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PETROBRAS

Workshop: Scientific Machine Learning (SciML) and Data-Driven Model Reduction for Reservoir Simulation

Eduardo Gildin
Petroleum Engineering Department at
Texas A&M University

Cenpes, Rio de Janeiro, August 11-15, 2025



**Source: DALLE-E 3 using “Decarbonization
in the Oil Industry”**



**Source: DALLE-E 3 using “Decarbonization
in the Oil Industry for NetZero”**

Your job: transport sand - Which one should you pick??



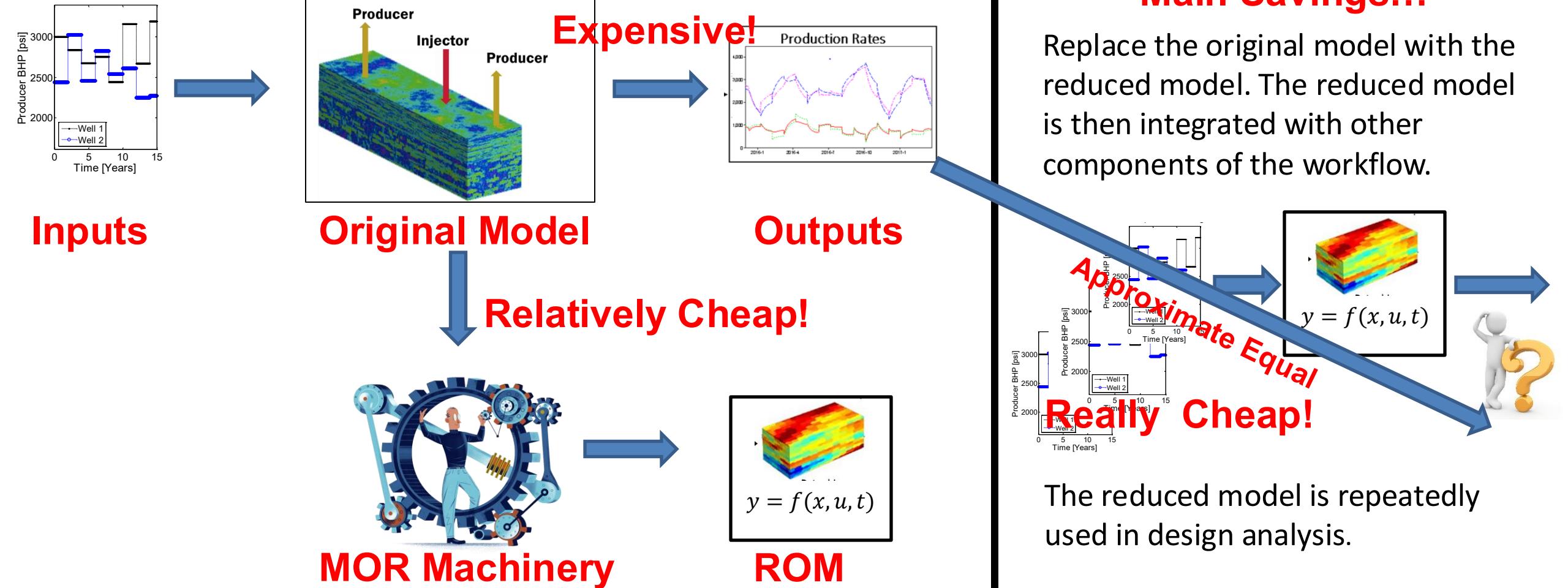
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Basic Idea



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The Holy Grail



→ Create a robust and scalable framework using **generalizable proxy models for fast computations leveraging reservoir simulation**

- “Theoretically” proven to work “all the time” → possible?
- Potentially include a reservoir simulator and production data
- Leading to fast, reliable, and interpretable simulations used in many reservoir management workflows
- Endow data-driven proxy models with features closely related to the ones encountered in nature, especially conservation laws.
- Attain scalability for very large problems (cheap training in offline mode, and cheap online computations)

Computational Cost



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Methods to reduce computational cost in the simulation can be classified in a broader sense as:

Reduce the cost of forward simulations (posteriori evaluations)

Surrogate models, reduced-order models, multiscale, upscaling

Reduce the input space dimension

Parameterizations: KL, DCT, sparsity-based, PC, HOSVD

Reduce the number of forward simulations

Efficient sampling: MCMC, DOE, etc.

HPC in Reservoir Simulation and Optimization

Complementary to the above methodologies

What is Model Order Reduction (MOR)?



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Find the lowest-complexity (dimensional) model, i.e., a *simplified model* that can capture the dominant behavior of the system of interest at a lower cost.

Physics-based (Dimension Reduction, Order Reduction) → Given a physical problem with dynamics described by the states $x \in \mathbb{R}^n$ where n is the dimension of the state space.

Because of redundancies, complexity, etc., we want to describe the dynamics of the system using a reduced number of states, that is $x \in \mathbb{R}^r, r \ll n \dots$

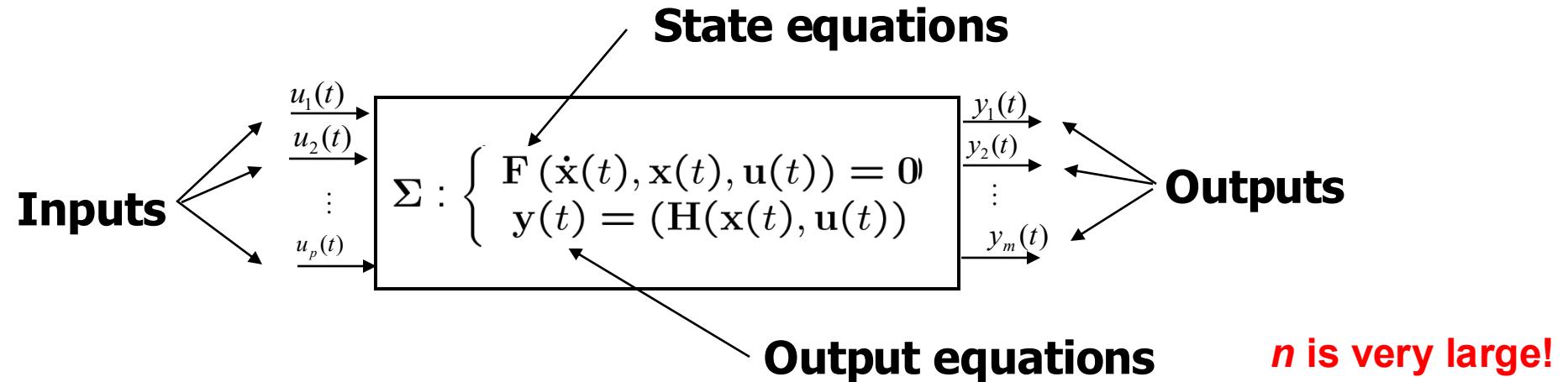
... by projecting a given High-Dimensional computational Model (HDM) on a subspace constructed after learning something about the system of interest

MODEL REDUCTION PROBLEM



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- Given



- linear time-invariant (LTI):

$$\Sigma : \begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ y(t) = Cx(t) + Du(t) \end{cases} \Leftrightarrow \Sigma = \left[\begin{array}{c|c} A & B \\ \hline C & D \end{array} \right] \in \mathbb{R}^{(n+p) \times (n+m)}$$

Projection-Based MOR



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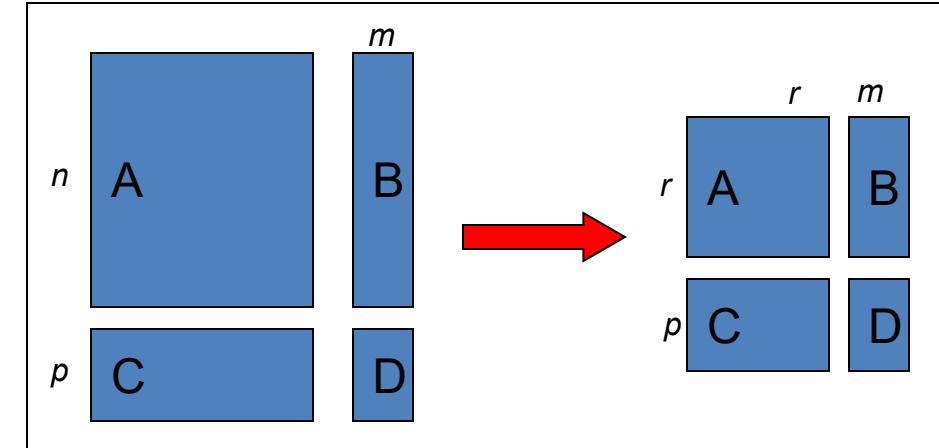
Approximate the states by a linear combination of basis vectors

$$\mathbf{x} \approx \sum_{i=1}^r \mathbf{V}_i x_{r_i}$$

$$\Sigma_r : \begin{cases} \dot{\mathbf{x}}_r(t) = \underbrace{\mathbf{W}^T \mathbf{A} \mathbf{V}}_{:=\mathbf{A}_r} \mathbf{x}_r(t) + \underbrace{\mathbf{W}^T \mathbf{B}}_{:=\mathbf{B}_r} \mathbf{u}(t) \\ \mathbf{y}_r(t) = \underbrace{\mathbf{C} \mathbf{V}}_{:=\mathbf{C}_r} \mathbf{x}_r(t) + \underbrace{\mathbf{D}}_{:=\mathbf{D}_r} \mathbf{u}(t) \end{cases}$$

Project

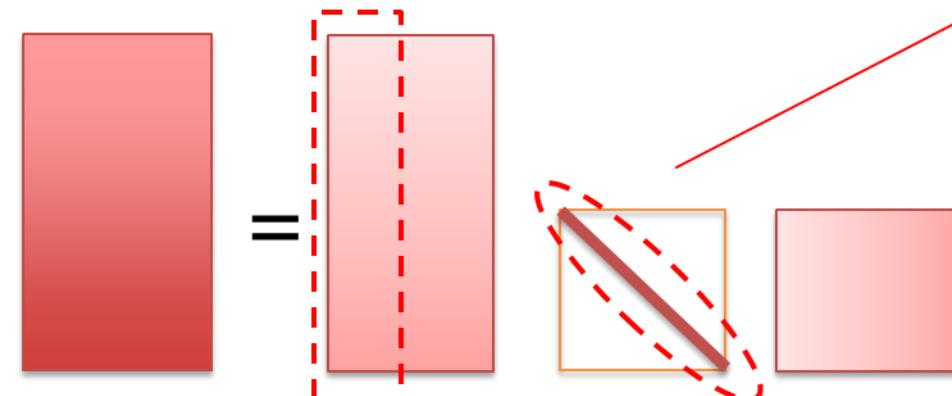
$$n \times 1 \left\{ \begin{bmatrix} \mathbf{x} \end{bmatrix} \approx \begin{bmatrix} \mathbf{V} \end{bmatrix} \begin{bmatrix} \mathbf{x}_r \end{bmatrix} \right\} r \times 1$$



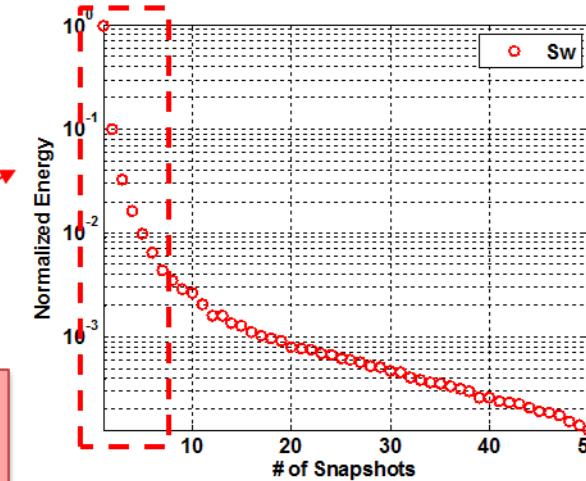
Principal Component Analysis (PCA) / Singular Value Decomposition (SVD)

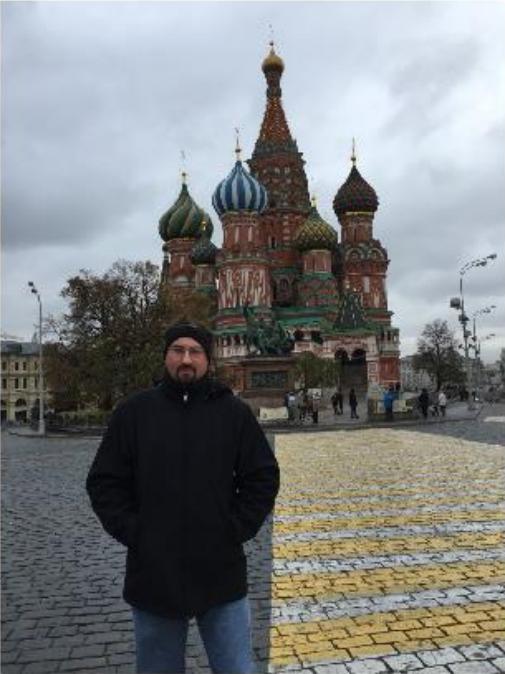
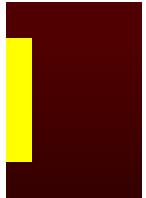
- Singular Value Decomposition

$$S = \mathbf{V} \Lambda \mathbf{W}^T$$



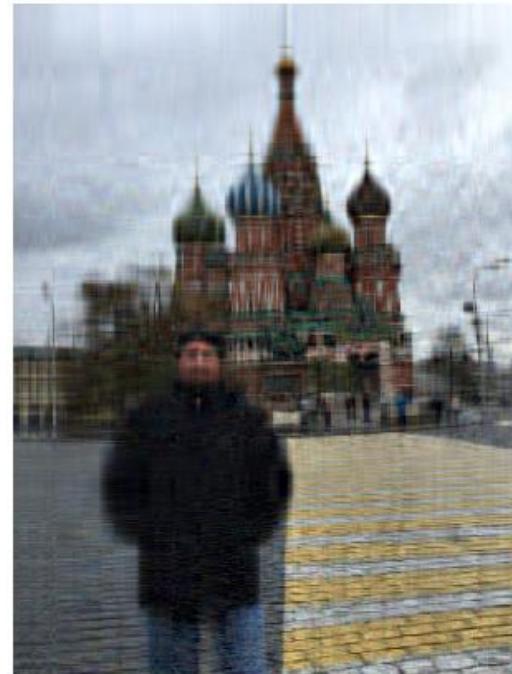
- Projection matrix ϕ : first m column of \mathbf{V} . ($m \ll n$)
(Kunisch and Volkwein 2001)



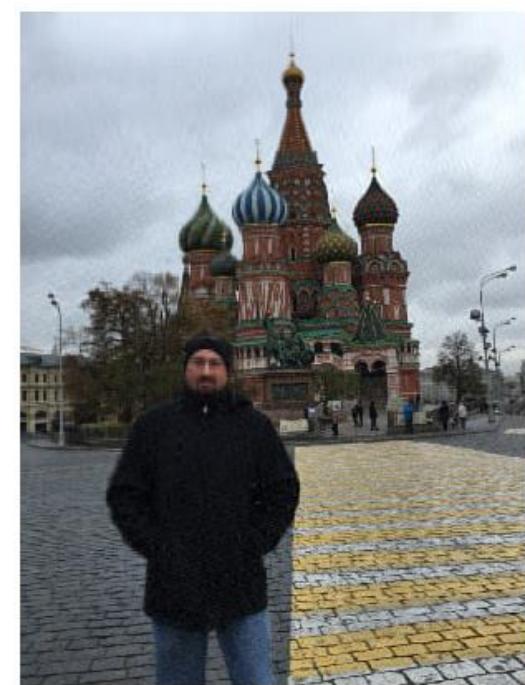


Size = 3264 X 2448

Image Compression



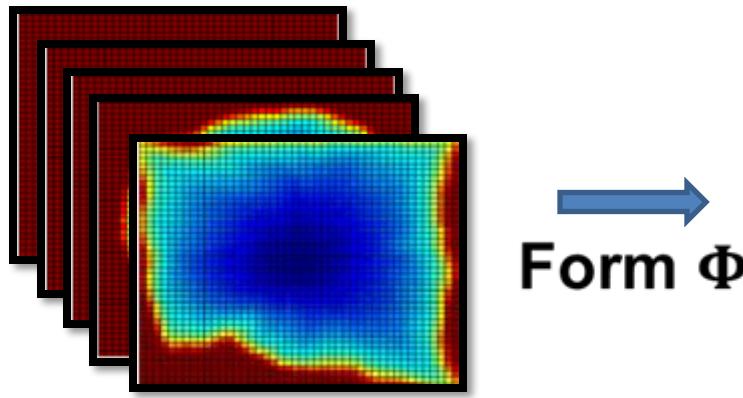
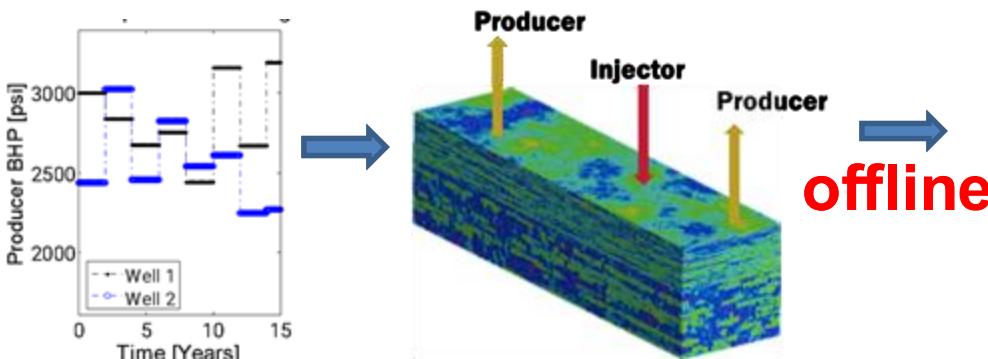
$k = 10$



$k = 100$



Projection-based ROM



$$[U, S, V] = SVD(X)$$

$$\mathbf{R}(\mathbf{x}^{n+1}, \mathbf{x}^n, \mathbf{u}^{n+1}) = \mathbf{F}(\mathbf{x}^{n+1}) + \mathbf{A}(\mathbf{x}^{n+1}, \mathbf{x}^n) + \mathbf{Q}(\mathbf{x}^{n+1}, \mathbf{u}^{n+1})$$
$$\mathcal{J} = \frac{\partial \mathcal{R}}{\partial \mathbf{x}}$$

$\mathbf{x} \rightarrow$ state (pressures, saturations)

$$\dot{\mathbf{x}} = f(\mathbf{x}) + g(\mathbf{x})\mathbf{u}$$

$$\mathbf{r} = \dot{\mathbf{x}}_r - f(\Phi \mathbf{x}_r) - g(\Phi \mathbf{x}_r)\mathbf{u}$$

$$\dot{\mathbf{x}}_r = \Phi^T f(\Phi \mathbf{x}_r) + \Phi^T g(\Phi \mathbf{x}_r)\mathbf{u}$$

Approximate

$$\mathbf{x} \approx \Phi \mathbf{x}_r$$

$$\Phi \in \mathbb{R}^{N \times r}$$

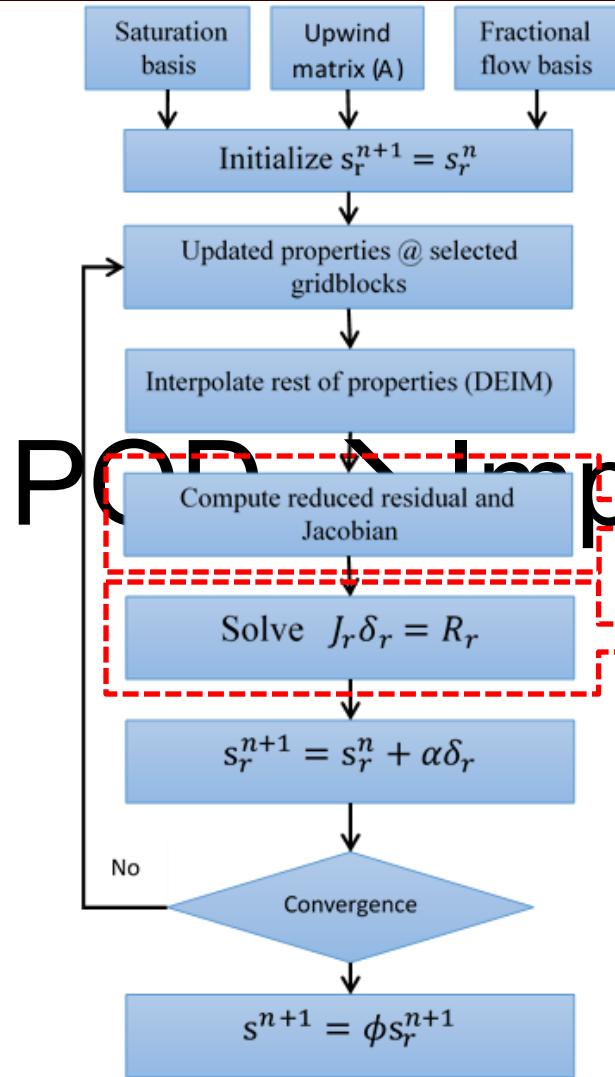
$$\Phi = \mathbf{U}[:, 1:r]$$

Project

$$\Psi^\top \mathbf{r} = 0$$

(Galerkin: $\Psi = \Phi$)

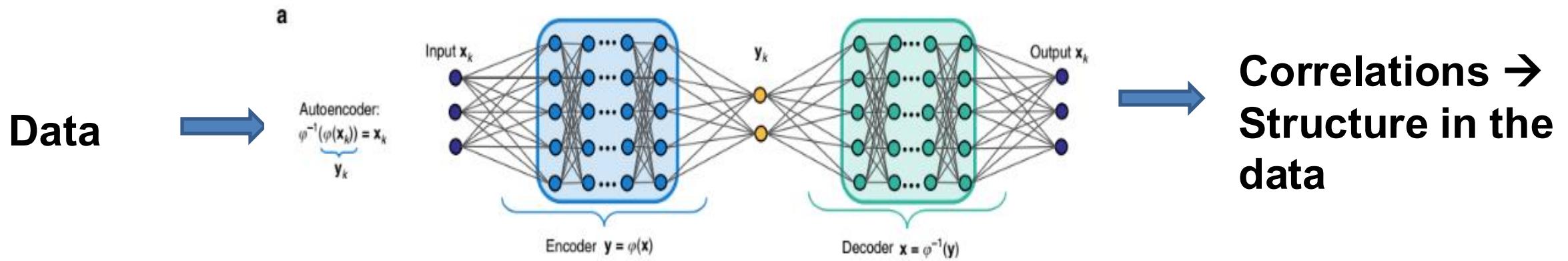
Question → how to find proper projections?



$$\begin{aligned} R_r &= \phi^T R \\ J_r &= \phi^T J \\ \delta_r &= J_r^{-1} R_r \end{aligned}$$

SVD is an old machine learning technique!

- Physics-based (projection-based) MOR can be seen as a physics enabled machine learning
 - Training → solve physics-based models (simulation) → snapshots **(need first principles)**
 - Machine learning: Identify structure in data (SVD?)
 - Reduction → projection **(need first principles)**



Why do you need MOR?



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Minimum data → Fast modeling

Fast simulation → Amenable to optimization under uncertainty (multiple realizations)

Parametric simulations → 1,000's of simulation

Applicable to large fields

Real-time reservoir management

MOR only pays off in workflows that require multiple calls of the reduced order model(s)

Tools for MOR and beyond



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MOR wiki → https://en.wikipedia.org/wiki/Model_order_reduction#Overview

SLICOT → <http://www.slicot.org/>
<https://github.com/SLICOT>

PyMOR → <https://pymor.org/>

MORLAB → <https://www.mpi-magdeburg.mpg.de/projects/morlab>

MATLAB – Control Toolbox →
<https://www.mathworks.com/help/control/ug/about-model-order-reduction.html>

pyDMD → <https://mathlab.sissa.it/pydmd>

libROM → <https://www.librom.net/>

pylibROM → <https://github.com/LLNL/pylibROM>

skrom → <https://scikitrom.github.io/>

Suggested Material/Reading



1. [GIL] Eduardo Gildin. Lecture Notes
2. [RAG] Jean Ragusa. Lecture Notes
3. [PYT1] Rick Muller. *A Crash Course in Python for Scientists*. <https://nbviewer.jupyter.org/gist/rpmuller/5920182>
4. [PYT2] Hans Petter Langtangen. *A Primer on Scientific Programming with Python*. Springer 2016
5. [MAT] Cleve Moler. *Numerical Computing with MATLAB*. SIAM 2004.
6. [MOR1] *Model Reduction and Approximation: Theory and Algorithms* edited by Peter Benner, Albert Cohen, Mario Ohlberger, Karen Willcox. SIAM 2017
7. [MOR2] Athanasios C. Antoulas. *Approximation of Large-Scale Dynamical Systems*. SIAM 2006
8. [MOR3] Daniel Wirtz. *Model Reduction for Nonlinear Systems: Kernel Methods and Error Estimation*. epubli GmbH, 2014.
9. [MOR4] *Model Reduction of Parametrized Systems*. Edited by Peter Benner, Mario Ohlberger, Anthony Patera, Gianluigi Rozza, Karsten Urban. Springer, 2014.
10. [MOR5] Reduced Order Methods for Modeling and Computational Reduction edited by Alfio Quarteroni, Gianluigi Rozza. Springer, 2014.
11. [MOR 6] Steven L. Brunton and J. Nathan Kutz. *Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control*. 1st Edition, Cambridge University Press; 2019.
12. [MOR 7] J. N. Kutz, S. L. Brunton, B. Brunton, J.L. Proctor. *Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems*. SIAM-Society for Industrial and Applied Mathematics, 2016
13. [DD_SUR1] Nathan Kutz, *Data-Driven Modeling & Scientific Computation: Methods for Complex Systems & Big Data*. 1st Edition, OUP Oxford, 2013
14. [DD_SUR2] A. I. J. Forrester, A. Sobester, A. Keane, *Engineering Design via Surrogate Modelling: A Practical Guide* 1st Edition, 2008 John Wiley & Sons, Ltd
15. [DD-SUR2] Andy Keane, Prasanth Nair. *Computational Approaches for Aerospace Design: The Pursuit of Excellence*



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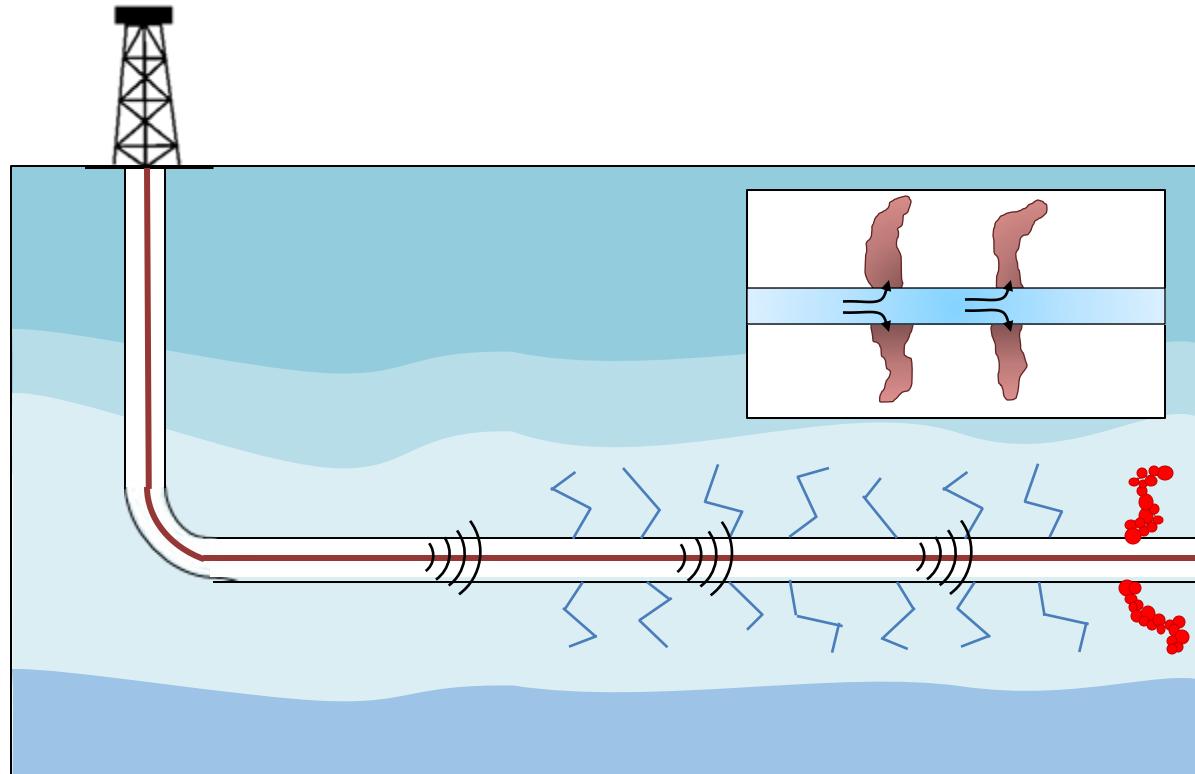
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MOR- Applications

Needs/Challenges

Subsurface Measurements Provide an Understanding of Fracture Propagation, Geometry and Its Interactions

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Distributed Acoustic Sensing

Microseismic

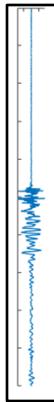
1. Data size → Big data
2. Data quality → Signal-to-Noise ratio (S/N)
3. Interpretability → Geometry/Propagation

1 well and 27 stages: 1.35 TB

A Tensor Is a D-way Array Or Multidimensional Collection Of Numbers

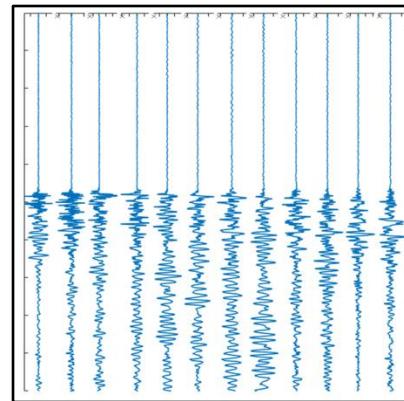
First-order tensor

Vector, $d=1$



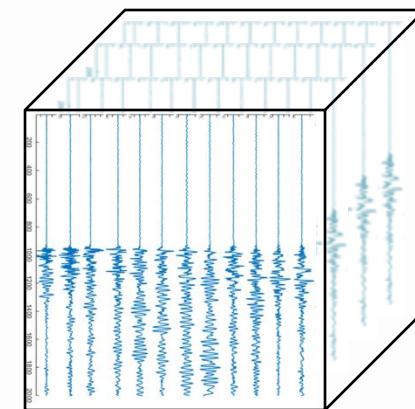
Second-order tensor

Matrix, $d=2$



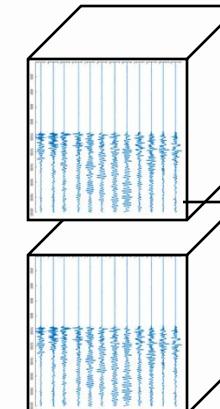
Third-order tensor

$d=3$



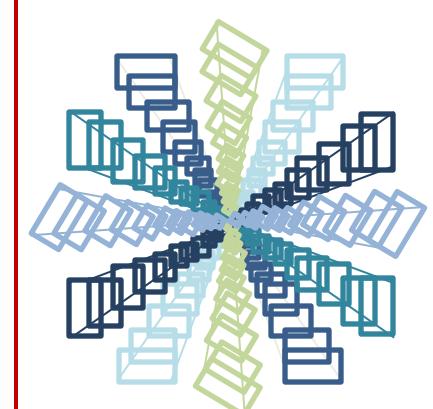
Fourth-order tensor

$d=4$



d -order tensor

$d > 3$

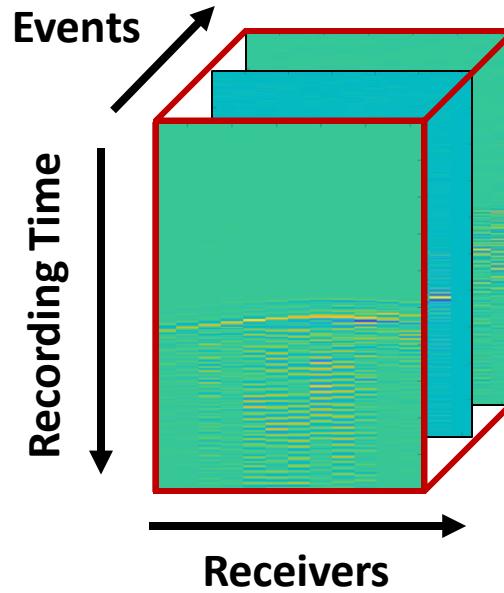


Synthetic and field data

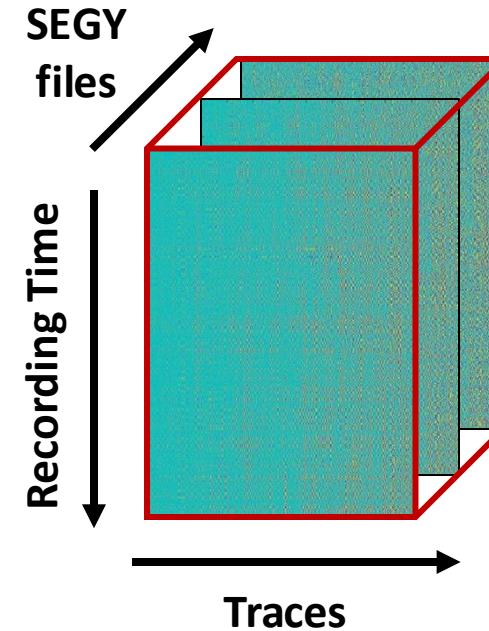
- Gonzalez, Keyla, Gildin, Eduardo, and Richard L. Gibson. "Improving Microseismic Denoising Using 4D (Temporal) Tensors and High-Order Singular Value Decomposition." Paper presented at the SPE/AAPG/SEG Unconventional Resources Technology Conference, Houston, Texas, USA, July 2021.
- Brankovic, M.; Gildin, E.; Gibson, R.L.; Everett, M.E. A Machine Learning-Based Seismic Data Compression and Interpretation Using a Novel Shifted-The GORE Consortium algorithm. Appl. Sci. 2021, 11, 4874.

HOSVD Compresses Data To a 70-80% Without Losing Any Significant Information

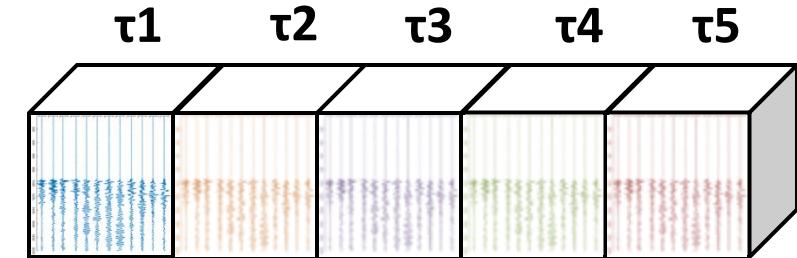
3D synthetic
microseismic tensor



3D field
DAS tensor

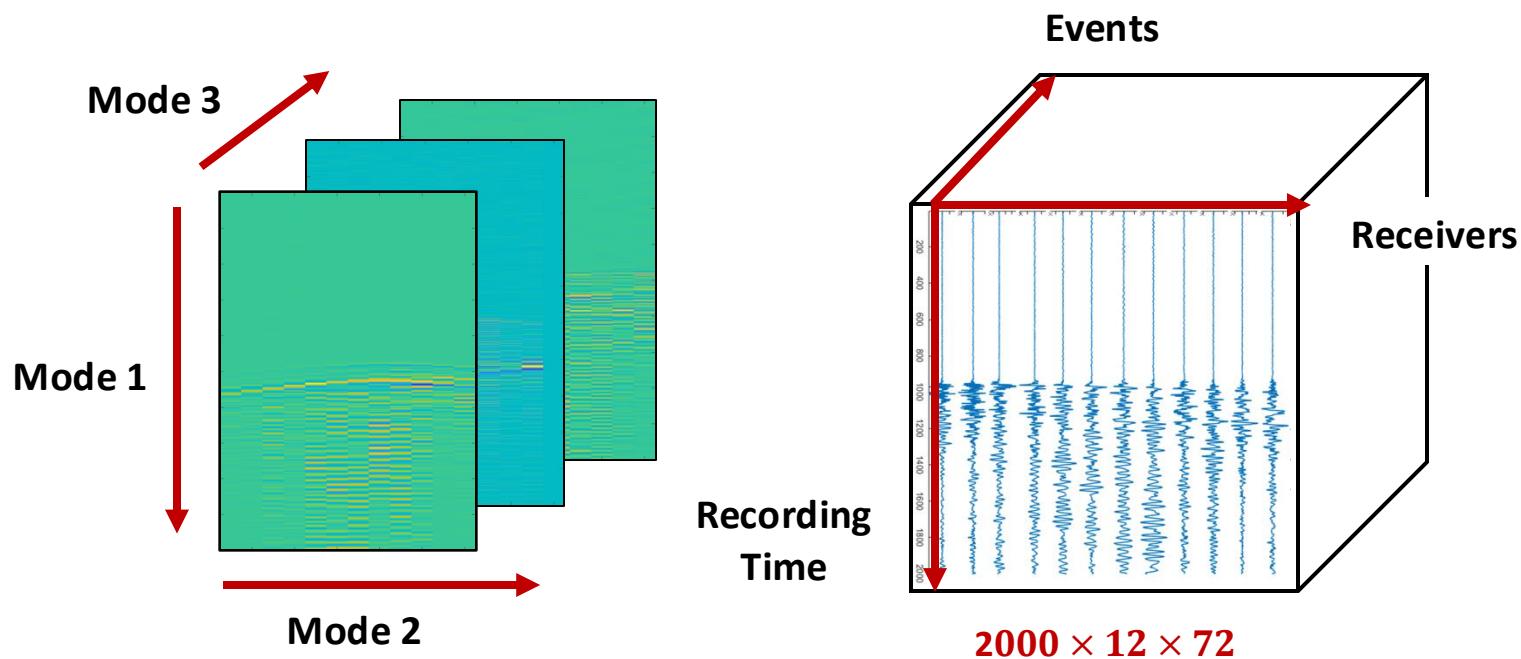


4D microseismic
tensor



Microseismic Datasets Can Be Arranged Into Multidimensional Arrays For Tensor Decomposition

3D synthetic microseismic tensor

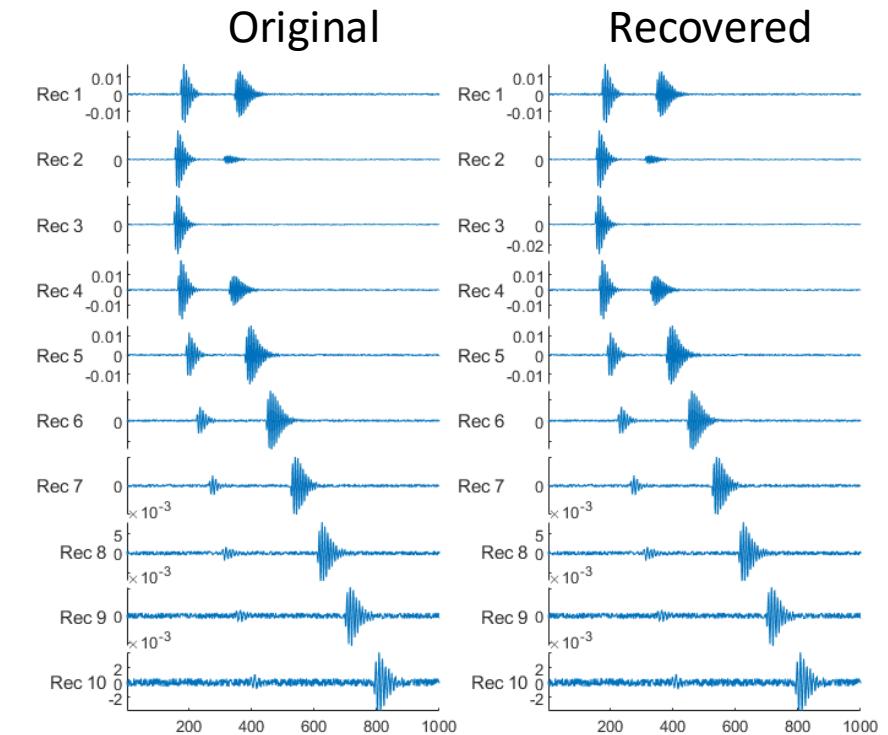
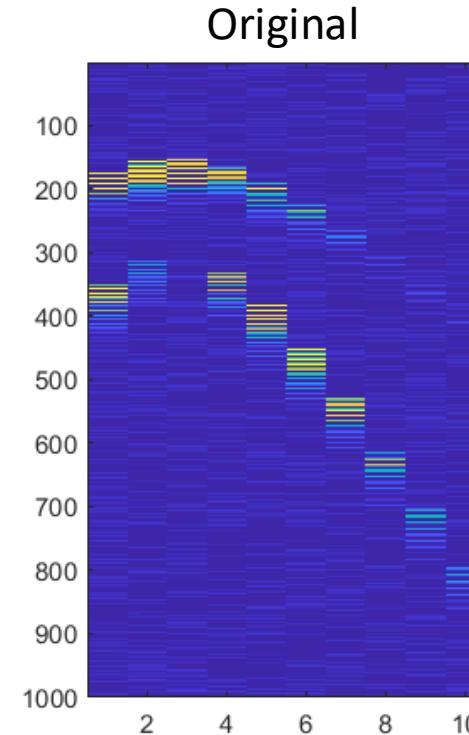
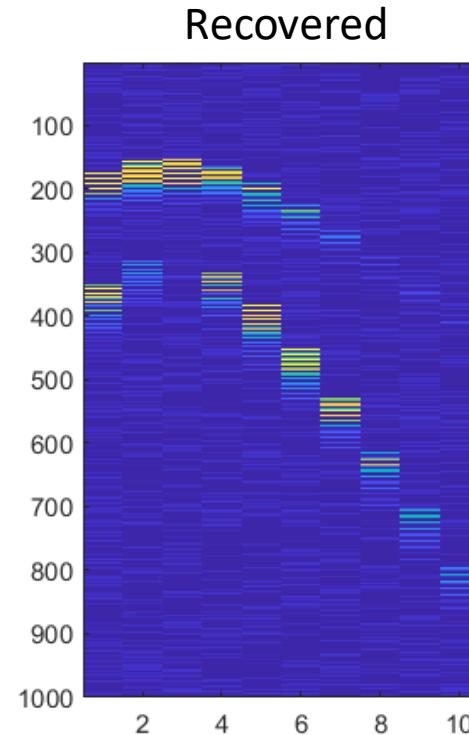


- 2000 milliseconds recording time
- 12 geophones
- 72 (x-y-z) event locations

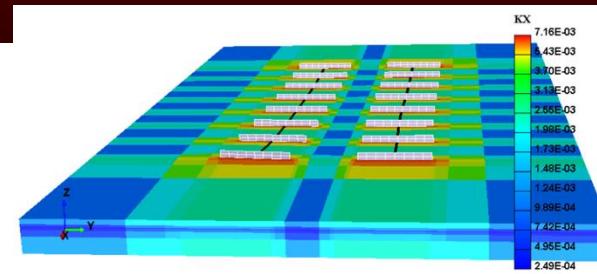
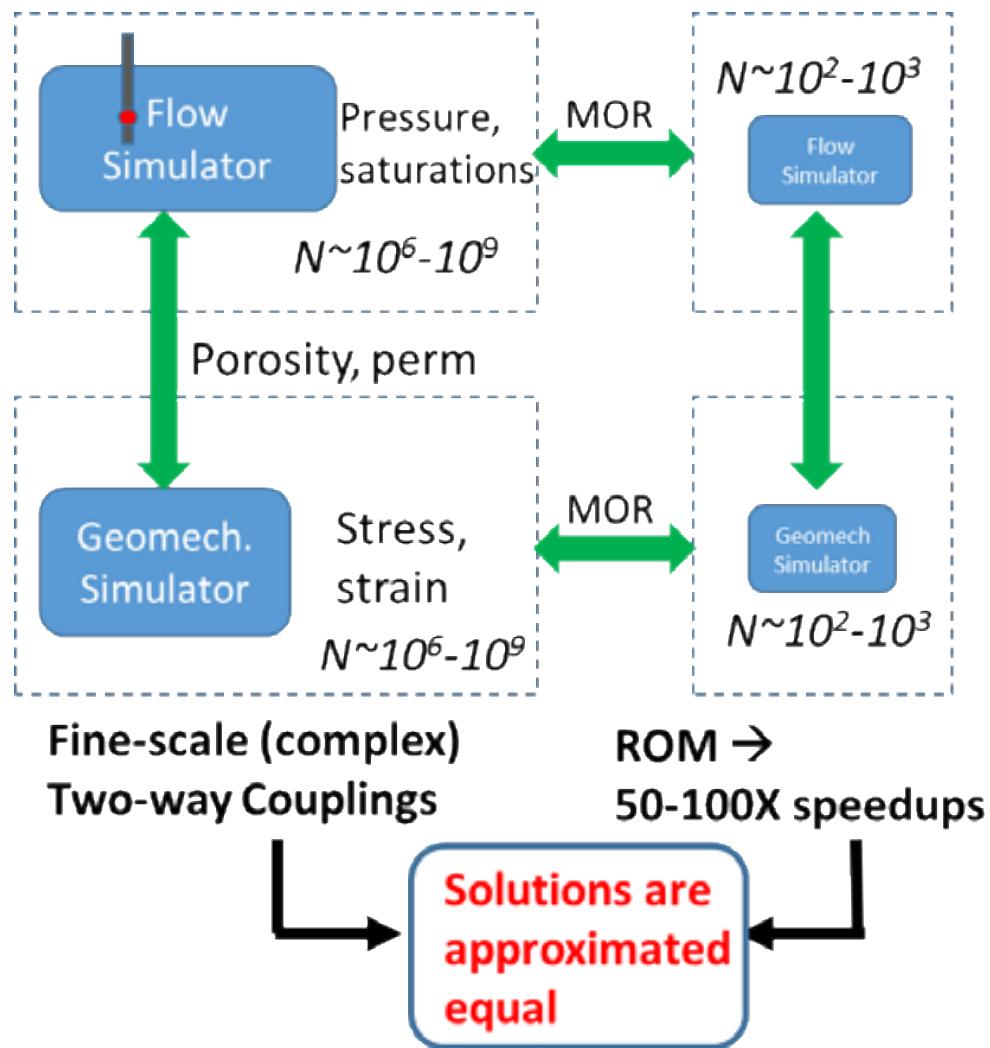
HOSVD Effectively Compresses Time 1 While Maintaining The Original Seismic Information

Tol: 0.079 – CR: 82.8%

Time 1

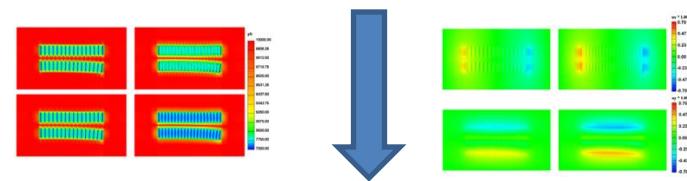


ROM for Flow and Geomechanics



Snapshots:

- Pressure, saturations
- displacements



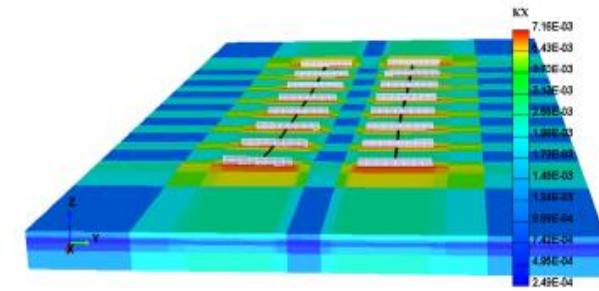
Apply:

- POD-DEIM
- TDEIM

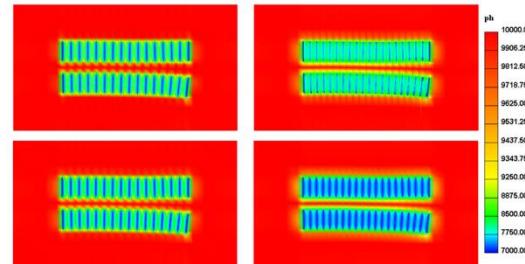
ROM for Coupled Flow and Geomechanics



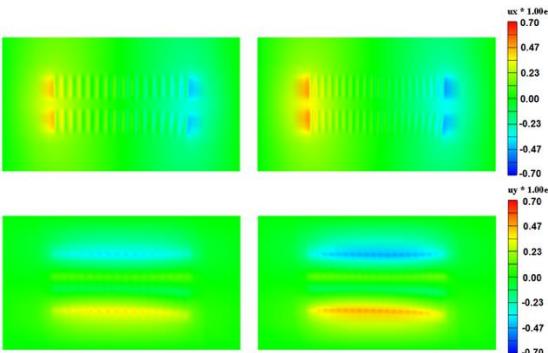
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16 fracs Pressure 24 fracs



Displacements



ROM's performance: flow only

#	$N^{(x)}$	$\tilde{n}^{(x)}$	$\tau_{\text{POD}}^{(x)} [\%]$	FOM runtime	ROM runtime	$\ \Delta\ _{rms}^{(p)}$	$\ \Delta\ _{rms}^{(S_w)}$	Speedup
8	49152	8	93.3	19.2	0.70	0.0032	0.0001	27.5
16	98304	8	93.3	49.4	1.36	0.0035	0.0001	36.2
24	147456	8	93.3	124.9	2.45	0.0040	0.0001	50.8

Error Mean square
Pressure/Saturation

When it works!

ROM's performance: coupled problem

#	$N^{(u_h)}$	$\tilde{n}^{(u_h)}$	$\tau_{\text{POD}}^{(u_h)} [\%]$	FOM runtime	ROM runtime	$\ \Delta\ _{rms}^{(u_h)}$	Speedup
8	78962	14	30.0	20.7	0.69	5.18e-8	30.0
16	157554	14	30.0	51.8	1.52	3.99e-8	38.2
24	236146	14	30.0	156.2	3.05	1.04e-7	51.2

$N \rightarrow$ number of degree of freedom (DOF) for the fine scale

$n \rightarrow$ number of DOF for the reduced model

FOM \rightarrow full order model

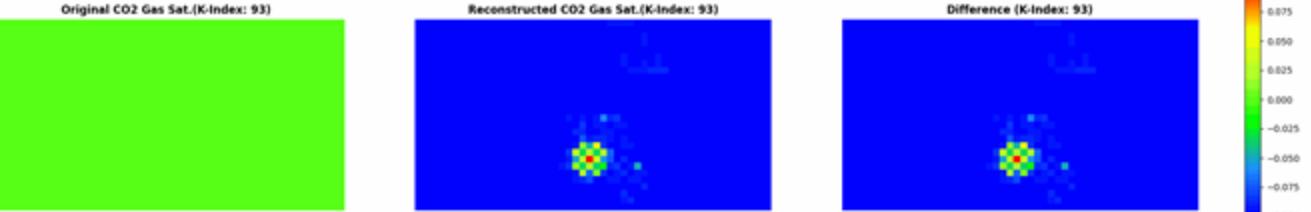
Sparse DMD Method for CCS



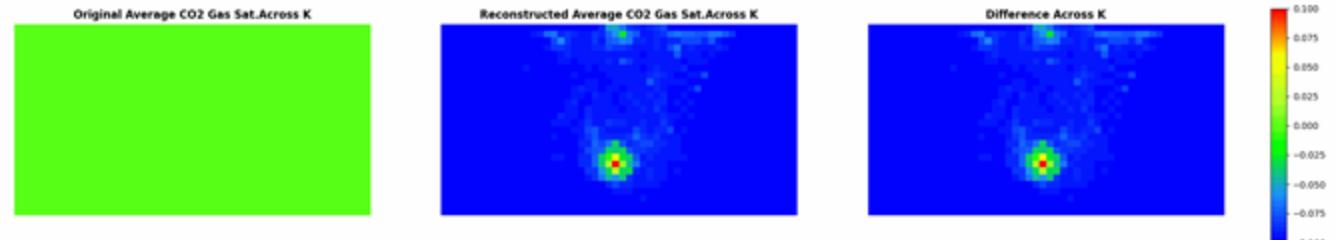
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Time Step: 0

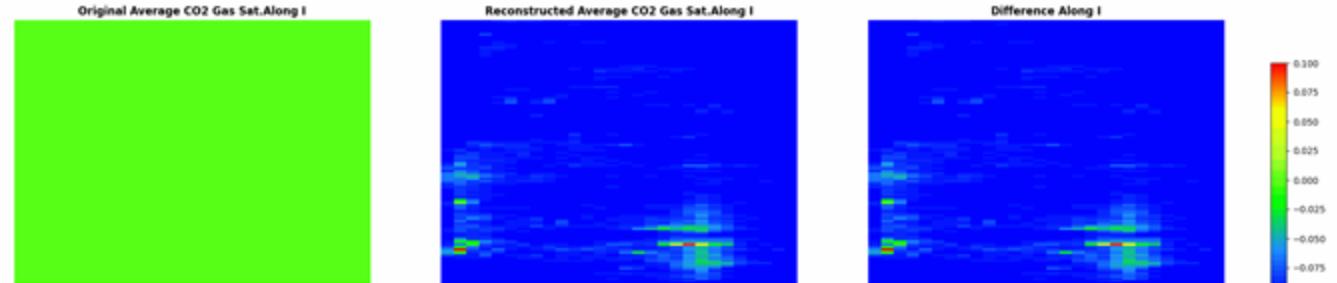
CO₂ Saturation map (top view, layer 93)



CO₂ Average Saturation map – all layers (top view)

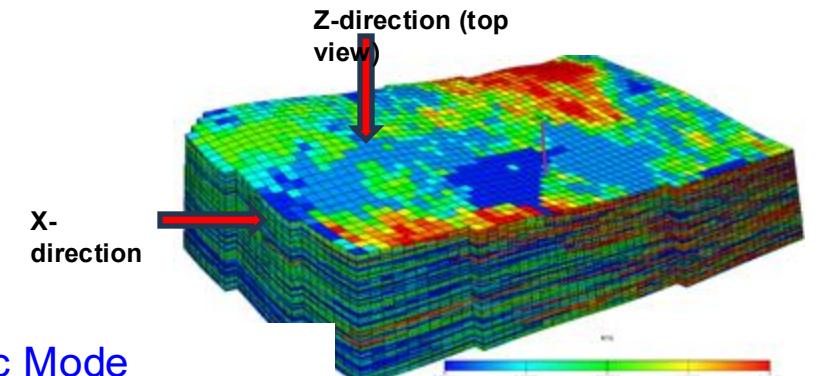


CO₂ Average Saturation map – all ith index (x-direction)



Results : CO₂ plume evolution

	Numerical model	Sp-DMD
Run time (seconds)	6000 (approx. 2hrs)	123 secs



[Rapid Geological CO₂ Storage Forecast and Optimization: A Data-driven Dynamic Mode Decomposition Model Order Reduction Approach](#)

D Voulanas, E Gildin - arXiv preprint arXiv:2407.20541, 2024

Deep-Koopman/Bilinear Formulation



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Reservoir eqs.

$$\dot{x} = f_1(x) + f_2(x)u$$

Koopman operator (Deep Neural Network): $x_k = \varphi(x)$

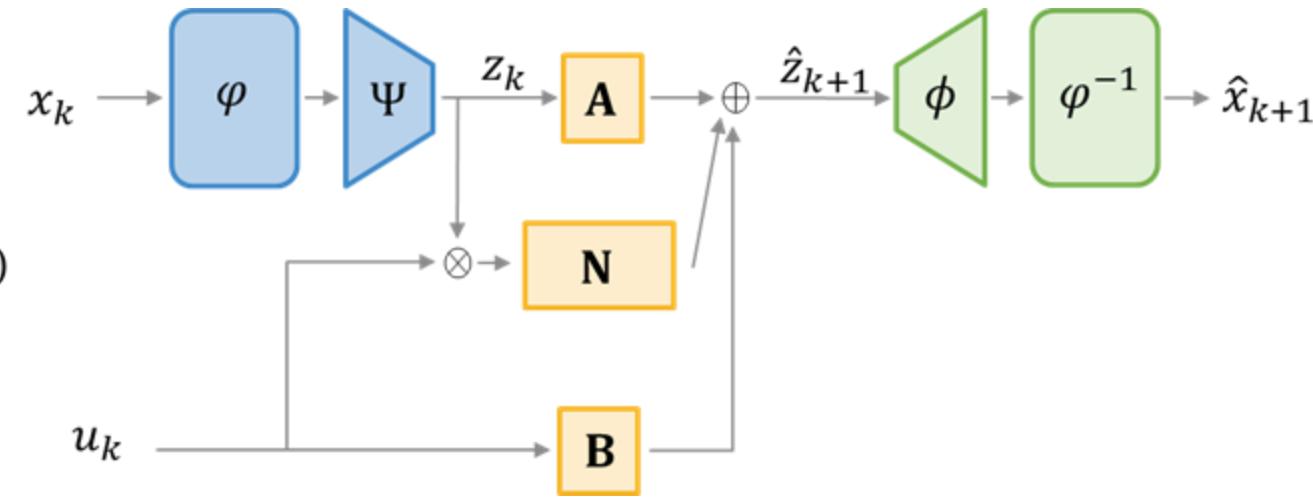
Bilinear eqs.

$$\dot{x}_k = Ax_k + N(u \otimes x) + Bu$$

Projections Φ and Ψ

Reduced-order eqs.

$$\dot{x}_r = \bar{A}x_r + \bar{N}(u \otimes x_r) + \bar{B}u$$



MRST - Matlab

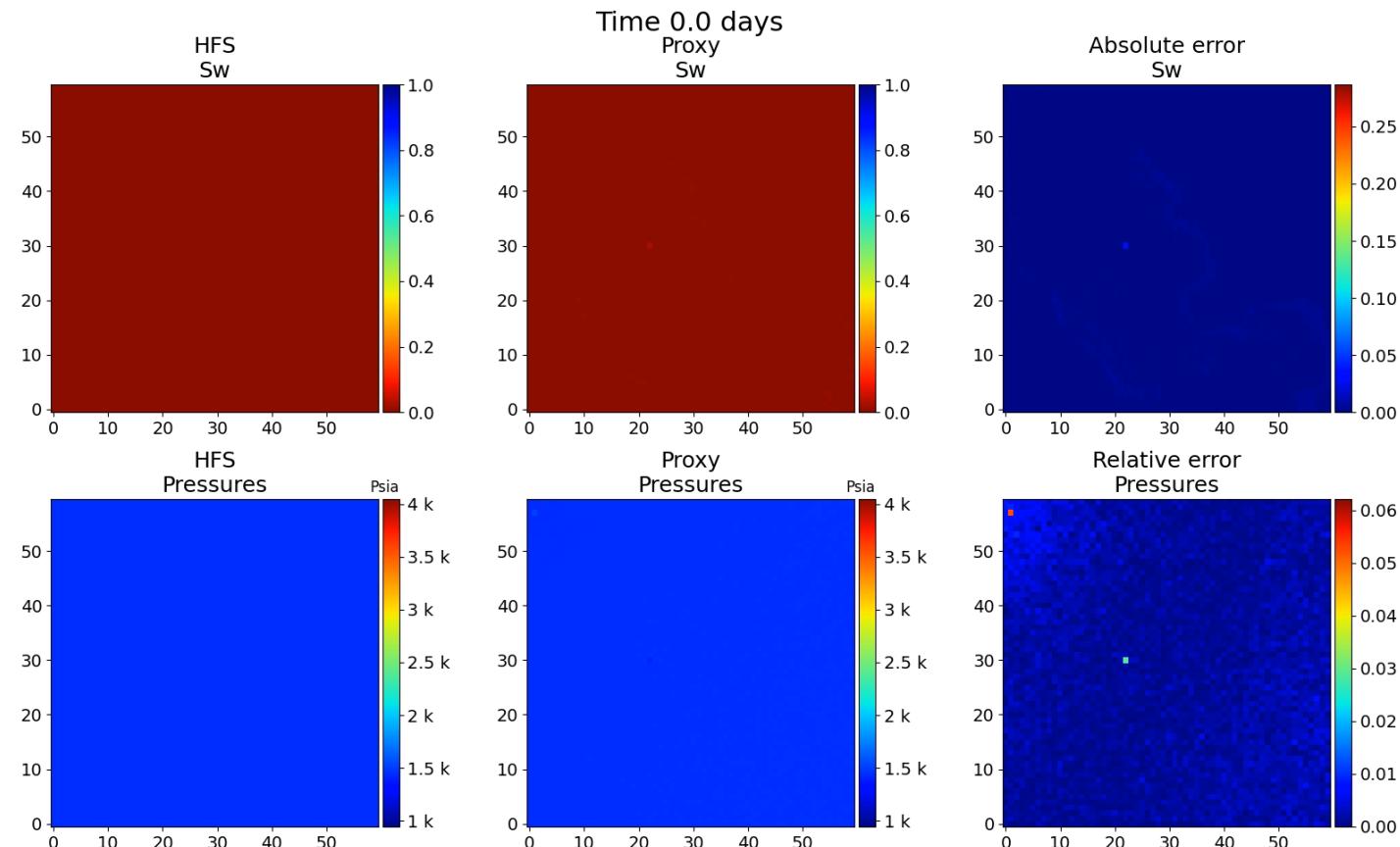
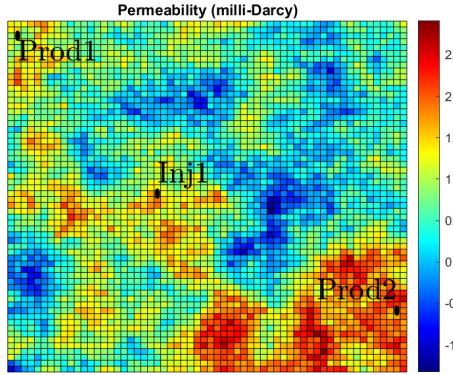
1 simulation ≈ 45 sec
320 simulations ≈ 4 hours

Proxy - Python

1 simulation ≈ 0.39 sec
320 simulations ≈ 40 sec

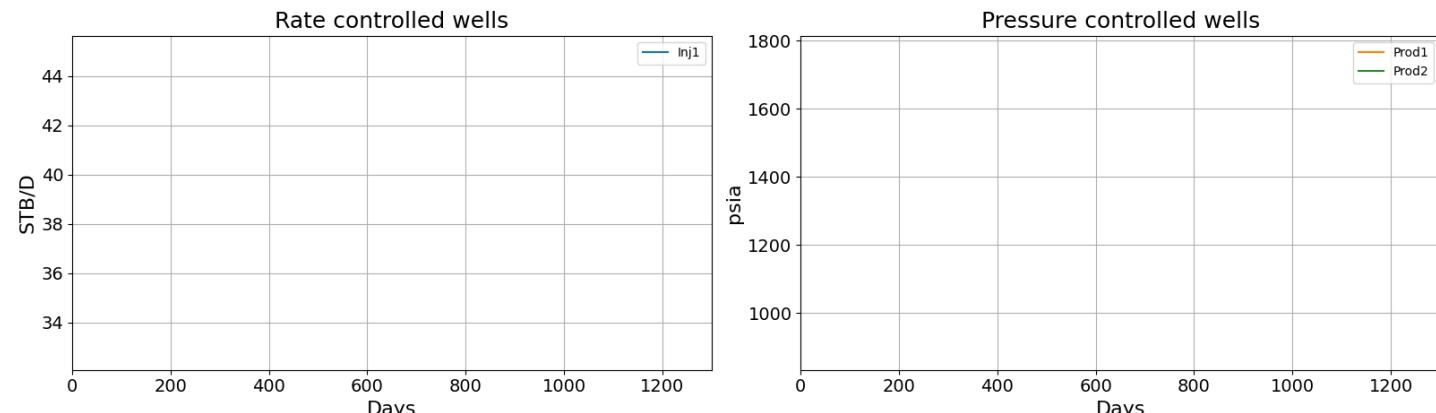
Solution → Formulate a robust Koopman framework
→ Theoretically sound
→ Linear, Bilinear, non-linear

Results: Time evolution

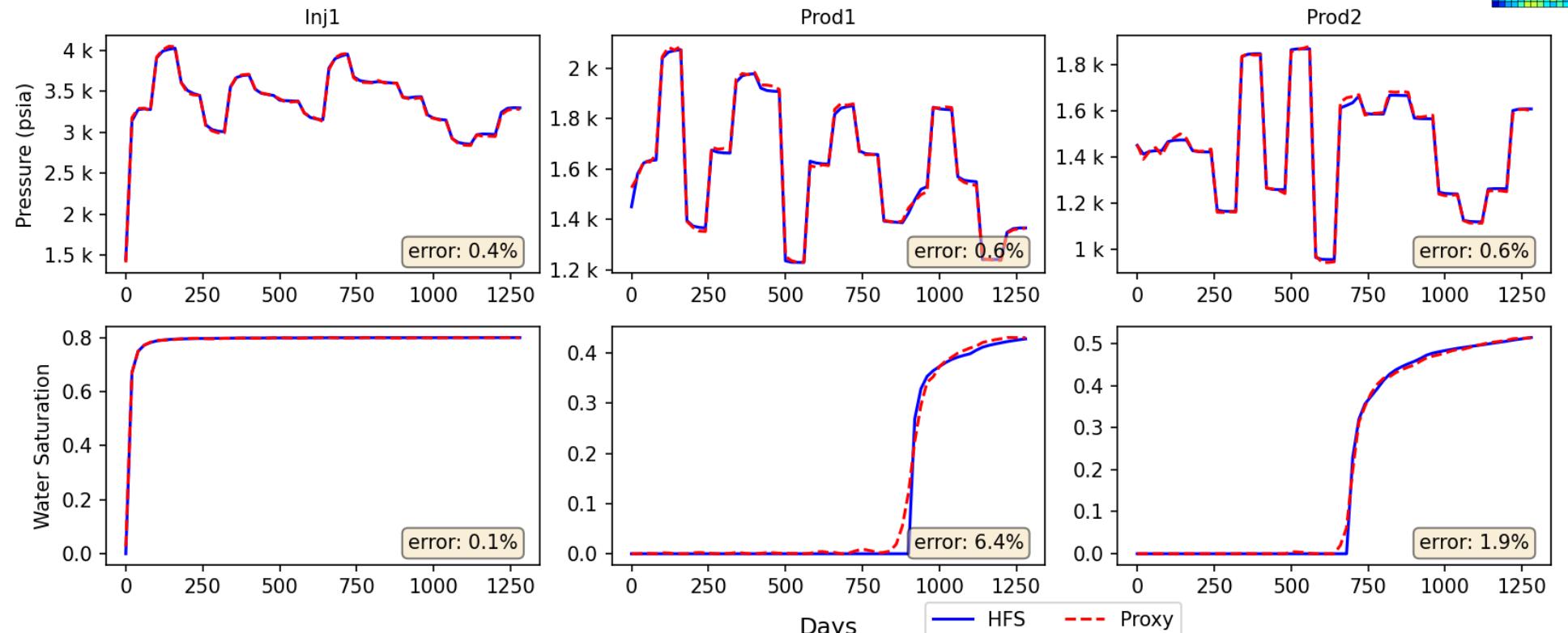
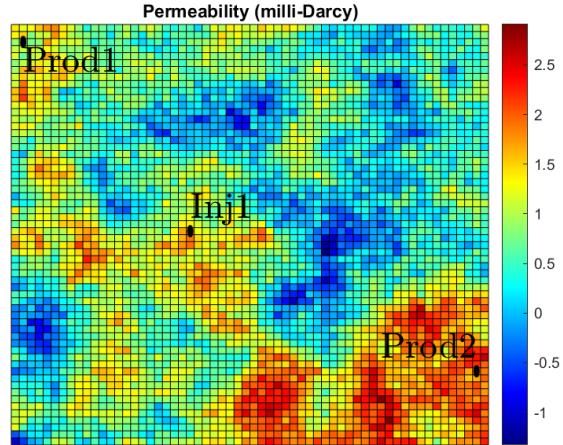


Performance comparison
(CPU Intel Xeon 3GHz – 1 core)

MRST - Matlab	Proxy - Python
1 simulation \approx 45 sec	1 simulation \approx 0.39 sec
320 simulations \approx 4 hours	320 simulations \approx 40 sec



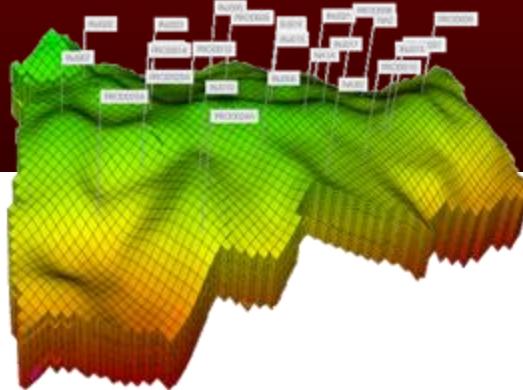
Results: States at well locations



$$\text{error} = \frac{\sum_k \|x_k - \hat{x}_k\|_1}{\sum_k \|x_k\|_1}$$

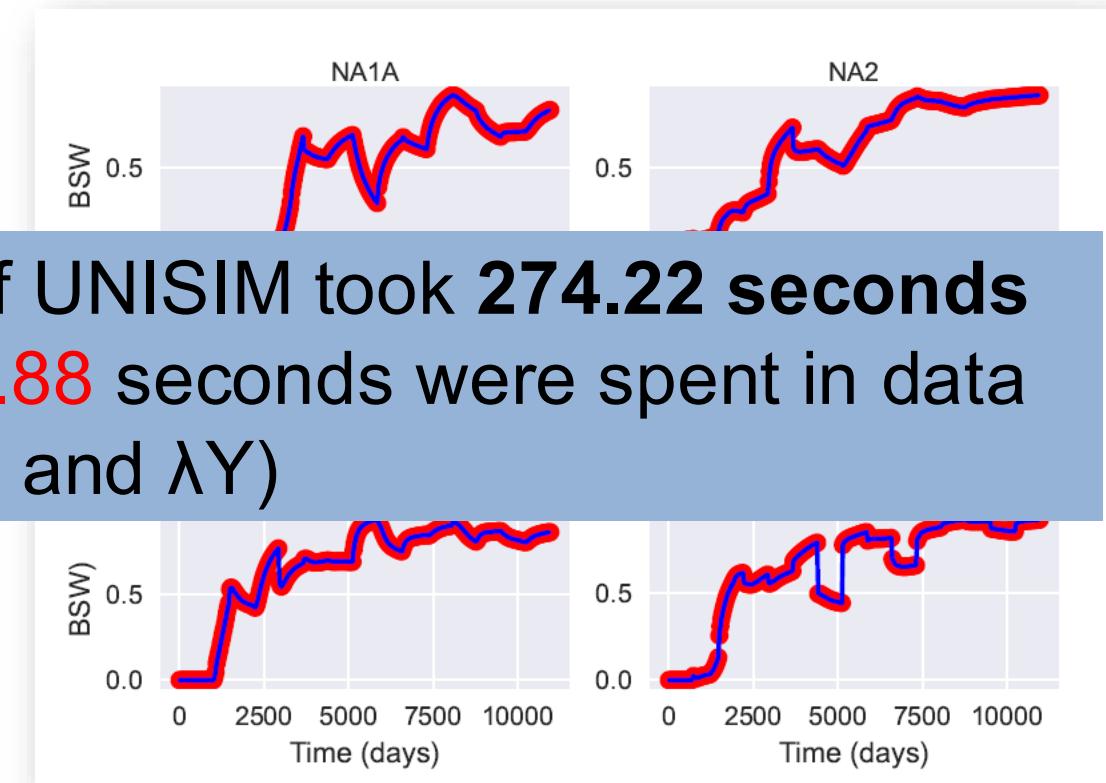
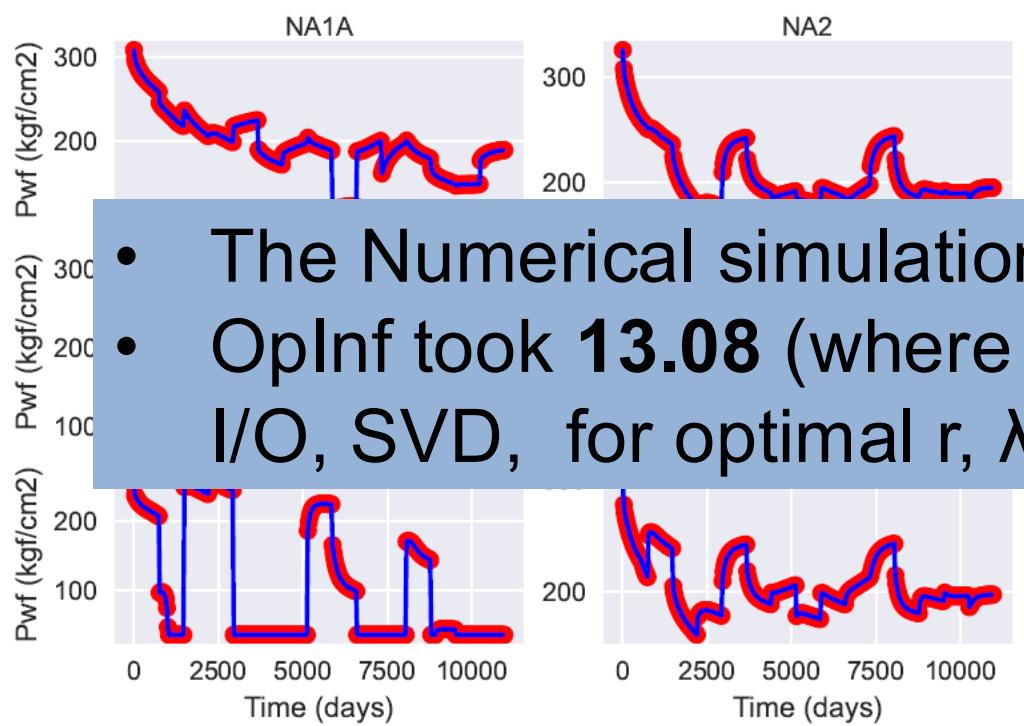
Results = 2 phase

r=25



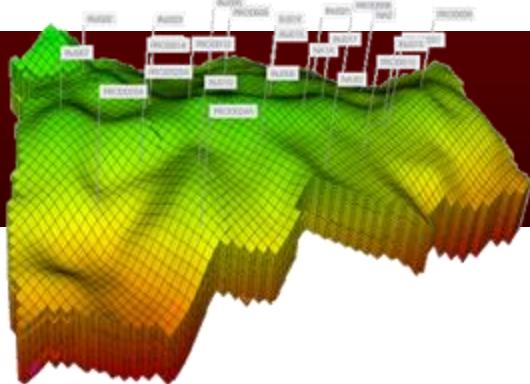
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Petroleum Engineering
Two Phase Model: Unisim

$$81 \times 58 \times 20 \\ = 93,960 \text{ cells}$$

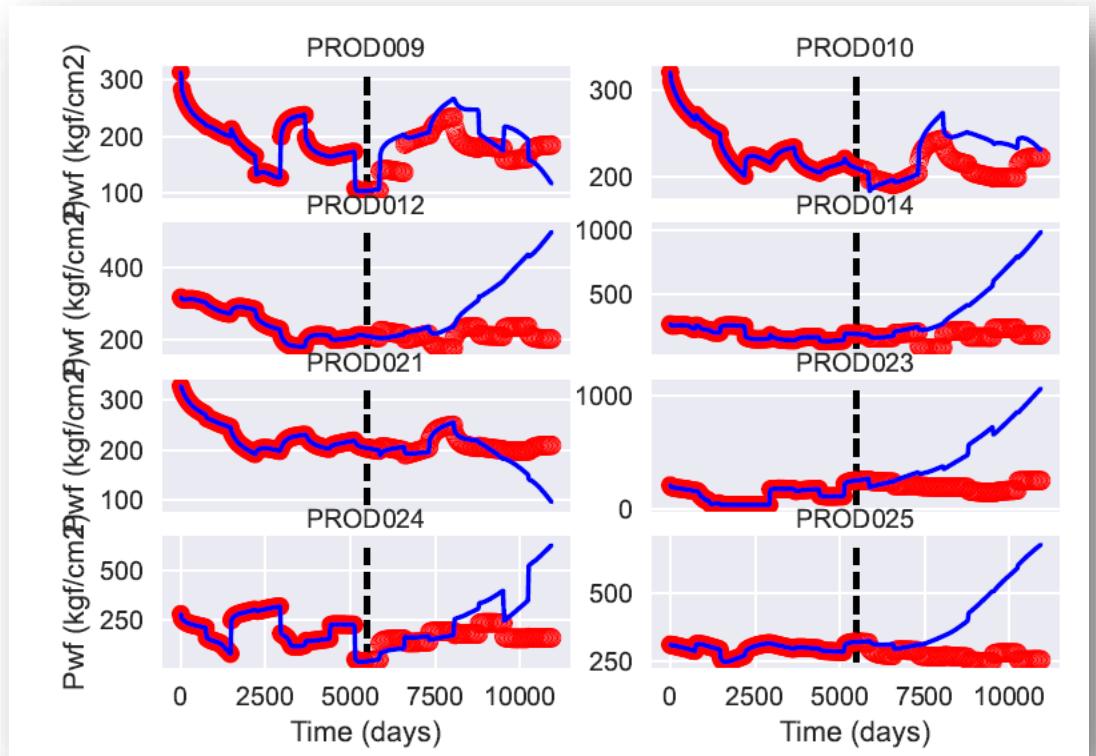
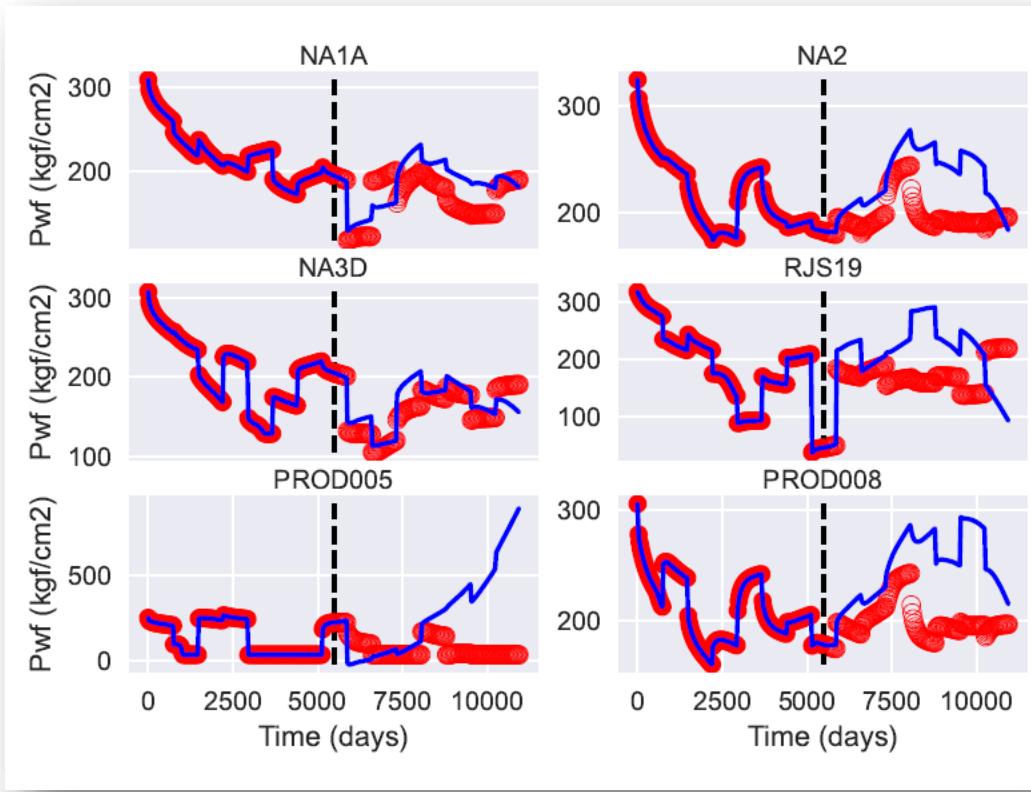


- The Numerical simulation of UNISIM took **274.22 seconds**
- Oplnf took **13.08** (where **10.88** seconds were spent in data I/O, SVD, for optimal r, λX , and λY)

Application



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Two Phase Model: Unisim

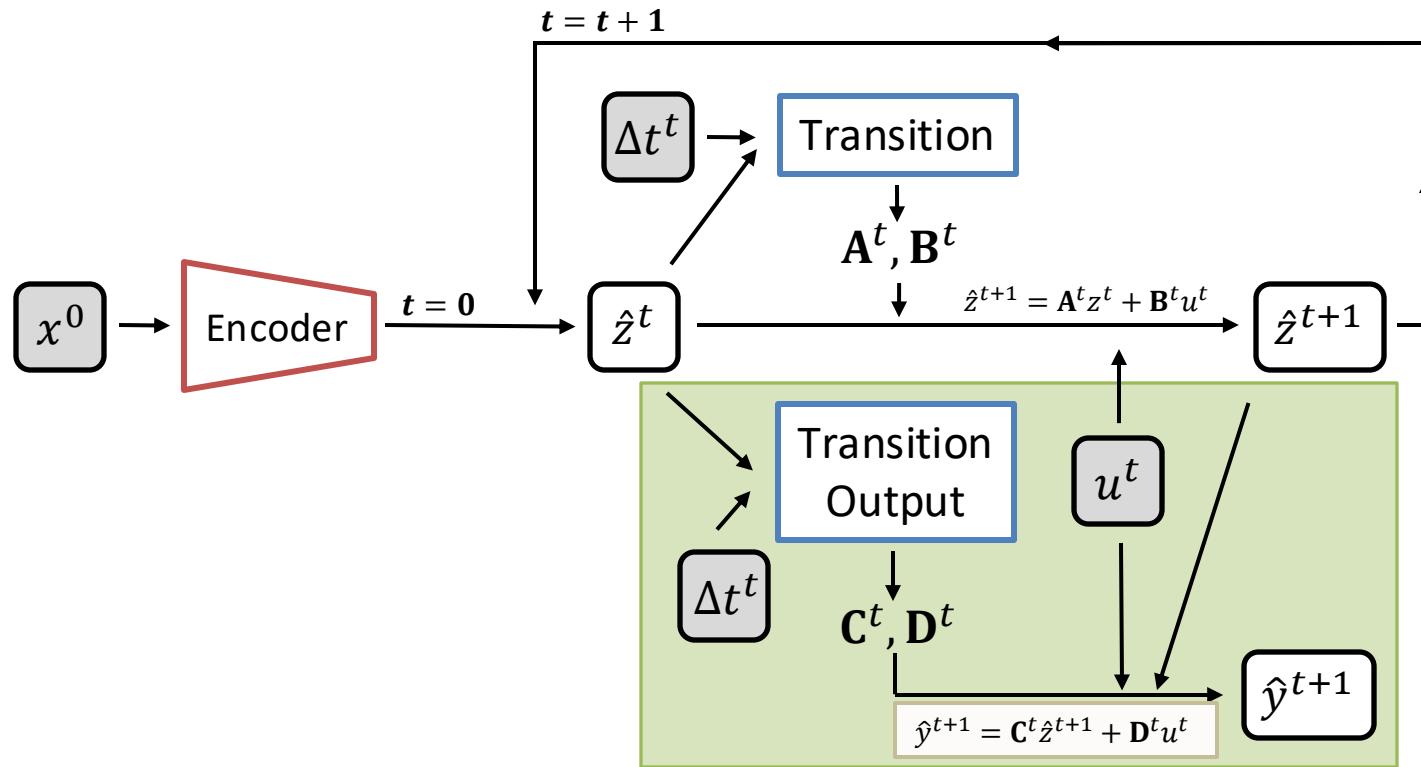


E2CO – Embed to Control and Observe*



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For reservoir simulation we are interested on the **model outputs** (e.g. well flow rates), not only on the states



Manuel Watter, Jost Tobias Springenberg, Joschka Boedecker and Martin Riedmiller., Embed to Control: A Locally Linear Latent Dynamics Model for Control from Raw Images. 2015.
[www.arxiv.org/abs/1506.07365](https://arxiv.org/abs/1506.07365).

Z.L. Jin, Y. Liu and L.J. Durlofsky, Deep-learning-based surrogate model for reservoir simulation with time-varying well controls. Journal of Petroleum Science and Engineering (2020), doi: <https://doi.org/10.1016/j.petrol.2020.107273>. and

Do not account for output

$$\begin{cases} z^{n+1} &= A^n z^n + B^n u^n \\ y^{n+1} &= C^n z^{n+1} + D^n u^n \end{cases}$$

E2CO

New architecture with Physical loss functions

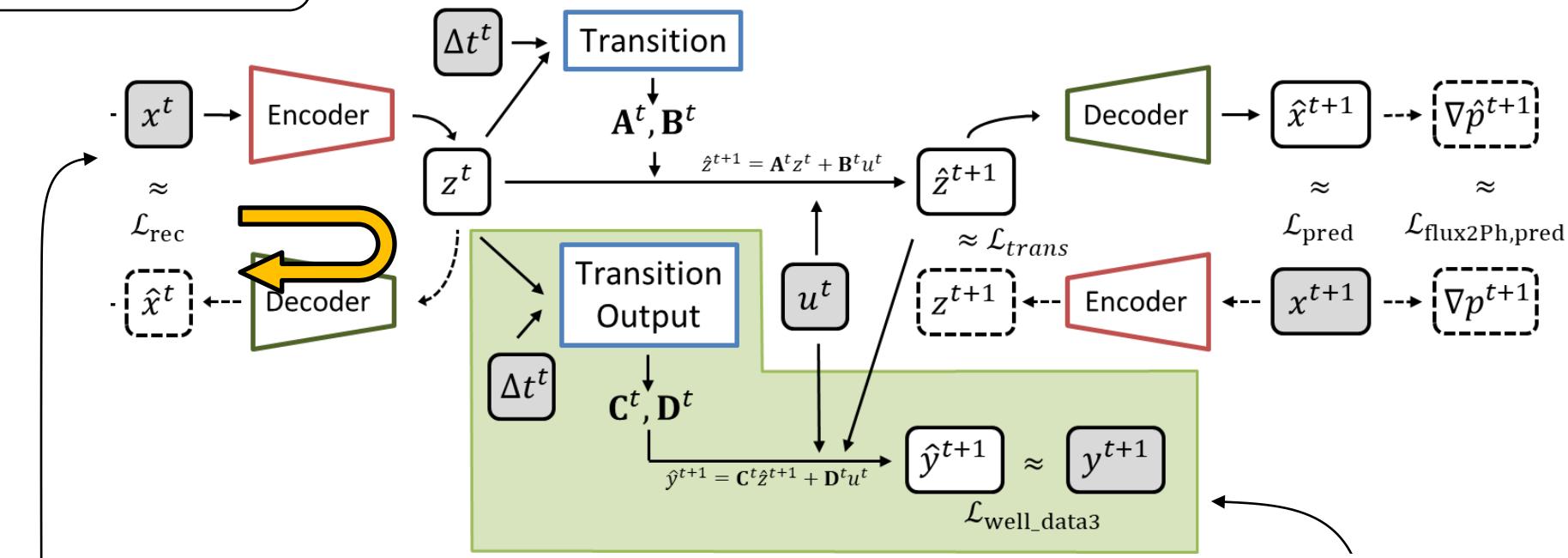
* Coutinho EJR, Dall'Aqua M and Gildin E (2021) Physics-Aware Deep-Learning-Based Proxy Reservoir Simulation Model Equipped With State and Well Output Prediction. *Front. Appl. Math. Stat.* 7:651178. doi: 10.3389/fams.2021.651178

E2CO – How to Train?



Loss Function
 $\mathcal{L}_{\text{rec}} = \|x^t - \hat{x}^t\|$

$$(\mathcal{L}_{\text{flux2Ph}})_i = (\mathcal{L}_{\text{flux2Ph,rec}})_i + (\mathcal{L}_{\text{flux2Ph,pred}})_i,$$



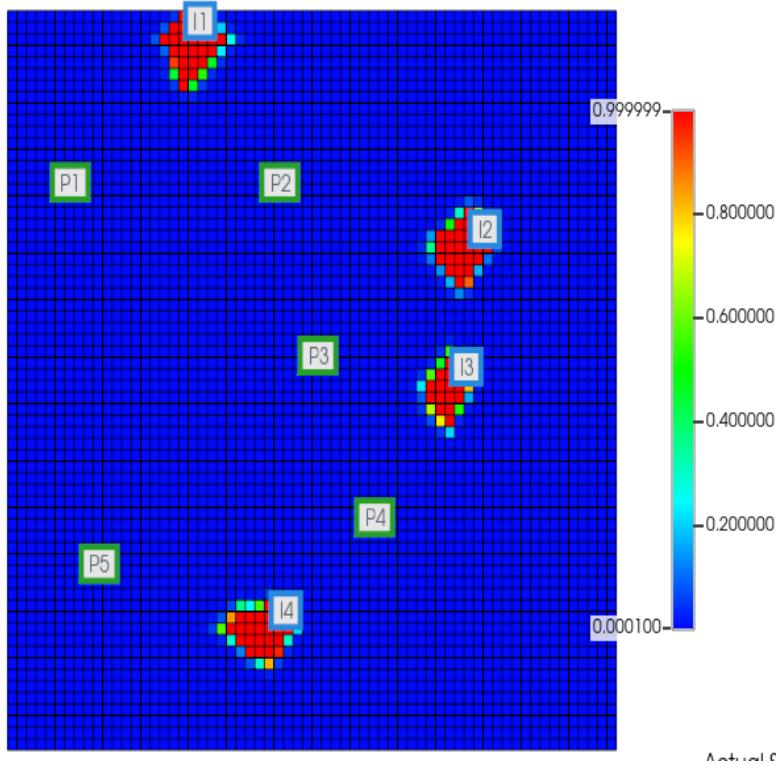
$$(\mathcal{L}_{\text{flux2Ph,rec}})_i = k \left\{ \left\| k_{r,o}(S_w^t) \nabla p^t - k_{r,o}(\hat{S}_w^t) \nabla \hat{p}^t \right\|_2^2 + \left\| k_{r,w}(S_w^t) \nabla p^t - k_{r,w}(\hat{S}_w^t) \nabla \hat{p}^t \right\|_2^2 \right\}_i,$$

$$(\mathcal{L}_{\text{flux2Ph,pred}})_i = k \left\{ \left\| k_{r,o}(S_w^{t+1}) \nabla p^{t+1} - k_{r,o}(\hat{S}_w^{t+1}) \nabla \hat{p}^{t+1} \right\|_2^2 + \left\| k_{r,w}(S_w^{t+1}) \nabla p^{t+1} - k_{r,w}(\hat{S}_w^{t+1}) \nabla \hat{p}^{t+1} \right\|_2^2 \right\}_i,$$

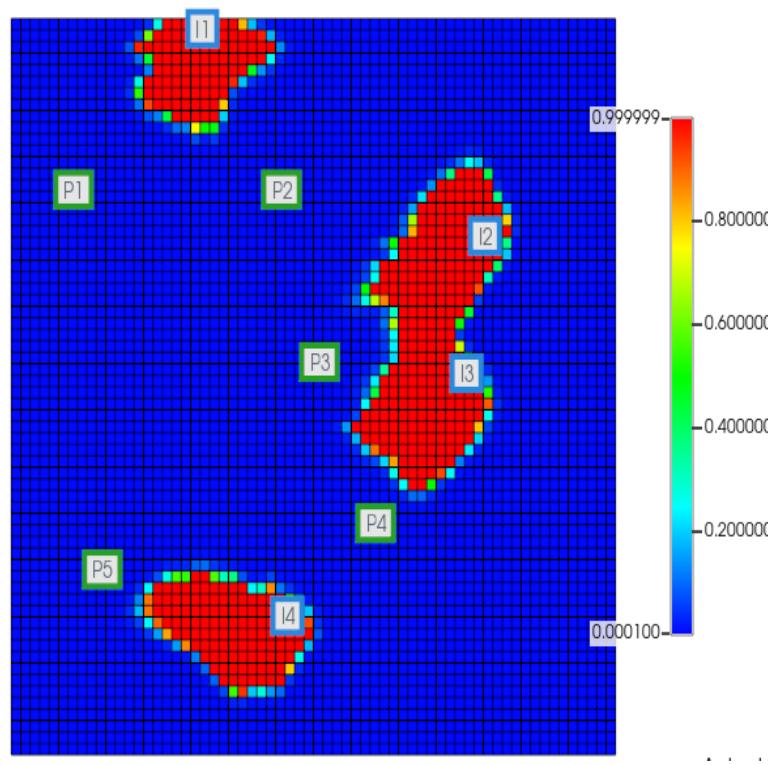
CO₂ plume behavior -Risk of leakages



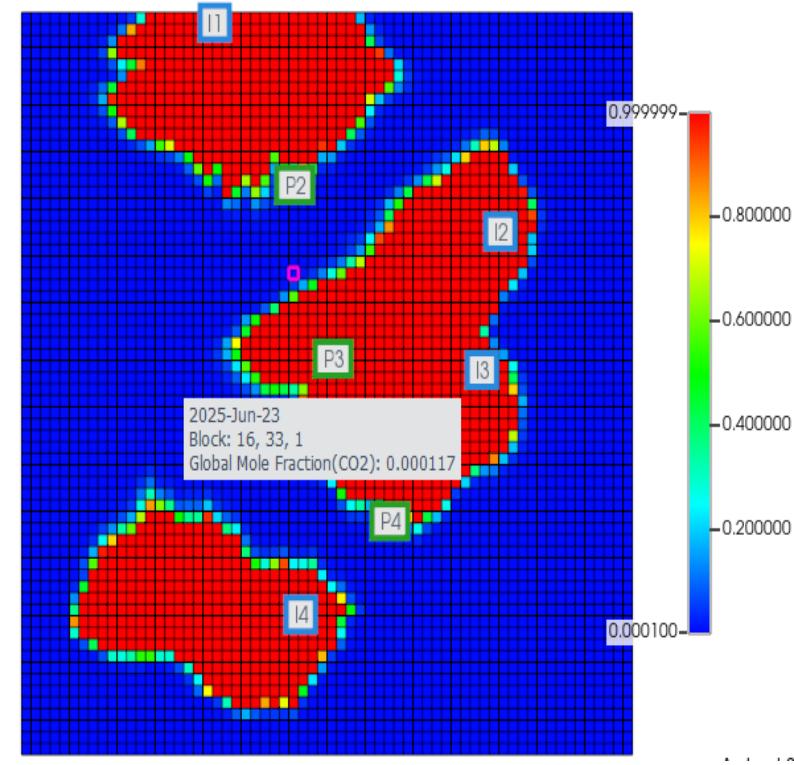
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Mole fraction at 100day



Mole fraction at 600day



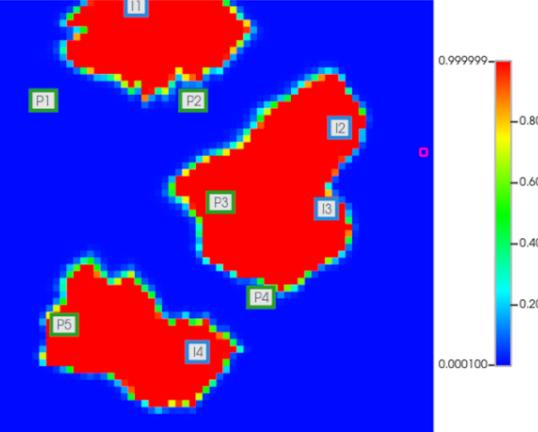
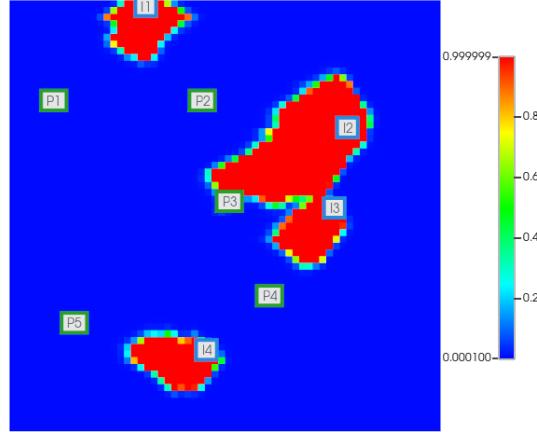
Mole fraction at 2000day

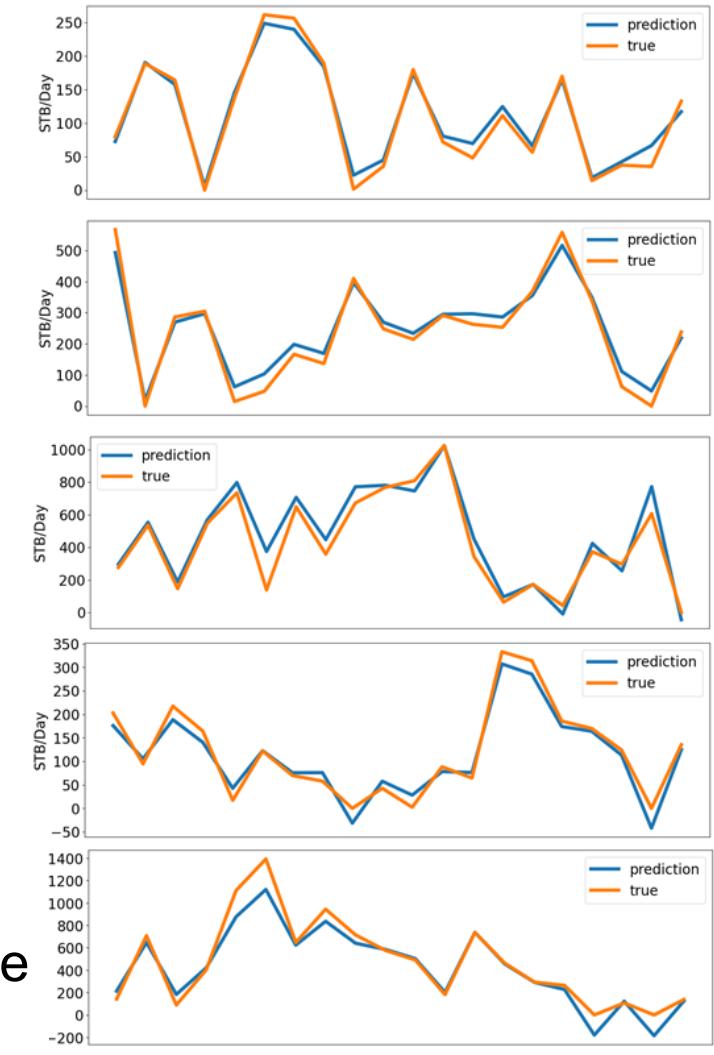
Transfer learning-based physics-informed convolutional neural network for simulating flow in porous media with time-varying controls. J. Chen, E Gildin, JE Killough, *Mathematics* 12 (20), 2024

E2CO for CCS - Optimal Injection scenario



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Full-order Simulation, sec	E2CO	
	Training, sec	Inference, sec
120~130	~ 3 hours (200 epochs, batch size 4)	2.86 (for 100 testing samples)
		
Base Case	Optimal Scenario	

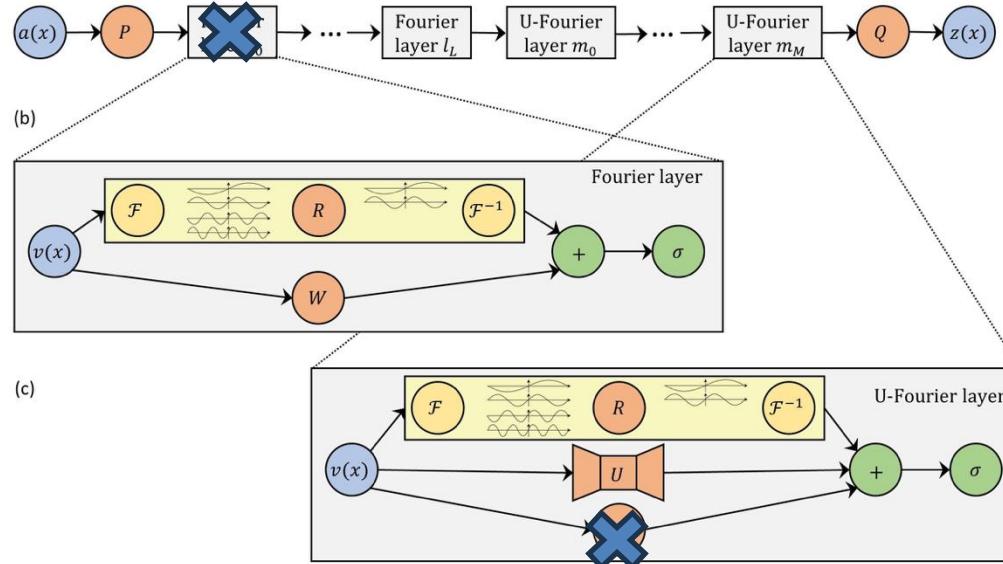


Optimization of pressure management strategies for geological CO₂ storage using surrogate model-based reinforcement learning, J Chen, E Gildin, G Kompantsev, *International Journal of Greenhouse Gas Control* 138, 2024

NEURAL OPERATORS - RESIDUAL U-NET

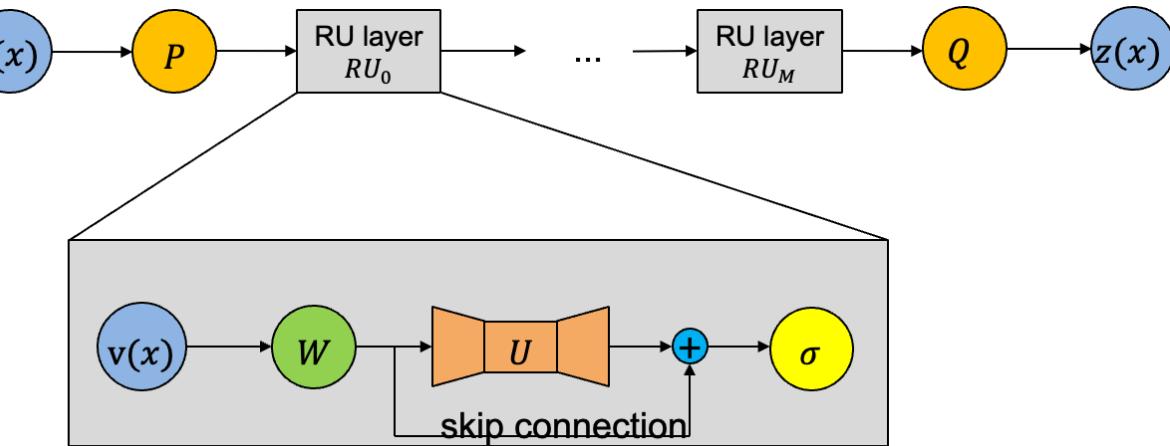
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Wen et al, U-FNO - an enhanced Fourier neural operator-based deep-learning model for multiphase flow [Advances in Water Resources](#)
Volume 163, May 2022, 104180



OUR model is 40% faster to train than U-FNO

The residual connection replaces the Fourier block.



Added skip connection

- In contrast to Fourier, there is no lost information when considering the high modes only, because the skip connection will retain all information.
- 3RU-NET includes 3 RU layers
- 5RU-NET includes 5 RU layers

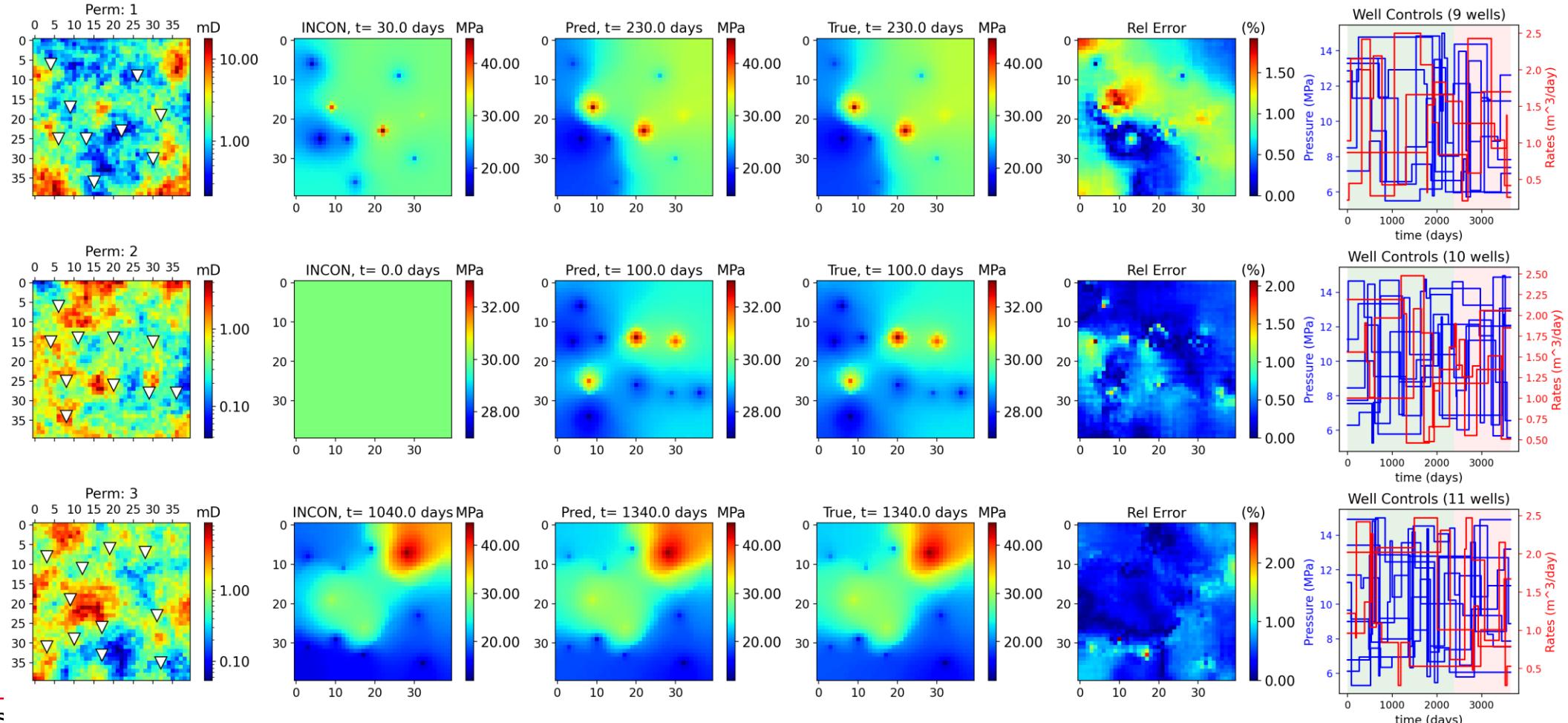
Neural operator-based proxy for reservoir simulations considering varying well settings, locations, and permeability field. D. Badawi and E. Gildin. *Computers & Geosciences* 196, 2025

U-FNO – Pressure Predictions



- 3500 training samples, 500 validation , 200 testing
- Training and validation samples have 6 wells (4 producers, 2 injectors)
- **Testing samples could have from 3 up to 12 wells.**

4hrs training

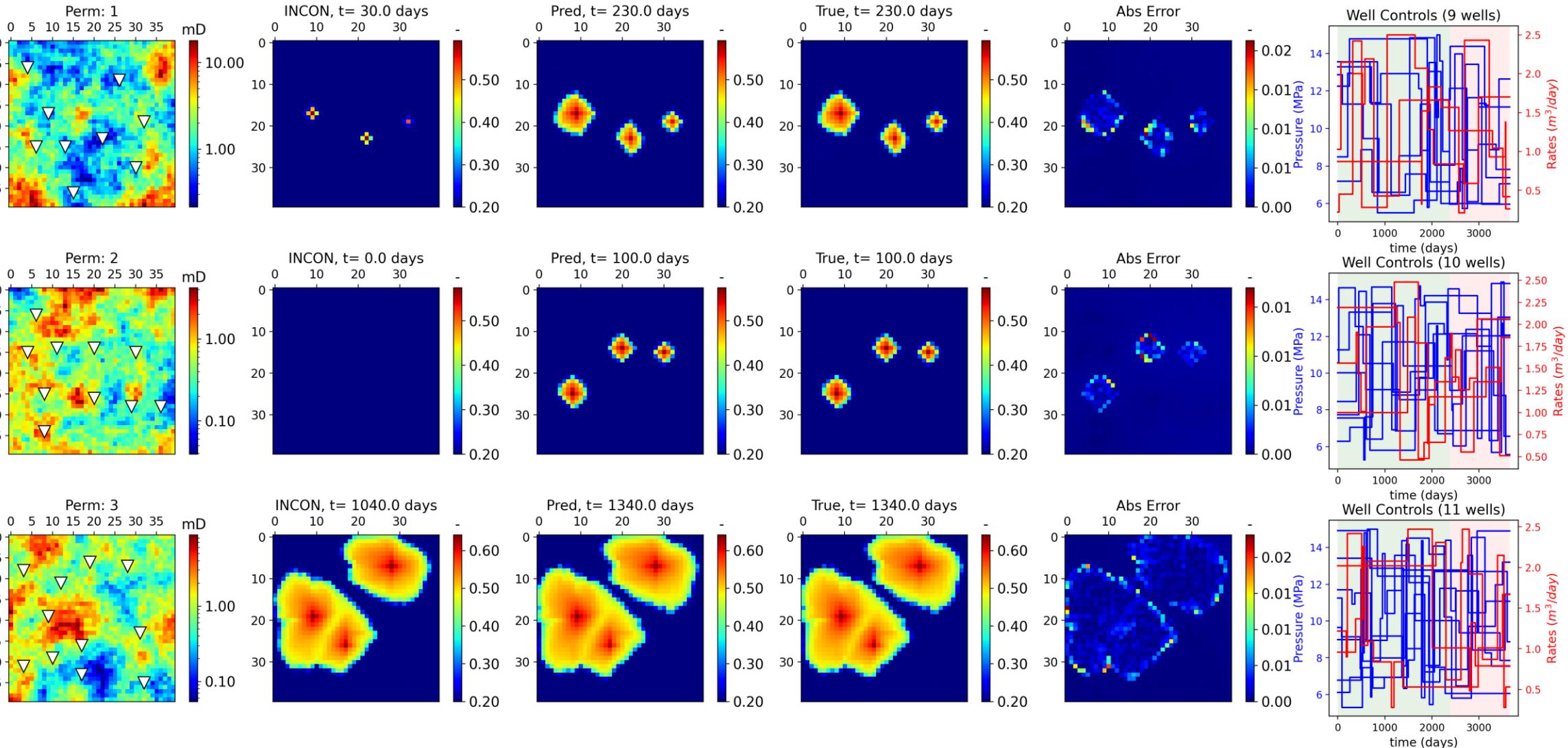




U-FNO – Saturation Predictions



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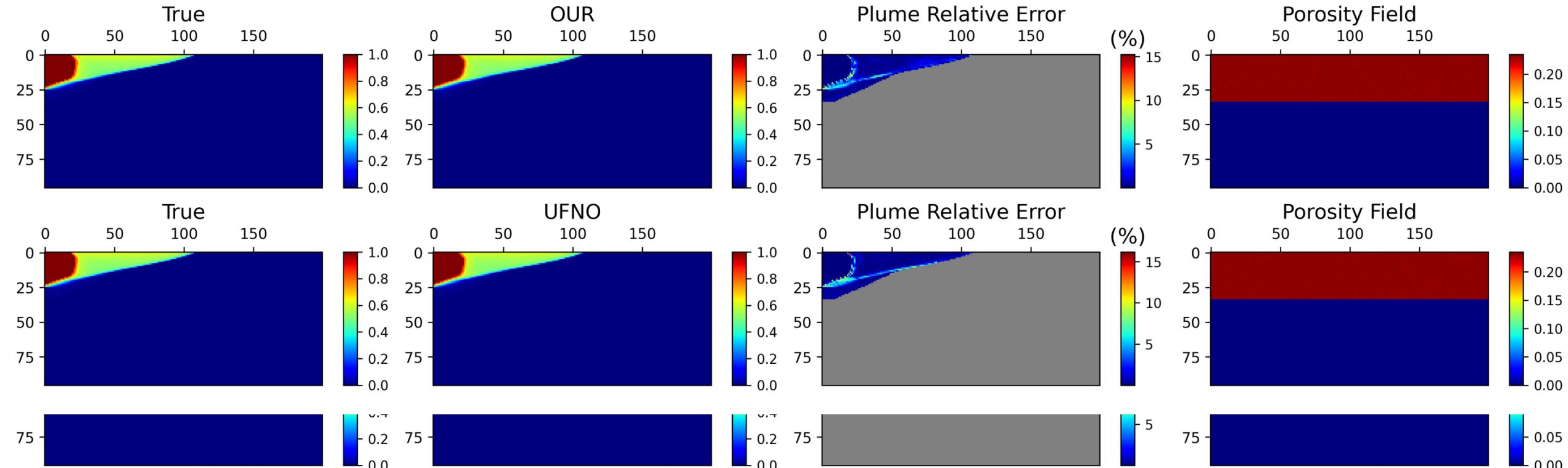


OURS vs U-FNO BENCHMARKING – SATURATION PREDICTION



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Benchmarking our model against U-FNO →
with the same dataset used in the U-FNO paper (CCS case)



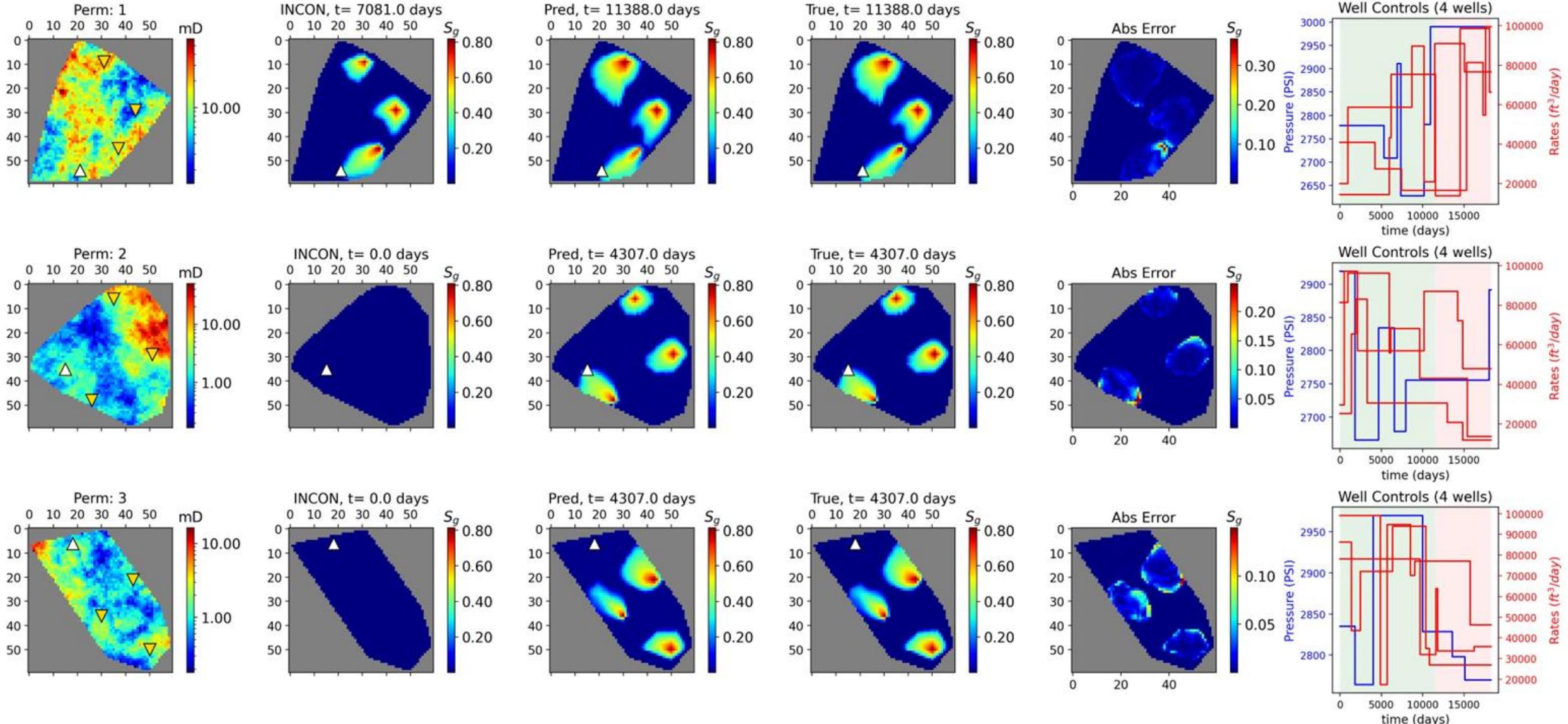
Wen et al, U-FNO - an enhanced Fourier neural operator-based deep-learning model for multiphase flow Advances in Water Resources Volume 163, May 2022, 104180



MODIFIED U-NET – CO₂ STORAGE



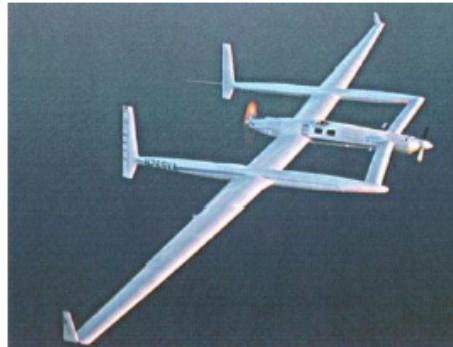
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I Other Applications of MOR



- ✿ Compute-intensive science and applications
 - parametric studies, stochastic analysis, uncertainty analysis
 - multidisciplinary modeling, multiscale modeling
 - multidisciplinary design optimization, optimal control, ...



"[If I am not getting the NASTRAN answer after 4 hours on a Cray, then God is sending me the message I have the wrong design]"

Burt Rutan, 1993



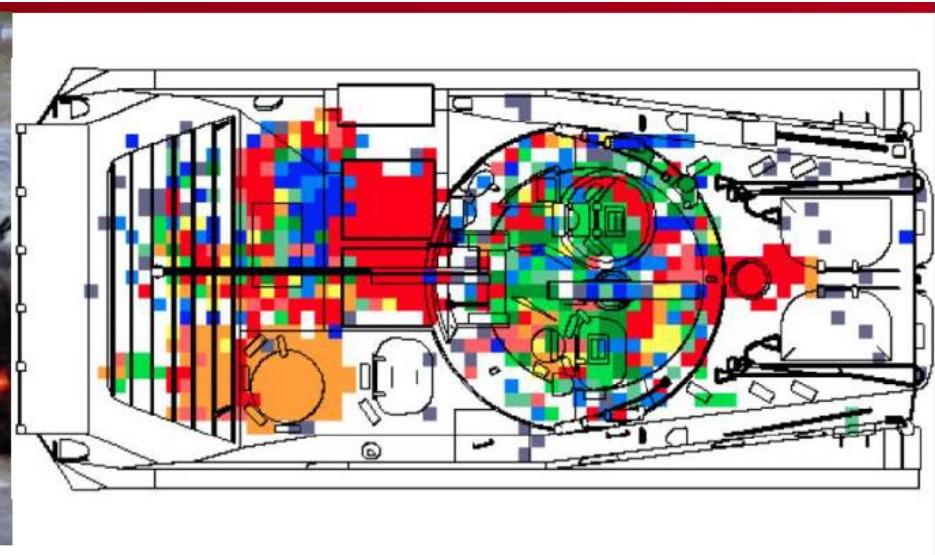
- ✿ Time-critical applications (technology & industrial representatives)
 - embedded systems, virtual reality, robotic surgery
 - Boeing, Intel, Toyota, VW, ANSYS, ESI, ..
- ✿ Funding agencies (omnipresent in most recent initiatives)
 - CENTER OF EXCELLENCE: Multi-Fidelity Modeling of Combustion Instabilities

Other Applications of MOR



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Explosion – Under Body Blast (Charbel Farhat)



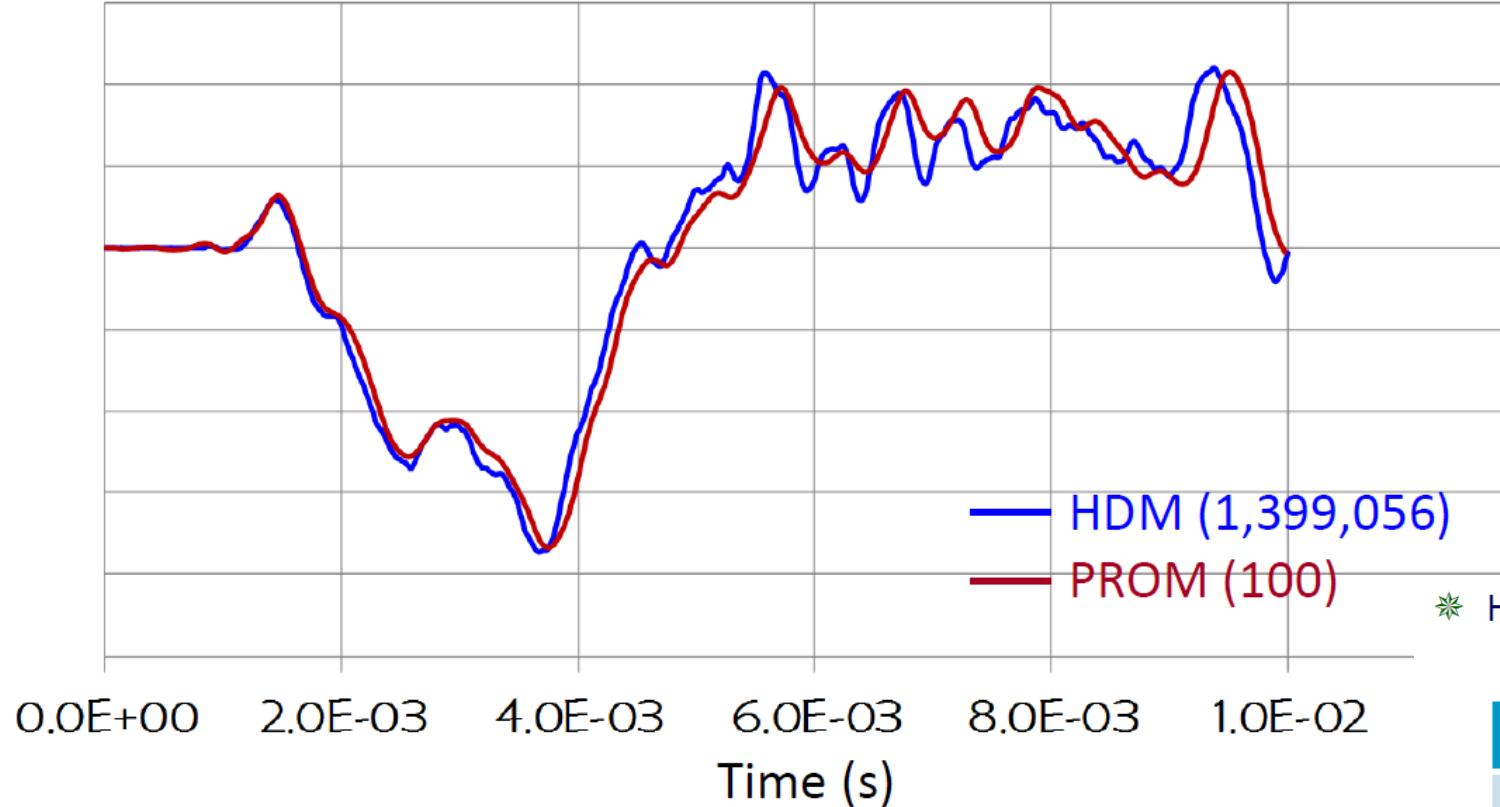
Non linear FEM

233,276 nodes
236,995 elements
~ 1.4 millions dofs



**MOR →
POD-based PMOR
 $d = 100$**

Node 263000 – u_x



* HDM: 128 cores of a Linux cluster — PROM: 16 cores

Model	Wall clock time	Speedup
HDM (1,399,056)	1.25×10^5 s (34.72 hrs)	
PROM (100)	4.32 s	28,935

→ CPU time speed-up = 231,481!



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Other Applications of MOR

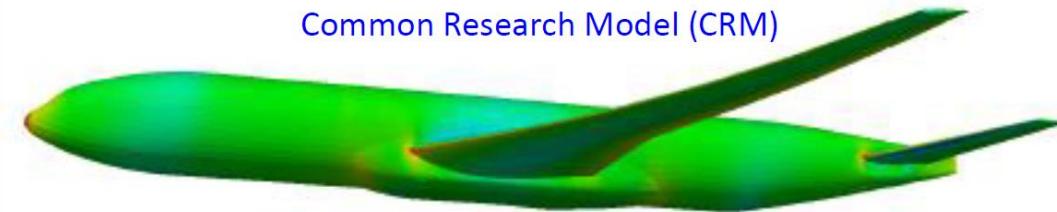


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Aircraft Design – aerodynamics (see Farhat, Willcox, etc)



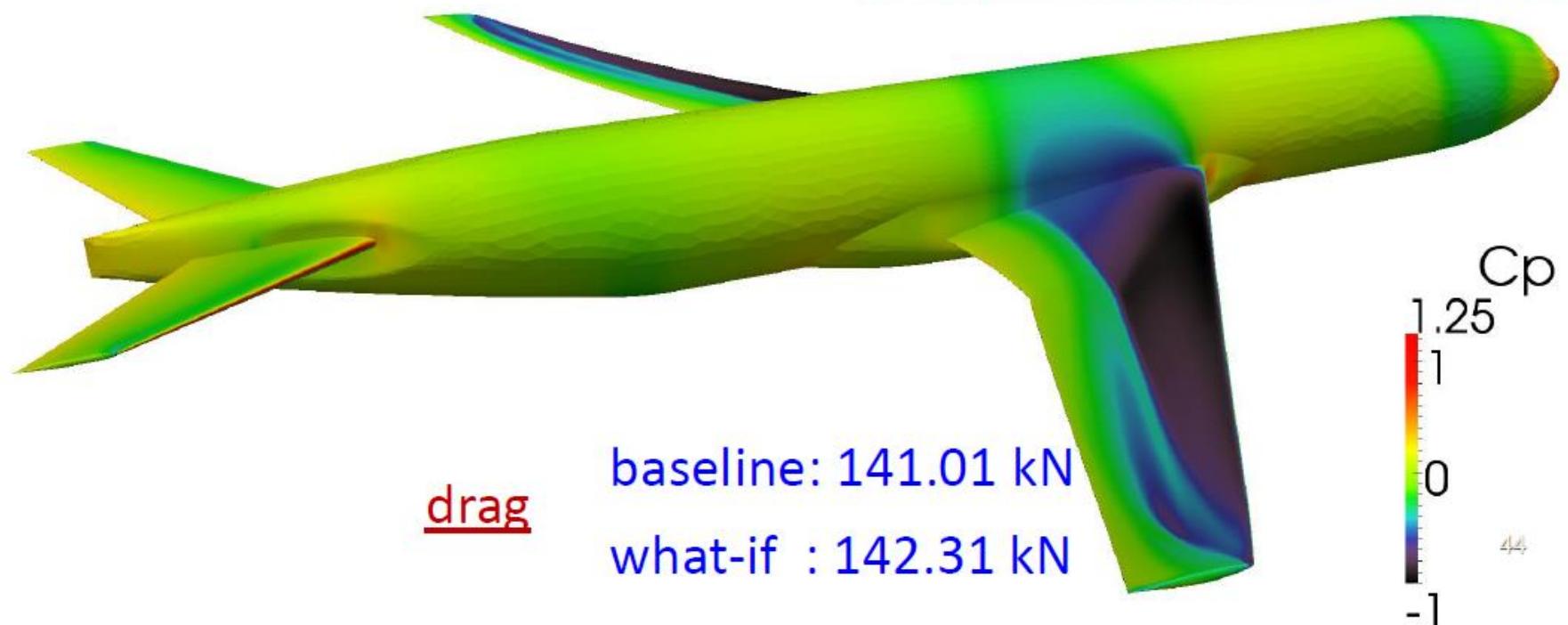
Common Research Model (CRM)



- ★ Excalibur (Cray XC40, ARL)
 - 1,024 cores assigned to each sampled configuration
 - 2 hrs wall-clock time per sampled configuration
 - 2 hrs wall-clock time for constructing global ROB
(embarrassingly parallel computations)
 - 3 mns wall-clock time for constructing and hyper reducing
the global ROM on 1,024 cores
- wall-clock time investment: 2.05 hrs on 24,576 cores

Example

- parameter point at the center of the database
- “real-time” prediction (*laptop*): 29 s (deform reduced mesh)
30 s (ROM soln)
78 s (HDM mesh morphing)
32 s (HDM soln reconstruction)
170 s (< 3 mins) wall-clock time



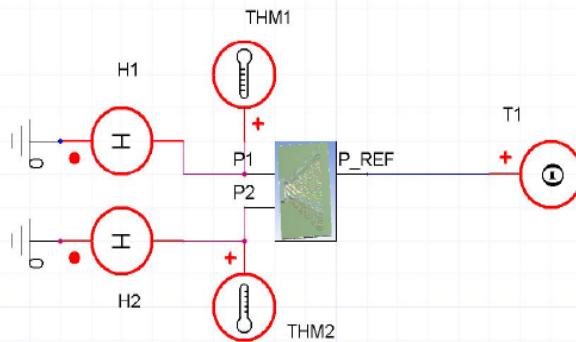
Other Applications



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Electro-Thermic Simulation of Integrated Circuit (IC)

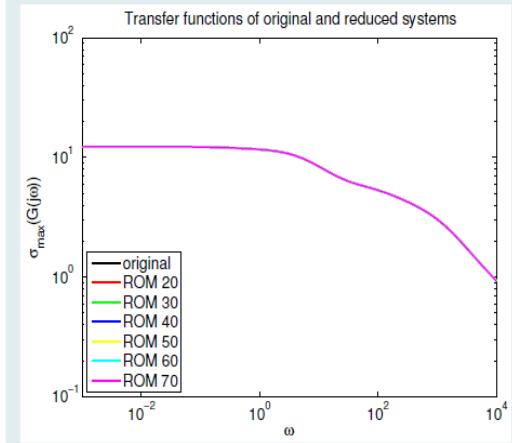
- SIMPLORER® test circuit with 2 transistors.



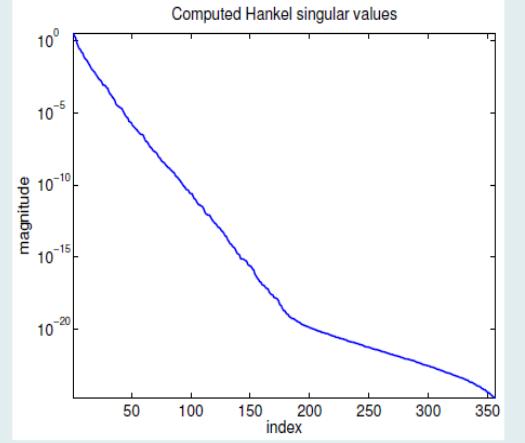
- Conservative thermic sub-system in SIMPLORER:
voltage \rightsquigarrow temperature, current \rightsquigarrow heat flow.
- Original model: $n = 270.593, m = p = 2 \Rightarrow$
Computing time (on Intel Xeon dualcore 3GHz, 1 Thread):
 - Main computational cost for set-up data $\approx 22\text{min}$.
 - Computation of reduced models from set-up data: 44–49sec. ($r = 20\text{--}70$).
 - Bode plot (MATLAB on Intel Core i7, 2,67GHz, 12GB):
 7.5h for original system , $< 1\text{min}$ for reduced system.

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Bode Plot (Amplitude)



Hankel Singular Values





Run Example in Matlab

- See My_First_MOR_Simulator_(Naive).zip

- Data Science alone (data-driven only) may have unintended consequences for complex Multiphysics applications
- Let's call "**Data-Physics Models**"
- Reduced order models → computed by projection
- Simpler approaches are desired
- I believe we can attain 1000X speedups with the tools we have so far for reservoir simulation alone
- Challenges: coupled flow and other processes → ever increasing complexities