Eigenviolence and other fixes to ENDF/B-VII.1 covariances

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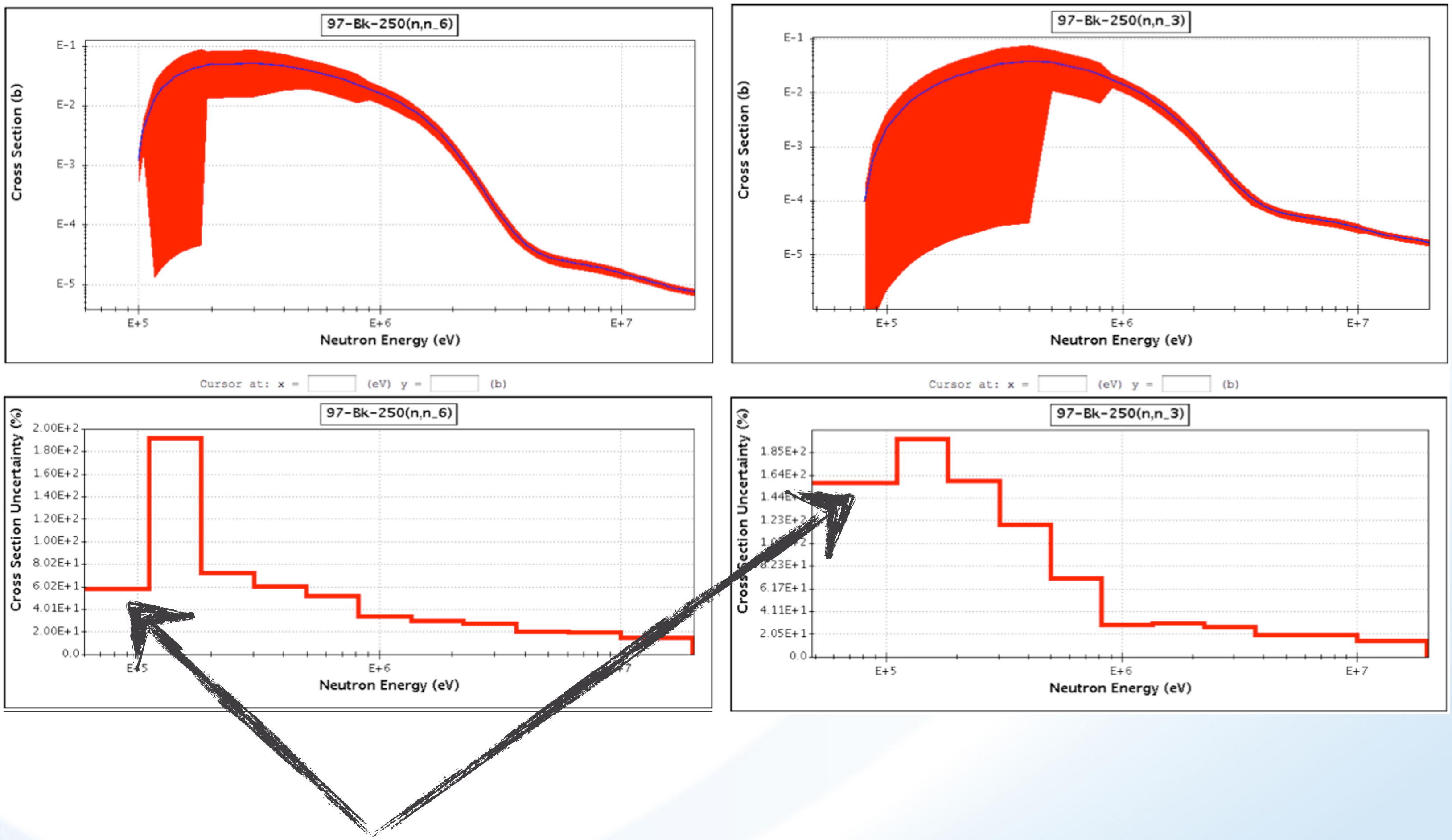
a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

Outline

- Cosmetic fixes to thresholds
  - All JENDL-4.0 actinides
  - 243,244m1Am
- Attempted to render all covariance matrices positive definite
  - Why these changes are important and for whom
  - What I did
  - Trouble nuclei: natC, 10,11B, 9Be, and those that could not be fixed...
  - Violence done to standards evaluations
- Summaries of changes

Cosmetic change to thresholds



1st bin supposed to be below threshold, but sometimes misses a little.
We set variance to be equal to 1st non-zero variance

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Why positive definiteness important

- The most common approach to Monte-Carlo uncertainty propagation is to do a eigenvalue decomposition of the covariance matrix:

$$\mathbf{\Delta^2}\sigma = \sum_i \vec{v}_i^T \lambda_i \vec{v}_i$$

- Then vary in the dominant eigen-directions:

$$\vec{\sigma} = \vec{\sigma_0} + \xi\sqrt{\lambda_i}\vec{v}_i$$

- Requires *real* uncertainties, if covariance diagonal, would have: $\lambda_i = \Delta^2\sigma_i$
- Approach used in LLNL's kiwi package & by Kent Parsons in LANL studies.

Eigenviolence

- Easiest thing is to reconstruct covariance matrix, w/o negative eigenvalues:

$$\mathbf{\Delta^2}\sigma = \sum_{i,\lambda_i \geq 0} \vec{v}_i^T \lambda_i \vec{v}_i$$

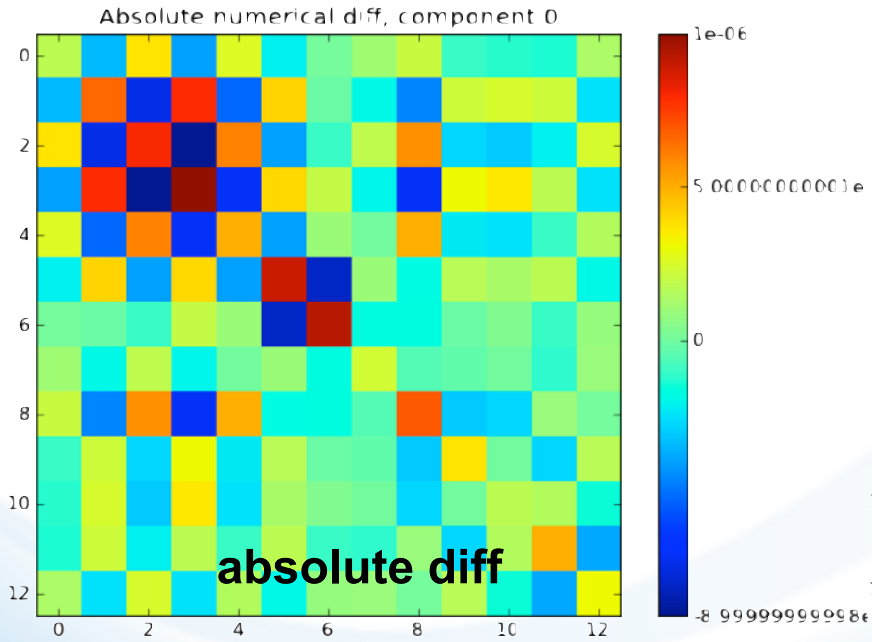
- Occasionally, finite precision of ENDF fields allow fake negative eigenmodes to occur, so should through away small positive modes too:

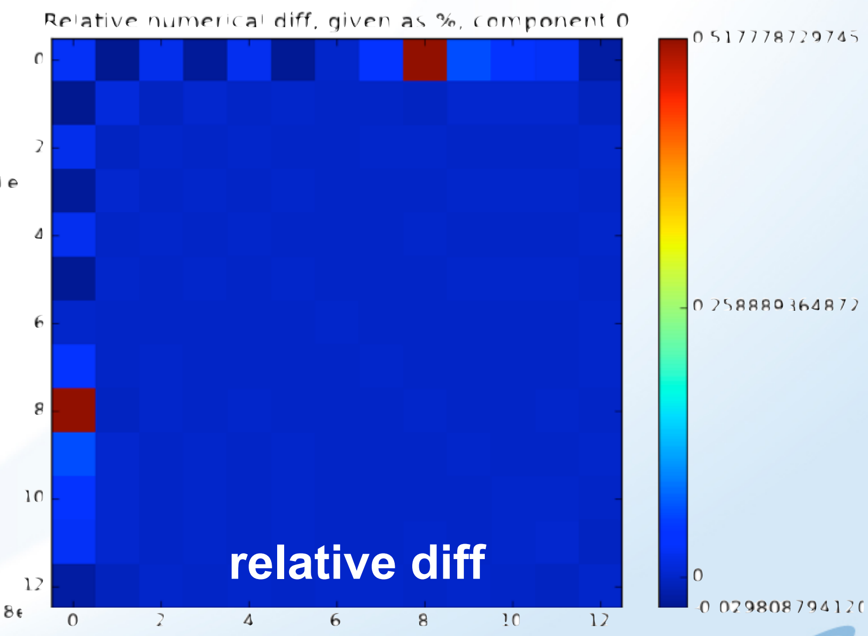
$$\mathbf{\Delta^2}\sigma = \sum_{i,\lambda_i \geq \varepsilon} \vec{v}_i^T \lambda_i \vec{v}_i$$

- If plan to invert matrix, this is good idea anyway

These changes are essentially cosmetic changes

- This is difference between new and old covariance matrices for $^1H(n,g)$
- Greatest absolute difference is barely detectable at ENDF precision in diagonal elements





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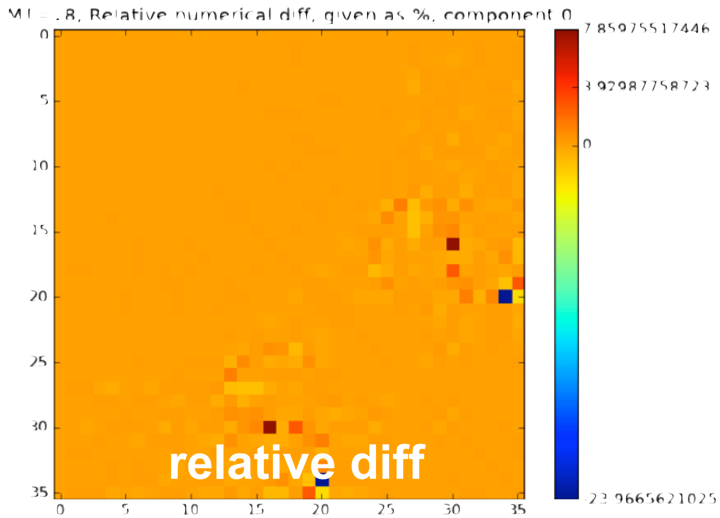
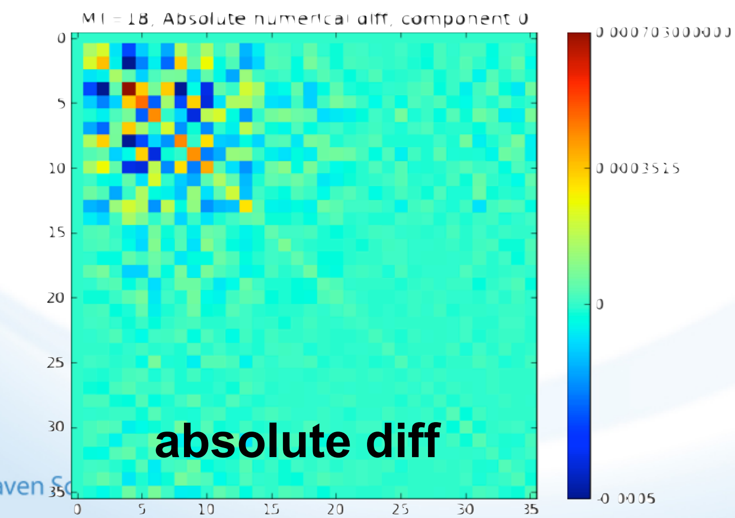
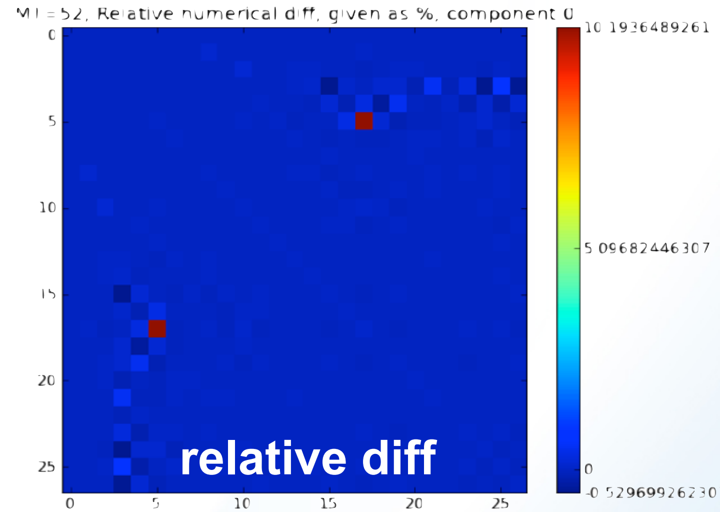
More sample changes

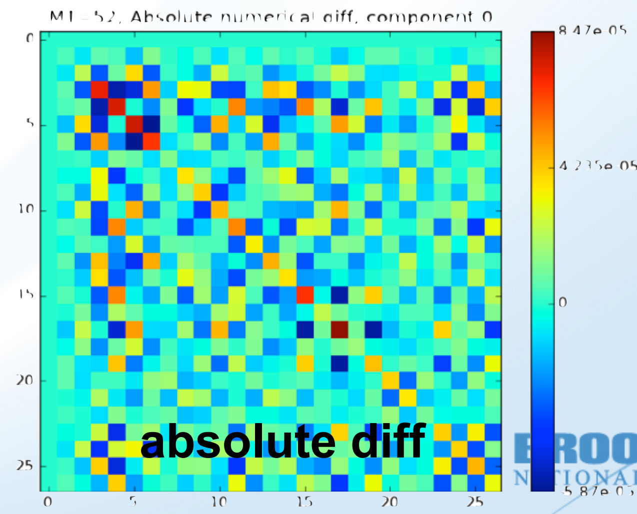
$^{229}Pa(n,f)$





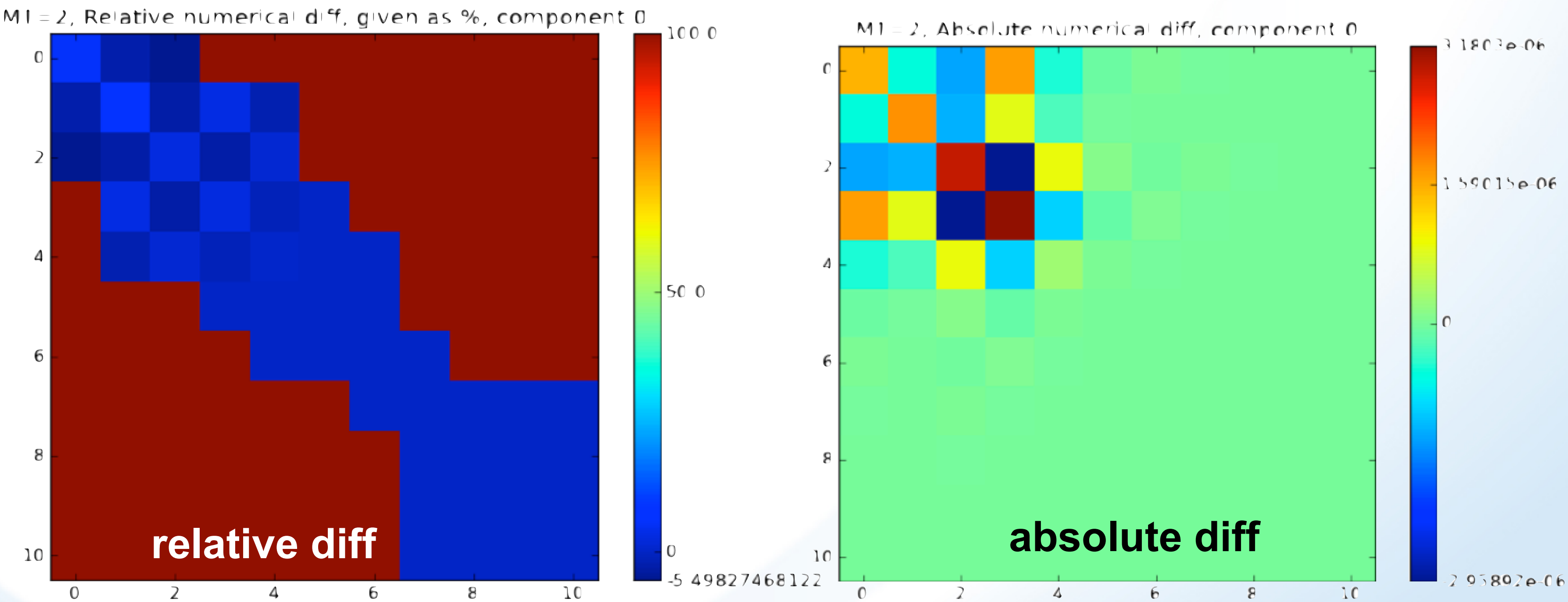
$^{229}Pa(n,n_2)$





For some nuclei, the change was more than cosmetic, but the covariances were in need of a facelift

$^{nat}C(n,el)$

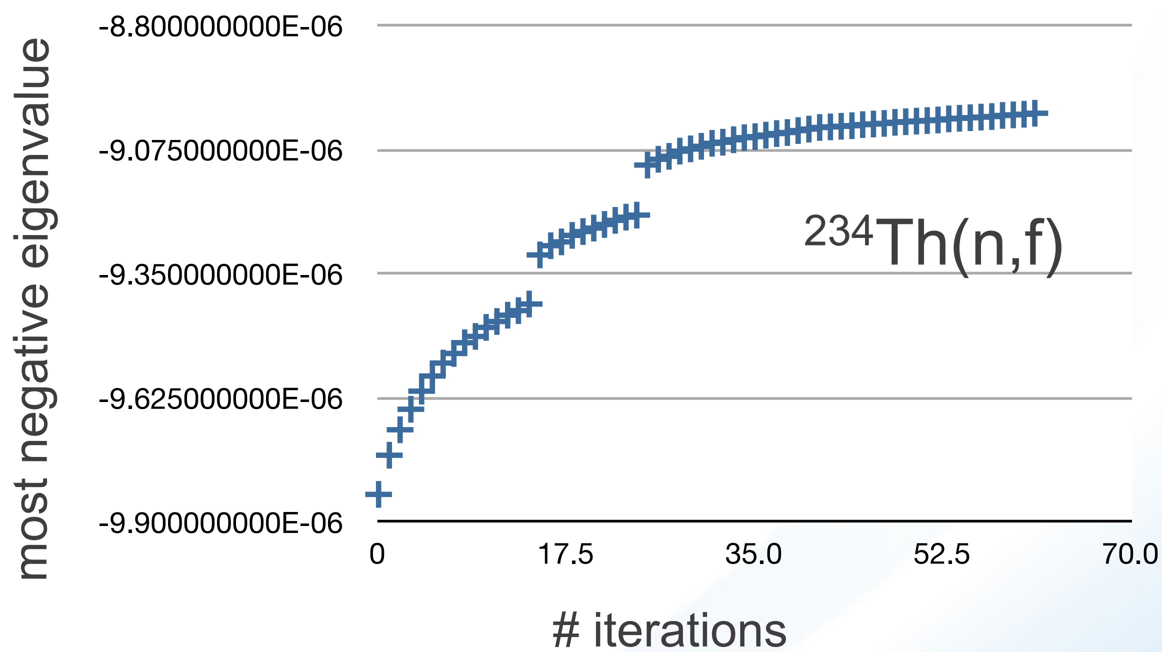


Note: this is a standards cross section

Similar sized changes for ^{9}Be, $^{10.11}B$, ^{54}Fe, ^{59}Co

Sometimes removing the negative eigenvalues wasn't possible

- Tough cutting, even into small positive eigenvalues wasn't enough; iterating doesn't help either



- ^{234}Th, ^{238}U, ^{239}Np, ^{250}Cm, ^{251,253,255}Es(n,f), ^{254m1}Es(n,n$_2$) impacted

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Summary of changes to standards evaluations

- ^{1}H(n,el): unchanged, did change (n,g)
- ^{3}He(n,p): untouched
- ^{6}Li(n,t): unchanged, did change (n,el)
- ^{10}B(n,a): unchanged, did change (n,el), (n,tot)
- ^{nat}C(n,el): Changed (n,el) and (n,tot), cosmetic only!
- ^{197}Au(n,g): untouched
- ^{235}U(n,f): unchanged, did change (n,2n), (n,g)
- ^{238}U(n,f): Changed (n,f) and (n,non), cosmetic only!
- (^{239}Pu(n,f)): unchanged, did change (n,2n), (n,g), (n,non)

Summary of rest of library

- Large changes: ^{9}Be, $^{10.11}$B, ^{54}Fe, ^{59}Co
- Small changes to many reactions:
  - ^{23}Na, ^{46,48}Ti, ^{89}Y, $^{90-96}$Zr, ^{95}Nb, ^{99}Tc, $^{101-103,106}$Ru, ^{103}Rh, $^{106-108}$Pd, ^{127,129}I, ^{132,134}Xe;
  - Rare Earths: ^{139}La, ^{141}Ce, ^{147}Pm, ^{149,151,152}Sm, ^{153,155}Eu, $^{152-160}$Gd, $^{166-170}$Er;
  - ^{191,193}Ir, $^{204-208}$Pb, ^{209}Bi;
  - Actinides: $^{225-227}$Ac, $^{227-234}$Th, $^{229-232}$Pa, $^{230-232}$U, $^{236-246}$Pu, $^{234-239}$Np, ^{240}Am, $^{240-250}$Cm, $^{245-250}$Bk, $^{246,248-254}$Cf, $^{251-255}$Es, ^{255}Fm
- Unfixable: ^{234}Th, ^{238}U, ^{239}Np, ^{250}Cm, ^{251,253,255}Es(n,f), ^{254m1}Es(n,n_2)
- Note: No apparent common factors causing bad eigenvalues