

Investigating Effects of Sensitivity Uncertainties

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7th International Serpent Group Meeting

Gainesville, FL USA

November 5th-10th, 2017



PAUL SCHERRER INSTITUT



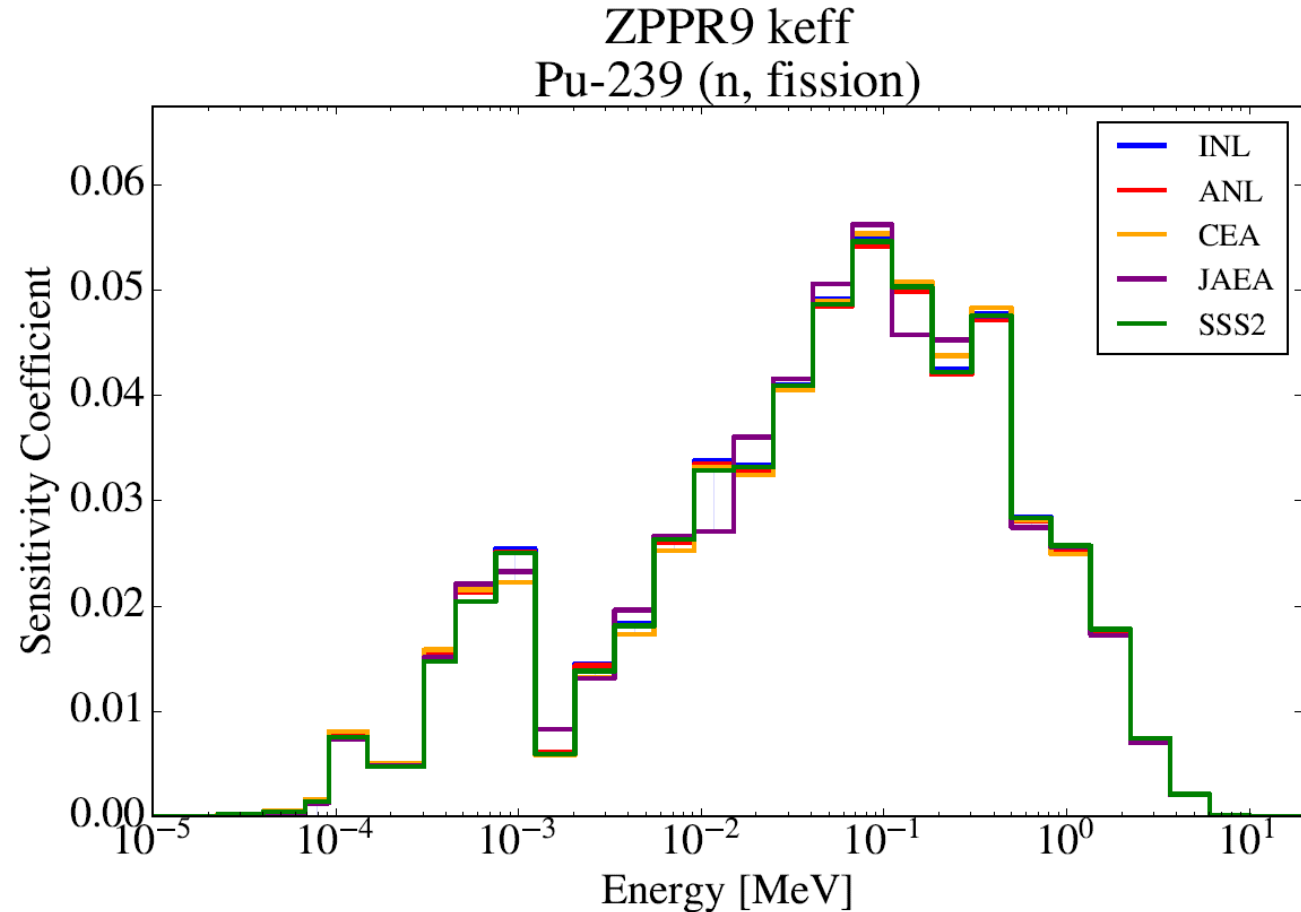
Introduction

- Want to use Serpent2.1.29 to do uncertainty quantification and data assimilation
- Means calculate sensitivities with Serpent
- Monte Carlo codes offer advantages for data assimilation
- No approximations in geometry, angle, energy
- For deterministic codes, need expert judgement to quantify these uncertainties
- Bias between C and E can be accurately quantified:
 1. Nuclear data uncertainty
 2. Experimental uncertainty
 3. Statistical uncertainty from Monte Carlo
- Advantages come with CPU-time disadvantages: sensitivity statistical uncertainties
- How do I efficiently use CPU time? Number of particle histories?

Sensitivity Profiles

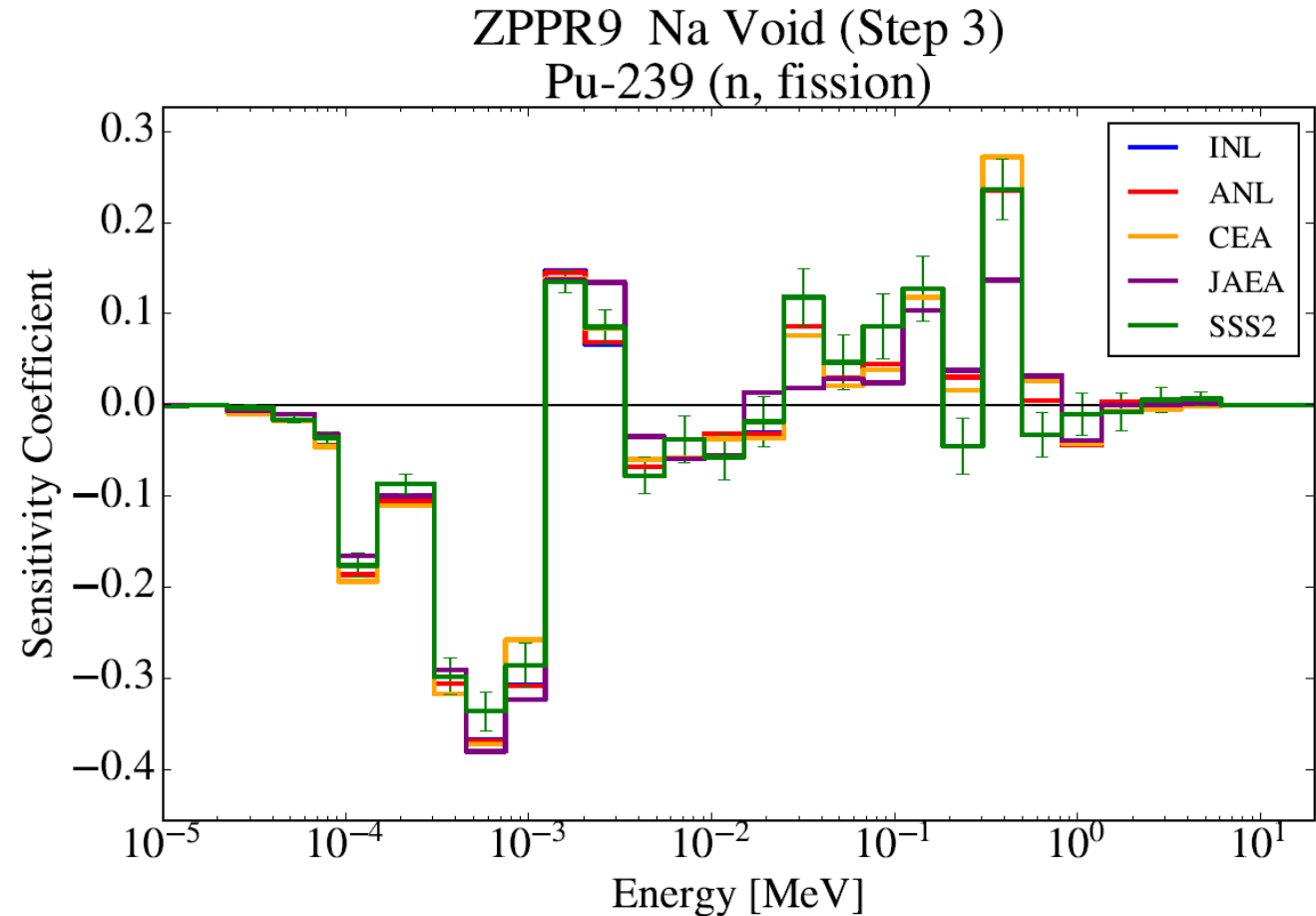
Sometimes have low
uncertainty...

Probably too particles



Sensitivity Profiles

Sometimes a bit
bigger uncertainty...



Sensitivity Profiles

Sometimes even
bigger...

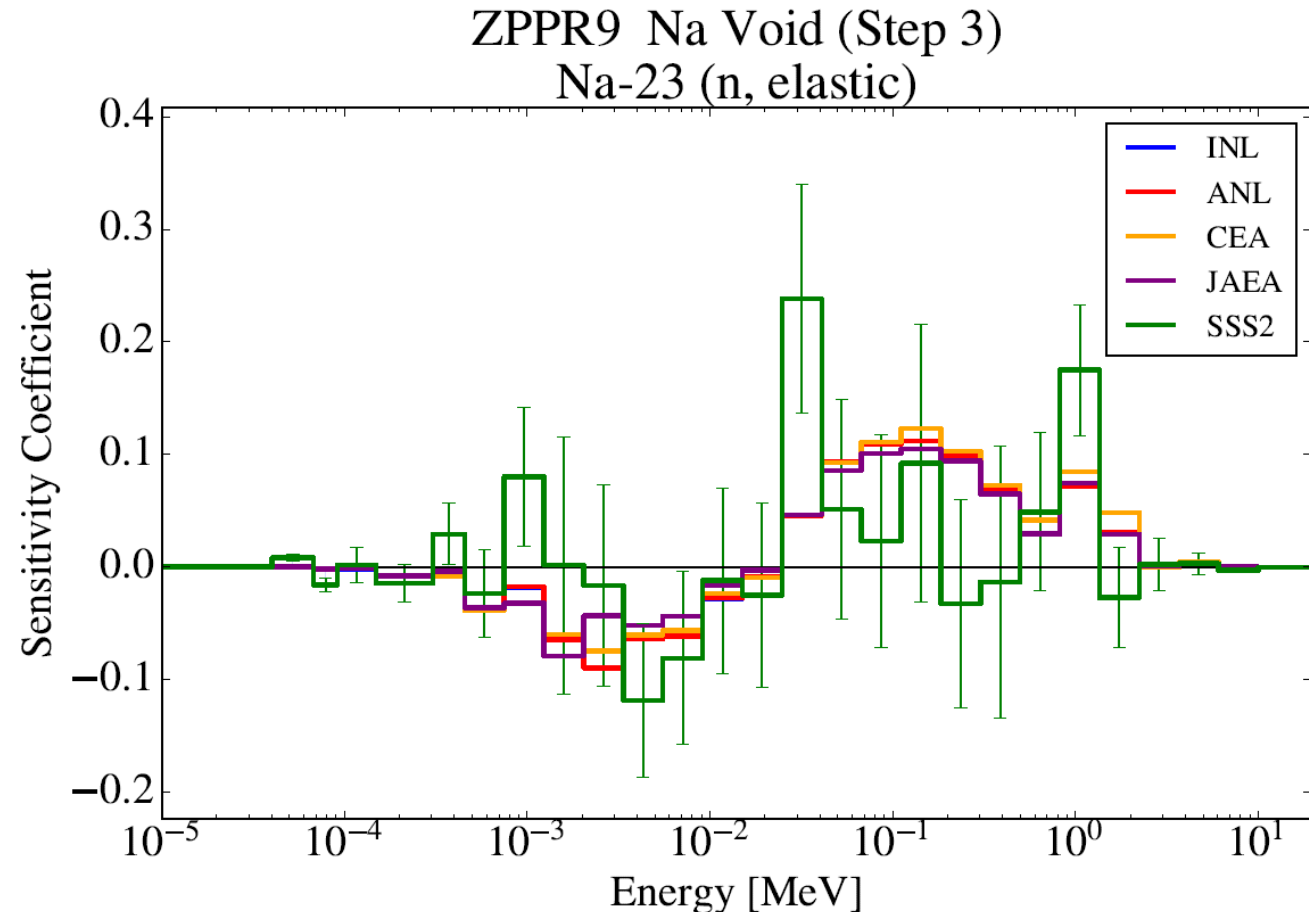
But what's too big?



How much should I
reduce the uncertainty?



How long to run
Serpent?



Outline

- I don't know how long I need to run Serpent!
- When are the sensitivities acceptable?
- When can I stop a simulation once the sensitivities are good enough for the given application?
- It's too hard to look at the sensitivities individually
 - Can have thousands!
 - Some are important and some aren't!
- Can we define a STOP criterion?
- Should be simple, global, and not require setting up data assimilation problem
- Makes Serpent more competitive with deterministic codes by eliminating CPU waste



Approach

- Take simple Jezebel Pu-239 benchmark
 - k_{eff}
 - F28/F25
 - F49/F25
 - F37/F25
- Save the sensitivity coefficients at ever 2 million particles
- Use them in uncertainty quantification and data assimilation
- Propose a convergence criterion

What/Why? Data Assimilation

- Comparing experiment vs. code have inherent bias from
 1. Methods' uncertainties: Monte Carlo or deterministic methods
 2. Modeling approximations
 3. Nuclear data uncertainties
- Uncertainties create a difference, or bias, between code and experiment:

$$bias = \frac{C}{E}$$

- Data Assimilation is method to treat nuclear data uncertainties and their effects

Prior information + Experimental Benchmarks = Posterior Information

Nuclear Data + Experiments = Posterior Nuclear Data

What/Why? Data Assimilation

- What do you get from applying data assimilation?
 1. Reduce the bias and the bias's uncertainty → may be able to reduce conservatism
 2. Give feedback to nuclear data evaluators reevaluating important nuclide/reaction pairs
- How does data assimilation address nuclear data uncertainties?
 1. “Consolidate” calculated and experimental responses. Assimilate integral experiments
 2. Adjust nuclear data and/or calculated/experimental responses

Effects on Linear Approximation

- Recall that sensitivities are just slopes from first-order perturbation theory

$$\mathcal{C}(\sigma) = \mathcal{C}(\sigma_0) + \frac{\partial \mathcal{C}}{\partial \sigma} (\sigma - \sigma_0) + \dots$$

$$\mathcal{C}(\sigma) \approx \mathcal{C}(\sigma_0) + S(\sigma - \sigma_0)$$

- When we use Serpent, we'll have three sources of uncertainty
 1. Mean value: $\mathcal{C}(\sigma_0)$
 2. Nuclear Data: σ_0
 3. Sensitivity coefficients: S

Effects on Linear Approximation

- Mean value uncertainty comes from the plain Serpent run
- The “Sandwich Rule” is the propagation of moments of first-order perturbation theory assuming nuclear data are the random variables

$$M_C = SM_\sigma S^T$$

- First-order propagation of moments assuming sensitivities are random variables

$$M_C = \Delta\sigma M_S \Delta\sigma$$

Effects on Linear Approximation

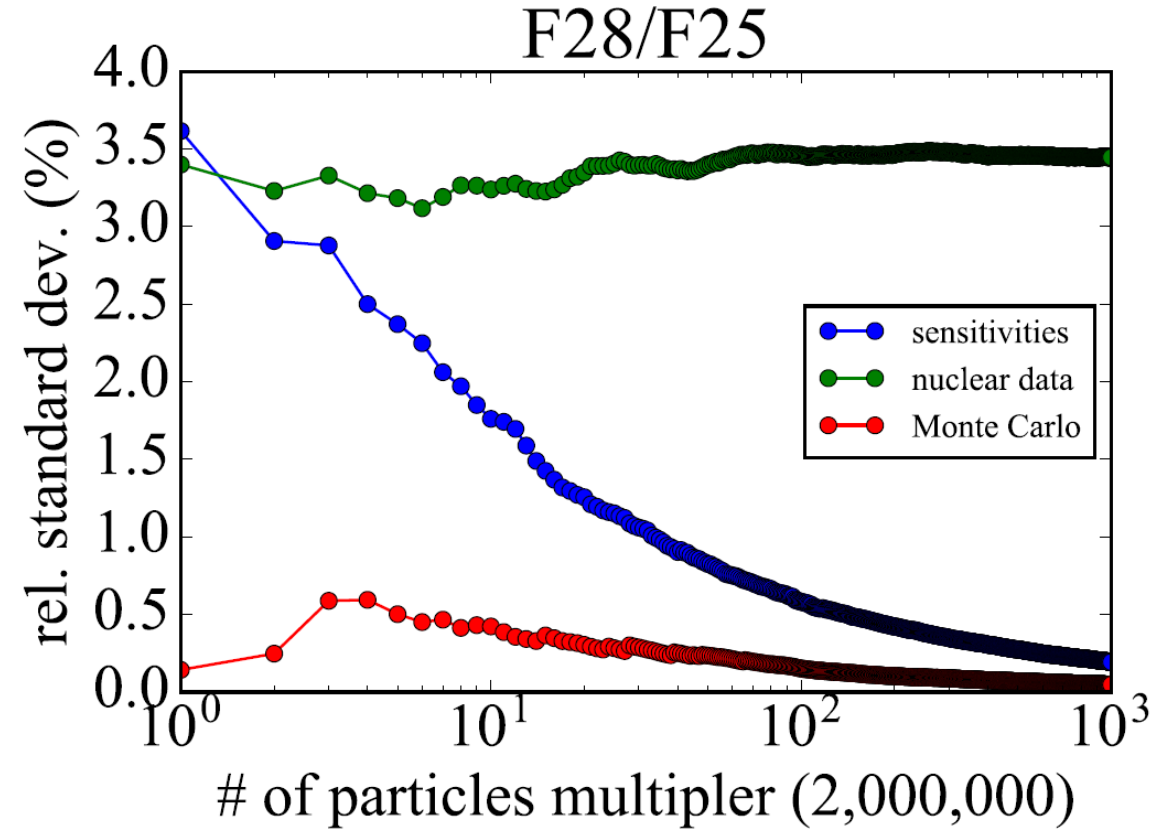
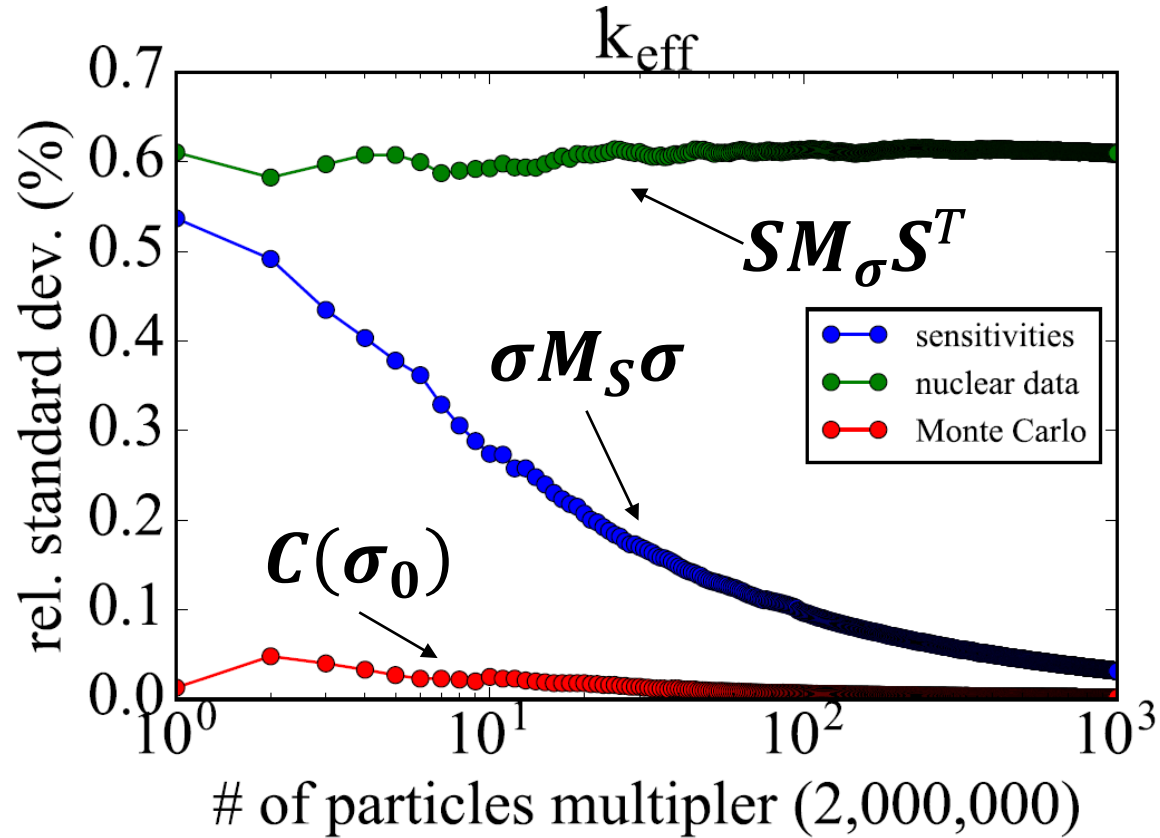
- To estimate uncertainty from three sources, need
 - S from Serpent calculation
 - M_σ from nuclear data library
 - M_S from Serpent (uncertainties associated with S)
 - $\Delta\sigma$ which is unknown.

$$M_C = SM_\sigma S^T$$

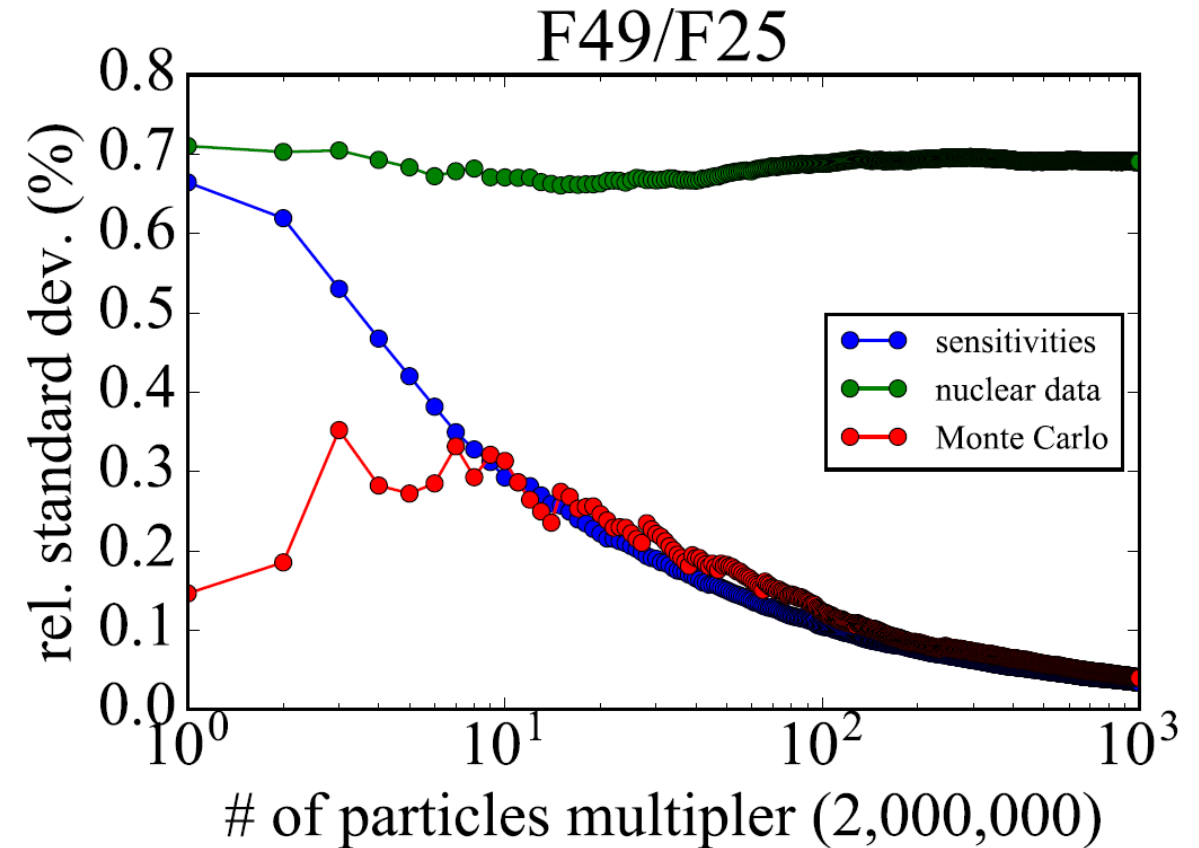
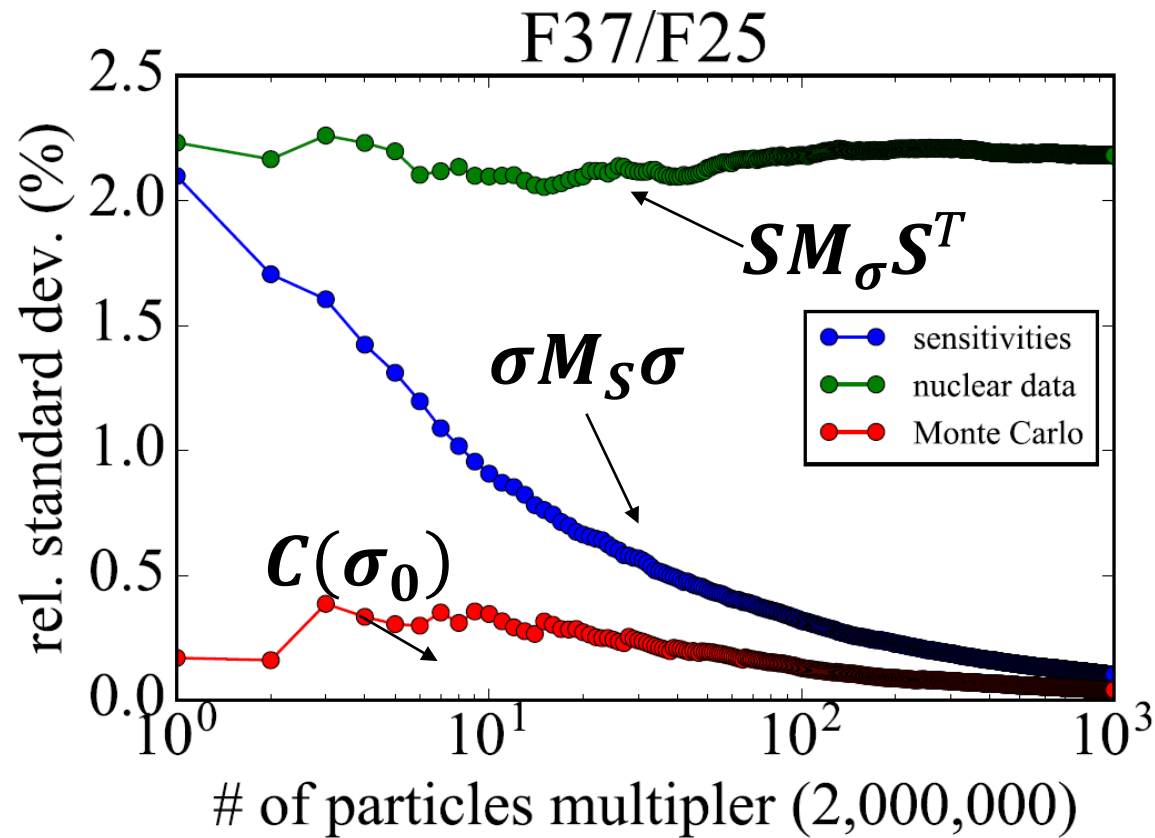
$$M_C = \Delta\sigma M_S \Delta\sigma$$

- Effect of S uncertainties is proportional to $\Delta\sigma$
- For now, assume 100% change in sigma $\longrightarrow M_C = \sigma M_S \sigma$
- Definitely an overestimation of uncertainty, but the goal is **STOP** criterion

Effects on Linear Approximation



Effects on Linear Approximation



STOP! Criterion

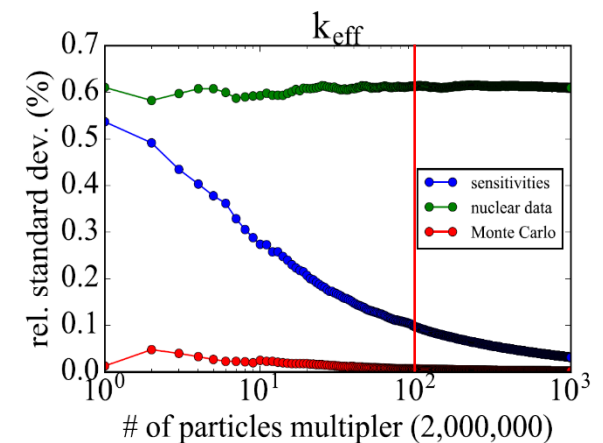
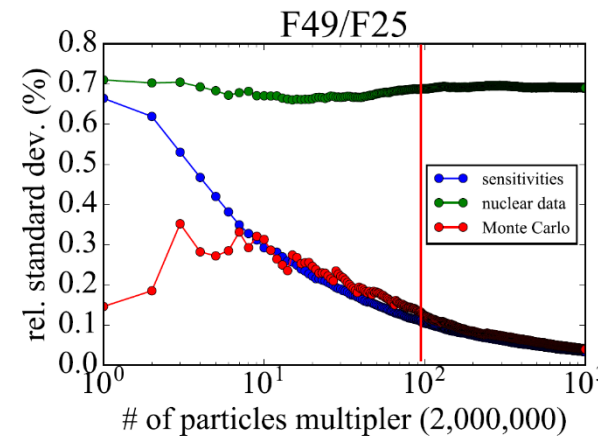
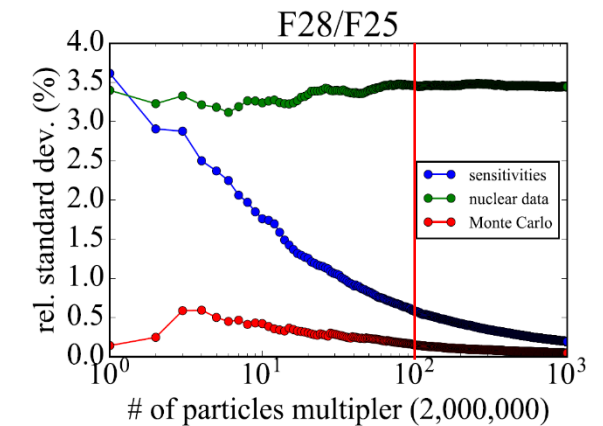
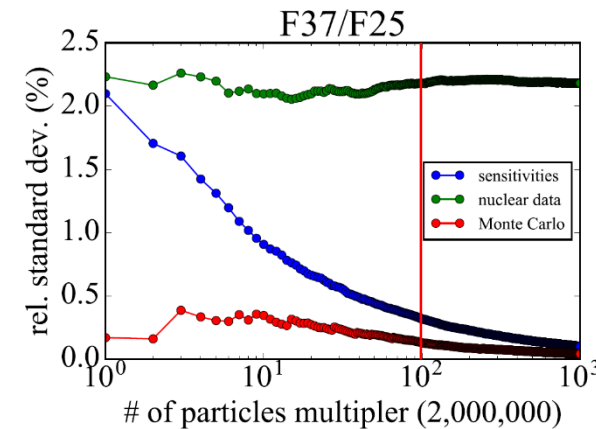
- Uncertainty from nuclear data is converged once

$$SM_{\sigma}S^T \gg \Delta\sigma M_S \Delta\sigma + C(\sigma_0)$$

- Assuming $\Delta\sigma = \sigma$** , results from this test case showed convergence when

$$SM_{\sigma}S^T = 0.2(\sigma M_S \sigma + C(\sigma_0))$$

- Corresponds to ~200 million particles
- Meets our goals for our criterion
 - Simple to calculate
 - Global parameter
 - Does not need data assimilation



Effects on Data Assimilation

- Have uncertain sensitivities plugged into DA equations
- How do they affect
 - Posterior calculated values?

$$\mathbf{C}' = \mathbf{C}_0 + \mathbf{S}(\boldsymbol{\sigma}' - \boldsymbol{\sigma})$$

$$\mathbf{M}'_{\mathbf{C}} = \mathbf{S}\mathbf{M}'_{\boldsymbol{\sigma}}\mathbf{S}^T$$

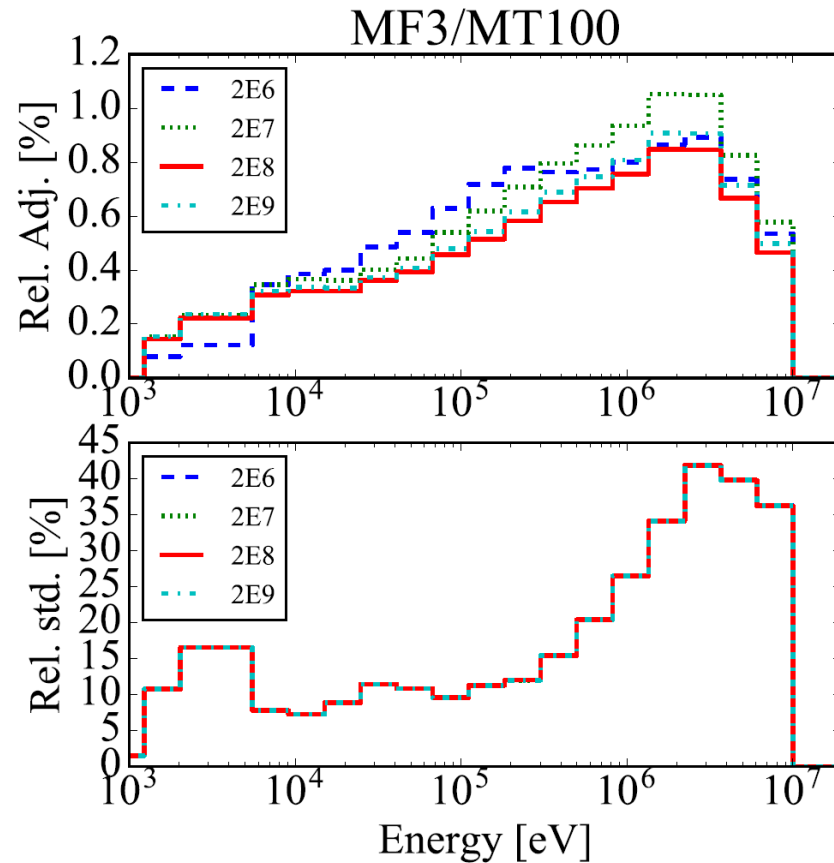
- Posterior nuclear data?

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathbf{M}_{\boldsymbol{\sigma}}\mathbf{S}^T[\mathbf{S}\mathbf{M}_{\boldsymbol{\sigma}}\mathbf{S}^T + \mathbf{M}_{EM}]^{-1}[\mathbf{E} - \mathbf{C}(\boldsymbol{\sigma})]$$

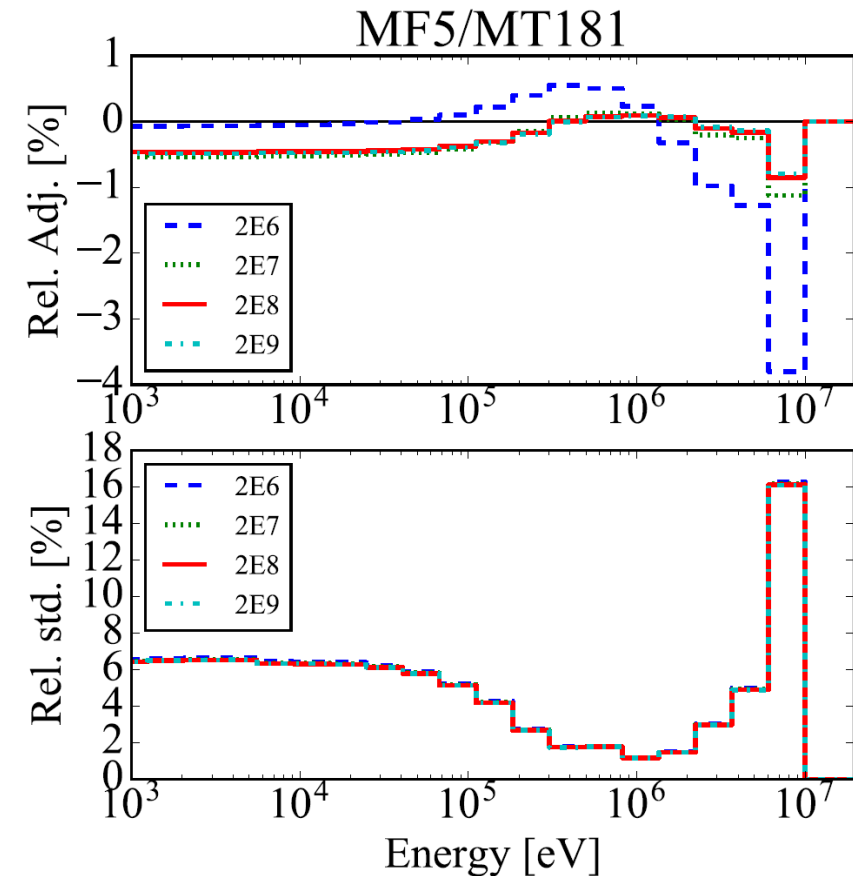
$$\mathbf{M}'_{\boldsymbol{\sigma}} = \mathbf{M}_{\boldsymbol{\sigma}} - \mathbf{M}_{\boldsymbol{\sigma}}\mathbf{S}^T[\mathbf{S}\mathbf{M}_{\boldsymbol{\sigma}}\mathbf{S}^T + \mathbf{M}_{EM}]^{-1}\mathbf{S}\mathbf{M}_{\boldsymbol{\sigma}}$$

- Look first at posterior nuclear data
- Does **STOP** criterion work?

Posterior Nuclear Data

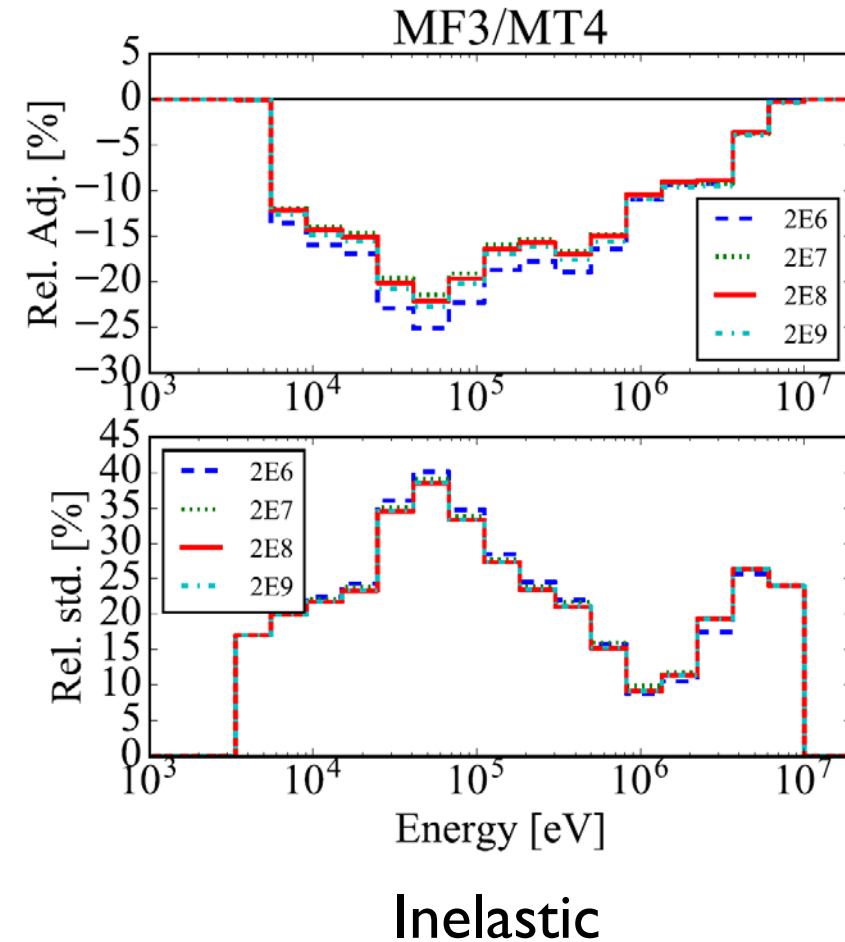
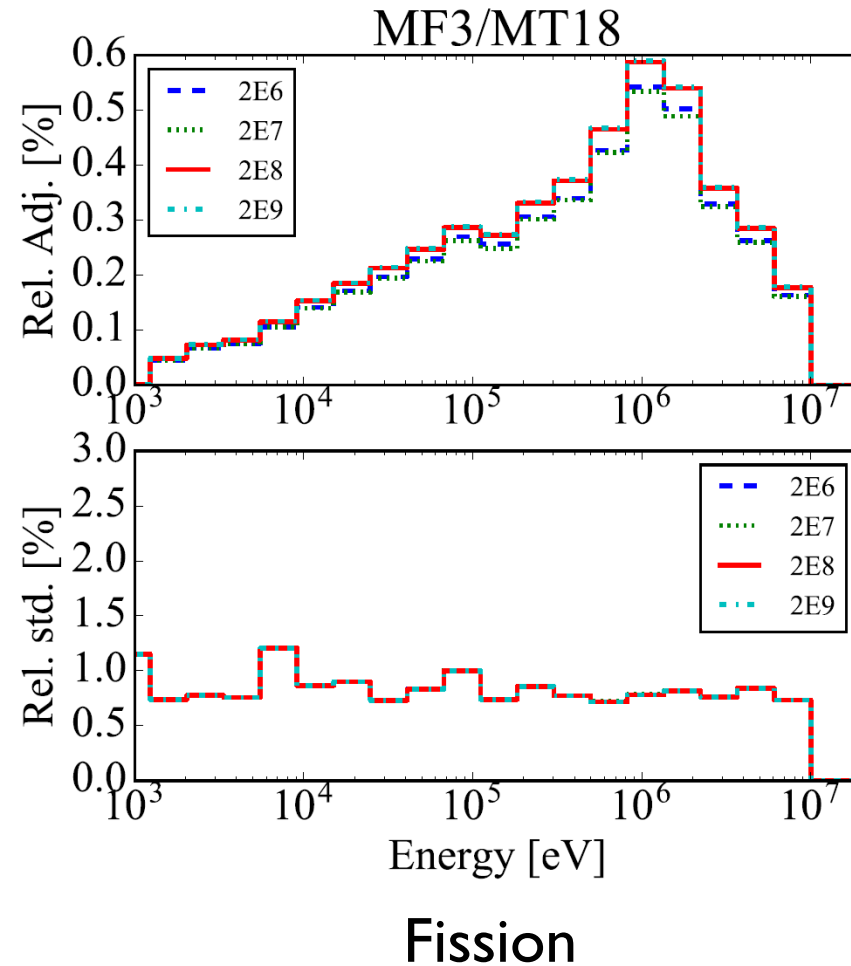


Capture



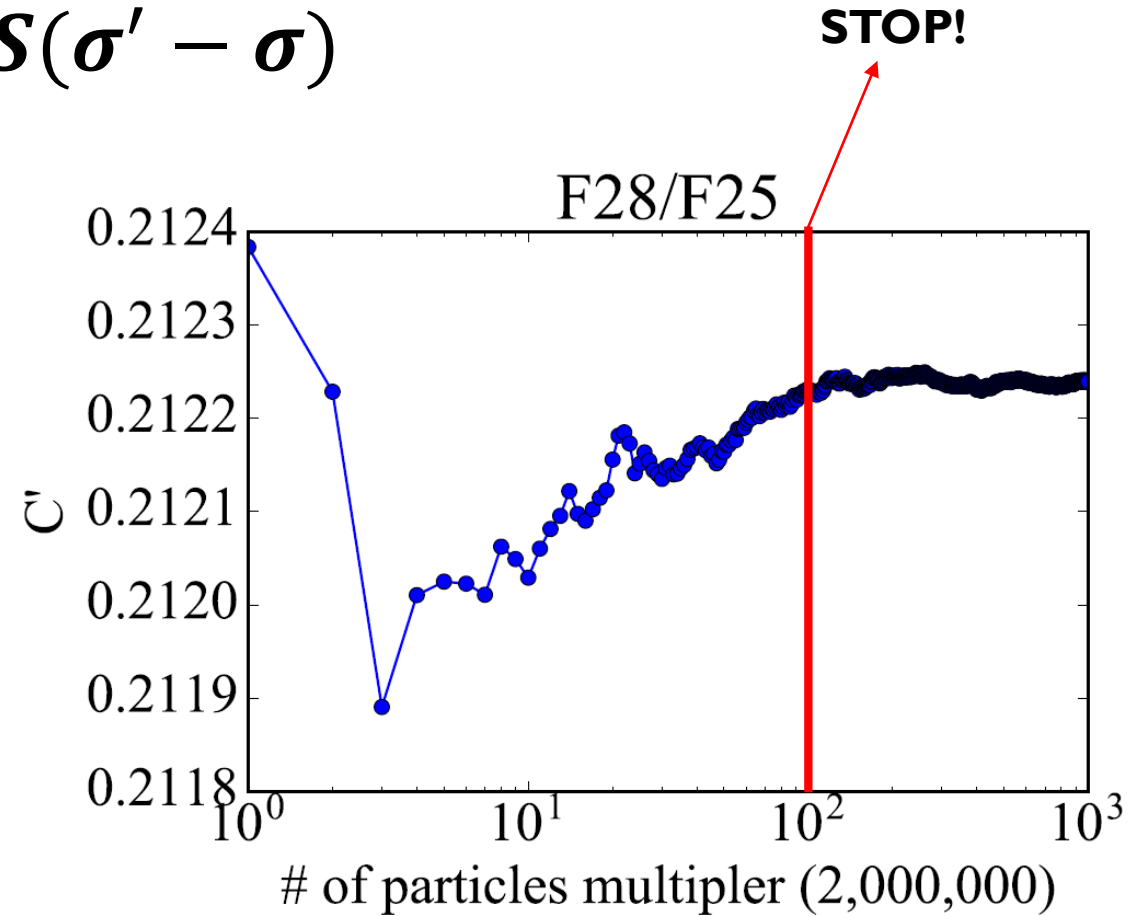
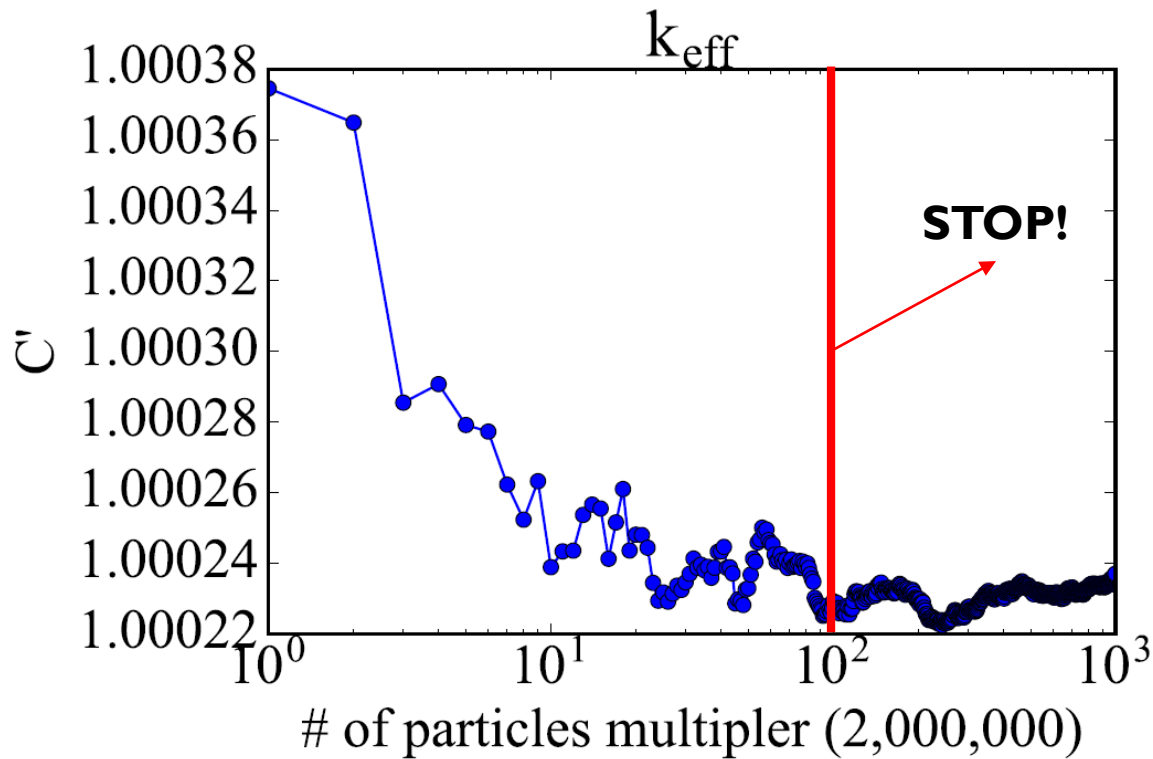
Fission Spectrum

Posterior Nuclear Data



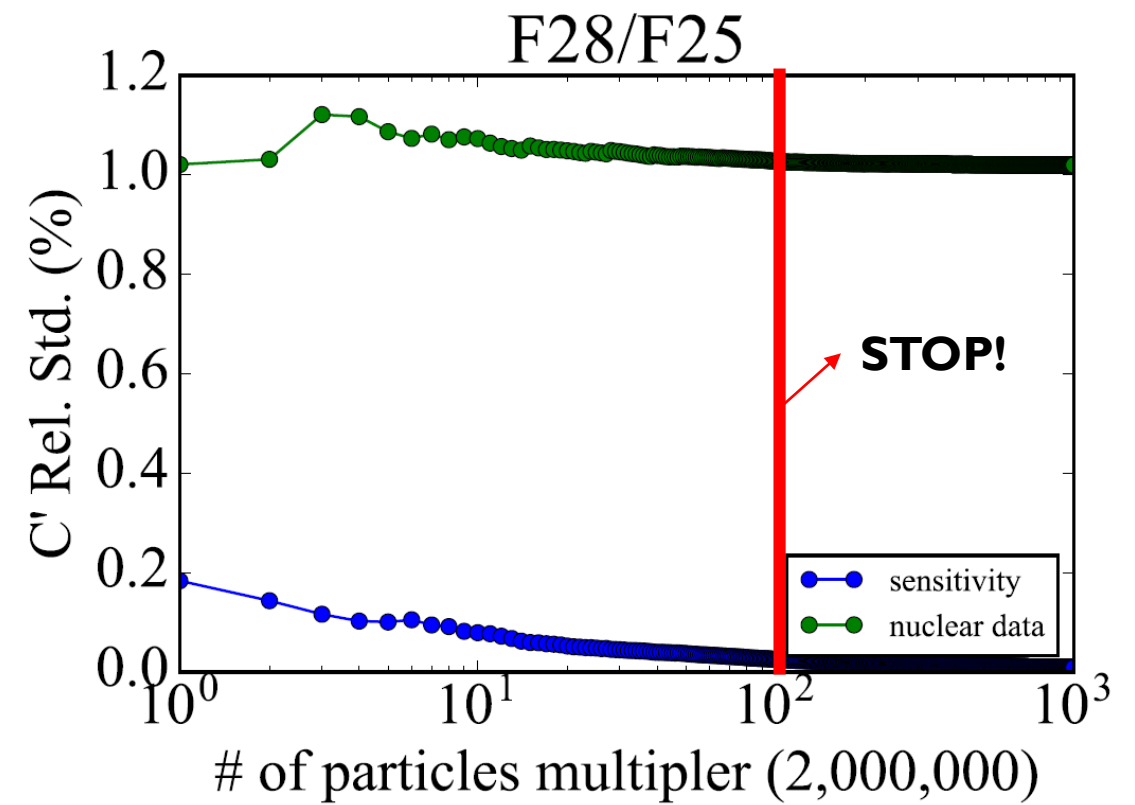
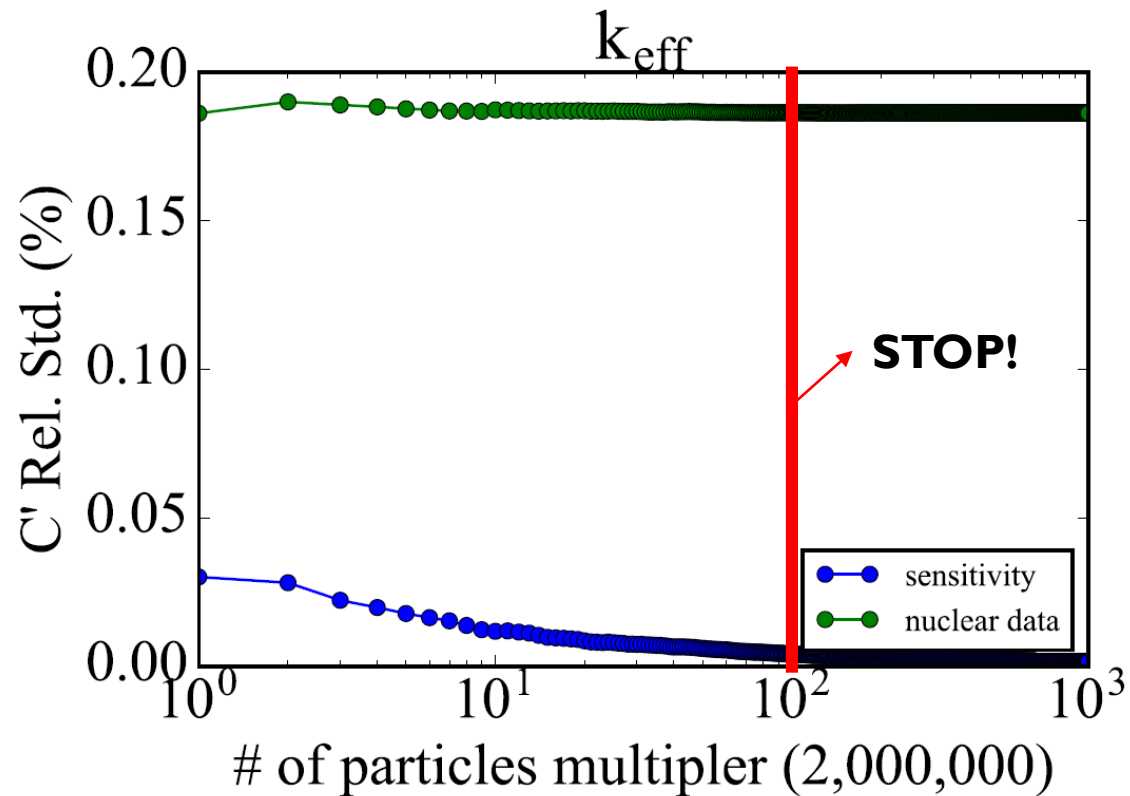
Posterior C

$$C' = C_0 + S(\sigma' - \sigma)$$



Posterior C Uncertainty

$$M'_C = SM'_\sigma S^T$$



DA Conclusions

- We see fluctuations in posterior distributions for C and for nuclear data
- But posteriors are remarkably inflexible to sensitivity uncertainty
- Fluctuations are diluted by other terms in the equations
- Our **STOP!** criterion was very effective
- At 200 million particles
 - Convergence of posterior nuclear data
 - Convergence of posterior C
 - Well past convergence of posterior C uncertainty

$$\sigma' = \sigma + M_{\sigma} S^T [S M_{\sigma} S^T + M_{EM}]^{-1} [E - C(\sigma)]$$

$$M'_{\sigma} = M_{\sigma} - M_{\sigma} S^T [S M_{\sigma} S^T + M_{EM}]^{-1} S M_{\sigma}$$

Conclusions

- Characterization of the effects of sensitivity uncertainties
- First step towards proposing a STOP! Criterion

$$SM_{\sigma}S^T = 0.2(\sigma M_S \sigma + C(\sigma_0))$$

- Data assimilation posteriors not heavily influenced by sensitivity uncertainties (2nd order effect)
- Realistic estimation uncertainty in first-order perturbation theory from uncertain sensitivities
- Can now plan large-scale simulations with Serpent for data assimilation and efficiently use CPU time

Conclusions

- Request as user
- Formulation assumes that nuclear data and sensitivities are uncorrelated.
- Best formulation would include correlations

$$M_C = \begin{bmatrix} S \\ \Delta\sigma \end{bmatrix} \begin{bmatrix} M_\sigma & M_{\sigma S} \\ M_{S\sigma} & M_S \end{bmatrix} \begin{bmatrix} S \\ \Delta\sigma \end{bmatrix}^T$$

- Can we compute the correlations between S and $\Delta\sigma$, or at least between S
- Would give most theoretically consistent results