# **Digital Twins in the era of** generative AI — Application to **Geological CO<sub>2</sub> Storage**

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**Georgia Tech College of Engineering** School of Electrical and Computer Engineering



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<sup>5</sup> now at Devito Codes

**MI4Seismic** 



# **Digital Twins in the era of** generative AI — Application to Geological CO<sub>2</sub> Storage



## Georgia Institute of Technology

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#### ML4Seismic



Why Geological Carbon Storage?



### Drivers geological CO<sub>2</sub> storage

- To keep temperatures below the 1.5-1.7°C rise, we need to safely store
  - ► 7 8 GtCO<sub>2</sub>/ yr by 2050
  - cumulatively 350 1200 GtCO<sub>2</sub> by 2100

- Requires *commissioning* of 7000 8000 offshore "Sleipners", @1 Mt/yr by 2050 deployment of 300 – 400 wells per year
  - monitoring of CO<sub>2</sub> migration to control subsurface distribution & verification
  - assurance of safe operations
  - transfer of liability to national governments at end of life cycle



# **Risk profiles**

#### Uncertainties & risk storage model

- highest at start
- diminish when more time-lapse data is collected

#### **Containment** risk increases

- ▶ w/ amount of CO<sub>2</sub> stored
- ► w/ size area undergoing pressure changes

There can be **NO** lapse in monitoring because

- any lack of *transparency* conformance
- ▶ will lead in loss in *confidence* by the *general* public

#### High-fidelity time-lapse information needs to be collected regularly over long periods of time!



#### uncertainty profile

#### containment risk profile





Wood et. al, Locked away – geological carbon storage, The Royal Society, October 2022 Ringrose, Philip. How to store CO2 underground: Insights from early-mover CCS Projects, 2020.

### Challenges monitoring Geological CO<sub>2</sub> Storage in Saline Aquifers

#### **Regulators & general public require transparency & assurances that** supercritical CO<sub>2</sub> stays put in the storage complex

- reservoir simulations alone are uncertain due to large variability permeability
- risk profile storage & containment highest at start & at end
- there is a need for reproducibility for transparency

#### **Develop low-cost monitoring & control system for CO<sub>2</sub> plumes**

- that is uncertainty aware
- maximally captures information collected over many decades
- attains accuracy needed to detect early onset leakage
- capable of risk mitigation via control

#### Systematic assessment of risks using techniques from uncertainty quantification.





![](_page_5_Picture_21.jpeg)

### **Digital Twins** from concept to reality

spans its lifecycle, is updated from real-time data, and uses simulation, machine learning and reasoning to help decision-making."

Innovation accelerating open-source software platform that

- makes data-informed predictions on future CO<sub>2</sub> plume behavior
- produces time-lapse data-consistent CO<sub>2</sub> predictions
- Is uncertainty aware & allows for scenario testing & control
- Informs on how much & where to collect data, thus reducing CCS monitoring costs

![](_page_6_Picture_7.jpeg)

![](_page_6_Picture_9.jpeg)

Møyner, O., et.al. 2023. Sintefmath/Jutul.jl: V0.2.5 (version v0.2.5). Zenodo. <u>https://doi.org/10.5281/zenodo.7775759</u> Luporini, F., et. al. 2022. devitocodes/devito: v4.6.2 (v4.6.2). Zenodo. <u>https://doi.org/10.5281/zenodo.6108644</u> Witte, P., et.al. 2020. slimgroup/JUDI.jl: DOI release (v2.0.2). Zenodo. <u>https://doi.org/10.5281/zenodo.3878711</u> Witte, P., et.al. 2021. slimgroup/InvertibleNetworks.jl: v2.1.0 (v2.1.0). Zenodo. <u>https://doi.org/10.5281/zenodo.5761654</u>

### **Open Source** scalable 2/3D code

#### Flow simulations:

- ► Jutul.jl
- JutulDarcy.jl

#### Wave simulations & imaging:

- Devito
- ► JUDI.jl

#### **Machine learning:**

- InvertibleNetworks.jl
- ► Flux.jl

![](_page_7_Picture_11.jpeg)

![](_page_7_Picture_12.jpeg)

![](_page_7_Picture_13.jpeg)

# Jutul JutulDarcy

![](_page_7_Picture_15.jpeg)

![](_page_7_Picture_16.jpeg)

### **Digital Twin** enabling technologies

#### **Key innovations:**

- Learned leakage detection\*
- Generative Geostatistical Modeling (GGM)\*
- Learned FWI w/ WISE: Full-waveform Inference w/ Subsurface Extensions\*
- Learned flow *imaging* via *coupled* flow-seismic\*
- Uncertainty-aware Digital Twin that allows for
  - controlled CO<sub>2</sub> injectivity rate
  - optimized CO<sub>2</sub> monitor well placement

\*Will be integrated into the Digital Twin for Underground CO<sub>2</sub> Storage

![](_page_8_Picture_13.jpeg)

# Learned leakage detection

![](_page_9_Picture_1.jpeg)

### **Explainable Leakage Detection** simulation-based training deep neural classifier

#### proxy model wavespeed, density

![](_page_10_Picture_2.jpeg)

reservoir model permeability, porosity

![](_page_10_Picture_4.jpeg)

![](_page_10_Picture_5.jpeg)

#### class activation mapping

![](_page_10_Figure_7.jpeg)

Huseyin Tuna Erdinc, Abhinav P. Gahlot, Ziyi Yin, Mathias Louboutin, and Felix J. Herrmann, "De-risking Carbon Capture and Sequestration with Explainable CO2 Leakage Detection in Time-lapse Seismic Monitoring Images", in AAAI 2022 Fall Symposium: The Role of AI in Responding to Climate Challenges, 2022

Ziyi Yin, Huseyin Tuna Erdinc, Abhinav Prakash Gahlot, Mathias Louboutin, and Felix J. Herrmann, "De-risking geological carbon storage from high resolution time-lapse seismic to explainable leakage detection", 2022

#### **CO**<sub>2</sub> dynamics time-lapse models wavespeed, density concentration, pressure pressure induced leakage fault regular two-phase flow deep neural classifier time-lapse imaging time-lapse (difference) data

![](_page_10_Figure_12.jpeg)

![](_page_10_Picture_13.jpeg)

![](_page_10_Picture_14.jpeg)

![](_page_10_Picture_15.jpeg)

![](_page_10_Picture_16.jpeg)

![](_page_10_Picture_17.jpeg)

# Generative Geostatistical Modeling (GGM)

![](_page_11_Picture_1.jpeg)

### Learning from examples w/ Generative Al

#### **Training:**

![](_page_12_Picture_2.jpeg)

![](_page_12_Figure_3.jpeg)

![](_page_12_Picture_4.jpeg)

#### **Sampling:**

![](_page_12_Picture_6.jpeg)

![](_page_12_Picture_7.jpeg)

![](_page_12_Picture_8.jpeg)

![](_page_12_Picture_9.jpeg)

![](_page_12_Picture_10.jpeg)

![](_page_12_Picture_11.jpeg)

![](_page_12_Picture_13.jpeg)

### Learned Geology from proxy Earth models

![](_page_13_Picture_1.jpeg)

**Training:** 

#### Sampling:

![](_page_13_Picture_4.jpeg)

![](_page_13_Picture_5.jpeg)

![](_page_13_Picture_6.jpeg)

![](_page_13_Picture_7.jpeg)

![](_page_13_Picture_8.jpeg)

![](_page_13_Picture_9.jpeg)

#### **Generative Geostatistical Modeling** training data augmentation

![](_page_14_Figure_1.jpeg)

![](_page_14_Figure_2.jpeg)

#### after training

Rafael Orozco, Mathias Louboutin, and Felix J. Herrmann, "Towards generative seismic kriging with normalizing flows", ML4SEISMIC Partners Meeting. 2023.

#### observed seismic

![](_page_14_Picture_6.jpeg)

![](_page_14_Picture_7.jpeg)

![](_page_14_Picture_8.jpeg)

![](_page_14_Figure_10.jpeg)

0

1

2

3

Lateral position [Km]

5

6

0.0

![](_page_14_Picture_11.jpeg)

![](_page_14_Picture_13.jpeg)

# Learned FWI w/ WISE

![](_page_15_Picture_2.jpeg)

#### **Full-waveform inference** posterior distribution

### velocity model

![](_page_16_Figure_2.jpeg)

fails because mapping is too complex

Ziyi Yin, Rafael Orozco, Mathias Louboutin, and Felix J. Herrmann, "WISE: Full-waveform Inference with Subsurface Extensions", ML4SEISMIC Partners Meeting. 2023.

#### observed data

![](_page_16_Picture_6.jpeg)

![](_page_16_Picture_7.jpeg)

![](_page_16_Picture_8.jpeg)

![](_page_16_Picture_9.jpeg)

#### **Full-waveform inference** posterior w/ physics-based summary statistic

### velocity model

![](_page_17_Figure_2.jpeg)

migration preserves information as long as migration-velocity model is sufficiently accurate

Rafael Orozco, Ali Siahkoohi, Gabrio Rizzuti, Tristan van Leeuwen, and Felix J. Herrmann, "Adjoint operators enable fast and amortized machine learning based **Bayesian uncertainty guantification**", in SPIE Medical Imaging Conference, 2023.

![](_page_17_Figure_5.jpeg)

![](_page_17_Picture_7.jpeg)

#### **Full-waveform inference** "approximate" posterior

### velocity model

![](_page_18_Figure_2.jpeg)

![](_page_18_Figure_3.jpeg)

![](_page_18_Figure_4.jpeg)

![](_page_18_Picture_5.jpeg)

#### **Full-waveform inference** summary statistics = RTM + subsurface offset

### sample velocity model

![](_page_19_Figure_2.jpeg)

![](_page_19_Picture_3.jpeg)

### subsurface offset gathers

![](_page_19_Picture_5.jpeg)

#### Training conditional Normalizing Flow (CNF)

![](_page_20_Figure_1.jpeg)

$$\hat{\theta} = \underset{\theta}{\operatorname{arg\,min}} \frac{1}{N} \sum_{\substack{N=1}}^{N} \frac{1}{N} \sum_{n=1}^{N} \sum_{n=$$

Train *amortized* CNF on N training pairs  $\{\mathbf{x}^{(n)}, \mathbf{y}^{(n)}\}_{n=1}^{N}$  with

$$\left( \|f_{\theta}(\mathbf{x}^{(n)};\mathbf{y}^{(n)})\|_{2}^{2} - \log \left|\det \mathbf{J}_{f_{\theta}}\right| \right)$$

![](_page_20_Picture_8.jpeg)

### Ground-truth velocity model

1000 E N 2000

3000

0

()

### 1000

2000 3000 4000 5000 6000 X [m]

![](_page_21_Picture_4.jpeg)

#### **Posterior samples** summary statistics = RTM

Z [m]

![](_page_22_Picture_1.jpeg)

#### layers are inconsistent and disconnected

#### 3000 4000 5000 6000 X [m]

![](_page_22_Picture_4.jpeg)

#### **Posterior samples** summary statistics = extended RTM w/ 50 offsets layers are more consistent and connected

### 1000 E N 2000

#### 3000 0

1000

#### 2000 3000 4000 5000 6000 X [m]

![](_page_23_Picture_5.jpeg)

#### **Conditional mean** *summary* statistics = RTM

![](_page_24_Picture_1.jpeg)

3000

0

### 1000

2000 3000 4000 5000 6000 X [m]

![](_page_24_Picture_4.jpeg)

#### **Conditional mean** *summary* statistics = *extended* RTM w/ 50 offsets

## $1000^{-1}$ Z [m] 2000

#### 3000 0

1000

![](_page_25_Picture_4.jpeg)

![](_page_25_Picture_6.jpeg)

#### **Uncertainty Quantification** standard deviation

1000 Z [m] 2000

3000

()

0

#### 1000 2000

3000

![](_page_26_Picture_5.jpeg)

![](_page_26_Picture_6.jpeg)

#### SLIM 🔶 ML4Seismic

![](_page_26_Figure_8.jpeg)

### Histogram

![](_page_27_Figure_1.jpeg)

![](_page_27_Figure_2.jpeg)

![](_page_27_Picture_4.jpeg)

#### **Forward UQ RTMs from posterior samples migration-velocity models**

 $1000^{-1}$ Z [m]  $2000^{-1}$ 

0

### 3000

U

#### 2000 1000

![](_page_28_Picture_4.jpeg)

![](_page_28_Picture_6.jpeg)

# Learned flow imaging via coupled two-phase flow-seismic

![](_page_29_Picture_1.jpeg)

![](_page_30_Figure_0.jpeg)

minimize Ζ

K

![](_page_30_Picture_5.jpeg)

#### InvertibleNetworks.jl

![](_page_30_Picture_7.jpeg)

Li, D., Xu, K., Harris, J. M., & Darve, E. (2020). Coupled time-lapse full-waveform inversion for subsurface flow problems using intrusive automatic differentiation. Water Resources Research, 56, e2019WR027032. Mathias Louboutin, Ziyi Yin, Rafael Orozco, Thomas J. Grady II, Ali Siahkoohi, Gabrio Rizzuti, Philipp A. Witte, Olav Møyner, Gerard J. Gorman, and Felix J. Herrmann, "Learned multiphysics inversion with differentiable programming and machine learning", The Leading Edge, vol. 42, pp. 452–516, 2023.

Ziyi Yin, Rafael Orozco, Mathias Louboutin, and Felix J. Herrmann, "Solving multiphysics-based inverse problems with learned surrogates and constraints", Advanced Modeling and Simulation in Engineering Sciences, vol. 10, 2023. Møyner, Olav, Martin Johnsrud, Halvor Møll Nilsen, Xavier Raynaud, Kjetil Olsen Lye, and Ziyi Yin. 2023. Sintefmath/Jutul.jl: V0.2.5 (version v0.2.5). Zenodo. https://doi.org/10.5281/zenodo.7775759.

 $\|\mathscr{F} \circ \mathscr{R} \circ \mathscr{S}_{\theta^*} \circ \mathscr{G}_{\mathbf{W}^*}(\mathbf{Z}) - \mathbf{d}\|_2^2$ 

![](_page_30_Picture_11.jpeg)

![](_page_30_Picture_12.jpeg)

![](_page_30_Picture_13.jpeg)

### **Unseen ground-truth permeability**

Z [m] U X [m]

![](_page_31_Picture_2.jpeg)

# 

![](_page_31_Picture_4.jpeg)

![](_page_31_Picture_6.jpeg)

#### **Initial permeability** case 1

U

#### 1000

2000 X [m]

![](_page_32_Picture_4.jpeg)

![](_page_32_Picture_6.jpeg)

![](_page_32_Picture_7.jpeg)

### **Inversion progress**

![](_page_33_Figure_1.jpeg)

![](_page_33_Figure_2.jpeg)

![](_page_33_Picture_3.jpeg)

# Digital Twin w/ generative Al

![](_page_34_Picture_2.jpeg)

### **Time-lapse data** modalities

permeability

![](_page_35_Picture_2.jpeg)

![](_page_35_Picture_3.jpeg)

![](_page_35_Picture_4.jpeg)

#### seismic images from noisy data w/ SNR 8.0 dB

![](_page_35_Picture_6.jpeg)

![](_page_35_Picture_7.jpeg)

![](_page_35_Picture_8.jpeg)
Møyner, Olav, Martin Johnsrud, Halvor Møll Nilsen, Xavier Raynaud, Kjetil Olsen Lye, and Ziyi Yin. 2023. Sintefmath/Jutul.jl: V0.2.5 (version v0.2.5). Zenodo. https://doi.org/10.5281/zenodo.7775759.

# **Time-lapse data** modalities $p(\mathbf{K}), p(\mathbf{x}_0)$ **CO**<sub>2</sub> saturation







### seismic images + well data





Ardizzone, Lynton, et al. "Conditional Invertible Neural Networks for Guided Image Generation." (2019). Radev, Stefan T., et al. "BayesFlow: Learning complex stochastic models with invertible neural networks." IEEE transactions on neural networks and learning systems 33.4 (2020) Cranmer, Kyle, Johann Brehmer, and Gilles Louppe. "The frontier of simulation-based inference." Proceedings of the National Academy of Sciences 117.48 (2020): 30055-30062

# Simulation-based inference w/ conditional Normalizing Flows (CNFs)

Given simulated training pairs  $(\mathbf{x}, \mathbf{y})$ 

- $\blacktriangleright$  amortized training of CNFs to sample from the posterior  $p(\mathbf{x} \mid \mathbf{y})$  for any  $\mathbf{y}$
- $\blacktriangleright$  when trained, CNFs solve inference problems by generating samples  $\mathbf{x} \sim p(\mathbf{x} | \mathbf{y}^*)$
- $\blacktriangleright$  samples are conditioned on observed data,  $y^*$

# $\mathbf{X} \sim p(\mathbf{X} \mid \mathbf{y})$



# *Dynamic* simulation-based inference



# Sequential Bayesian Inference dynamical model for CO<sub>2</sub> plumes



# Approach: sample from posterior at previous time step, k - 1, and use it as a *prior* for the *current* time step, k.

Tatsis, Konstantinos E., Vasilis K. Dertimanis, and Eleni N. Chatzi. "Sequential bayesian inference for uncertain nonlinear dynamic systems: A tutorial." arXiv preprint arXiv:2201.08180 (2022). Kruse, Jakob, et al. "HINT: Hierarchical invertible neural transport for density estimation and Bayesian inference." Proceedings of the AAAI Conference on Artificial Intelligence. Vol. 35. No. 9. 2021

## At time index k-1

- $\blacktriangleright \mathbf{X}_{k-1}$  state (CO<sub>2</sub> saturation)
- $\blacktriangleright$  **y**<sub>k-1</sub> observed time-lapse data
- *M* dynamics operator
- $\mathcal{H}$  observation operator



# **Learned Sequential Bayesian Inference** given $\mathbf{y}_{k-1}^*$ generate training samples $(\mathbf{x}_k, \mathbf{y}_k) \sim p(\mathbf{x}_k, \mathbf{y}_k)$



# $\hat{\theta} = \arg\min_{\theta} \frac{1}{N} \sum_{n=1}^{N} \left( \|f_{\theta}(\mathbf{x}_{k}^{(n)}; \mathbf{y}_{k})\|_{n=1}^{N} \right)$

Create training ensemble by sampling

► prev. state 
$$\mathbf{x}_{k-1} \sim p(\mathbf{x}_{k-1} | \mathbf{y}_{k-1}^*)$$

• permeability  $\mathbf{K} \sim p(\mathbf{K})$ 

Applying dynamics  $\mathbf{x}_k = \mathcal{M}(\mathbf{x}_{k-1}, \mathbf{K})$ 

Simulating data  $\mathbf{y}_k = \mathscr{H}(\mathbf{x}_k)$ 

$$\sum_{k=1}^{n} |\mathbf{x}_{k}, \mathbf{y}_{k}| \sim p(\mathbf{x}_{k}, \mathbf{y}_{k}) \text{ via}$$

$$\sum_{k=1}^{n} |\mathbf{y}_{k}|^{2} - \log \left| \det \mathbf{J}_{f_{\theta}} \right|$$



# Learned Sequential Bayesian Inference sample from posterior $\mathbf{x}_k \sim p(\mathbf{x}_k | \mathbf{y}_k^*)$



Sample from posterior  $\mathbf{x}_k \sim p(\mathbf{x}$ with  $\mathbf{z} \sim N(0, I)$ .

#### Note: implicitly sampled from

$$p(\mathbf{x}_k | \mathbf{y}_k, \mathbf{y}_{1:k-1}) = \frac{p(\mathbf{y}_k | \mathbf{x}_k) p(\mathbf{x}_k | \mathbf{y}_{1:k-1})}{p(\mathbf{y}_k | \mathbf{y}_{1:k-1})}$$

 $p(\mathbf{x}_{k} | \mathbf{y}_{1:k-1}) = \mathbb{E}_{\mathbf{x}_{k-1} \sim p(\mathbf{x}_{k-1} | \mathbf{y}_{1:k-1})} \left[ p(\mathbf{x}_{k} | \mathbf{x}_{k-1}) \right]$ 

Marginalizes over

• previous state  $\mathbf{x}_{k-1}$ 

► permeability K

$$\mathbf{x}_k | \mathbf{y}_k^*$$
) via  $\mathbf{x}_k = f_{\hat{\theta}}^{-1}(\mathbf{z}; \mathbf{y}_k^*)$ 



# Example – inference w/ time-lapse seismic images & pressure data







Kruse, Jakob, et al. "HINT: Hierarchical invertible neural transport for density estimation and Bayesian inference." *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 35. No. 9. 2021.





# **Generating ground-truth data** for single fixed $\mathbf{K}^* \sim p(\mathbf{K}), \mathbf{x}_0^* \sim p(\mathbf{x}_0)$













# **Digital Twin** inferred CO<sub>2</sub> saturations conditioned on time-lapse well & seismic data

#### ground truth



#### error between truth & inferred



#### inferred mean



#### 3.2Km

#### inferred variance





# More realistic example



## **Samples** permeability distribution





3.2Km



## **Ground-truth & observations** plumes & imaged seismic

### ground-truth CO<sub>2</sub> plume



#### observed seismic



3.2Km



## Assimilated plumes ground-truth vs. inferred CO<sub>2</sub> plumes

### ground-truth CO<sub>2</sub> plumes



## inferred w/ seismic CO<sub>2</sub> plumes



## UQ errors & inferred standard deviation

#### errors w.r.t. ground-truth



### inferred standard deviations



# **Digital shadow**



Check also president's column in the Leading Edge, November 2023

# Digital Twin w/ controlled injectivity



# Fracture risk

- Initial state: DT of 0.05 ± 0.01m<sup>3</sup>/s injectivity
- leads to over pressure after 1920 days of injection
- rock fractures due to over pressure denoted by red areas
- unacceptable risk









Ringrose, Philip. "How to store CO2 underground: Insights from early-mover CCS projects." (2020): 978-3. Møyner, Olav, Martin Johnsrud, Halvor Møll Nilsen, Xavier Raynaud, Kjetil Olsen Lye, and Ziyi Yin. 2023. Sintefmath/Jutul.jl: V0.2.5 (version v0.2.5). Zenodo. https://doi.org/ 10.5281/zenodo.7775759.



Develop a numerical scheme to

- ensure induced reservoir pressure remains below the fracture *pressure* with *high* probability
- adapt the injection rate

Make use of

- Jutul.jl's numerical reservoir simulations
- modern non-convex constrained optimization techniques
- In numerical approximation of the gradient



# **Reservoir simulations** control at timestep k = 3

Add pressure to state  $\mathbf{x}_k =$  $\mathbf{p}_k$ 

Given injectivity,  $q_k$ , simulate state,  $\mathbf{X}_{k+1}$ , via

$$\mathbf{x}_{k+1} = \mathscr{M}(\mathbf{x}_k, \mathbf{K}; q_k)$$

for  $\mathbf{K} \sim p(\mathbf{K})$ 

- exceeds fracture pressure regularly at timestep k = 4
- $\blacktriangleright$  need to control injectivity,  $q_k$



# Optimized injection rates

#### Solve

## max $q_k \Delta t$ subject to $\mathbf{x}_{k+1}['p'] < \mathbf{p}_{max}$ where $\mathbf{x}_{k+1} = \mathcal{M}(\mathbf{x}_k, \mathbf{K}; q_k)$ $q_k$ with reservoir simulations over time interval $t = k\Delta t$ to $t = (k + 1)\Delta t$ • use finite-differences to approximate $\frac{\partial \mathbf{x}_{k+1}}{\partial \mathbf{x}_{k+1}}$ $\partial q_k$ $\blacktriangleright$ impose constraint for fracture pressure, $\mathbf{p}_{max}$ , via log-barrier method

- use Armijo linesearch
- ► solve w/ until tolerance  $\epsilon < 10^{-3}$
- requires on average 30 reservoir simulations



# Optimized w/o vs. w/ control

Saturation at current time



Difference between pressure at current time and hydro





Difference between pressure at current time and hydro





# Is the control beneficial?

### Without controlled injection rate:

44.3% of the samples during the next time step fracture

## With controlled injection rate:

2.34% of the samples during the next time step fracture

**Conclusion: Controlling injection decreases risk of fracture.** 





# Digital Twin w/ optimized well locations



# Situation

## Two types of time-lapse CO<sub>2</sub> plume observations

### direct but local – borehole(s)









# Problem

CO<sub>2</sub> project lasts years thus can drill more wells but:

## many location options



Operators deciding well locations should be informed by

- Current knowledge of the CO<sub>2</sub> plumes
- physics simulations of plume forecasts





# Solution: Bayesian experimental design

- Chose experiment design W that allows for  $\ensuremath{\textit{maximal}}$  information gain
  - $\mathbf{y} = \mathbf{W}(\mathbf{u})$
- quantified by the Kullback-Leibler divergence:
  - $D_{KL}(p(\mathbf{x} | \mathbf{y}) | | p(\mathbf{x})).$
- Expected information gain (EIG) averages over all possible designs
  - $EIG(\mathbf{W}) = \mathbb{E}_{p(\mathbf{y}|\mathbf{W})} \left[ D_{KL}(p(\mathbf{x}|\mathbf{y}) | | p(\mathbf{x})) \right].$

Go, Jinwoo, and Tobin Isaac. "Robust expected information gain for optimal Bayesian experimental design using ambiguity sets." Uncertainty in Artificial Intelligence. PMLR, 2022.



Hoffmann, Till, and Jukka-Pekka Onnela. "Minimizing the Expected Posterior Entropy Yields Optimal Summary Statistics." arXiv preprint arXiv:2206.02340 (2022).

# Relation conditional neural density & EIG

Maximizing the expected posterior density is equivalent to maximizing the expected information gain

## Thus optimizing under the posterior density objective will increase the EIG!

- $\max_{\mathbf{W}} EIG(\mathbf{W}) = \mathbb{E}_{p(\mathbf{y}|\mathbf{W})} \left[ D_{KL}(p_{\theta}(\mathbf{x} | \mathbf{y}, \mathbf{W}) | | p(\mathbf{x})) \right] = \mathbb{E}_{p(\mathbf{y}|\mathbf{W})} \left[ \mathbb{E}_{p(\mathbf{x}|\mathbf{y})} \left[ \log p_{\theta}(\mathbf{x} | \mathbf{y}) \log p(\mathbf{x}) \right] \right]$ 
  - $= \mathbb{E}_{p(\mathbf{y}|\mathbf{W})} \left[ \mathbb{E}_{p(\mathbf{x}|\mathbf{y})} \left[ \log p_{\theta}(\mathbf{x}|\mathbf{y}) \right] \right] \text{ law of total expectation}$
  - =  $\mathbb{E}_{p(\mathbf{x},\mathbf{y}|\mathbf{W})} \left[ \log p_{\theta}(\mathbf{x}|\mathbf{y}) \right]$  same as neural posterior objective!



# **Proposed method**

As usual, prepare posterior learning algorithm:  $\{\mathbf{x}^{(n)}, \mathbf{y}^{(n)}\}_{i=1}^{N}$ Instead of optimizing only network parameters:

$$\hat{\theta} = \arg\max_{\theta} \frac{1}{N} \sum_{n=1}^{N} \left( -\|f_{\theta}(\mathbf{x}^{(n)}; \mathbf{y}^{(n)})\|_{2}^{2} + \log \left|\det \mathbf{J}_{f_{\theta}}\right| \right).$$

Jointly optimize experiment design, W, –i.e., by

$$\hat{\theta}, \, \hat{\mathbf{W}} = \underset{\theta, \mathbf{W}}{\operatorname{arg\,max}} \, \frac{1}{N} \sum_{i=1}^{N} \left( -\|f_{\theta}(\mathbf{x}^{(n)}; \mathbf{W} \odot \mathbf{y}^{(n)})\|_{2}^{2} + \log \left| \det \mathbf{J}_{f_{\theta}} \right| \right).$$



# **Proposed method**

Optimize for probability *density* of well placement

- well budget agnostic
- decide number of wells post-hoc
- easier optimization
- stochastic sampling during training avoids local minima

Wu, Sixue, Dirk J. Verschuur, and Gerrit Blacquière. "Automated seismic acquisition geometry design for optimized illumination at the target: A linearized approach." *IEEE Transactions on Geoscience and Remote Sensing* 60 (2021) Bengio, Yoshua, Nicholas Léonard, and Aaron Courville. "Estimating or propagating gradients through stochastic neurons for conditional computation." *arXiv:1308.3432* (2013).






























# ground-truth CO<sub>2</sub>



#### inference error



#### inference mean







# ground-truth CO<sub>2</sub>



#### inference error



#### inference mean







# ground-truth CO<sub>2</sub>



#### inference error



#### inference mean







# ground-truth CO<sub>2</sub>



#### inference error



#### inference mean







# Improvement on baseline

# Our algorithm places wells near or at optimal locations as measured by error







# **Digital Twin**





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