Bayesian Learning of Multifidelity Surrogate Networks (MFNets): MCMC and Variational Inference Approaches

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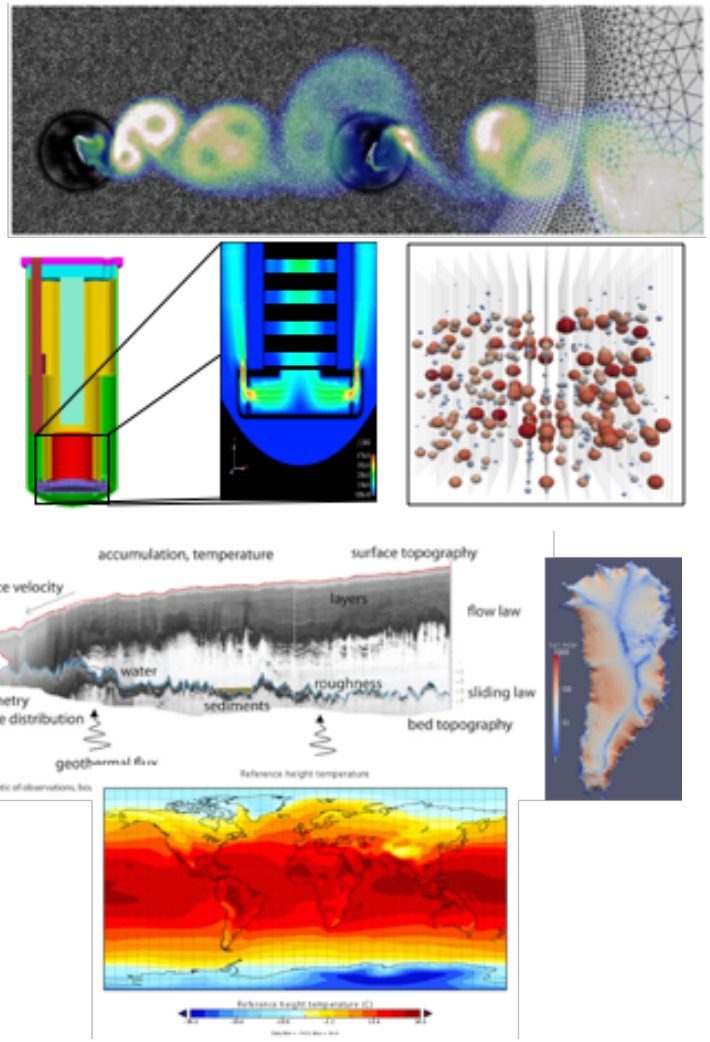
Uncertainty quantification for high-fidelity models

- Determine uncertainty on HF models
  - Expectation, variance
  - Probability of failures
- Severe simulation budget constraints
  - High dimensional PDEs
  - Large-scale computing resources
- Model complexity increases dimensionality
- HF models $\rightarrow$ UQ more important
  - Less validation, study, and analysis
  - Greater exploitation of nonlinearities
  - Uncertainty due to model form, initial conditions, and operating conditions

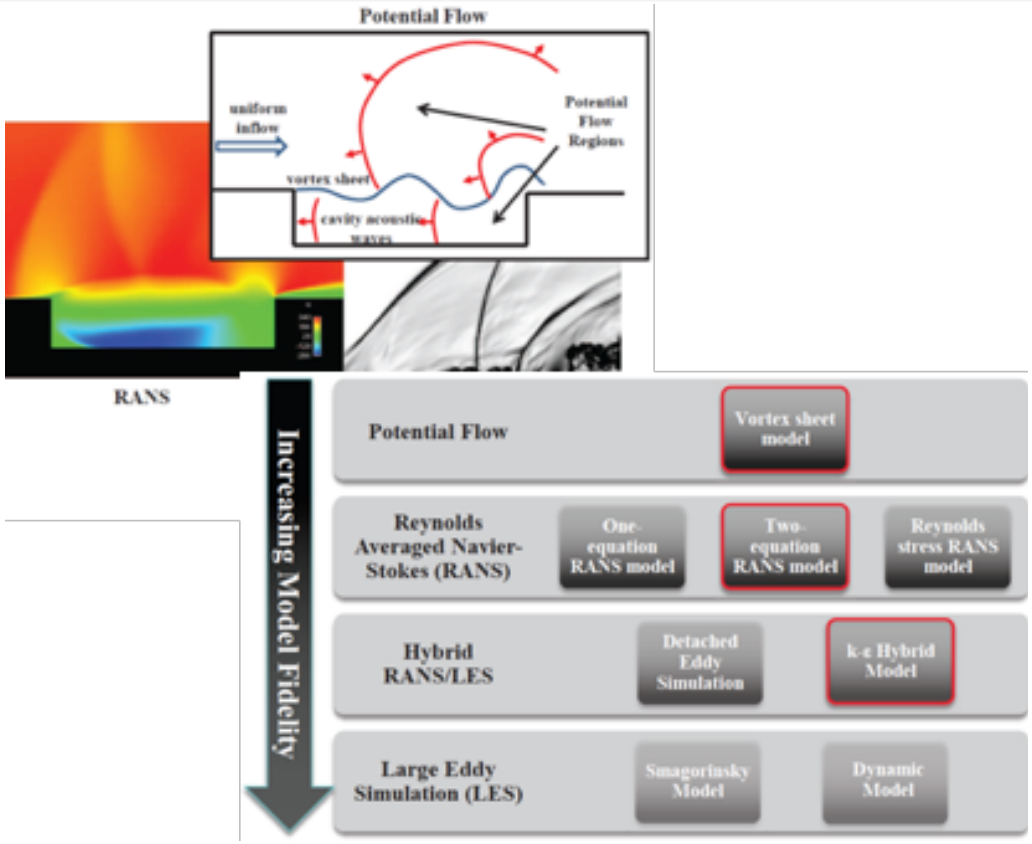


Leveraging multiple models/simulation sources

Key idea

We almost never have just ***one*** model, instead we develop many over the course of a study/analysis. Can we leverage these?

- Sources
  - Hierarchy of fidelities
  - Ensemble of peer models
  - Discretization levels
  - Experimental data



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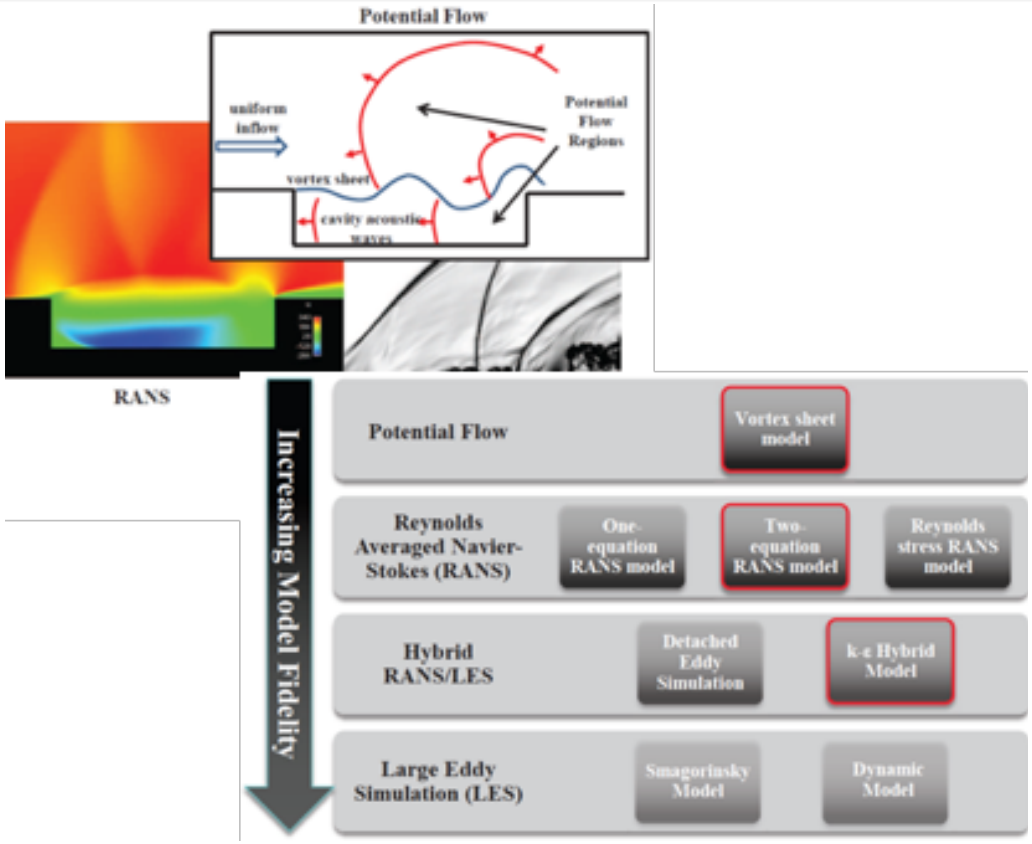

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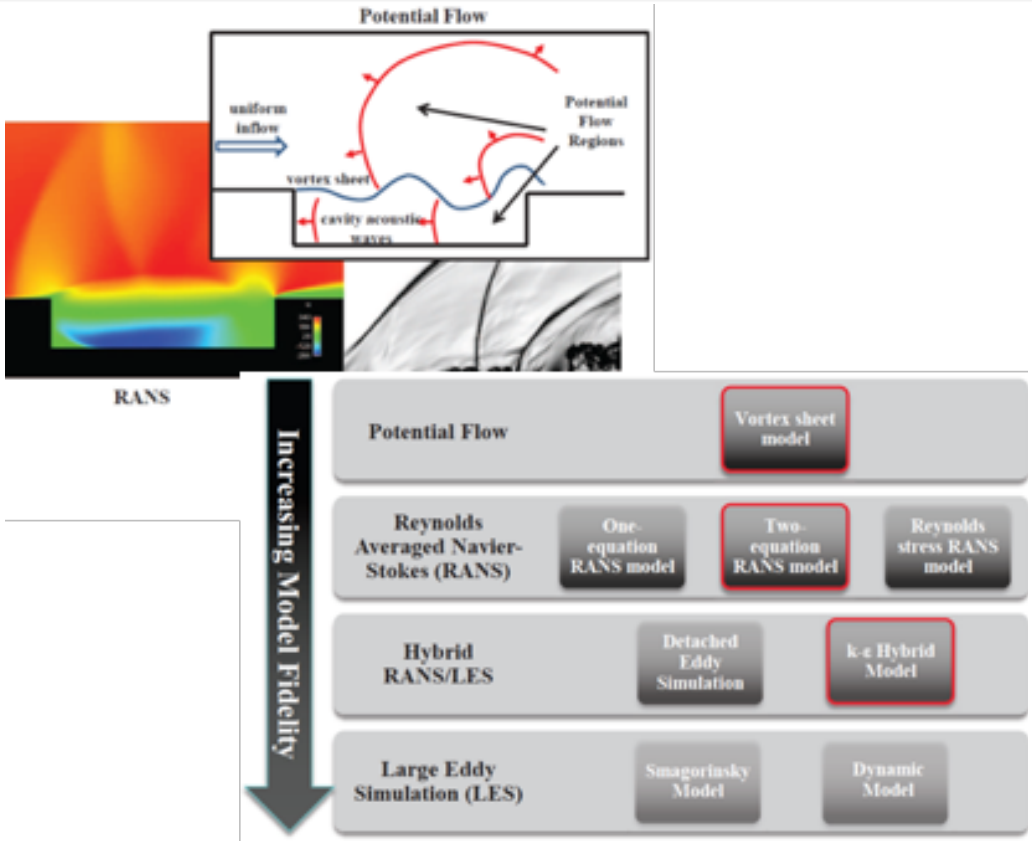

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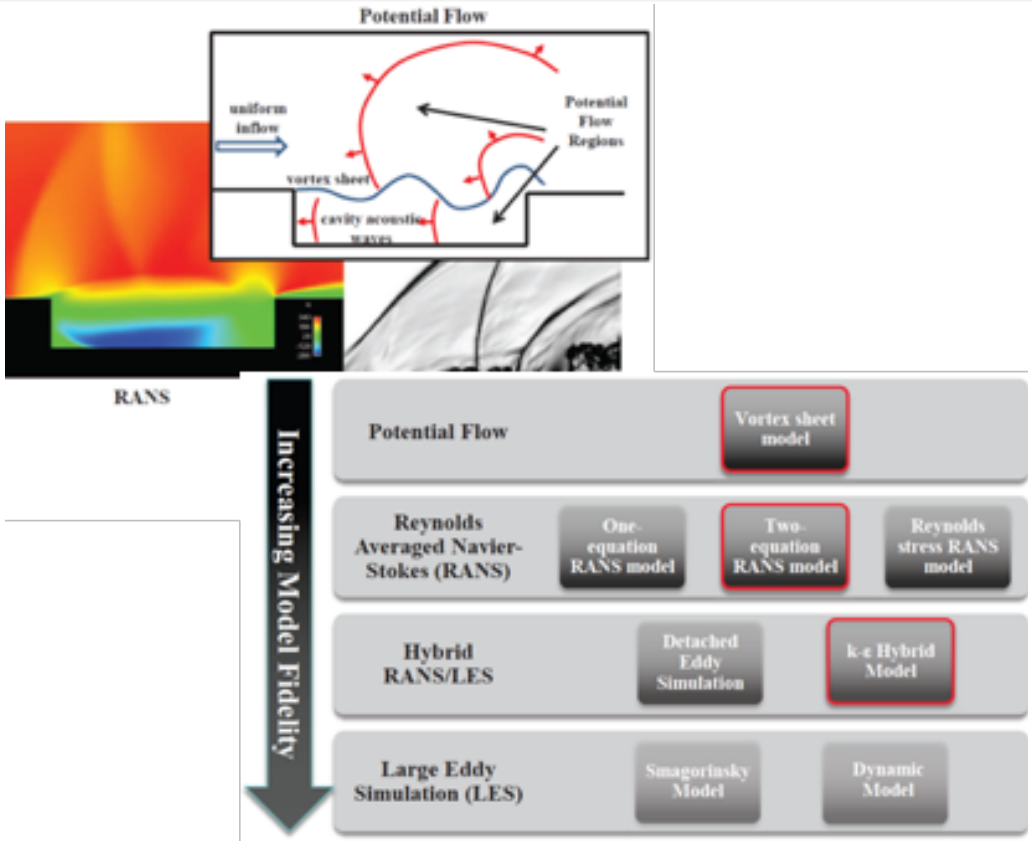

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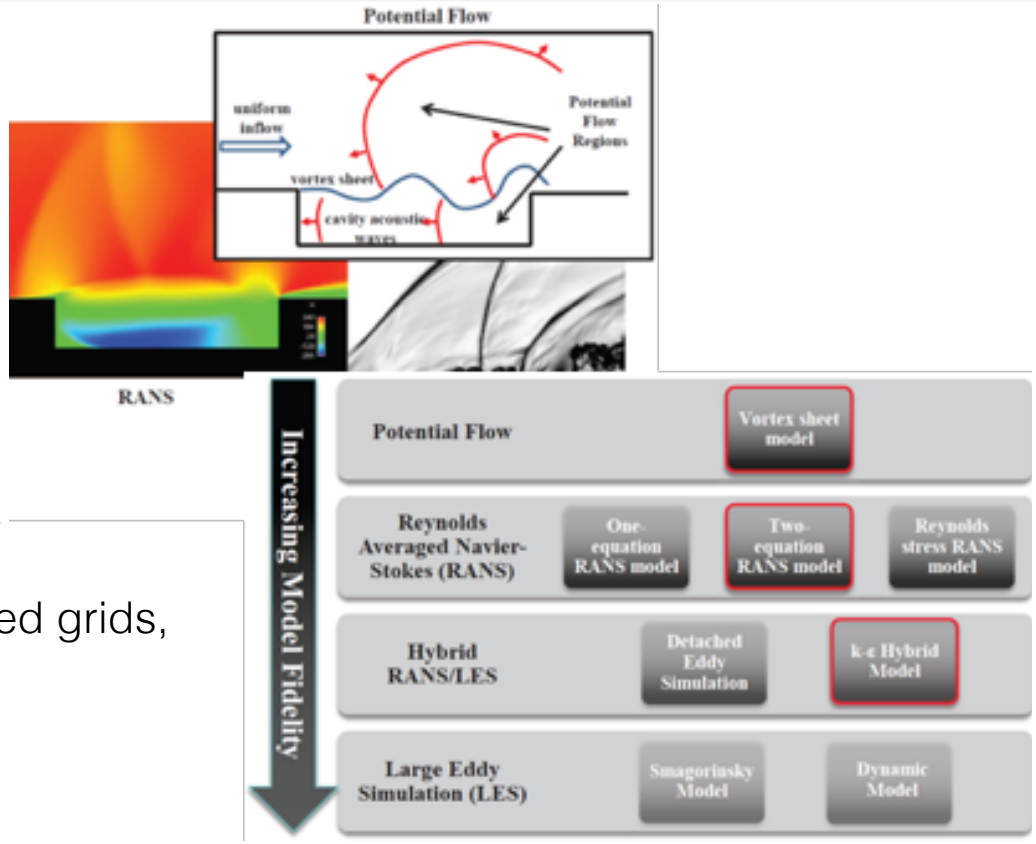

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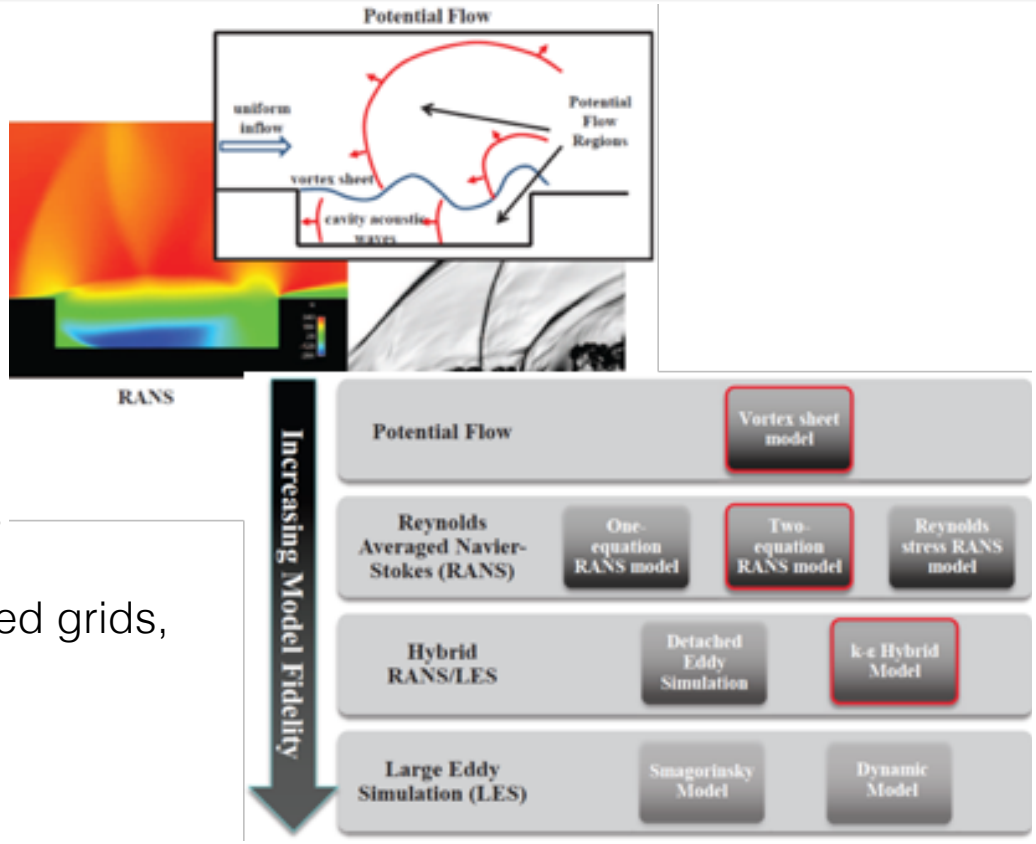
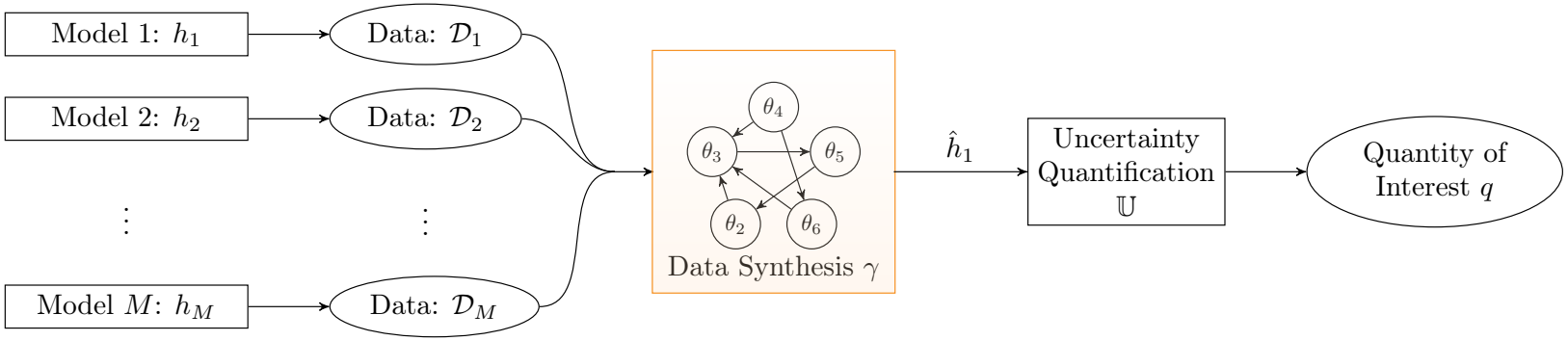
  - Lack of assumed relationships



Contribution in this talk

Problem: *A-priori* structural assumptions (hierarchical or otherwise) between models can lack robustness and limit efficiency

Contribution: A new modeling framework for multi-fidelity surrogate models that can flexibly adapt to variety of situations



Outline

- Multifidelity methods for enhancing surrogate approaches
  - Overview of existing approaches
  - A graph-based formulation: MFNets
  - Examples
- Probabilistic MFNets

The standard approach: autoregressive (recursive) modeling

Two-model case

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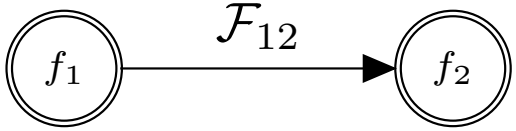

$$f_2 = \mathcal{F}_{12}[f_1] + \delta_2$$

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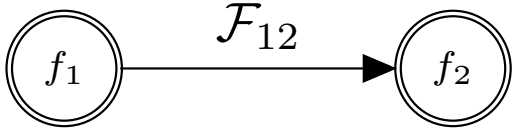
   - Recursive co-kriging: Kennedy and O'Hagan, Gratiet and Garnier



$$\delta_2 = f_2 - \mathcal{F}_{12}[f_1]$$

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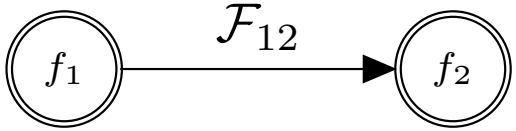

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Learning Requirements

- Things to learn: f_1, $\mathcal{F}_{12}$, δ_2
- If any are nonlinearly parameterized, then not a Gaussian process!

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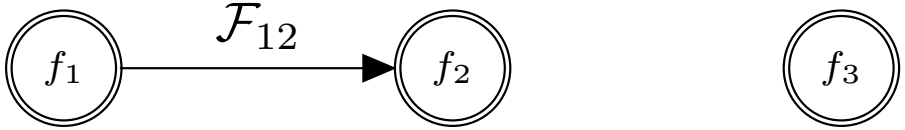

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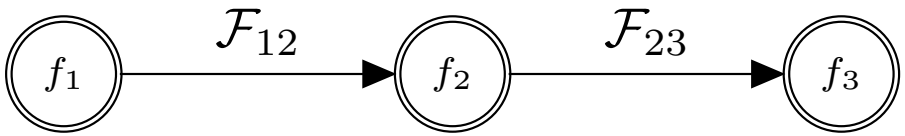
General case

1. Introduce a third (higher fidelity) information source
2. Again establish a recursive relationship

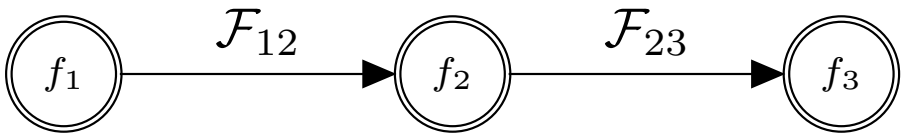


$$f_3 = \mathcal{F}_{23}[f_2] + \delta_3 = \mathcal{F}_{23}\left[\mathcal{F}_{12} f_1 + \delta_2\right] + \delta_3$$

The standard approach: autoregressive (recursive) modeling

General case

1. Introduce a third (higher fidelity) information source
2. Again establish a recursive relationship
3. Again learn the discrepancy



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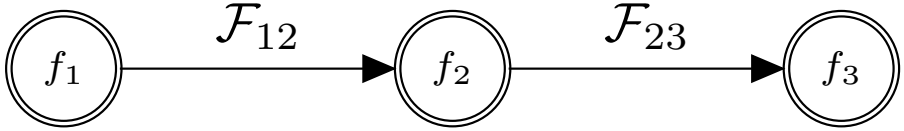

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Challenges

- Many existing techniques require nested sample points and step-wise optimization [Gratiet 2014, Perdikaris 2017]
- Many existing techniques that assume separable $\mathcal{F}_{ij}[f_i] = \rho_{ij}(x) f_i(x)$ treat parameters of ρ_{ij} as hyperparameters that are optimized separately to retain Gaussianity.

Why do we need another paradigm?

1. Not all information sources are obviously hierarchical
   - Depends on QoI
   - Peer models are common
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   - MIMC [Haji-Ali 2016] vs. MLMC [Giles 2008]
   - Generalized ACV [Gorodetsky 2020] vs. recursive control variate approaches (MFMC) [Peherstorfer 2016]
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3. Need more training algorithms to consider non-GP cases and non-nested sampling

Multifidelity Networked Surrogate Models (MFNets)

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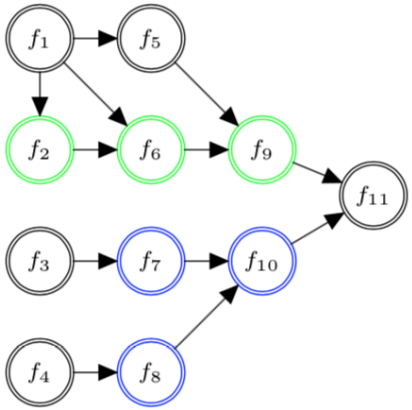
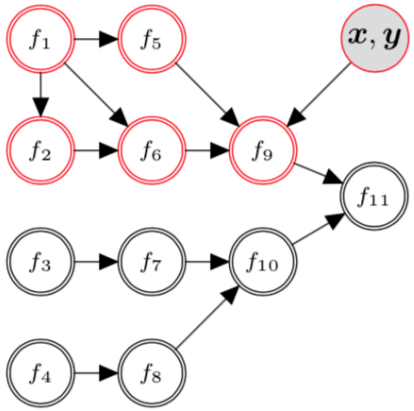
Main idea: model relationships between surrogate outputs

An MFNet is a DAG $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with nodes representing information sources $\mathcal{V} = \{f_1, \ldots, f_M\}$ and directed edges $\mathcal{E} = \{(j \to i)\}$ representing their relationships

$$f_i(x) = \sum_{j \in \text{pa}(i)} \mathcal{F}_{ji}[f_j(x)] + \delta_i(x).$$



(a) Sample structure of a multifidelity surrogate.



(b) Evaluating (10) for $k = 9$ requires data from f_9 and traversing the ancestors of f_9 (depicted in red).

Figure 1: An example DAG used to define a multifidelity surrogate. This structure exhibits a complicated relationship between each function and the high-fidelity f_{11}. Both hierarchical and peer relationships are exhibited within these networks. For instance the left panel shows an example of hierarchical structure $(f_2 \to f_6 \to f_9)$ in green and example of peer structure $(f_7 \to f_{10}, f_8 \to f_{10})$ in blue.

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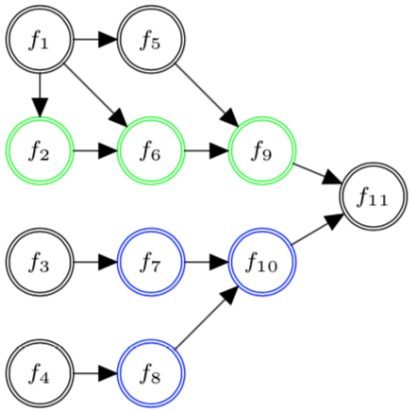

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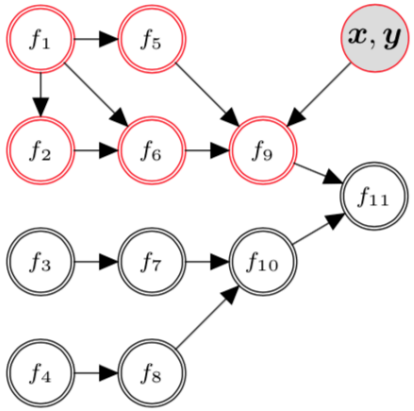

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Training: setting up the log posterior

- Log likelihood:
  - Root node approximation $f_k = V_k^T(x)\beta_k$

$$-\log p(\boldsymbol{y}_k \mid \boldsymbol{x}; \beta_k) = \frac{n}{2}\log 2\pi + n\log\sigma_k + \frac{1}{2\sigma_k^2}\left\|\boldsymbol{y}_k - V_k^T(\boldsymbol{x})\,\beta_k\right\|_2^2$$

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- Independent exponential family prior $p(\theta) = g(\theta)\exp(\phi^T(\theta)\nu)$

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- DAG structure enables fast and efficient backpropagation for gradient computation

Synthetic example with stochastic models

$$f_k(x) = \left(2 + (2x_1^5 + 2x_2^5)\Delta_1 + 3x_1x_2 + (x_1^2 + x_2^2 + 5x_1^2x_2^2)\Delta_2 + 0.5x_1 + 0.5x_2\right)(1 + \mathbb{E}[\mathcal{N}(0,1)]),$$

	Δ_1	Δ_2	N (Monte Carlo)
f_1	0	0	5
f_2	0	0	10
f_3	0	0	100
f_4	0	1	5
f_5	0	1	10
f_6	0	1	100
f_7	1	1	5
f_8	1	1	10
f_9	1	1	100

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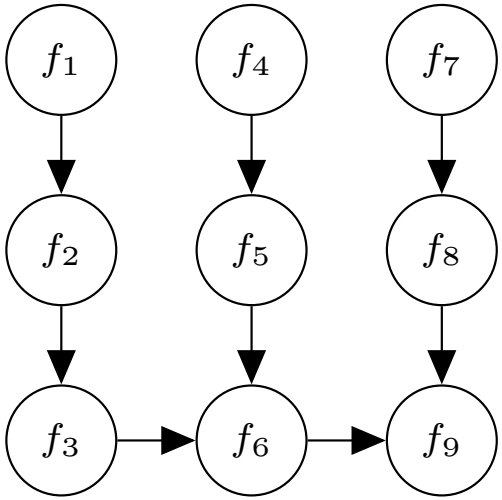
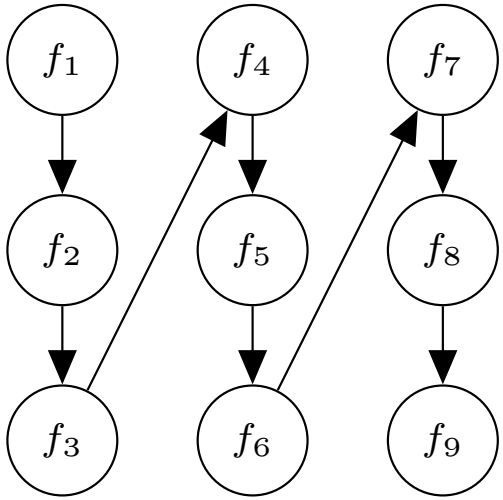
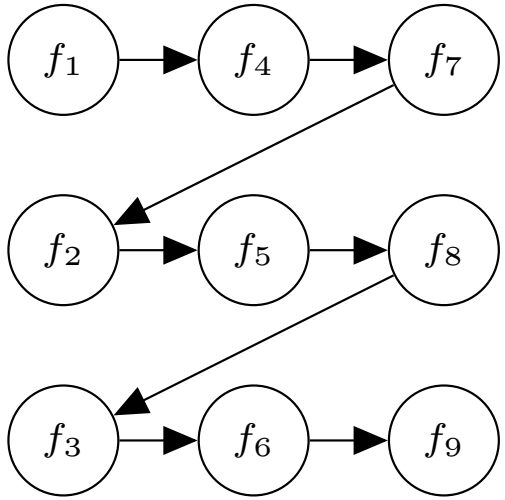


(a) Natural ordering



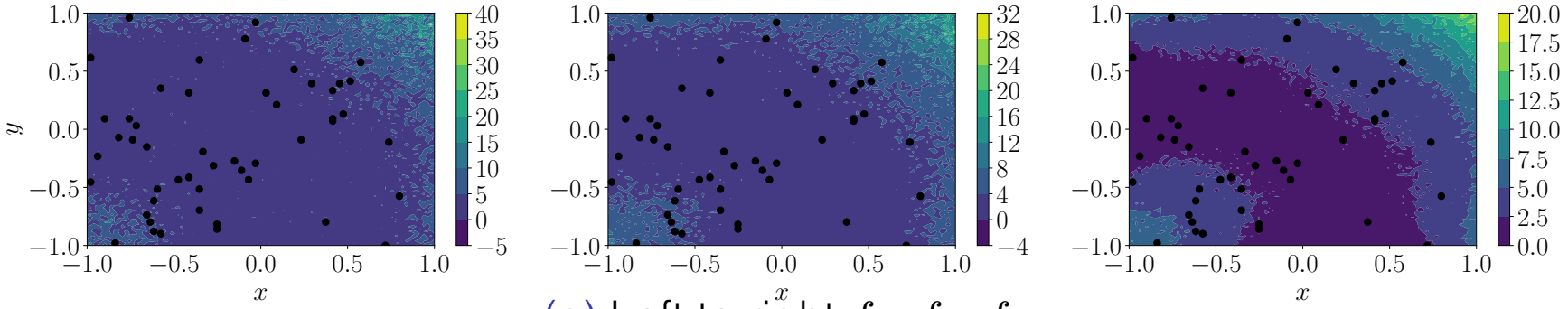
(b) Hierarchical ordering by model fidelity Δ first



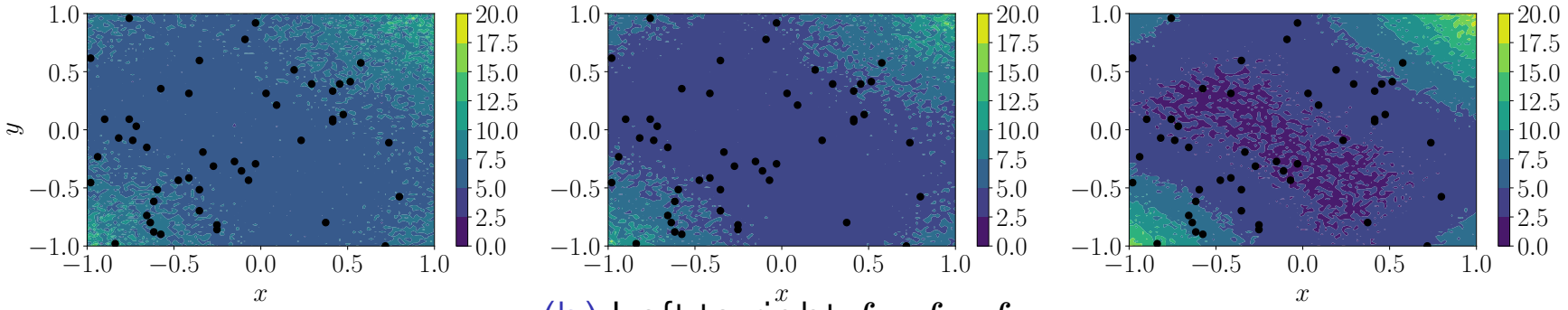
(c) Alternate Hierarchical ordering by noise fidelity N first.

Figure: Analytical noise test case: models' natural structure versus two candidate hierarchical orderings.

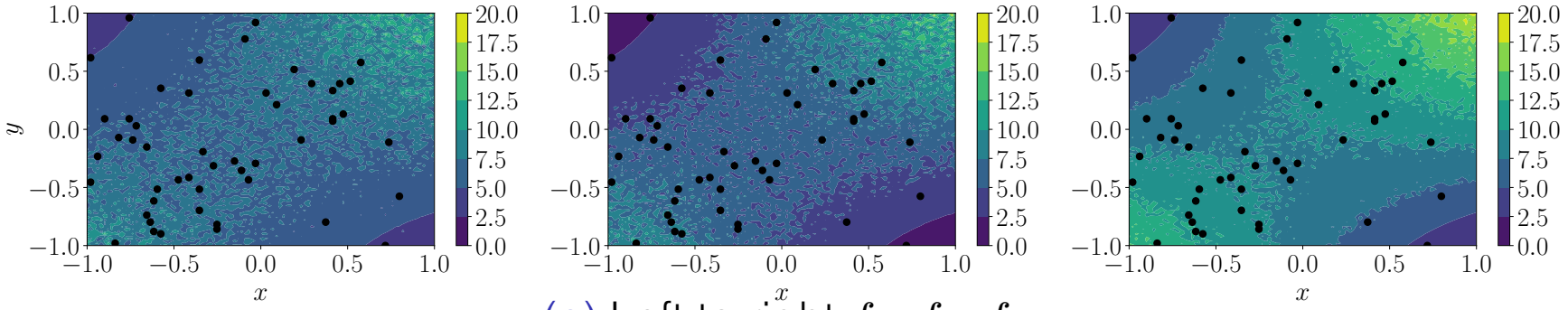
Synthetic response surfaces



(a) Left to right f_7, f_8, f_9



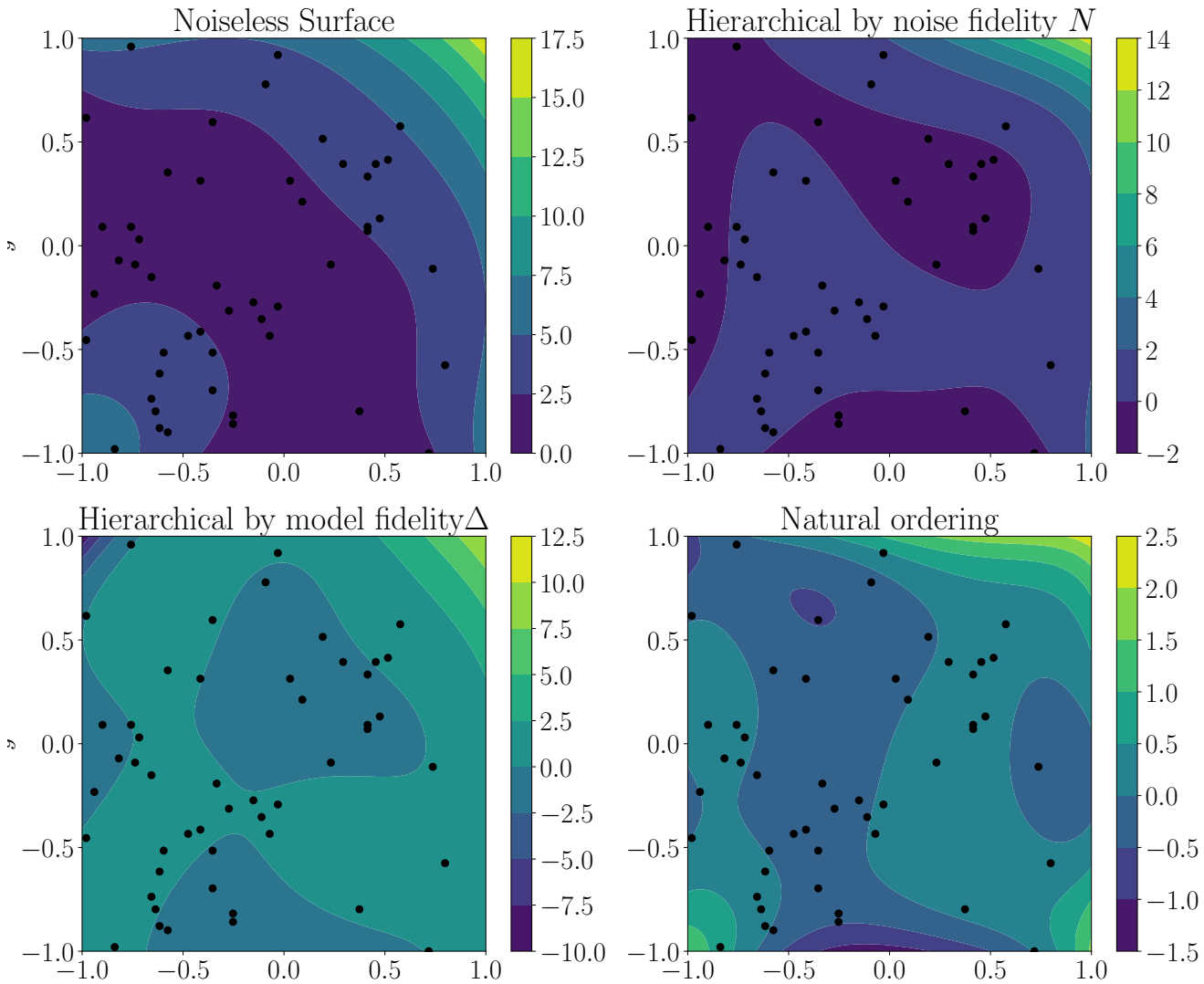
(b) Left to right f_4, f_5, f_6



(c) Left to right f_1, f_2, f_3

Highest fidelity model and pointwise errors

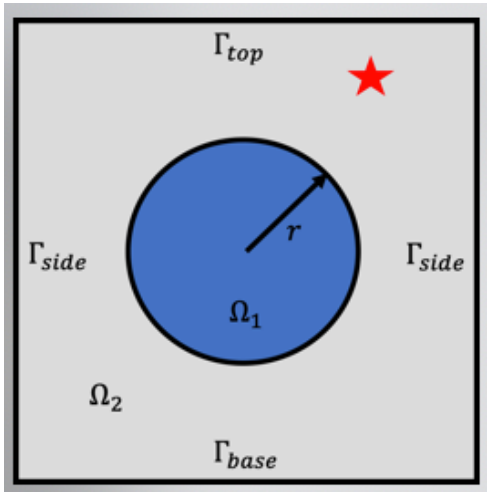
Natural ordering obtains order of magnitude lower errors



Thermal block

$$\begin{cases} -\text{div}(\kappa(\mu_0)\nabla u(\boldsymbol{\mu})) = 0 & \text{in } \Omega, \\ u(\boldsymbol{\mu}) = 0 & \text{on } \Gamma_{top}, \\ \kappa(\mu_0)\nabla u(\boldsymbol{\mu}) \cdot \mathsf{n} = 0 & \text{on } \Gamma_{side}, \\ \kappa(\mu_0)\nabla u(\boldsymbol{\mu}) \cdot \mathsf{n} = \mu_1 & \text{on } \Gamma_{base}. \end{cases}$$

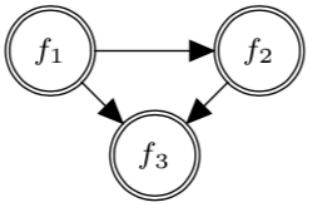
$$\kappa(\mu_0) = \begin{cases} \mu_0 & \text{in } \Omega_1, \\ 1 & \text{in } \Omega_2, \end{cases}$$



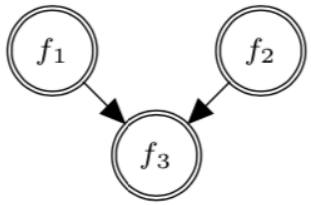
1. Three models: two finite element models with different mesh resolution, and reduced order model.
2. Constructed using RBniCS [Hesthaven, Rozza, Samm, 2015]
3. Predict temperature at (0.5, 0.8)

Thermal block results

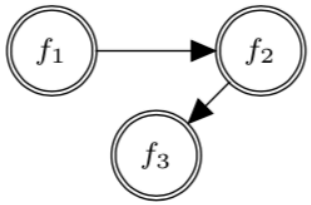
Non-recursive solution is best over 85% realizations of training data



(a) Full

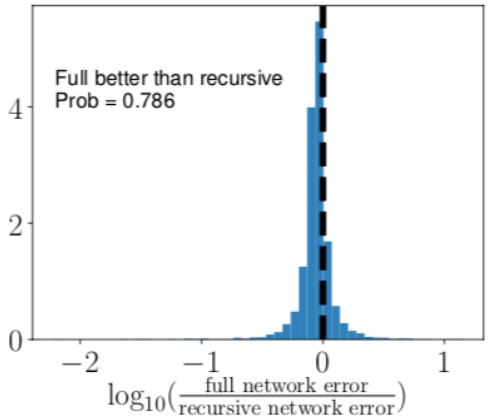


(b) Peer

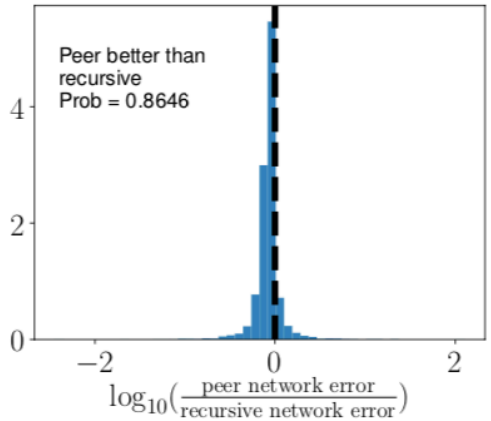


(c) Hierarchical

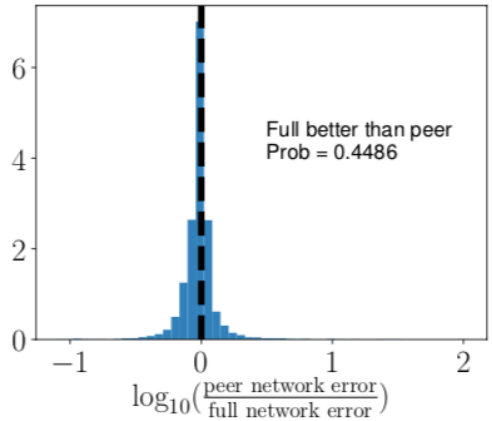
Figure 9: Thermal block model network structures.



(a) Full vs. hierarchical/recursive.



(b) Peer vs. hierarchical/recursive.



(c) Peer vs. full.

Probabilistic approaches

Questions:

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1. Can we extend our approaches to probabilistic learning?

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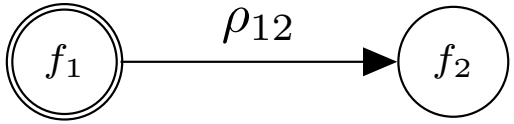
Next: A description and visualization of challenges

Non-identifiability in the posterior
Analytic expansion of two-model case

- Consider the two-function graph with linear parameterizations



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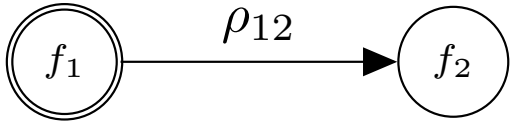

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$$f_1(x) = V_1^T(x)\beta_1$$

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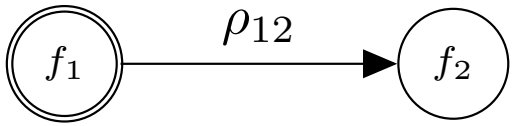

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$$\begin{aligned} f_2(x) &= \rho_{12}(x) f_1(x) + \delta_2(x) \\ &= \left(W_{12}^T(x)\alpha_{12}\right) V_1^T(x)\beta_1 + V_2^T(x)\beta_2 \\ &= \left(W_{12}^T \otimes V_1^T\right)(x)\left(\alpha_{12} \otimes \beta_1\right) + V_2^T(x)\beta_2 \end{aligned}$$

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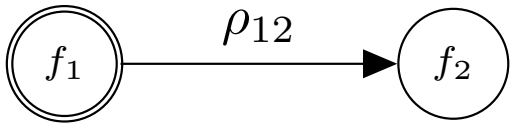

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- Explicit example with linear 1D models

$$\begin{aligned} f_2(x) &= \left(\alpha_{12,0} + \alpha_{12,1}x\right)\left(\beta_{1,0} + \beta_{1,1}x\right) + \beta_{2,0} + \beta_{2,1}x \\ &= \alpha_{12,1}\beta_{1,1}x^2 + \left(\alpha_{12,0}\beta_{1,1} + \alpha_{12,1}\beta_{10} + \beta_{2,1}\right)x + \left(\beta_{2,0} + \alpha_{12,0}\beta_{1,0}\right) \end{aligned}$$

Non-identifiability in the posterior
Manifold of equal probabilities

$$f_1(x) = \beta_{1,0} + \beta_{1,1}x$$
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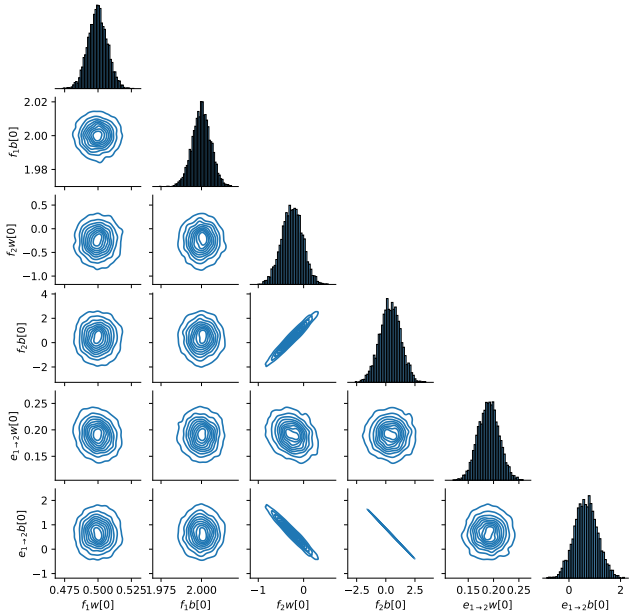
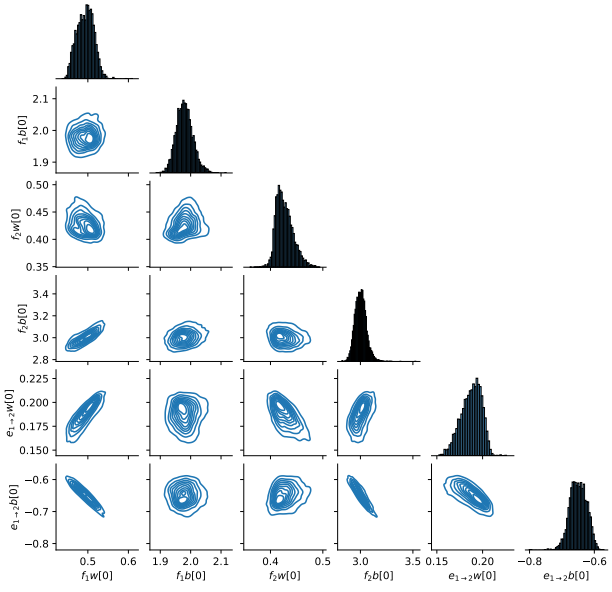
4. 3 unknowns and 2 equations $\rightarrow$ 1 dimensional null space

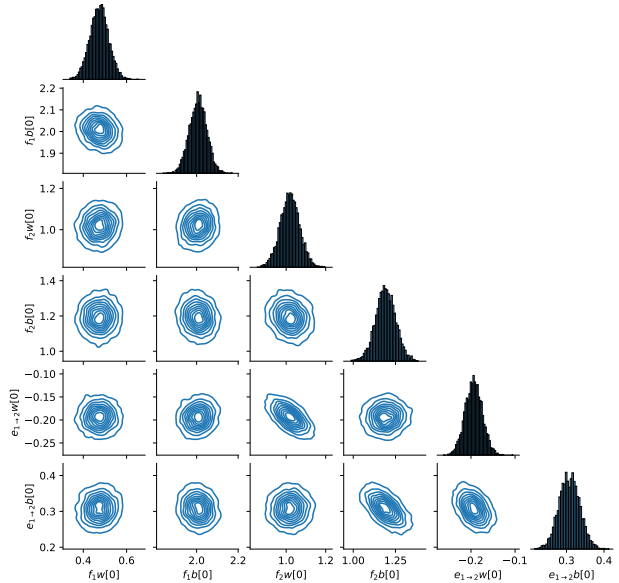
Non-identifiability in the posterior
HMC vs. Inverse Autoregressive Normalizing Flow vs. Normal



(a) HMC



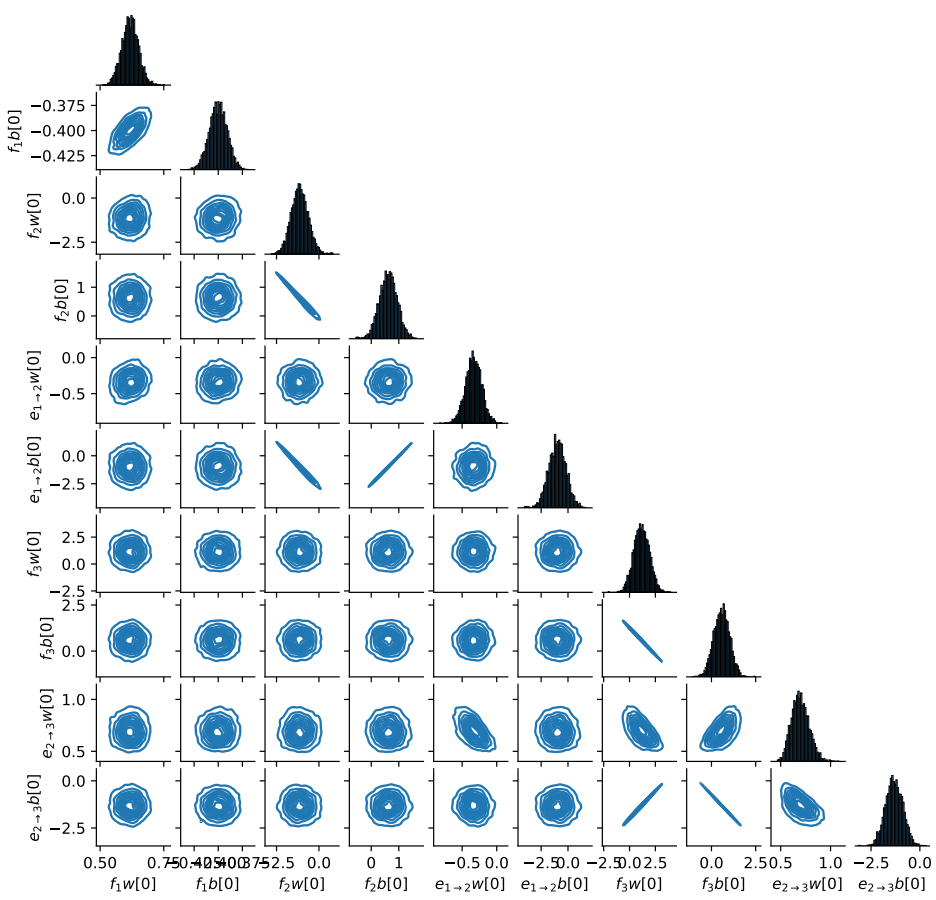
(b) IAF



(c) Multivariate Normal

Non-identifiability in the posterior

3D case: variational inference misses manifold



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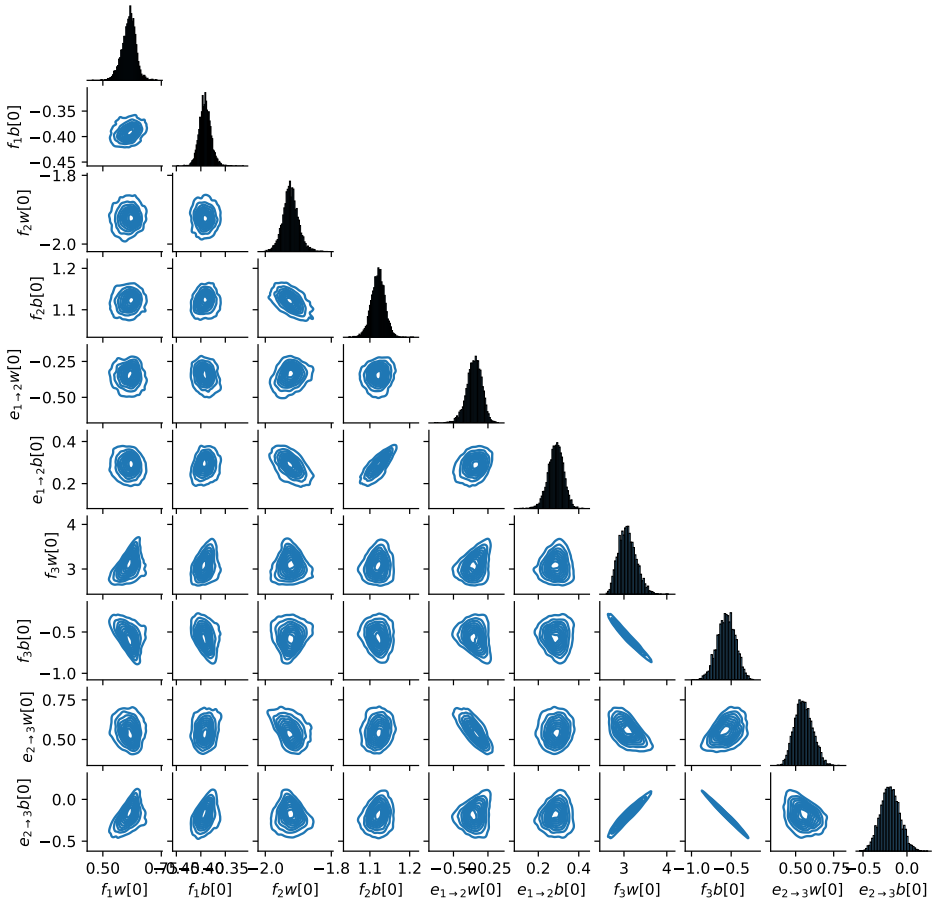

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- Code: `http://github.com/goroda/MFNetsSurrogates`

Acknowledgements

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