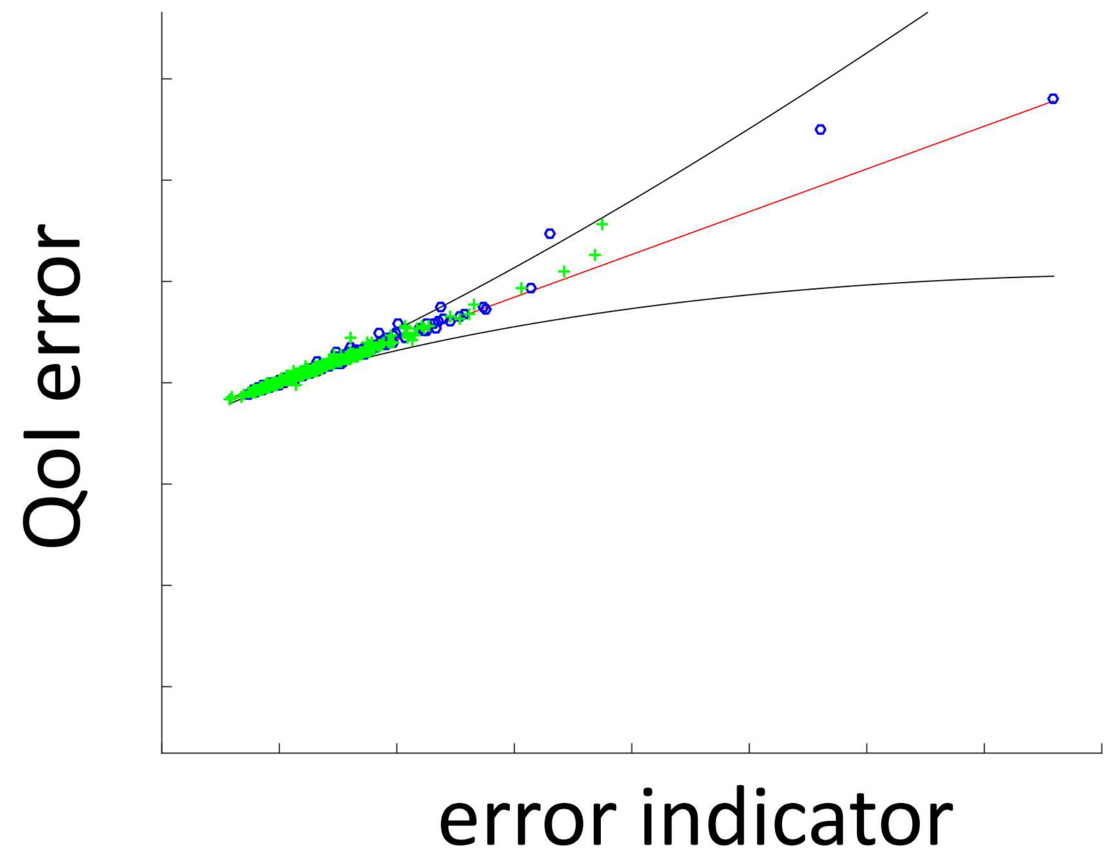
SAND2018-4585C

Integrating reduced-order models in Bayesian inference via stochastic error models

$$\underbrace{\tilde{\mathbf{q}}_{\mathrm{HFM}}(\boldsymbol{\mu})}_{\text{stochastic}} = \underbrace{\mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu})}_{\text{deterministic}} + \underbrace{\tilde{\delta}(\boldsymbol{\mu})}_{\text{stochastic}}$$



Kevin Carlberg[*], **Wayne Uy**[^], **Fei Lu**[†], **Matthias Morzfeld**[Δ]

[*]Sandia National Laboratories, [^]Cornell University,
[†]Johns Hopkins University, [Δ]University of Arizona

SIAM Conference on Uncertainty Quantification
April 19, 2018

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Surrogate modeling in UQ

inputs $\boldsymbol{\mu}$ → *high-fidelity model* → *outputs* $\mathbf{q}_{\mathrm{HFM}}$

- high-fidelity-model (HFM) noise model: $\mathbf{q}_{\mathrm{meas}} = \mathbf{q}_{\mathrm{HFM}}(\boldsymbol{\mu}) + \varepsilon$
- measurement noise ε has probability distribution $\pi_{\varepsilon}(\cdot)$
- HFM likelihood: $\pi_{\mathrm{HFM}}(\mathbf{q}_{\mathrm{meas}} \mid \boldsymbol{\mu}) = \pi_{\boldsymbol{\varepsilon}}(\mathbf{q}_{\mathrm{meas}} - \mathbf{q}_{\mathrm{HFM}}(\boldsymbol{\mu}))$

inputs $\boldsymbol{\mu}$ → *surrogate model* → *outputs* $\mathbf{q}_{\mathrm{surr}}$

- surrogate noise model: $\mathbf{q}_{\mathrm{meas}} = \mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu}) + \varepsilon$
  - inconsistent with HFM noise model
- surrogate likelihood: $\pi_{\mathrm{surr}}(\mathbf{q}_{\mathrm{meas}} \mid \boldsymbol{\mu}) = \pi_{\boldsymbol{\varepsilon}}(\mathbf{q}_{\mathrm{meas}} - \mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu}))$
  - inconsistent with HFM noise model

$$\mathbf{q}_{\mathrm{HFM}}(\boldsymbol{\mu}) = \mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu}) + \delta(\boldsymbol{\mu})$$

How can we account for the error $\delta(\boldsymbol{\mu})$?

Surrogate modeling in UQ: existing work

Simply replace high-fidelity with surrogate
[Xiu and Karniadakis, 2002; Marzouk and Najm, 2009; Frangos et al., 2010; Nguyen et al., 2010; Li, Marzouk, 2014; Cui et al., 2015]

+ straightforward, can optimize surrogate
- does not account for surrogate error
- inconsistent with HFM noise model

Multifidelity model management [Peherstorfer, Willcox, Gunzberger, 2016]

- Forward UQ [Giles, 2008; Ng and Willcox, 2014; Narayan et al., 2014; Teckentrup et al., 2015; Peherstorfer et al., 2016]
- Inverse UQ [Christen and Fox, 2005; Efendiev et al., 2006; Cotter et al., 2013; Cui et al., 2013]

+ guaranteed convergence to high-fidelity UQ analysis
- many queries of high-fidelity model

Stochastic model of the surrogate error

- Surrogate itself is stochastic [Bilionis, Zabaras, 2012; Moustapha et al., 2016]
- Construct a stochastic error model
  [Ng and Eldred, 2012; Drohmann and C., 2015; Manzoni, Pagani, Lassila, 2016; Trehan, C., Durlofsky, 2017]

+ no queries of high-fidelity model
+ rigorous: accounts for surrogate epistemic uncertainty
- does not converge to high-fidelity UQ analysis

Surrogate modeling in UQ

$$\mathbf{q}_{\text{HFM}}(\boldsymbol{\mu}) = \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}) + \boldsymbol{\delta}(\boldsymbol{\mu})$$

- HFM noise model: $\mathbf{q}_{\text{meas}} = \mathbf{q}_{\text{HFM}}(\boldsymbol{\mu}) + \boldsymbol{\varepsilon}$
$$= \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}) + \boldsymbol{\delta}(\boldsymbol{\mu}) + \boldsymbol{\varepsilon}$$
- HFM likelihood: $\pi_{\text{HFM}}(\mathbf{q}_{\text{meas}} \,|\, \boldsymbol{\mu}) = \pi_{\boldsymbol{\varepsilon}}(\mathbf{q}_{\text{meas}} - \mathbf{q}_{\text{HFM}}(\boldsymbol{\mu}))$
$$= \pi_{\boldsymbol{\varepsilon}}(\mathbf{q}_{\text{meas}} - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}) - \boldsymbol{\delta}(\boldsymbol{\mu}))$$

\+ equivalent to high-fidelity-model formulation

− not practical: the error $\boldsymbol{\delta}(\boldsymbol{\mu})$ is deterministic but generally unknown

Idea: *stochastic model $\tilde{\delta}(\mu)$ for the error that models its uncertainty*

$$\underbrace{\tilde{\mathbf{q}}_{\text{HFM}}(\boldsymbol{\mu})}_{\text{stochastic}} = \underbrace{\mathbf{q}_{\text{surr}}(\boldsymbol{\mu})}_{\text{deterministic}} + \underbrace{\tilde{\boldsymbol{\delta}}(\boldsymbol{\mu})}_{\text{stochastic}}$$

- stochastic HFM noise model: $\mathbf{q}_{\text{meas}} = \tilde{\mathbf{q}}_{\text{HFM}}(\boldsymbol{\mu}) + \boldsymbol{\varepsilon}$
$$= \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}) + \tilde{\boldsymbol{\delta}}(\boldsymbol{\mu}) + \boldsymbol{\varepsilon}$$
- stochastic HFM likelihood: $\pi_{\widetilde{\text{HFM}}}(\mathbf{q}_{\text{meas}} \,|\, \boldsymbol{\mu}) = \pi_{\boldsymbol{\varepsilon}+\tilde{\boldsymbol{\delta}}}(\mathbf{q}_{\text{meas}} - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}))$

\+ consistent with HFM noise model

\+ practical if the stochastic error model $\tilde{\delta}$ is computable

Questions

- What properties do we want in a stochastic error model?
- How does a stochastic error model affect Bayesian inference?
- What is the optimal stochastic error model?
- How can we construct a stochastic error model for reduced-order models?

Questions

- **What properties do we want in a stochastic error model?**
- How does a stochastic error model affect Bayesian inference?
- What is the optimal stochastic error model?
- How can we construct a stochastic error model for reduced-order models?

Stochastic error model

$$\underbrace{\tilde{\mathbf{q}}_{\mathsf{HFM}}(\boldsymbol{\mu})}_{\text{stochastic}} = \underbrace{\mathbf{q}_{\mathsf{surr}}(\boldsymbol{\mu})}_{\text{deterministic}} + \underbrace{\tilde{\delta}(\boldsymbol{\mu})}_{\text{stochastic}}$$

- Forward UQ: $\pi_{\mathsf{HFM}}(\mathbf{q}_{\mathsf{meas}} \mid \boldsymbol{\mu}) = \pi_{\boldsymbol{\varepsilon}}(\mathbf{q}_{\mathsf{meas}} - \mathbf{q}_{\mathsf{HFM}}(\boldsymbol{\mu}))$

  $\pi_{\widetilde{\mathsf{HFM}}}(\mathbf{q}_{\mathsf{meas}} \mid \boldsymbol{\mu}) = \pi_{\boldsymbol{\varepsilon}+\tilde{\delta}}(\mathbf{q}_{\mathsf{meas}} - \mathbf{q}_{\mathsf{surr}}(\boldsymbol{\mu}))$

- Inverse UQ: $\pi_{\mathsf{post}}^{\mathsf{HFM}}(\boldsymbol{\mu} \mid \mathbf{q}_{\mathsf{meas}}) \propto \pi_{\mathsf{prior}}(\boldsymbol{\mu})\pi_{\boldsymbol{\varepsilon}}(\mathbf{q}_{\mathsf{meas}} - \mathbf{q}_{\mathsf{HFM}}(\boldsymbol{\mu}))$

  $\pi_{\mathsf{post}}^{\widetilde{\mathsf{HFM}}}(\boldsymbol{\mu} \mid \mathbf{q}_{\mathsf{meas}}) \propto \pi_{\mathsf{prior}}(\boldsymbol{\mu})\pi_{\boldsymbol{\varepsilon}+\tilde{\delta}}(\mathbf{q}_{\mathsf{meas}} - \mathbf{q}_{\mathsf{surr}}(\boldsymbol{\mu}))$

- Desired properties in stochastic error model $\tilde{\delta}(\boldsymbol{\mu})$
  1. cheaply computable: similar cost to evaluating the surrogate
  2. low variance: introduces as little uncertainty as possible

$$\lim_{\mathrm{Var}(\tilde{\delta})\to 0} \pi_{\widetilde{\mathsf{HFM}}}(\mathbf{q}_{\mathsf{meas}} \mid \boldsymbol{\mu}) = \pi_{\mathsf{HFM}}(\mathbf{q}_{\mathsf{meas}} \mid \boldsymbol{\mu})$$

$$\lim_{\mathrm{Var}(\tilde{\delta})\to 0} \pi_{\mathsf{post}}^{\widetilde{\mathsf{HFM}}}(\boldsymbol{\mu} \mid \mathbf{q}_{\mathsf{meas}}) = \pi_{\mathsf{post}}^{\mathsf{HFM}}(\boldsymbol{\mu} \mid \mathbf{q}_{\mathsf{meas}})$$

  3. validated: correctly models the epistemic uncertainty in the error

Questions

- What properties do we want in a stochastic error model?
- How does a stochastic error model affect Bayesian inference?
- **What is the optimal stochastic error model?**
- How can we construct a stochastic error model for reduced-order models?

Stochastic error model

$$\underbrace{\tilde{\mathbf{q}}_{\text{HFM}}(\boldsymbol{\mu})}_{\text{stochastic}} = \underbrace{\mathbf{q}_{\text{surr}}(\boldsymbol{\mu})}_{\text{deterministic}} + \underbrace{\tilde{\delta}(\boldsymbol{\mu})}_{\text{stochastic}}$$

- Forward UQ: $\pi_{\text{HFM}}(\mathbf{q}_{\text{meas}} \mid \boldsymbol{\mu}) = \pi_{\varepsilon}(\mathbf{q}_{\text{meas}} - \mathbf{q}_{\text{HFM}}(\boldsymbol{\mu})$

  $\pi_{\widetilde{\text{HFM}}}(\mathbf{q}_{\text{meas}} \mid \boldsymbol{\mu}) = \pi_{\varepsilon+\tilde{\delta}}(\mathbf{q}_{\text{meas}} - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}))$
- Inverse UQ: $\pi^{\text{HFM}}_{\text{post}}(\boldsymbol{\mu} \mid \mathbf{q}_{\text{meas}}) \propto \pi_{\text{prior}}(\boldsymbol{\mu})\pi_{\varepsilon}(\mathbf{q}_{\text{meas}} - \mathbf{q}_{\text{HFM}}(\boldsymbol{\mu}))$

  $\pi^{\widetilde{\text{HFM}}}_{\text{post}}(\boldsymbol{\mu} \mid \mathbf{q}_{\text{meas}}) \propto \pi_{\text{prior}}(\boldsymbol{\mu})\pi_{\varepsilon+\tilde{\delta}}(\mathbf{q}_{\text{meas}} - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}))$

Homoscedastic $\tilde{\delta}(\boldsymbol{\mu})$

- **Low-variance error model**: $\text{Var}(\tilde{\delta}(\boldsymbol{\mu}) + \varepsilon) \approx \text{Var}(\varepsilon)$
  - *Forward UQ.* measurements certain: $D_{\text{KL}}(\pi_{\text{HFM}} \,\|\, \pi_{\widetilde{\text{HFM}}})$ small
  - *Inverse UQ.* data informative: $D_{\text{KL}}(\pi^{\text{HFM}}_{\text{post}} \,\|\, \pi^{\widetilde{\text{HFM}}}_{\text{post}})$ small
- **High-variance error model:** $\text{Var}(\tilde{\delta}(\boldsymbol{\mu}) + \varepsilon) \gg \text{Var}(\varepsilon)$
  - *Forward UQ*: measurements uncertain: $D_{\text{KL}}(\pi_{\text{HFM}} \,\|\, \pi_{\widetilde{\text{HFM}}})$ large
  - *Inverse UQ*: data uninformative: $D_{\text{KL}}(\pi_{\text{prior}} \,\|\, \pi^{\widetilde{\text{HFM}}}_{\text{post}})$ small

Heteroscedastic $\tilde{\delta}(\boldsymbol{\mu})$

- measurements certain, data informative for $\boldsymbol{\mu}$ where surrogate trusted

Questions

- What properties do we want in a stochastic error model?
- How does a stochastic error model affect Bayesian inference?
- **What is the optimal stochastic error model?**
- How can we construct a stochastic error model for reduced-order models?

Case 1: Deterministic error model

Proposition [Manzoni, Pagani, Lassila, 2014]

If the following conditions hold:

1. $\varepsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$
2. The error model $\tilde{\delta}(\boldsymbol{\mu})$ is deterministic
3. The error model satisfies

$$\|\mathbf{q}_{\text{meas}}(\boldsymbol{\mu}) - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}) - \tilde{\delta}(\boldsymbol{\mu})\| < \|\mathbf{q}_{\text{HFM}}(\boldsymbol{\mu}) - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu})\|, \quad \forall \boldsymbol{\mu} \in \mathcal{D}$$

then

$$D_{\text{KL}}(\pi_{\text{HFM}} \,\|\, \pi_{\widetilde{\text{HFM}}}) < D_{\text{KL}}(\pi_{\text{HFM}} \,\|\, \pi_{\text{surr}}), \quad \forall \boldsymbol{\mu} \in \mathcal{D}$$

– Deterministic error model violates property 3 (validation)

Case 2: Gaussian, homoscedastic error model

Proposition [C., Uy, Lu, Morzfeld, 2018]

If the following conditions hold:

1. $\varepsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$,
2. Error model is Gaussian and homoscedastic
$$\tilde{\boldsymbol{\delta}}(\boldsymbol{\mu}) \sim \mathcal{N}(\tilde{\mathbf{m}}(\boldsymbol{\mu}), \tilde{\sigma}^2 \mathbf{I}), \quad \forall \boldsymbol{\mu} \in \mathcal{D}$$
3. Error model is unbiased $\mathrm{E}[\tilde{\mathbf{m}}(\boldsymbol{\mu})] = \boldsymbol{\delta}(\boldsymbol{\mu}), \ \forall \boldsymbol{\mu} \in \mathcal{D}$,

then

$$\max_{\tilde{\sigma}^2} \mathrm{E}_{\text{prior}}[D_{\text{KL}}(\pi_{\text{HFM}} \,\|\, \pi_{\text{surr}}) - D_{\text{KL}}(\pi_{\text{HFM}} \,\|\, \pi_{\widetilde{\text{HFM}}})]$$

is positive and is attained at

$$\tilde{\sigma}_\star^2 = \frac{1}{n_s} \mathrm{E}_{\text{prior}}[\|\mathbf{q}_{\text{HFM}}(\boldsymbol{\mu}) - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}) - \tilde{\mathbf{m}}(\boldsymbol{\mu})\|^2]$$

+ Suggests error-model noise can be computed as sample variance

$$\tilde{\sigma}^2 = \frac{1}{n_s} \mathrm{E}_{\text{data}}[\|\mathbf{q}_{\text{HFM}}(\boldsymbol{\mu}) - \mathbf{q}_{\text{surr}}(\boldsymbol{\mu}) - \tilde{\mathbf{m}}(\boldsymbol{\mu})\|^2]$$

− Homoscedasticity may violate property 3

Case 3: Gaussian, heteroscedastic error model

Proposition [C., Uy, Lu, Morzfeld, 2018]

Let $\{\mathcal{D}_i\}_{i=1}^{M}$ be a non-overlapping partition of the parameter space $\mathcal{D}$.
If the following conditions hold:

1. $\varepsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$,
2. Error model is Gaussian and heteroscedastic such that
$$\tilde{\boldsymbol{\delta}}(\boldsymbol{\mu}) \sim \mathcal{N}(\tilde{\mathbf{m}}(\boldsymbol{\mu}), \tilde{\sigma}_i{}^2 \mathbf{I}), \quad \forall \boldsymbol{\mu} \in \mathcal{D}_i$$
3. Error model is unbiased $\mathrm{E}[\tilde{\mathbf{m}}(\boldsymbol{\mu})] = \boldsymbol{\delta}(\boldsymbol{\mu})$, $\forall \boldsymbol{\mu} \in \mathcal{D}$,

then

$$\max_{\tilde{\sigma}_i^2} \mathrm{E}_{\mathrm{prior}}[D_{\mathrm{KL}}(\pi_{\mathrm{HFM}} \,\|\, \pi_{\mathrm{surr}}) - D_{\mathrm{KL}}(\pi_{\mathrm{HFM}} \,\|\, \pi_{\widetilde{\mathrm{HFM}}})\mathbf{1}_{\mathcal{D}_i}(\boldsymbol{\mu})]$$

is positive and is attained at

$$\tilde{\sigma}_{i,\star}^2 = \frac{1}{n_s} \mathrm{E}_{\mathrm{prior}}[\|\mathbf{q}_{\mathrm{HFM}}(\boldsymbol{\mu}) - \mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu}) - \tilde{\mathbf{m}}(\boldsymbol{\mu})\|^2 \mid \mathcal{D}_i]$$

+ Error-model noise should be computed as sample variance over regions

$$\tilde{\sigma}_i^2 = \frac{1}{n_s} \mathrm{E}_{\mathrm{data}}[\|\mathbf{q}_{\mathrm{HFM}}(\boldsymbol{\mu}) - \mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu}) - \tilde{\mathbf{m}}(\boldsymbol{\mu})\|^2 \mid \mathcal{D}_i]$$

+ Heteroscedasticity can satisfy property 3

Questions

- What properties do we want in a stochastic error model?
- How does a stochastic error model affect Bayesian inference?
- What is the optimal stochastic error model?
- **How can we construct a stochastic error model for reduced-order models?**

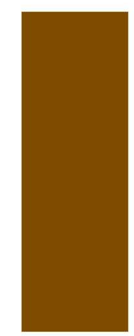
Reduced-order modeling

High-fidelity model

$$\mathbf{r}(\mathbf{x};\boldsymbol{\mu}) = 0, \quad \mathbf{q}_{\mathrm{HFM}}(\boldsymbol{\mu}) = \mathbf{q}(\mathbf{x}(\boldsymbol{\mu});\boldsymbol{\mu})$$

Reduced-order model

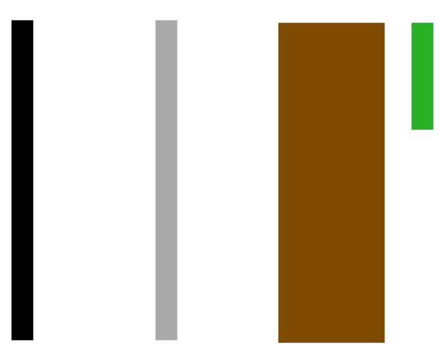
- **Offline:** construct low-dimensional basis $\boldsymbol{\Phi}$



- **Online:** construct low-dimensional basis

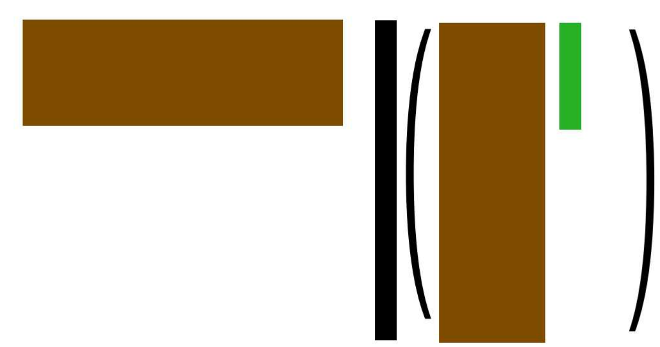
1. Reduce number of unknowns

$$\mathbf{x} \approx \mathbf{x} = \boldsymbol{\Phi}\hat{\mathbf{x}}$$



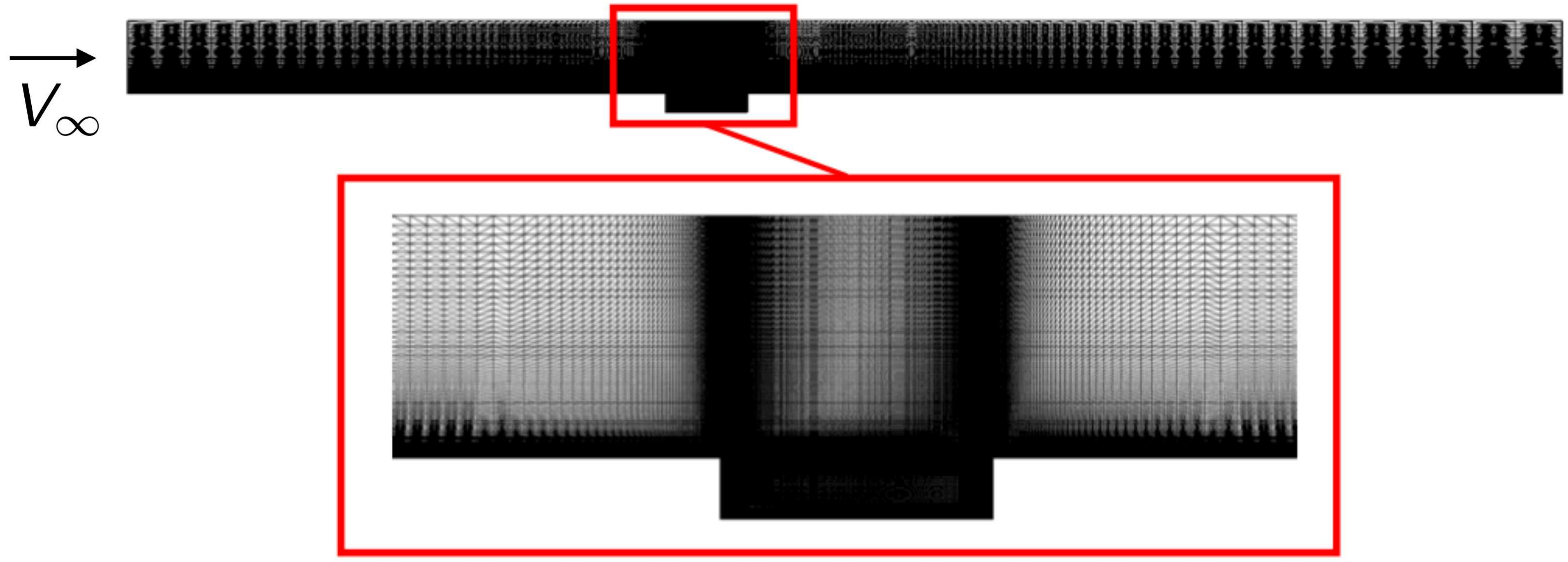
2. Reduce number of equations

$$\boldsymbol{\Phi}^T\mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}};\boldsymbol{\mu}) = \mathbf{0}$$



$$\boldsymbol{\Phi}^T\mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}};\boldsymbol{\mu}) = \mathbf{0}, \quad \mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu}) = \mathbf{q}(\boldsymbol{\Phi}\hat{\mathbf{x}}(\boldsymbol{\mu});\boldsymbol{\mu})$$

ROM demonstration: turbulent cavity



- Unsteady Navier–Stokes
- Re = 6.3 x 10^6
- M_∞ = 0.6

Spatial discretization
- 2nd-order finite volume
- DES turbulence model
- 1.2×10^6 degrees of freedom

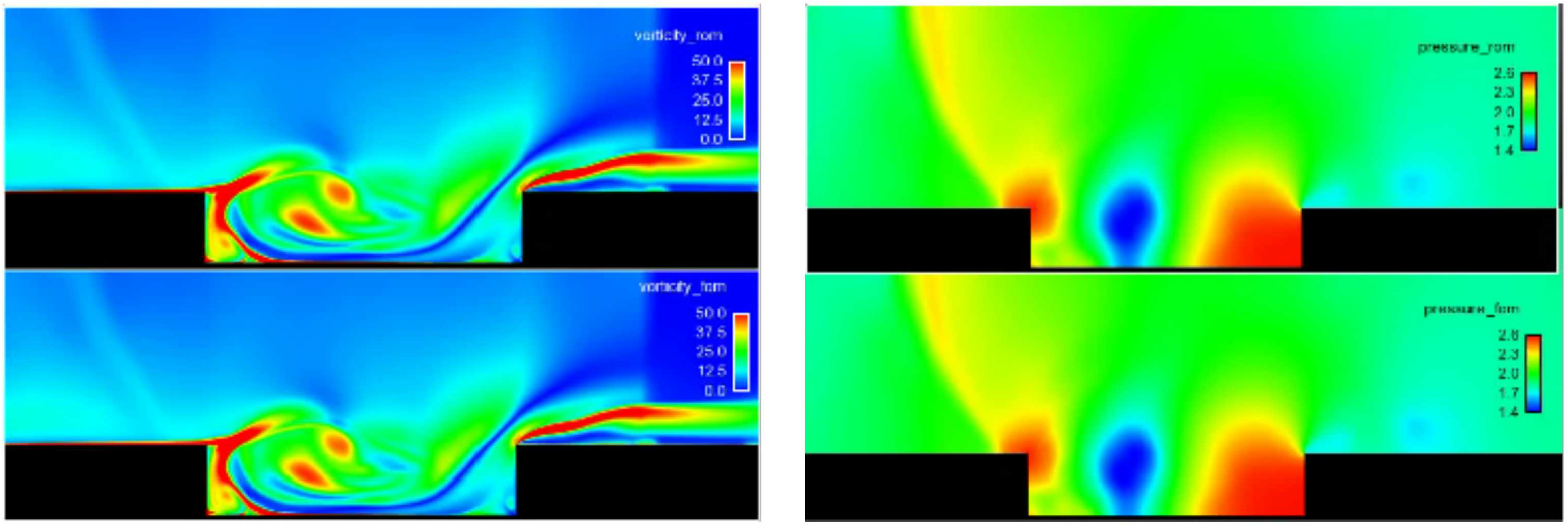
Temporal discretization
- 2nd-order BDF
- Verified time step $\Delta t = 1.5 \times 10^{-3}$
- 8.3×10^3 time instances

Turbulent-cavity results [C., Barone, Antil, 2017]

vorticity field *pressure field*

GNAT ROM
dim: 179
32 min, 2 cores

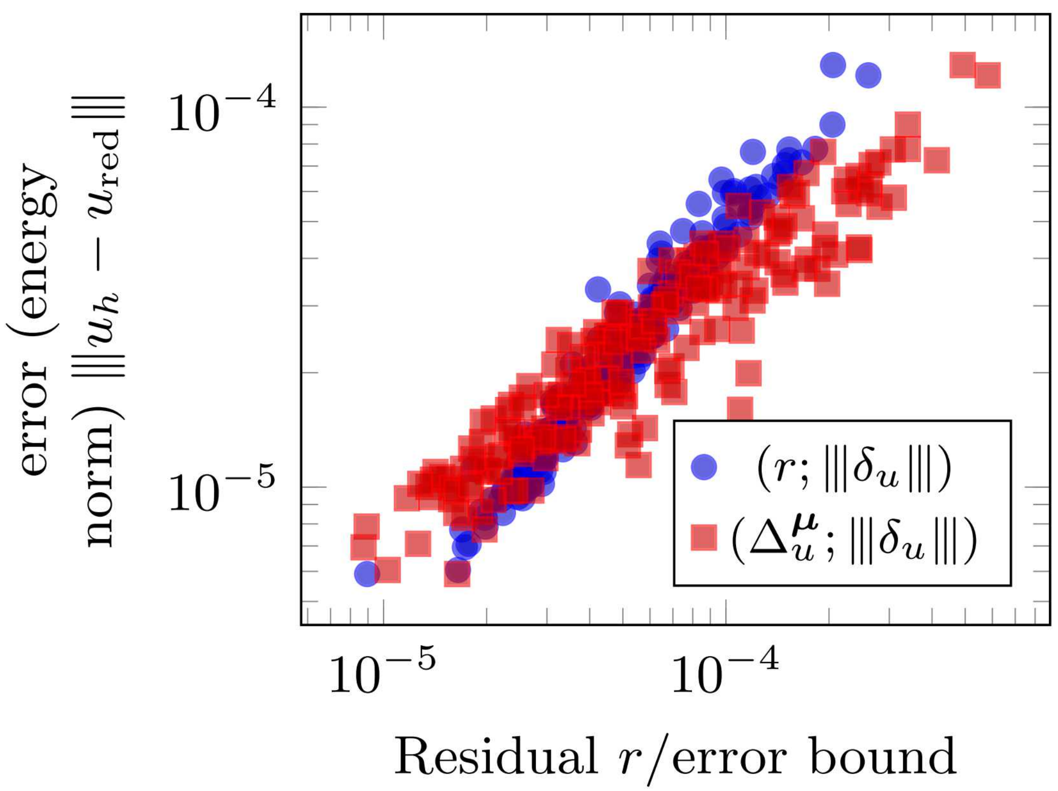
high-fidelity
dim: 1.2M
5 hours, 48 cores

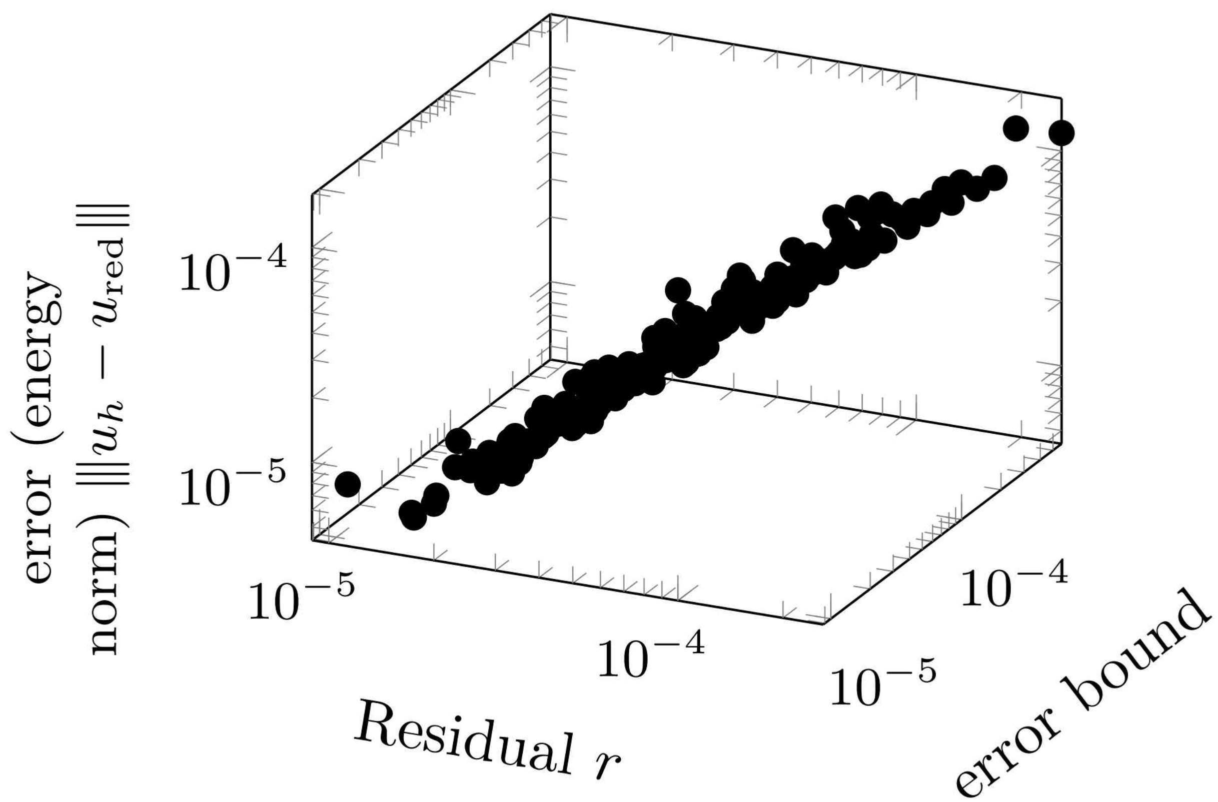


+ *<1% error*
+ *229X computational-cost reduction*

How can we construct an error model for the ROM?

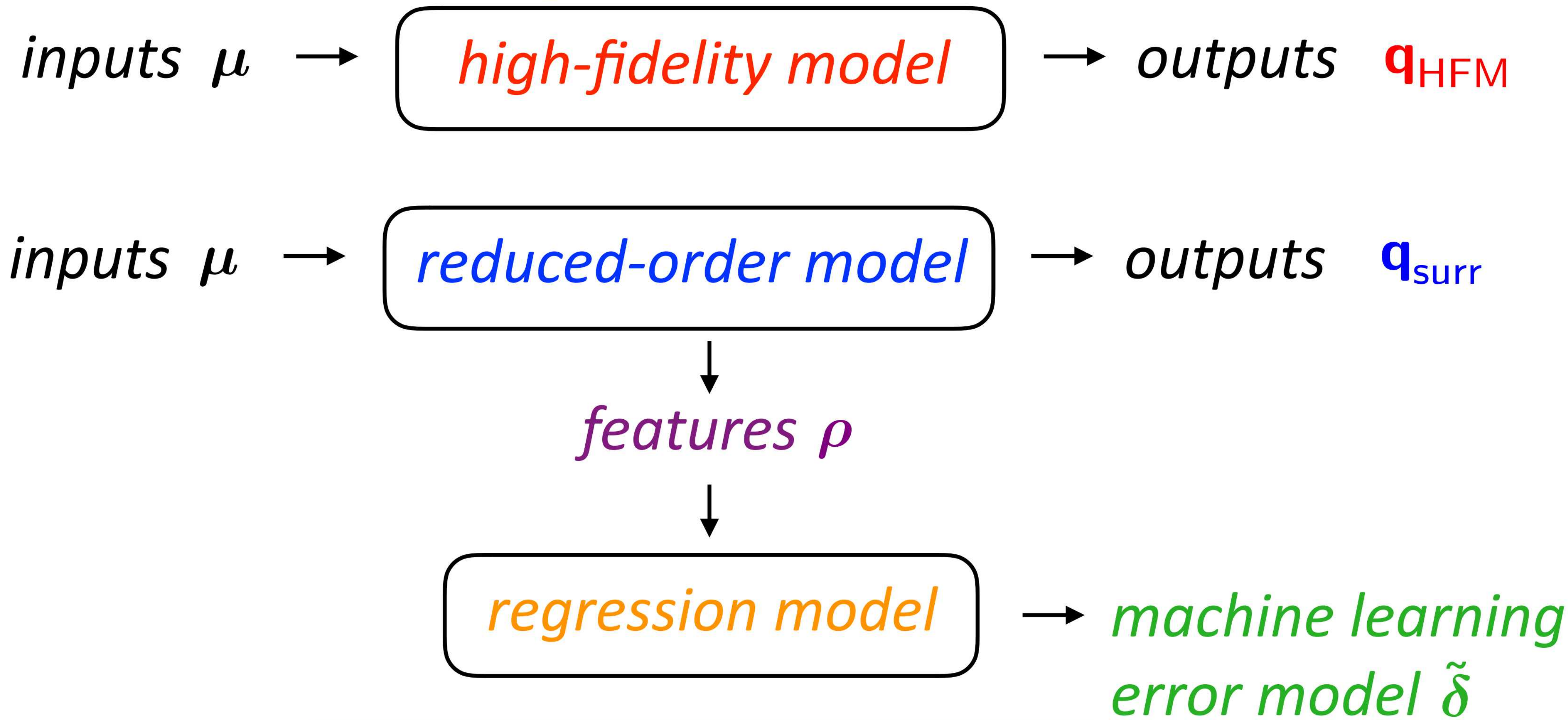
Key observation





ROMs generate cheaply computable error indicators that correlate with the ROM error

Machine-learning error models



$$\underbrace{\tilde{\mathbf{q}}_{\text{HFM}}(\boldsymbol{\mu})}_{\text{stochastic}} = \underbrace{\mathbf{q}_{\text{surr}}(\boldsymbol{\mu})}_{\text{deterministic}} + \underbrace{\tilde{\delta}(\boldsymbol{\mu})}_{\text{stochastic}}$$

How to determine features ρ and regression model?

- ➔ Approximated dual-weighted residuals and Gaussian-process regression
  [Drohmann, C., 2015; Pagani, C., Manzoni, 2018] **Pagani: Wed, 3pm, MS79**
- Large number of physics-informed features and high-dim regression
  [Trehan, C., Durlofsky, 2017; Freno, C., 2018] **Freno: Wed, 5:30pm, MS93**

Feature: dual-weighted residual [Drohmann, C., 2015]

- Approximate HFM output to first order

$$q_i(\mathbf{x}) \approx q_i(\boldsymbol{\Phi}\hat{\mathbf{x}}) + \frac{\partial q_i}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})(\mathbf{x} - \boldsymbol{\Phi}\hat{\mathbf{x}}) \quad (1)$$

- Approximate HFM residual to first order

$$\mathbf{0} = \mathbf{r}(\mathbf{x}) \approx \mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}}) + \frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})(\mathbf{x} - \boldsymbol{\Phi}\hat{\mathbf{x}})$$

- Solve for the error

$$\mathbf{x} - \boldsymbol{\Phi}\hat{\mathbf{x}} \approx -\left[\frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})\right]^{-1} \mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}}) \quad (2)$$

- Substitute (2) in (1)

$$q_i(\mathbf{x}) - q_i(\boldsymbol{\Phi}\hat{\mathbf{x}}) \approx \mathbf{y}_i{}^T \mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}})$$

with the dual solution $\mathbf{y}_i$ satisfying

$$\frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})^T \mathbf{y}_i = \frac{\partial q_i}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})^T$$

Feature: dual-weighted residual [Drohmann, C., 2015]

$$q_i(\mathbf{x}) - q_i(\boldsymbol{\Phi}\hat{\mathbf{x}}) \approx \mathbf{y}_i{}^T \mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}})$$

$$\frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})^T \mathbf{y}_i = \frac{\partial q_i}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})^T$$

- Want to avoid HFM-scale solves, so approximate dual as

$$\mathbf{y}_i \approx \tilde{\mathbf{y}}_i = \boldsymbol{\Phi}_i \hat{\mathbf{y}}_i$$

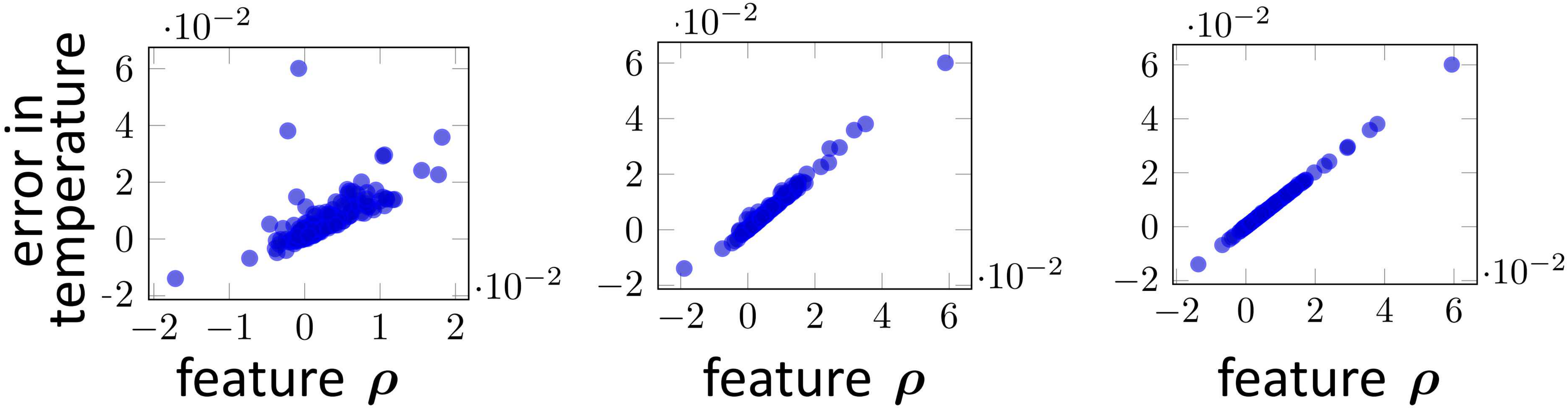
and construct ROM for the dual

$$\boldsymbol{\Phi}_i{}^T \frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})^T \boldsymbol{\Phi}_i \hat{\mathbf{y}}_i = \boldsymbol{\Phi}_i{}^T \frac{\partial q_i}{\partial \mathbf{x}}(\boldsymbol{\Phi}\hat{\mathbf{x}})^T$$

- **One feature**: $q_i(\mathbf{x}) - q_i(\boldsymbol{\Phi}\hat{\mathbf{x}}) \approx \rho_i = \tilde{\mathbf{y}}_i{}^T \mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}}) = \hat{\mathbf{y}}_i{}^T \boldsymbol{\Phi}_i{}^T \mathbf{r}(\boldsymbol{\Phi}\hat{\mathbf{x}})$
- **Regression model**: Gaussian process [Rasmussen, Williams, 2006]

Application 1: Poisson equation [Drohmann, C., 2015]

- *quantity of interest:* temperature at a point



$\mathbf{\Phi}_i$ *dimension 10* $\mathbf{\Phi}_i$ *dimension 15* $\mathbf{\Phi}_i$ *dimension 20*

+ *uncertainty control:* variance reduced as columns added to $\mathbf{\Phi}_i$

Error model summary

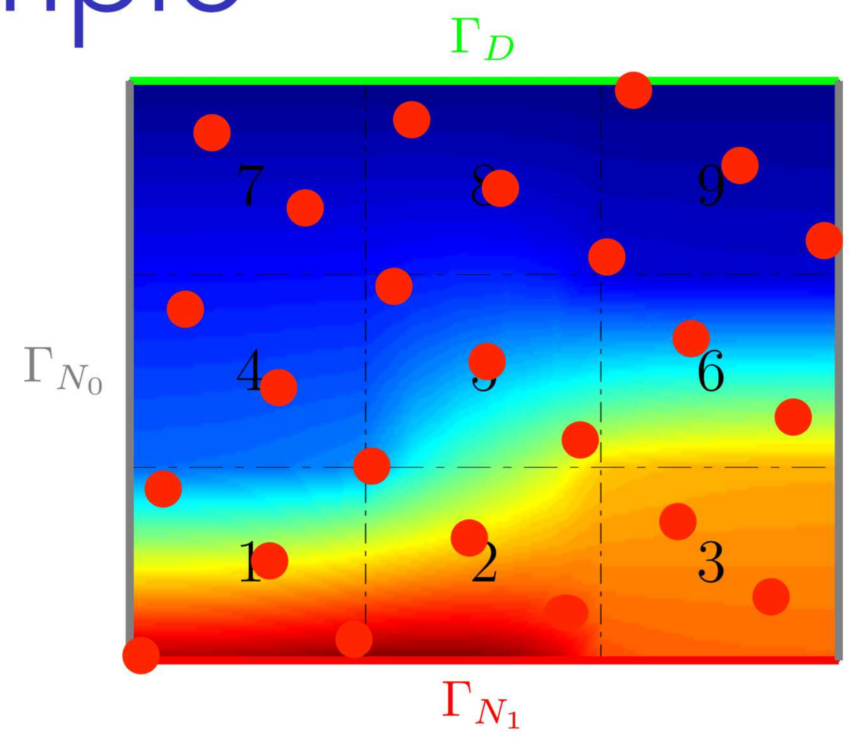
- Desired properties in error model
  1. cheaply computable: approximated dual-weighted residual
  2. low variance: possible from ROM-generated error indicator
  3. validated: accurately models error distribution on a test set

- Error-model noise should be computed as sample variance over regions

$$\tilde{\sigma}_i^2 = \frac{1}{n_s} \mathrm{E}_{\mathrm{data}}[\| \mathbf{q}_{\mathrm{HFM}}(\boldsymbol{\mu}) - \mathbf{q}_{\mathrm{surr}}(\boldsymbol{\mu}) - \tilde{\mathbf{m}}(\boldsymbol{\mu}) \|^2 \,|\, \mathcal{D}_i]$$

  - Gaussian process satisfies this for $\mathcal{D}_i = \{\boldsymbol{\mu} \,|\, \boldsymbol{\rho}(\boldsymbol{\mu}) = \boldsymbol{\rho}_i\}$

Numerical example



$$\triangle c(x;\boldsymbol{\mu})u(x;\boldsymbol{\mu}) = 0 \text{ in } \Omega \qquad \boldsymbol{x}(\boldsymbol{\mu}) = 0 \text{ on } \Gamma_D$$

$$\nabla c(\boldsymbol{\mu})\boldsymbol{x}(\boldsymbol{\mu}) \cdot n = 0 \text{ on } \Gamma_{N_0} \qquad \nabla c(\boldsymbol{\mu})\boldsymbol{x}(\boldsymbol{\mu}) \cdot n = 1 \text{ on } \Gamma_{N_1}$$

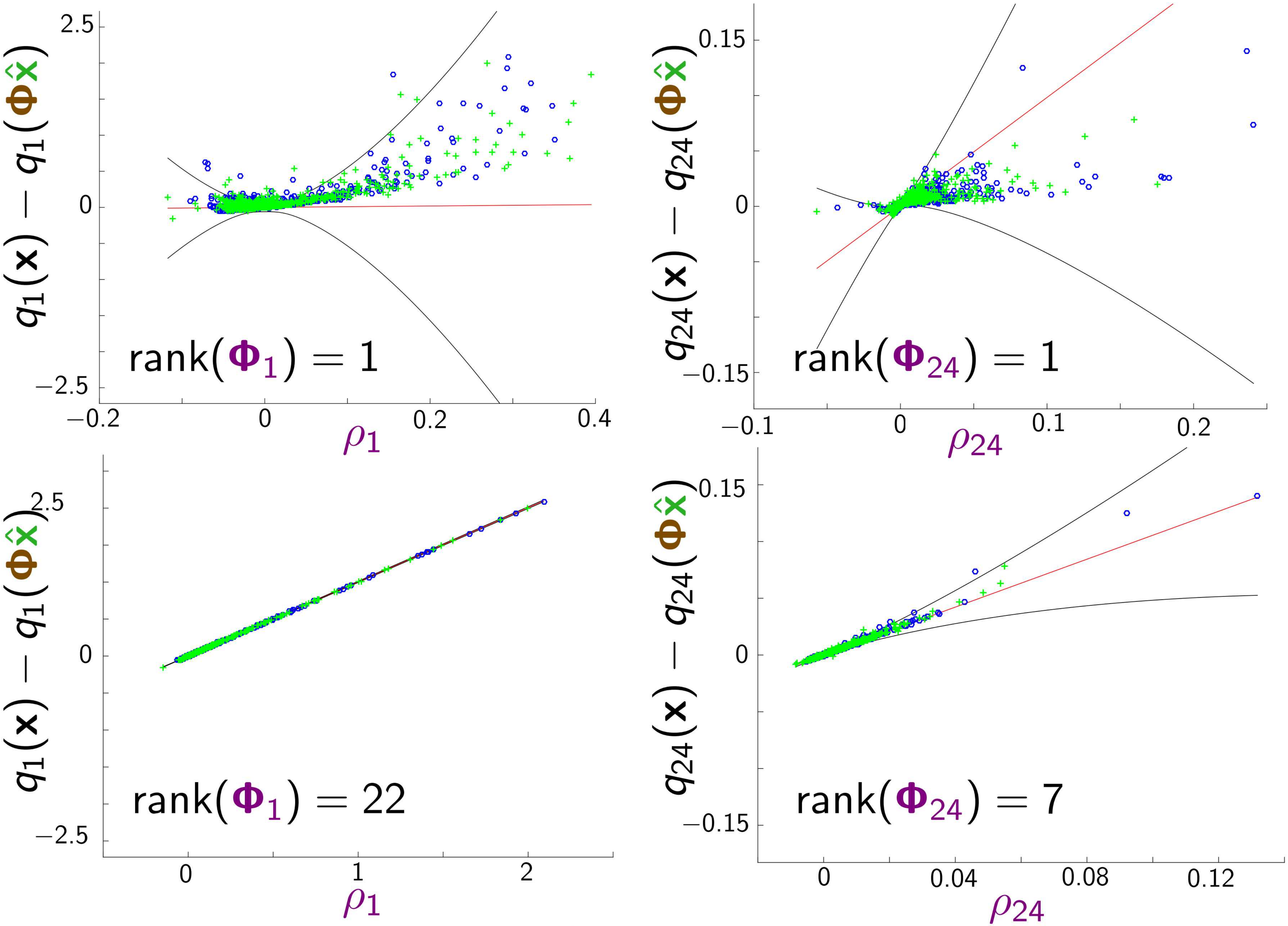
- Inputs $\boldsymbol{\mu} \in [0.1, 10]^9$ define diffusivity in *c* in subdomains
- Outputs **q** are 24 measured temperatures
- ROM constructed via RB-Greedy [Patera and Rozza, 2006]
- $\pi_{\text{prior}}(\boldsymbol{\mu})$: Gaussian with variance 0.1
- $\boldsymbol{\varepsilon} \sim \mathcal{N}(0, 1 \times 10^{-3})$
- Posterior sampling: 1×10^5 samples w/ implicit sampling [Tu et al., 2013]

Machine learning error models

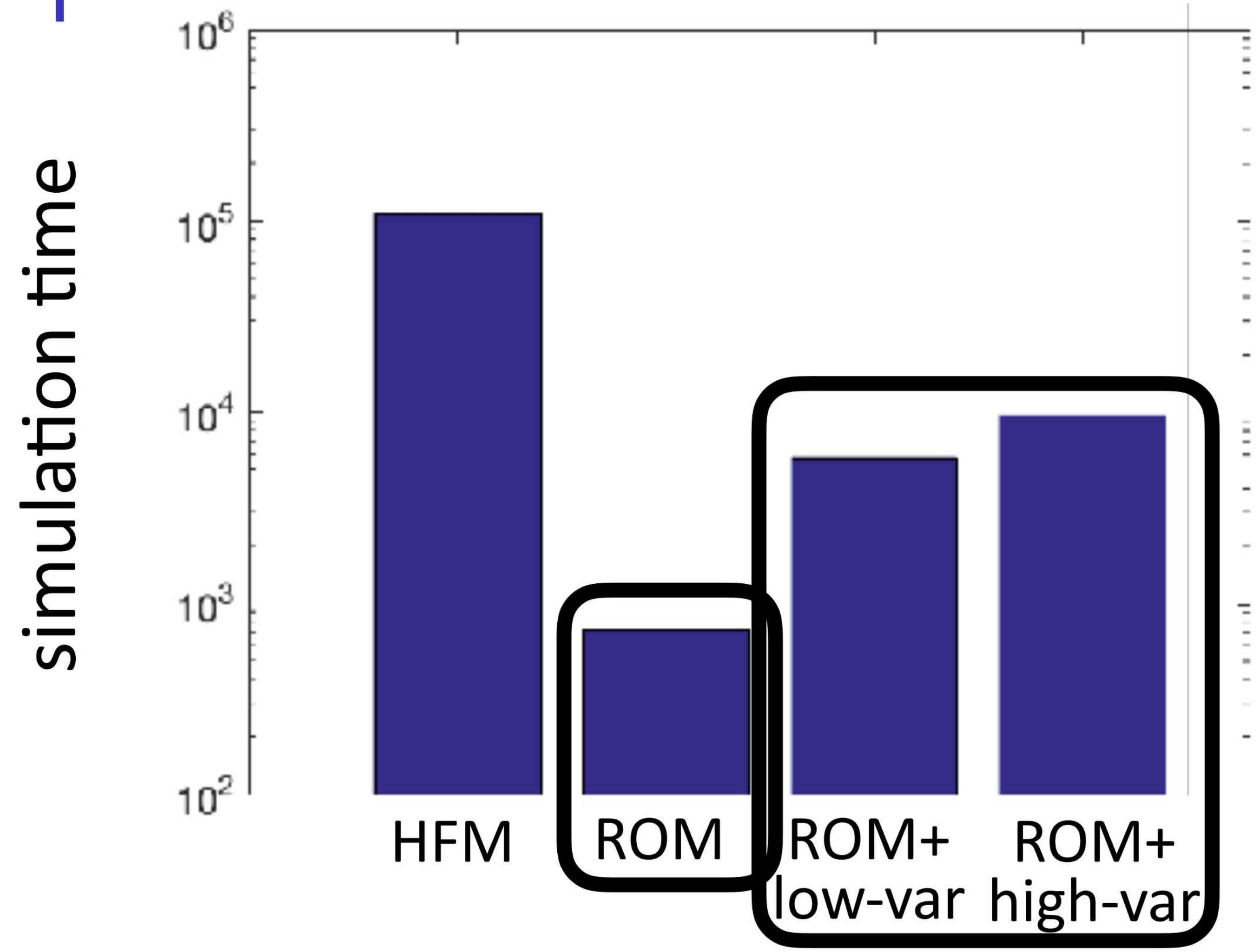
$$\tilde{\delta}_i(\boldsymbol{\mu}) \sim \mathcal{N}(\beta\rho_i(\boldsymbol{\mu}), \alpha_1 + \alpha_2|\rho_i(\boldsymbol{\mu})|^{\alpha_3})$$

high
variance
cheap

low
variance
costly

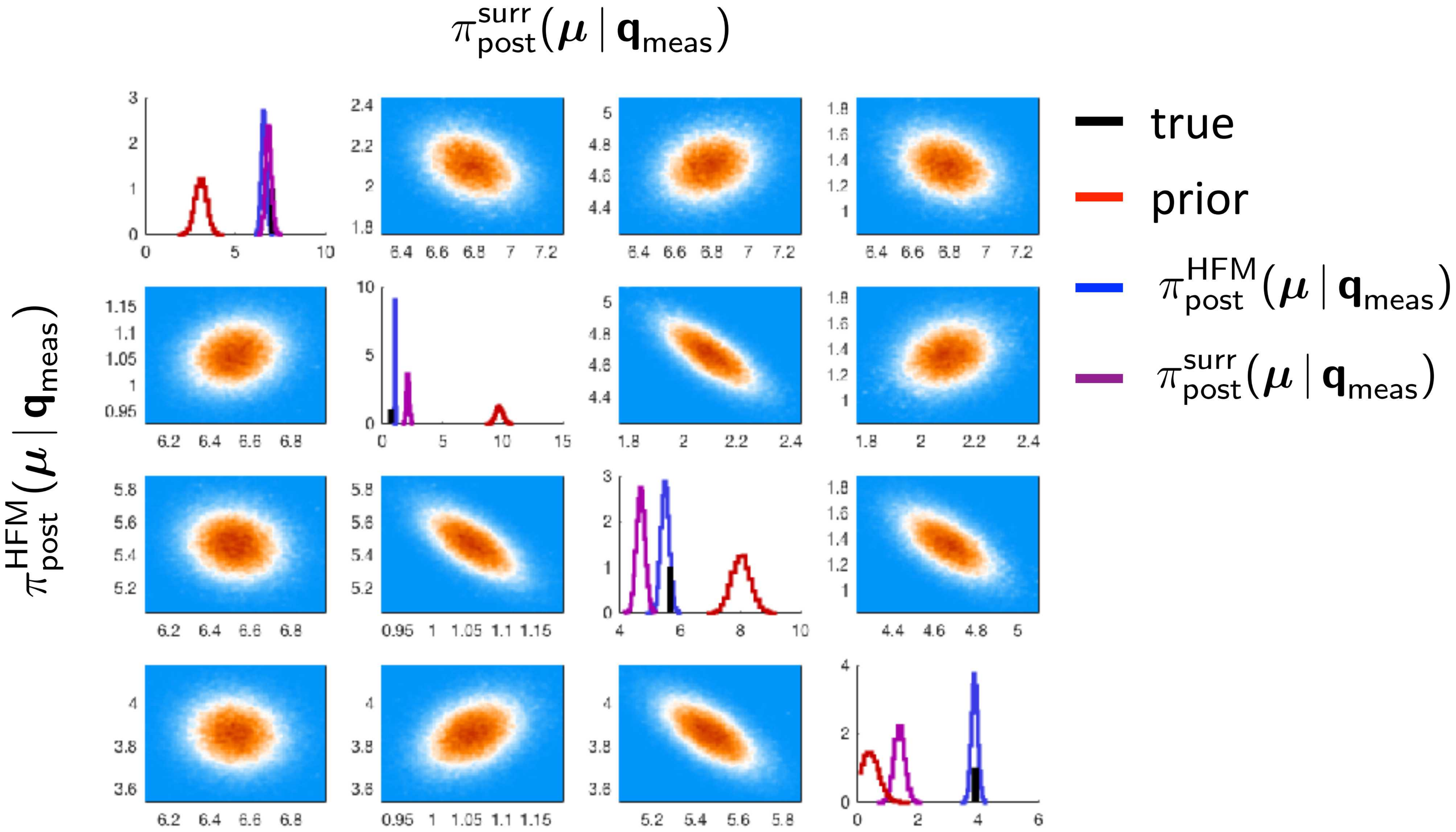


Wall-time performance



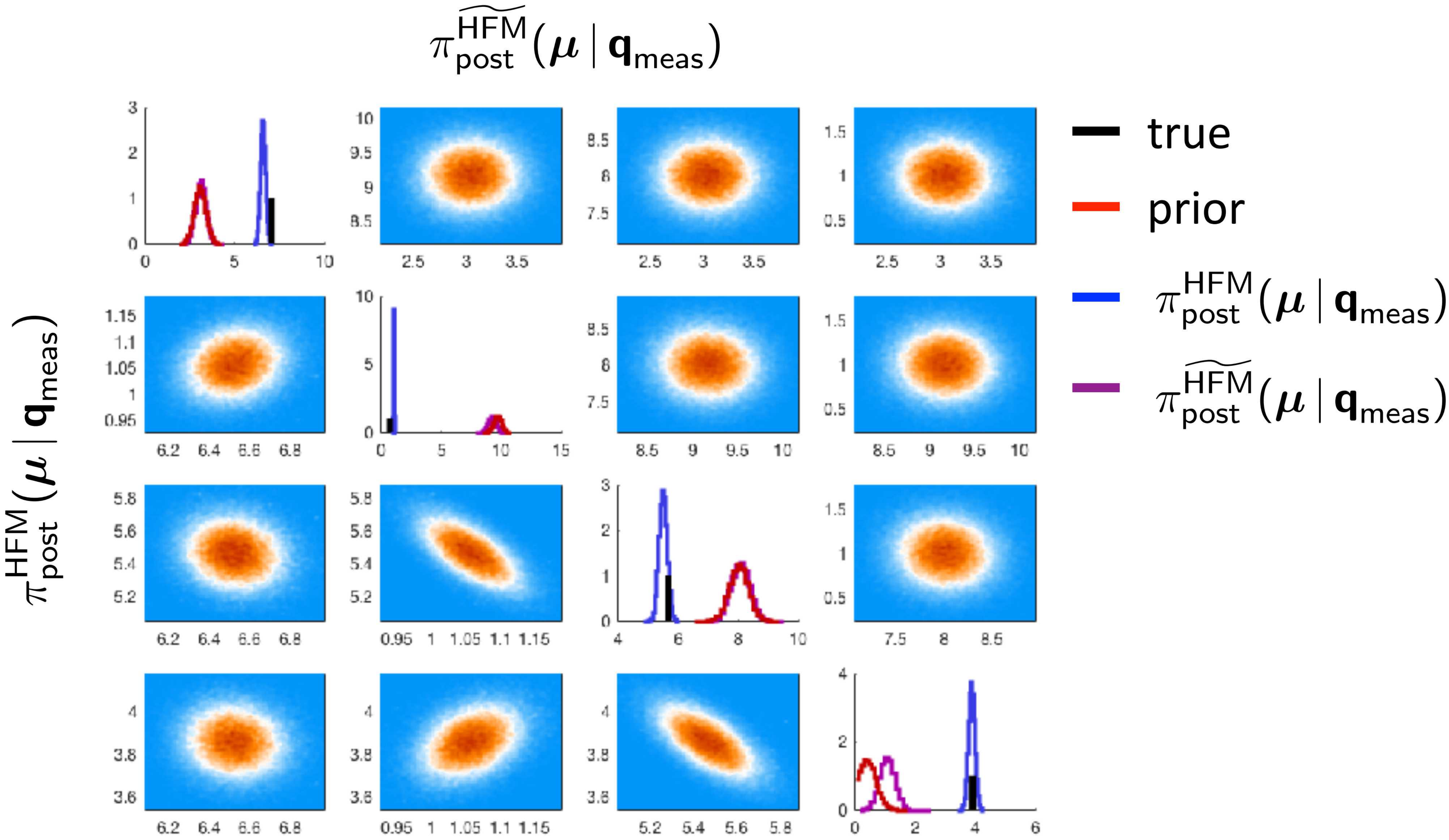
- ROM:
  + cheapest
  - inconsistent formulation
- ROM + error models:
  + cheaper than HFM
  - more expensive than ROM
  + consistent formulation

Posteriors: ROM



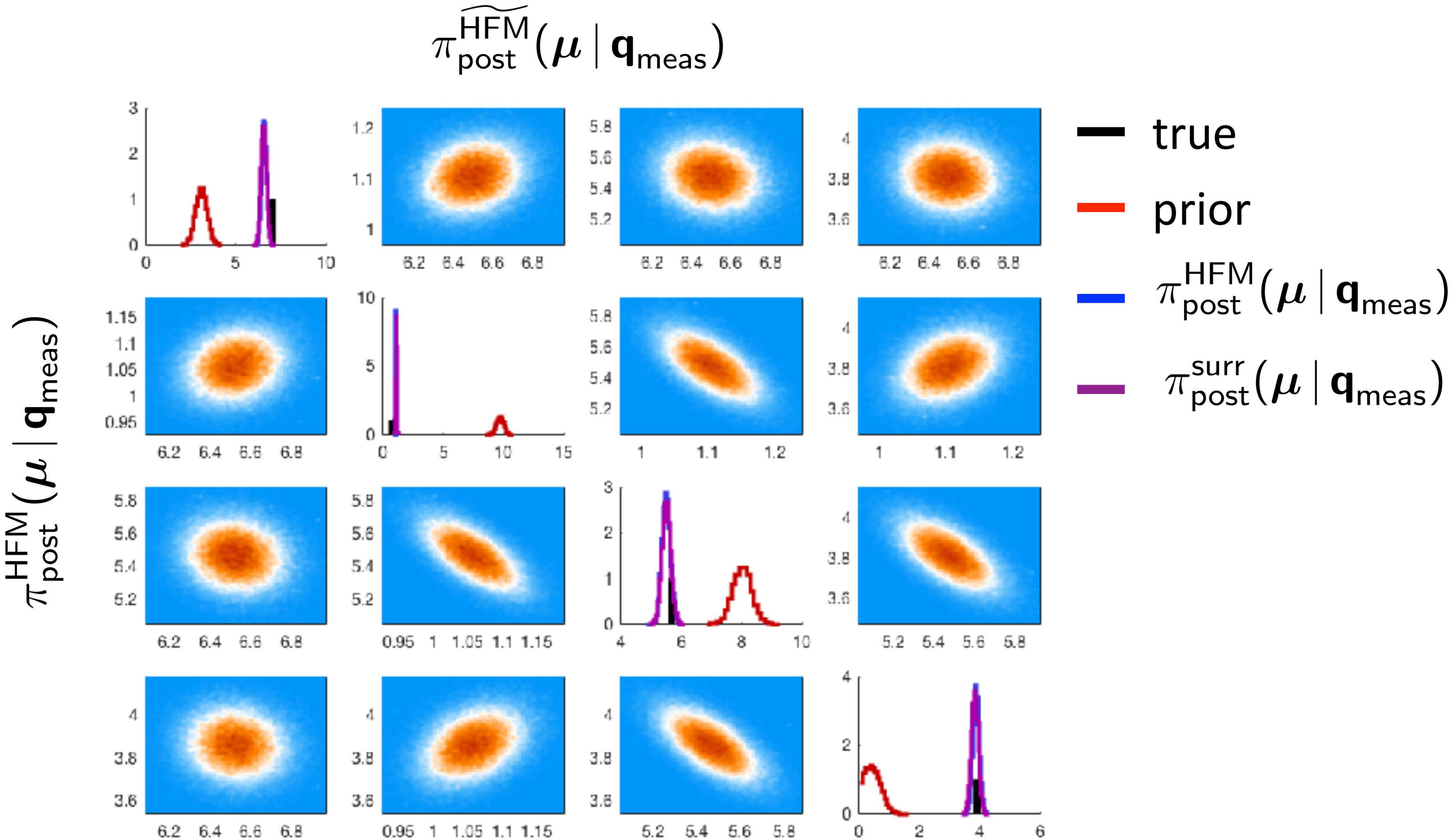
+ HFM posterior: close to **true parameters**
- ROM posterior: far from prior and **true parameters**

Posteriors: ROM + high-variance error model



+ ROM + high-var error model posterior: close to prior

Posteriors: ROM + low-variance error model



+ ROM + low-var error model posterior: close to HFM posterior

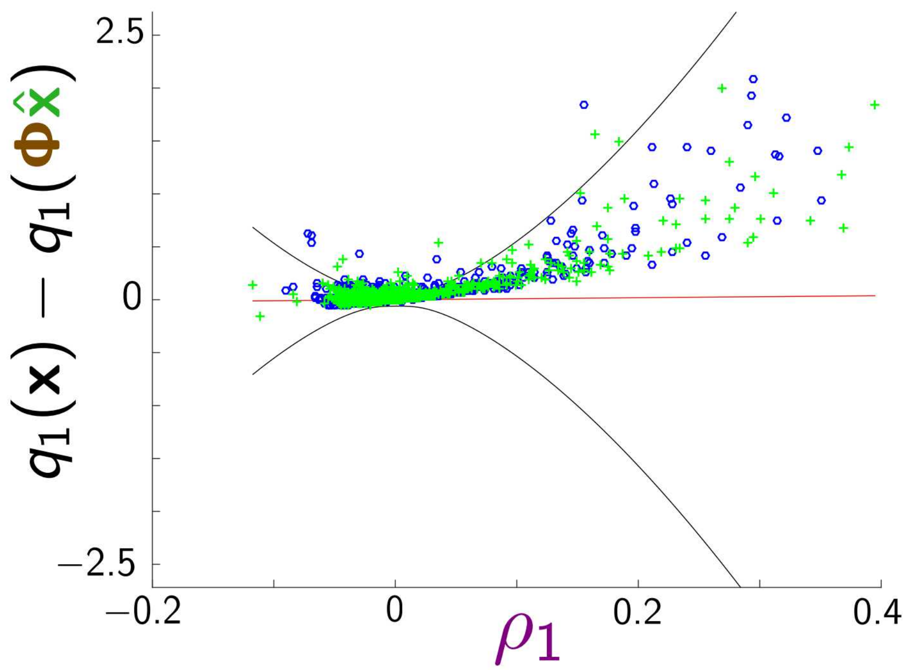
Summary

- What properties do we want in a stochastic error model?
  - Cheaply computable, low variance, validated
- What is the optimal stochastic error model?
  - Error-model variance should be the sample variance over regions
- How does a stochastic error model affect Bayesian inference?
  - High-variance: close to prior; low-variance: close to HFM posterior
- How can we construct a stochastic error model for reduced-order models?
  - Machine-learning error models based on error-indicator features

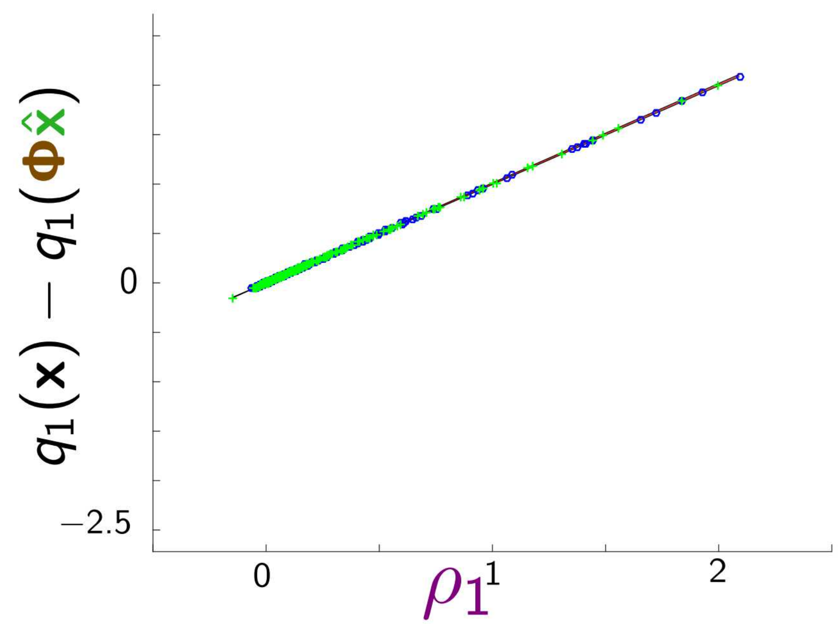
Questions?

References

- C, Uy, Lu, Morzfeld. Rigorous integration of reduced-order models in Bayesian inference via stochastic error models, *in preparation*, 2018.
- Trehan, C, and Durlofsky. Error modeling for surrogates of dynamical systems using machine learning. International Journal for Numerical Methods in Engineering, 112(12):1801–1827, 2017.
- Drohmann and C. The ROMES method for statistical modeling of reduced- order-model error. SIAM/ASA Journal on Uncertainty Quantification, 3(1):116–145, 2015.



high-variance error model



low-variance error model

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.