Propagating Nuclear Reaction Uncertainties from Databases to Applications

INT Program: Bayesian Methods in Nuclear Physics

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Many thanks to George Papadimitriou, Perry Chodash, Caleb Mattoon and Joe Wasem

June 29, 2016

LLNL-PRES-696059
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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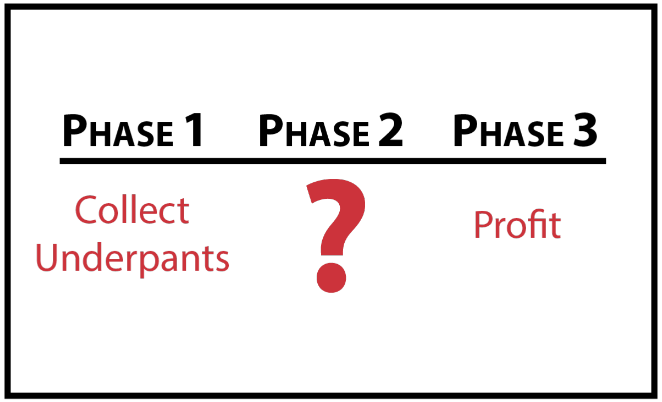
Overview (in three easy steps)

- Step 1 – Brief discussion on several applications where nuclear reactions play a pivotal role (nuclear reactors, asteroid deflection, NIF/Omega diagnostics)
- Step 2 – Discussion of the nuclear databases (good, bad, & ugly) used for applications and how uncertainties are currently handled
- Step 3 – Application results and quoting final state uncertainties



PHASE 1	PHASE 2	PHASE 3
Collect Underpants	?	Profit

How databases handle/propagate uncertainties is an open question and discussion/suggestions would be greatly appreciated

Nuclear reactors in a nutshell

- 14% of the world's electricity is provided by nuclear reactors, and as much as 75% in some countries, such as France
- Efficiency and safety are at the center of any reactor implementation
- This is usually quantified in terms of the neutron multiplication factor, k_{eff}
  - $k_{eff} < 1$, subcritical
  - $k_{eff} = 1$, critical (where reactors like to be)
  - $k_{eff} > 1$, supercritical (fission rate grows exponentially/dangerously)
- k_{eff} calculated via neutron transport codes which use nuclear reaction databases
  - Here we explore Monte Carlo transport (Mercury), which has its own set of uncertainties

Annular Core Research Reactor
(Sandia National Laboratories)

(Courtesy of Perry Chodash)

k_{eff} is most dependent on nuclear reaction cross-sections and uncertainty quantification is of upmost importance for this quantity

Asteroid deflection and nuclear option

- 10,505 known asteroids within 900k km of Earth , 1445 within 35k km. Of this 10,505, 867 have diameter > 1km

Green: Deflect without nuke

Blue: Disrupt with nuke

Orange: Essentially screwed

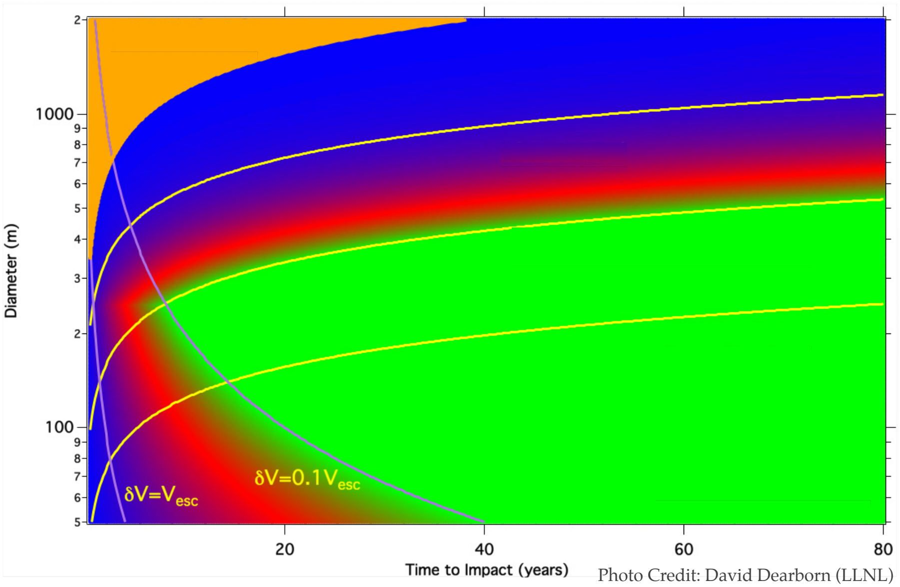


Photo Credit: David Dearborn (LLNL)

- Feb 2013: Chelyabinsk impact
  - Size: 20 m
  - 1500 injuries

- Neutron transport and energy deposition play pivotal role for nuclear option, as neutrons can deposit large amounts of energy deeper in asteroid, leaving the largest impact

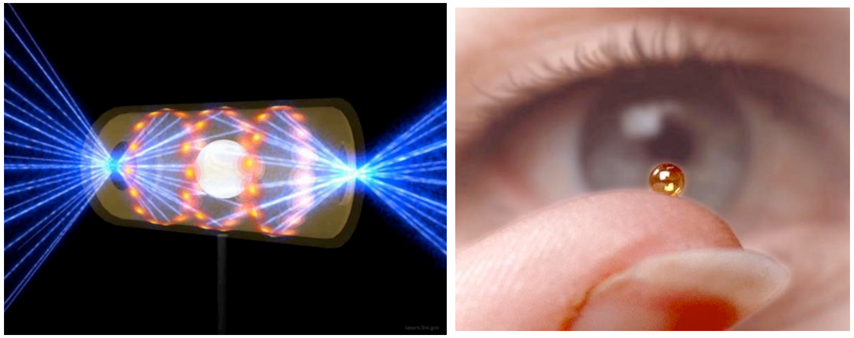
- Current estimates do not take nuclear uncertainties into account (i.e. the plot of scenarios to the left likely has appreciable uncertainty)

Uncertainty in nuclear reactions can lead to uncertainty in final results which could change political strategies for various threats.

Diagnostics for laser experiments (NIF, Omega, …)

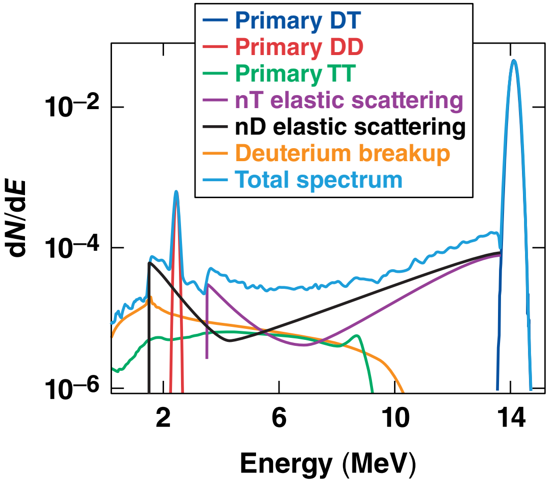
- For inertial confinement fusion (ICF) experiments, neutrons and gamma rays from nuclear reactions provide most prompt diagnostics (window into what is going on)

(Photos from LLNL)

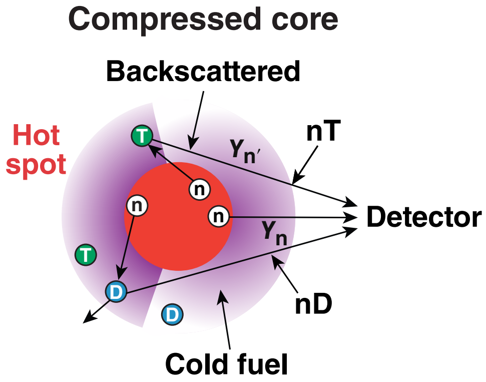


Neutrons → Yield, Asymmetries, Temp.

Gammas → Reactions, turbulence/mix



(Figures from C. Forrest 2015 DPP presentation)



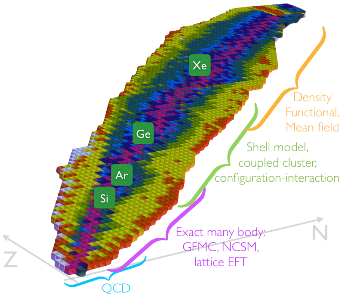
- Neutron-deuteron interactions are largest source of uncertainty, in particular deuteron breakup: D(n,2n)p
- Large final state discrepancies found among nuclear data/evaluations
- Experimentalists at LLE in Rochester have started performing nuclear cross-section measurements on Omega to further explore issues

See 2015 DPP talk and Ph.D thesis of Chad Forrest for more info

Proper uncertainty of deuteron reactions required to accurately diagnose NIF implosions

Data flow, input data, and databases

Computational Theory



(From Will Detmold presentation)

Experiment

(FRIB)

Continuous Energy Evaluations

R-matrix

Optical Models

Hauser-Feshbach

Databases

ENDF

ENDL

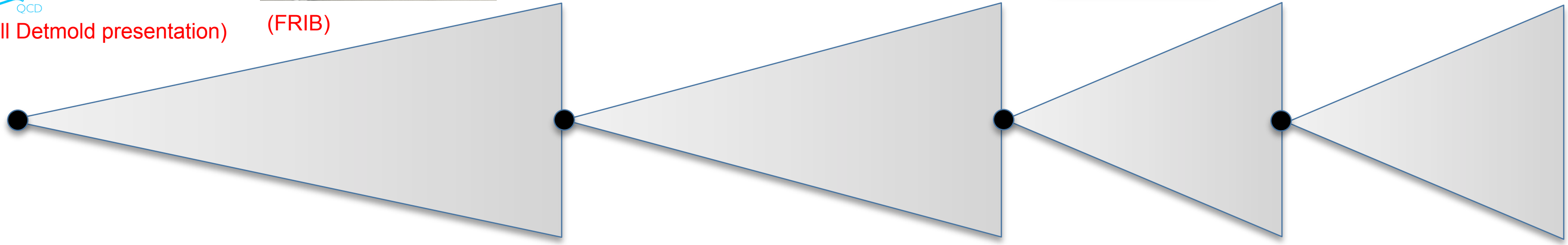
…

Applications

Reactors

NIF

…

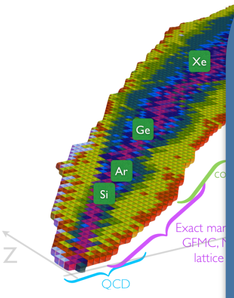


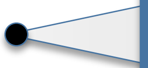
- Basic data flow: data expands (distributions, correlations, etc.) in each field and then is consolidated at "node" before being handed off to next field as input
- Experiment in consolidated into database (EXFOR) for evaluators (would be nice to have similar database for computational theory calculations of nuclear reactions and/or have more evaluators use such data)
- Evaluations are consolidated into nuclear databases (ENDF, ENDL, etc.)

Key question of talk: what minimized set of information is needed at each node to accurately quantify uncertainty at each stage of the calculation?

Data flow, input data, and databases

Computational Th





BEWARE:

Bugs and Errors can creep in at every processing stage of calculation!!

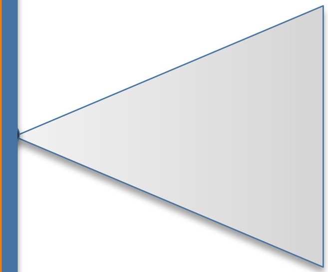
As convenient as databases are, care needs to be taken and one should perform sanity checks often!!

Applications

Reactors

NIF

…

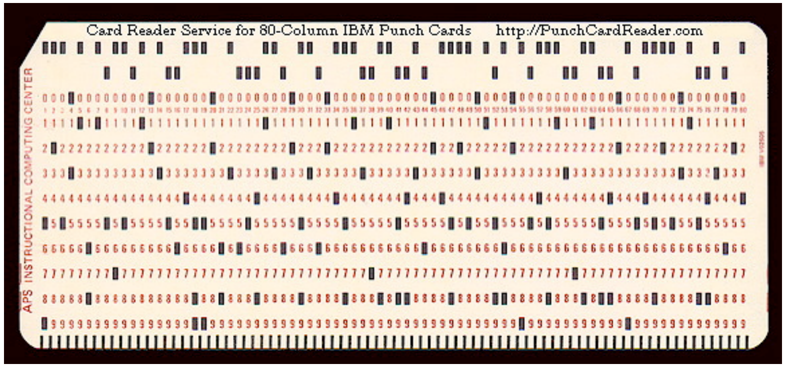


- Basic data flo … ode” before being handed off to
- Experiment in … e for computational theory calculatio
- Evaluations are consolidated into nuclear databases (ENDF, ENDL, etc.)

Key question of talk: what minimized set of information is needed at each node to accurately quantify uncertainty at each stage of the calculation?

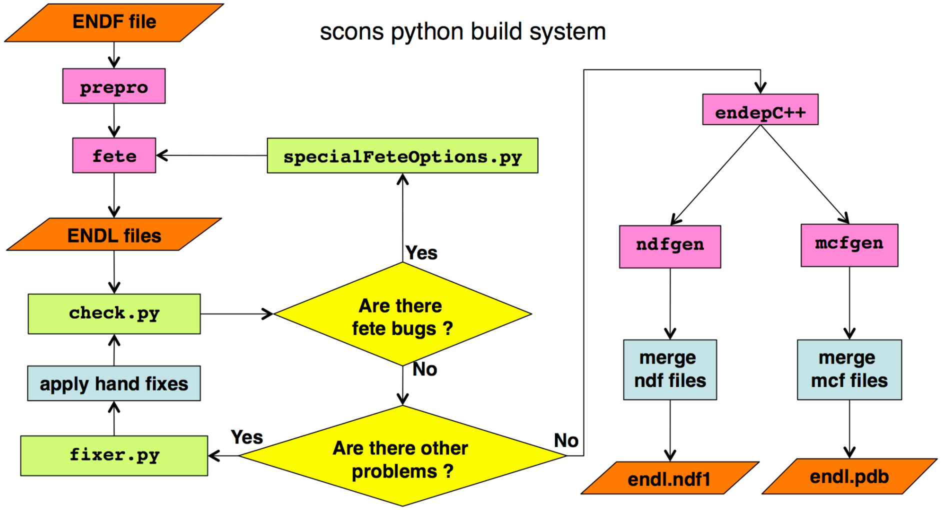
The ENDL present and GND future

- At LLNL we use ENDL format (1959), which was designed for compactness in order to fit on 70-byte punch cards



- Compactness leads to physics limitations
  - Only point-wise data
  - Only stores two-body c.o.m. frame angular data
  - Stores limited gamma data for 2+ step reactions

(From ENDL2011 documentation)


scons python build system

ENDF file

`prepro`

`fete`

`specialFeteOptions.py`

ENDL files

`check.py`

Are there fete bugs ?

Yes

No

apply hand fixes

`fixer.py`

Are there other problems ?

Yes

No

`endepC++`

`ndfgen`

`mcfgen`

merge ndf files

merge mcf files

endl.ndf1

endl.pdb

- Processing complicated and poorly documented, thus bugs abound
  - Example:
    - Many evaluations do not conserve energy
    - Needed kludge is implemented to fix this, but fix introduced a bug that led to massive errors in outgoing gammas

- ENDL not unique in this regard; ENDF and other databases/processing codes have just as many if not worse processing bugs

Uncertainties can come from bugs/errors, but these too need to be accounted for in the end

The ENDL present and GND future

- At LLN
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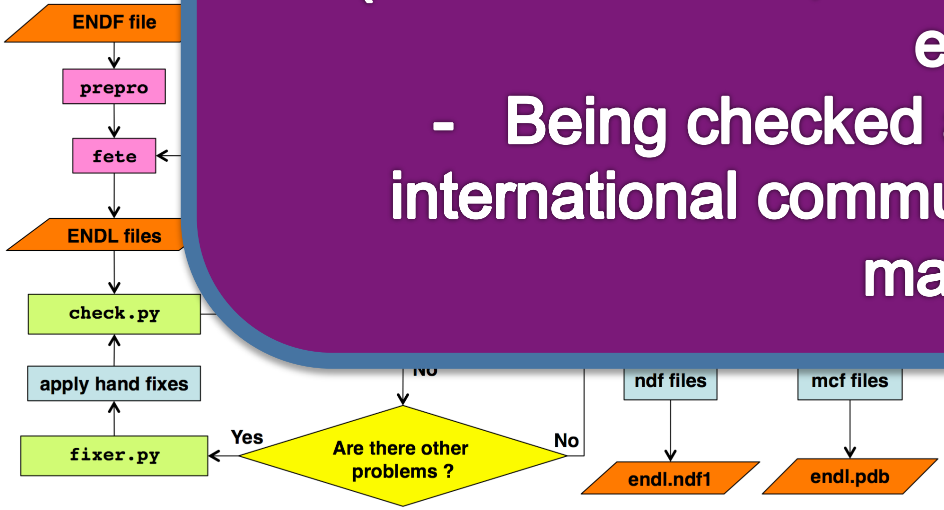
GND aims to fix many of these database issues:

- Will include far more comprehensive physics (direct reactions, double diff. cross-sections, etc.)
- Being checked and developed by international community (10+ years in the making)



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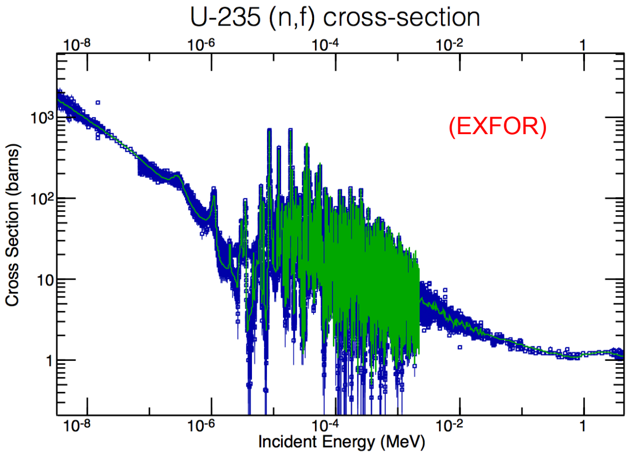
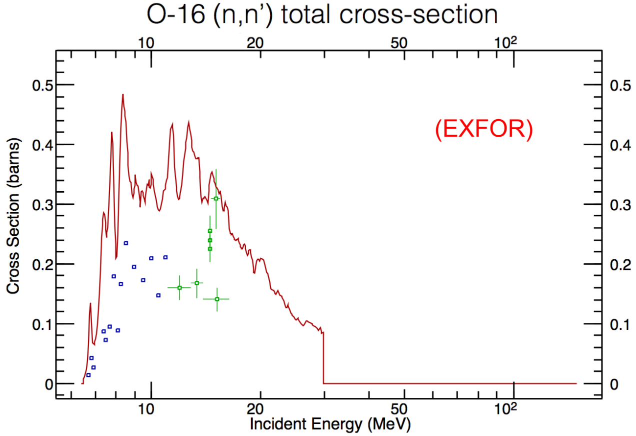
Uncertainties can come from bugs/errors, but these too need to be accounted for in the end

Not all data should be treated the same



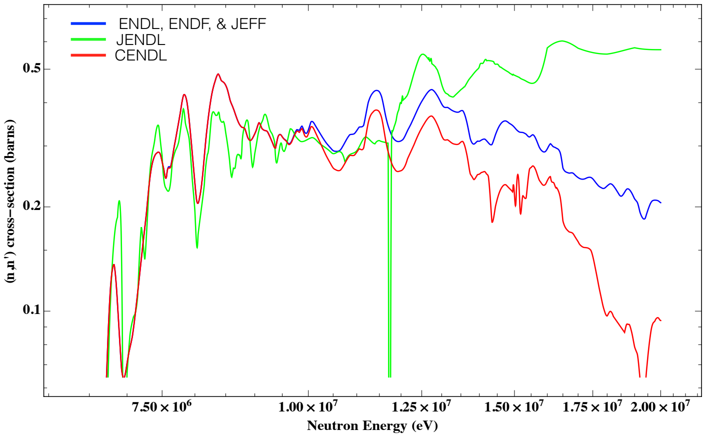


- Some channels have large amounts of data, such as ^{235}U(n,f), which gives evaluators high confidence in evaluations (at the few percent level)

- Most channels have little or no data, such as ^{16}O(n,n'). In this particular case, evaluation derived indirectly from combination of R-Matrix/H-F fits of ^{16}O(n,tot), ^{16}O(n,elas), and ^{12}C(α,n). Huge, uncontrolled uncertainty.

- Different evaluation in Japan (JENDL) and China (CENDL) differ greatly from US (ENDF) and Europe (JEFF)

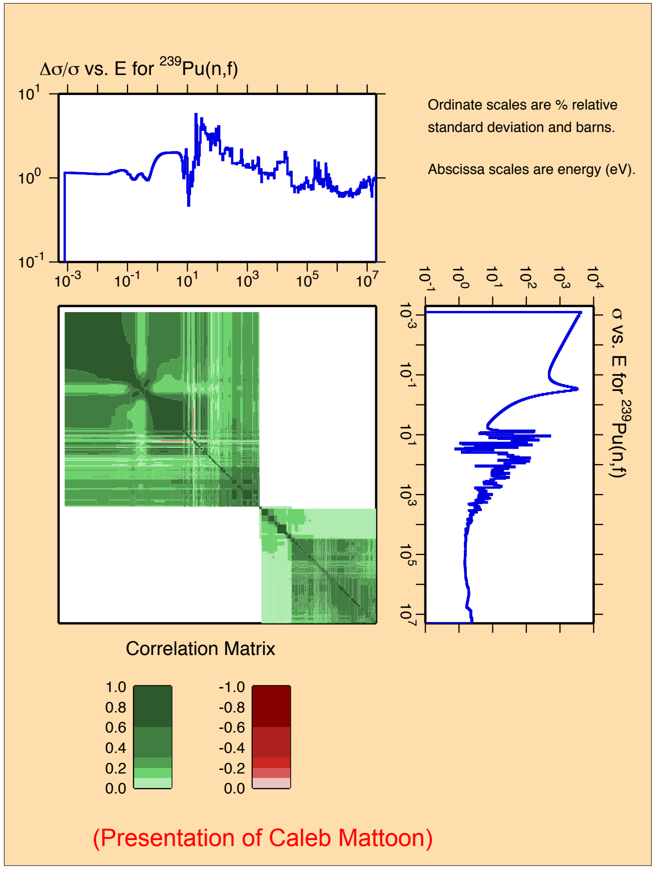
O-16 (n,n') cross-section different databases



Without uncertainties, nuclear database treats these as equally valid evaluations

Database covariance matrices and variations

- With many of the point-wise evaluations in each channel [(n,elas), (n,n'), (n,2n), (n,f)], the databases store a covariance matrix
- Processing code (kiwi) take this covariance, sample from a Gaussian distribution on each principle vector, and then rotate back to determine a new variation/realization of the data (i.e. a new database with correlated Gaussian variations)
- Current ENDL data format does not have cross-channel/isotope covariances (GND will allow for this) and currently can only do Gaussian variations (no specification of distributions is given)



Ordinate scales are % relative standard deviation and barns.

Abscissa scales are energy (eV).

(Presentation of Caleb Mattoon)

Channels with covariance matrices allow us to make new database with correlated Gaussian variation of those channels

Database covariance matrices and variations

Technical description of what code does:

- From the covariance matrix M get eigenvalues λ and eigenvectors Λ (where i^{th} column of Λ is the vector corresponding to λ_i)
- Variation vector R:

$$R_i = \sum_j \eta_j \Lambda_{j,i} \qquad \eta_j = \sqrt{\lambda_j} V_j$$

Realization
Type = vector

Eigenvector
Type = vector

Weight
Type = number

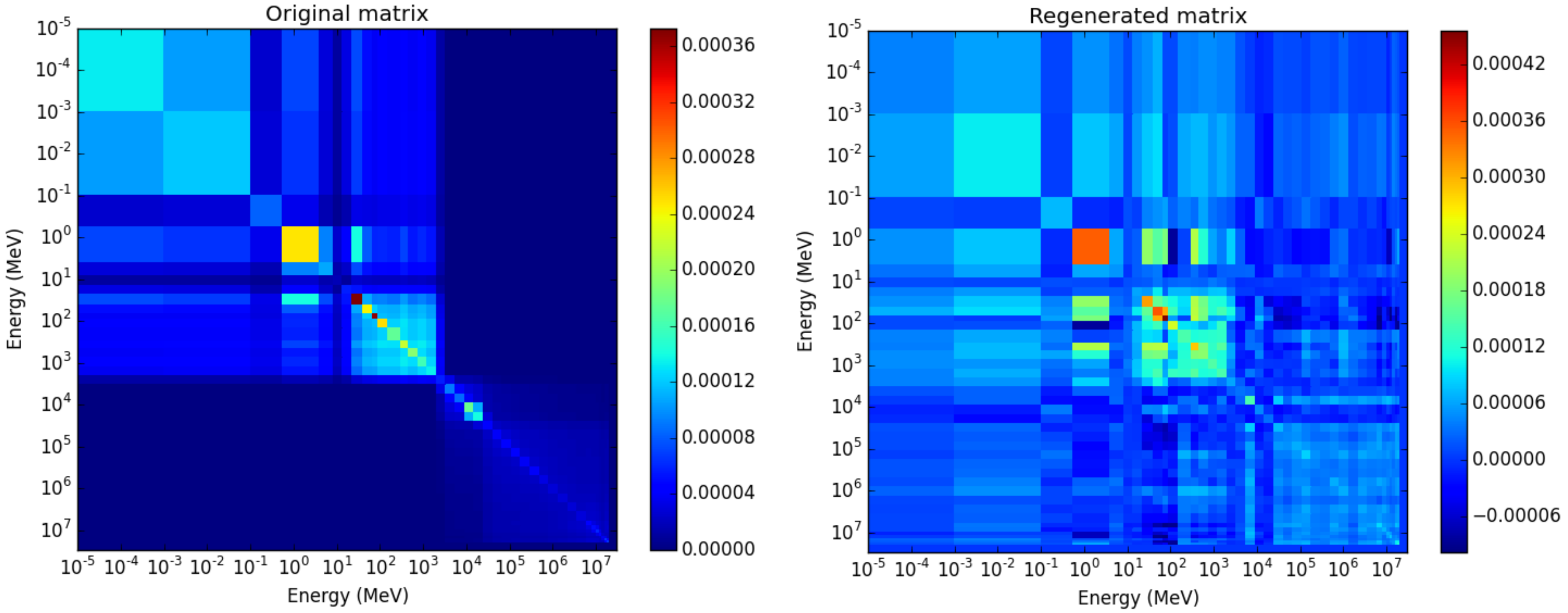
Eigenvalue
Type = number

Random (Gaussian-distributed)
Type = number

(Thanks to Caleb Mattoon for spelling this out for me)

Covariance of many realizations (variations) R-vectors reproduces covariance matrix M

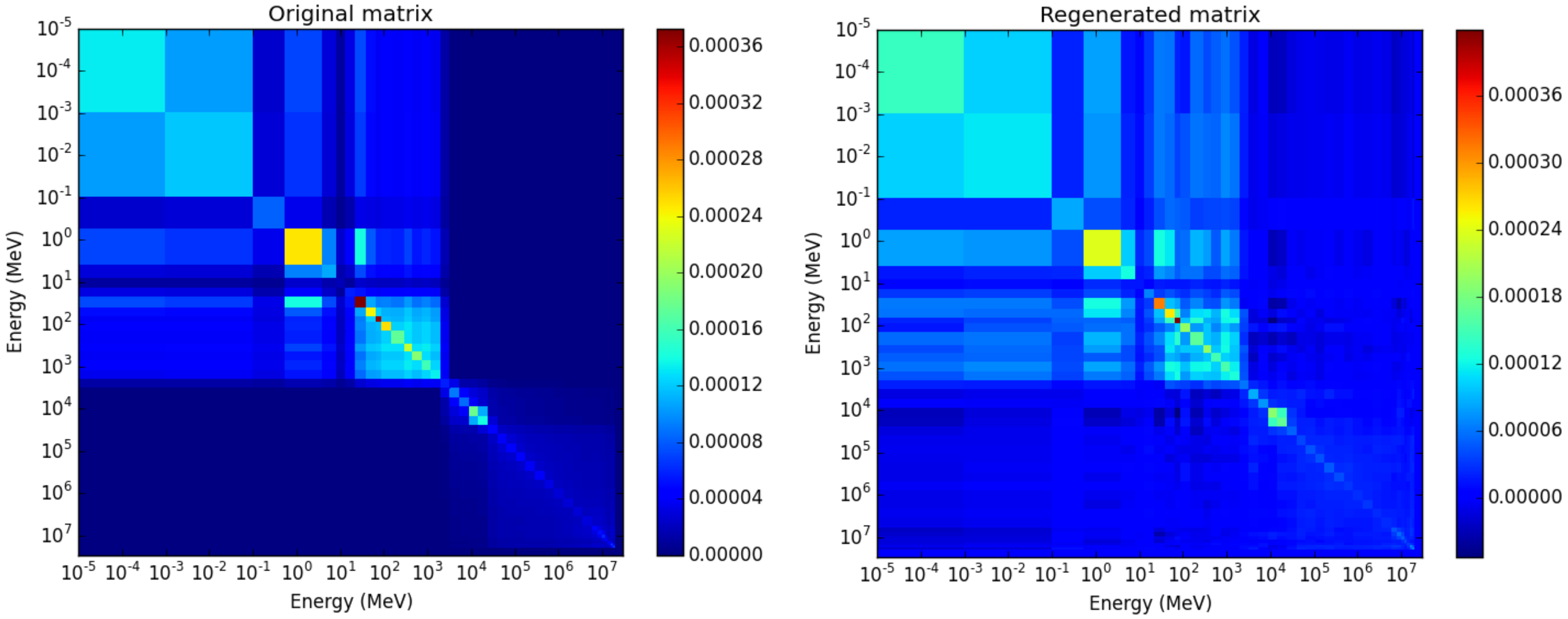
Covariance example for ^{239}Pu(n,f)



after 10 realization iterations

(Slide from Caleb Mattoon)

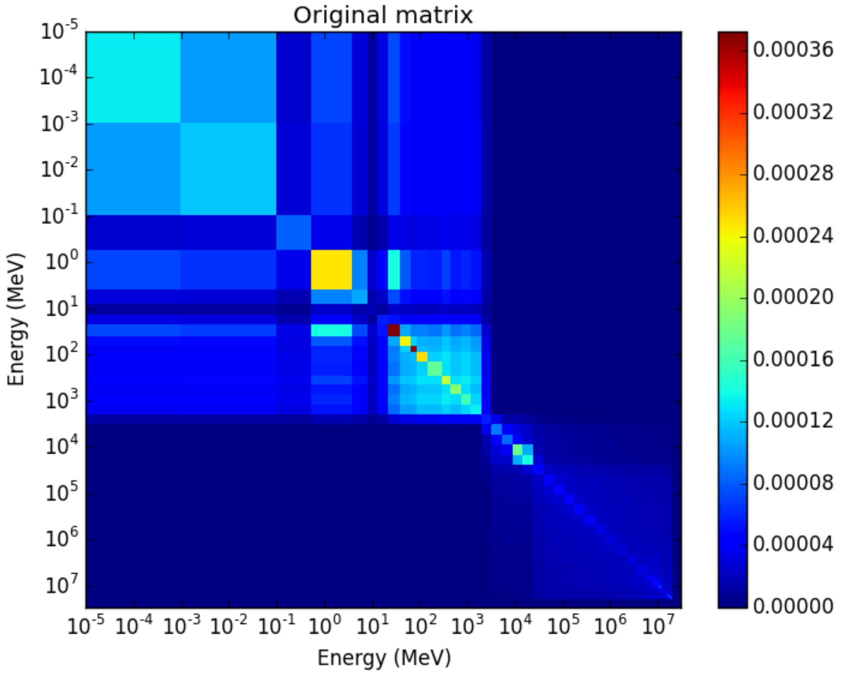
Covariance example for ^{239}Pu(n,f)



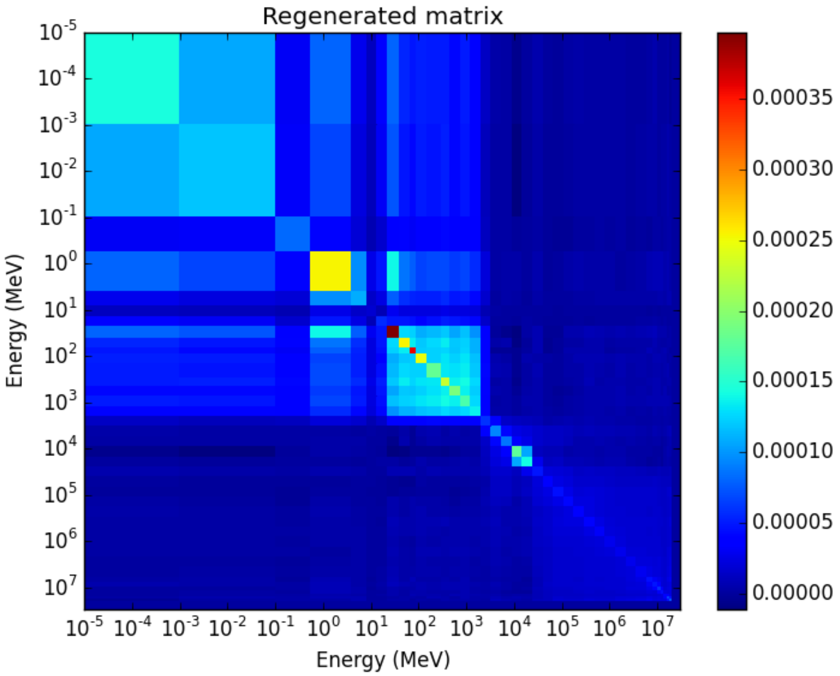
after 100 realization iterations

(Slide from Caleb Mattoon)

Covariance example for ^{239}Pu(n,f)



Original matrix

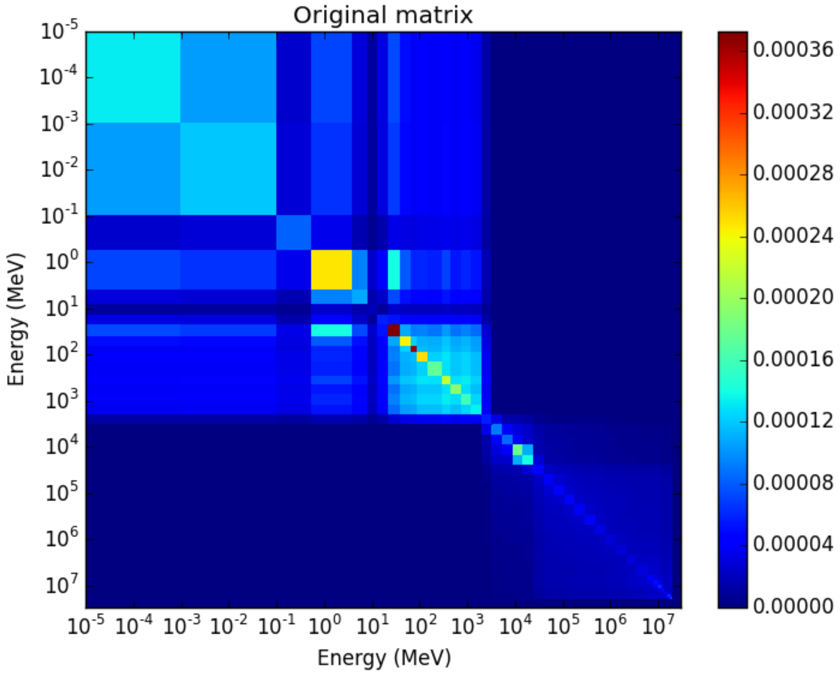


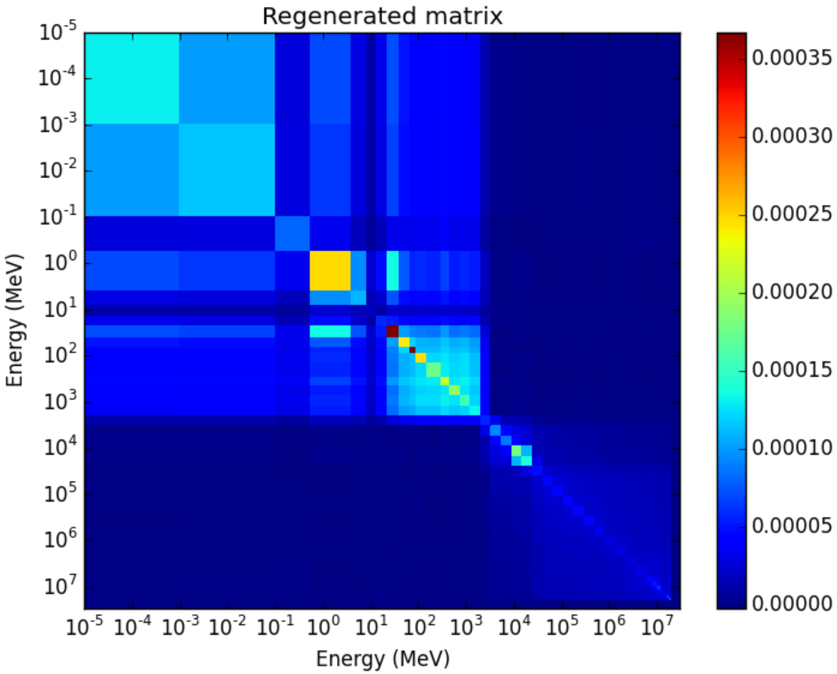
Regenerated matrix

after 1000 realization iterations

(Slide from Caleb Mattoon)

Covariance example for ^{239}Pu(n,f)





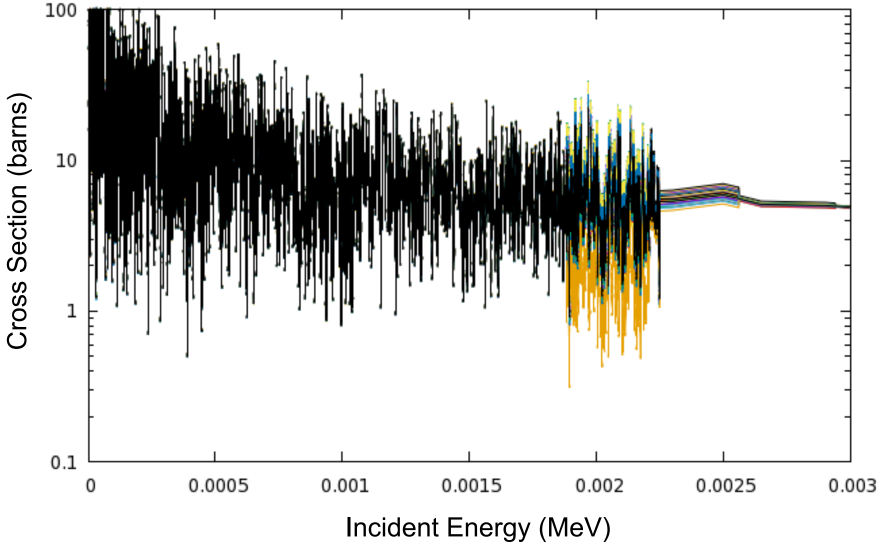
after 10K realization iterations

(Slide from Caleb Mattoon)

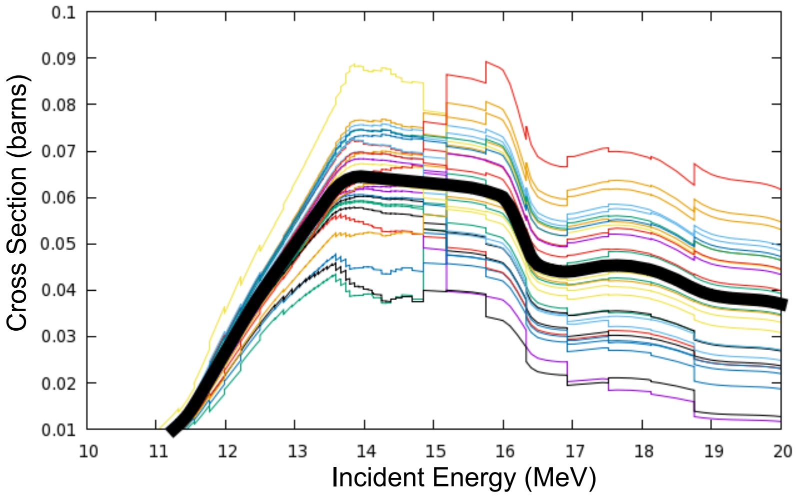
Gaussian variation examples

- Dark line is original evaluation and colored lines are 30 variations
- As expected, ^{235}U (n,f) does not vary much (< 1%) in low energy regime

^{235}U (n,f)



^{16}O (n,n')

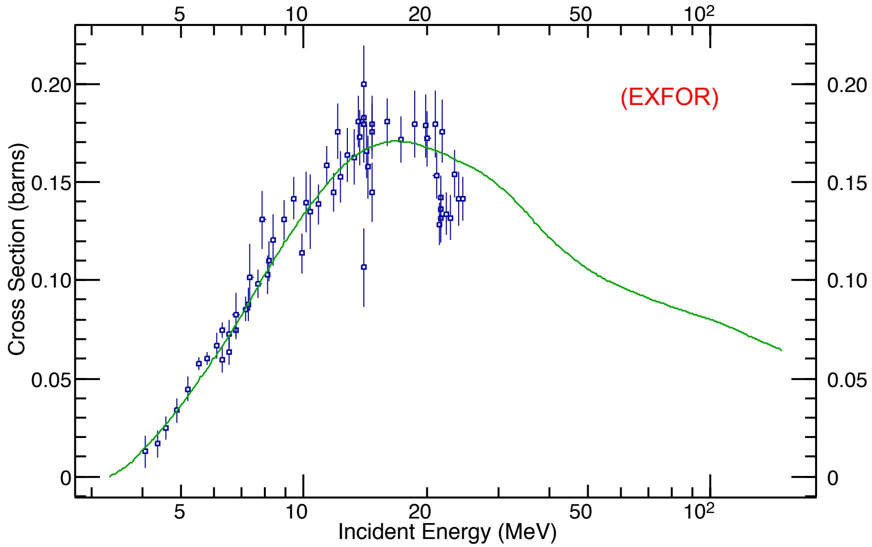


- Variations much more significant for high energies of ^{16}O (n,n'), not dissimilar from spread of different evaluations

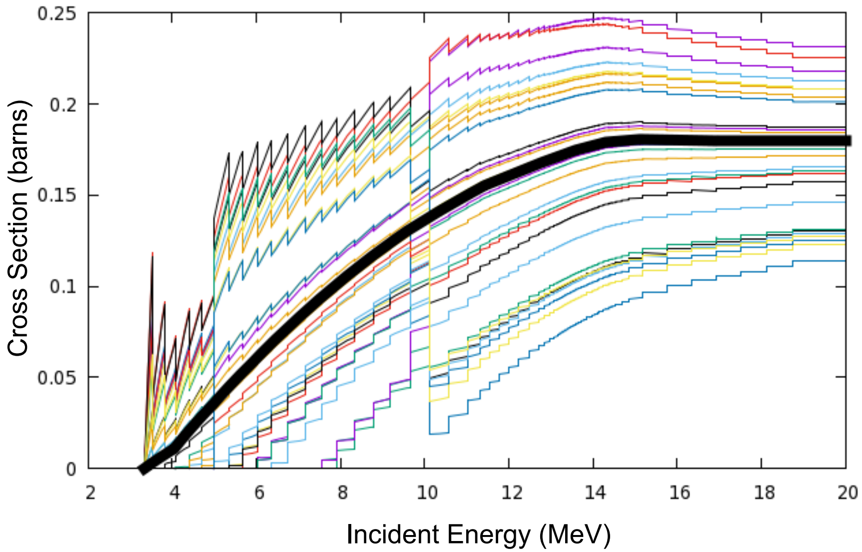
For many channels and isotopes, variations largely reflect (known) uncertainties in evaluations and rarely underestimate uncertainties

Some covariance matrices give “excessive” uncertainty

D (n,2n) – Exp & Eval



D (n,2n) – Variations & Eval



- Not uncommon to overestimate uncertainties
- In the case of D (n,2n), there is ample experimental data and a “reasonable” evaluation, but covariance in database suggests factors of 5 uncertainty across energy range
- Evaluation still not ideal (N-body phase space model as opposed to Fadeev methods or pionless EFT), and puzzles still remain in final state neutron energy distributions (large uncertainty source I do not cover here)

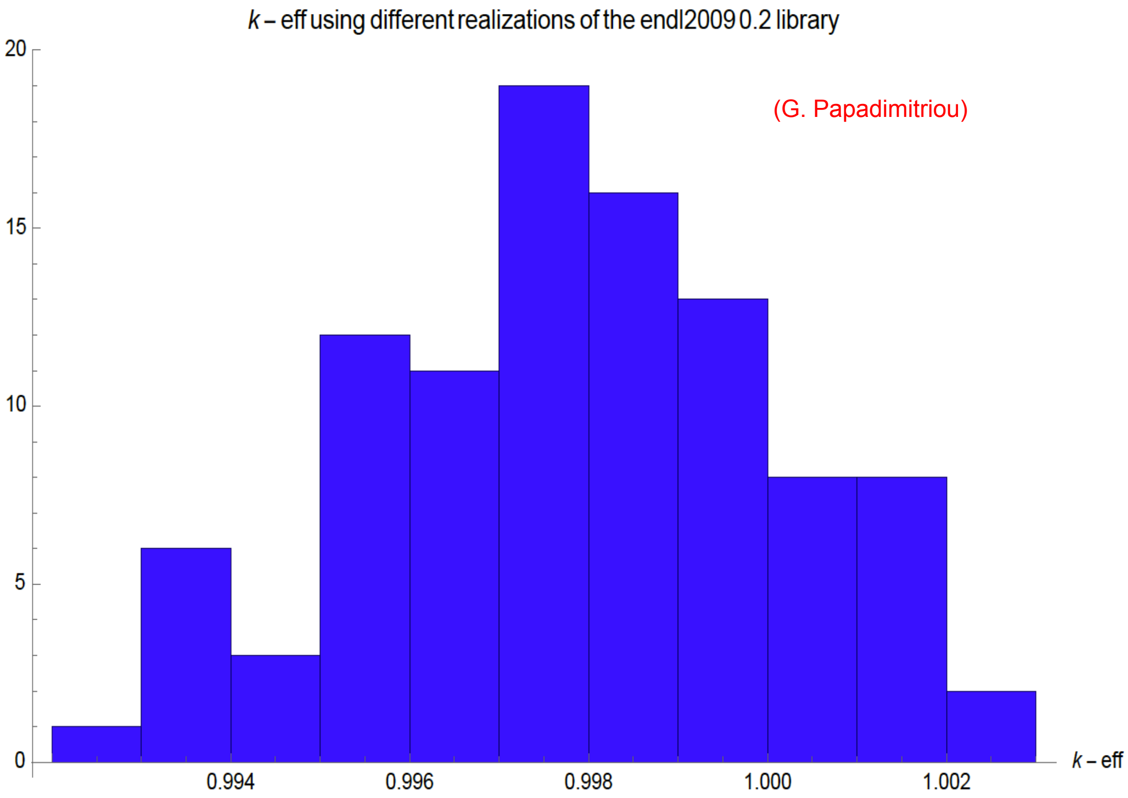
Being “overly-conservative” in uncertainty estimation can be equally detrimental

Reactor example: k_{eff} for different data variations

Based on initial code by Perry Chodash

Work by George Papadimitriou

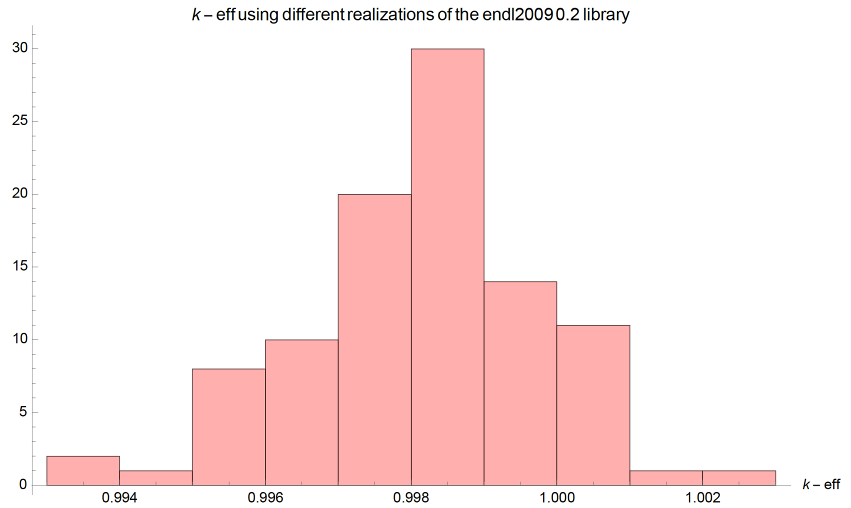
- 100 k_{eff} calculations of ACRR reactor using Monte Carlo Transport and 100 variations of nuclear database
- Varied all isotopes in reactor; channels (n,n'), (n,2n), (n,f), (n,p), (n,d),(n,t),(n,γ)
- Example of a reactor setup where $\langle k_{eff} \rangle$ is subcritical, but nuclear uncertainties allow for supercritical possibilities
- While differences look small to non-experts, reactor experts do not consider this spread "small"



Nuclear reaction uncertainties can play a significant role in k_{eff} and accurate representation of result distribution also important

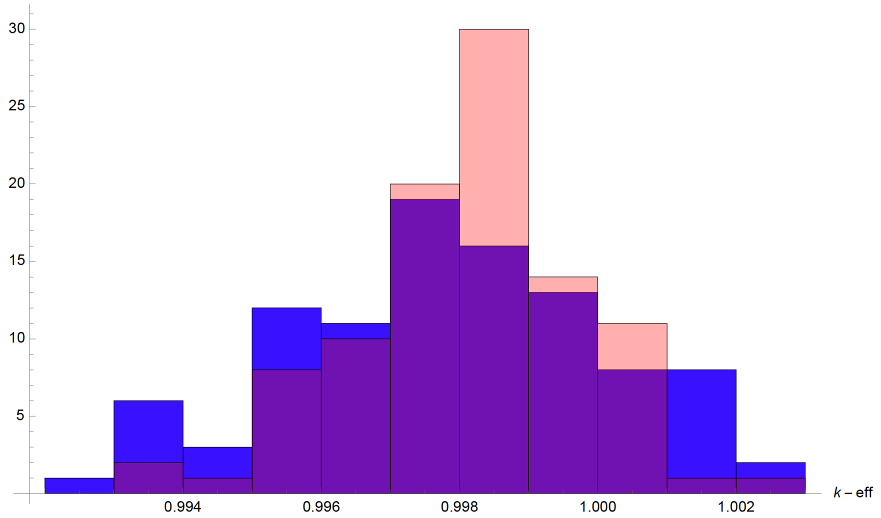
Reactor example: k_{eff} for different data only varying ^{9}Be(n,2n)

- Can single out individual channels for variations
- ^{9}Be(n,2n) ^{8}Be has large cross-section for low energy neutrons (reactor has 35% enriched UO_2-BeO fuel)



(G. Papadimitriou)

Only the ^{9}Be (n,2n) cross-section was varied.



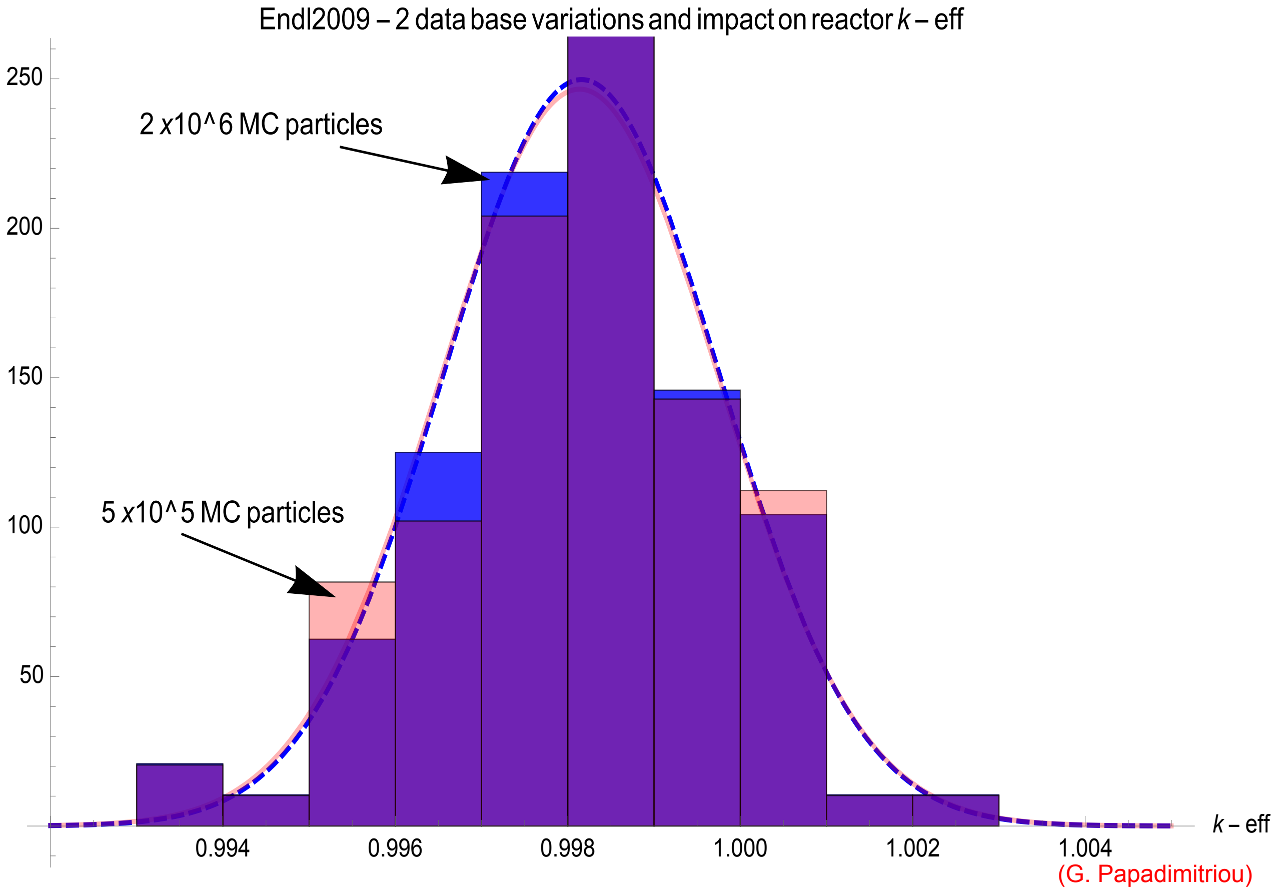
Only the ^{9}Be (n,2n) variations vs. all variations.

(G. Papadimitriou)

While spread is larger when all isotopes are varied, it is clear ^{9}Be(n,2n) uncertainty important (i.e. would need to improve evaluation/data on uncertainty to reduce reactor uncertainty)

Reactor example: Separate sources of uncertainty

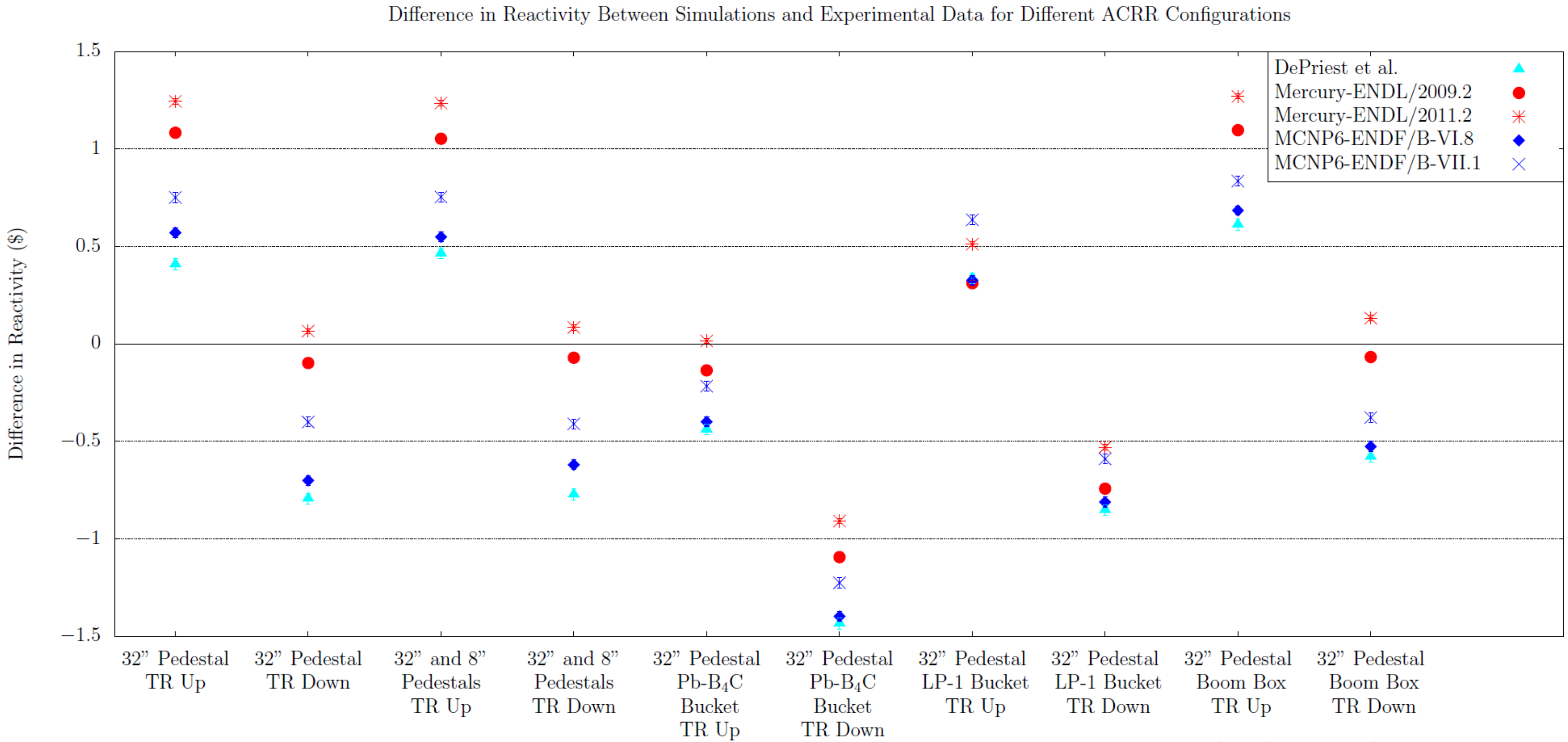
- Two sources of statistical uncertainty: nuclear evaluation uncertainty and Monte Carlo (MC) transport uncertainty
- In principle, MC transport uncertainty scales with square root of the number of sample particles
- Only way to separate the two uncertainties is to increase MC samples and see how distribution changes



(G. Papadimitriou)

Since width does not change with MC samples, spread due almost entirely to nuclear data uncertainty (would need improve reaction experiment or reaction theory)

Reactor example: k_{eff} comparing different databases & processing codes



(Slide from Perry Chodash's presentation)

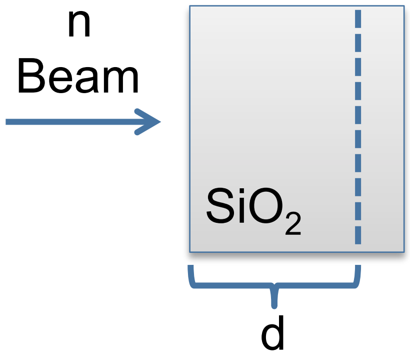
Many issues remain, when comparing different databases/transport codes (red vs. blue) and the comparison with experiment.

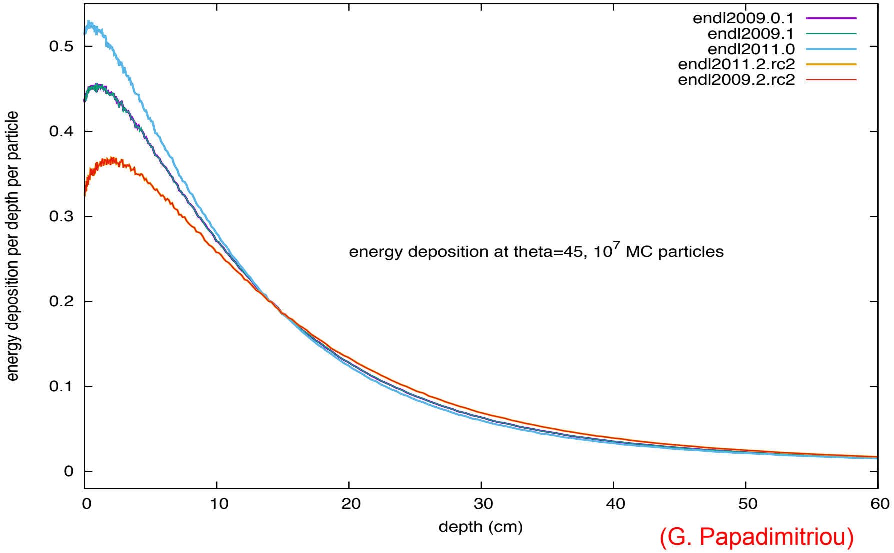
Asteroid deflection example: Energy deposition on SiO$_2$

Based on initial code by Rob Managan

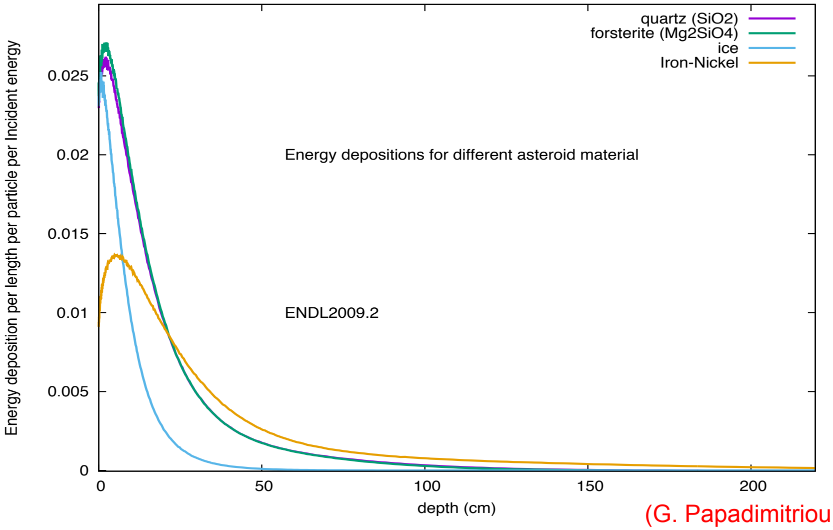
Work by George Papadimitriou

- Attempt to figure out the energy deposition of a neutron beam at a fixed energy as a function of depth in the target asteroid material (we will focus on SiO$_2$).
- Large gamma energy upon neutron capture, (n,γ), allows for deep energy deposition, but (n,p) and (n,α) interactions reduce energy deposited as it takes energy to pry particles from bound state





(G. Papadimitriou)

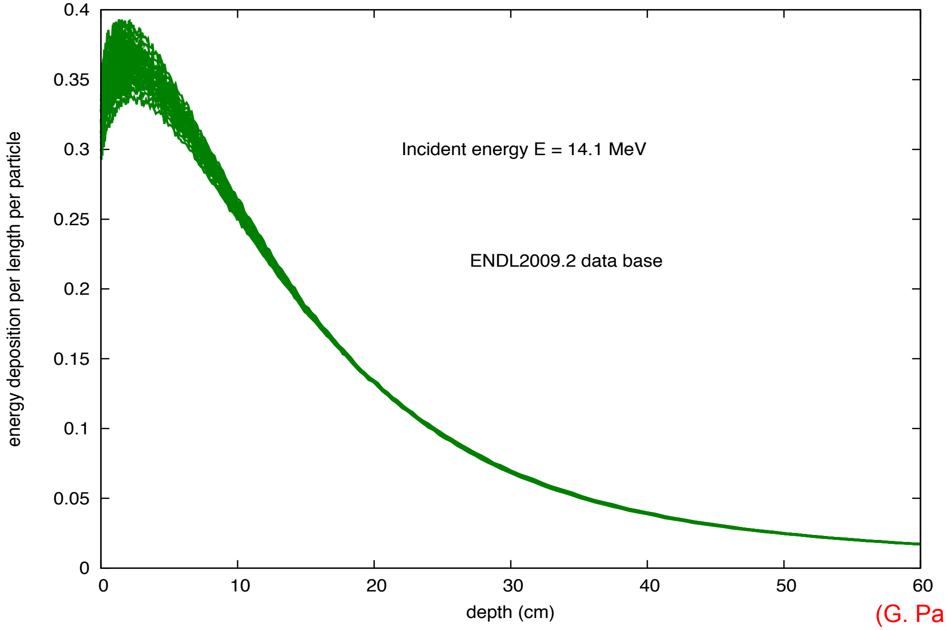


(G. Papadimitriou)

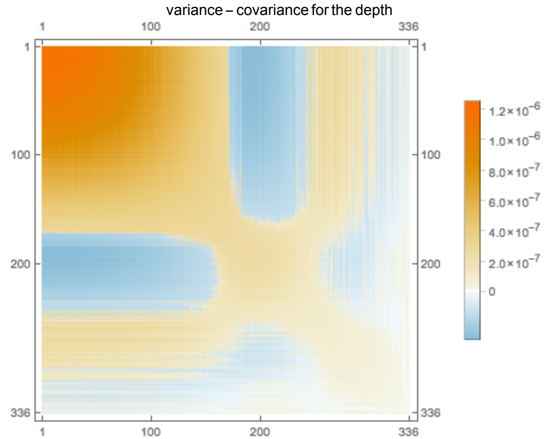
Neutron can deposit energies up to a few meters deep.
Calculations also allow for detailed checks of database/processing codes.

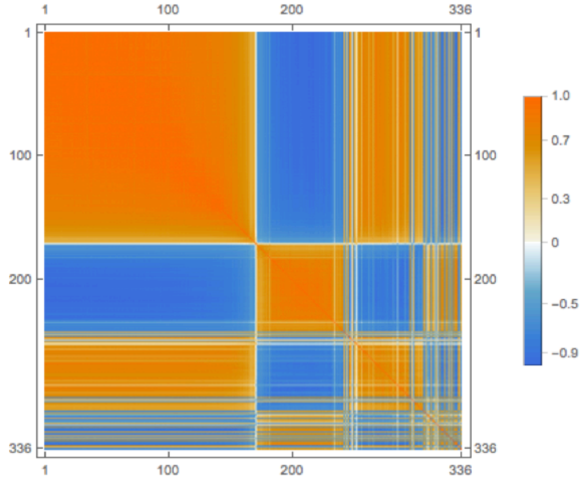
Asteroid deflection example: Energy deposition on SiO_2 with data variations and final covariance

- Ran multiple energy deposition calculations with 100 variations on ^{28}Si and ^{16}O reactions
- Calculate covariance matrix, which can be used in next stage of asteroid calculations



(G. Papadimitriou)



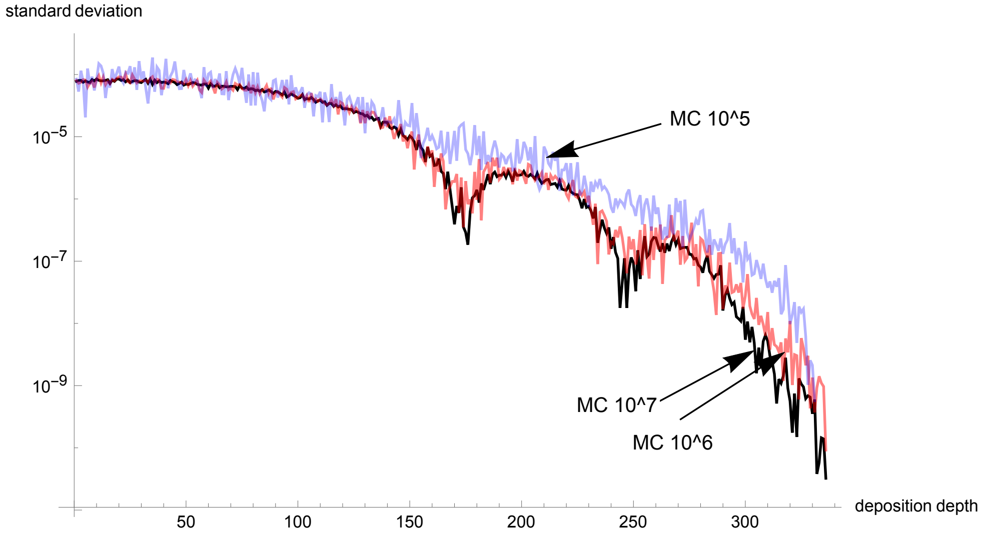


(G. Papadimitriou)

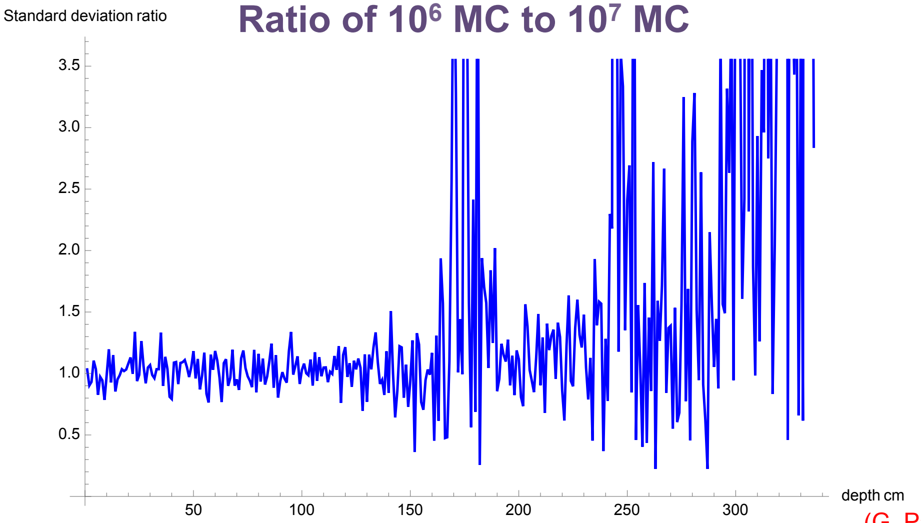
Final covariance and correlation matrices show regions of high correlation

Asteroid deflection example: Separating out different sources of uncertainty

- Plots show variance of diagonal elements of covariant matrix for different sample Monte Carlo particles and the ratio of two of the curves



(G. Papadimitriou)


Ratio of 10^6 MC to 10^7 MC

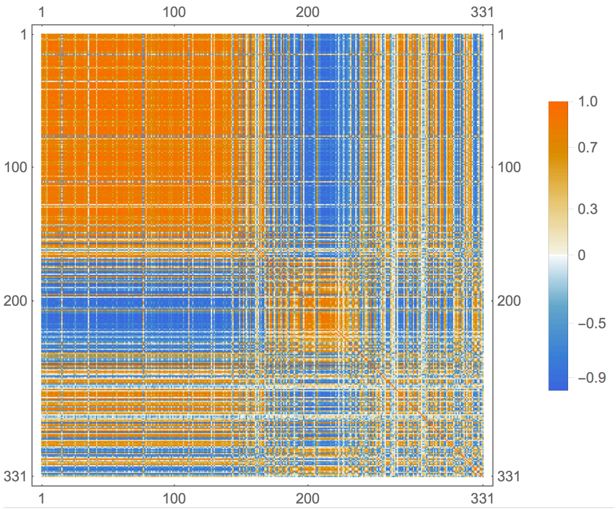
(G. Papadimitriou)

- Different energies have different uncertainty sources
- In left plot, if the variance ratio is around 1, uncertainty is due to nuclear data. If larger than 1 (on the order of 3), uncertainty can be adressed with more Monte Carlo transport samples (i.e. more computer time)

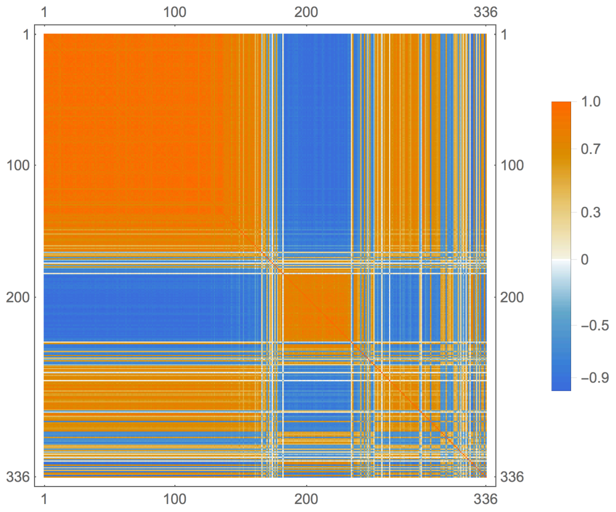
Most regions are limited by nuclear reaction uncertainties, but several regions could improve with more Monte Carlo transport samples

Asteroid deflection example: Separating out different sources of uncertainty

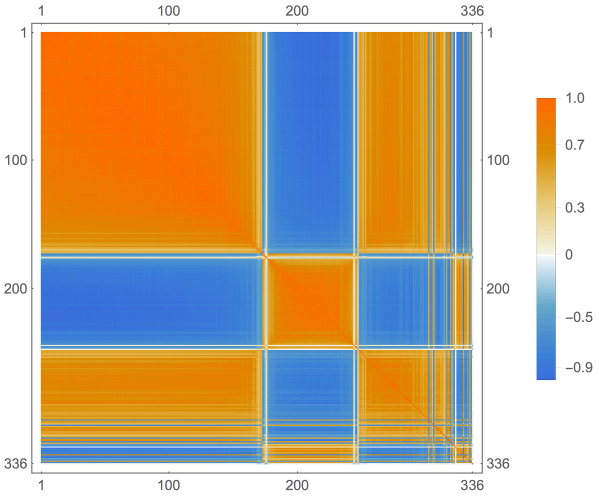
10^5 MC samples



10^6 MC samples



10^7 MC samples



(G. Papadimitriou)

Correlations in data become more clear with more resolved transport.
Also, covariance matrix gives a good qualitative metric for MC resolution.

Closing Thoughts

- The primary goal of this talk was to show explicit examples of how applications use nuclear physics and uncertainties

- At the crux of all issues are the double-edge swords called databases
  - On one hand, the summary and consolidation of data is a must for going forward to an application
  - Unfortunately, discarded information and bugs/errors largely complicate matters

- Current uncertainty prescription in nuclear database: covariance matrices for many isotopes and channels
  - Applications used these covariance matrices to make new varied database and rerun their calculations dozens of times
  - Variations of cross-channel and cross-isotope covariances (coming in GND)
  - Currently no info on distributions are stored

Uncertainty quantification in applications is of top importance in many fields and any suggestions would be greatly appreciated

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