

Everything flows

Bridging fluid flows and data assimilation through entropy and stochasticity

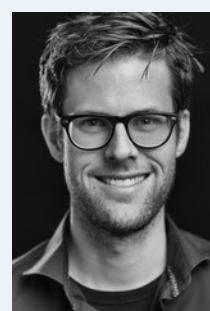
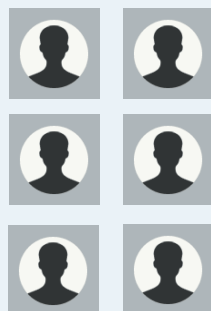
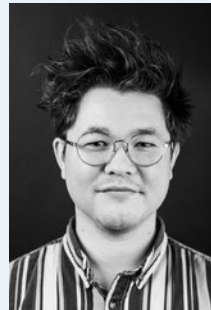
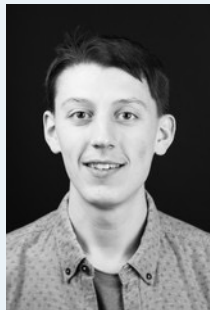
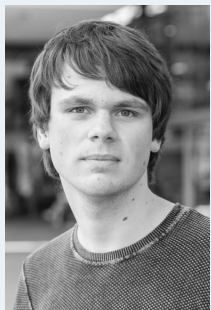
Benjamin Sanderse

IPAM, April 16, 2026

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The Scientific Computing group @CWI

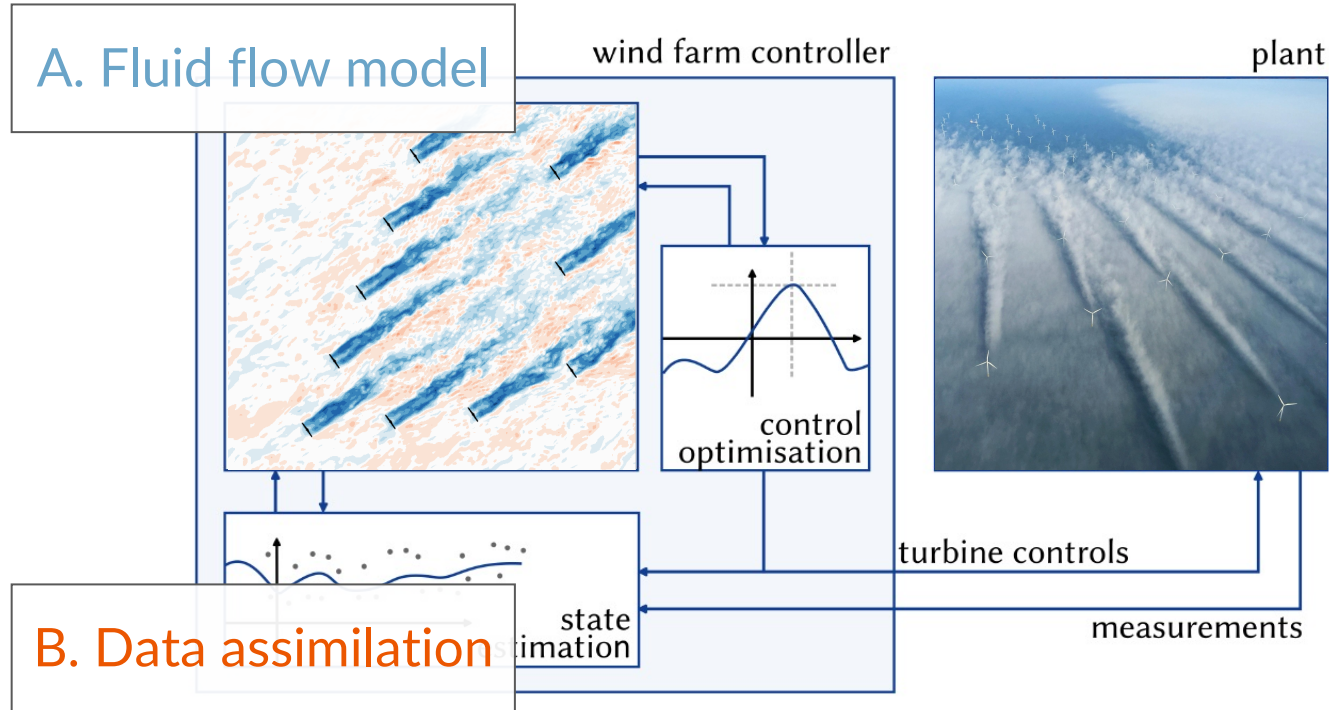


MSc students

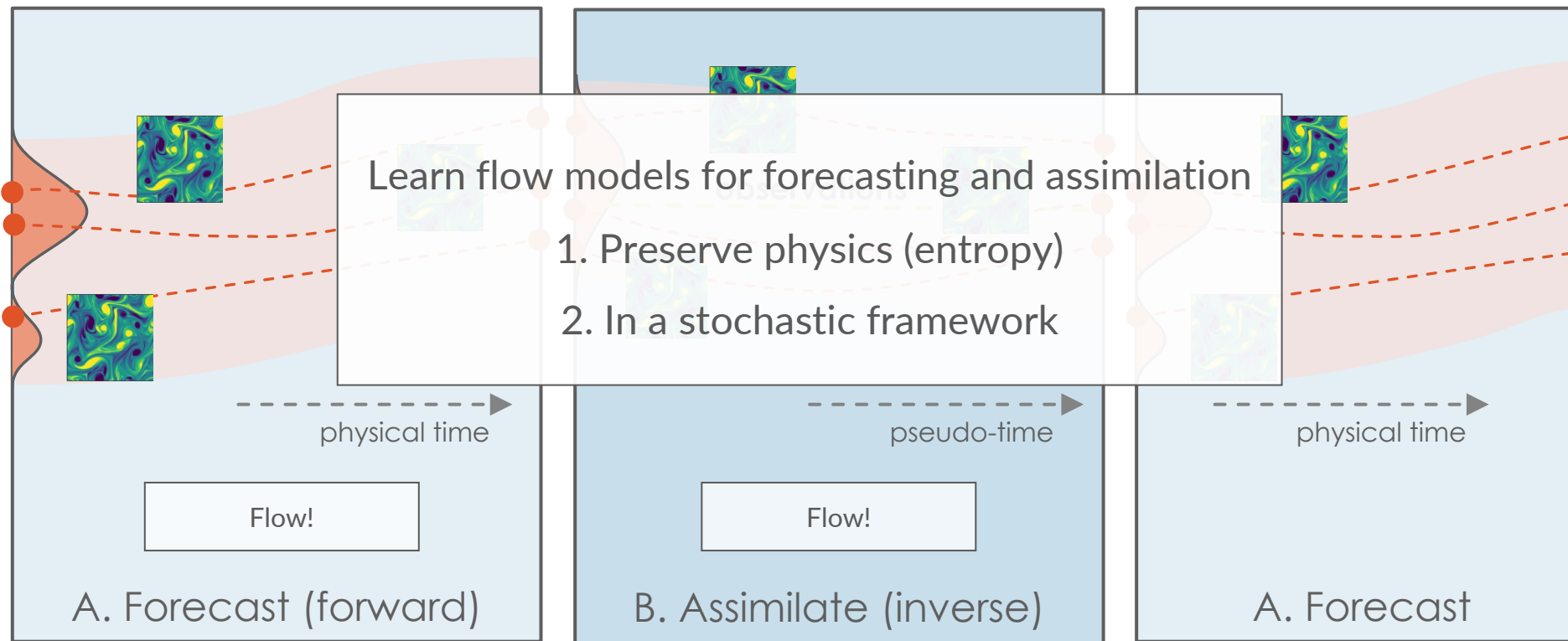
PhD candidates & postdocs

Staff

Fluid flows in energy applications



Summary: probabilistic forecasting and assimilation



A. Fluid flow model

True dynamics

Navier-Stokes (non-linear PDE)

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ p \mathbf{I} + \rho \mathbf{v} \otimes \mathbf{v} \\ \mathbf{v}(E+p) \end{pmatrix} = \nabla \cdot \begin{pmatrix} 0 \\ \boldsymbol{\tau} \\ \boldsymbol{\tau} \cdot \mathbf{v} + \mathbf{q} \end{pmatrix}$$

Reduce dimension:

1. Discretize
2. Filter: remove small scales
3. Close (e.g. neural net)

Learnt model

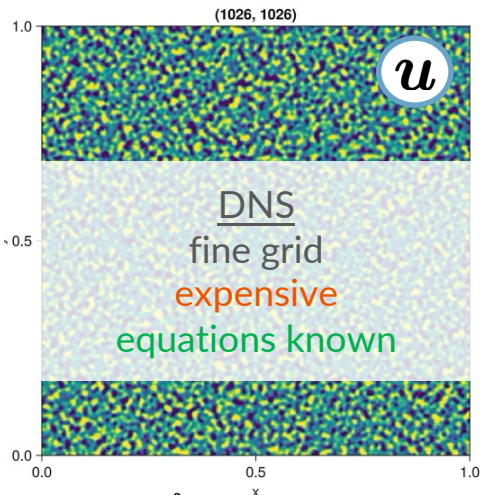
Neural LES model

$$\frac{d\bar{\mathbf{u}}}{dt} = \mathbf{f}(\bar{\mathbf{u}}) + \mathbf{m}(\bar{\mathbf{u}}; \theta)$$

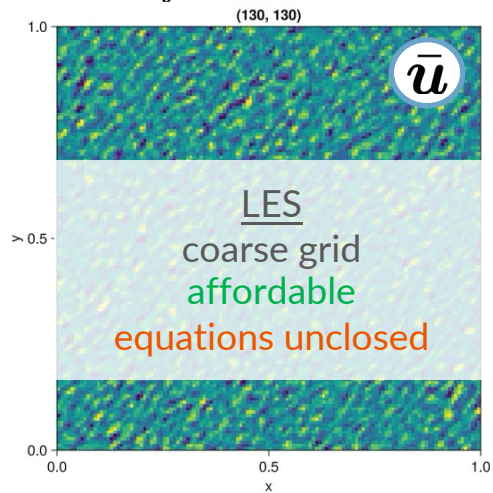
Structure (entropy)

Stable and physical solutions

$$s = -\rho \ln \left(\frac{p}{\rho^\gamma} \right) \quad \frac{d}{dt} \int_{\Omega} s \, d\Omega \leq 0$$



$$\bar{\mathbf{u}} = \int \mathbf{u}(\xi, t) G(x, \xi) d\xi$$



The closure problem - interpretations

DNS: \mathbf{u}

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u})$$

LES: $\bar{\mathbf{u}}$

$$\frac{d\bar{\mathbf{u}}}{dt} = \mathbf{f}(\bar{\mathbf{u}}) + \mathbf{m}(\bar{\mathbf{u}}; \theta)$$

$$\mathbf{m}(\bar{\mathbf{u}}; \theta) \approx \mathcal{C}(\bar{\mathbf{u}}, \mathbf{u}) = \overline{\nabla \cdot (\mathbf{u} \otimes \mathbf{u})} - \nabla \cdot (\bar{\mathbf{u}} \otimes \bar{\mathbf{u}})$$

- Learning missing physics (model discovery, model error)
- PDE-constrained optimization problem: minimize loss function s.t. PDE holds

$$\mathcal{L}_{\theta}^{\text{prio}}(\bar{\mathbf{u}}^*, \mathbf{u}^*) = \|\mathbf{m}(\bar{\mathbf{u}}^*; \theta) - \mathbf{C}(\mathbf{u}^*, \bar{\mathbf{u}}^*)\|^2$$

$$\mathcal{L}_{\theta}^{\text{post}}(\bar{\mathbf{u}}_{\theta}, \bar{\mathbf{u}}^*) = \|\bar{\mathbf{u}}_{\theta} - \bar{\mathbf{u}}^*\|^2$$

- Inverse problem: non-uniqueness, ill-posed

SciML approaches for closure models

Foundations of Data Science



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SCIENTIFIC MACHINE LEARNING FOR CLOSURE MODELS IN MULTISCALE PROBLEMS: A REVIEW

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ROMIT MAULIK^{✉3} AND SHADY E. AHMED^{✉2}

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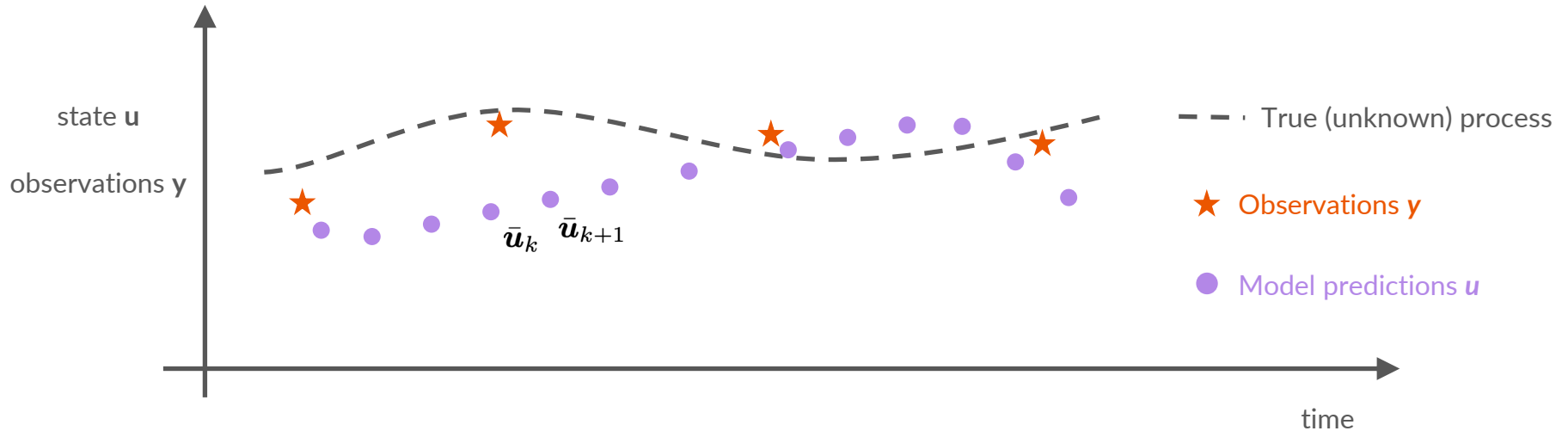
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Westgate Building, University Park, 16802, PA, USA

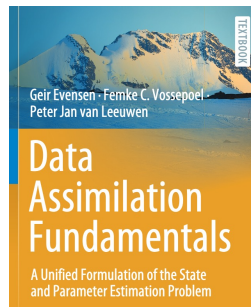
ABSTRACT. Closure problems are omnipresent when simulating multiscale systems, where some quantities and processes cannot be fully prescribed despite their effects on the simulation's accuracy. Recently, scientific machine learning approaches have been proposed as a way to tackle the closure problem, combining traditional (physics-based) modeling with data-driven (machine-learned) techniques, typically through enriching differential equations with neural networks. This paper reviews the different reduced model forms, distinguished by the degree to which they include known physics, and the different objectives of a priori and a posteriori learning. The importance of adhering to physical laws (such as symmetries and conservation laws) in choosing the reduced model form and choosing the learning method is discussed. The effect of spatial and temporal discretization and recent trends toward discretization-invariant models are reviewed. In addition, we make the connections between closure problems and several other research disciplines: inverse problems, Mori-Zwanzig theory, and multi-fidelity methods. In conclusion, much progress has been made with scientific machine learning approaches for solving closure problems, but many challenges remain. In particular, the generalizability and interpretability of learned models is a major issue that needs to be addressed further.

Data assimilation

- The learned model $\mathbf{m}(\bar{\mathbf{u}}; \theta)$ is trained on limited “offline” DNS data and needs calibration
- The state might need corrections, too



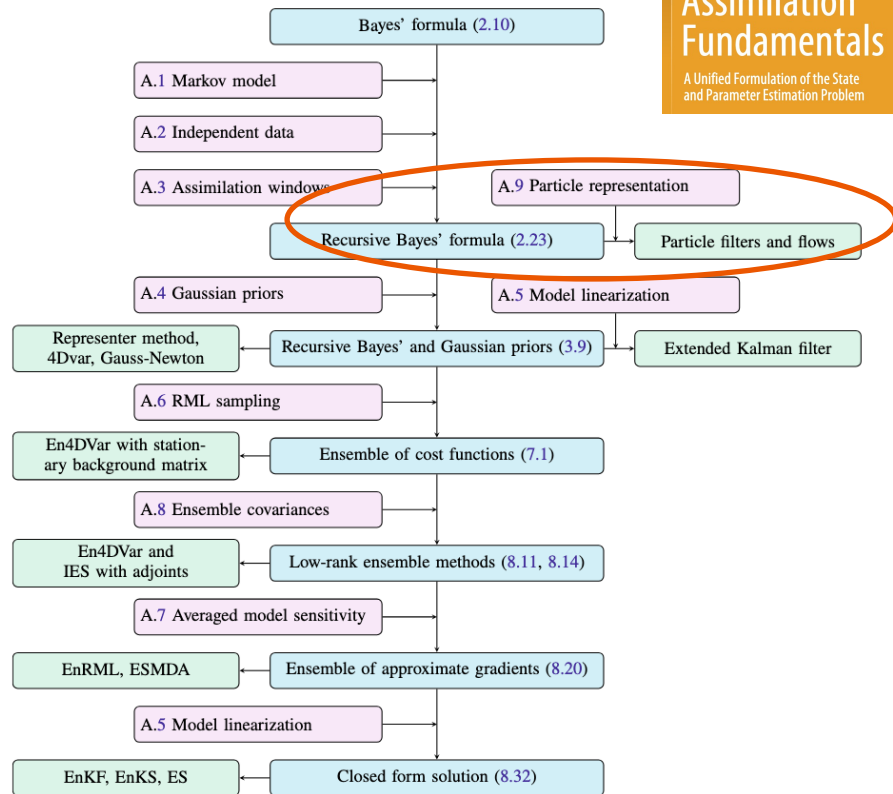
Data assimilation



- Interested in **filtering distribution**:

$$p(\bar{\mathbf{u}}^{n+1} | \mathbf{y}^{1:n+1}) \propto p(\mathbf{y}^{n+1} | \bar{\mathbf{u}}^{n+1}) p(\bar{\mathbf{u}}^{n+1} | \mathbf{y}^{1:n})$$

- Data assimilation = Bayesian inference
- Use particles, solve Bayes in pseudo-time



B. Data assimilation

True dynamics

Bayes -> Fokker-Planck (linear!)

$$\frac{\partial p_\tau}{\partial \tau} + \nabla \cdot (p_\tau \mathbf{c}) = 0 \quad \mathbf{c} = \nabla \ln \left(\frac{q(\bar{\mathbf{u}})}{p_\tau(\bar{\mathbf{u}})} \right)$$

Reduce dimension

1. Filtering formulation
2. Discretize (particles)
3. Close (kernel)

Learnt model

Particle flow filter, flow matching, neural ODE, ... :

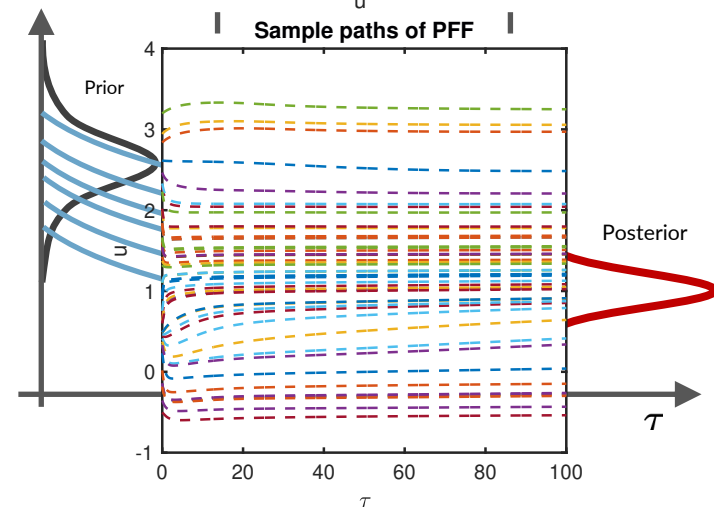
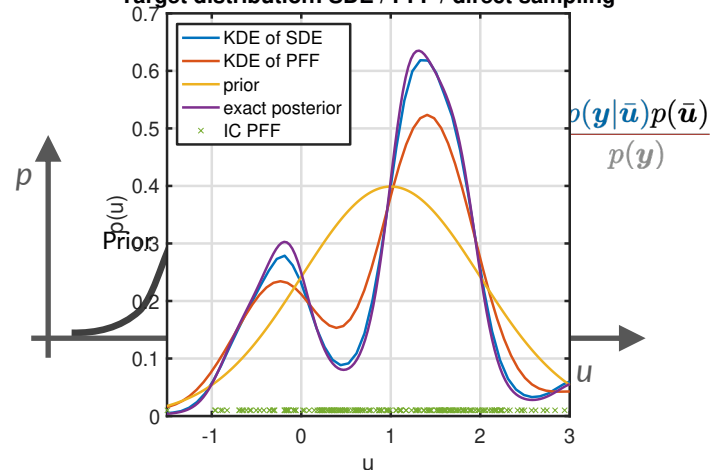
$$\frac{d\bar{\mathbf{u}}}{d\tau} = \mathbf{g}(\bar{\mathbf{u}}; \theta)$$

Structure (entropy)

Distance to posterior (KL-divergence)

$$d = -p_\tau \ln \left(\frac{q}{p_\tau} \right) \quad \frac{dD_{\text{KL}}}{d\tau} = - \int p_\tau \mathbf{c} \cdot \mathbf{c} d\Omega \leq 0$$

Target distribution: SDE / PFF / direct sampling



	A. Fluid flow model (forward)	B. Data assimilation (inverse)
True dynamics	Navier-Stokes $\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ p \mathbf{I} + \rho \mathbf{v} \otimes \mathbf{v} \\ \mathbf{v}(E+p) \end{pmatrix} = \nabla \cdot \begin{pmatrix} 0 \\ \boldsymbol{\tau} \\ \boldsymbol{\tau} \cdot \mathbf{v} + q \end{pmatrix}$	Bayes / Fokker-Planck $\frac{\partial p_{\boldsymbol{\tau}}}{\partial \boldsymbol{\tau}} + \nabla \cdot (p_{\boldsymbol{\tau}} \mathbf{c}) = 0 \quad \mathbf{c} = \nabla \ln \left(\frac{q(\bar{\mathbf{u}})}{p_{\boldsymbol{\tau}}(\bar{\mathbf{u}})} \right)$
	<div style="border: 1px solid black; padding: 5px; display: inline-block;">Filter, discretize, close</div>	<div style="border: 1px solid black; padding: 5px; display: inline-block;">Filter, discretize, close</div>
Learnt model	Neural LES model $\frac{d\bar{\mathbf{u}}}{dt} = \mathbf{f}(\bar{\mathbf{u}}) + \mathbf{m}(\bar{\mathbf{u}}; \theta)$	Particle flow filter (PFF) $\frac{d\bar{\mathbf{u}}}{d\boldsymbol{\tau}} = \mathbf{g}(\bar{\mathbf{u}}; \theta)$
Entropy function	$s = -\rho \ln \left(\frac{p}{\rho^\gamma} \right) \quad \frac{d}{dt} \int_{\Omega} s \, d\Omega \leq 0$	$d = -p_{\boldsymbol{\tau}} \ln \left(\frac{q}{p_{\boldsymbol{\tau}}} \right) \quad \frac{d}{d\boldsymbol{\tau}} \int d \, d\Omega \leq 0$

Structure preservation: entropy



*“You should call it entropy, for two reasons.
In the first place your uncertainty function has been used in statistical mechanics
under that name, so it already has a name.
In the second place, and more important, **no one really knows what entropy is,
so in a debate you will always have the advantage.**”*

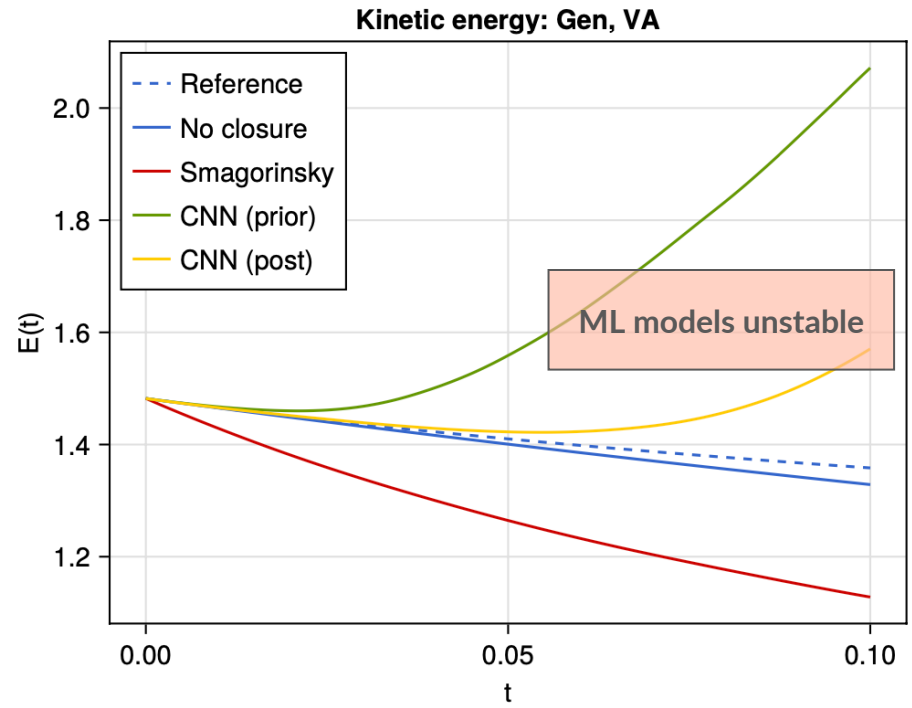
Von Neumann's advice to Shannon

Neural closure models suffer from instability

LES: $\frac{d\bar{u}}{dt} = f(\bar{u}) + m(\bar{u}; \theta)$

Instabilities occur:

- even with a-posteriori training
- even with perfect (DNS) training data
- even without chaotic behavior



Learning flow models

Structure-preserving parameterization

Discretization consistency

NN architectures that preserve symmetries

Hard
constraints

Probabilistic models via stochastic differential equations

Change loss function: a-posteriori learning

Soft
constraints

Preserve structure: entropy

- Conservation law:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \frac{\partial \mathbf{f}^v(\mathbf{u})}{\partial x} \quad \times \eta(\mathbf{u}) = \frac{\partial s}{\partial \mathbf{u}}$$

- Convex

Note “math - physics clash”:

! Mathematical entropy **decreases**

! Energy can be an entropy function

- Pro

stability condition

- Conservation (inviscid):

\int_{Ω}

$$\frac{d\mathcal{S}[\mathbf{u}]}{dt} = 0$$

- Dissipation (shocks/diffusion):

$$\frac{d\mathcal{S}[\mathbf{u}]}{dt} \leq 0$$

$$\mathcal{S}[\mathbf{u}] := \int_{\Omega} s(\mathbf{u}) dx$$

Example: compressible Euler

$$\sigma(\mathbf{u}) = \ln(p/\rho^\gamma)$$

$$p(\mathbf{u}) = \left(E - \frac{1}{2}u^2\right) (\gamma - 1)$$

- PDE (hyperbolic)
- Entropy function
- Entropy variables
- Global **entropy conservation**

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (E + p)u \end{bmatrix} = 0$$

$$s(\mathbf{u}) = \frac{-\rho \sigma}{\gamma - 1}$$

$$\eta(\mathbf{u}) = \frac{\partial s}{\partial \mathbf{u}} = \begin{bmatrix} \frac{\gamma - \sigma}{\gamma - 1} - \frac{\rho u^2}{2p} \\ \rho u / p \\ -\rho / p \end{bmatrix}$$

$$\frac{d\mathcal{S}[\mathbf{u}]}{dt} = \frac{d}{dt} \int_{\Omega} \frac{-\rho \sigma}{\gamma - 1} dx = 0$$

Why entropy? (physics)

Stability

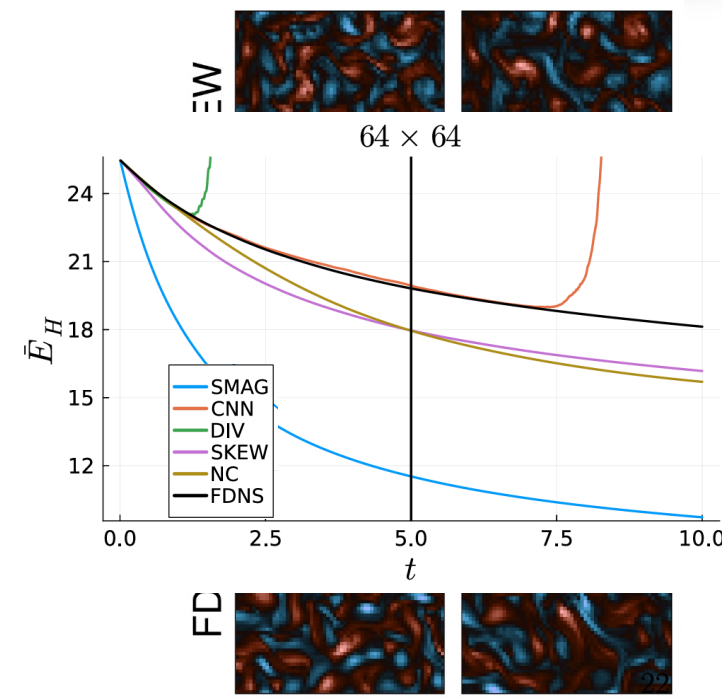
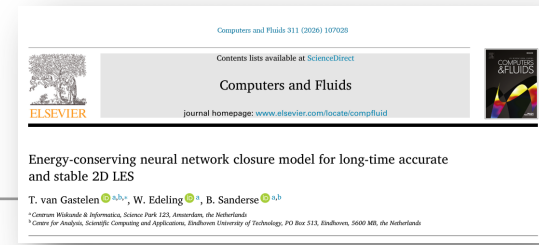
Physically admissible solutions

Structure-preserving closure (1)

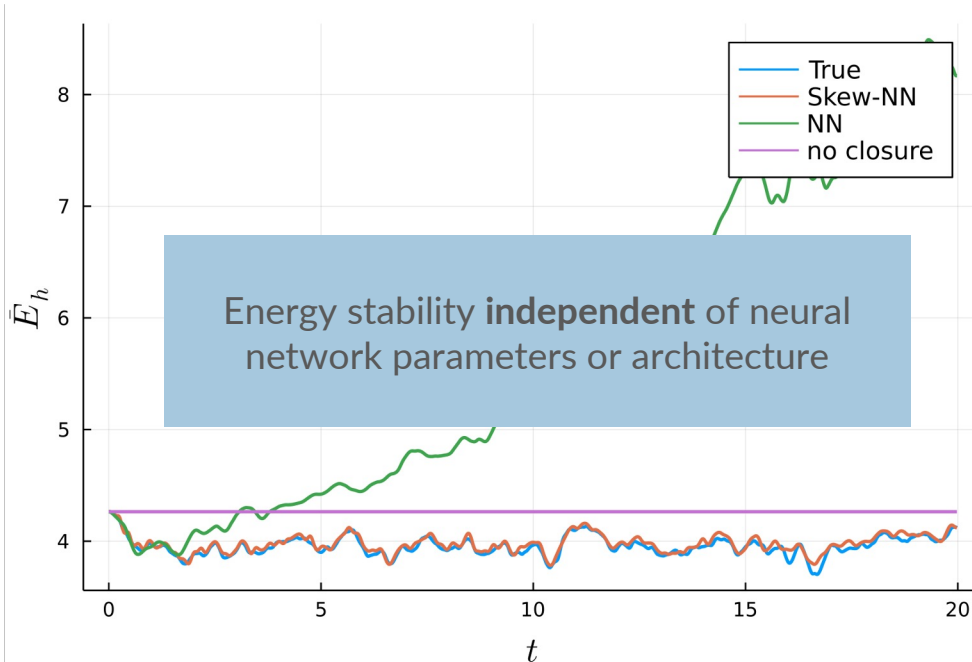
- LES: $\frac{d\bar{\mathbf{u}}}{dt} = \mathbf{f}(\bar{\mathbf{u}}) + \mathbf{m}(\bar{\mathbf{u}}; \theta)$
- New skew-symmetric parameterization:

$$\mathbf{m}(\bar{\mathbf{u}}; \theta) = (\mathbf{K} - \mathbf{K}^T)\bar{\mathbf{u}} - \mathbf{Q}^T \mathbf{Q} \bar{\mathbf{u}}$$
 neural networks: $\mathbf{K} = \mathbf{K}(\bar{\mathbf{u}}; \theta) \quad \mathbf{Q} = \mathbf{Q}(\bar{\mathbf{u}}; \theta)$
- Entropy stability guaranteed: $\bar{\mathbf{u}}^T \mathbf{m}(\bar{\mathbf{u}}; \theta) \leq 0$

Compatibility condition satisfied by construction
- Similar parameterization possible for data assimilation (?)



Structure-preserving closure (2)



Extended neural closure model

$$\frac{d}{dt} \begin{bmatrix} \bar{\mathbf{v}} \\ \mathbf{s} \end{bmatrix} = \begin{bmatrix} \mathbf{f}(\bar{\mathbf{v}}) \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{m}_\theta^v(\bar{\mathbf{v}}, \mathbf{s}) \\ \mathbf{m}_\theta^s(\bar{\mathbf{v}}, \mathbf{s}) \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{m}_\theta^v(\bar{\mathbf{v}}, \mathbf{s}) \\ \mathbf{m}_\theta^s(\bar{\mathbf{v}}, \mathbf{s}) \end{bmatrix} = \mathcal{K}_\theta(\bar{\mathbf{v}}, \mathbf{s}) \begin{bmatrix} \bar{\mathbf{v}} \\ \mathbf{s} \end{bmatrix}$$

Skew-symmetric “matrix” \mathcal{K} leads to exact energy conservation:

$$\frac{d\bar{E}_h(\bar{\mathbf{v}})}{dt} + \frac{d\frac{1}{2}\|\mathbf{s}\|^2}{dt} = 0$$

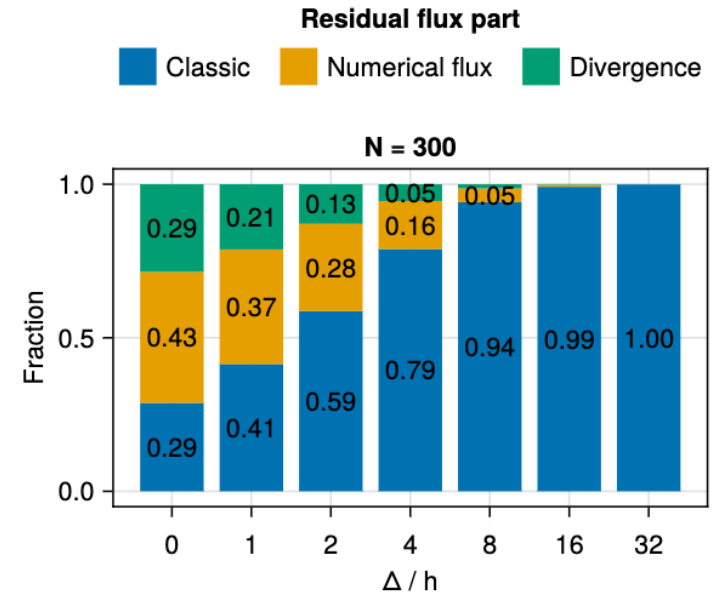
Discretization matters!

- LES is a combined physical-numerical model with **two filters**:
 - A **physical filter**
 - A **discretization-induced filter**

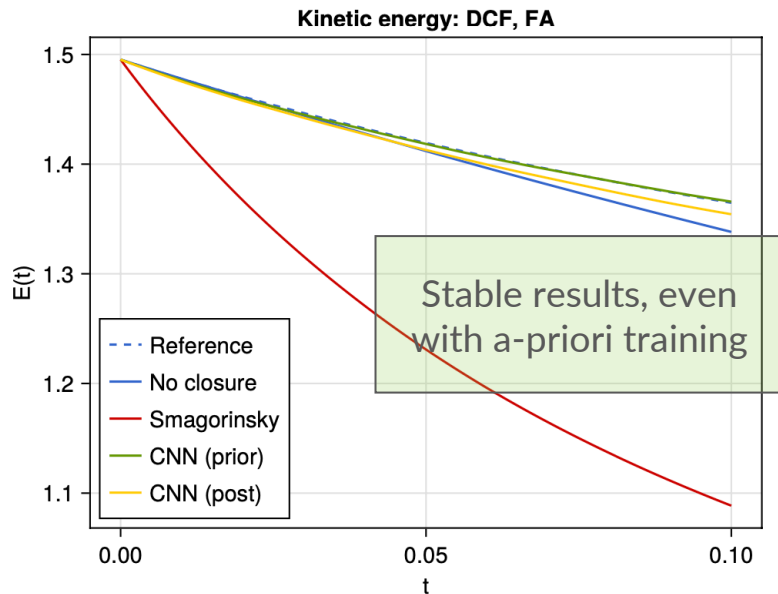
- The closure expression consists of **physical terms and discretization terms**

$$\mathbf{m}(\bar{\mathbf{u}}; \theta) \approx \mathcal{C}(\bar{\mathbf{u}}, \mathbf{u}) = \overline{\nabla \cdot (\mathbf{u} \otimes \mathbf{u})} - \nabla \cdot (\bar{\mathbf{u}} \otimes \bar{\mathbf{u}})$$

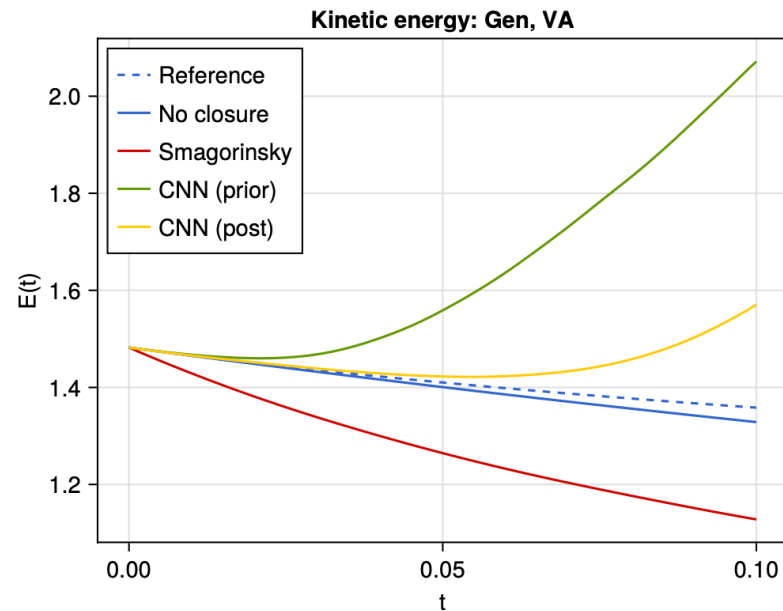
- A good closure model should incorporate both



New discretization-consistent filter



Discretization-consistent filter



Standard filter

Other structure: symmetries

- **Symmetries** can be incorporated into NNs:

- Group-equivariant CNNs
- Graph NNs
- **Tensor-basis NNs:**

$$\mathbf{m}(\bar{\mathbf{u}}; \theta) = \nabla \cdot \tau^{\text{TB}}, \quad \tau^{\text{TB}} = \Delta^2 \sum_k \alpha_k(\lambda) \mathbf{T}^{(k)}$$

- **Many open questions**

- Which symmetries are most important?
- Continuous vs. discrete symmetries

Harnessing Equivariance: Modeling Turbulence with Graph Neural Networks
Marius Kurz^{a*}, Andrea Beck^b, Benjamin Sandese^{a,c}

PHYSICS OF FLUIDS 29, 015105 (2017)

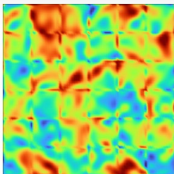
Physical consistency of subgrid-scale models for large-eddy simulation of incompressible turbulent flows

Comparison of data-driven symmetry-preserving closure models for large-eddy simulation

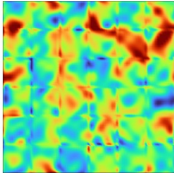
Syver Døving Agdestein^{a,b*}, Benjamin Sandese^b

^aScientific Computing Group, Centrum Wiskunde & Informatica, Science Park 121, Amsterdam, 1098 XG, The Netherlands
^bCentre for Analysis, Scientific Computing and Applications, Delft University of Technology, PO Box 512, Delft, 2600 MB, The Netherlands

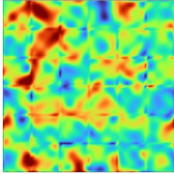
U_0



↓ $\Delta t = 10$

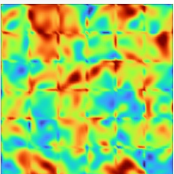


↓ $\rho_{\frac{\pi}{2}}(\cdot)$

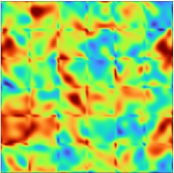


$\rho_{\frac{\pi}{2}}(\mathcal{T}_{\mathcal{M}}(U_0))$

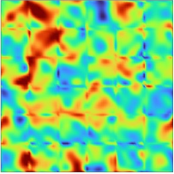
U_0



↓ $\rho_{\frac{\pi}{2}}(\cdot)$



↓ $\Delta t = 10$



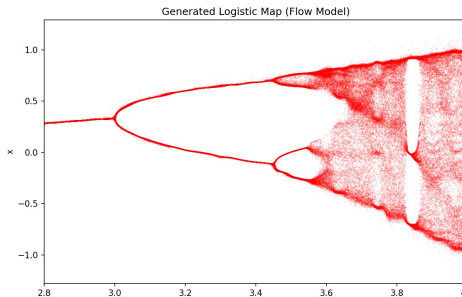
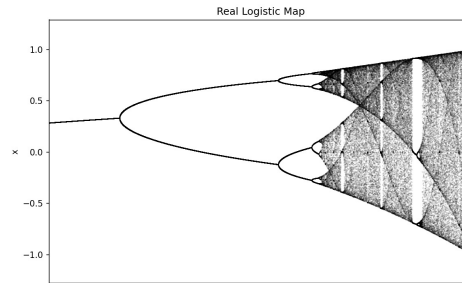
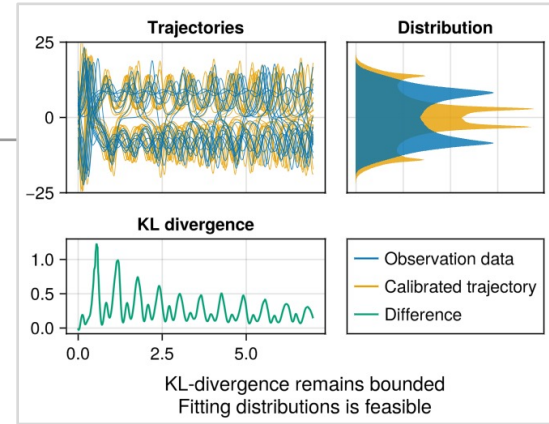
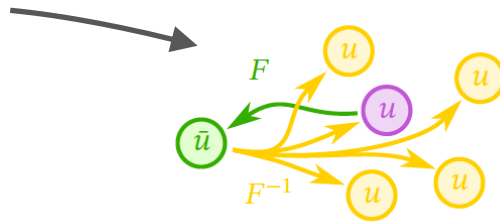
$\mathcal{T}_{\mathcal{M}}(\rho_{\frac{\pi}{2}}(U_0))$

=

Structure-preserving stochastic models

Why stochastic?

- Turbulence is chaotic, interested in **statistics**
- Effect of **non-uniqueness**
- **Uncertainty quantification**
- **Model missing physics**
- Explore distributions, bifurcations



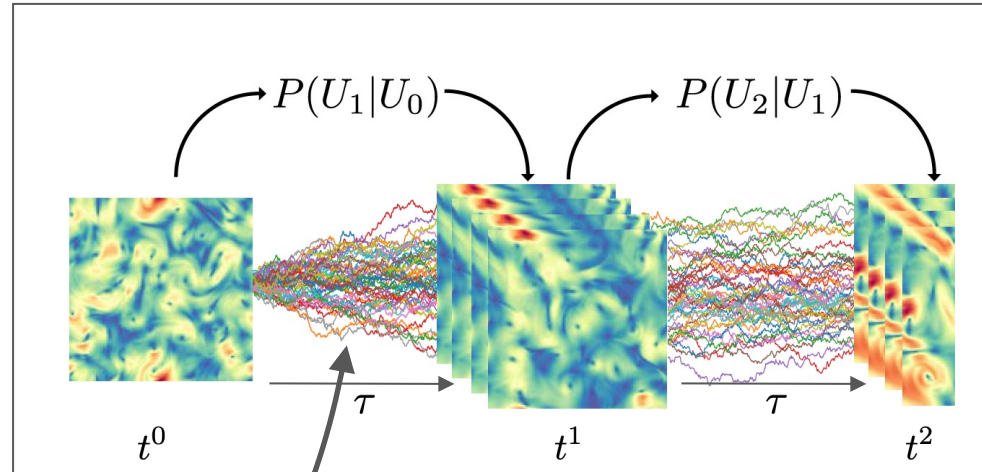
Stochastic forecasting for turbulence

- Each time step, solve an SDE in pseudo-time
- Simulate **ensemble**
- Need to find drift + diffusion

Generative modeling

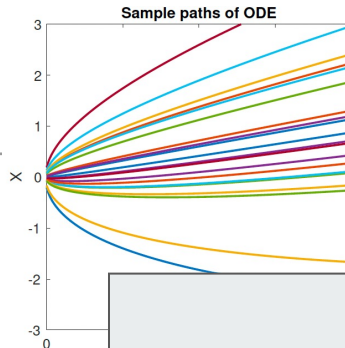
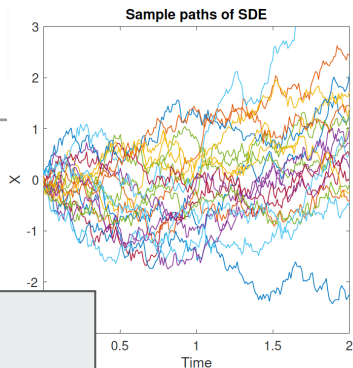


Finding SDEs



$$d\bar{\mathbf{u}}_t = (\mathbf{f}(\bar{\mathbf{u}}_t) + \mathbf{m}_\theta(\bar{\mathbf{u}}_t))dt + \sigma(t)d\mathbf{W}_t$$

The "trinity"



SDE

$$d\mathbf{x}_t = \mathbf{b}(\mathbf{x}_t)dt + g(t)d\mathbf{w}_t$$

ODE

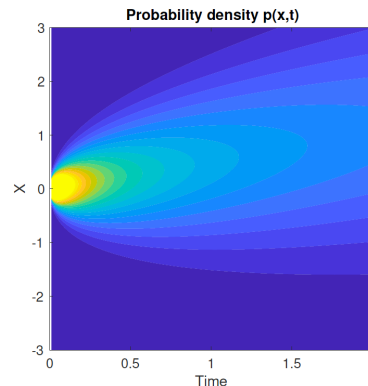
$$\frac{d\mathbf{x}_t}{dt} = \mathbf{c}(\mathbf{x}, t)$$

$$\mathbf{c}(\mathbf{x}, t) = \mathbf{b}(\mathbf{x}) - \frac{1}{2}g^2(t)\nabla_{\mathbf{x}} \ln p(\mathbf{x}, t)$$

implied distribution

Fokker-Planck

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = -\nabla \cdot (\mathbf{b}(\mathbf{x})p(\mathbf{x}, t)) + \nabla \cdot \left(\frac{1}{2}g^2(t)\nabla p(\mathbf{x}, t) \right)$$



Finding the drift in the SDE

Stochastic interpolants (SI) [1]:

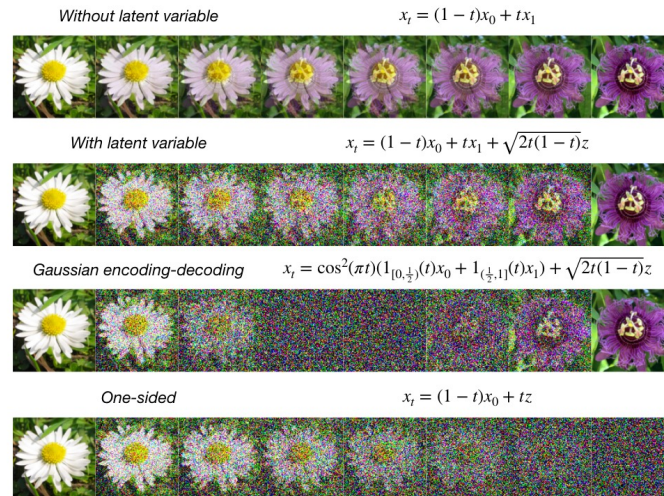
- Interpolate between flow fields
- Related to flow matching [2]

Finding the drift is **similar to a-priori training** (no adjoints etc.):

$$L(\theta) = \int_0^1 \mathbb{E} [|\mathbf{b}_\theta(\mathbf{I}_\tau(\mathbf{x}_0, \mathbf{x}_1), \tau) - \mathbf{R}_\tau(\mathbf{x}_0, \mathbf{x}_1)|^2] d\tau$$

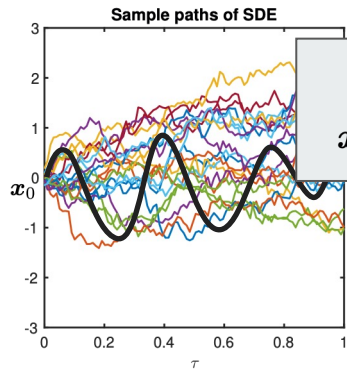
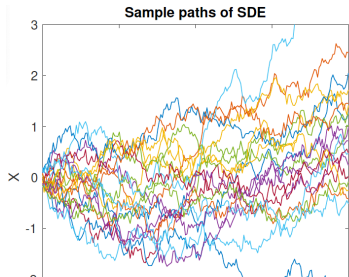
$$\mathbf{x}_\tau \approx \mathbf{I}_\tau(\mathbf{x}_0, \mathbf{x}_1) = \alpha_\tau \mathbf{x}_0 + \beta_\tau \mathbf{x}_1 + \gamma_\tau \mathbf{W}_\tau$$

$$d\bar{\mathbf{u}}_t = (\mathbf{f}(\bar{\mathbf{u}}_t) + \mathbf{m}_\theta(\bar{\mathbf{u}}_t))dt + \sigma(t)d\mathbf{W}_t$$



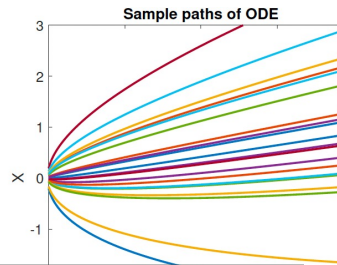
[1] Albergo, Michael S., Nicholas M. Boffi, and Eric Vanden-Eijnden. "Stochastic interpolants: A unifying framework for flows and diffusions." arXiv:2303.08797 (2023).

[2] Y. Lipman, M. Tancik, and J. Lu, Flow matching for generative modelling, arXiv:2210.02747, 2022.



Stochastic interpolant

$$\mathbf{x}_\tau \approx I_\tau(\mathbf{x}_0, \mathbf{x}_1) = \alpha_\tau \mathbf{x}_0 + \beta_\tau \mathbf{x}_1 + \gamma_\tau \mathbf{W}_\tau$$



SDE

$$d\mathbf{x}_t = \mathbf{b}(\mathbf{x}_t)dt + g(t)d\mathbf{w}_t$$

ODE

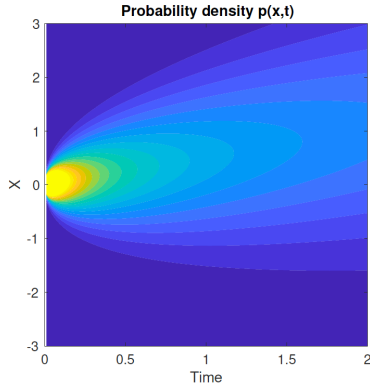
$$\frac{d\mathbf{x}_t}{dt} = \mathbf{c}(\mathbf{x}, t)$$

$$\mathbf{c}(\mathbf{x}, t) = \mathbf{b}(\mathbf{x}) - \frac{1}{2}g^2(t)\nabla_{\mathbf{x}} \ln p(\mathbf{x}, t)$$

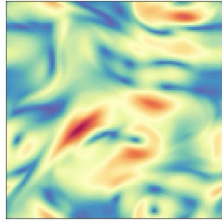
implied distribution

Fokker-Planck

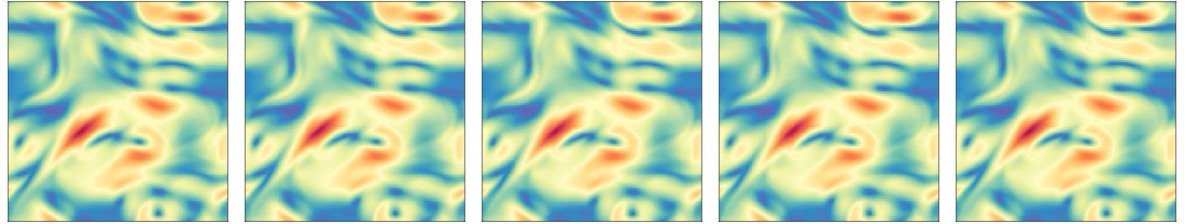
$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = -\nabla \cdot (\mathbf{b}(\mathbf{x})p(\mathbf{x}, t)) + \nabla \cdot \left(\frac{1}{2}g^2(t)\nabla p(\mathbf{x}, t) \right)$$



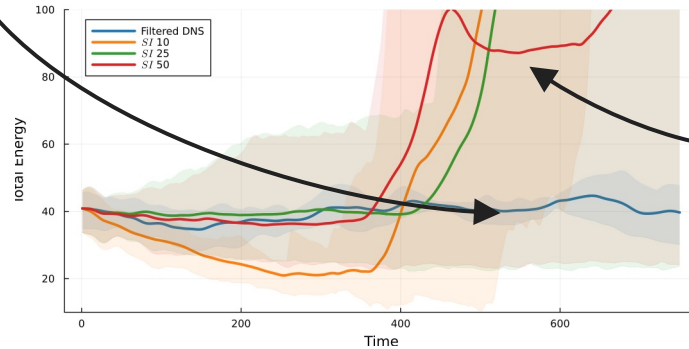
Vanilla stochastic interpolant results



Ground truth
(filtered DNS)



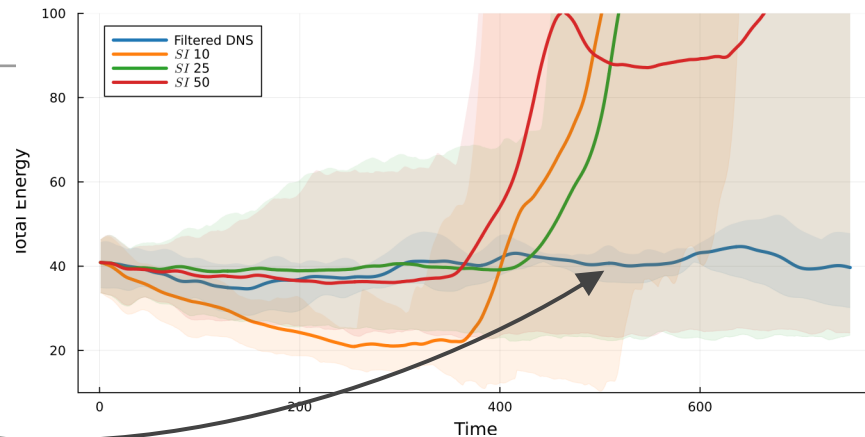
Example realizations



Vanilla SIs have **unphysical energy behavior**

Structure-preserving SI

- Should not enforce energy stability on individual trajectories
 - Flow only statistically energy stable
- **Idea:** tune the α_τ, β_τ coefficients for energy consistency:



$$L_{\text{energy}}(\alpha_\tau, \beta_\tau) = \int_0^1 \mathbb{E}_{(\mathbf{x}_0, \mathbf{x}_1)} \left[d \left[\frac{1}{2} \|\mathbf{I}_\tau(\mathbf{x}_0, \mathbf{x}_1)\|_2^2 \right] - k_\tau(\mathbf{x}_0, \mathbf{x}_1) \right] d\tau$$

Need Ito's lemma

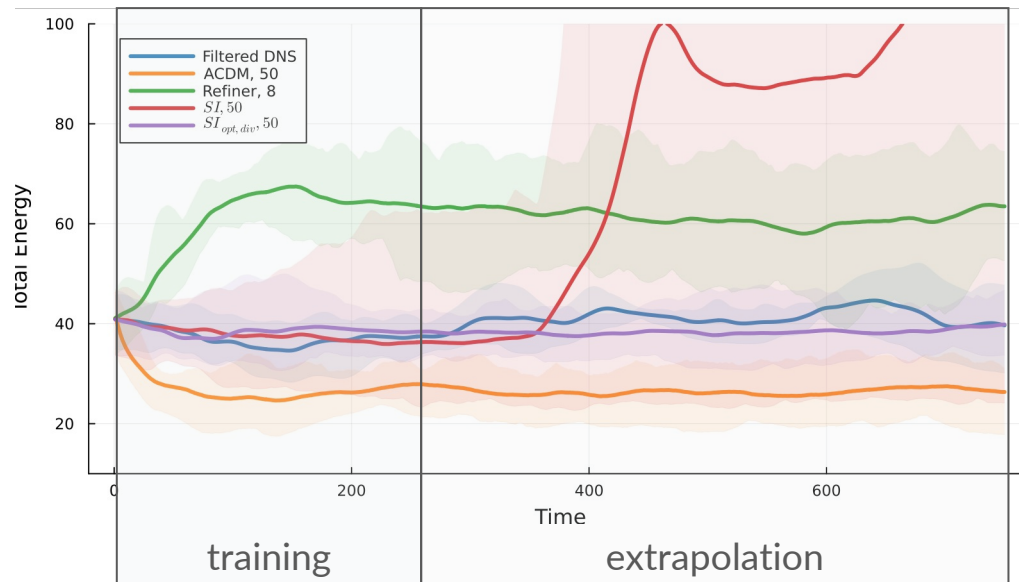
Desired rate of change

Structure-preserving SI

- New parameterization of interpolant promotes stability
- Long roll-outs possible

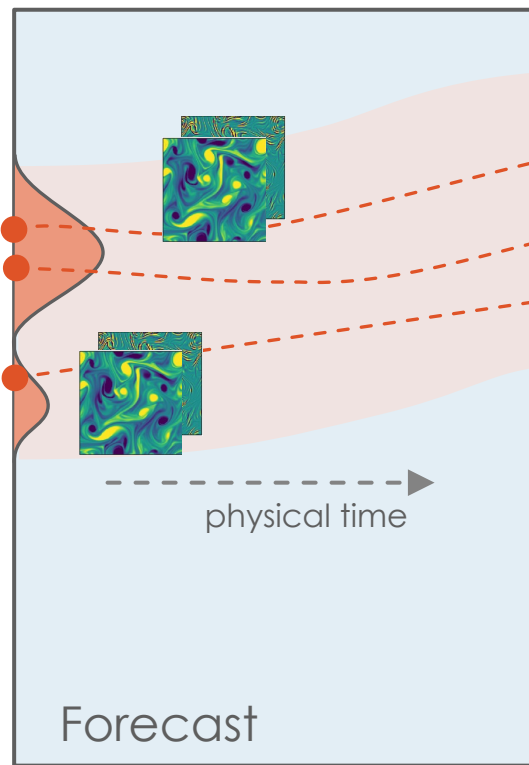
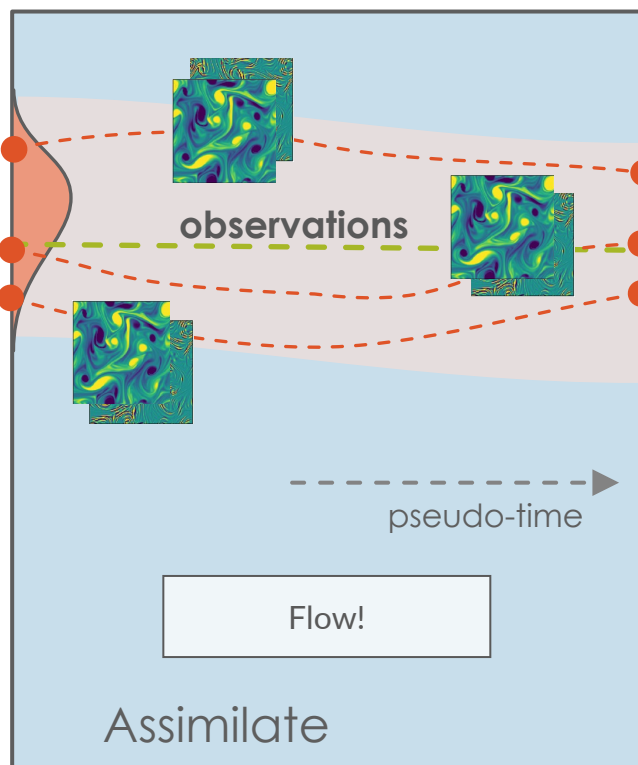
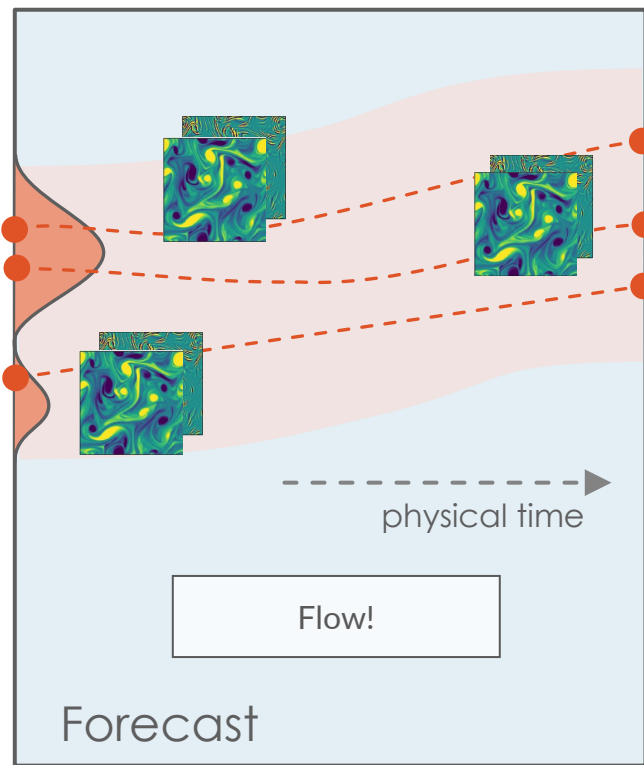
Implications for data assimilation:

- Stochastic interpolants can be adapted to Bayesian inference
- Stable and physics aware inference
- Combined framework for forward and inverse problem



	A. Fluid flow model	B. Data assimilation
True dynamics	Navier-Stokes $\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ p \mathbf{I} + \rho \mathbf{v} \otimes \mathbf{v} \\ \mathbf{v}(E + p) \end{pmatrix} = \nabla \cdot \begin{pmatrix} 0 \\ \boldsymbol{\tau} \\ \boldsymbol{\tau} \cdot \mathbf{u} + \mathbf{q} \end{pmatrix}$	Bayes / Fokker Planck $\frac{\partial p_\tau}{\partial \tau} + \nabla \cdot (p_\tau \mathbf{c}) = 0 \quad \mathbf{c} = \nabla \ln \left(\frac{q(\bar{\mathbf{u}})}{p_\tau(\bar{\mathbf{u}})} \right)$
Learnt model	Neural LES model $\frac{d\bar{\mathbf{u}}}{dt} = \mathbf{f}(\bar{\mathbf{u}}) + \mathbf{m}(\bar{\mathbf{u}}; \theta)$	Particle flow filter $\frac{d\bar{\mathbf{u}}}{d\tau} = \mathbf{g}(\bar{\mathbf{u}}; \theta)$
Structure (entropy)	Stable and admissible solutions	Distance to target (posterior)
Stochastic	Probabilistic (UQ); model error; chaoticity; regularization $d\bar{\mathbf{u}}_t = (\mathbf{f}(\bar{\mathbf{u}}_t) + \mathbf{m}_\theta(\bar{\mathbf{u}}_t))dt + \sigma(t)d\mathbf{W}_t$	Explore phase space; ugly posteriors; bifurcations $d\bar{\mathbf{u}}_\tau = \mathbf{g}_\theta(\bar{\mathbf{u}})d\tau + \sigma(\tau)d\mathbf{W}_\tau$

Everything flows



Connecting to plasma fusion

- Approximations (averaging, collisions, etc.) made in fusion models (Vlasov-Poisson/Maxwell/gyrokinetic) introduce model error that can (should?) be modelled stochastically
- The forward kinetic equation in fusion is a nonlinear FP equation with an associated entropy function
 - > *implied SDE?*
 - > *even tighter integration of forward and inverse problem?*
- Learned (chaotic!) models require calibration (data assimilation), *especially in the case of control*