Advancing Earth System Model Calibration
A diffusion-based method

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Need an efficient UQ method for earth system model calibration

- U.S. Department of Energy's earth system model, land model, ELM simulates ecosystem's response to climate change.
- ELM involves 65+ parameters whose values need to be estimated for accurate model prediction.
- Current uncertainty quantification (UQ) methods are computationally expensive.
- We introduced a diffusion-based uncertainty quantification (DBUQ) method for efficient parameter estimation and model calibration.

DBUQ method

- DBUQ is a score-based diffusion method.
- It draws parameter posterior samples by formulating a generative model *F*, $X|Y \approx F(Y, Z; \theta)$

Our DBUQ method for parameter uncertainty quantification

Input: Prior sample set $\mathcal{D}_{\text{prior}} = \{(x_j, y_j)\}_{j=1}^{J}$;

Output: Trained generative model $F(Y, Z; \theta)$;

Procedure:

1. **for** $m = 1, \dots, M$
   - Estimate score function using Monte Carlo estimation through Eq. (13)–(15);
   - Solve the ODE in Eq. (16) with the estimated score function;
   - Obtain one sample (x_m, y_m, z_m) in the dataset $\mathcal{D}_{\text{label}}$;

   end
2. Train a NN to approximate the generative model $X = F(Z, Z; \theta)$ using the training data $\mathcal{D}_{\text{label}} = \{(x_m, y_m, z_m)\}_{m=1}^{M}$.

Generate parameter posterior samples: for a given observation y, evaluate the trained F at standard Gaussian samples Z to generate parameter posterior samples to approximate the target distribution $p(X|Y = y)$

Advantages of DBUQ

Computationally and memory efficient
Amortized Bayesian inference

- Formulate a supervised learning problem to estimate the sample generator *F*;
  - After the generator is trained, it can quickly generate numerous parameter posterior samples for any given observations;
- Use MC method to estimate the score function;
  - Computationally efficient;
- Solve a reverse ODE based on the estimated score function to generate the labeled data to train *F*;
  - Computationally and memory efficient as solving the ODE only needs to store the initial and terminal states of the transport path;

➢ DBUQ can be generally applied to site-specific earth system model calibration on a global scale, paving the way for more effective and timely climate impact analyses.

An illustrative examples of DBUQ

Problem

We use a simple 1D problem to illustrate our DBUQ method. The forward model $g(X)$ in the likelihood function of Eq. (2) is defined by

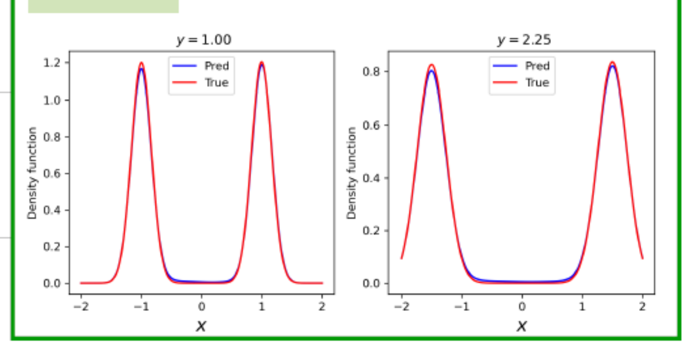
$$g(X) = X^2,$$

where the prior distribution of X is defined by a uniform distribution $\mathcal{U}([-2, 2])$ in the domain $[-2, 2]$. The observation variable Y is defined by

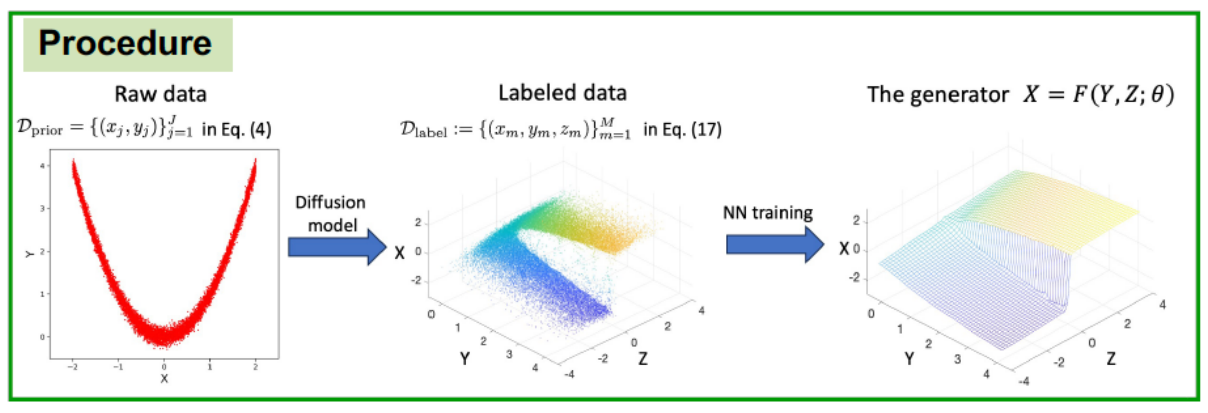
$$Y = g(X) + \varepsilon,$$

where ε follows the Gaussian distribution $\mathcal{N}(0, \sigma^2)$ with $\sigma = 0.1$.

Result



Procedure



- Multimodal distributions can be common for earth system model parameter estimation;
- It is challenging for UQ methods to capture all the possible modes;
- DBUQ accurately approximates the target bi-modal distributions;
- DBUQ is also computationally efficient, taking < 2min.

Apply DBUQ to improve ELM calibration

- Problem: Use DBUQ to estimate 8 ELM parameters;
- Observation: Annual averaged latent heat flux (LH) for 5 years at the Missouri Ozark AmeriFlux site in 2006-2010;
- Prior sample: 1000 paired samples $\mathcal{D}_{\text{prior}} = \{(x_j, y_j)\}_{j=1}^{J}$
- Two case studies:
  - Synthetic case for method verification
  - Real observations application
- Compare DBUQ with MCMC for performance evaluation

Parameter name	Parameter range
rootb_par	[0.5, 4]
slatop	[0.01, 0.05]
flnr	[0.1, 0.4]
frootcn	[25, 60]
froot_leaf	[0.3, 1.5]
br_mr	[1.5e-6, 4e-6]
crit_dayl	[35000, 45000]
crit_onset_gdd	[600, 1000]

DBUQ

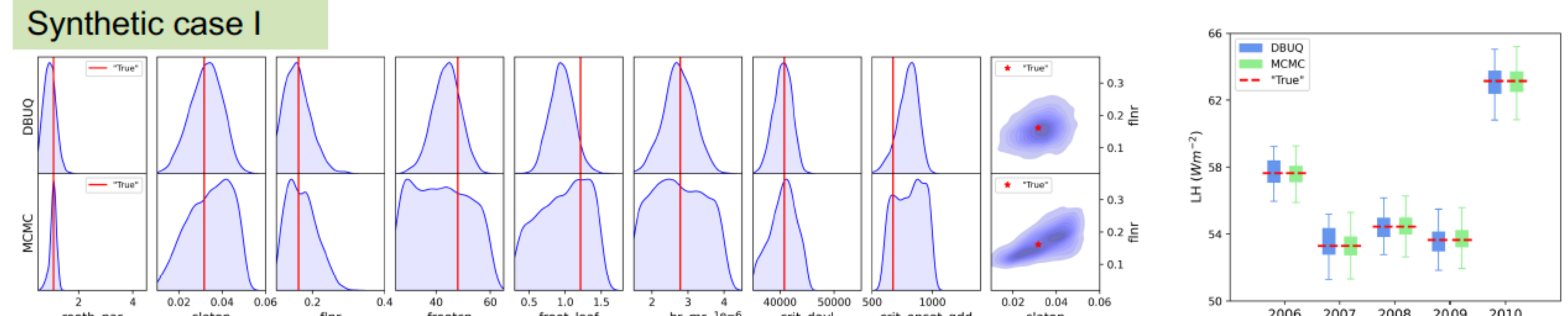
- Input: 1000 prior samples $\mathcal{D}_{\text{prior}} = \{(x_j, y_j)\}_{j=1}^{J}$
- Output: **a trained generator** which can be quickly evaluated to generate target samples for any given observations;
- Computing time: < 10 min for solving both cases
- **Particularly suitable for site-specific earth system model calibration at a global scale** due to its computational efficiency and amortized inference.

MCMC

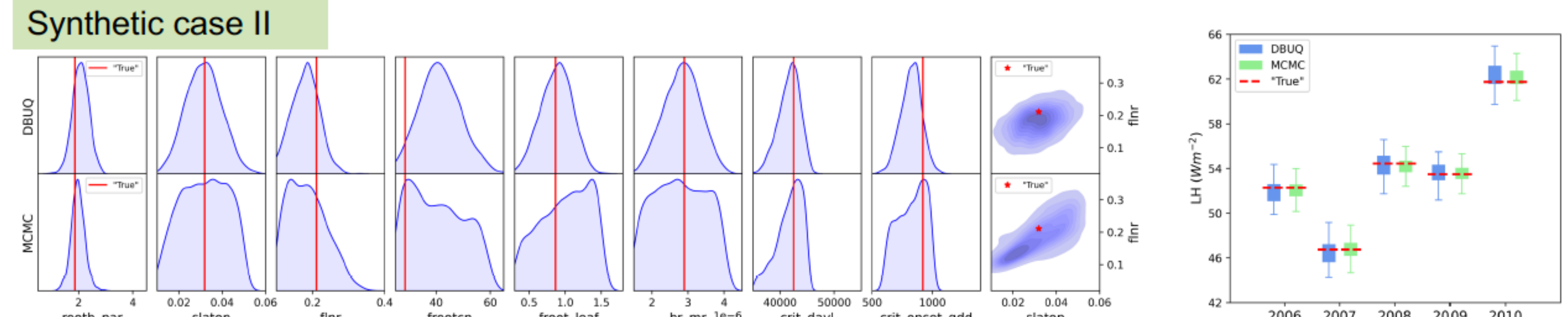
- Input: 1000 prior samples $\mathcal{D}_{\text{prior}} = \{(x_j, y_j)\}_{j=1}^{J}$
- Procedure: build a surrogate model on the prior samples, and then perform MCMC simulations on the surrogate;
- Output: **a set of posterior samples;** For a different observation, we need to re-run MCMC;
- Computing time: ~ 5 hours for one case to generate the same number of posterior samples as DBUQ.

DBUQ accurately estimates parameter PDFs

Synthetic case I



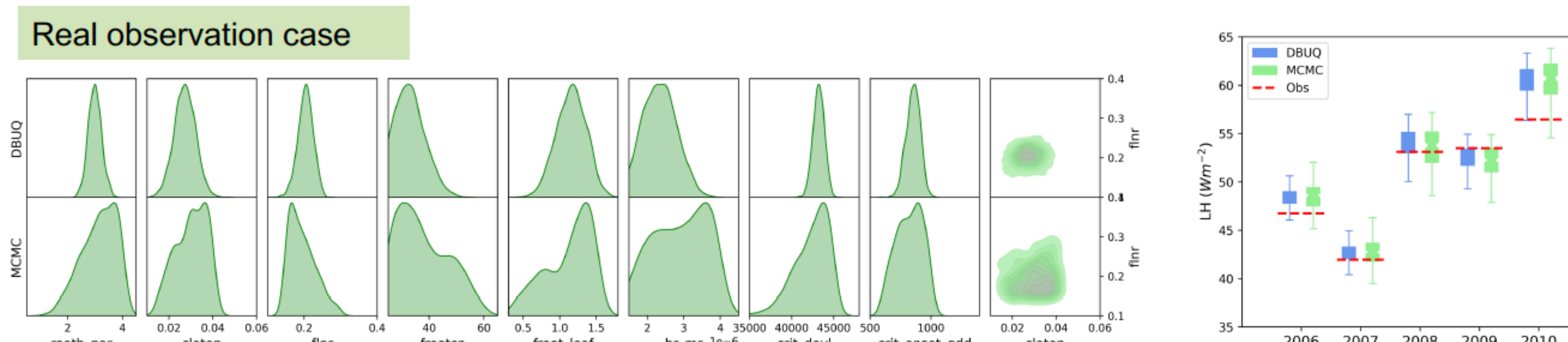
Synthetic case II



- DBUQ shows high accuracy in approximating the parameter posterior distributions.
  - Similar to the MCMC results, both accurately estimate the "true" parameter values with high probability.
- DBUQ demonstrates an accurate model calibration, as the prediction samples simulated from the parameter posterior samples are closely around the "true" observation.

DBUQ achieves 30X speedup than MCMC

Real observation case



- DBUQ again shows high accuracy in approximating the parameter posterior distributions.
  - Similar to the MCMC results in estimating both the marginal and joint PDFs.
- DBUQ demonstrates an accurate model calibration, as the prediction samples simulated from the parameter posterior samples are closely around the observation.
- Note, DBUQ achieves the similar accurate results with MCMC but using much less computational time.
  - DBUQ: 10 min for all the three case studies;
  - MCMC: 5 hours for one case studies;