Bayesian Monte-Carlo Framework: New Methods for Resonance Parameter Evaluation

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Assumptions or approximations used with Bayes' Theorem

1. The *model and* the prior PDF of *data* are assumed to be *perfect*
2. The model is approximated by its 1st order (*linear*) expansion
3. Prior and posterior PDFs are approximated by *normal* PDFs.

- We recognize that 1. is equivalent to constraining the *posterior* expectation values of δ, and of its covariance matrix, to 0:

$$z \equiv \begin{pmatrix} P \\ D \end{pmatrix}$$

$$\delta \equiv \delta(z, T(P)) \equiv T(P) - D$$

$$\langle \delta \rangle' = 0 \qquad \mathbf{\Delta}' \equiv \langle (\delta - \langle \delta \rangle')(\delta - \langle \delta \rangle')^{\mathsf{T}} \rangle' = \mathbb{0}$$

- We remove 1. by letting evaluator choose values of $\langle \delta \rangle'$ and $\mathbf{\Delta}'$
- 2. and 3. can be removed by Metropolis-Hastings Monte Carlo

Overview of approximations used by ORNL codes

Code name	$\langle\delta\rangle'$	Δ'	Prior/Post PDF	Cost Function	Minimization
SAMMY	0	0	Normal/Normal	$\chi^2(z=(P,T(P)),\langle z\rangle,\boldsymbol{C})$	Linear, iterative
TSURFER	0	0	Normal/Normal	$-\|\|-$	Linear, 1 step
BMC	Any	Any	Any/any	$X^2(z,\langle z\rangle,\boldsymbol{C},T(P),\lambda,\boldsymbol{\Lambda})$	MHMC

- Bayes' theorem with arbitrary constraints:

$$\boldsymbol{\Lambda}=\boldsymbol{\Lambda}(\langle\delta\rangle',\boldsymbol{\Delta}',\langle z\rangle,\boldsymbol{C})$$
$$\lambda=\lambda(\langle\delta\rangle',\boldsymbol{\Delta}',\langle z\rangle,\boldsymbol{C})$$

$$p'(z|\beta,\gamma)=p'(z|\gamma,\beta)=N'\mathcal{L}(\beta|z,\gamma)\times p(z|\gamma)$$

$$\mathcal{L}(\beta|z,\gamma)\leftarrow\mathcal{L}(\langle\delta\rangle',\boldsymbol{\Delta}'|z,\gamma)=e^{-\frac{1}{2}(\delta-\lambda)^{\dagger}\boldsymbol{\Lambda}^{-1}(\delta-\lambda)}$$

$$\begin{aligned}\beta &\leftarrow \{\text{any constraints on } \textit{posteriors} \text{ imposed by } \textit{evaluator}\},\\ \gamma &\leftarrow \{\text{any parameters needed to define the prior PDF, } p(z|\gamma)\}\end{aligned}$$

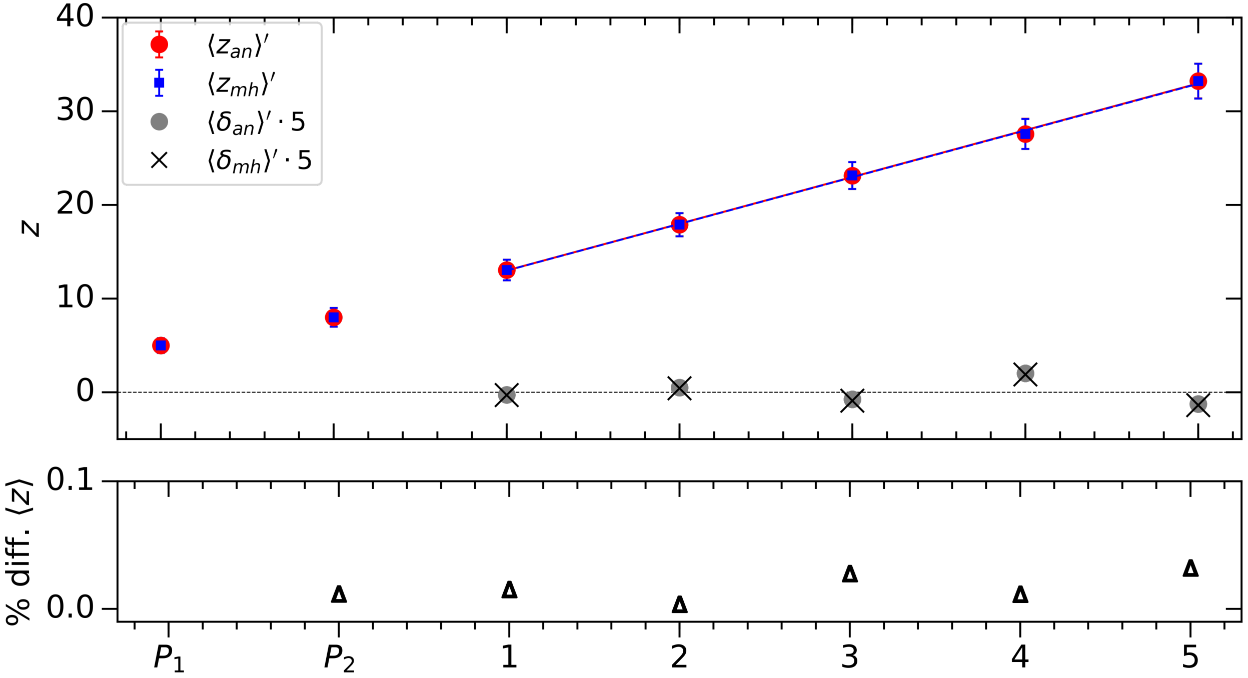
- GLS is recovered, i.e., $X^2\rightarrow\chi^2$, for $(\Lambda=\lambda=0)\leftarrow(\Delta'=\langle\delta\rangle'=0)$.

Metropolis Hastings Monte Carlo (MHMC) Algorithm

$N \leftarrow$ iterations ▷ necessary number of iterations for convergence
$i \leftarrow 0$
$z_0 \leftarrow$ arbitrary values ▷ z_i can be of arbitrary dimension
while $i < (N + 1)$ **do**
  Generate random candidate sample z' from $g(z'|z_i)$
  $A = \min\left(1, \frac{p(z')}{p(z_i)} \frac{g(z_i|z')}{g(z'|z_i)}\right)$
  Generate random value of u from uniform distribution between $(0, 1)$
  if $u < A$ **then**
    $z_{i+1} \leftarrow z'$
  else
    $z_{i+1} \leftarrow z_i$
  $i \leftarrow i + 1$

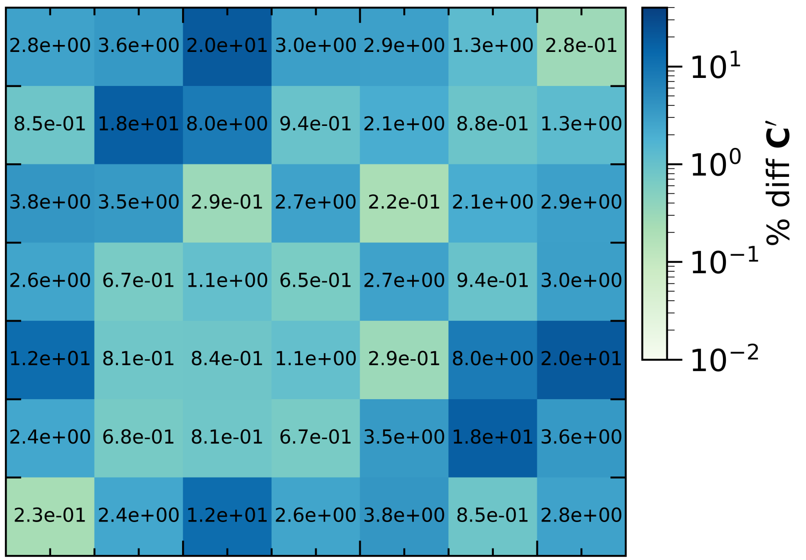
Analytical solutions: Linear model

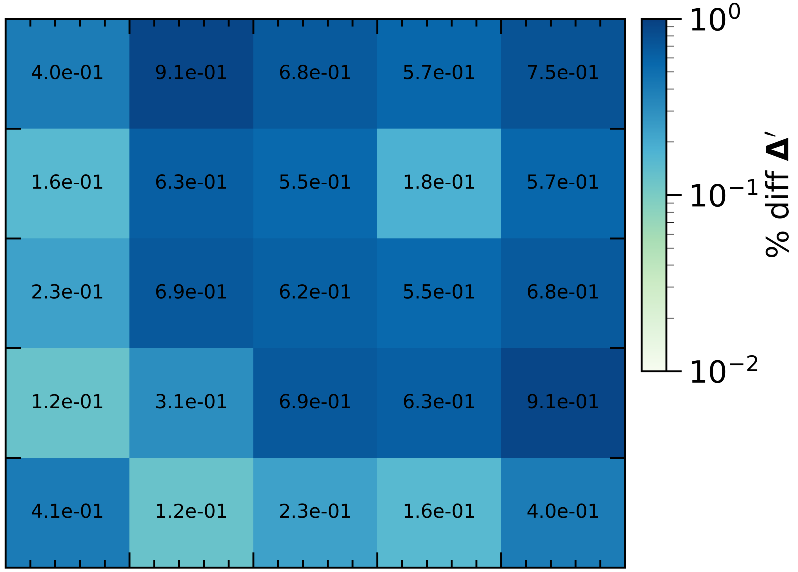
$$T(P) = P_1x + P_2$$



- We validate the framework with linear models
- The upper plot shows the perfect (within statistical uncertainty) agreement between the analytical and MHMC values for $\langle z\rangle'$ and $\langle \delta\rangle'$
- The lower plot shows that the difference between the analytical and MHMC $\langle z\rangle'$ is not $> 0.06\%$ for any element of z

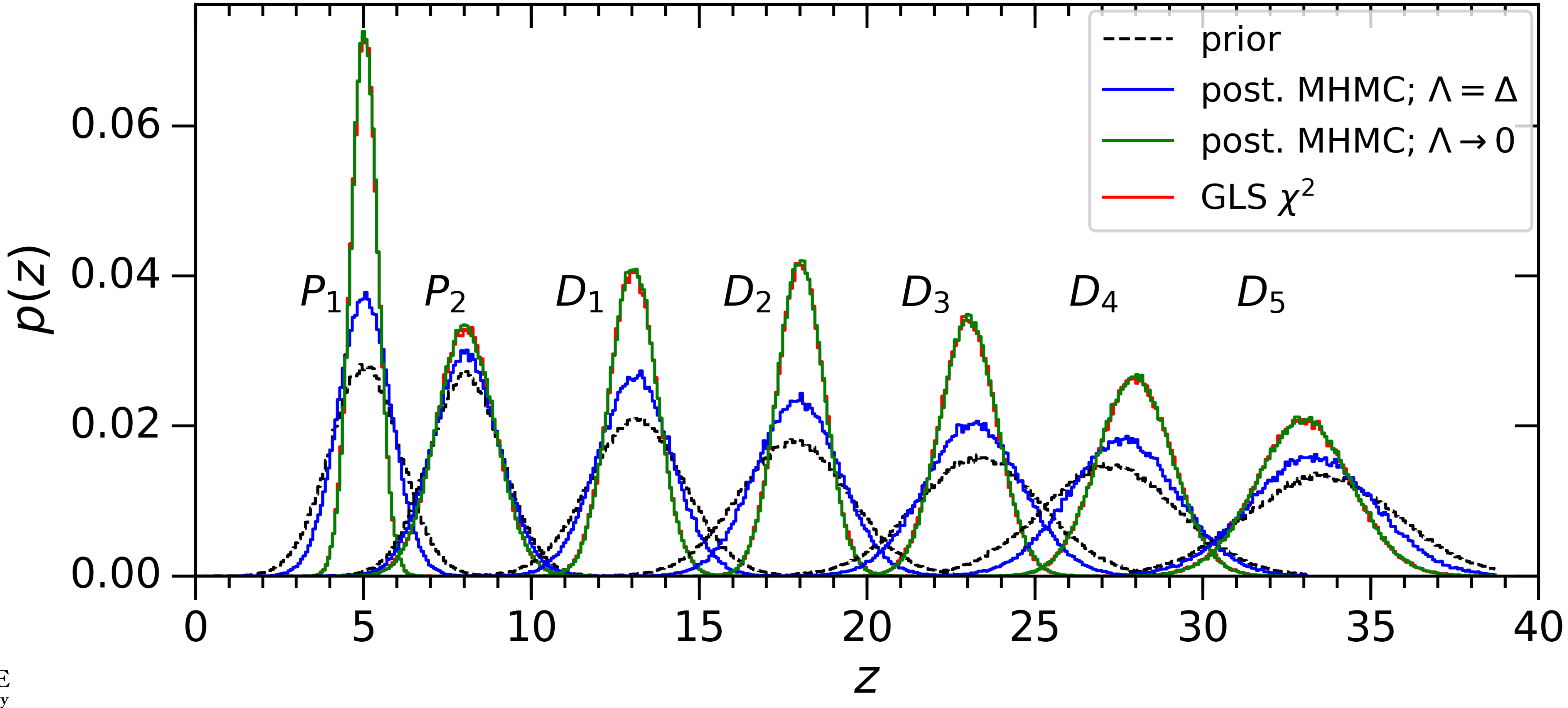
- Diagonal of $\boldsymbol{C}'$ matches analytical to within $< 0.6\%$, off-diagonal requires more iterations
- $\boldsymbol{\Delta}'$ matches well throughout





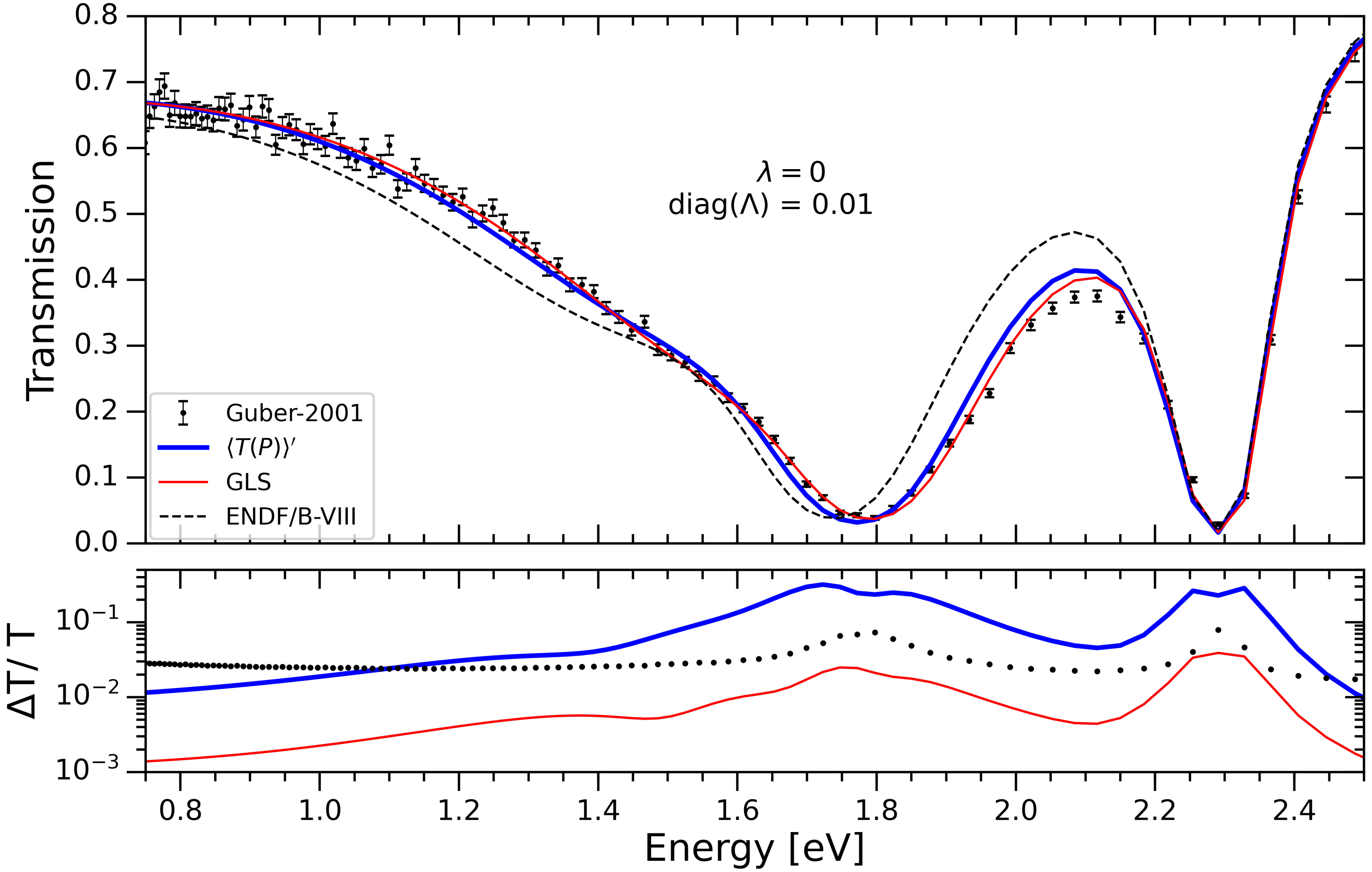
Comparison to GLS: Linear Model

- Case $\Lambda = \Delta$: solves for $\mathbf{\Delta}' = \mathbf{\Delta}/2$ **and** $\langle\boldsymbol{\delta}\rangle' = \langle\boldsymbol{\delta}\rangle/2$ by using $\Lambda = \Delta$ and $\lambda = 0$
- Case $\Lambda \rightarrow 0$: solves for $\mathbf{\Delta}' = \mathbf{0}$ **and** $\langle\boldsymbol{\delta}\rangle' = \mathbf{0}$ by using $\Lambda \rightarrow 0$ and $\lambda \rightarrow 0$ (matches GLS)
  - Demonstrates the effect of the GLS assumption: $\langle\delta\rangle' = 0, \Delta' = 0$

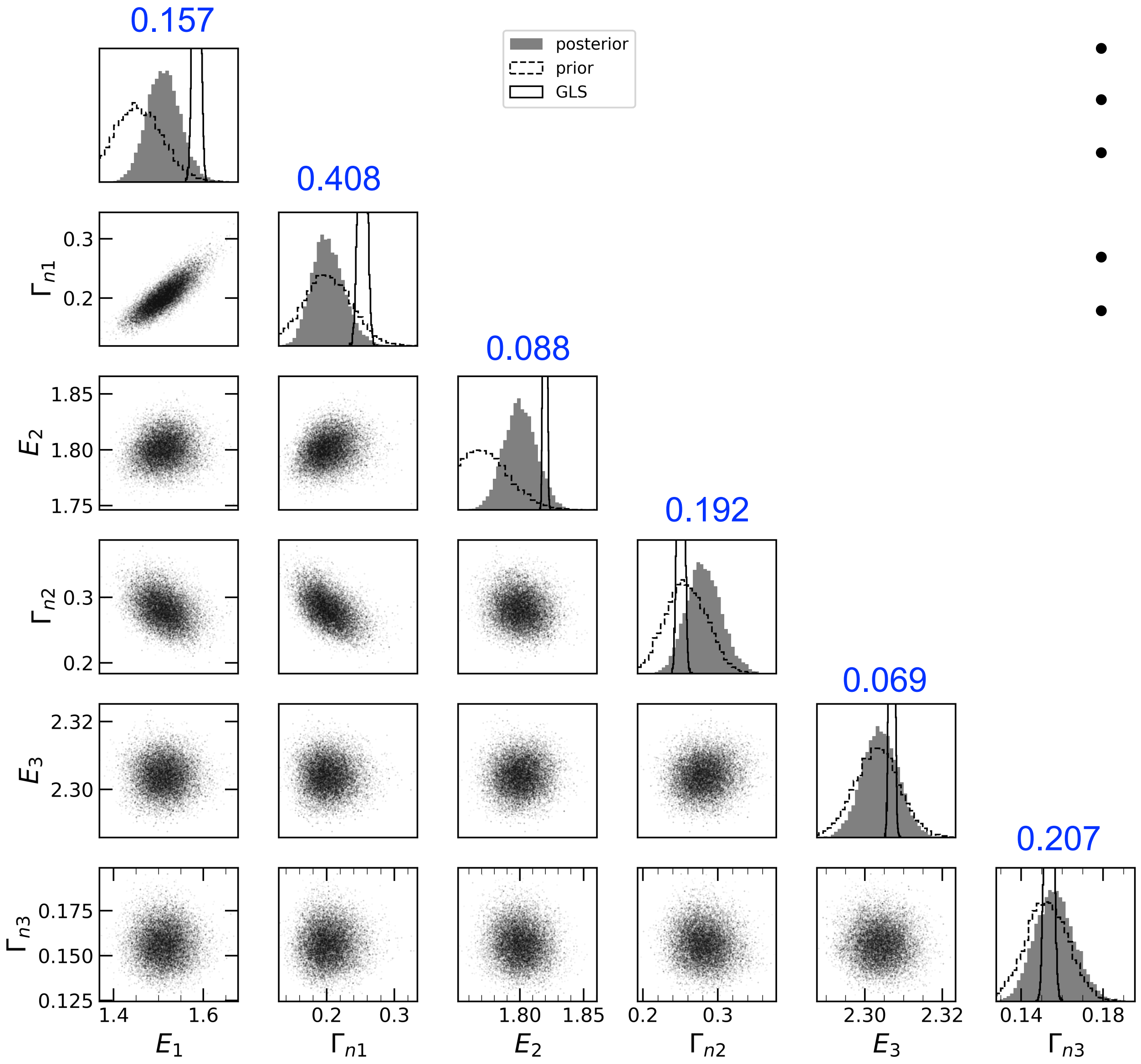


Application to RRR evaluation: U-233

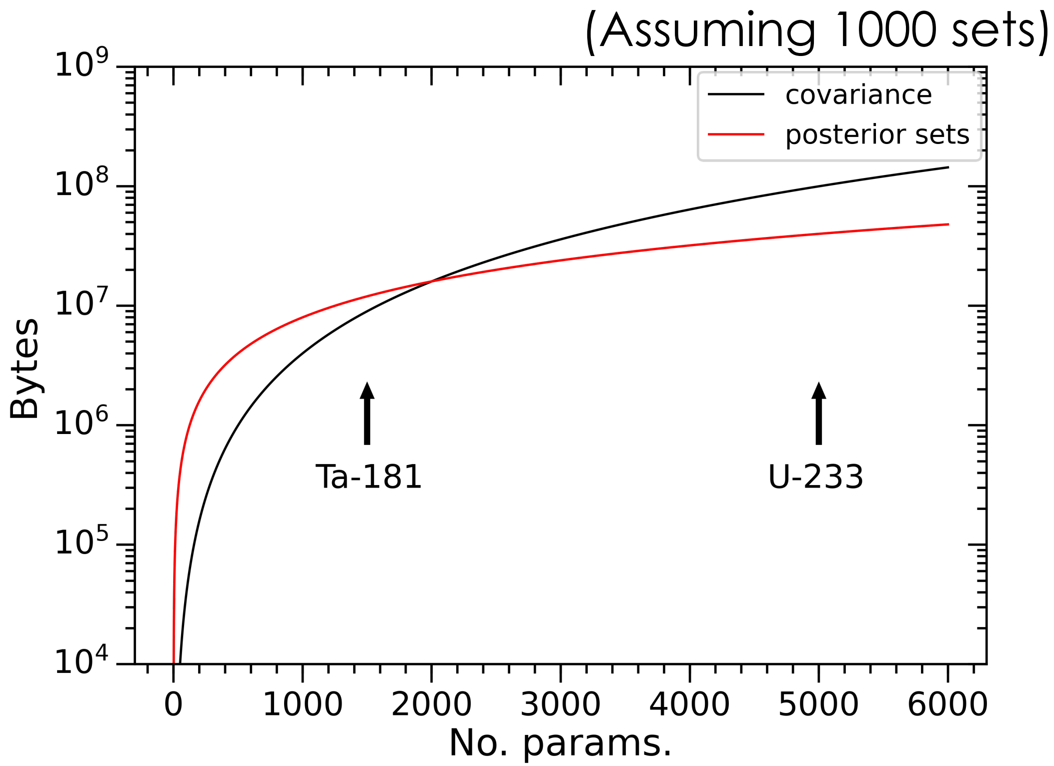
- Fit 3 resonances allowing the energy eigenvalues and neutron widths to vary
- The explicit application of $\mathbf{\Delta}' \neq 0$ gives the evaluator control over model/data defects (background, normalization, etc.)
- Uncertainty on model now envelopes the data



Uncertainty analysis: covariance and beyond



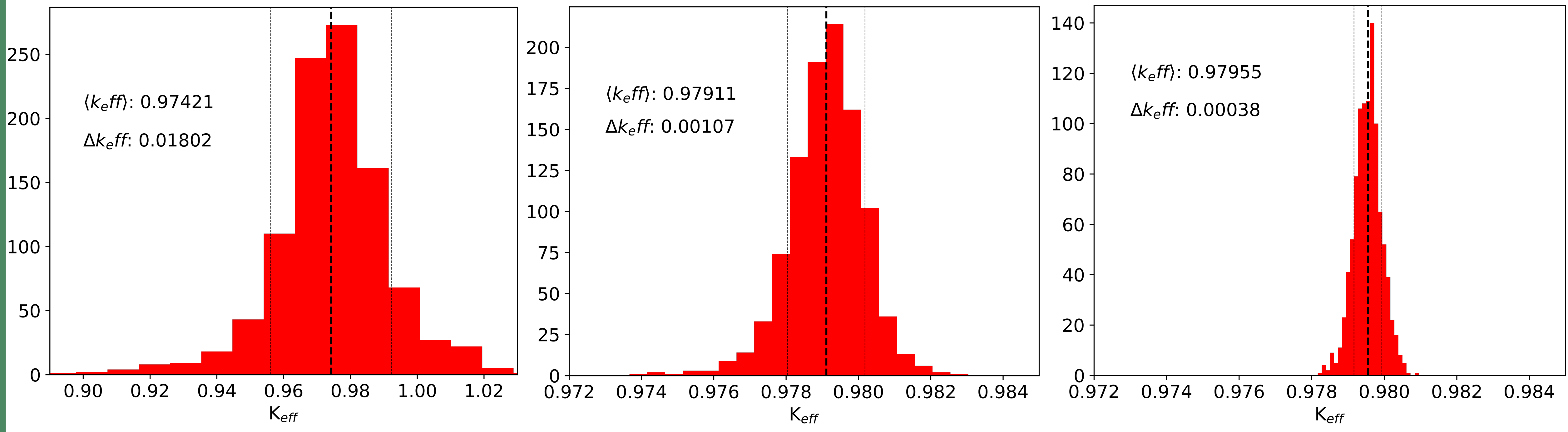
- 6 resonance parameters
- ~30,000 posterior sets make up PDF
- Posterior PDFs compared to GLS (black) and prior (black-dashed) PDFs
- Instead of storing covariance, store posterior sets
- All PDFs are positively skewn (blue)



The Impact on Reactors

- Example: U233-SOL-INTER-001
- We randomly sample ENDF/B-VIII.0 File 32
- Issues exposed: non-linearity (sensitivities), non-normality (PDFs)
- Take-away: small change in RP uncertainty can lead to large changes in Δk_{eff}

MC samples from: File 32, File 32 divided by 4, File 32 divided by 8



k_{eff} uncertainty is decreasing significantly faster than linear scaling would imply

Considerations

- BMC evaluation is a tool to address:
  - **Imperfect data & models**
  - **non-linear models**
  - **non-normal PDFs**
- ENDF-6 format does not allow non-normal parameter PDFs
  - Storing posterior sets allows for: variance, covariance, skewness, etc.
- To better predict criticality we could:
  - Document non-normal parameter PDFs (i.e. asymmetric uncertainty)
  - Consider non-linear sensitivity of k_{eff} to resonance parameters
  - Reduce uncertainty in key resonance parameters

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Additional Slides

MC *vs.* linear approx. for Δk_{eff} of U233-SOL-INTER-001-001

- MC reveals large deviation from non-linearity for ENDF/B-VIII.0 U-233 File 32