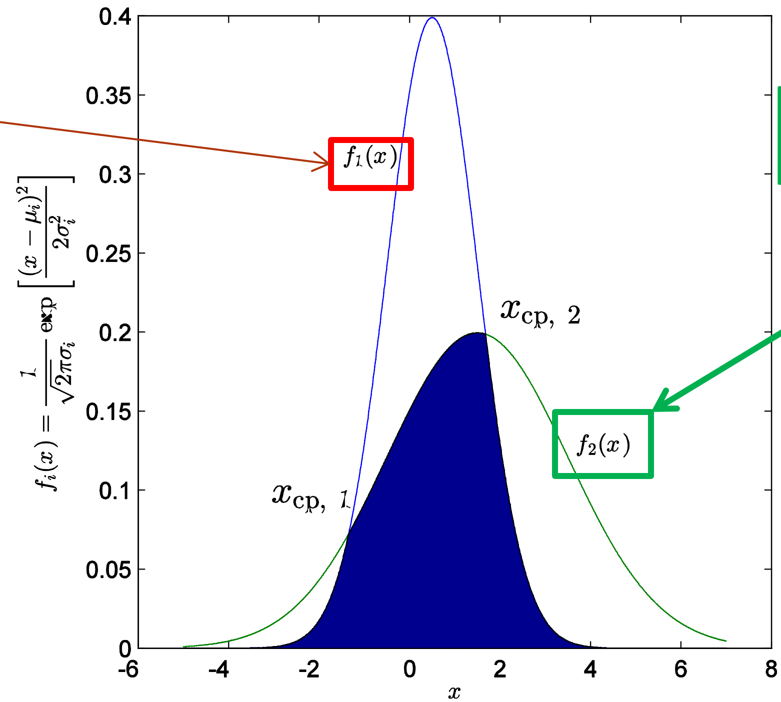
- Calculation and Analysis Procedure



Calibration based on MCNP Simulations

- Calibration
  - MC quantities of interest (QOIs): given in forms of normal distributions
  - Score estimation: overlaps of QOI distributions
    - It measures how close each realization is to the reference QOI

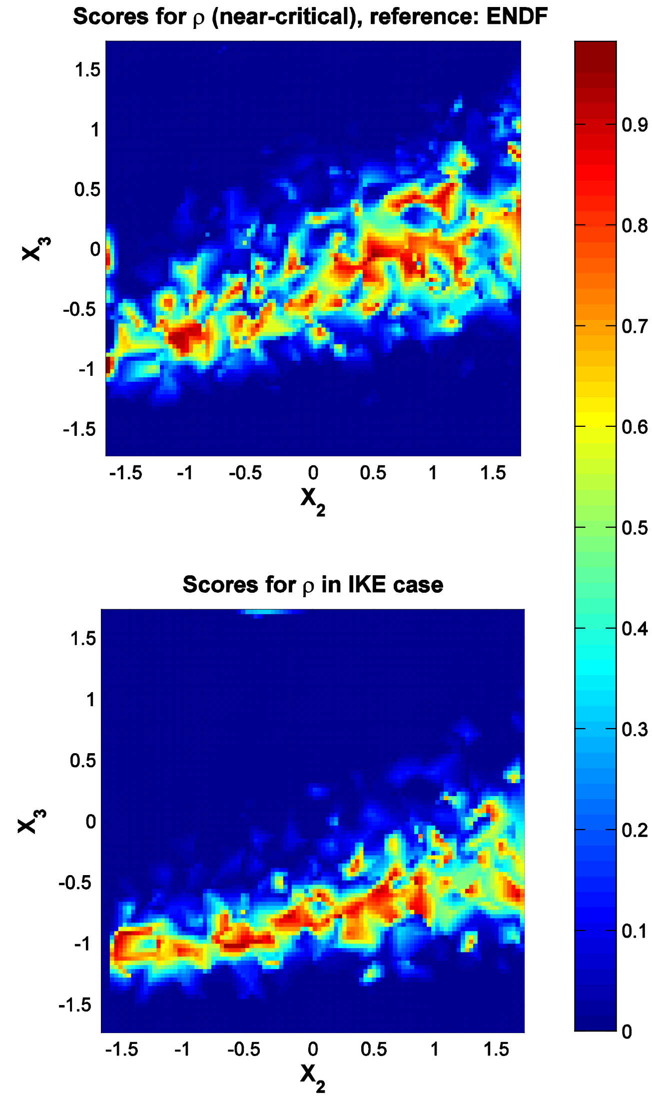
Target distribution for QOI



Particular realization distribution for QOI

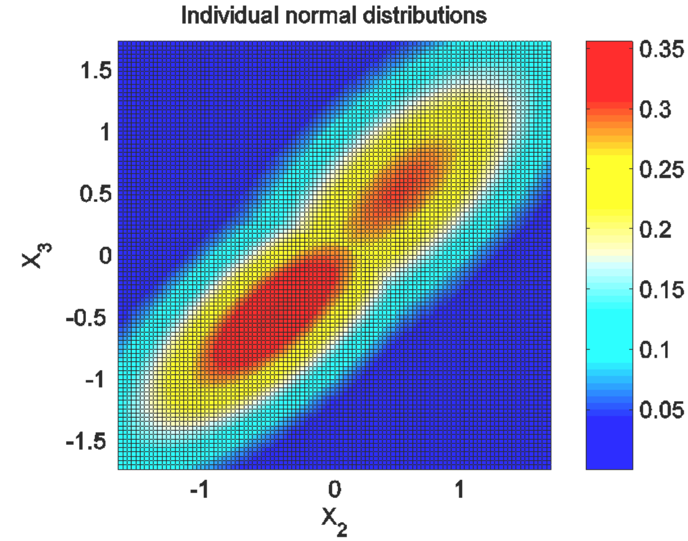
Calibration based on MCNP Simulations

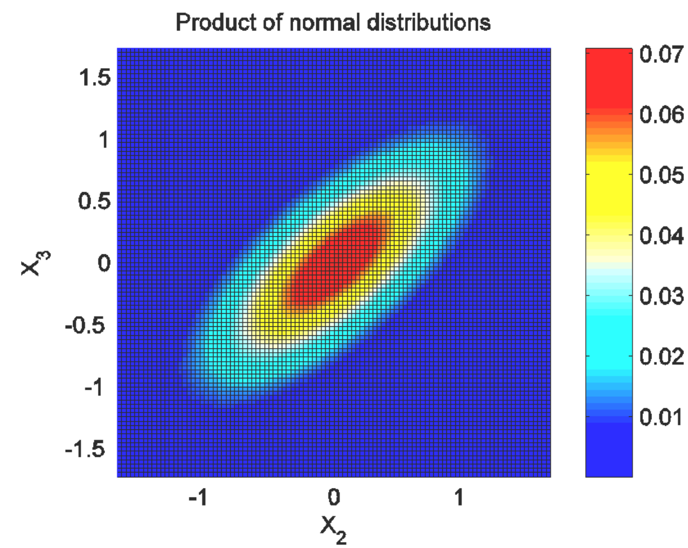
- Score Estimation for Calibration
  - ENDF and IKE scattering data were used as calibration examples
  - X_2: standardized form of branching ratio of acoustic mode to optical mode in H in ZrH_x
  - X_3: standardized form of optical peak position in H in ZrH_x
  - They have different high score regions
- What if we have multiple QOIs sensitive to proposed parameters?



Calibration based on MCNP Simulations

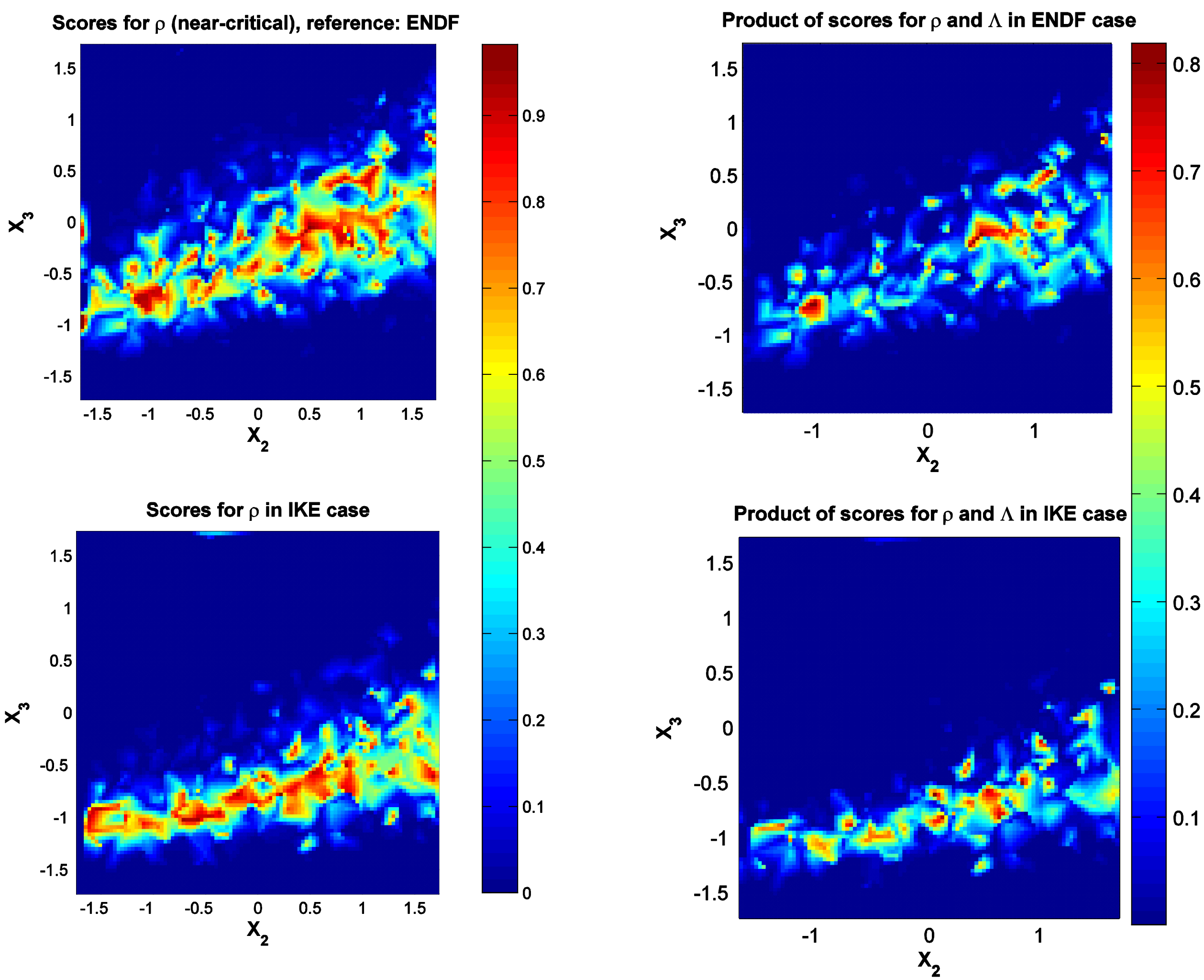
- Score Estimation for Calibration
  - ENDF and IKE scattering data were used as calibration examples
  - They have different high score regions
- What if we have multiple QOIs sensitive to proposed parameters?
  - Multiplications of multiple score distributions
  - Calibrated parameter ranges shrink





Calibration based on MCNP Simulations

- An example of the products



Conclusions and Future Work

- Model tests:
  - It would be reasonable to hypothesize PPS models for ZrH_x phonon spectra
- Methodology:
  - NJOY-MCNP chain is compatible with this UQ study;
  - ANOVA and cross-validations are effective to determine the main-factor affecting QOIs and find the relationship between the parameters and QOIs;
  - Score estimation may be appropriate to take the calibration.
- QOI sensitivities:
  - Several QOIs (e.g. ρ, $\alpha_{T_{\mathrm{fuel}}}$, Λ, etc.) are found to be sensitive to proposed parameters
- Future work:
  - Investigate in-core neutron detectors to further constrain the parameters in the model.
  - Calibrate parameters for TRIGA reactor at TAMU for different temperatures.
  - Tabulate $S(\alpha, \beta, T)$ for TRIGA reactor at TAMU

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- Thank you!