Structure in Learning (& MICDE)

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What are some successes in "AI for Science" ?

- Materials property descriptions, discovery & design
- Protein structure
- Drug discovery, Genetics
- Imaging and segmentation (in most discipline)
- Clustering/Classification (in most disciplines)

Why the above problems?

- Discreteness (or "discretizability") of underlying spaces
  ➔ Text, graphs, categorization, binarization, sequences, etc
- "Discoverability" of somewhat universal features
- Diverse, (mostly) complete and high quality data
- Data standardization
- Modularity of tasks
- Deficiencies in existing methods!
- We know what questions to ask !!

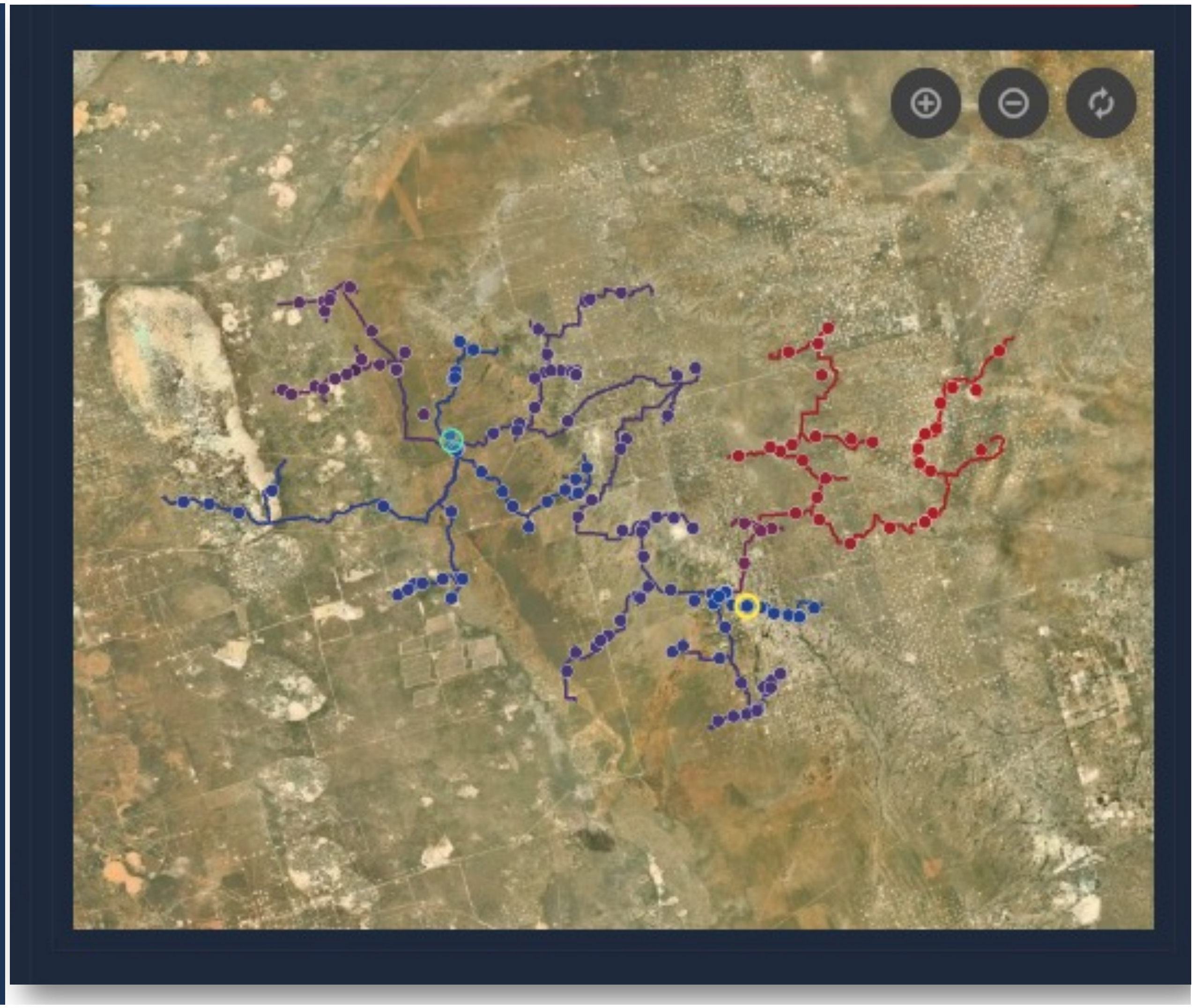
Confidential | Not for redistribution

Case study

Optimizing gas delivery in complex well networks

https://demo.geminus.ai/network

Geminus



Case study

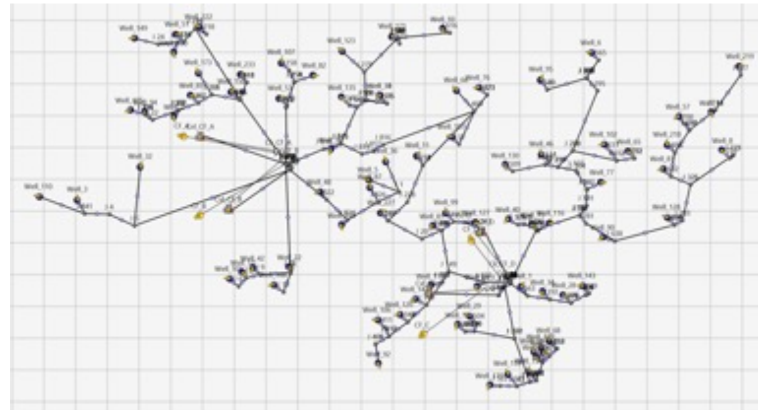
Optimizing gas delivery in complex well networks

https://demo.geminus.ai/network

Geminus

Context

- Goal to maximize revenue by finding ideal gas distribution across multiple sales points
- Limited by short decision time scales, network complexity, and sensor data sparseness



Solution

- AI models matching simulation accuracy used for rapid ”what-if” analysis and optimization of distribution to multiple sales points
- Intelligent advisor app powered by AI model provides interactive capabilities, in real time

Dimensionality	168 control inputs

Impact

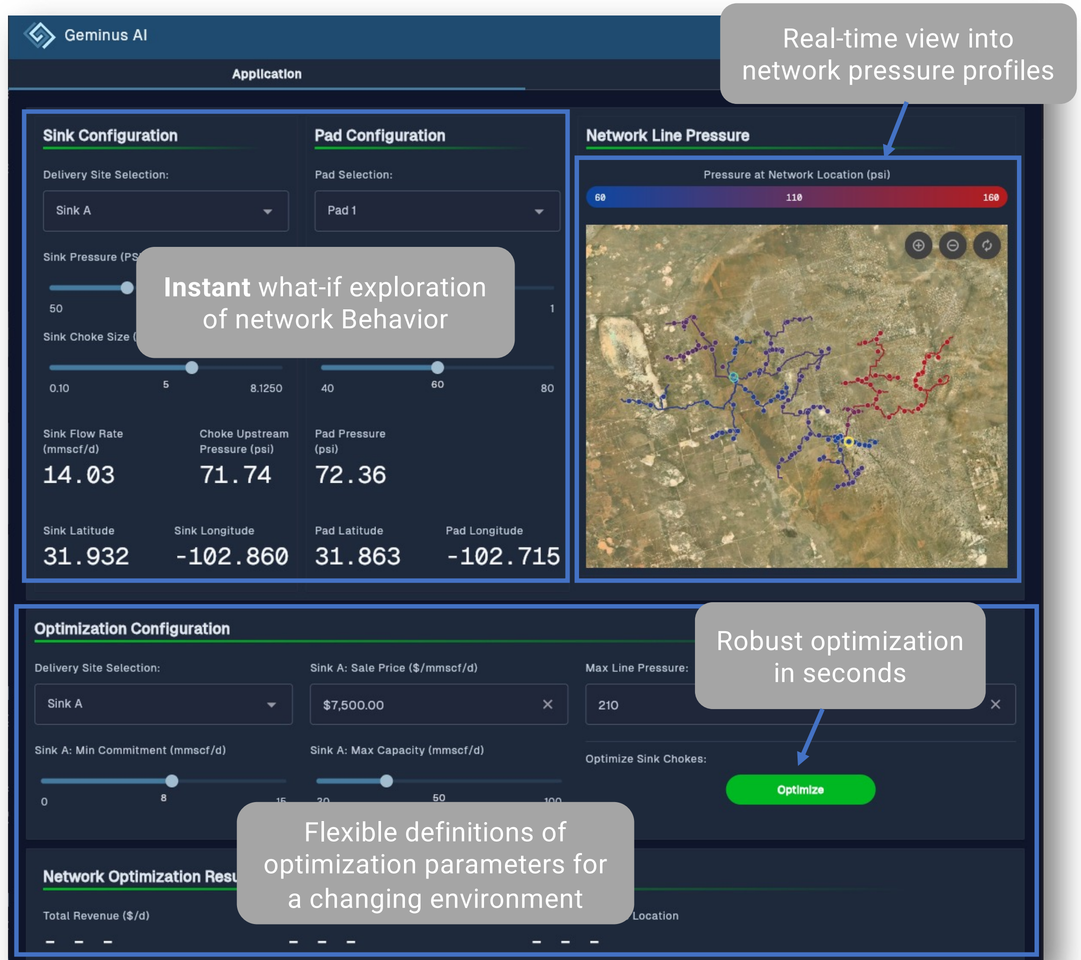
- Ability to optimize online in short decision time frames (near real time) handling high dimensionality
- Easily adaptable to changes in network topology

Interactive Demo

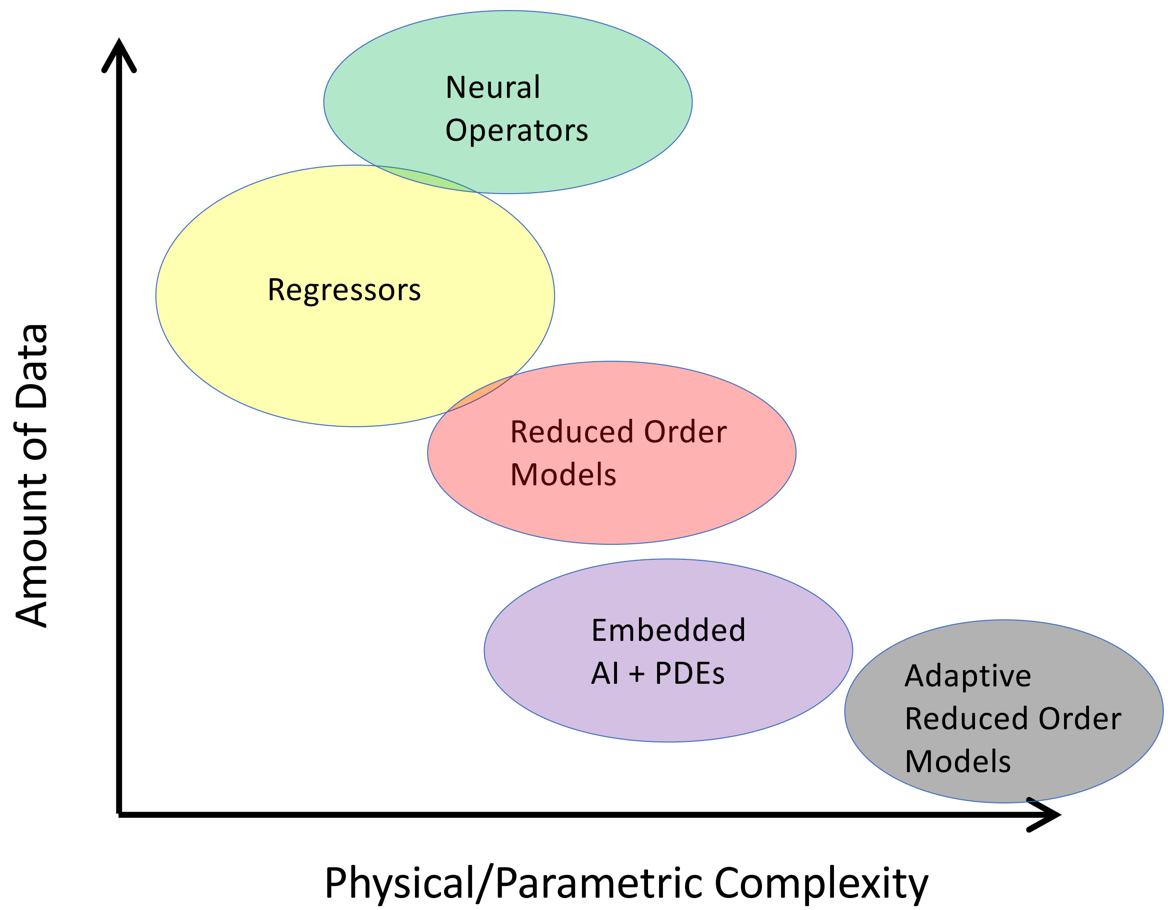
Geminus-powered intelligent advisor for well network optimization

https://demo.geminus.ai/network

Geminus



What about PDEs, dynamical systems (and other complex spatio-temporal processes?)



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Multi-scale, Multi-physics, Complexity : An Example

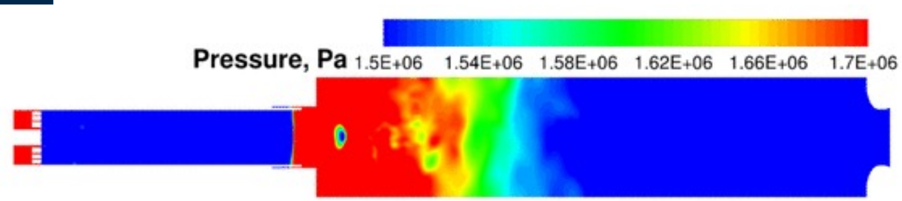
- Non-linear, Multi-scale multi-physics interactions : acoustics, flow & reaction
- Flow – Large coherent structures + small shear layer dynamics
- Reaction – Highly intensive, distributed & intermittent thin flame
- High sensitivity to parameter changes

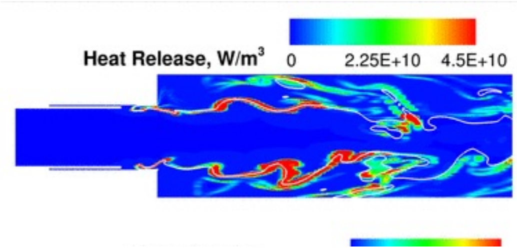
$$\frac{\partial Q}{\partial t}+\frac{\partial F_i}{\partial x_i}+\frac{\partial F_{v,i}}{\partial x_i}=H$$

$$Q=\begin{pmatrix}\rho\\ \rho u_i\\ \rho h^0-p\\ \rho Y_l\end{pmatrix},\ F_i=\begin{pmatrix}\rho u_i\\ \rho u_i u_j\\ \rho u_i h^0\\ \rho u_i Y_l\end{pmatrix},\ F_{v,i}=\begin{pmatrix}0\\ \tau_{ij}\\ u_j\tau_{ji}+q_i\\ \rho V_{i,l}Y_l\end{pmatrix},\ H=\begin{pmatrix}0\\ 0\\ 0\\ \dot{\omega}_l\end{pmatrix}$$

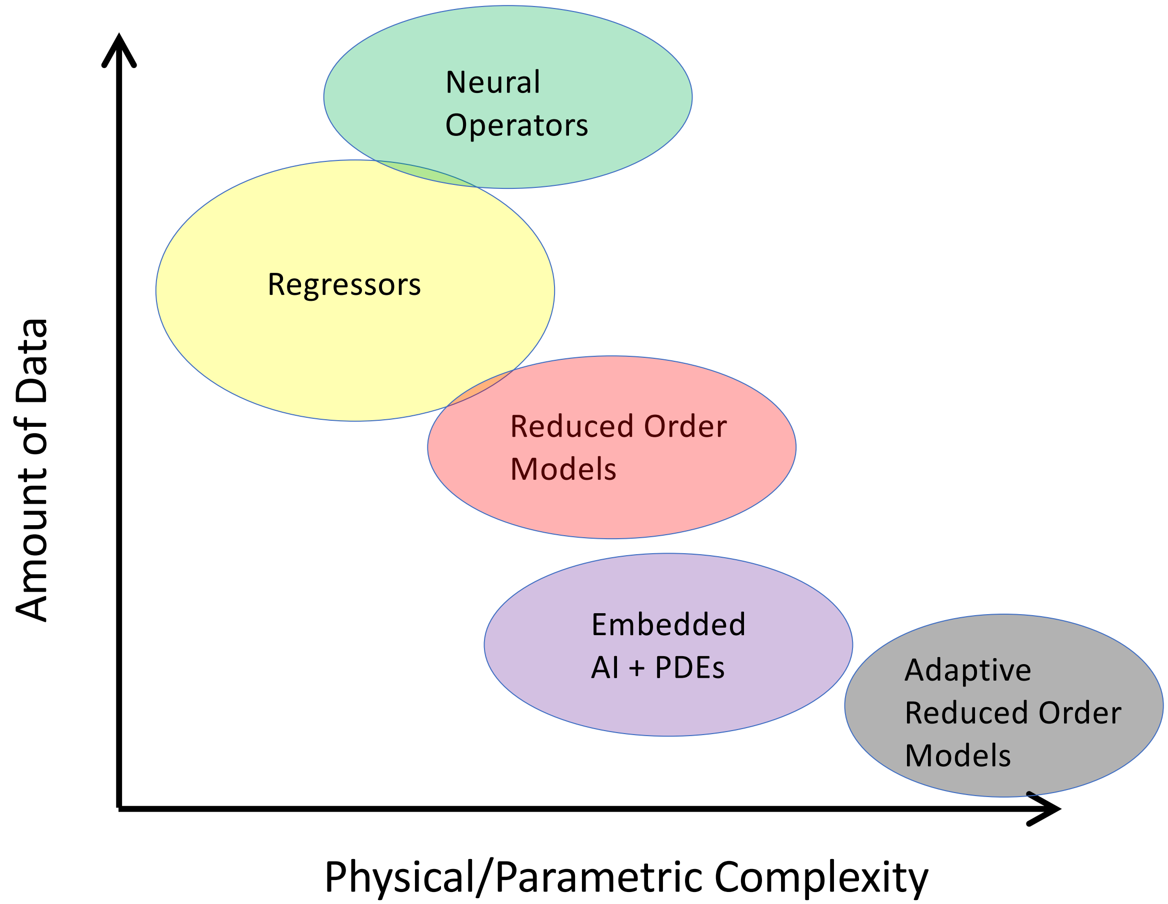
Highly nonlinear and stiff source term :

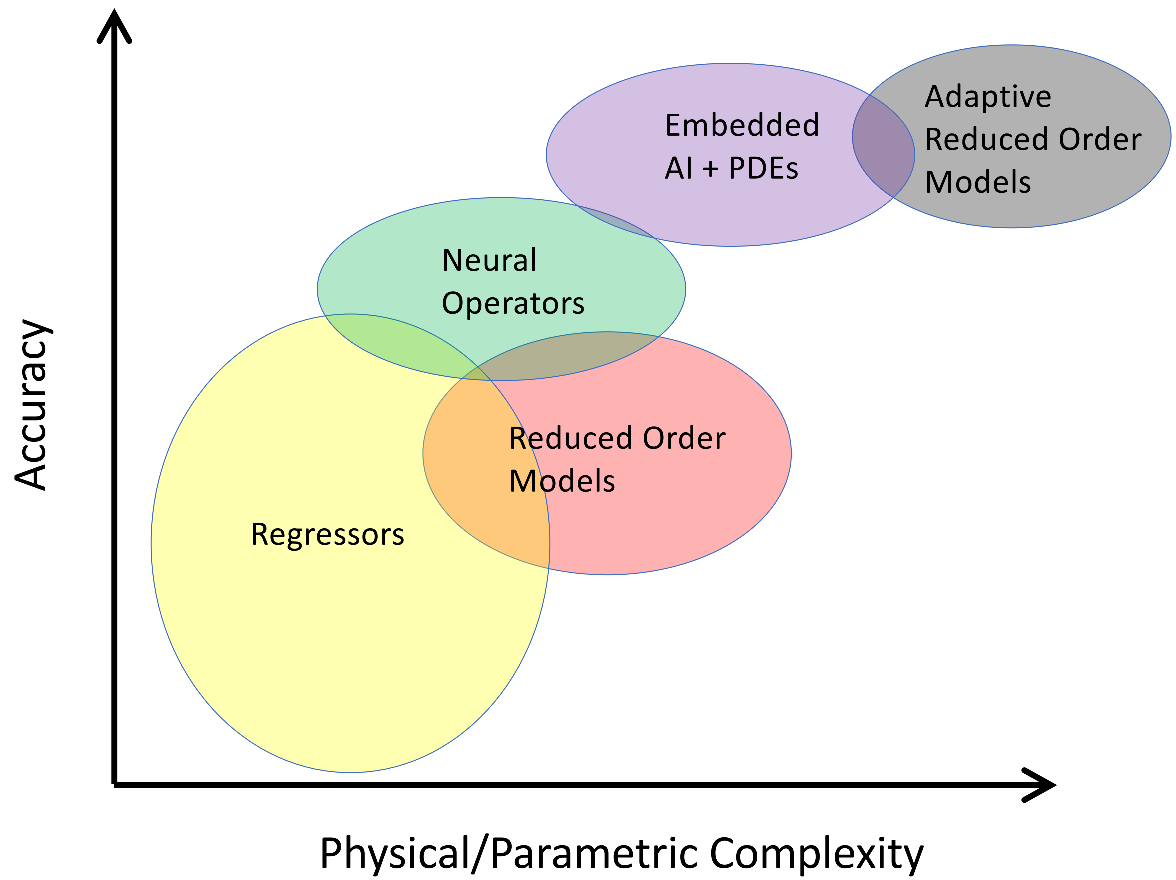
$$e.g.,\ \dot{\omega}_1=\frac{\rho Y_1}{M_1}AT^b\exp\left(\frac{-E_a}{R_u T}\right)[\frac{\rho Y_1}{M_1}]^{0.2}[\frac{\rho Y_2}{M_2}]^{1.3}$$



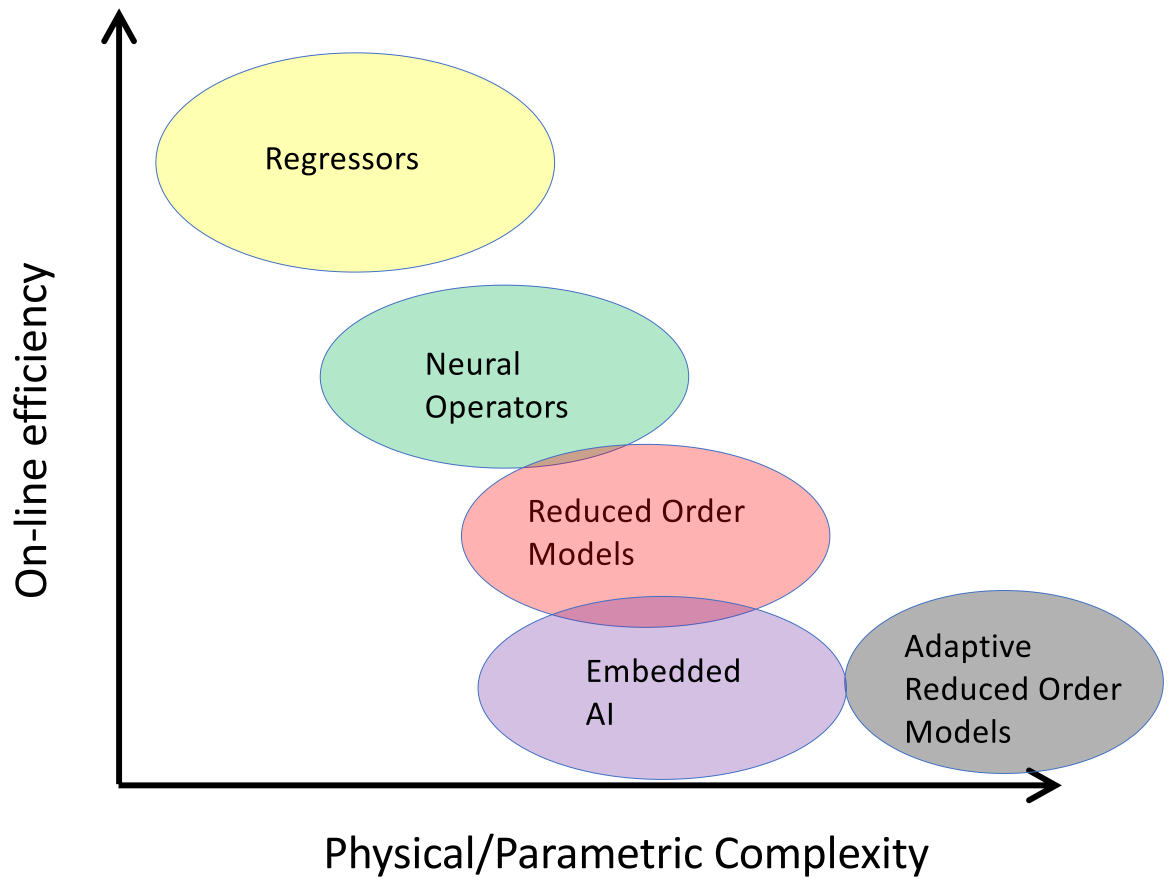


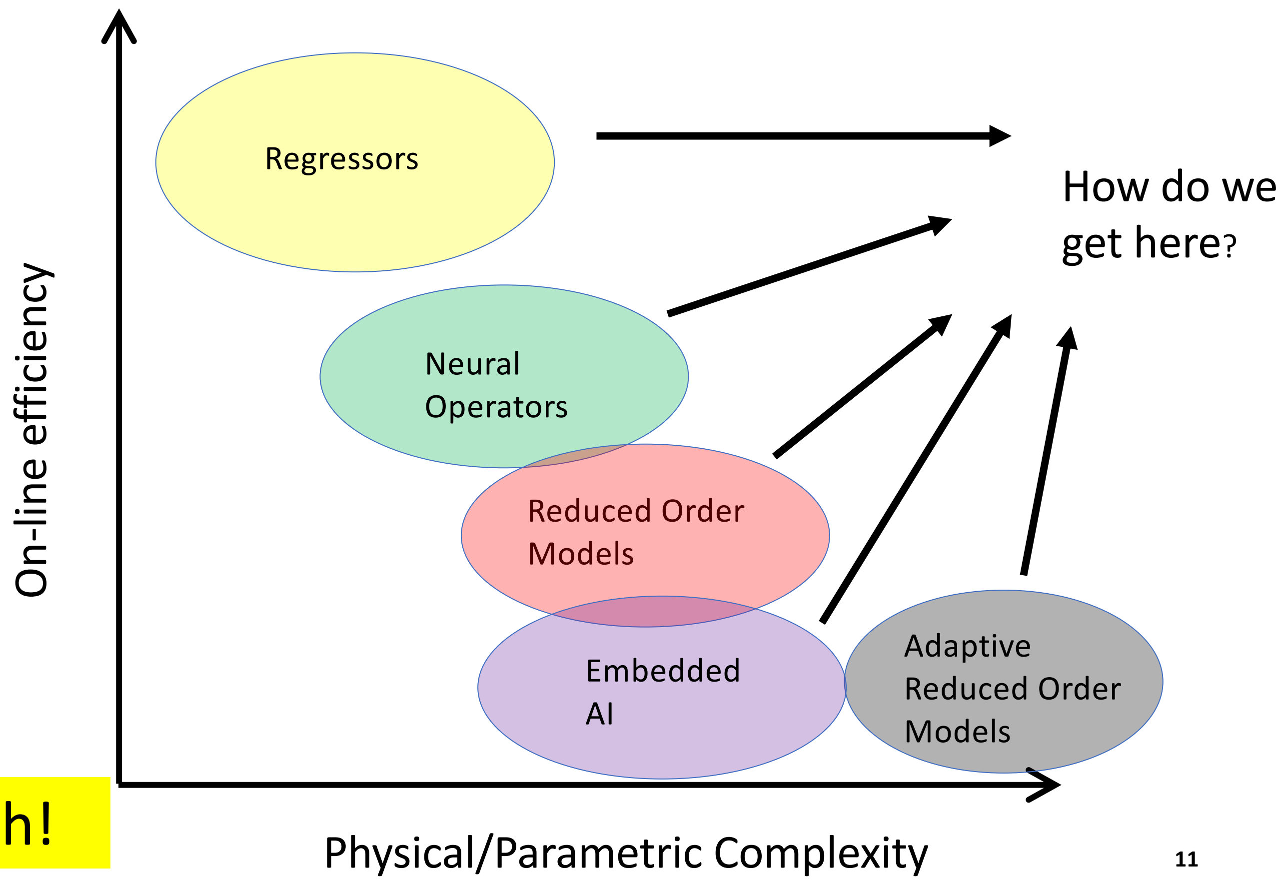
What about PDEs, dynamical systems (and other complex spatio-temporal processes?)





Accuracy
Embedded
AI + PDEs
Adaptive
Reduced Order
Models
Neural
Operators
Reduced Order
Models
Regressors
Physical/Parametric Complexity


On-line efficiency
Regressors
Neural
Operators
Reduced Order
Models
Embedded
AI
Adaptive
Reduced Order
Models
Physical/Parametric Complexity


Regressors
Neural Operators
Reduced Order Models
Embedded AI
Adaptive Reduced Order Models
How do we get here?
On-line efficiency
Physical/Parametric Complexity

Bar is high!

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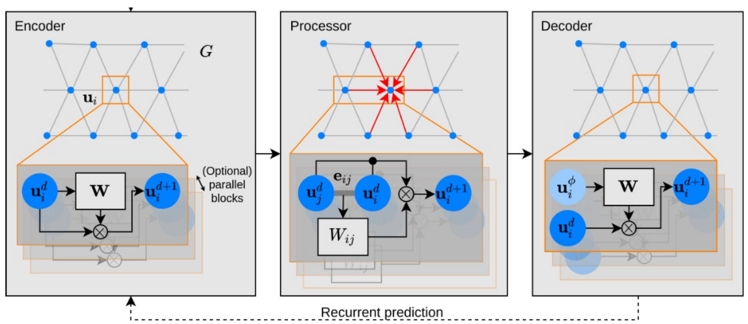
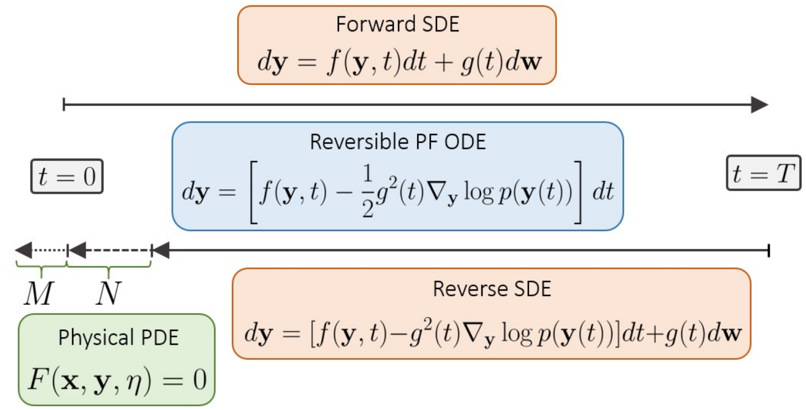
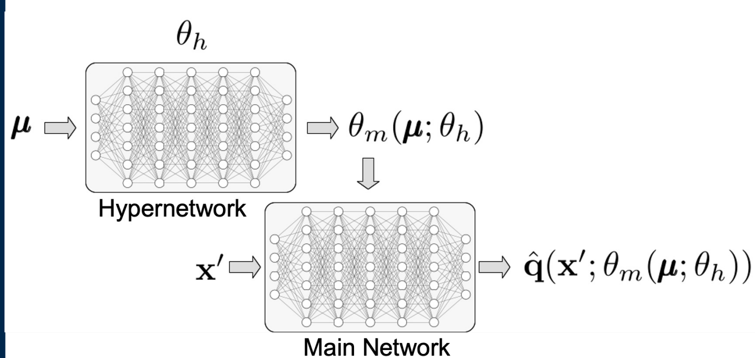
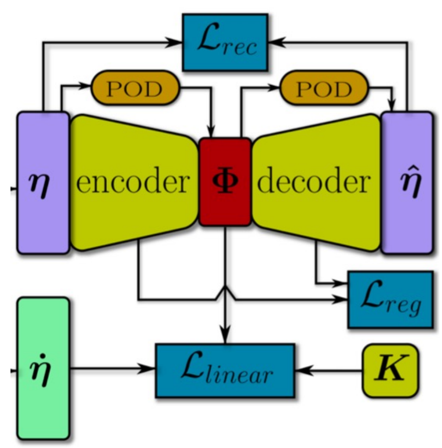
How to get there? Structure in Learning





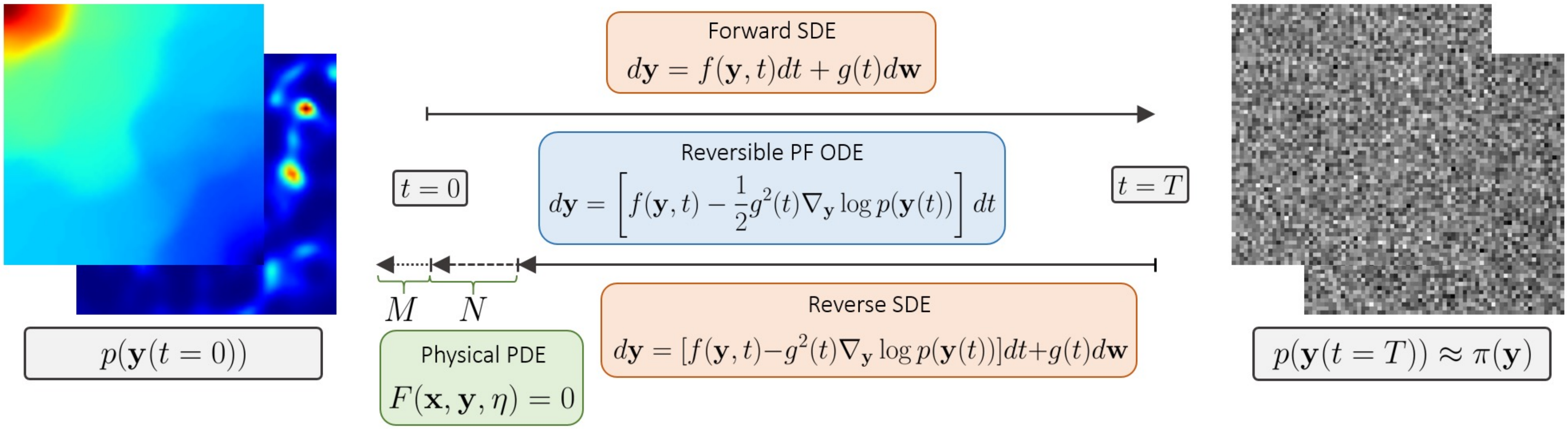




Enforcing Physical Consistency in Score-based diffusion models

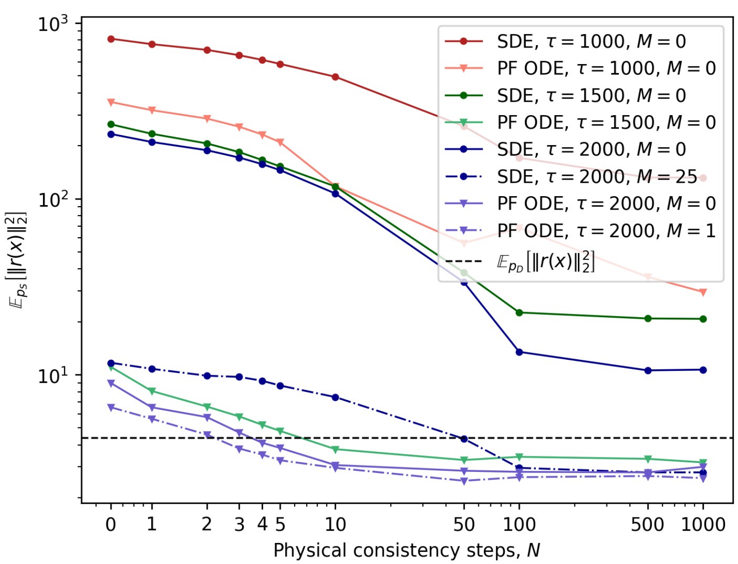
- Minimize physical PDE residual $\mathbf{r} = F(\mathbf{x}, \mathbf{y}, \eta)$

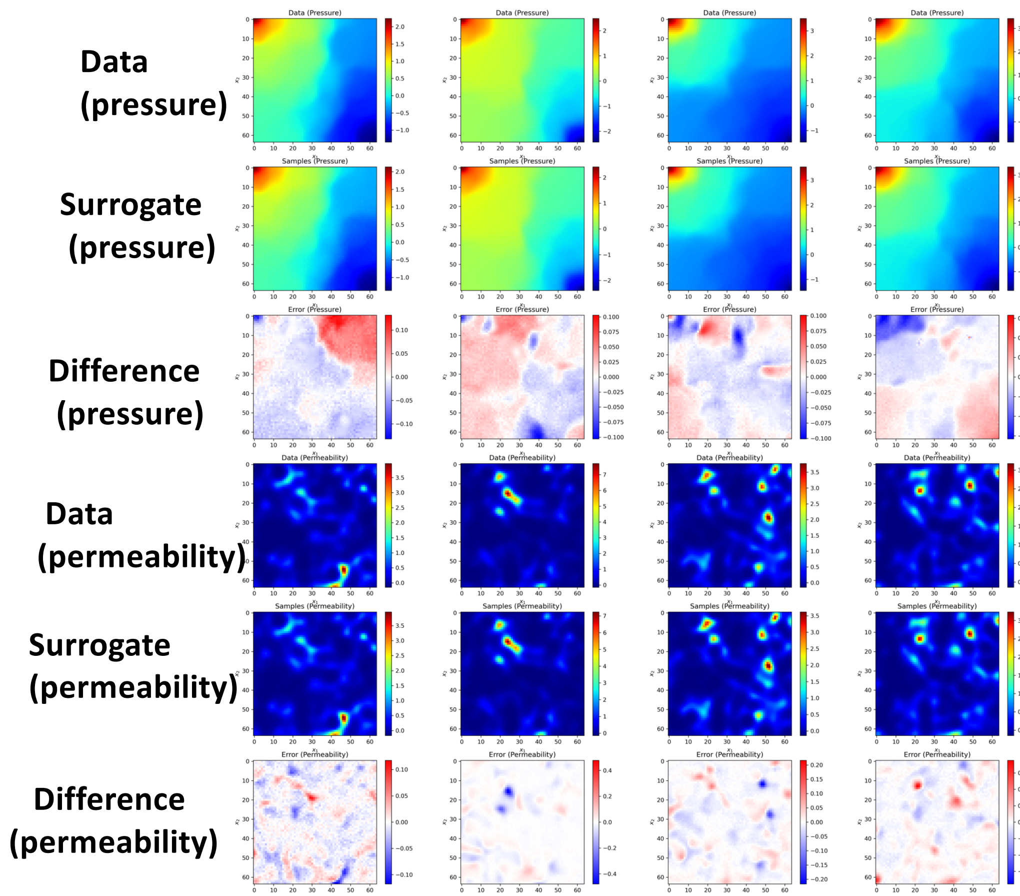
- Step in negative gradient direction during SDE / PF ODE solve: $\mathbf{y}_{i-1} = \mathrm{Solver}(\mathbf{y}_i, t_i) - 2\epsilon \mathbf{r} \nabla_{\mathbf{y}} \mathbf{r}$



Example: Darcy Flow

- Examples of single sample generation for conditional input
- All generated samples have physical residuals similar to or less than data samples





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Conditional Parameterization I

- Standard dense layer of width w:

$$f(\mathbf{h};\Theta) = \sigma(\mathbf{W}\mathbf{h} + \mathbf{b}),$$
$$\mathbf{W} \in \mathbb{R}^{n_h \times w}, \mathbf{b} \in \mathbb{R}^{w}.$$

- How to fit $f(\mathbf{h}) = \mathbf{h}^2$?

What if W = h, b=0, σ = 1?

How can we formalize, generalize this?

Jiayang Xu, Aniruddhe Pradhan, and Karthikeyan Duraisamy (2021). "Conditionally Parameterized, Discretization-Aware Neural Networks for Mesh-Based Modeling of Physical Systems". In: *Advances in Neural Information Processing Systems* 34

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Application to generalized unstructured meshes

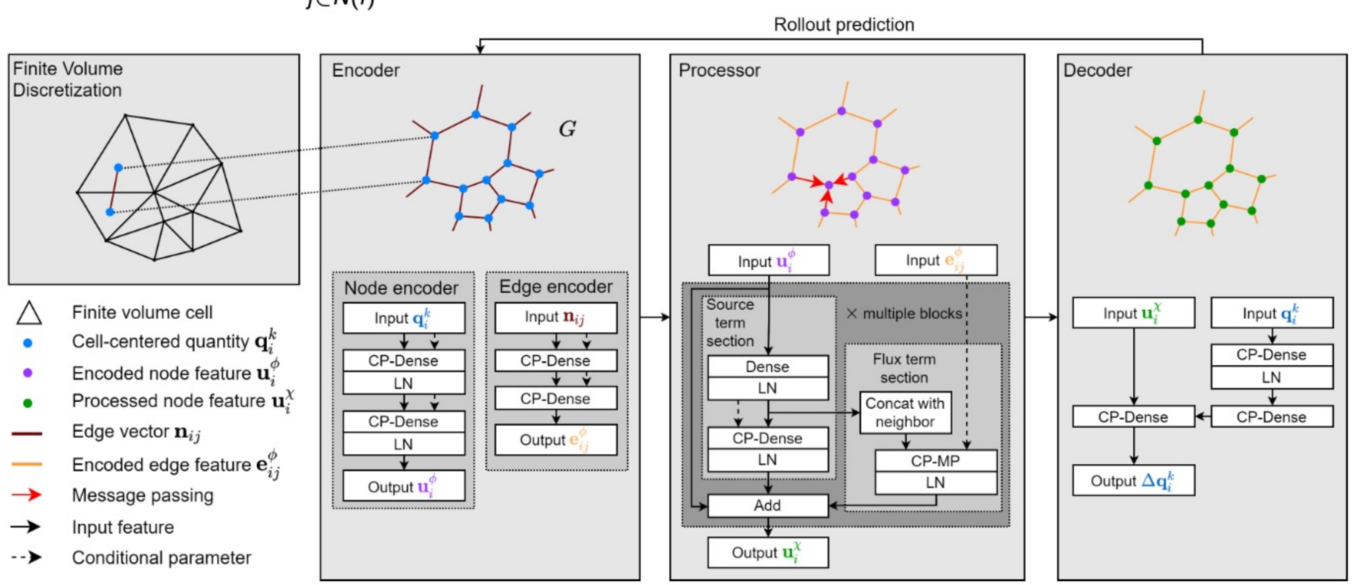
Encoder-processor-decoder architecture with CP-dense and CP-message passing layers:

- Flux term modeled by CP-message passing:

$$\mathbf{W}_{ij} = \sigma\left(\langle \mathbf{W}, \mathbf{e}_{ij} \rangle + \mathbf{B}\right), \mathbf{h}_i^{\mathrm{CPMP}} = \sum_{j \in N(i)} w_{ij} \sigma\left(\langle \mathbf{W}_{ij}, [\mathbf{u}_i; \mathbf{u}_j] \rangle\right). \tag{15}$$

- Contrasted with standard message passing with node-edge concatenation:

$$\mathbf{s}_i = \sum_{j \in N(i)} \sigma\left(\langle \mathbf{W}_1, [\mathbf{u}_i; \mathbf{u}_j; \mathbf{e}_{ij}] \rangle + \mathbf{b}_1\right), \mathbf{h}_i^{\mathrm{MP}} = \sigma\left(\langle \mathbf{W}_2, [\mathbf{u}_i; \mathbf{s}_i] \rangle + \mathbf{b}_2\right). \tag{16}$$



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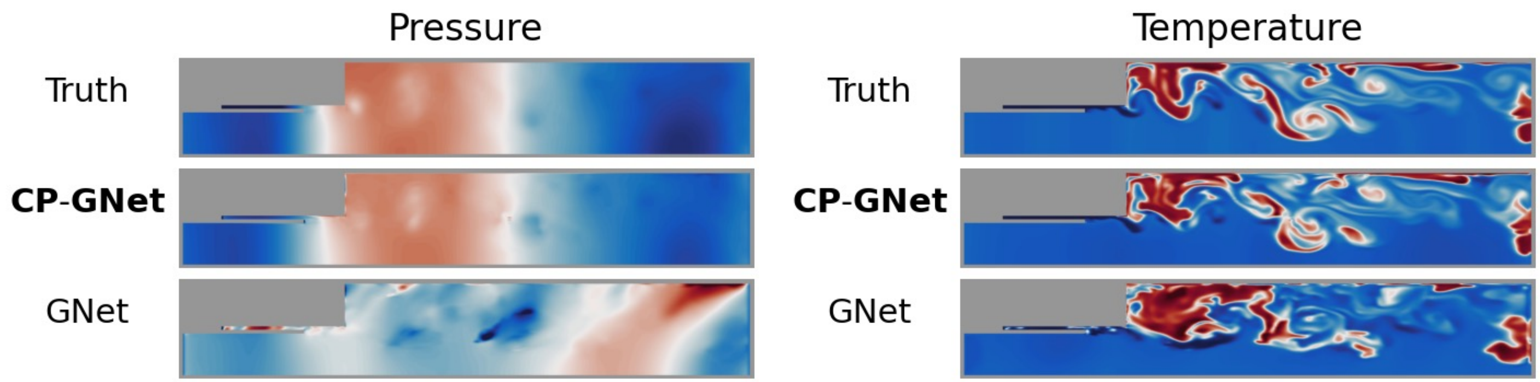
Rocket Combustion



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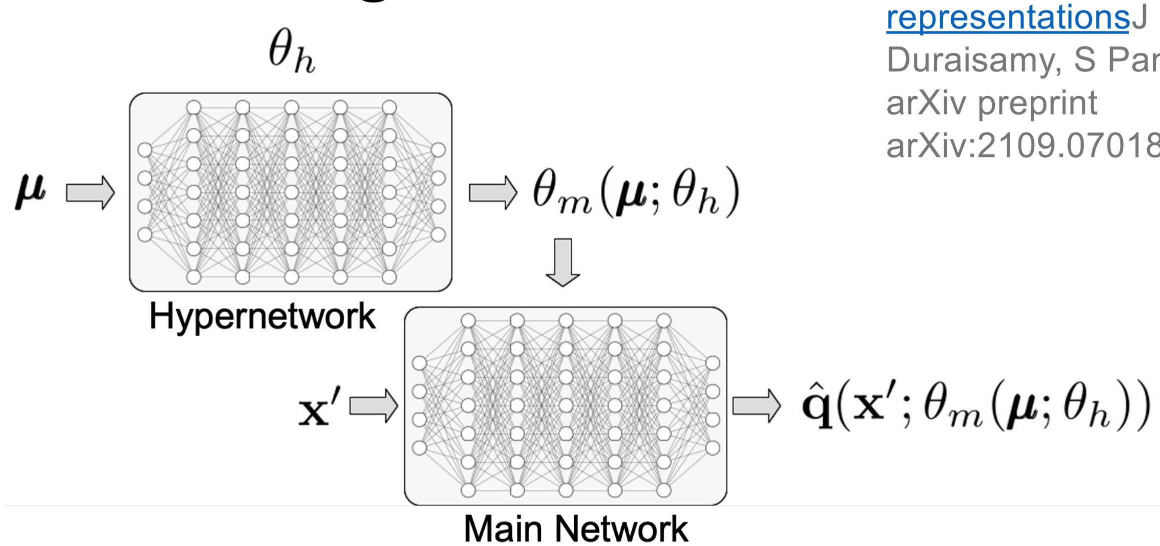
Discretization-independent Surrogate modeling

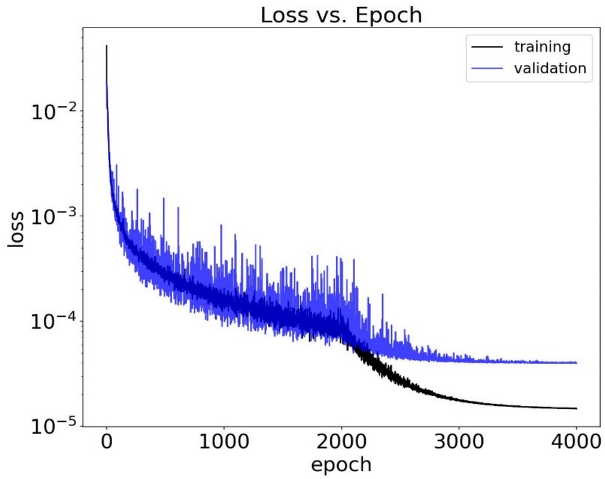
[Discretization-independent surrogate modeling over complex geometries using hypernetworks and implicit representations]J Duvall, K Duraisamy, S Pan arXiv preprint arXiv:2109.07018



$$\theta_m(\boldsymbol{\mu}) = N_h(\boldsymbol{\mu}; \theta_h)$$

$$\hat{\mathbf{q}}(\mathbf{x}'; \theta_m(\boldsymbol{\mu})) = N_m(\mathbf{x}'; \theta_m(\boldsymbol{\mu}))$$

Transonic Rotor w/Varying Speed and Geometry (DVH)



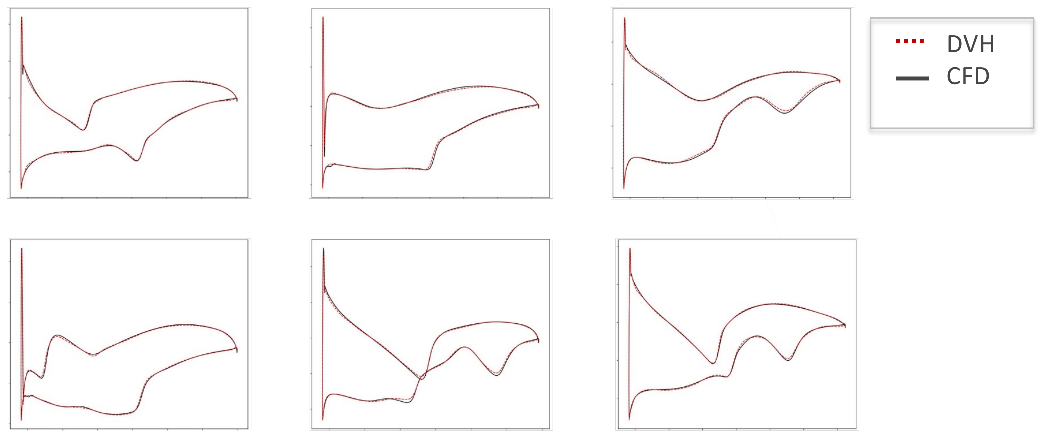
Main Network		Hypernetwork	
# Hidden Layers	# Nodes	# Hidden Layers	# Nodes
5	100	5	50

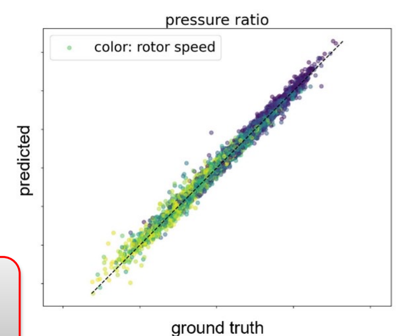
Hypernetwork inputs: $\boldsymbol{\mu} \in \mathbb{R}^9$

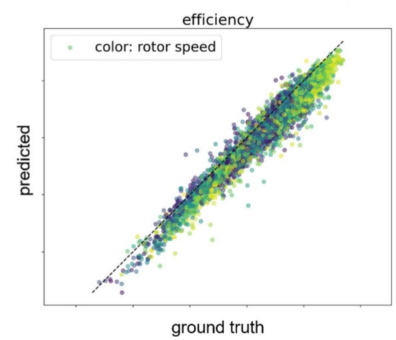
Main network inputs: $\mathbf{x}' = [x, y, \phi]^T$

Predicted variables: $\mathbf{q} = [\rho, p, u, v, w, k, \omega, E_0\rho]^{\mathrm{T}}$

Airfoil surface pressure distributions, all unseen

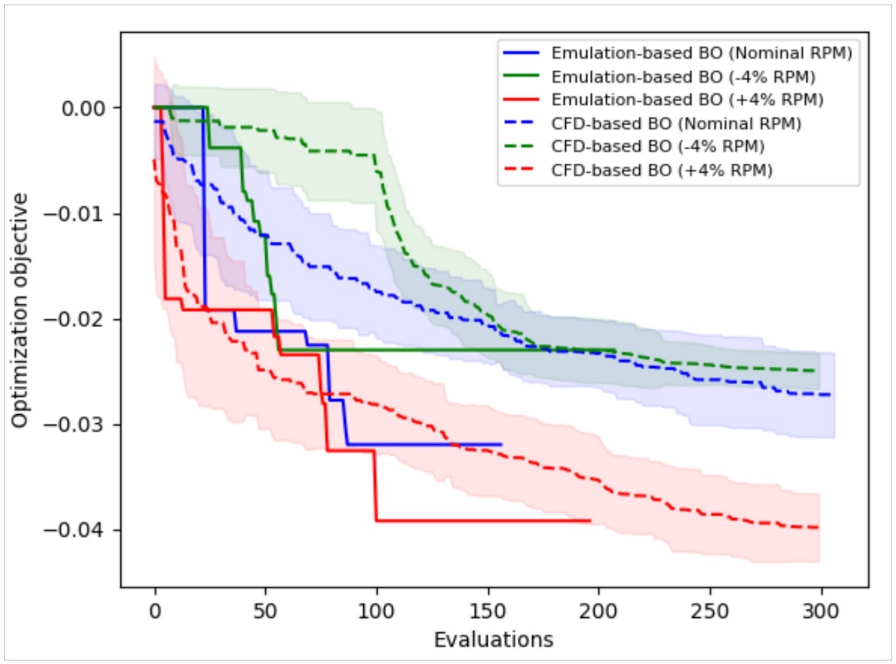


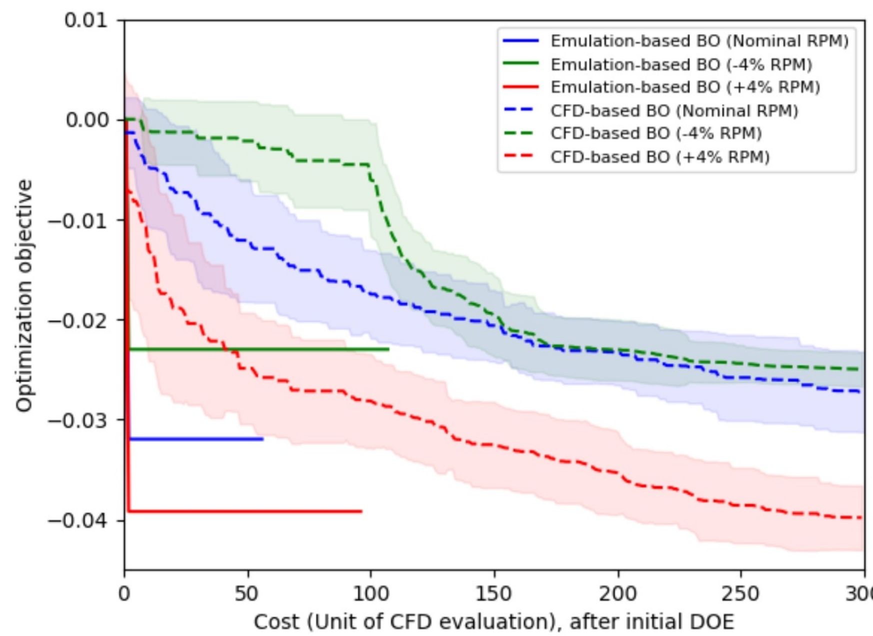




DVH generalizes well w/varying flow condition, training with 800 randomly selected cases (test on 9,200)

Emulator-driven design optimization at varying rotor speed





DVH achieves better or similarly-performing designs at a fraction of the online cost

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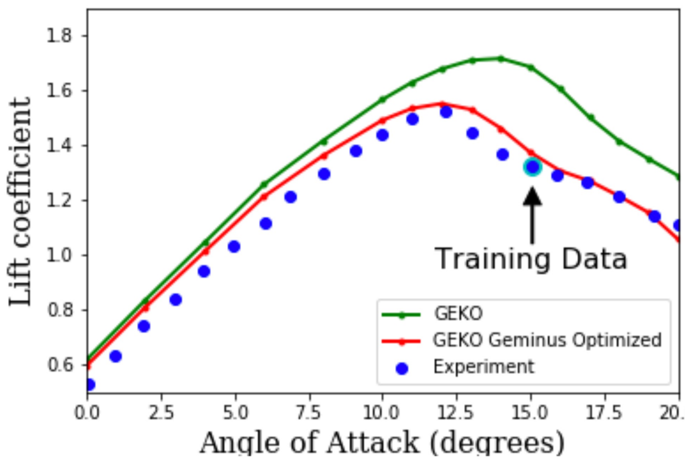
Embedded AI + Physics

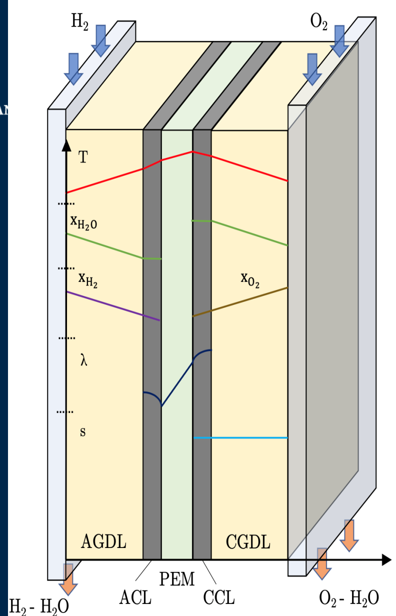
$$R(u, \beta \circ \eta(u), \alpha) = 0$$

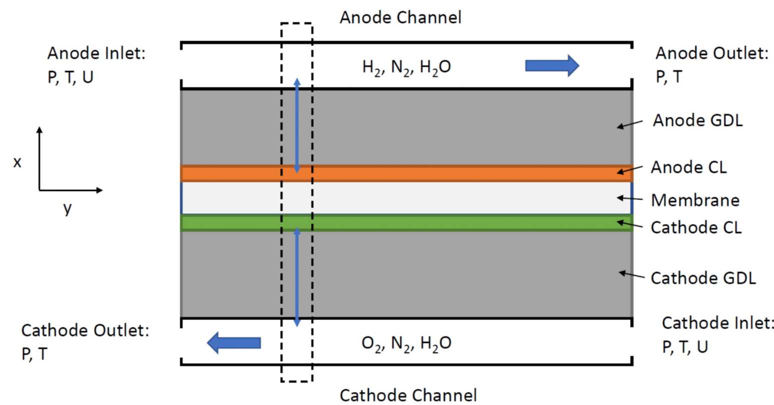
ML Augmentation



Physics constraints +
Physical consistency +
Information from data +
Interpolation in feature space =
Extrapolation in physical space

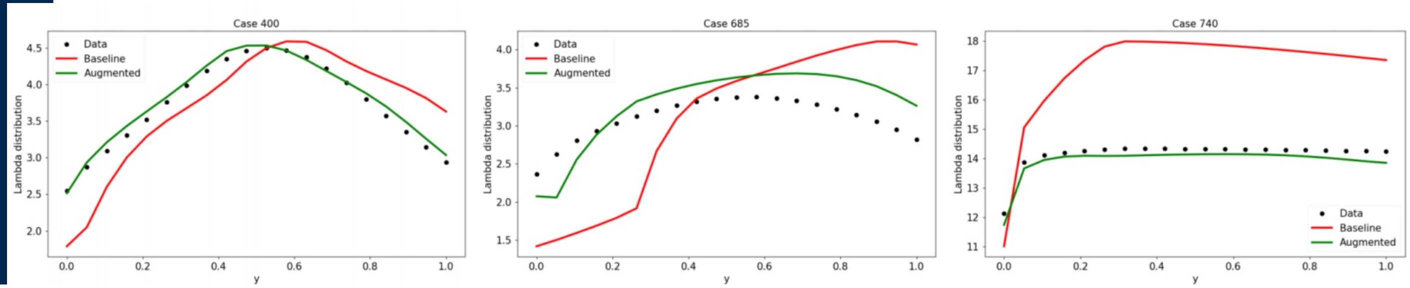
From detailed analysis model to engine control unit



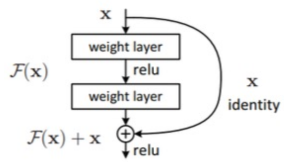


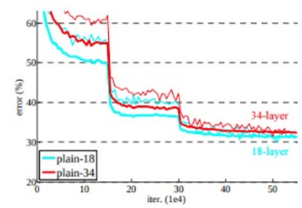
[A non-intrusive approach for physics-constrained learning with application to fuel cell modeling](#)
Srivastava, et al.
Computational Mechanics, 2023

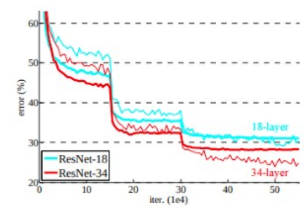
3D (High fidelity) to Augmented 1D (low-fidelity)
=
Design to Engine control unit

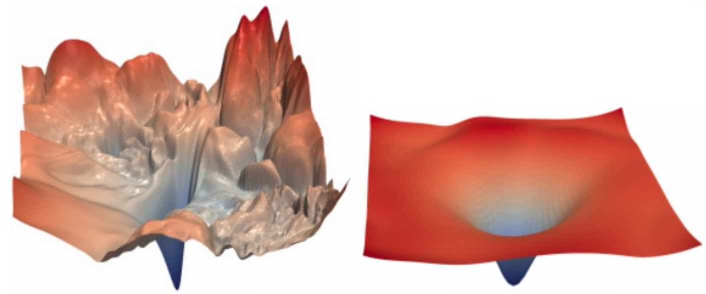


Enforcing structure for Learning : "DMD ResNet"









(a) without skip connections (b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

$$\boldsymbol{\Phi}_{svd}(\mathbf{z}) = \mathbf{z}\boldsymbol{\Lambda}\mathbf{V}_D, \quad \boldsymbol{\Psi}_{svd}(\boldsymbol{\Phi}) \triangleq \boldsymbol{\Phi}\mathbf{V}_D^\top\boldsymbol{\Lambda}^{-1},$$

$$\boldsymbol{\Phi}(\mathbf{z}) = \underbrace{\boldsymbol{\Phi}_{nn}(\mathbf{z})W_{enc,L} + b_{enc,L}}_{\text{nonlinear observables}} + \underbrace{\boldsymbol{\Phi}_{svd}(\mathbf{z})W_{enc,L}}_{\text{linear observables}},$$

$$\boldsymbol{\Psi}(\boldsymbol{\Phi}) = \underbrace{\boldsymbol{\Psi}_{nn}(\boldsymbol{\Phi})}_{\text{nonlinear reconstruction}} + \underbrace{\boldsymbol{\Psi}_{svd}(\boldsymbol{\Phi}W_{dec,1})}_{\text{linear reconstruction}},$$

Enforcing structure for Learning : Stability

We propose : (where $\zeta_1, \ldots, \zeta_{D-1}, \sigma_1, \ldots, \sigma_D \in \mathbb{R}$.)

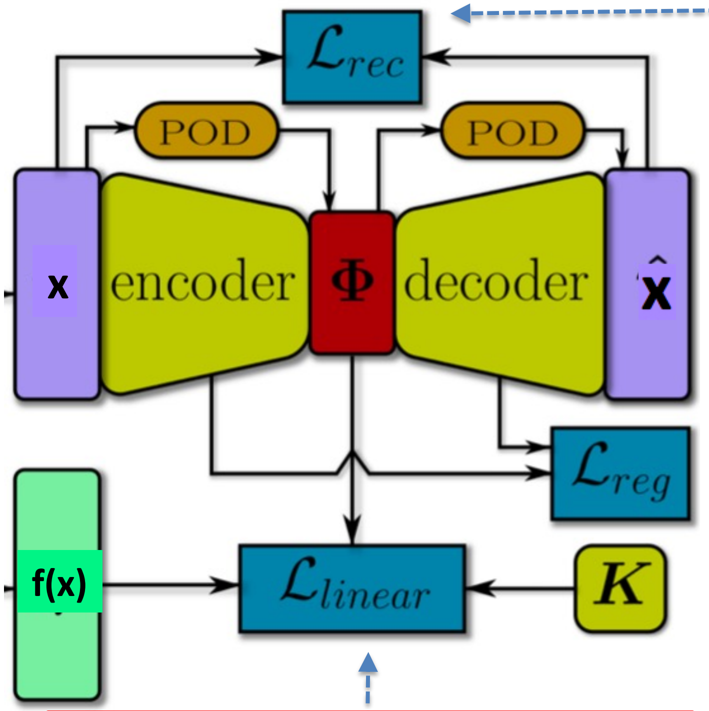
$$\mathbf{K}_{stable} = \begin{bmatrix} -\sigma_1^2 & \zeta_1 & & \\ -\zeta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \zeta_{D-1} \\ & & -\zeta_{D-1} & -\sigma_D^2 \end{bmatrix}, \qquad (5)$$

Theorem

$\forall D \in \mathbb{N}$, for any real square diagonalizable matrix $\mathbf{K} \in \mathbb{R}^{D\times D}$ that only has non-positive real part of the eigenvalues $D \geq 2$, there exists a set of $\zeta_1, \ldots, \zeta_{D-1}, \sigma_1, \ldots, \sigma_D \in \mathbb{R}$ such that $\mathbf{K}_{stable}$ is similar to $\mathbf{K}$ over $\mathbb{R}$. Moreover, for any $\zeta_1, \ldots, \zeta_{D-1}, \sigma_1, \ldots, \sigma_D \in \mathbb{R}$, the real part of the eigenvalue of $\mathbf{K}_{stable}$ is non-positive.

Unconditionally stable, and “expressive” $\rightarrow$ any diagonalizable matrix corresponding to a stable Koopman operator can be represented without loss of information

Use Math + physics + structure for Learning



$$\frac{1}{M}\sum_{i=1}^{M}\|\mathbf{\Psi}(\mathbf{\Phi}(\mathbf{x}_i)) - \mathbf{x}_i\|^2$$

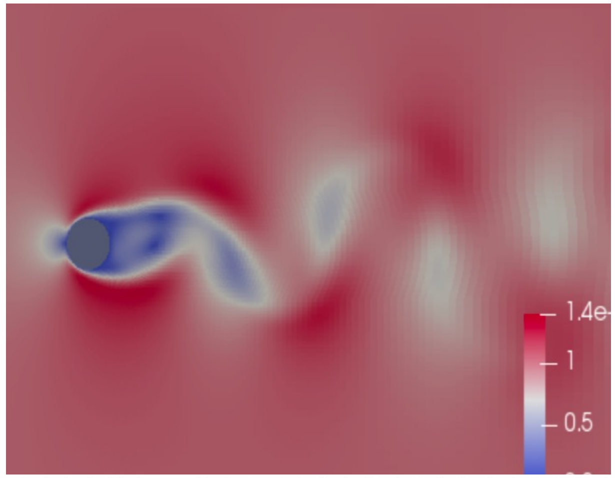
$$\begin{aligned}\mathbf{\Phi}(\boldsymbol{x}) &= \mathbf{\Phi}_{dmd}(\boldsymbol{x}) + \mathbf{\Phi}_{nn}(\boldsymbol{x}),\\ \mathbf{\Psi}(\mathbf{\Phi}) &= \mathbf{\Psi}_{dmd}(\mathbf{\Phi}(\boldsymbol{x})) + \mathbf{\Psi}_{nn}(\mathbf{\Phi}(\boldsymbol{x}))\end{aligned}$$

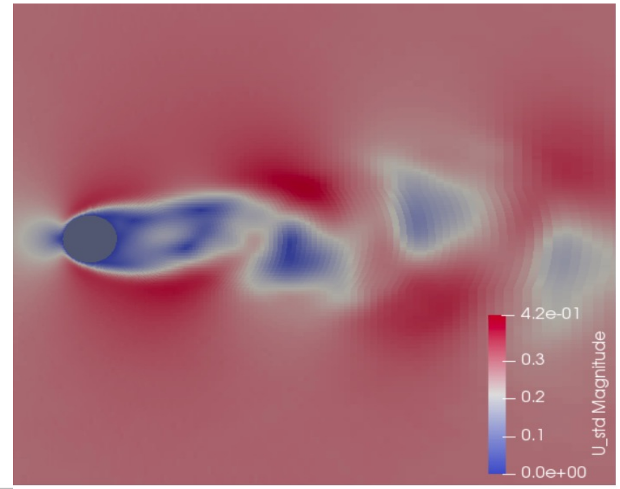
$$\frac{1}{M}\sum_{i=1}^{M}\|\mathbf{f}(\mathbf{x}_i)\cdot\nabla_{\mathbf{x}}\mathbf{\Phi}(\mathbf{x}_i) - \mathbf{\Phi}(\mathbf{x}_i)\mathbf{K}\|^2$$

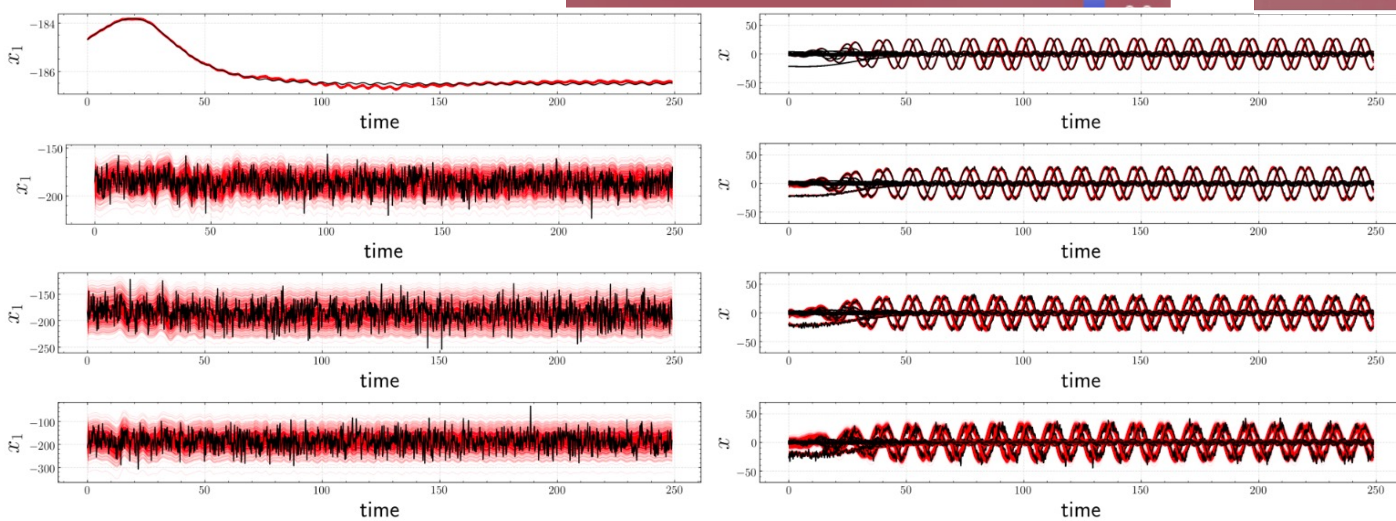
Pan. S. & Duraisamy, K., *Physics-Informed Probabilistic Learning of Linear Embeddings of Non-linear Dynamics With Guaranteed Stability*, SIAM J. of Applied Dynamical Systems, 2020.

Flow over cylinder: Prediction with uncertainties

•Gaussian white noise added







Physics-Informed Probabilistic Learning of Linear Embeddings of Non-linear Dynamics With Guaranteed Stability, Pan, S., and Duraisamy, K., SIADS, 2020

Relevant Efforts at UM

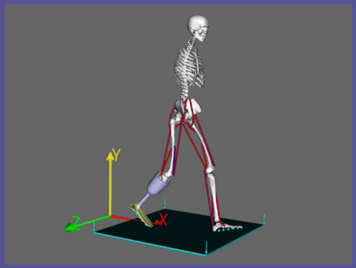
Centers & Initiatives

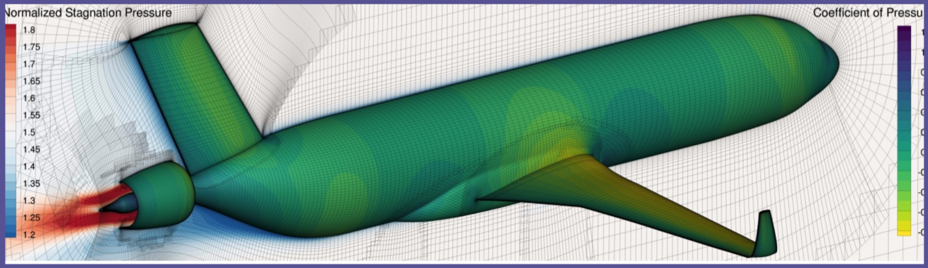
- Center for Data-driven Computational Physics [2015-]
- MIDAS Schmidt AI in Science Post doc program [2022-]
- Initiative on Scientific Foundation models - sciFM.ai [2023-]
- Major National Lab presence on Campus to collaborate on computational science + AI [2024-]
- MIDAS Data science Fellowships [2015-]

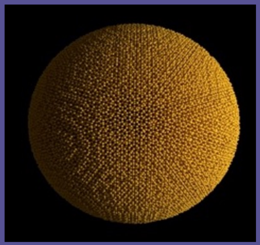
Center-scale grants

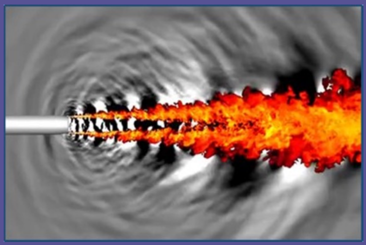
- $15 M Center on AI + Co-design for Energy
- $10 M NASA Center on Space weather modeling
- $3.5M NSF Major Research Instrumentation
- $5.0M NSF Data Infrastructure Building Blocks
- $5.17M NSF CRISP and Toyota Research Institute
- $5.8 M Air Force Center of Excellence on Reduced Order Modeling
- $5.4 M ARPA-E project on Digital Twins for Nuclear Reactors
- $7.5 M MURI on Climate impact on DoD installations

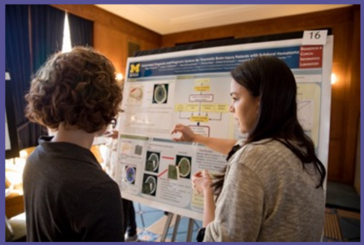
+ Many Others

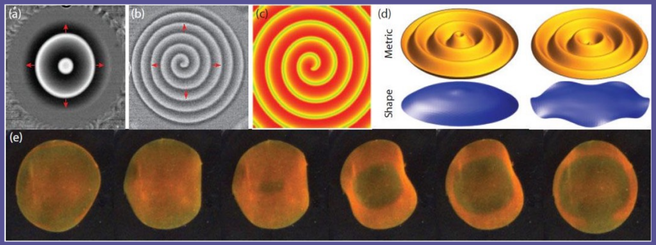












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Harvard AI4Science

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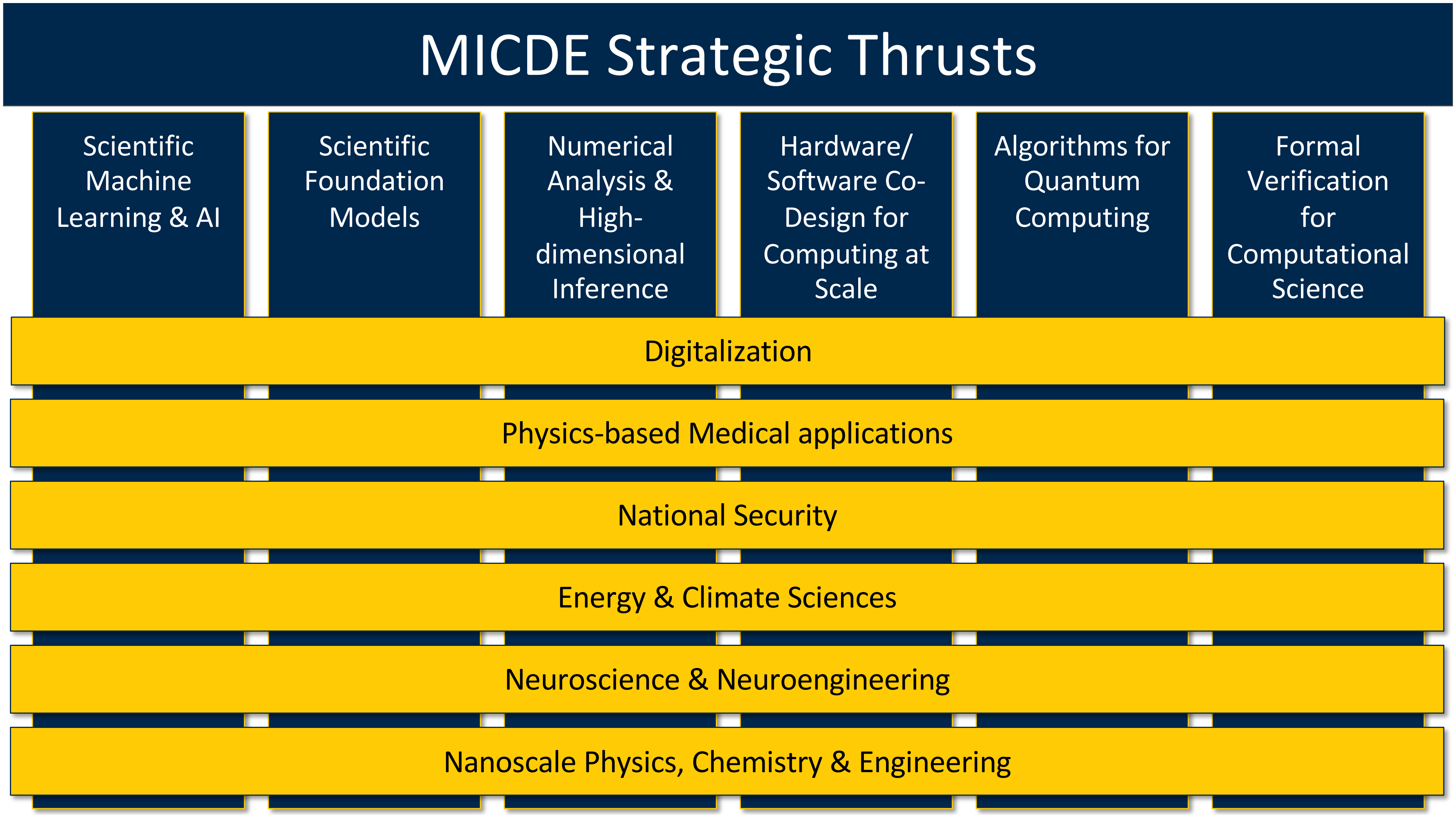
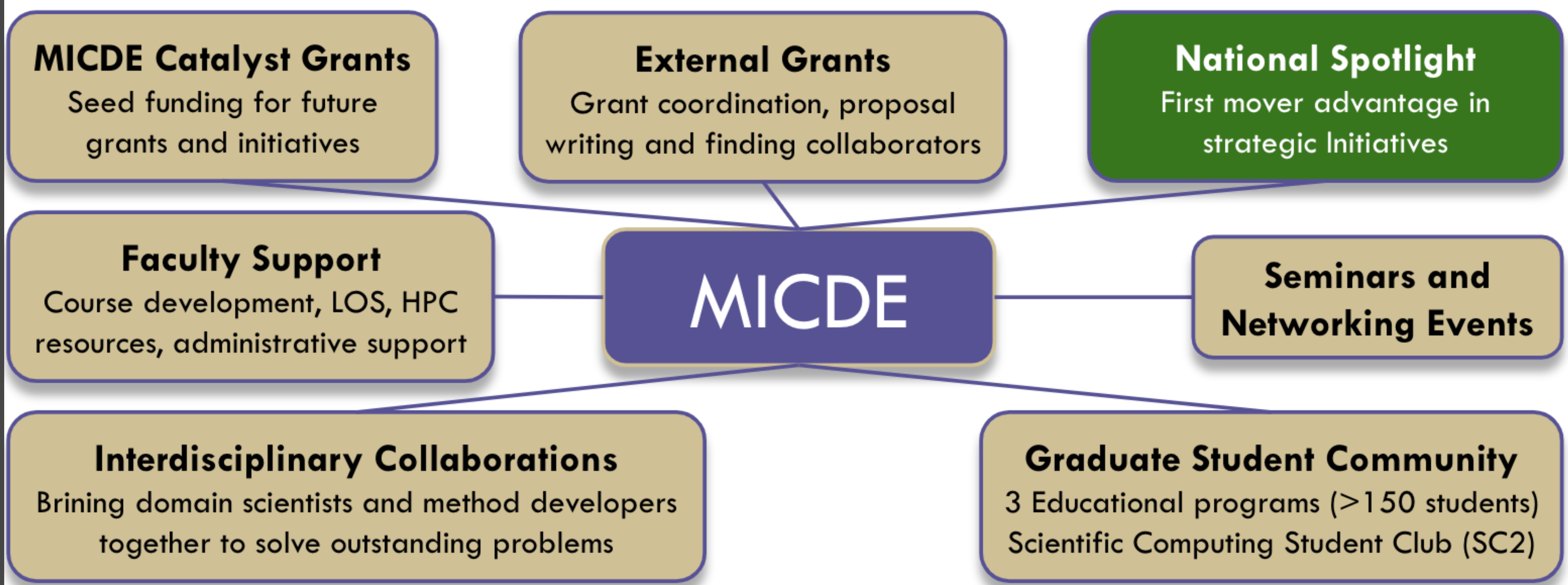

MICDE Strategic Thrusts
Scientific Machine Learning & AI
Scientific Foundation Models
Numerical Analysis & High-dimensional Inference
Hardware/ Software Co-Design for Computing at Scale
Algorithms for Quantum Computing
Formal Verification for Computational Science
Digitalization
Physics-based Medical applications
National Security
Energy & Climate Sciences
Neuroscience & Neuroengineering
Nanoscale Physics, Chemistry & Engineering


MICDE Catalyst Grants
Seed funding for future grants and initiatives
External Grants
Grant coordination, proposal writing and finding collaborators
National Spotlight
First mover advantage in strategic Initiatives
Faculty Support
Course development, LOS, HPC resources, administrative support
MICDE
Seminars and Networking Events
Interdisciplinary Collaborations
Brining domain scientists and method developers together to solve outstanding problems
Graduate Student Community
3 Educational programs (>150 students)
Scientific Computing Student Club (SC2)

MICDE Initiative: SciFM and GenAI for Science

- **Utilizing innovations in Generative AI models for scientific research**
- Kicked off by two MICDE Catalyst Grants supporting the development of scaling laws for training large language models (LLMs) for Molecular Discovery using Wafer-Scale Computing
- Thrust I: Designing LLMs for expediting materials discovery and molecular design by directly encoding scientific knowledge, applying BERT-based LLMs
- Thrust II: Creation of surrogate physics models by fine-tuning foundation models trained on multiple Partial Differential Equations
- 2024 INCITE Award from DOE of 200k GPU node-hours on Polaris

2024 MICDE Annual Conference

Topic: **Scientific Foundation Models (SciFM)**

Dates: April 2nd and 3rd, 2024

Where: Rackham Auditorium, Ann Arbor

SciFM are poised to have a similar transformative impact on science as Generative AI has had on natural language.

First of its kind dedicated exclusively to the exciting and nascent field of SciFM

Stellar lineup of speakers and panelists

2024 MICDE Annual Conference Lineup

Jason Pruet, Director of National Security AI, Los Alamos National Laboratory

Ian T. Foster, Director of Data Science and Learning Division, Argonne National Laboratory

Sanjeev Arora, Director of Princeton Language & Intelligence

Petros Koumoutsakos, Herbert S. Winokur, Jr. Professor of Computing in Science and Engineering, Harvard

Jonathan Carter, Associate Laboratory Director, Computing Sciences, Lawrence Berkeley National Laboratory

Animashree Anandkumar, Bren Prof. of Computing, Caltech

Rajesh Swaminathan, Partner, Khosla Ventures

Jean-Luc Cambier, Director of Research Programs, Office of the Secretary of Defense

Michael Mahoney, Leader of ML and Analytics Group, Lawrence Berkeley National Laboratory & UC Berkeley

Payel Das, Research Staff Member and Manager, AI Science, IBM T. J. Watson Research Center

and many more…

Check https://micde.umich.edu/SciFM24 for more details

SciFM 24 : Day 1

Hands-on Workshop by TPC

HPCwire

Since 1987 - Covering the Fastest Computers in the World and the People Who Run Them

- Home
- Topics
- Sectors

13, 2023

nal lab has started training a massive AI brain that could ultimately
e must-have computing resource for scientific researchers.

ational Laboratory (ANL) is creating a generative AI model called
T and is pouring a giant mass of scientific information into creating

is being trained on its Aurora supercomputer, which delivers more
f an exaflop performance at ANL. The system has Intel's Ponte
PUs, which provide the main computing power.

U-M Generative AI tools

AI Tools (https://genai.umich.edu/resources/tools)**:**

- U-M GPT (provides access to popular hosted AI models)
- U-M Maizey (using custom datasets for enriched experience)
- U-M GPT Toolkit (full control over AI environment and models)

Research (https://genai.umich.edu/resources/research):

- Initiative on Scientific Foundation Models: sciFM.ai

Training (https://genai.umich.edu/resources/training)

Check https://genai.umich.edu/ for more information