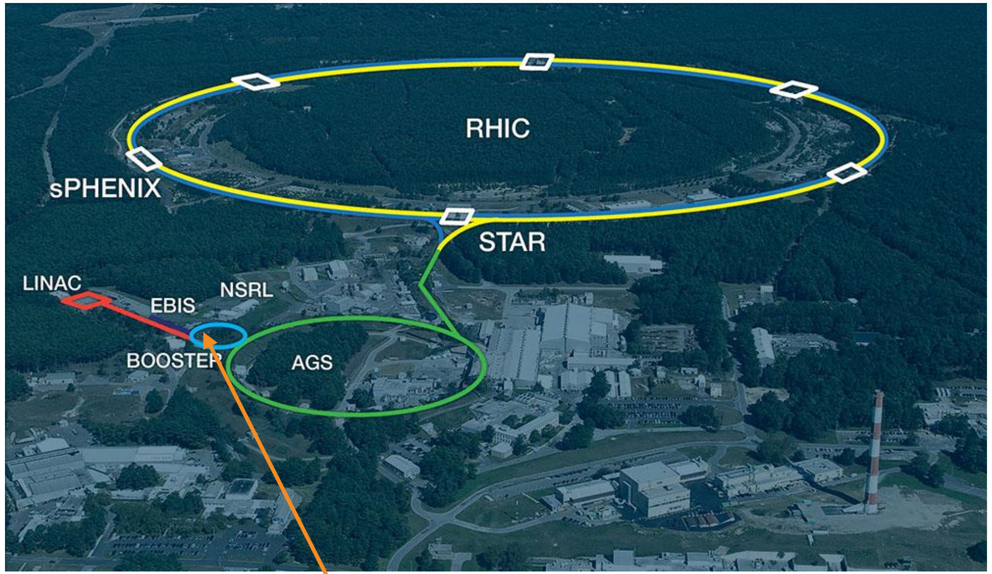
Machine-Learning–Accelerated Bayesian Uncertainty Quantification for Digital Twin Modeling and Control of the AGS Booster

Christopher Kelly

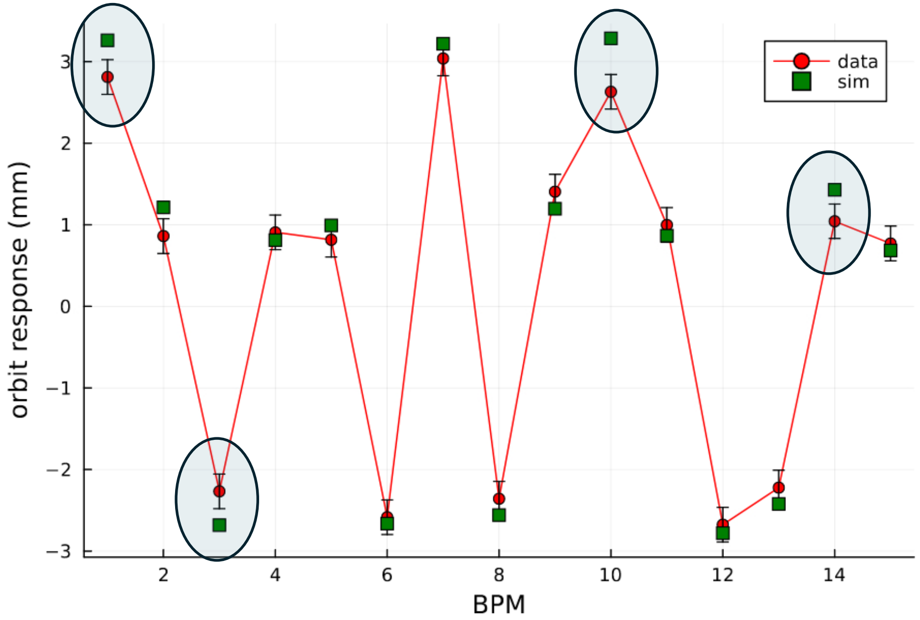
Computational Science Department

10/2?/25

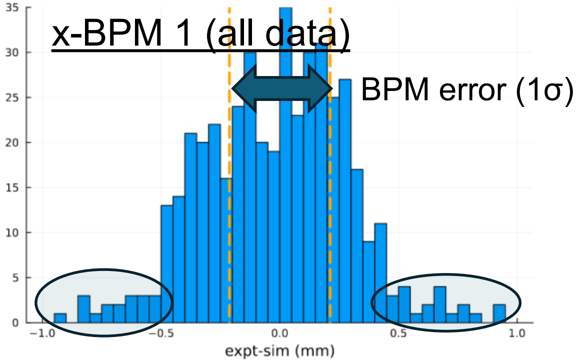
RHIC AGS Booster and Digital Twin

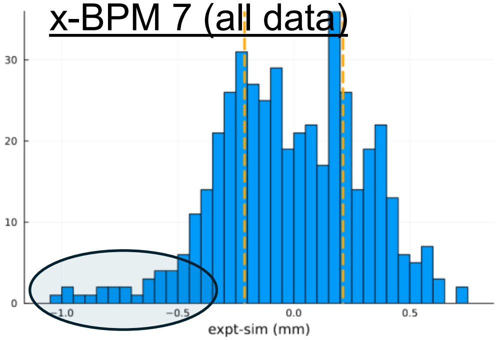


- Accurate beam control in AGS Booster is required to achieve high-quality beams for RHIC and EIC.
- A precise Digital Twin would enable more reliable beam control, improving physics output.
- Current best model of beam dynamics in RHIC is through the BMAD/TAO simulator.
- However, comparison of simulation to real beam orbit data shows discrepancies of unknown origin.
- **Use Bayesian Uncertainty Quantification (UQ) to study the discrepancies.**



Example orbit response to changing the strength of one of the corrector quadrupole magnets plotted versus the beam position monitor (BPM) index, showing deviation between simulation and real data,





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Bayesian UQ

"**Likelihood**": probability of data $\mathcal{D}$ given params Θ
normal dist. centered on simulation
$\sigma = \sqrt{2} \times \mathrm{bpm\ err.}$ (sqrt 2 due to orbit difference!)

"**Priors**": expert knowledge of *parameters*
(quantifies assumptions)

"**Posterior**": (output)
distribution of the parameters given the data

Bayes' Theorem

$$P(\Theta|\mathcal{D}) = \frac{P(\mathcal{D}|\Theta)P(\Theta)}{P(\mathcal{D})}$$

("Evidence" not needed for MCMC)

- "Inference" workflow:
  1. Identify (or introduce) a set of parameters to infer
  2. Decide on prior distributions and parameters
  3. Collect a set of data: complete orbit responses for different current settings (notably correctors)
  4. Sample posterior for params Θ via Bayes' theorem using Markov Chain Monte Carlo | **Use Julia "Turing" package**
  5. Study the posterior distributions of each parameter (assess errors, correlations, etc)
  6. Sample from posterior and likelihood function for specific current settings gives the "posterior predictive distribution" : **orbit response predictions with uncertainties**

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Parametrizing the unknown

- Many possible causes for discrepancies that are hard to directly quantify, e.g.
  - magnet misalignments,
  - power supply transfer function parameters
  - magnet nonlinearities
  - stray fields
- Rather than attempt to parametrize each source we introduce catch-all “nuisance parameters”
- Orbit most strongly depends on the 24 (x) + 24 (y) quadrupoles.
- Allow for per-quadrupole differences in the “**transfer function**” that maps quad current to magnetic field strength.
- Allow to vary by multiplicative “var” factors

$$T'(I^i_{\text{quad}}, I^i_{\text{dipo}}) = \text{var}_i \times T(I^i_{\text{quad}}, I^i_{\text{dipo}})$$

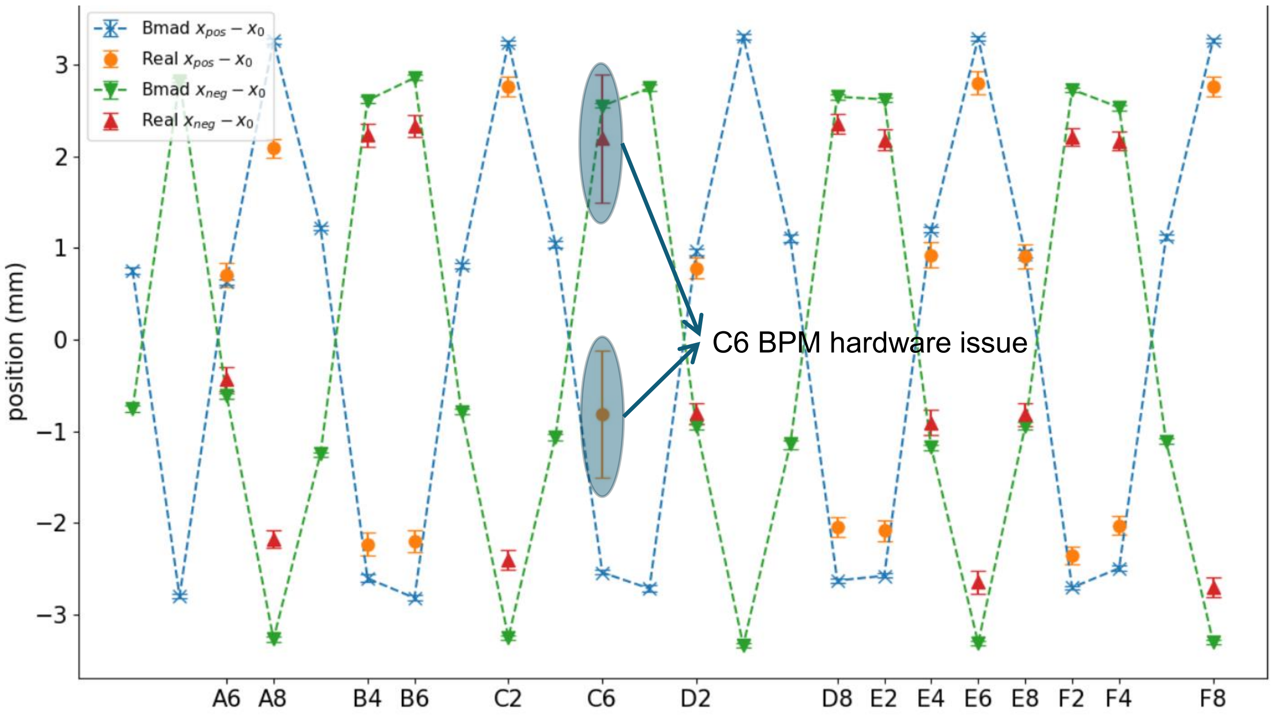
- Priors: lognormal centered on 1.0 (null)
- Prior width hard to guess due to unknowns: assume a few percent

```
function kqh_var(idipo, iqhc, var, qhstr1=0, qhstr2=0, quad="A2")

    klhc0 = 0.001818 #+ offset
    klhc1 = 9.080E-4 #* multf
    klhc2 = 6.657E-9
    klhc3 = 7.225E-12
    klhc4 = 3.239E-15
    klhc5 = 5.07E-19

    pl1 = ["A2", "A8", "C2", "C8", "E2", "E8"]
    ml1 = ["B2", "B8", "D2", "D8", "F2", "F8"]
    pl2 = ["A4", "B6", "C4", "D6", "E4", "F6"]
    ml2 = ["A6", "B4", "C6", "D4", "E6", "F4"]

    if quad in pl1
        iqh = idipo + ckc * (iqhc + bdot * iqhbd) + ckc2 * (qhstr1)
    elseif quad in ml1
        iqh = idipo + ckc * (iqhc + bdot * iqhbd) + ckc2 * (-qhstr1)
    elseif quad in pl2
        iqh = idipo + ckc * (iqhc + bdot * iqhbd) + ckc2 * (qhstr2)
    elseif quad in ml2
        iqh = idipo + ckc * (iqhc + bdot * iqhbd) + ckc2 * (-qhstr2)
    end

    b1lh = klhc0 + iqh * klhc1 + iqh^2 * klhc2 - iqh^3 * klhc3 + iqh^4 * klhc4 - iqh^5 * klhc5

    ckh = (1 - 0.00004179 * (bdot / bdipo(idipo))) * 1.00 * b1lh / (brho(idipo) * lenqh) * var

    return ckh
end
```

Dataset

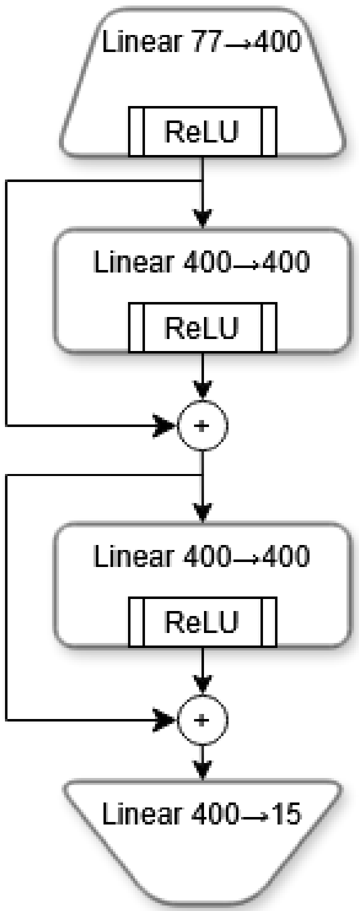
- Fix static magnet currents (up to power-supply fluctuations)
- Baseline setting with correctors set to 0A
- Vary each of the 24+24 corrector magnet currents in turn from 0A to +22A, -22A
- Record orbit for all BPMs before and after perturbation
- 2-5 repeat measurements for each setting
- (Applied data pruning to remove outliers associated with known faulty hardware.)
- Construct responses by taking the orbit difference between an initial and final setting.
    - Many possibly combinations

Horizontal (x) orbit response
Corrector A4 0A→+22A



Surrogate Model

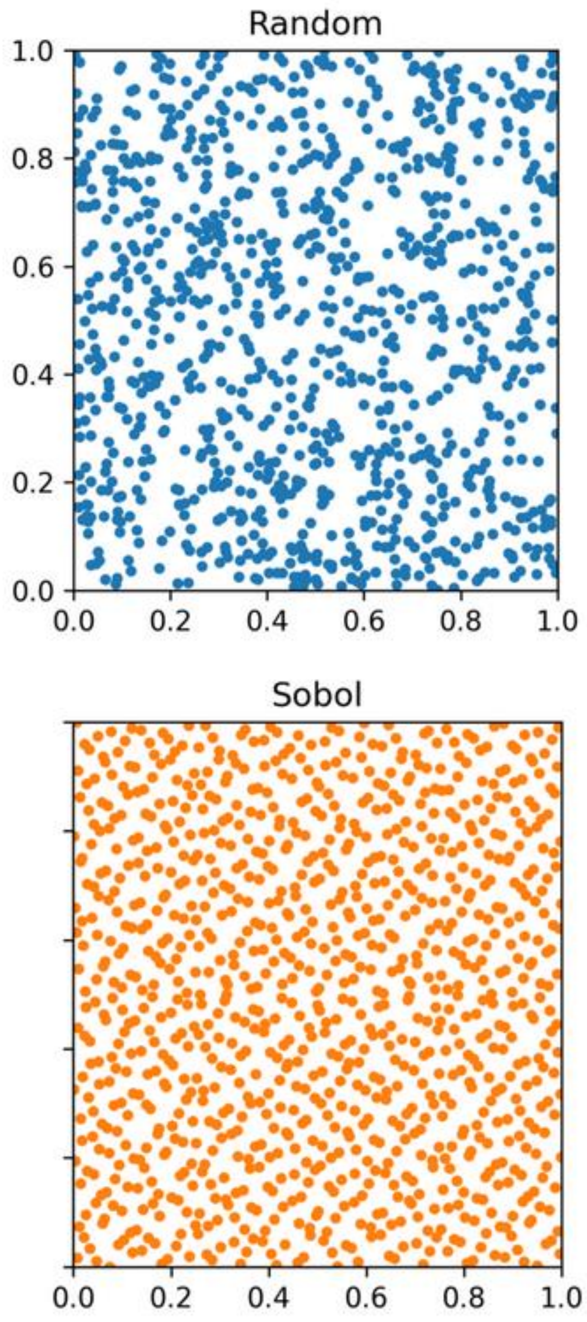
- Sampling the 48-dimensional parameter space is challenging and needs an efficient algorithm: "hybrid (aka Hamiltonian) Monte Carlo"
- This requires many simulation evaluations **including derivatives**
- Replace direct BMAD sim with machine-learned surrogate model
    - **Require highly accurate surrogate with MSE validation losses ~10^{-4} to be << BPM error (0.15mm)**
    - Train separate model for each plane
    - 77 input features and 15 (x), 18 (y) output features
    - 335,415 params residual neural network (RESNET)
    - Trained using Julia "Flux" package



The model architecture employed for this study

Surrogate data

- Use a Sobol pseudo-random uniform sampling scheme to sample the 77 input dimensions (for each plane)
  - More uniform than uniform-random
- Use data-derived ranges for static/corrector magnet currents
- Choosing ranges for the 48 “vars” nuisance parameters most challenging
  - Found increasing orbit instability / sim. failures as var range was made larger
    - Possibly due to unfortunate combinations of large vars, or
    - Orbit resonance effects
  - This could not be overcome even after intense hyperparameter optimization
  - **Needed to restrict var range to 0.94 – 1.06 to obtain sufficiently precise surrogate**
- Data subsampling required to restrict to vicinity of Booster tunes (x : 4.83±0.05,   y: 4.665±0.05)
- 2M samples generated, 820-870K surviving tune cut
- Achieved validation loss 3×10^{-4} (x), 1×10^{-4} (y)
- Corresponds to ±0.057mm, ± 0.017mm vs 0.15mm BPM error



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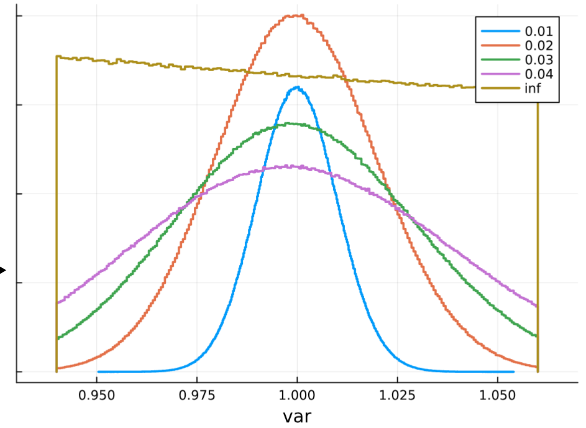
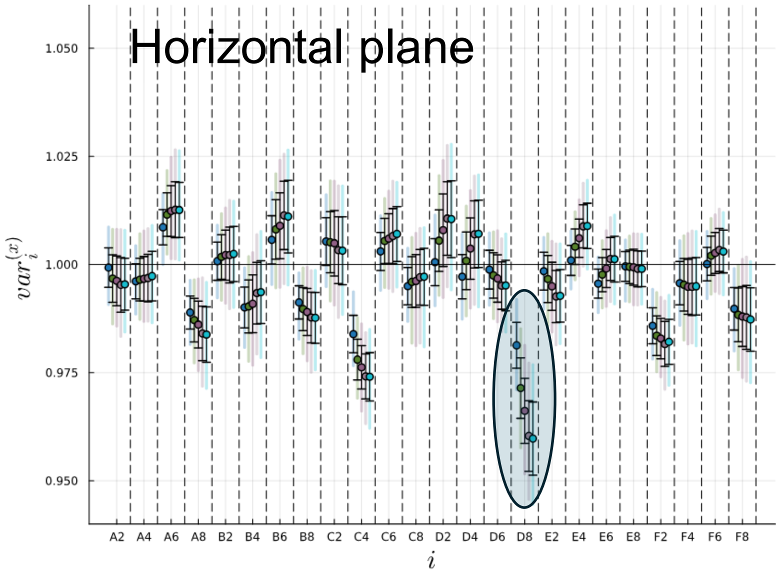
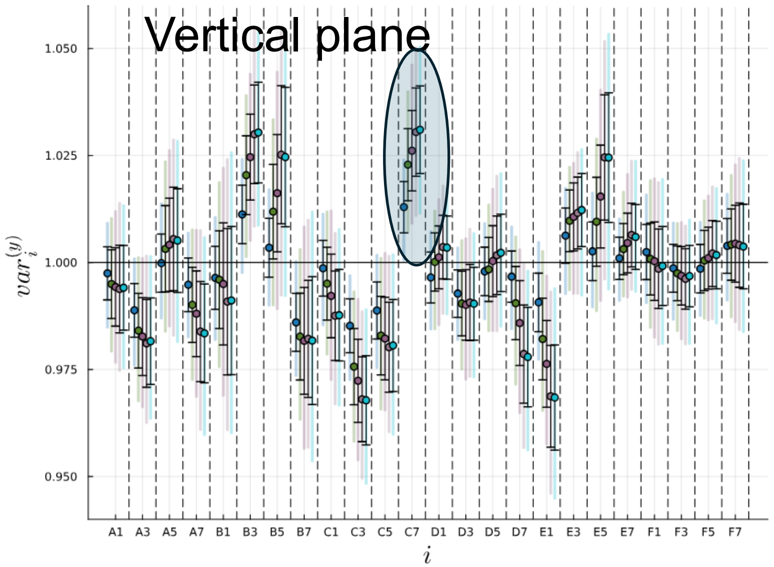
Prior sensitivity

- Lognormal prior width hard to estimate: how sensitive is our inference to the choice?
  - Perform a prior sensitivity study: $\sigma \in \{0.01, 0.02, 0.03, 0.04, \infty\}$
- Apply hard bound on prior distributions at [0.94,1.06] to account for surrogate validity
  - Distorts prior distributions for large σ≥0.04
- Use data subset where each corrector in turn kicked from 0A to +22A and -22A.





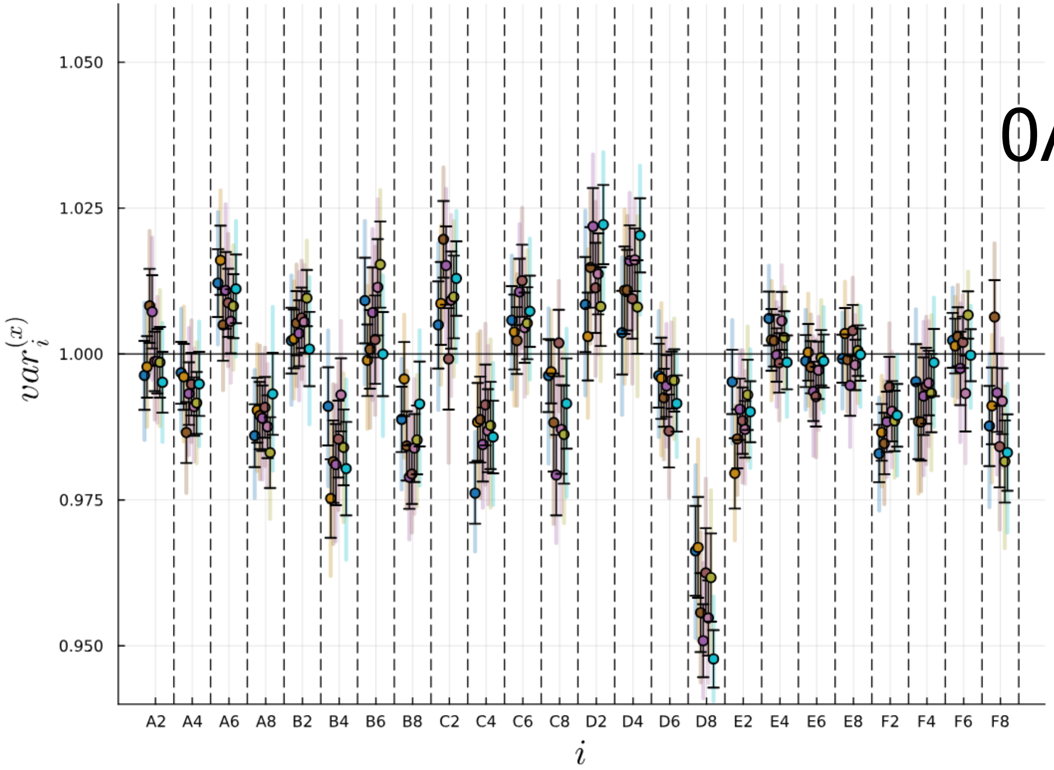
Error bars:
Inner: 68% conf
Outer: 95% conf



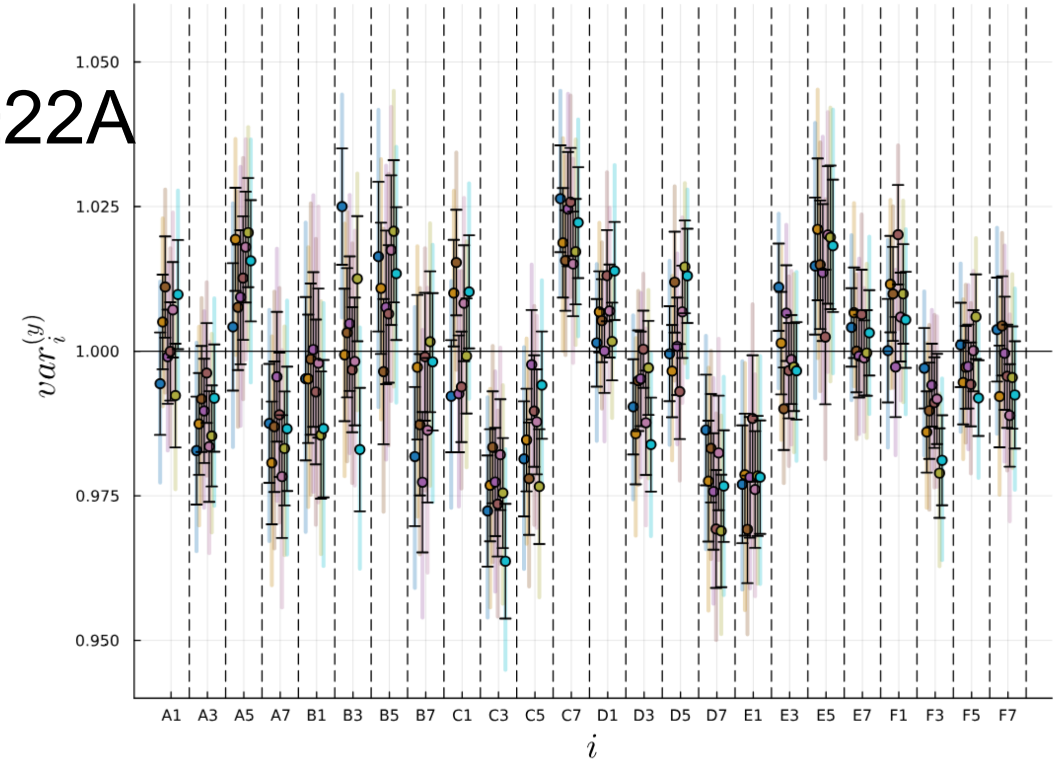
- Results generally stable under relaxing priors
- Stronger dependence on assumptions for some vars hints at near-flat directions in parameter space
- Some vars, particularly x-var “D8”, remain inconsistent with null result and move further away as priors relaxed – hints at real, physical cause?
- Choose σ=0.03 for final results as least constraining prior not overly distorted by truncation

Dataset dependence

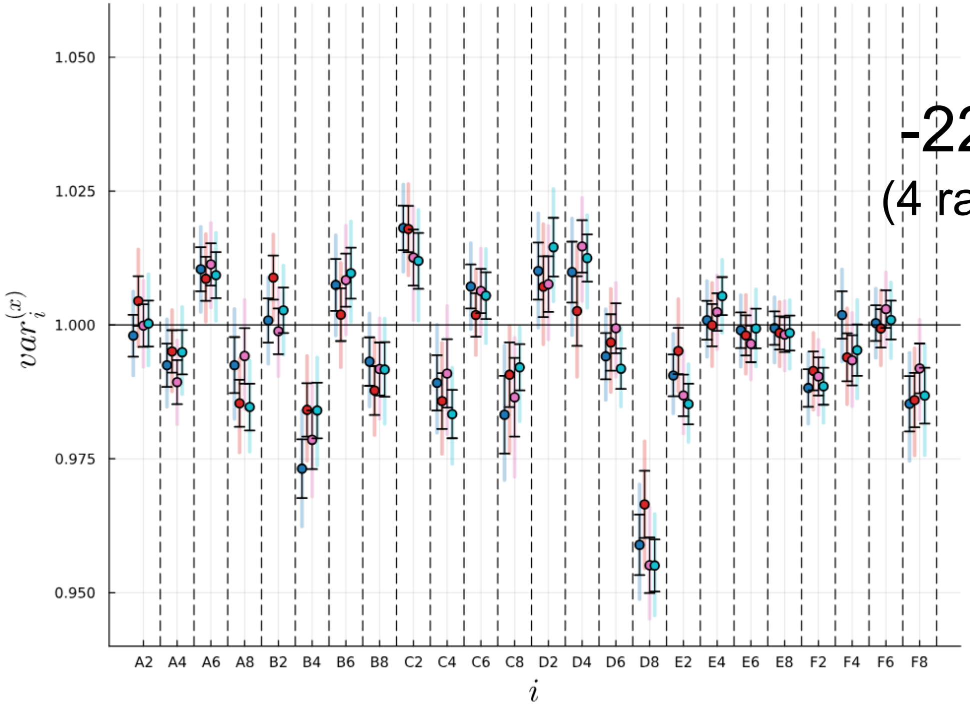
- "Pooling" all data together for inference makes analysis more susceptible to unmodeled systematic effects between different subset classes.
- Instead, we repeat the analysis for different data subsets to test for consistency
    - Randomly draw from repeat measurements for fixed corrector settings
    - **Consider multiple choices of initial and final current setting**



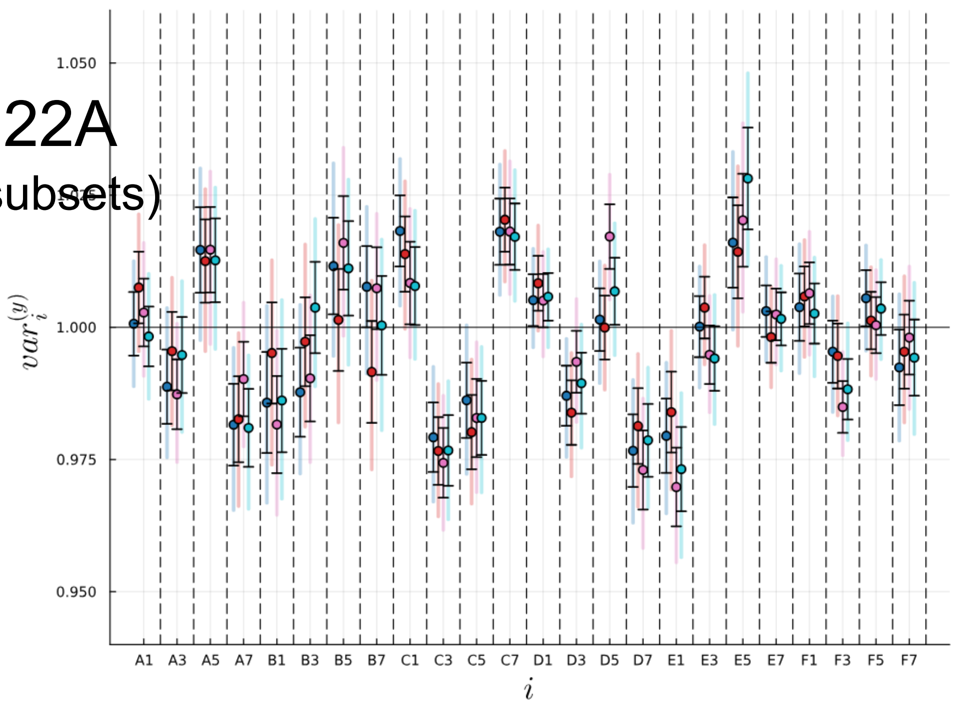
0A→±22A



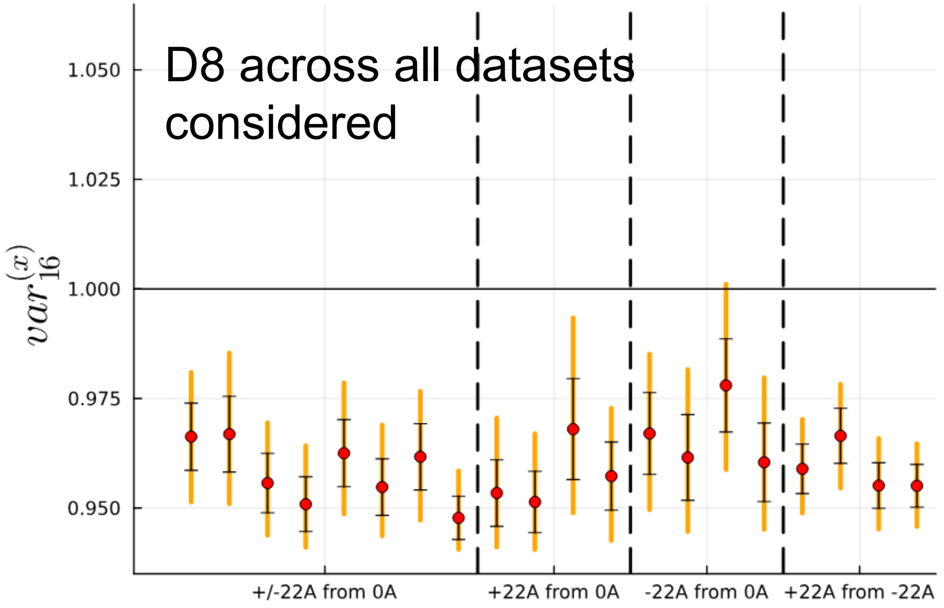
Excellent consistency



-22A→+22A
(4 random subsets)



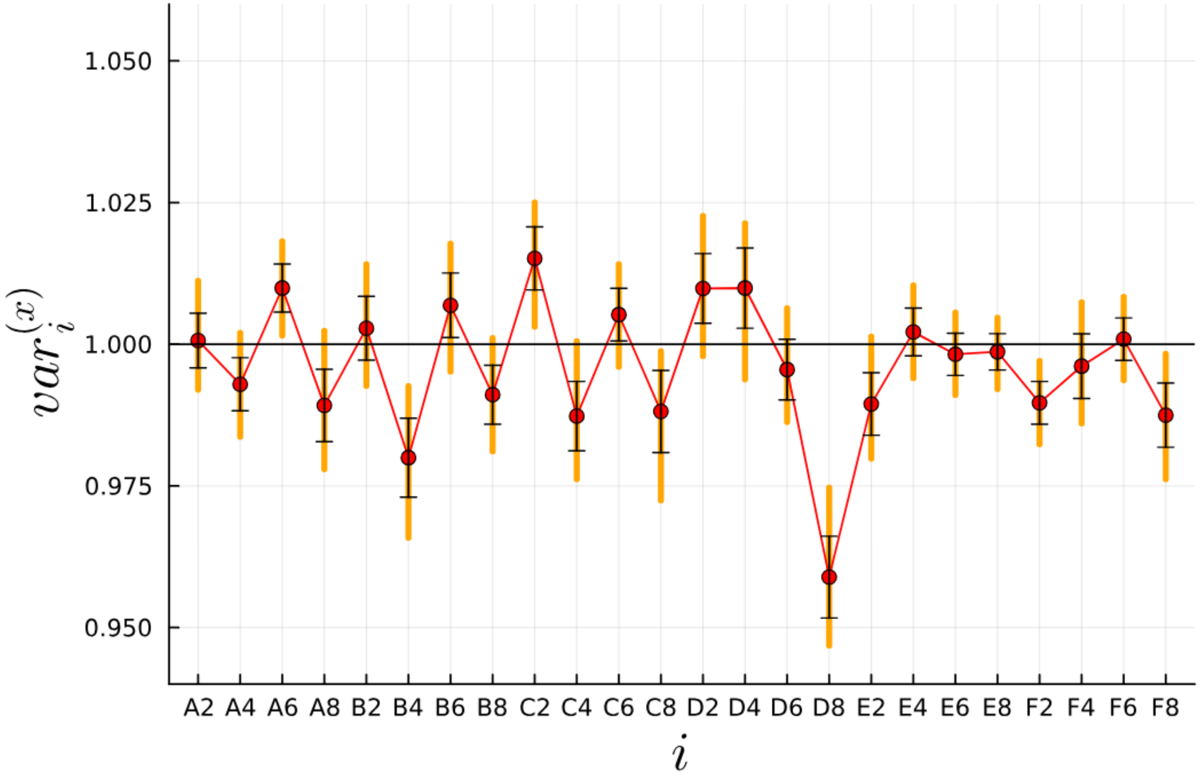
D8 across all datasets considered

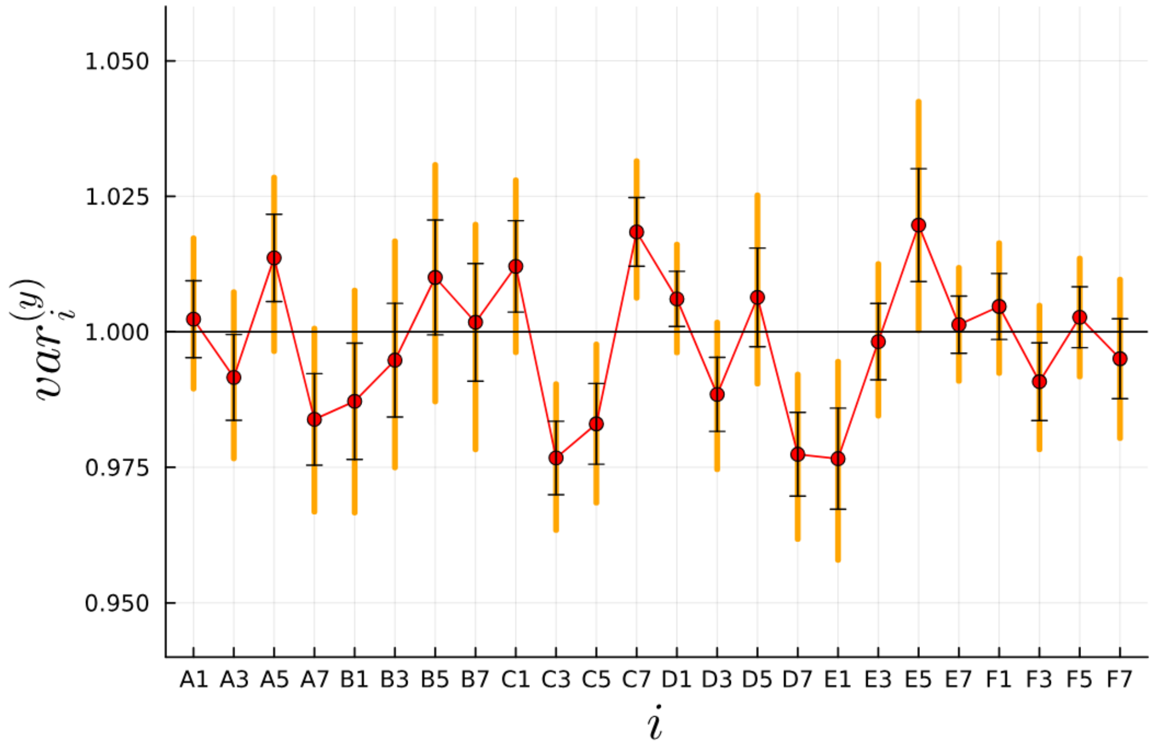


- Uncertainties significantly smaller for -22A→+22A subsets
- Likely because Digital Twin errors amplified by including two extreme corrector values

Final inference result

- Pool the four -22A→+22A results to account for dataset dependence





- Most results cluster around null result to within a few %
- D8 is notable exception
  - although close to prior lower bound, results strongly suggest data favors a low value

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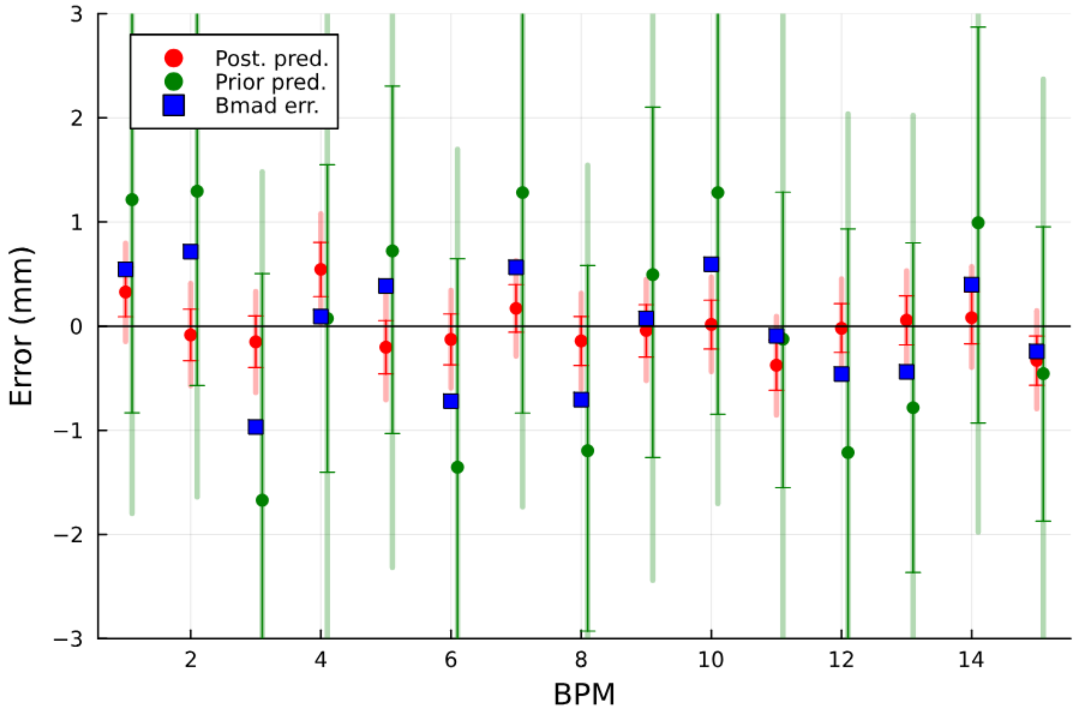
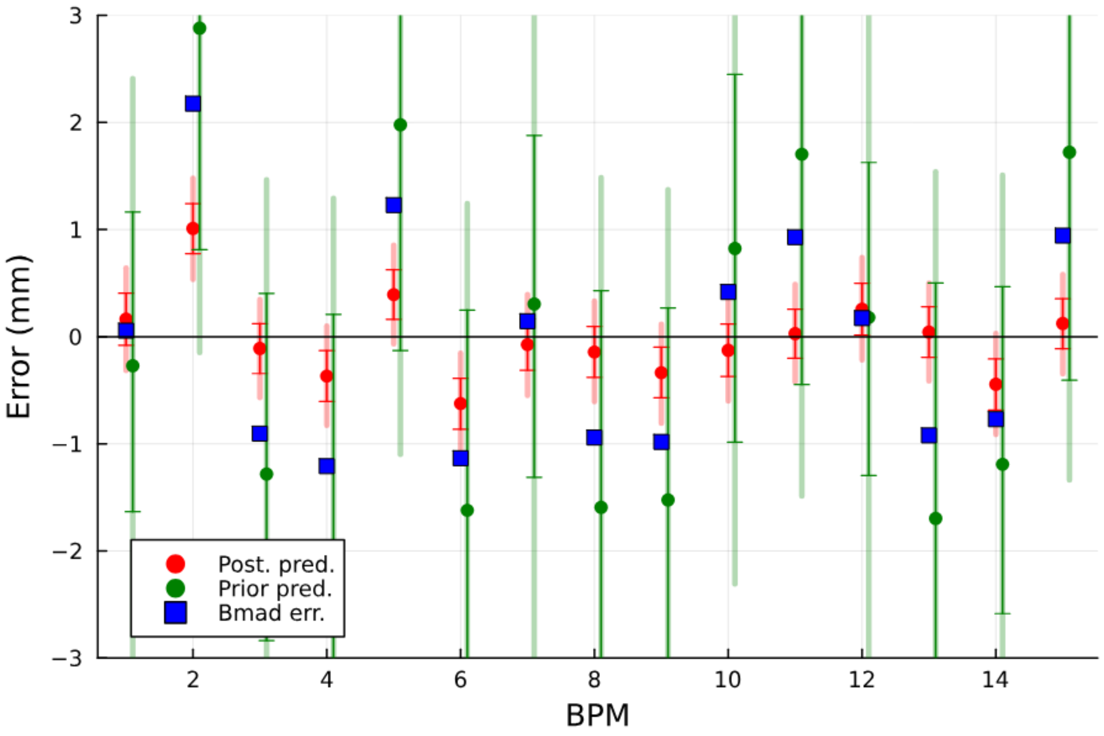
Posterior/prior predictions

- Two example orbit responses in the -22A→+22A subset





- General improvement in agreement between model and data

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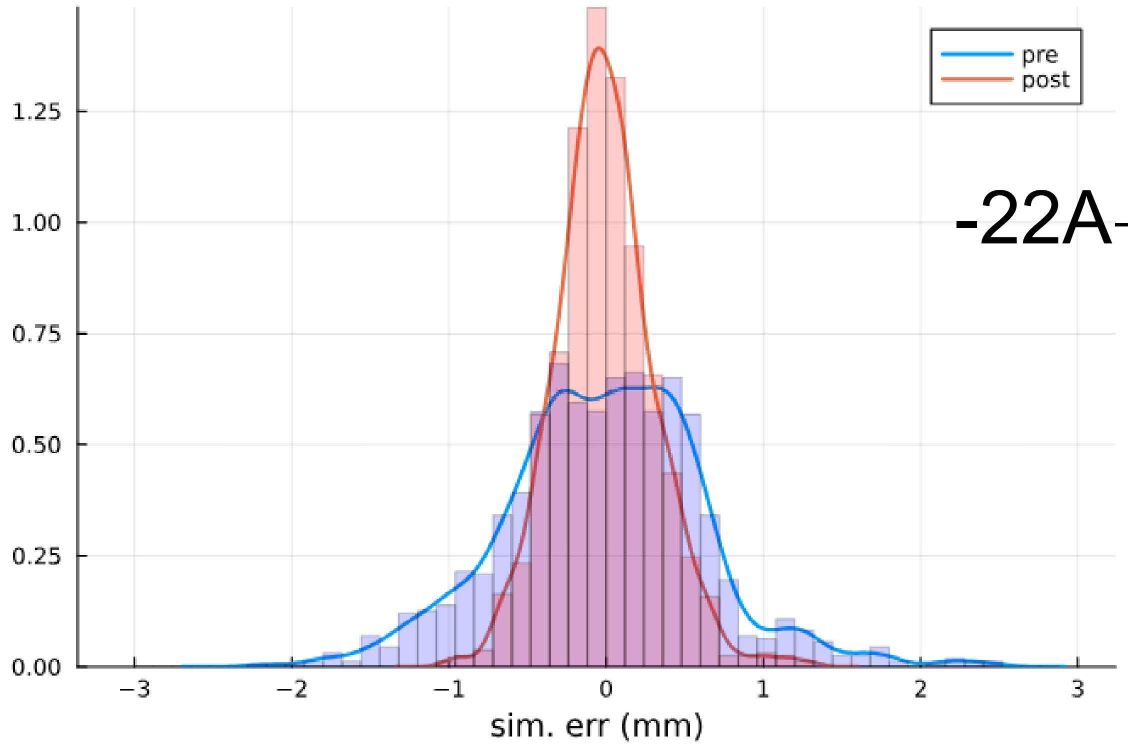
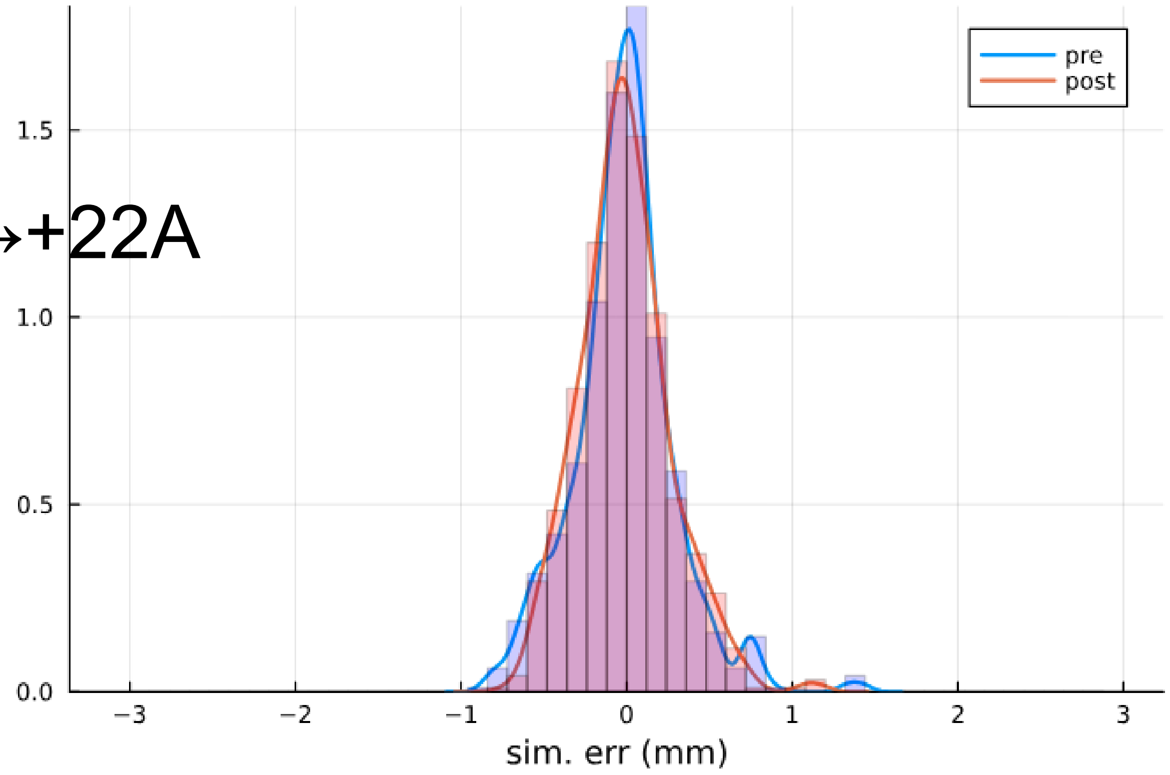
Point estimates

- Posterior predictions still use surrogate – possibility of additional error
- See if incorporating **central values** (point estimates) of var posteriors improved Bmad Digital Twin



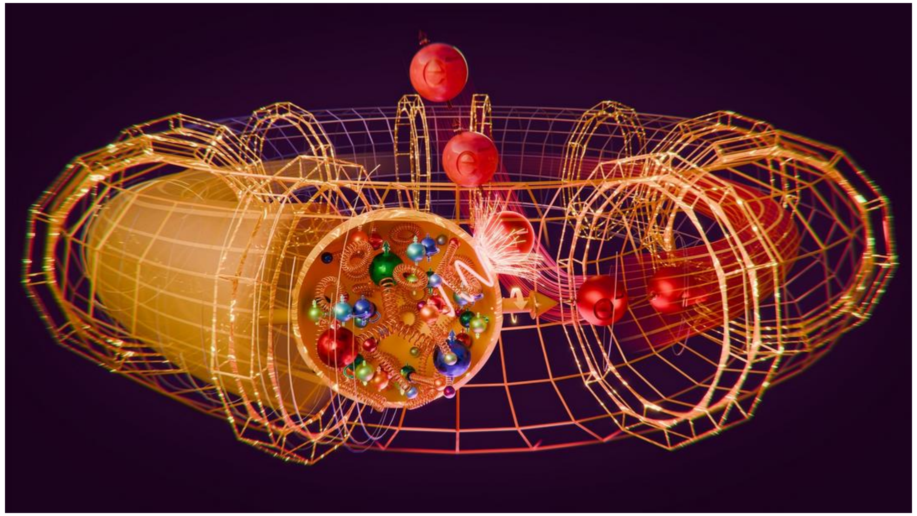
-22A→+22A



- Digital Twin error for -22A→+22A data considerably improved for horizontal plane!

Conclusions

- Introduction of magnet-dependent nuisance parameters constrained by data shows evidence of localized phenomenon that may help identify root cause.
- Including just the point-estimates significantly improves modeling errors.
- Bayesian UQ demonstrated as useful approach to quantifying error sources in accelerator Digital Twins.
- **AI/ML played a vital role in providing a fast, differentiable surrogate model of the simulation**
- Future research could be to include additional data
  - e.g. with different static magnet currents
  - or with more complicated corrector setups
  - Bayesian Optimal Experimental Design could be used to identify an optimal experiment to improve uncertainties
- Uncertainty-aware Digital Twin model could be used for improved beam control
  - Allow for assessing trade-offs of control actions with knowledge of uncertainty of modeling



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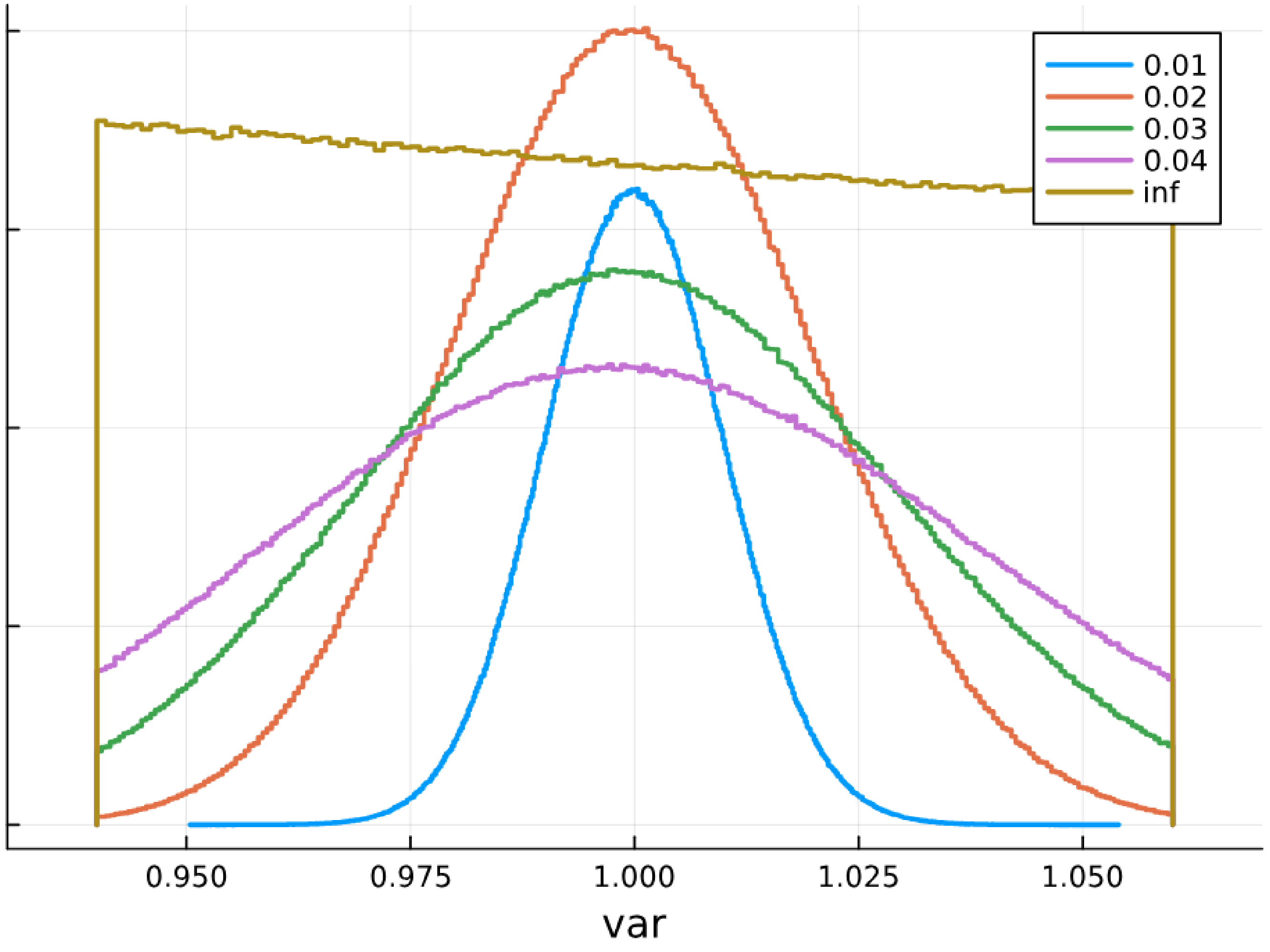
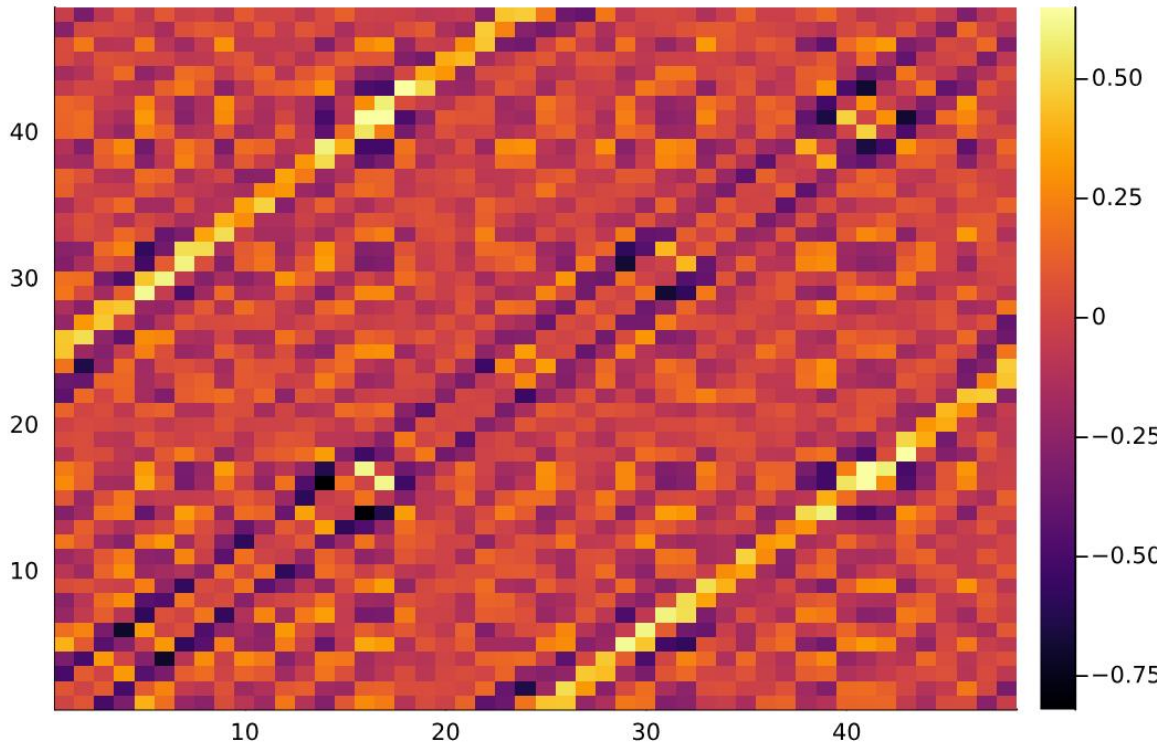
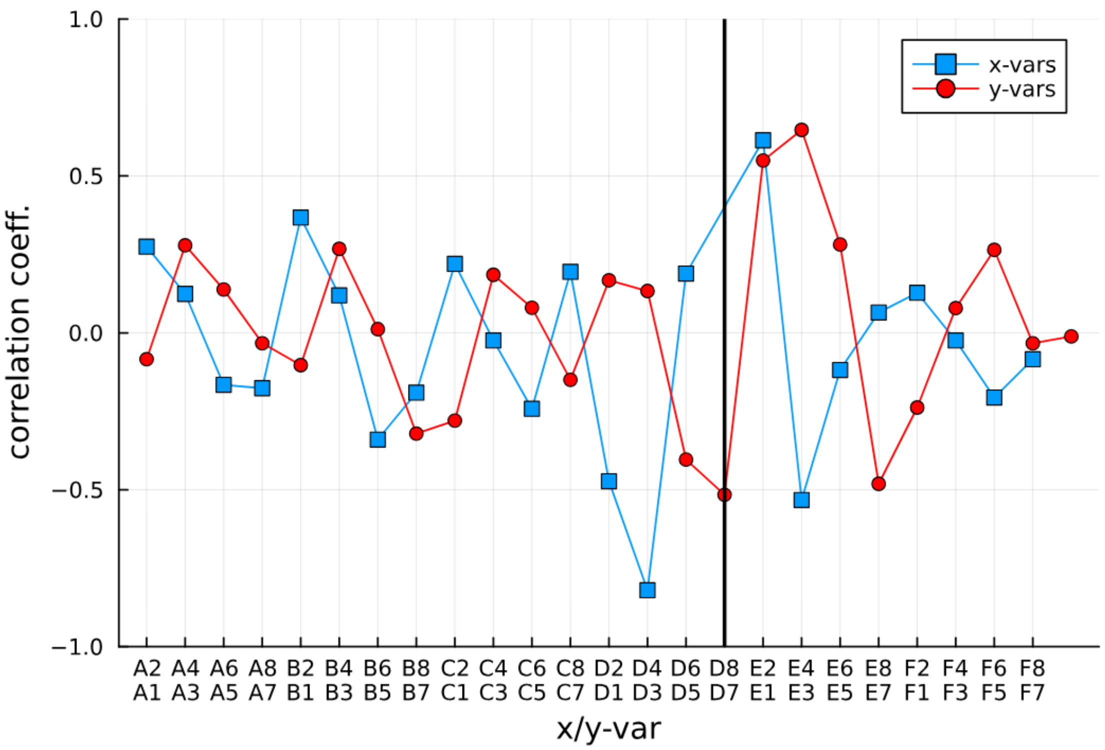
Effect of truncation on priors



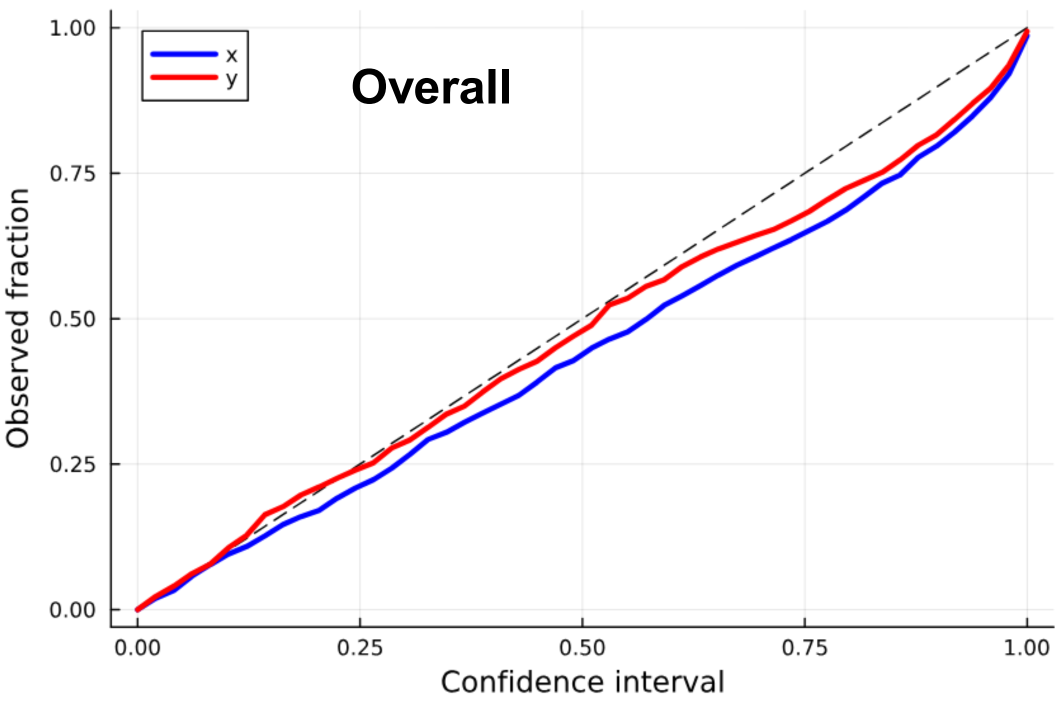
Correlation structure

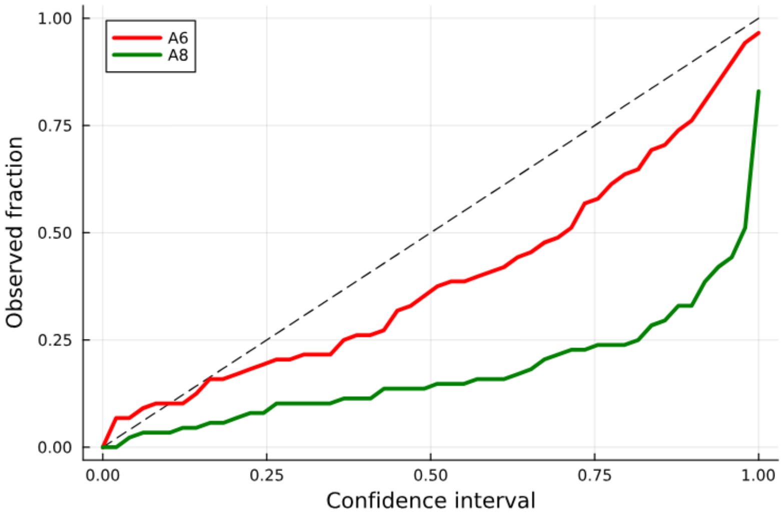


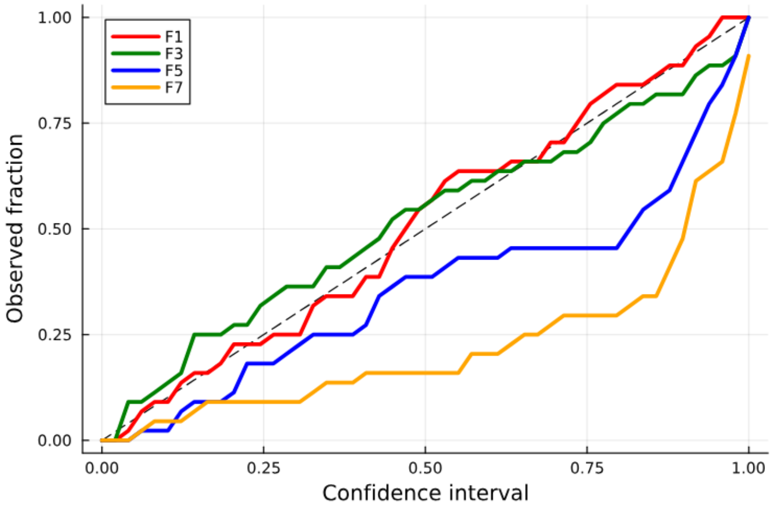


Calibration curve

- Question: are the remaining larger-than-errorbar differences in the posterior predictions due to unmodeled behavior?
- Compute fraction of data points within different confidence bands of the corresponding posterior predictive distribution
- Find data distribution is generally well described by our error bars







- Evidence of underestimation of errors (overconfidence) for some BPMS
  - Investigate in future