SAND2022-9339C

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Facilitating Atmospheric Source Inversion via Operator Regression

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Sandia National Laboratories

SIAM Mathematics of Planet Earth

July 15, 2022

U.S. DEPARTMENT OF ENERGY NNSA

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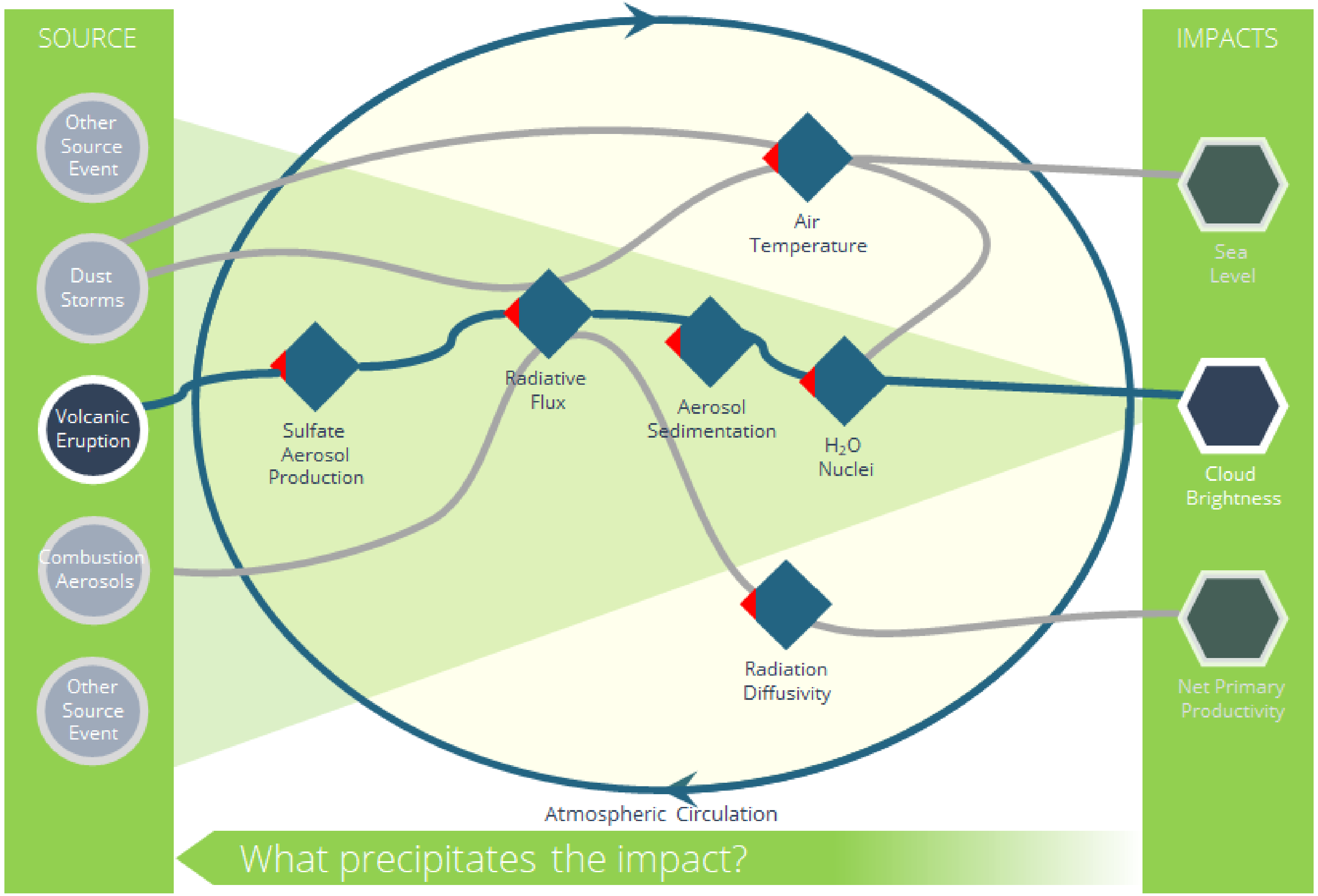
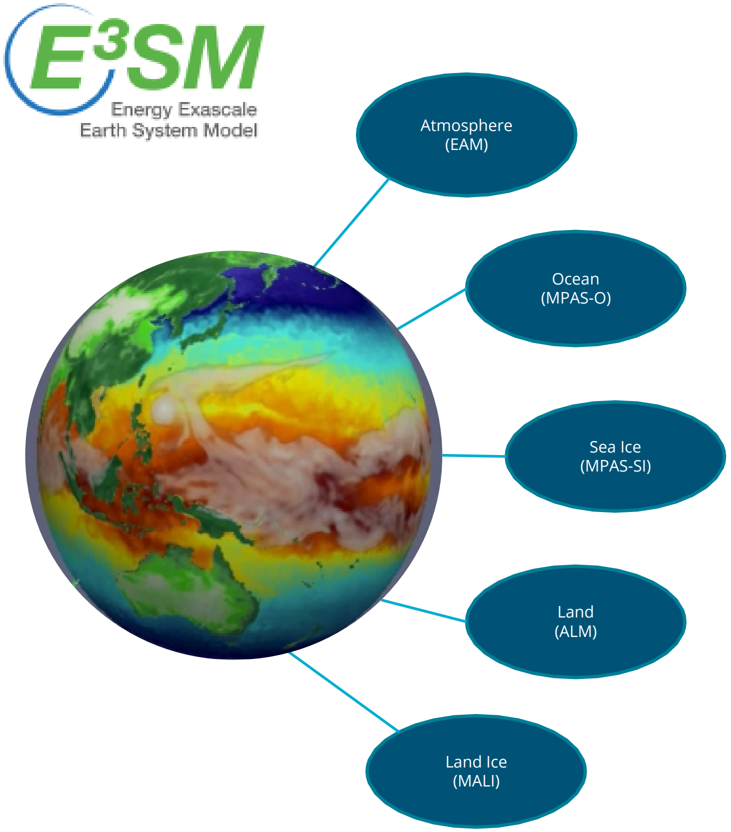
Atmospheric Source Inversion

- Inferring sources from impacts is ill-posed.
- Spatially localized sources create global impacts.
- Climate model complexity prohibits direct inversion.
- Operator surrogates may enable inversion.
- Spatiotemporal data improves information content.

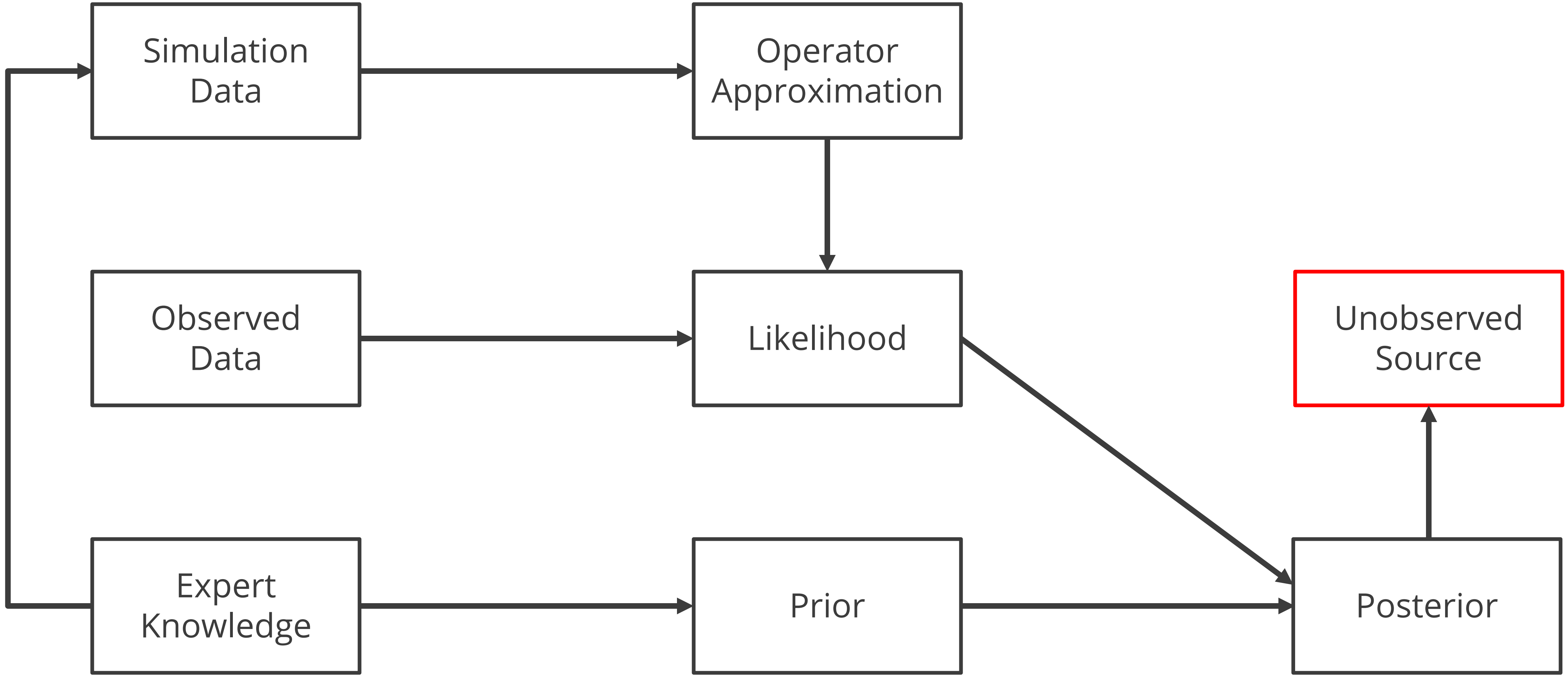


Goals and Tiered Verification



- Infer operators for tracer evolution generated by E3SM.
- Energy Exascale Earth System Model (E3SM) is developed by US DOE.
- Use operator surrogate to enable inversion.
- End goal: source inversion for Mount Pinatubo eruption.
- Question about data, dimension reduction, operator architecture, etc.
- Start with a synthetic SO_2 transport model infer a volcanic source.

Overview of the Workflow



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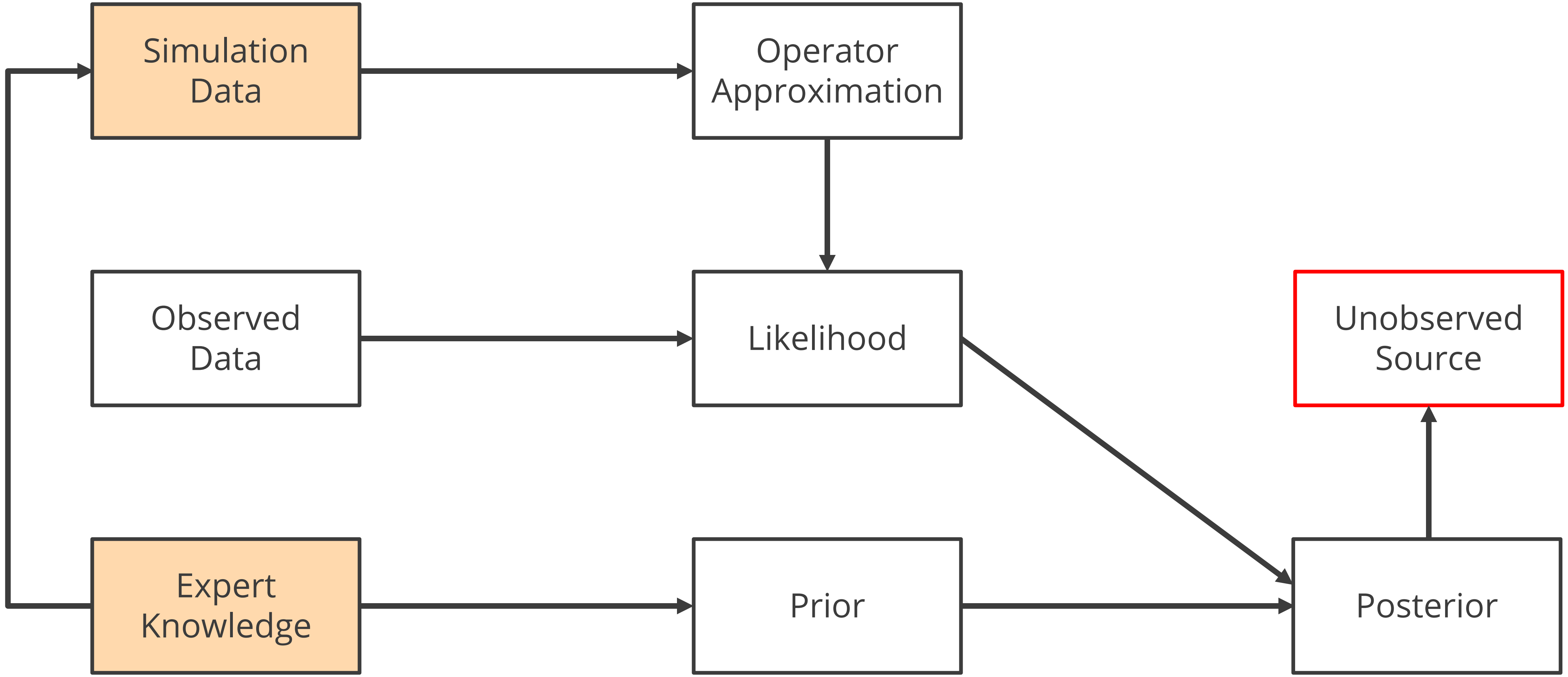
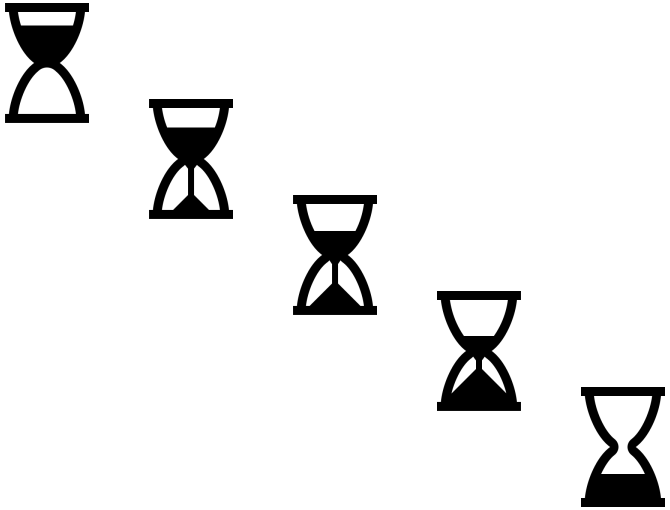


Simulation Data Generation

- Choose M possible sources over N time steps,
- sources $\mathbf{z}^m \in \mathbb{R}^N$ are functions of time,
- corresponding to the states $\mathbf{u}_0^m, \mathbf{u}_1^m, \ldots, \mathbf{u}_N^m \in \mathbb{R}^d$,
- for simulation runs $m = 1,2, \ldots, M$,
- where M is typically small.



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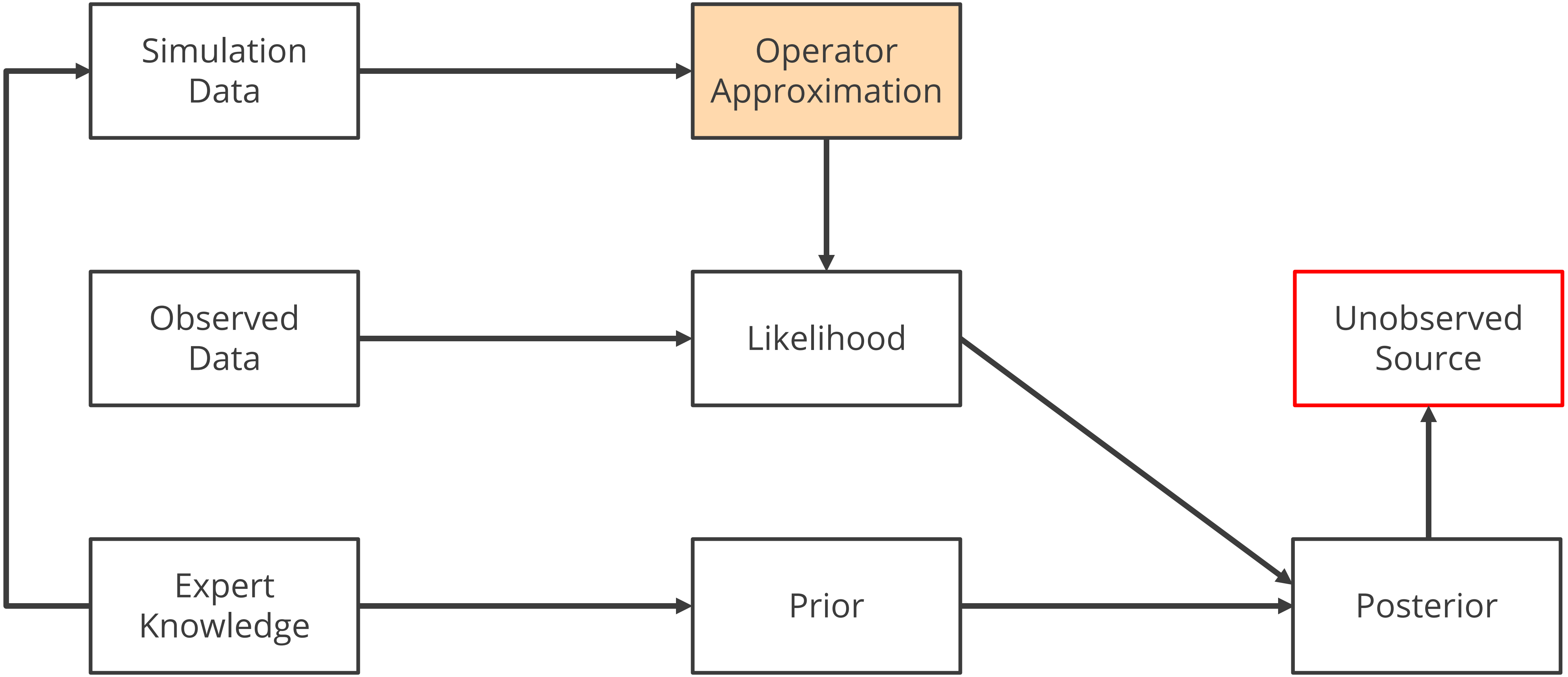


Operator Approximation: Learning Formulation

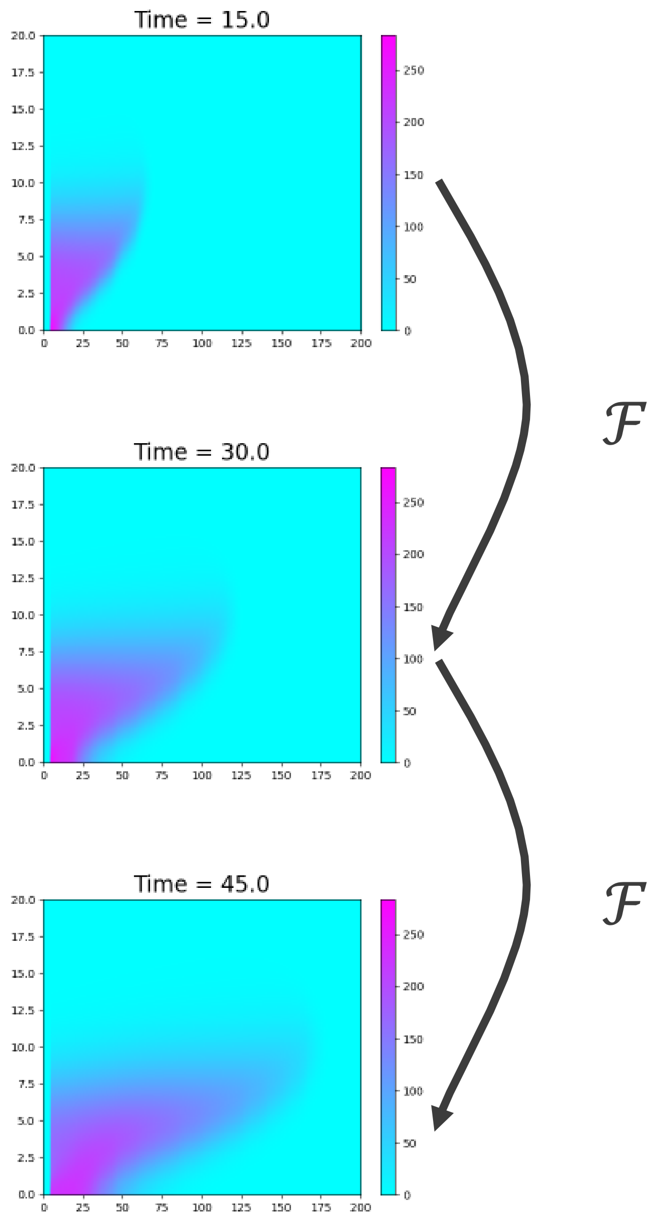
- Input the initial condition $\mathbf{u}_0$ and source $\boldsymbol{z}$,
- to predict time snapshots $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N \in \mathbb{R}^d$.
- Approximate the flow map

$$\mathbf{u}_{n+1} = \mathcal{F}(\mathbf{u}_n, z_n)$$

- and compose it to predict the time history

$$\mathbf{u}_{n+1} = \mathcal{F}(\mathcal{F}(\cdots \mathcal{F}(\mathcal{F}(u_0, z_0), z_1) \cdots, z_{n-1}), z_n)$$

- Given data pairs $\{(z_n^m, \mathbf{u}_n^m, \mathbf{u}_{n+1}^m)\}$, approximate $\mathcal{F}$.



Operator Approximation: Dimension Reduction

- Principal component analysis (PCA) to compress the spatial dimension.

State Snapshots | Modes

number of spatial nodes d

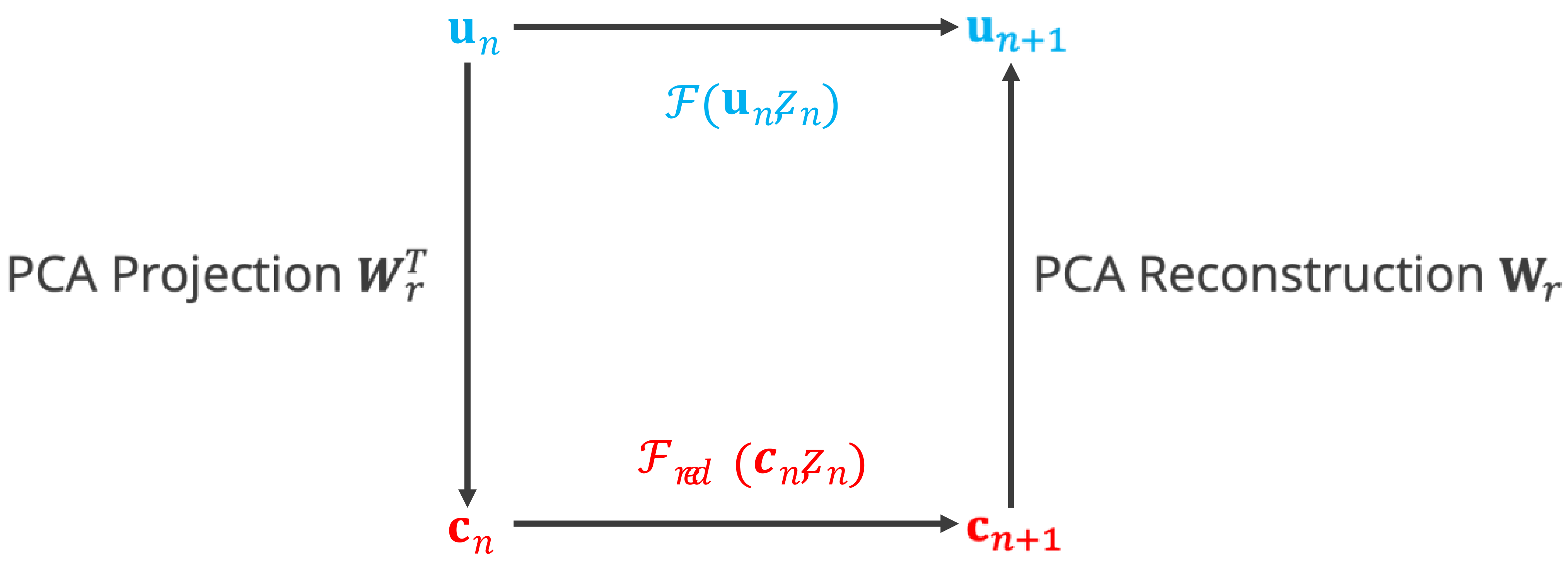
$$\begin{bmatrix} \mathbf{u}_0^1\ \mathbf{u}_1^1 \cdots \mathbf{u}_N^1\ \mathbf{u}_0^2 \cdots \mathbf{u}_N^2 \cdots \mathbf{u}_N^M \end{bmatrix} \approx \begin{bmatrix} \mathbf{W}_r \end{bmatrix} \begin{bmatrix} \boldsymbol{\Sigma}_r \end{bmatrix} \begin{bmatrix} \mathbf{V}_r^T \end{bmatrix}$$

Coordinates

number Of PCA modes r

$$\begin{bmatrix} \mathbf{c}_0^1\ \mathbf{c}_1^1 \cdots \mathbf{c}_N^1\ \mathbf{c}_0^2 \cdots \mathbf{c}_N^2 \cdots \mathbf{c}_N^M \end{bmatrix} = \begin{bmatrix} W_r^T \end{bmatrix} \begin{bmatrix} \mathbf{u}_0^1\ \mathbf{u}_1^1 \cdots \mathbf{u}_N^1\ \mathbf{u}_0^2 \cdots \mathbf{u}_N^2 \cdots \mathbf{u}_N^M \end{bmatrix}$$

Operator Approximation: Reduced Operator

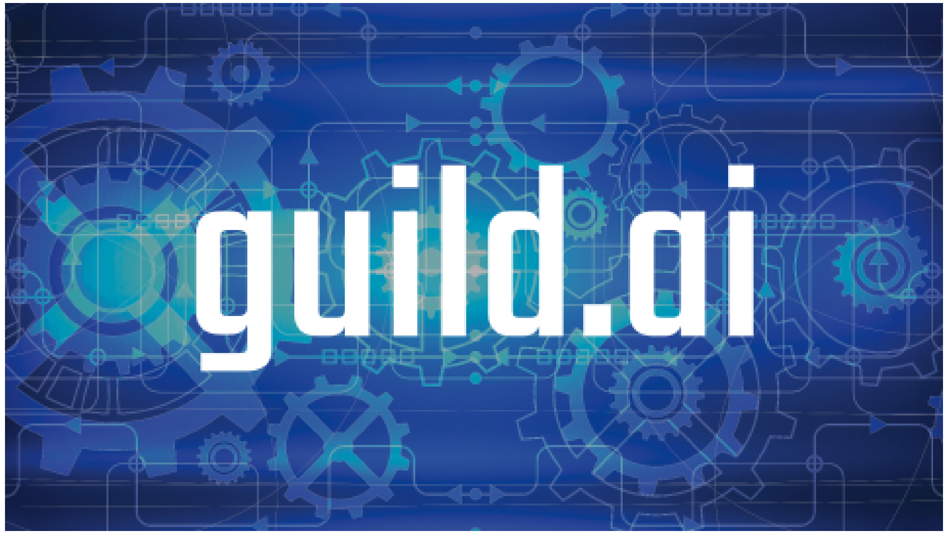


- The flow map $\mathcal{F}(\mathbf{u}_n, z_n)$ is defined in $\mathrm{d} = \mathcal{O}(10^5)$ dimensions.
- Learn a reduced operator $\mathcal{F}_{red}(\boldsymbol{c}_n, z_n)$ in $r = \mathcal{O}(10)$ dimensions.
- Approximate $\mathcal{F}_{red}(\boldsymbol{c}_n, z_n)$ via a Neural Network trained on time step pairs.

Operator Approximation: Network Architecture

$$c_{n+1} = \mathcal{F}_{red}(\boldsymbol{c}_n, z_n) = \boldsymbol{c}_n + \Delta t\, \mathcal{NN}(\boldsymbol{c}_n, z_n, \xi)$$

- Impose structure through PCA modes and time discretization.
- $\mathcal{NN}(\boldsymbol{c}_n, z_n, \xi)$ is a dense 2 layer feed forward network with parameters ξ.
- Many hyperparameters:
  - Number of PCA modes
  - Network depth
  - Activation function
  - Learning rate
  - Loss function
  - etc



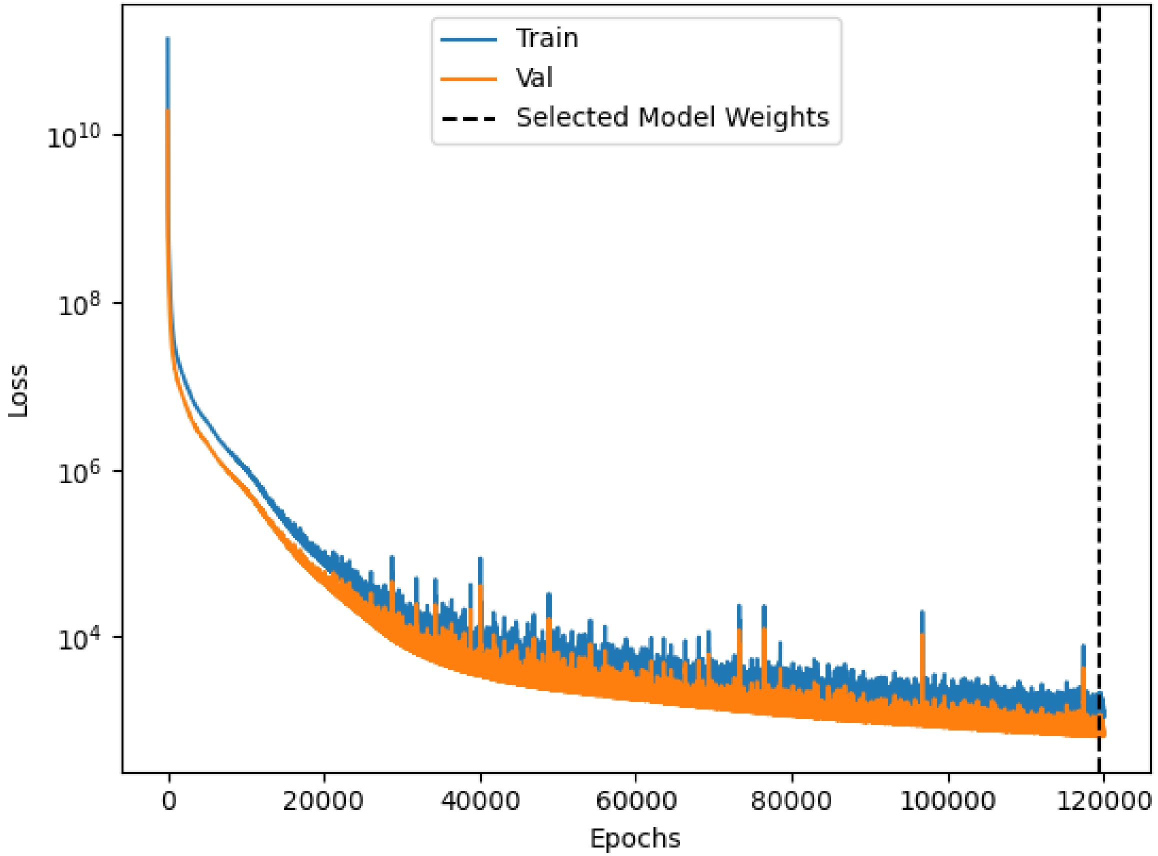
TensorFlow

Operator Approximation: Prediction, Loss, and Training

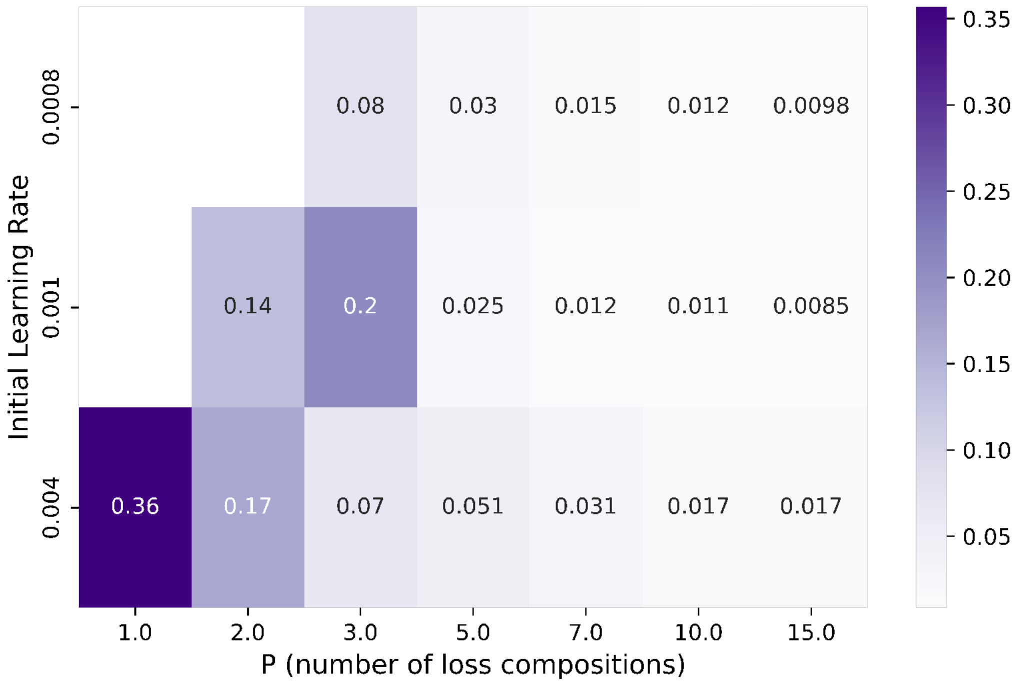
- Training data is all time steps $\{(z_n^m, \mathbf{c}_n^m, \mathbf{c}_{n+1}^m)\}$.
- Training loss is prediction error for p time steps:

$$Loss(\xi) = \sum_{m=1}^{M} \sum_{n=0}^{N-1} \sum_{p=1}^{P} \left\| \mathbf{c}_{n+p}^m - \mathcal{F}_{red}^{[p]}(\mathbf{c}_n^m, \mathbf{z}, \xi) \right\|^2$$

- $\mathcal{F}_{red}^{[p]}(\mathbf{c}_n^m, \mathbf{z}, \xi)$ denotes p compositions of $\mathcal{F}_{red}$.
- Guild enables efficient experiment tracking.
- Use validation set error to determine hyperparameters.

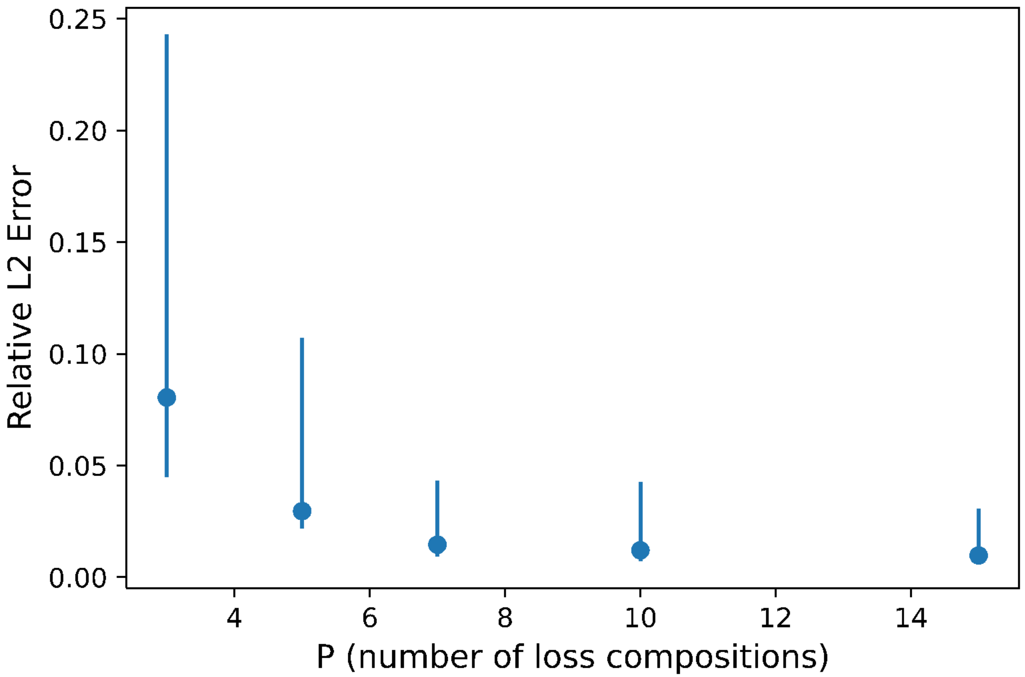


Operator Approximation: Experiment Tracker

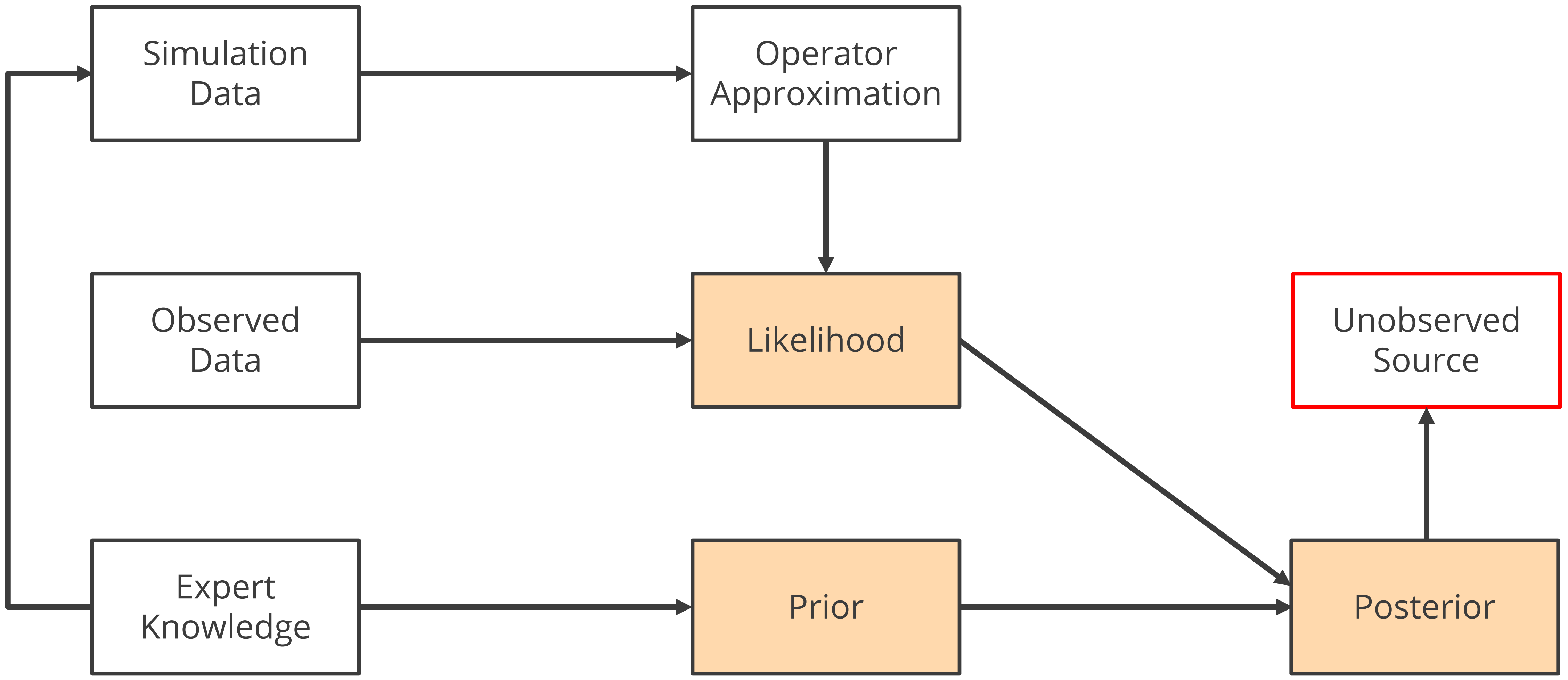


- Validation set relative error.
- Automation many training instances.
- Number of loss compositions is crucial.

- Error variability over 10 runs.
- Increasing P decreases variability.



Overview of the Workflow



Prior and Likelihood

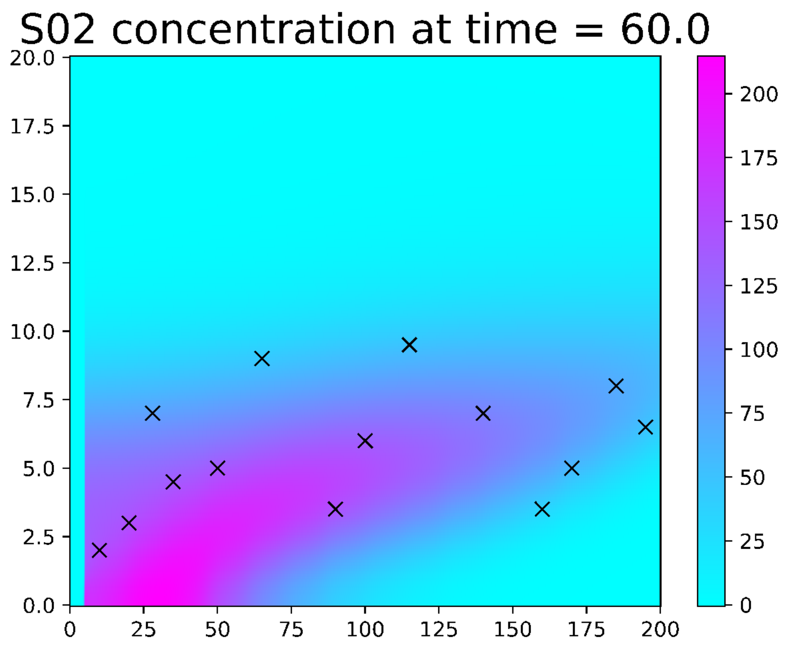
- Assume Gaussian prior and noise models:

$$\pi_{prior}(\mathbf{z}) \propto \exp(-\tfrac{1}{2}\|\mathbf{z} - \bar{\mathbf{z}}\|^2_{\boldsymbol{\Gamma}^{-1}_{prior}}) \qquad \pi_{like}(\mathbf{z}, \mathcal{D}) \propto \exp(-\tfrac{1}{2}\mathcal{M}(\mathbf{z}, \mathcal{D}))$$

- the misfit $\mathcal{M}$ depends on data $\mathcal{D} = [\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_N]$ as

$$\mathcal{M}(\mathbf{z}, \mathcal{D}) = \sum_{n=1}^{N} \left\| \mathcal{O}\mathbf{W}_r \mathcal{F}^{[n]}_{red}(\mathbf{c}_0, \mathbf{z}, \xi) - \mathbf{d}_n \right\|^2_{\boldsymbol{\Gamma}^{-1}_{noise}}$$

- with observation operator $\mathcal{O}$ illustrated by the x's,
- and model prediction $\mathbf{W}_r \mathcal{F}^{[n]}_{red}(\mathbf{c}_0, \mathbf{z}, \xi)$.



Maximum A Posteriori Probability (MAP) Point

- Bayes rule gives the posterior distribution,

$$\pi_{post} \propto \pi_{prior}\, \pi_{like}$$

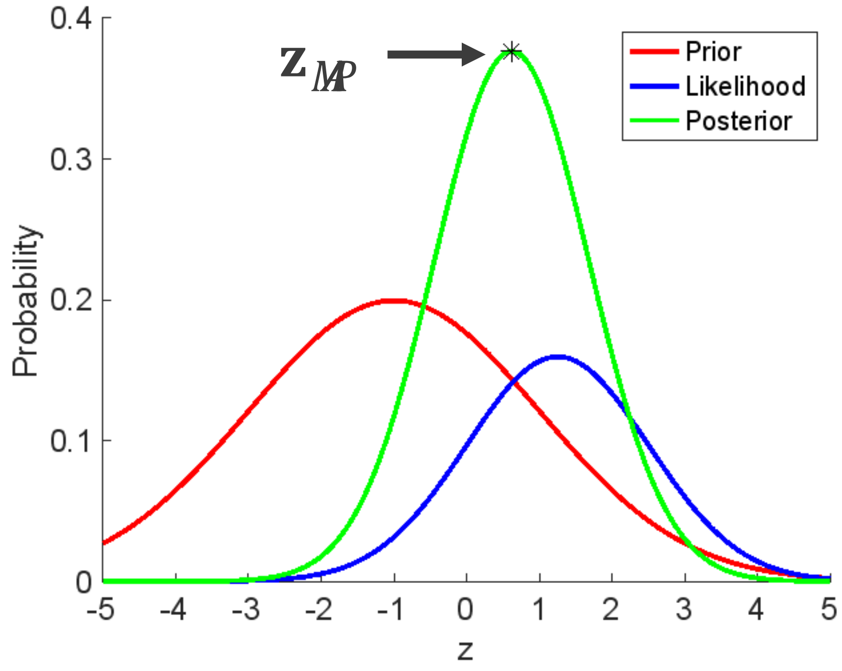
- to characterize the probability of the possible sources.

- Determine the maximum probability point,

$$\mathbf{z}_{MAP} = \underset{\mathbf{z}}{\operatorname{argmax}}\, \pi_{post}(\mathbf{z})$$

- or equivalently minimize the negative log of the posterior

$$\mathbf{z}_{MAP} = \underset{\mathbf{z}}{\operatorname{argmin}} \frac{1}{2} M(\mathbf{z}) + \frac{1}{2} \|\mathbf{z} - \bar{\mathbf{z}}\|^2_{\boldsymbol{\Gamma}^{-1}_{prior}}$$



Maximum A Posteriori Probability (MAP) Point

$$\mathbf{z}_{MAP} = \underset{\mathbf{z}}{\mathrm{argmin}} \frac{1}{2} M(\mathbf{z}) + \frac{1}{2} \|\mathbf{z} - \bar{\mathbf{z}}\|^2_{\boldsymbol{\Gamma}^{-1}_{prior}}$$

- Minimization using a Newton-CG Trust Region algorithm.
- Evaluate Neural Network Jacobian using algorithmic differentiation.
- Solve discretized adjoint equations to compute the exact gradient and Gauss-Newton Hessian.
- Cost per optimization iterate is one $\mathcal{NN}(\boldsymbol{c}_n, z_n, \xi)$ evaluation plus Jacobian for each time step.

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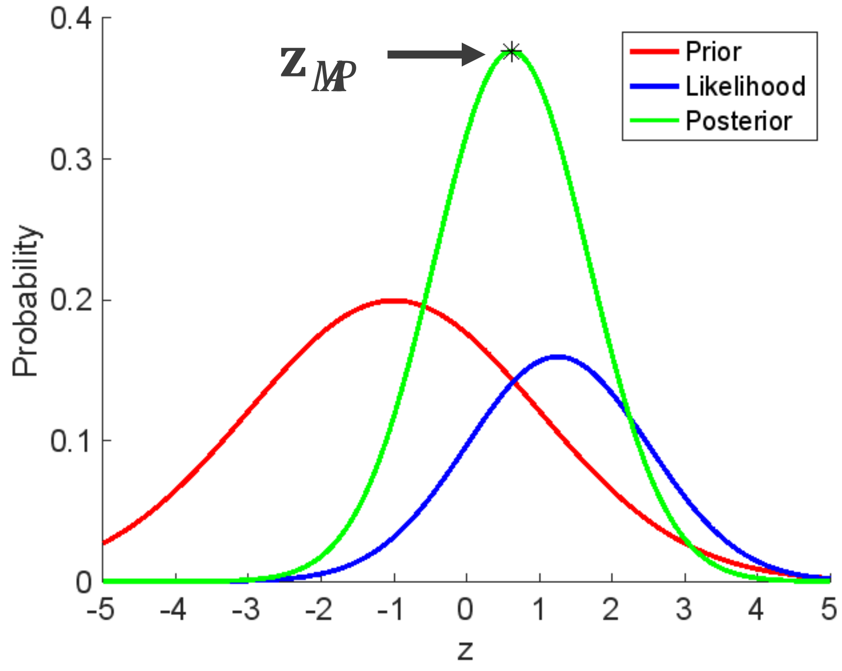
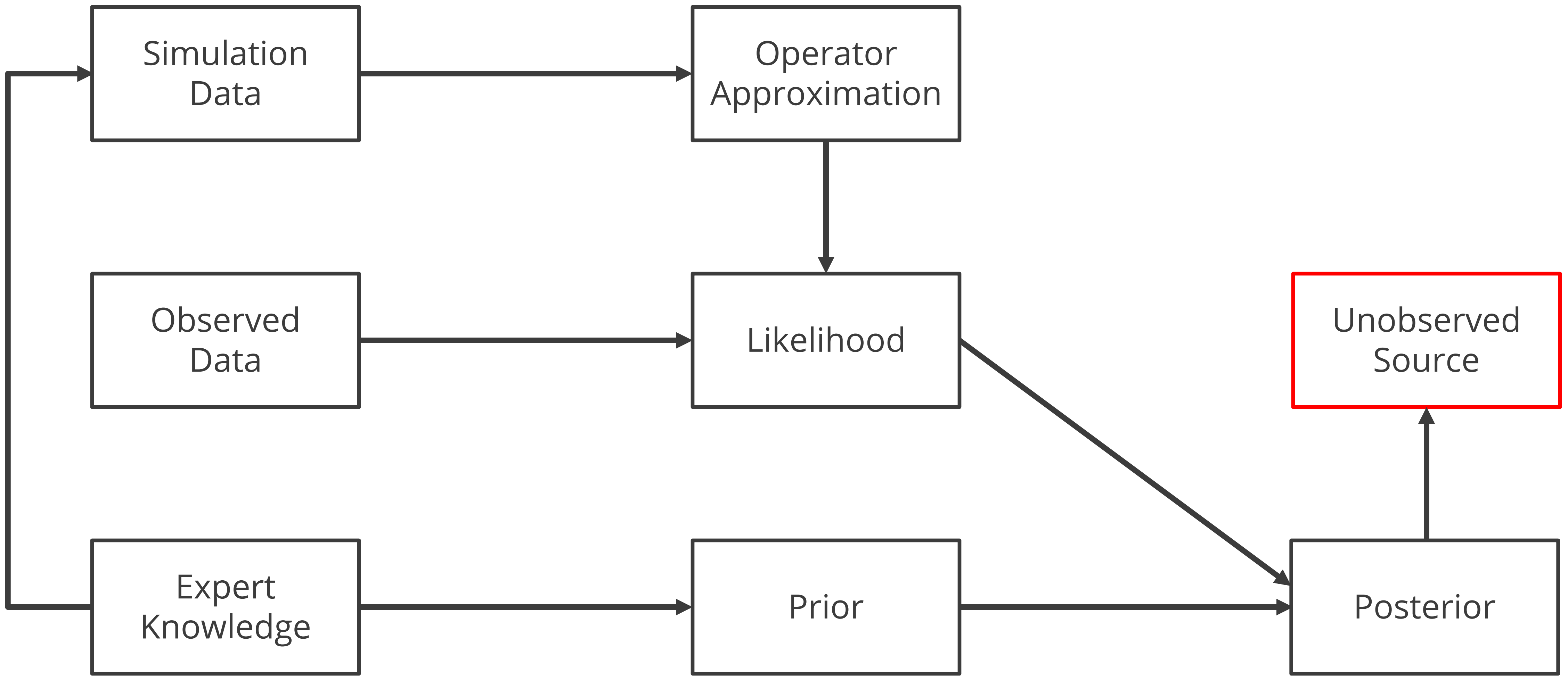
Posterior Sampling

$$\pi_{post} \propto \pi_{prior} \, \pi_{like}$$

- Laplace approximation: assume π_{post} is Gaussian.
- Mean is computed via optimization: $\mathbf{z}_{MAP}$.
- Covariance is the inverse Hessian of $-\log(\pi_{post})$ evaluated at $\mathbf{z}_{MAP}$.
- Leverage data sparsity for low rank approximation.
- Laplace approximation is an efficient first step.
- Markov Chain Monte Carlo methods are alternatives.



Overview of the Workflow



SO_2 Plume Model Problem

Change in SO2 concentration with respect to time

Diffusion

Wind

Gravity

Chemistry

Volcano source

$$\frac{\partial c}{\partial t} - \kappa \nabla^2 c + \boldsymbol{v} \cdot \nabla c - S\boldsymbol{e}_y \cdot \nabla c = R(c) + f \qquad \text{on } \Omega \times [0, T]$$

$$\nabla c \cdot \boldsymbol{n} = 0 \qquad \text{on } \partial\Omega \times [0, T]$$

$$c = 0 \qquad \text{on } \Omega \times \{0\}$$

No outflow

Zero initial SO2 concentration

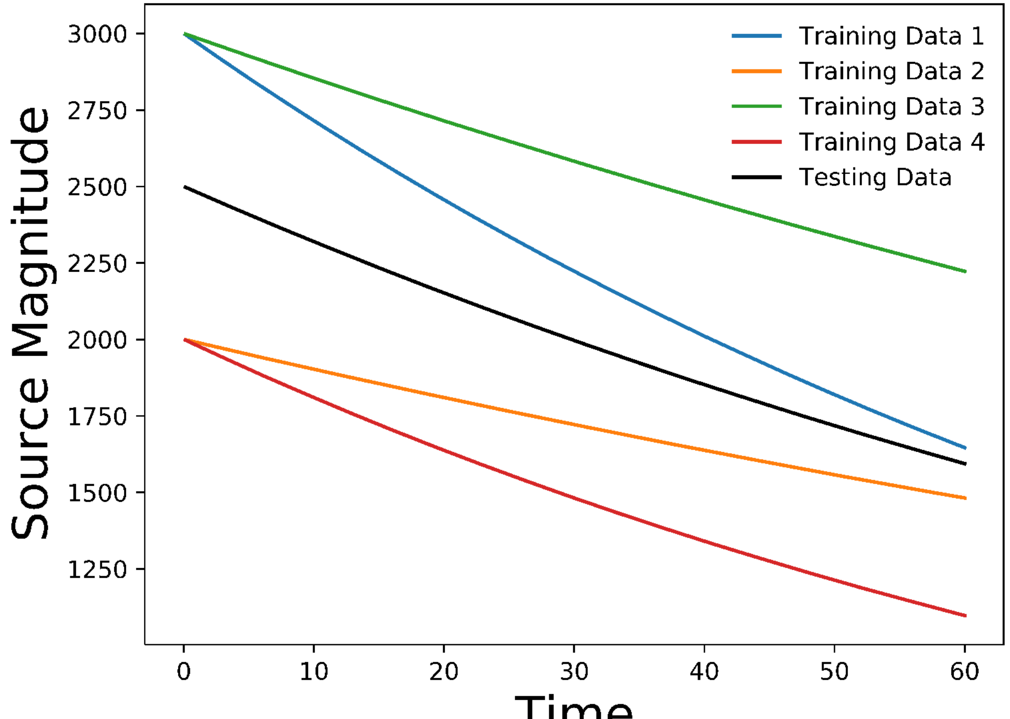
Data Generation

$$\frac{\partial c}{\partial t} - \kappa \nabla^2 c + \boldsymbol{v} \cdot \nabla c - S \boldsymbol{e}_y \cdot \nabla c = R(c) + f \qquad \text{on } \Omega \times [0, T]$$

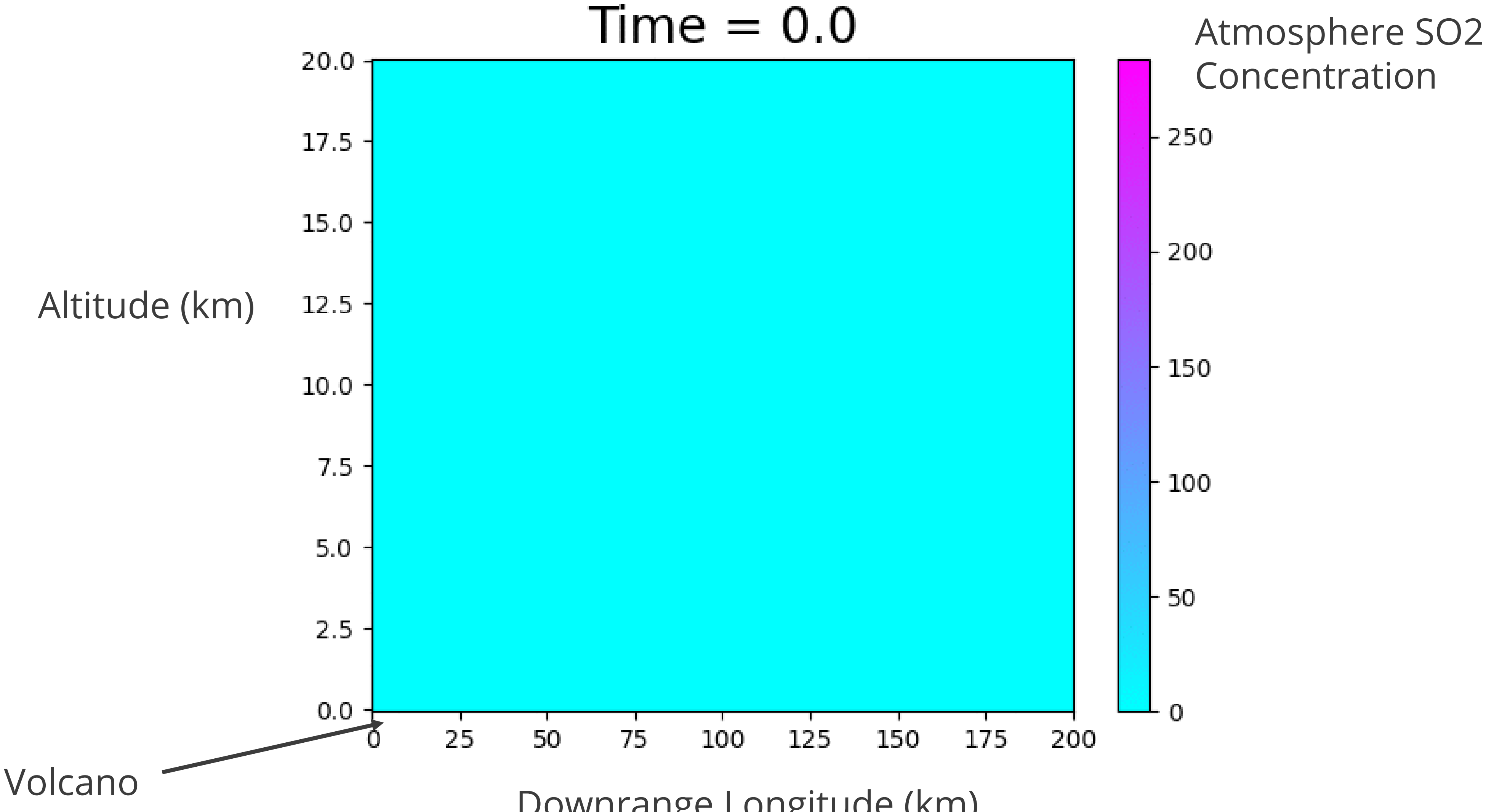
$$\nabla c \cdot \boldsymbol{n} = 0 \qquad \text{on } \partial\Omega \times [0, T]$$

$$c = 0 \qquad \text{on } \Omega \times \{0\}$$

- Training data from 3 different source terms.
- Validation data from a 4th source term.
- Testing data from a 5th source term.
- Train flow map approximation to infer testing data source.

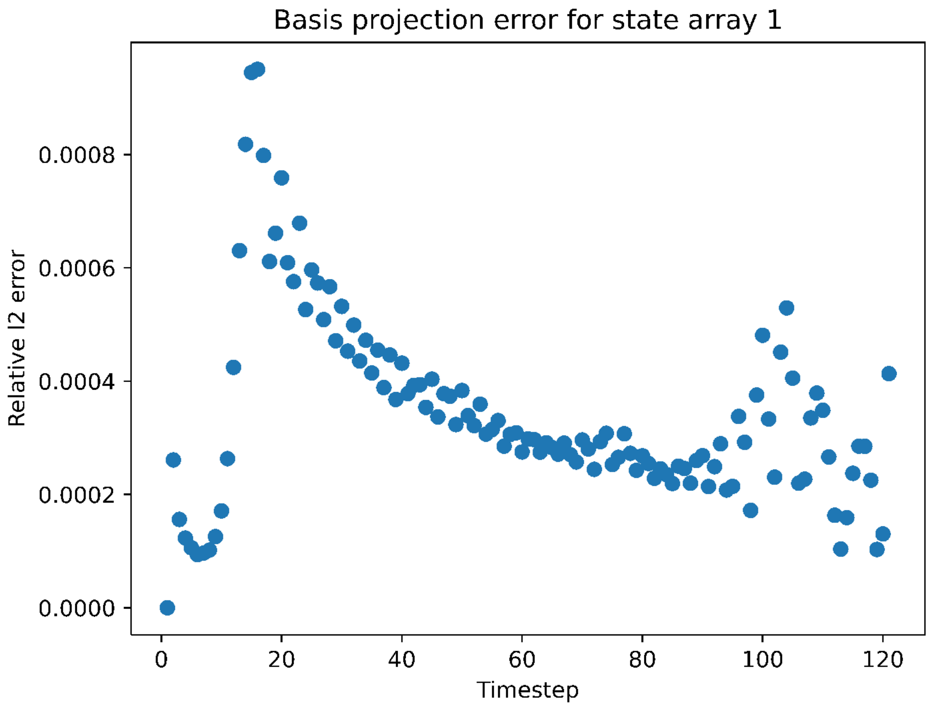


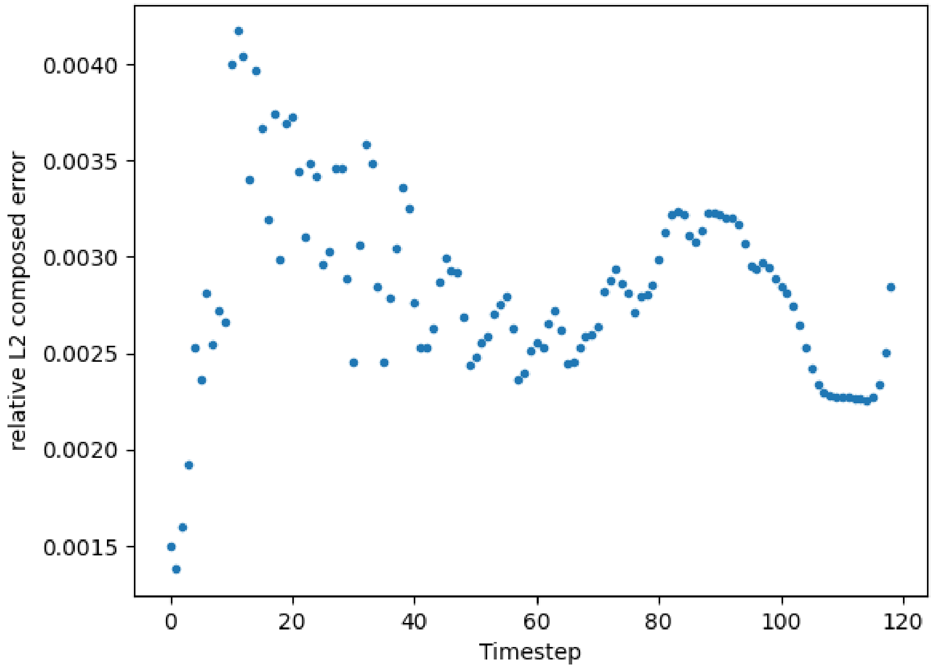
An Example of the Data



Operator Approximation

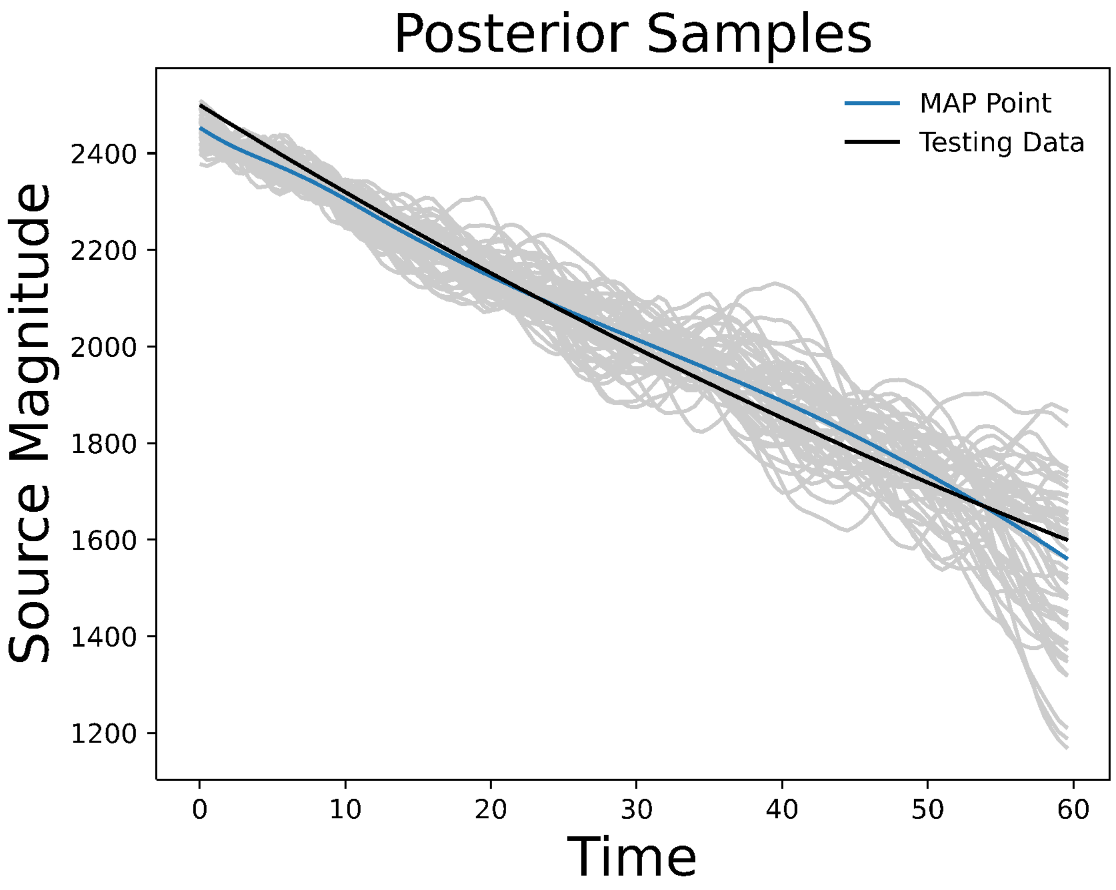
- Compress $\mathcal{O}(10^5)$ nodes to $\mathcal{O}(10^1)$ PCA modes with $\mathcal{O}(.01\%)$ relative error.





- Operator approximation achieves $\mathcal{O}(.4\%)$ prediction error.

Posterior Samples



- Black curve is the testing data.
- Blue curve is the MAP point.
- Grey curves are approximate posterior samples.
- Capture source well.
- Overestimates uncertainty later in time.

Conclusions and Ongoing Work

Next Steps

- Maturing hyperparameter optimization.
- Transitioning toward climate models and data.
- Advanced samplers for non-Gaussian posteriors.

End Goals

- Capturing spatial structure to better inform inversion.
- Identification of *pathways* to identify a reduced climate system.
- Final demonstration to characterize Mount Pinatubo eruption.