Structure-preserving learning of embedded, discrete closure models

Benjamin Sanderse, Syver Agdestein, Toby van Gastelen, Henrik Rosenberger, Hugo Melchers

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Woudschoten conference

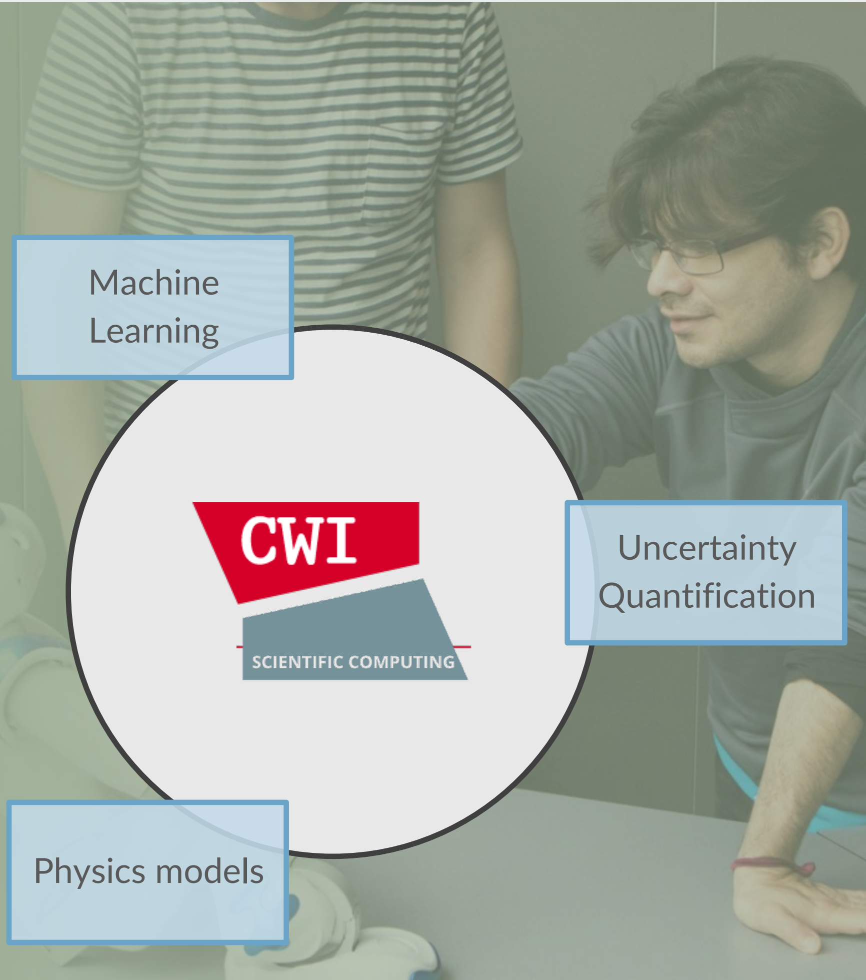
CWI

Scientific Computing group

Predictive science at the interface of ML, UQ and PDEs

Common theme: use physics knowledge to steer design of ML & UQ algorithms

- Closure models
- Reduced order models
- Bayesian inverse problems
- Neural networks



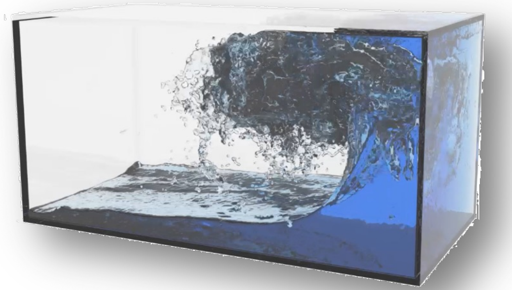
Scientific Computing and Machine Learning

- **SC for ML**
  approximation theory of neural networks; optimization theory; improve and understand NNs

- **SC by ML**
  improve existing SC methods, e.g. use NNs for matrix inversion

- **SC and ML**
  tight integration of SC and ML methods **- focus of this talk**

Typical applications: energy and climate

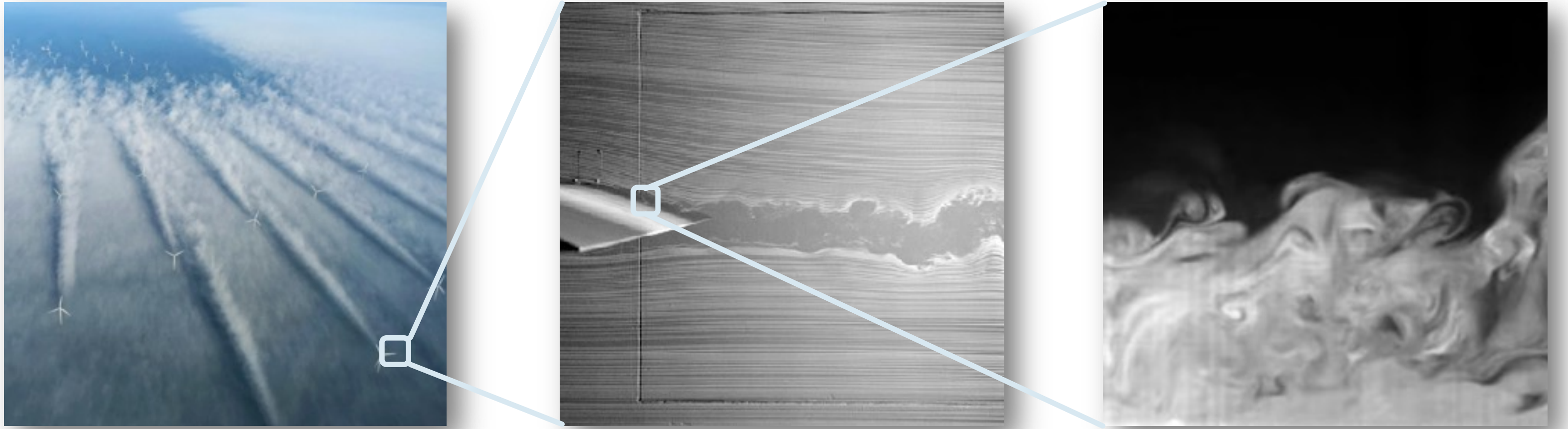


Sloshing of LNG

Offshore wind farms

Weather & climate

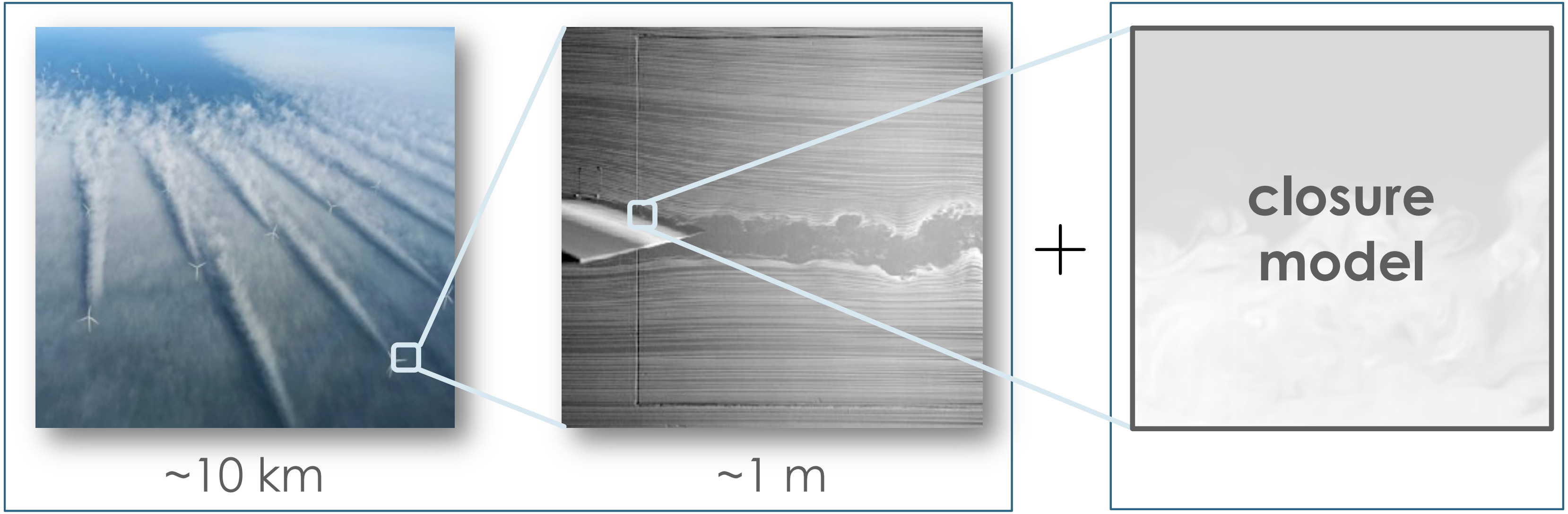
Many applications feature multiscale fluid flows



~10 km ~1 m ~1 mm

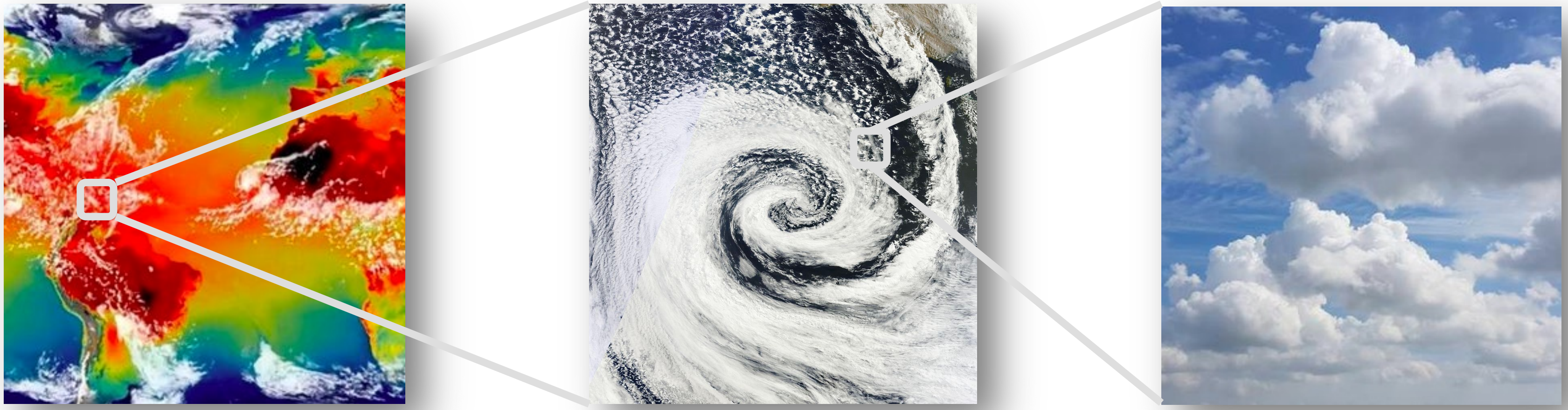
Simulating all scales with a computational model is unfeasible

Accurate and stable closure models needed



Closure model approximates effect of small scales on large scales

Closure problems occur in many fields

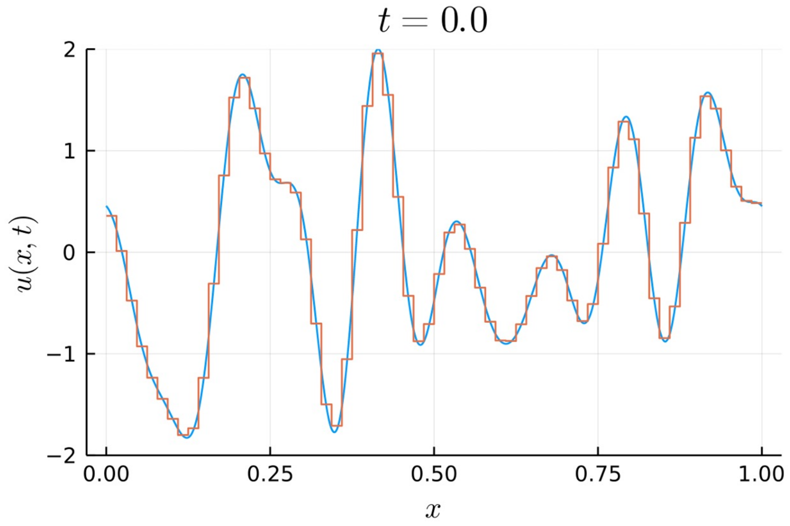


Resolving clouds in climate/weather models: “parameterization”

Example: "closure" with neural network

- Burgers' equation: $$\frac{\partial u}{\partial t} = -\frac{1}{2}\frac{\partial}{\partial x}\left(u^2\right) + \nu\frac{\partial^2 u}{\partial x^2}$$
- Small scales appear for small viscosity ν
- Aim: **accurate solutions on coarse grids**
- "Simple" machine learning approach:

$$\mathbf{u}(t + \Delta t) = \mathbf{u}(t) + \Delta t \cdot \mathrm{NN}(\mathbf{u}(t); \vartheta)$$

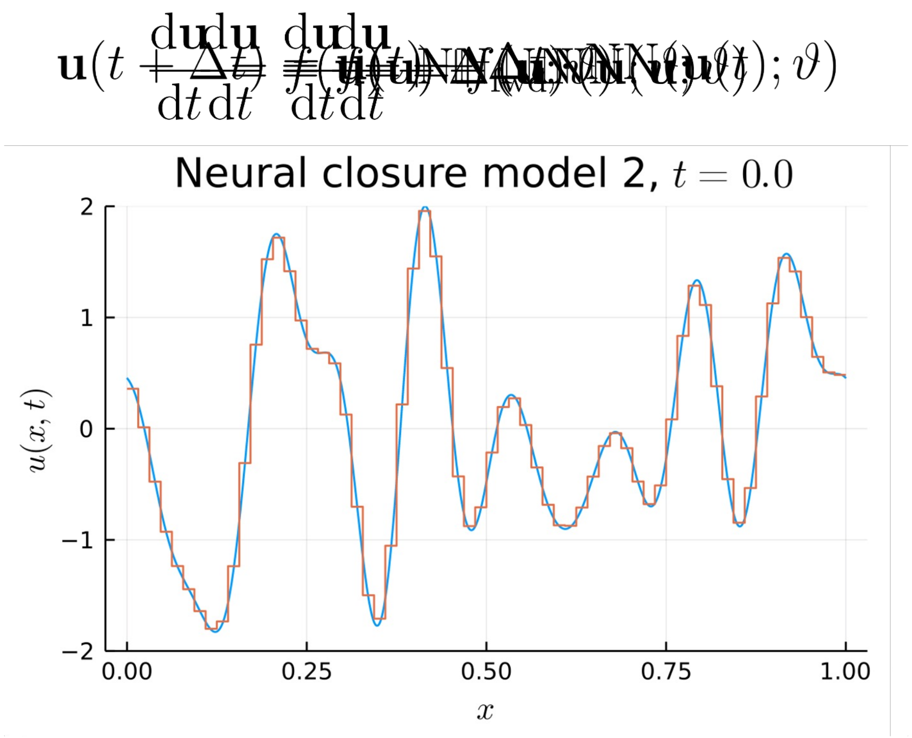


SciML approaches reduce error

increasing structure (“inductive bias”)

- Low-res model (“no closure”):
  0.10
- Basic ML model:
  0.087
- Neural ODE:
  0.041
- Neural closure model:
  0.029
- With momentum conservation:
  0.026

Including physics is most useful for small neural networks



Today’s talk

- **Structure-preserving closure models and stability**
- **Training procedures: derivative fitting vs. trajectory fitting**

“Discretize first” - “Preserve structure” – “Embedded learning”

- **Non-locality** in space and time (Mori-Zwanzig)
- **Stochastic** closure models
- **Reduced order models** and closure

Basics of closure modelling

- We consider PDEs describing many scales, e.g. the Navier-Stokes equations

$$\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{F}(\boldsymbol{u}) \qquad \boldsymbol{F}(\boldsymbol{u}) := -\nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{u}) - \nabla p + \nu \nabla^2 \boldsymbol{u}$$

- NS describes (too) many scales of motion for small viscosity ν

- Reduce range of scales by a **filtering** operation:

$$\bar{\boldsymbol{u}} = \mathcal{A}(\boldsymbol{u}) \qquad \mathcal{A}(\boldsymbol{u}) = \int \boldsymbol{u}(\xi, t) G(x, \xi) \mathrm{d}\xi \qquad \boldsymbol{u}' = \boldsymbol{u} - \bar{\boldsymbol{u}}$$

- **Aim**: use coarser meshes and larger time steps when solving for $\bar{\boldsymbol{u}}$

Basics of closure modelling

- Art: find a **closure model** with parameters θ s.t.

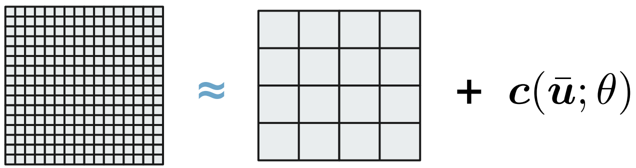
$$\boldsymbol{c}(\bar{\boldsymbol{u}};\theta) \approx \mathcal{C}[\mathcal{A},\mathcal{F}](\boldsymbol{u})$$

- Commutator error often due to nonlinearity, e.g. (Navier-Stokes):

$$\mathcal{C}[\mathcal{A},\mathcal{F}](\boldsymbol{u}) = \overline{\nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{u})} - \nabla \cdot (\bar{\boldsymbol{u}} \otimes \bar{\boldsymbol{u}})$$

- Finding $\boldsymbol{c}(\bar{\boldsymbol{u}};\theta)$ is an inverse problem which can have multiple solutions

- Common form: $\dfrac{\partial \bar{\boldsymbol{u}}}{\partial t} = \boldsymbol{F}(\bar{\boldsymbol{u}}) + \boldsymbol{c}(\bar{\boldsymbol{u}};\theta)$



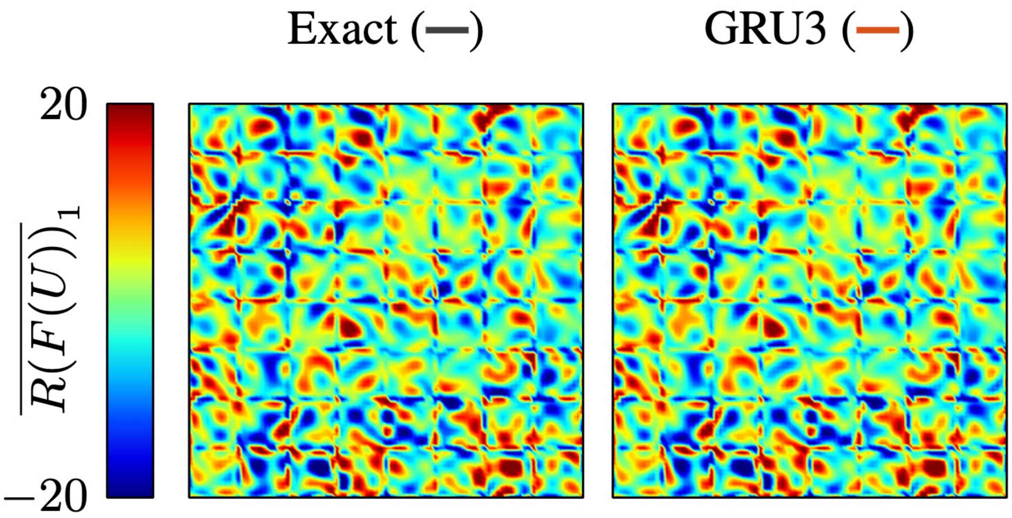
Basics of closure modelling

- Traditionally, closure model are formulated as **closed-form expressions** based on physical arguments
  - Smagorinsky model, gradient model, e.g. $\boldsymbol{c}(\bar{\boldsymbol{u}};\theta) = \nabla \cdot (\nu_T(\bar{\boldsymbol{u}}) S(\bar{\boldsymbol{u}}))$
  - Great interpretability; universal applicability highly limited
- Recent alternative:
  - Use **neural networks** to approximate the commutator error: $\boldsymbol{c}(\bar{\boldsymbol{u}};\theta) = \mathrm{NN}(\bar{\boldsymbol{u}};\theta)$

$$\theta = \mathrm{argmin}_\theta ||\mathrm{NN}(\bar{\boldsymbol{u}}_{\mathrm{ref}};\theta) - \mathcal{C}[\mathcal{A},\mathcal{F}](\boldsymbol{u}_{\mathrm{ref}})||_2^2$$

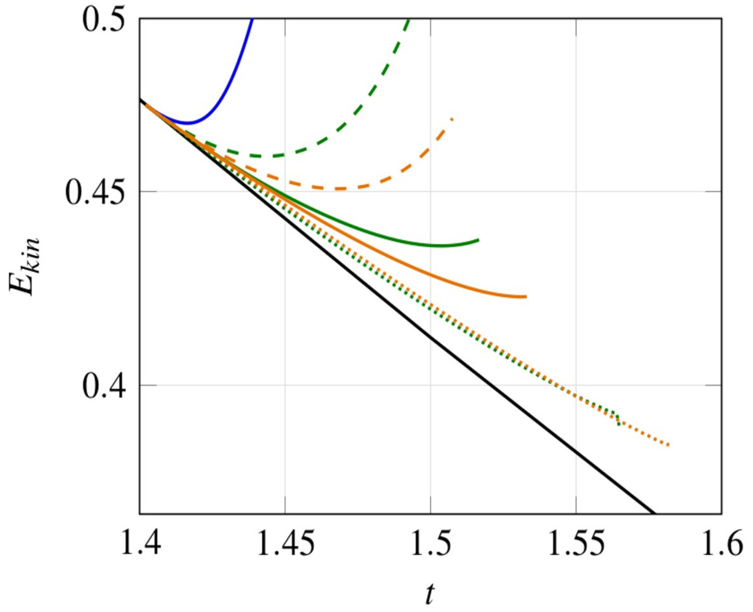
  - Issue: **difficult to get stable results**

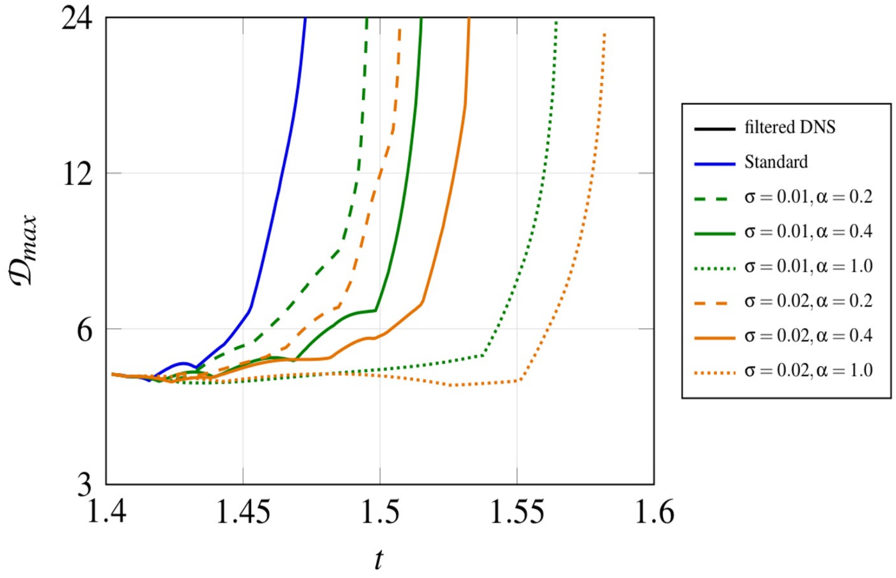
Neural-networks give great match...



Kurz & Beck, “A machine learning framework for LES closure terms”, 2021

… but give instabilities in the dynamical system





Kurz & Beck, “Investigating Model-Data Inconsistency in Data-Informed Turbulence Closure Terms”, 2020

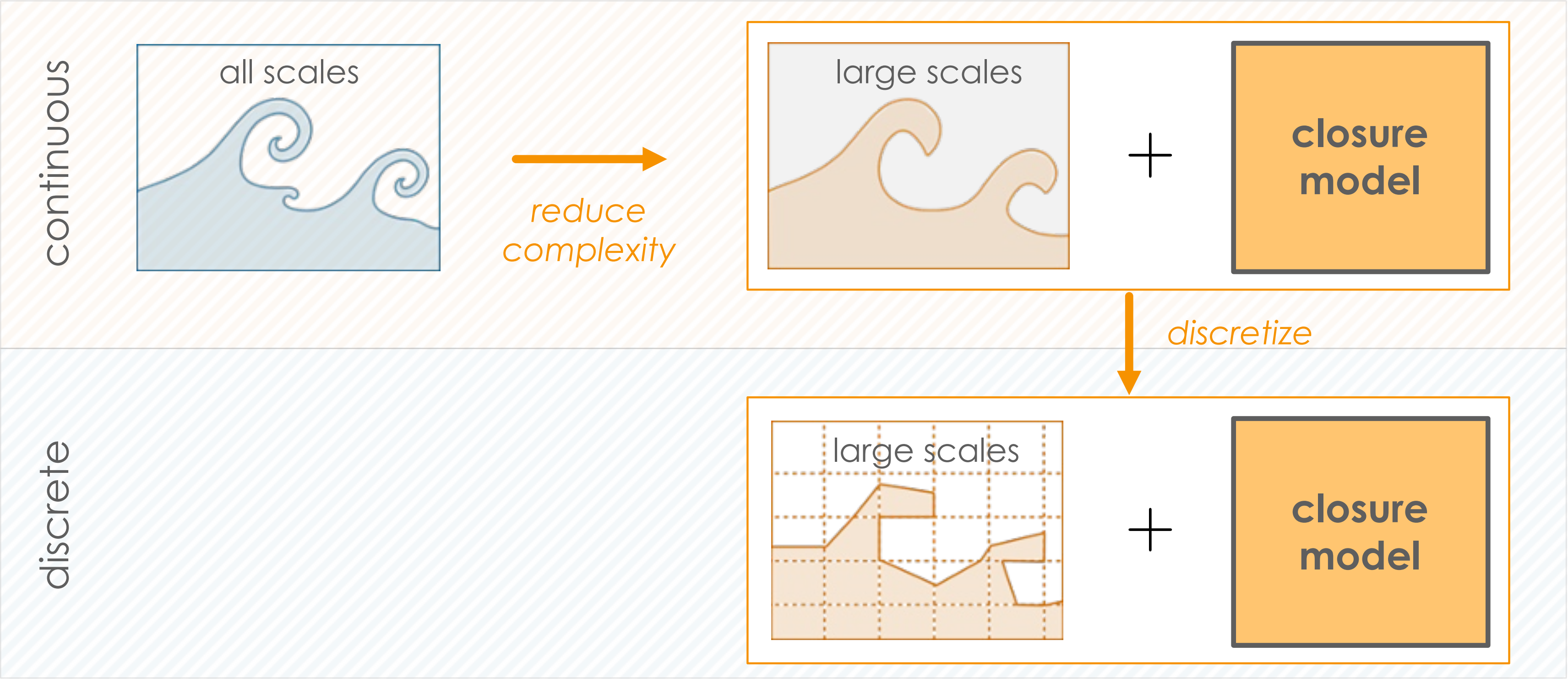
Tackling instability in dynamical systems with NNs

- “**Model-data inconsistency**” and **instability** common problem for ML-based closure models (mismatch training environment and prediction environment)

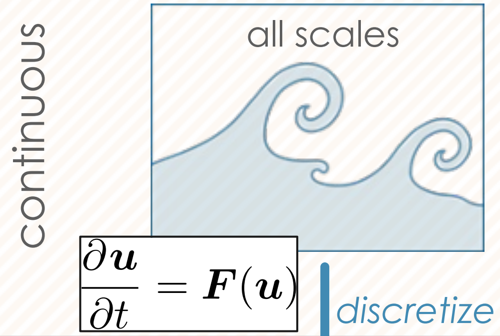
- Recent approaches:
  - Stability training on data with artificial noise (Kurz & Beck, 2021)
  - Minimizing (or eliminating) backscatter (Park & Choi, 2021)
  - Projection onto a stable basis (Beck et al., 2019)
  - Trajectory fitting (List et al., 2022; MacArt et al., 2021)
  - Reinforcement learning (Bae & Koumoutsakos, 2022; Kurz et al. 2022)

Our approach: “discretize first” + “preserve structure”

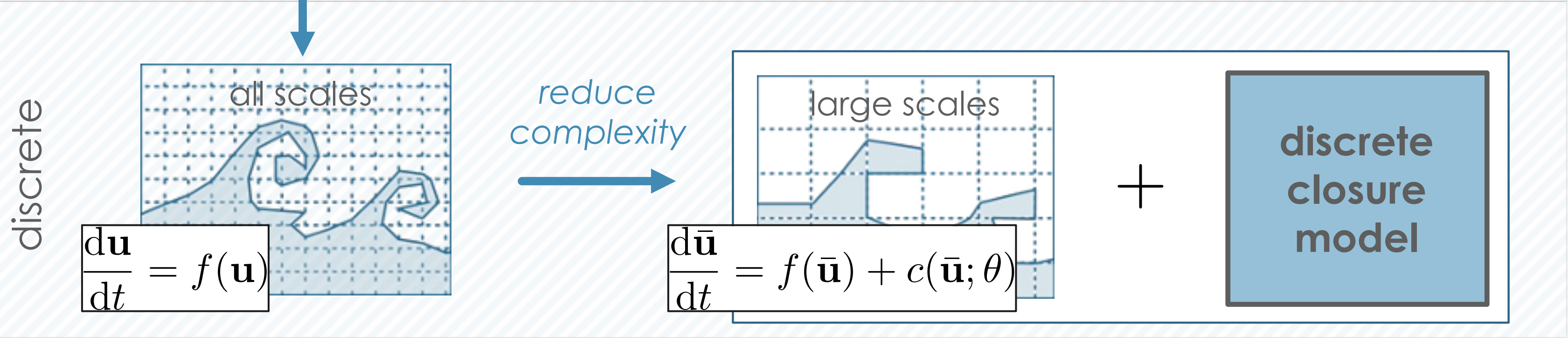
Common approach in closure modelling



New approach: discretize first



- Consistency training data and prediction environment
- Inverse problem easier on discrete level
- Closure models tailor-made to discretization
- Less regularity requirements
- Easier to handle boundary conditions



Example of “discretize first”: inferring a parameter

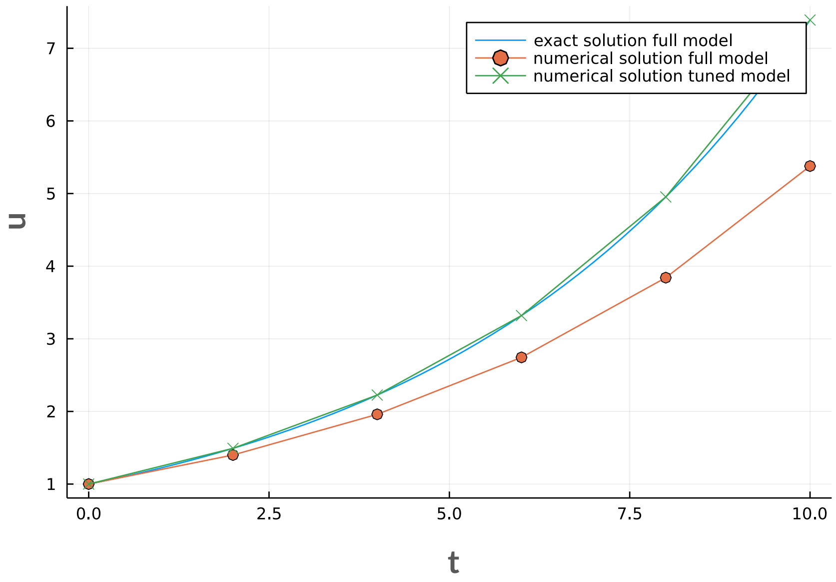
- Problem: find θ in the ODE $$\frac{\mathrm{d}u}{\mathrm{d}t} = \theta u$$
- Given: initial condition and reference solution $u_{\mathrm{ref}}(T)$
- Forward Euler discretization $$u^n = (1 + \Delta t\theta)^n u(0)$$
- Minimize loss function $$\begin{aligned}\mathcal{L}(u^n(\theta), u_{\mathrm{ref}}(T)) &= (u^n - u_{\mathrm{ref}}(T))^2 \\ &= ((1 + \Delta t\theta)^n u(0) - u_{\mathrm{ref}}(T))^2\end{aligned}$$

Example of “discretize first”: inferring a parameter

- True value: $\theta^* = 0.2$
- Forward Euler:

$$\theta_{\mathrm{FE}} = \frac{1}{\Delta t}\left(\left(\frac{u_{\mathrm{ref}}(T)}{u(0)}\right)^{1/n} - 1\right) \approx 0.245$$

- The “incorrect” parameter gives the **exact solution: it corrects the discretization error**



Example of “discretize first”: inferring a parameter

- Problem: find θ in the ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & \theta \\ -\theta & 0 \end{pmatrix}}_{A(\theta)} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

- Given: initial condition and reference solution $u_{\mathrm{ref}}(T)$

- RK3 discretization

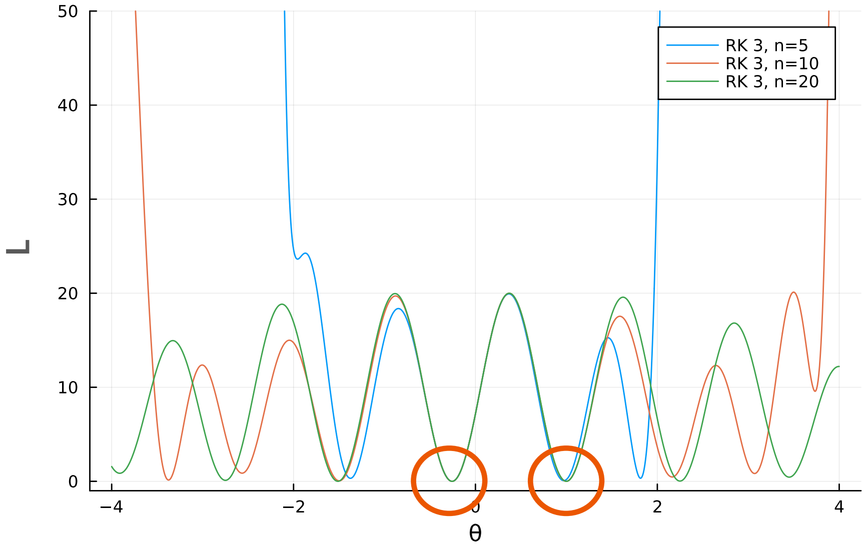
$$u^n = (I + \Delta t A(\theta) + \frac{1}{2}\Delta t^2 A(\theta)^2 + \frac{1}{6}\Delta t^3 A(\theta)^3)^n u(0)$$

- Minimize loss function

$$\mathcal{L}(u^n(\theta), u_{\mathrm{ref}}(T)) = \|u^n(\theta) - u_{\mathrm{ref}}(T)\|_2^2$$

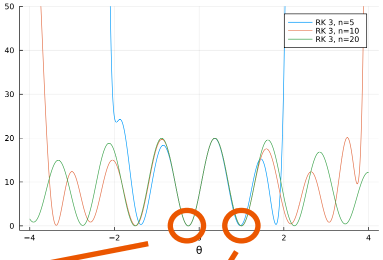
Example of "discretize first": inferring a parameter

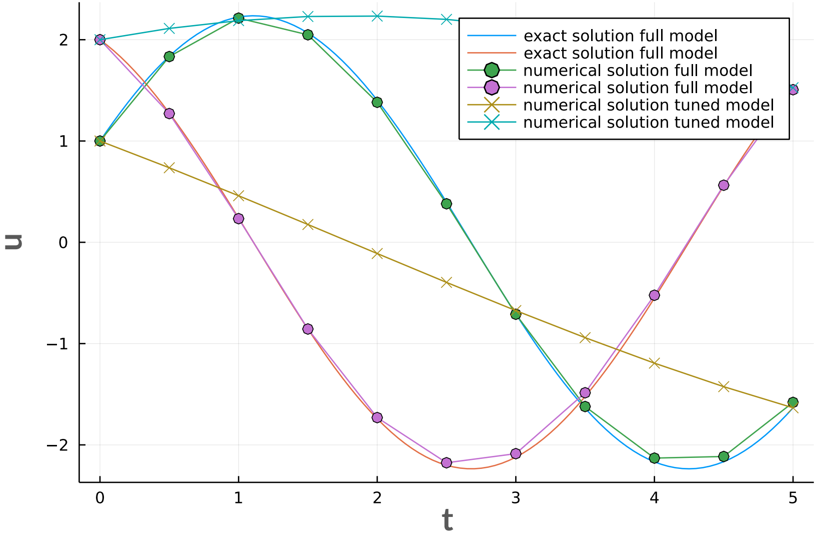
- Loss function high-order polynomial in θ
- Multiple local minima - *aliasing*
- Number of minima *increases* with number of time steps and with order of RK scheme

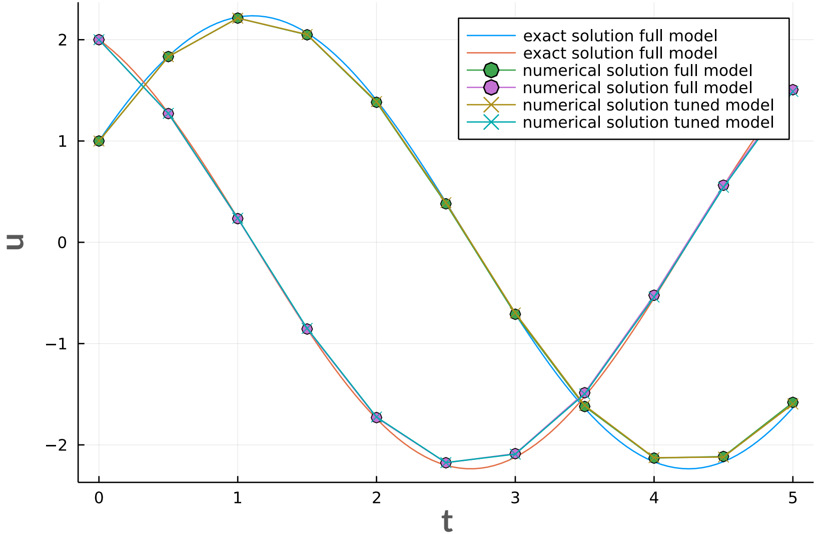


Inferring a parameter

- Loss function choice important
- Local minima can be tricky







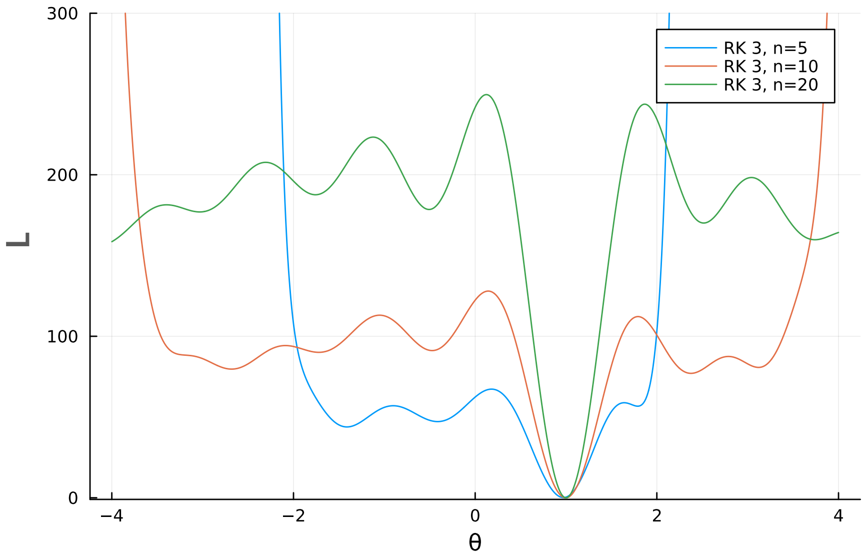
Example of "discretize first": inferring a parameter

- Adapt loss function

$$\mathcal{L}(u^n(\theta), u_{\text{ref}}) = \sum_{i=1}^{N_t} \|u^i(\theta) - u_{\text{ref}}(t_i)\|_2^2$$

- Clear global minimum

- We call this "**trajectory fitting**" – (more about this later)



Examples of preserving structure

- ODE formulation ("neural ODE")

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = \mathrm{NN}(\bar{\mathbf{u}};\theta)$$

- Closure model form ("neural closure model")

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = f(\bar{\mathbf{u}}) + \mathrm{NN}(\bar{\mathbf{u}};\theta)$$

- Conservation

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = f(\bar{\mathbf{u}}) + \nabla \cdot \mathrm{NN}(\bar{\mathbf{u}};\theta)$$

- Translation invariance

CNN architecture

- **Energy conservation**

Energy conservation implies stability

- Many PDEs, including Navier-Stokes, possess **secondary conservation laws**, such as energy or entropy, which give a **stability bound**

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{u}) = -\nabla p + \nu \nabla^2 \boldsymbol{u}$$

$$\Longrightarrow$$

$$\frac{\mathrm{d}K}{\mathrm{d}t} = -\nu \int_\Omega \nabla \boldsymbol{u} : \nabla \boldsymbol{u} \, \mathrm{d}\Omega$$

$$K := \frac{1}{2} \int \boldsymbol{u} \cdot \boldsymbol{u} \, \mathrm{d}\Omega$$

Idea: impose a similar structure on the filtered equations

Korteweg - de Vries equation

- Shallow water waves, solitons:

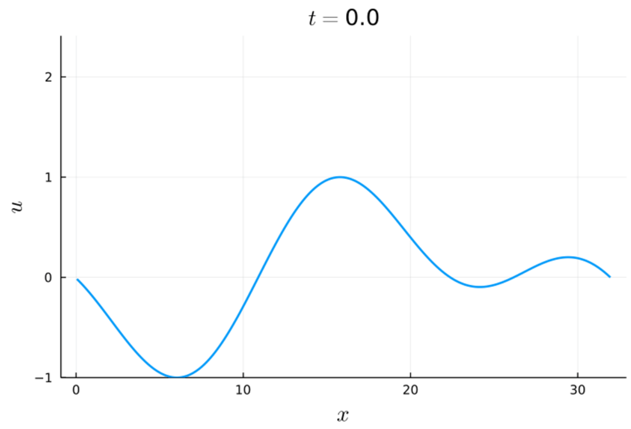
$$\frac{\partial u}{\partial t} + 3\frac{\partial u^2}{\partial x} = -\frac{\partial^3 u}{\partial x^3}$$

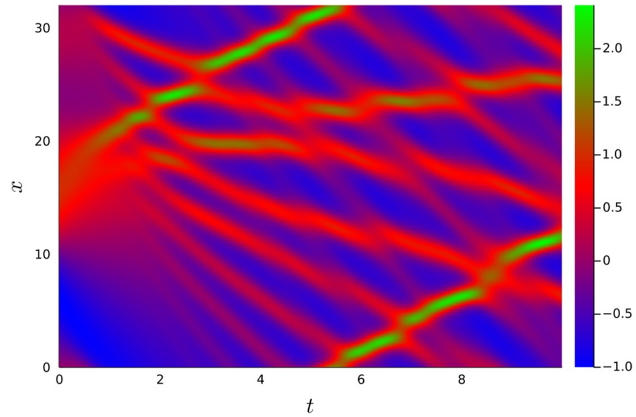
- Energy conservation (periodic BCs):

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\underbrace{\frac{1}{2}\int_\Omega u^2 d\Omega}_{=:E} = 0$$

- Discretized using skew-symmetric scheme:

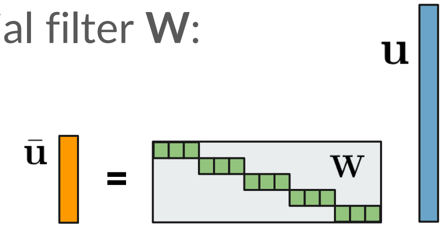
$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = -3\mathbf{G}(\mathbf{u}) - \mathbf{D}_3\mathbf{u} \qquad (\mathbf{u}, \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}) = 0$$



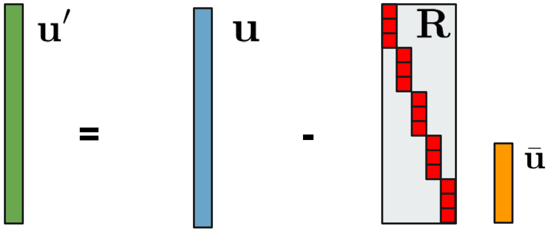


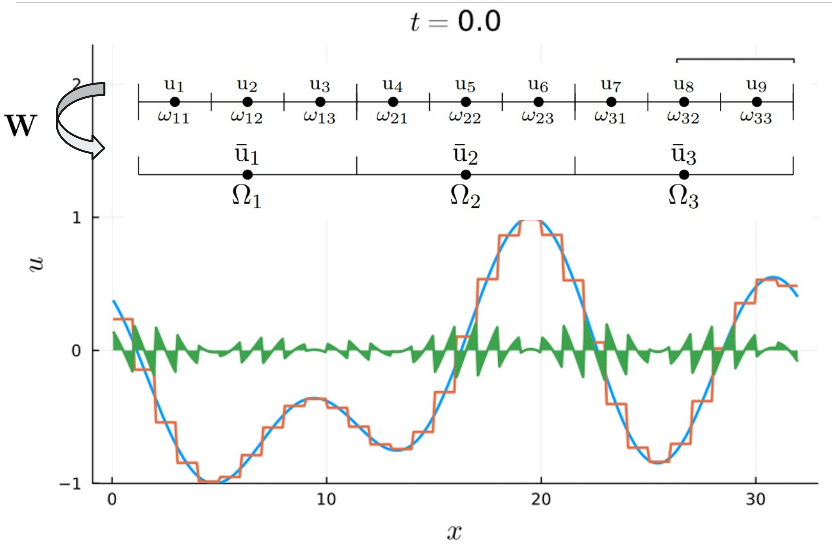
Discrete filtering and reconstruction

- Spatial filter **W**:



- Subgrid-scales defined via reconstruction operator **R**:





subgrid scales important near sharp gradients

Energy decomposition

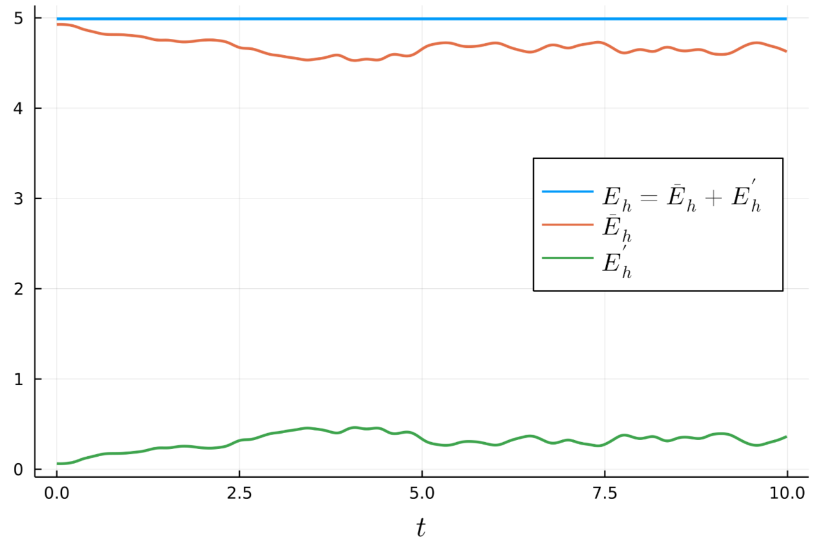
- Since **W R = I**, we can decompose the energy as:

$$E_h = \underbrace{\frac{1}{2}(\bar{\mathbf{u}}, \bar{\mathbf{u}})_\Omega}_{=:\bar{E}_h} + \underbrace{\frac{1}{2}(\mathbf{u}', \mathbf{u}')_\omega}_{=:E'_h}$$

- Time evolution:

$$\frac{\mathrm{d}E_h}{\mathrm{d}t} = \boxed{\frac{\mathrm{d}\bar{E}_h(\bar{\mathbf{u}})}{\mathrm{d}t}} + \boxed{\frac{\mathrm{d}E'_h(\mathbf{u}')}{\mathrm{d}t}} = 0$$

- **To use energy stability we need information about the small scales**



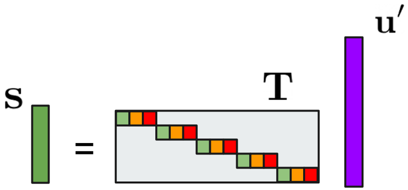
Total energy conserved, **large-scale energy not**

Subgrid compression

- Simulating **u'** is not feasible.
- Replace **u'** by **compressed (coarse-grid) variable s**

$$\frac{1}{2}(\mathbf{s},\mathbf{s})_\Omega \approx E'_h(\mathbf{u}')$$

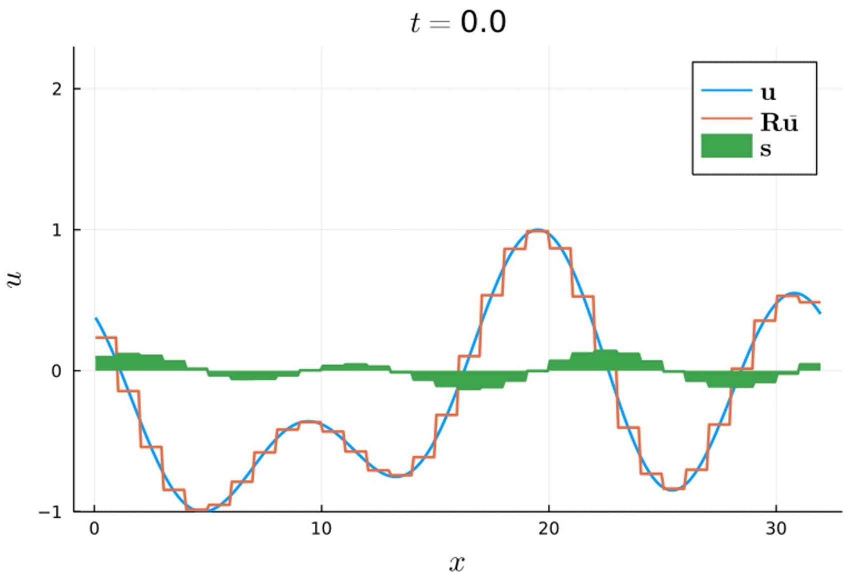
with linear compression **T**



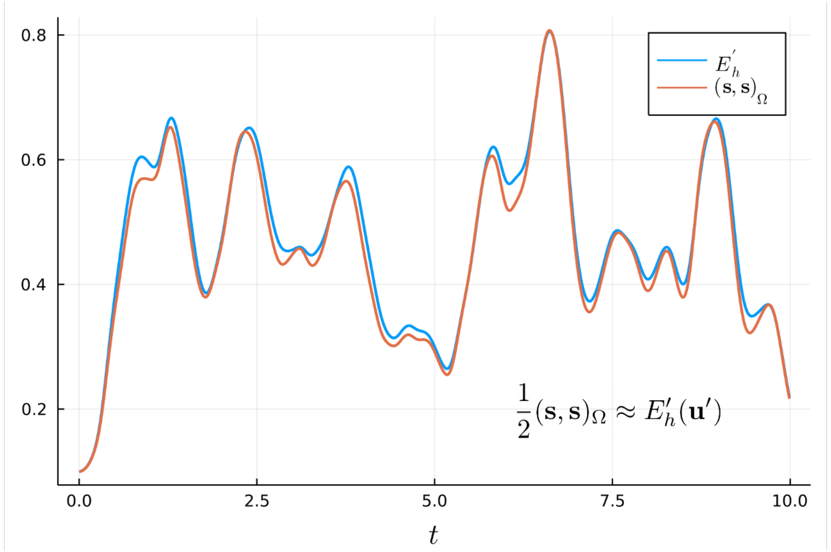
learned from

$$= \arg\min \sum_{d=1}^{\mathcal{D}} ||\frac{1}{2}\mathbf{s}_d^2 - \frac{1}{2}\mathbf{W}(\mathbf{u}'_d)^2||_2^2$$

Compressed variables learn effective subgrid content



compressed subgrid variable identifies sharp gradients



learned compression matches small scale energy closely

Energy-conserving closure model

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = f(\bar{\mathbf{u}}) + \underbrace{\overline{f(\mathbf{u})} - f(\bar{\mathbf{u}})}_{\approx c(\bar{\mathbf{u}};\theta)}$$

- Large scale dynamics with closure model
- Compressed small scale dynamics (latent variables)

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\bar{\mathbf{u}}\\ \mathbf{s}\end{bmatrix} = \begin{bmatrix}f(\bar{\mathbf{u}})\\ \mathbf{0}\end{bmatrix} + \begin{bmatrix}c_u(\bar{\mathbf{u}},\mathbf{s};\theta_u)\\ c_s(\bar{\mathbf{u}},\mathbf{s};\theta_s)\end{bmatrix}$$

"extended neural closure model"

- Energy conserving condition

$$\frac{\mathrm{d}\bar{E}_h(\bar{\mathbf{u}})}{\mathrm{d}t} + \frac{1}{2}\frac{\mathrm{d}(\mathbf{s},\mathbf{s})_\omega}{\mathrm{d}t} = 0$$

- Our proposal: learn **a skew-symmetric matrix** $\mathcal{K}$ with entries given by neural network outputs

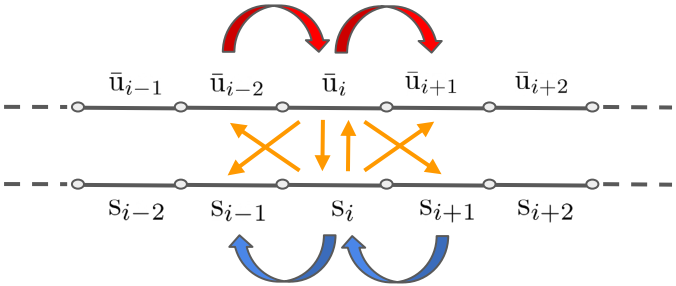
$$\begin{bmatrix}c_u(\bar{\mathbf{u}},\mathbf{s};\theta_u)\\ c_s(\bar{\mathbf{u}},\mathbf{s};\theta_s)\end{bmatrix} = \mathcal{K}(\bar{\mathbf{u}},\mathbf{s};\mathbf{\Theta})\begin{bmatrix}\bar{\mathbf{u}}\\ \mathbf{s}\end{bmatrix}$$

Skew-symmetric neural network

$$\begin{bmatrix} c_u(\bar{\mathbf{u}}, \mathbf{s}; \theta_u) \\ c_s(\bar{\mathbf{u}}, \mathbf{s}; \theta_s) \end{bmatrix} = \mathcal{K}(\bar{\mathbf{u}}, \mathbf{s}; \mathbf{\Theta}) \begin{bmatrix} \bar{\mathbf{u}} \\ \mathbf{s} \end{bmatrix}$$

- Intuition behind skew-symmetric closure model: **local energy exchanges**

$$\mathcal{K}(\bar{\mathbf{u}}, \mathbf{s}; \mathbf{\Theta}) = \begin{bmatrix} \mathbf{K}_1 & \mathbf{K}_2 \\ -\mathbf{K}_2^T & \mathbf{K}_3 \end{bmatrix}$$



- Skew-symmetric forms obtained by

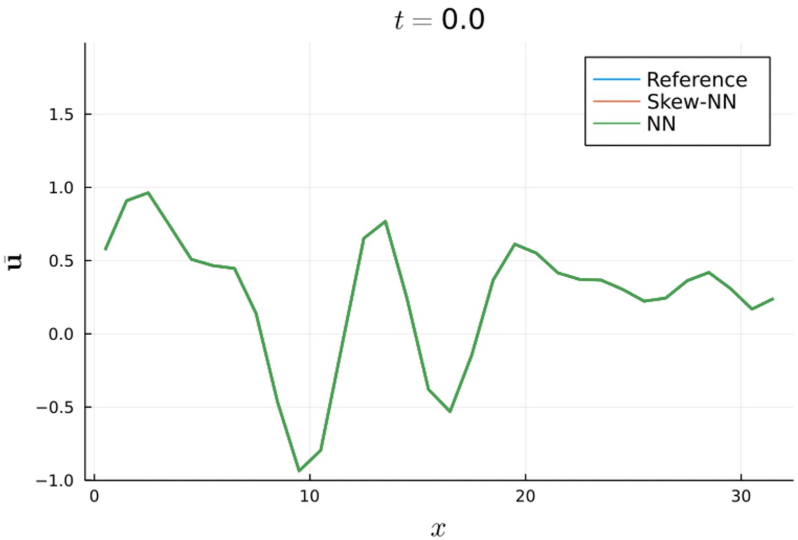
$$\mathbf{K}_1 = [\mathbf{M}_1(\theta), \mathbf{\Phi}_1(\theta), \mathbf{M}_2(\theta)]$$

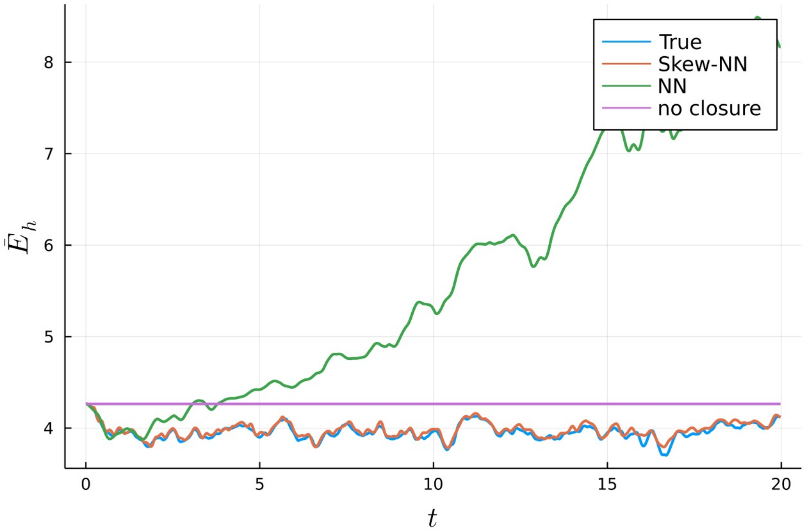
$$[\mathbf{A}, \mathbf{\Phi}, \mathbf{B}] := \mathbf{A}\mathbf{\Phi}\mathbf{B}^T - (\mathbf{A}\mathbf{\Phi}\mathbf{B}^T)^T$$

- $\mathbf{K}_2$ allows energy exchange between large and small scales

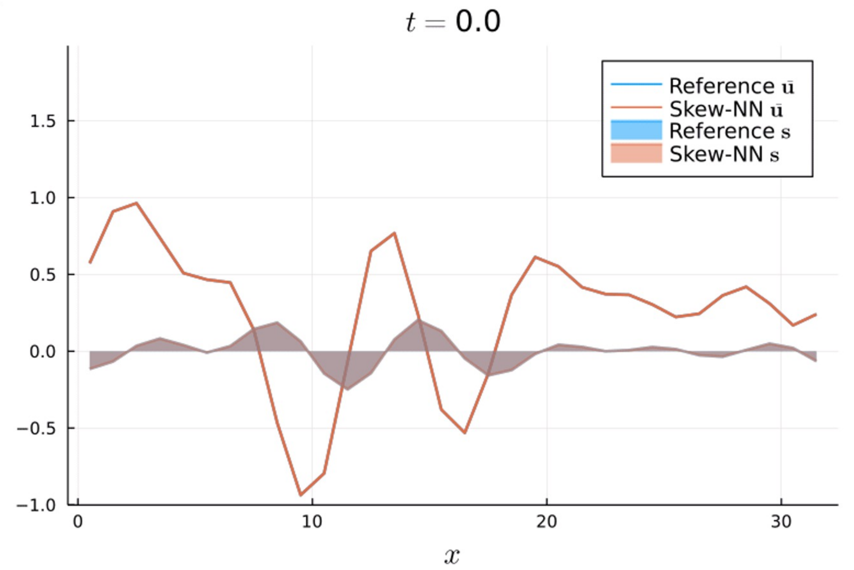
New closure model improves quality + stability

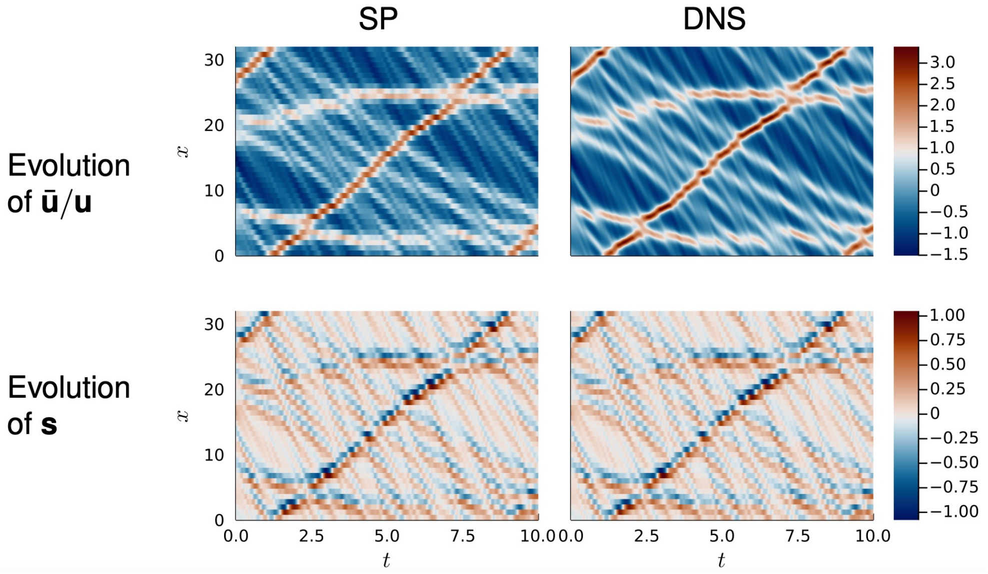
- Trained on different initial conditions, tested on unseen initial conditions
- Reduction from N = 600 to N = 30
- Compare to standard CNN





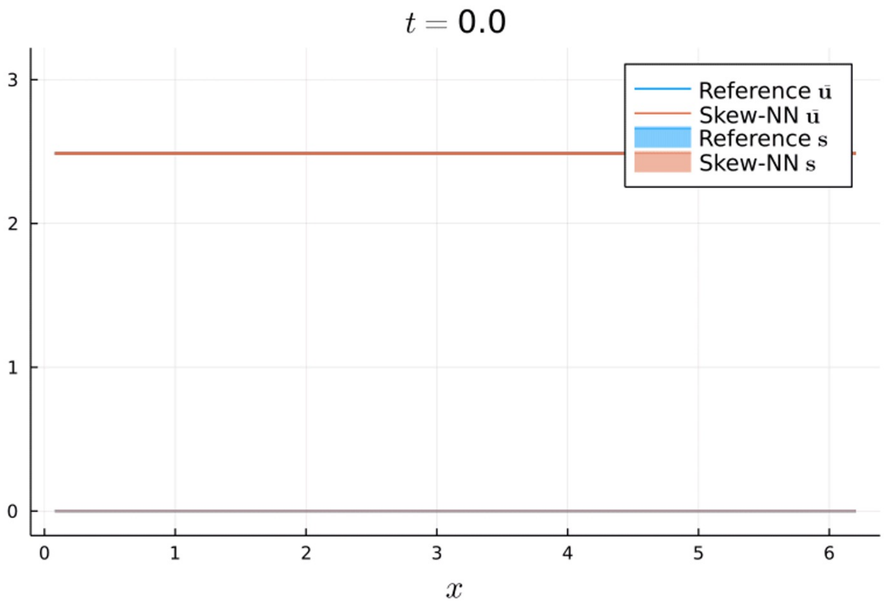
Evolution of subgrid content matches nicely





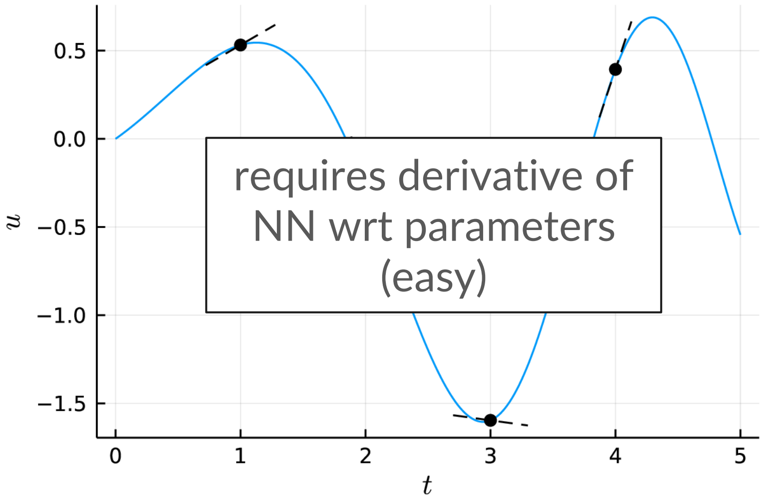
Extension to Burgers' equation

- Includes viscosity and time-dependent boundary conditions
- Reduction from N=1000 to N=40



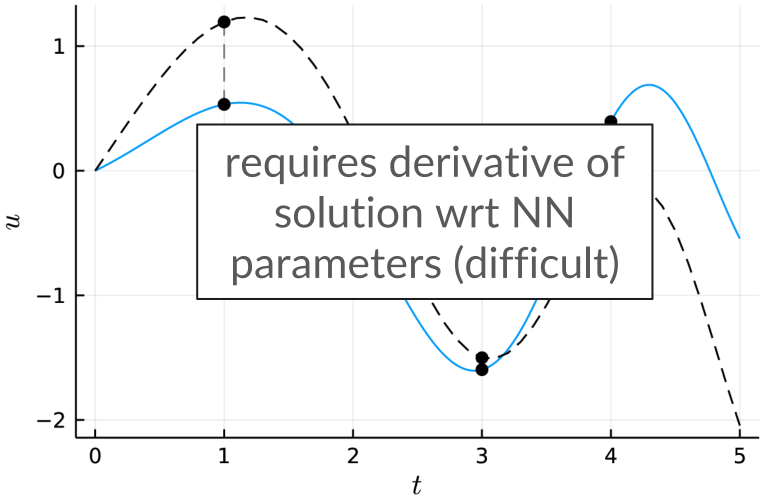
What about training neural closure models?

Training approaches for neural closure ODEs



derivative fitting

$$\text{Loss} = \left\| \left(\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} \right)_{\text{ref}} - \text{NN}(\mathbf{u}_{\text{ref}}; \vartheta) \right\|^2$$



trajectory fitting

$$\text{Loss} = \sum_{i=1}^{N_t} \left\| \mathbf{u}(t_i) - \mathbf{u}_{\text{ref}}(t_i) \right\|^2, \;\; \text{where} \;\; \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \text{NN}(\mathbf{u}; \vartheta)$$

$$\text{Loss} = \left\| \left(\frac{d\mathbf{u}}{dt}\right)_{\text{ref}} - \text{NN}(\mathbf{u}_{\text{ref}}; \vartheta) \right\|^2$$

Derivative fitting can be inaccurate (and unstable)

Theorem 3.2. *Let $\mathbf{u}_{\text{ref}}(t), t \geq 0$ be given, and let $\mathbf{u}(t), t \geq 0$ be the solution of the ODE $\frac{d\mathbf{u}}{dt} = NN(\mathbf{u}; \vartheta)$. If the following holds:*

$$a) \quad \left\| \frac{d}{dt}\mathbf{u}_{\text{ref}}(t) - NN(\mathbf{u}_{\text{ref}}(t); \vartheta) \right\| \leq \varepsilon,$$

$$b) \quad \| NN(\mathbf{a}; \vartheta) - NN(\mathbf{b}; \vartheta) \| \leq C \, \|\mathbf{a} - \mathbf{b}\| \,,$$

then the following error bound holds:

$$\|\mathbf{u}_{\text{ref}}(t) - \mathbf{u}(t)\| \leq \frac{\varepsilon}{C} \left(e^{Ct} - 1\right).$$

Based on the “Fundamental Lemma”, Hairer et al. (1993)

If a neural ODE:

- is given a good initial condition;
- approximates the derivative well and is Lipschitz;

Then, the resulting ODE solution may still be **inaccurate**

$$\text{Loss} = \sum_{i=1}^{N_t} \left\|\mathbf{u}(t_i) - \mathbf{u}_{\text{ref}}(t_i)\right\|^2, \text{ where } \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \text{NN}(\mathbf{u};\vartheta)$$

Trajectory fitting ("embedded learning")

- Trajectory fitting yields **stable results, tailor-made** to the discretization
- Derivatives of loss function computed via **sensitivity methods** $\frac{\mathrm{dLoss}}{\mathrm{d}\theta}$

1. Discretise-then-optimise:
   - Need **differentiable solver** (not always available, e.g. black box code)
2. Optimise-then-discretise
   - Solve adjoint equations (Chen et al. 2018)

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{y}^\top & = -\mathbf{y}^\top \frac{\partial}{\partial \mathbf{u}} \text{NN}(\mathbf{u}(t);\vartheta) \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{z}^\top & = -\mathbf{y}^\top \frac{\partial}{\partial \vartheta} \text{NN}(\mathbf{u}(t);\vartheta) \end{cases}$$

$$\frac{\mathrm{dLoss}}{\mathrm{d}\theta} = \mathbf{z}(0)$$

Comparison of approaches

trajectory fitting

	Derivative fitting	Discretise-then-optimise	Optimise-then-discretise
Terms that must be differentiable	NN	NN, f, and ODE solver	NN and f
Accuracy of computed gradients of loss function	Exact	Exact	Approximate
Can learn long-term accuracy	No	Yes	Yes
Requires time-derivatives of training data	Yes	No	No
Computational cost	Low	High	High

Several issues / design choices:

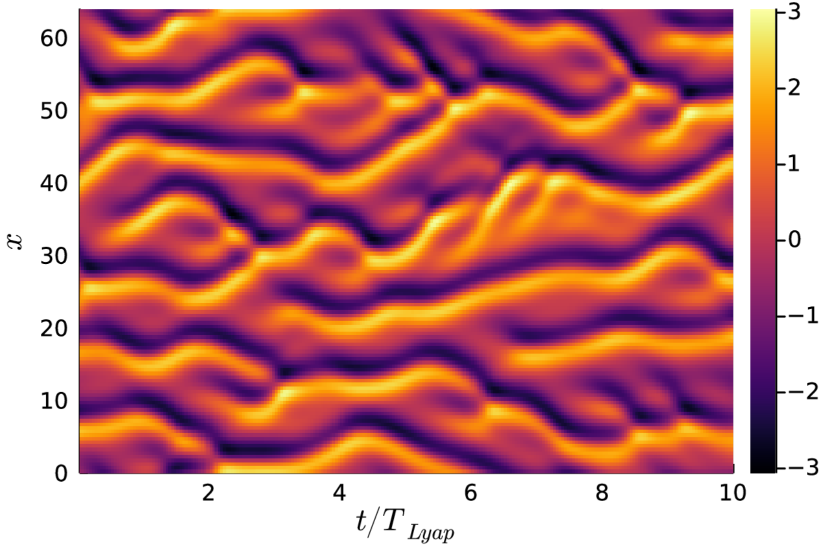
- Trajectory length / “unrolled time steps” in loss function
- Stiffness (backpropagation with implicit solvers more difficult)
- Chaotic systems
- Exploding /vanishing gradients

Kuramoto-Sivashinsky equation

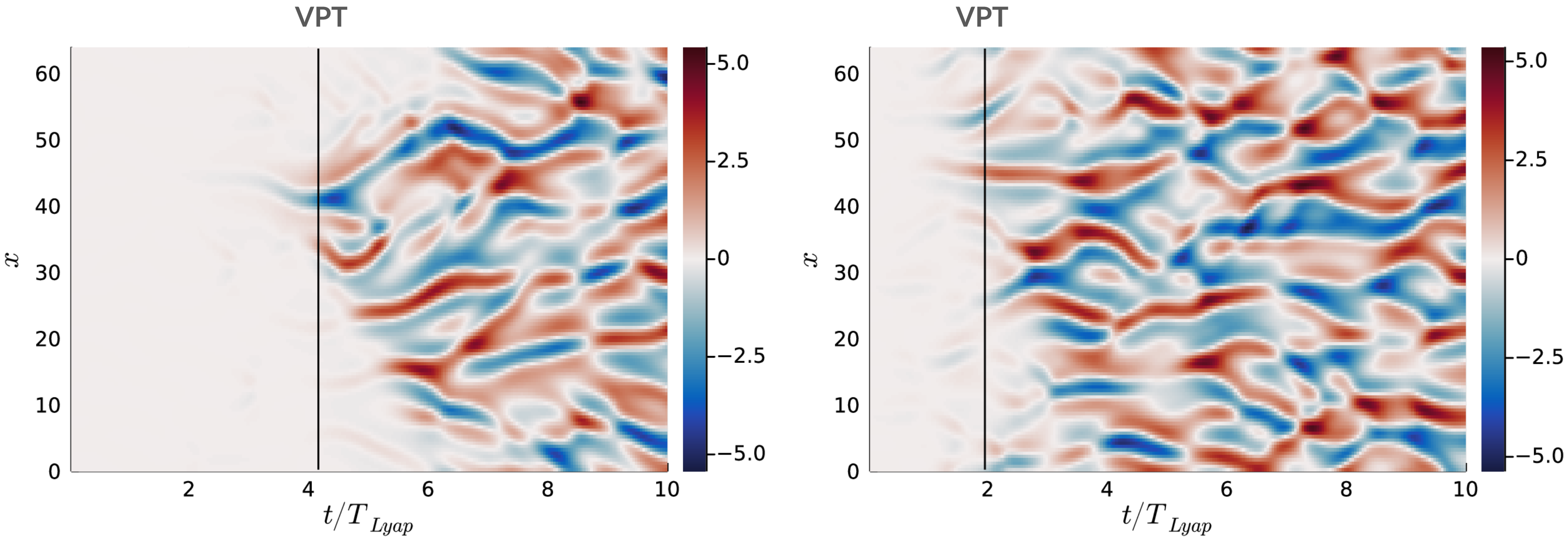
$$\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x}\left(u^2\right) = -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^4 u}{\partial x^4}$$

$$\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} = f(\bar{\mathbf{u}}) + \nabla \cdot \mathrm{NN}(\bar{\mathbf{u}};\theta)$$

- **Chaotic:**
  - Use Valid Prediction Time (VPT) to assess accuracy
  - Weighting of loss function to damp exponential increase in sensitivity
- **Stiff:**
  - Opt-Disc: **implicit** ESDIRK KenCarp47
  - Disc-Opt: **explicit** ETDRK4 in Fourier domain (Kassam & Trefethen 2005)
- Reduction 1024 -> 128



Effect of trajectory length, optimise-then-discretise



short trajectories

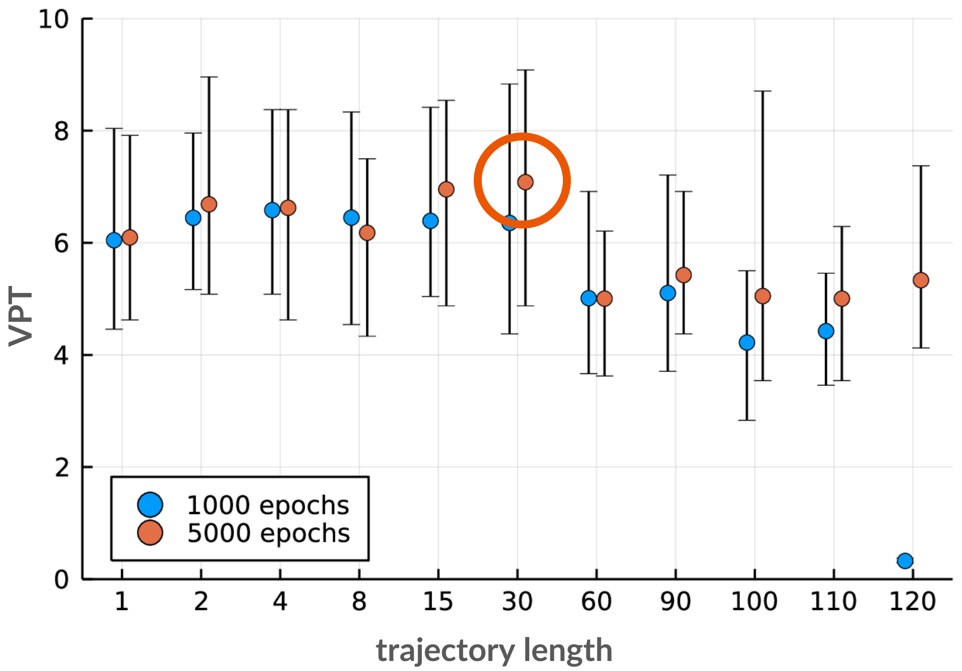
long trajectories

Valid prediction time, optimise-then-discretise

Training method		VPT Min	VPT Avg	VPT Max
Coarse ODE		1.17	1.93	3.00
Derivative fitting		4.17	5.36	7.54
Optimise-then-discretise	Short trajectories	4.08	5.84	8.29
	Long trajectories	2.38	3.38	4.67
Long trajectories, decaying error weights	$c = 0.5$	2.42	4.20	5.38
	$c = 1.0$	2.96	4.38	6.29
	$c = 1.5$	3.29	4.58	5.88
	$c = 2.0$	2.71	4.29	5.75

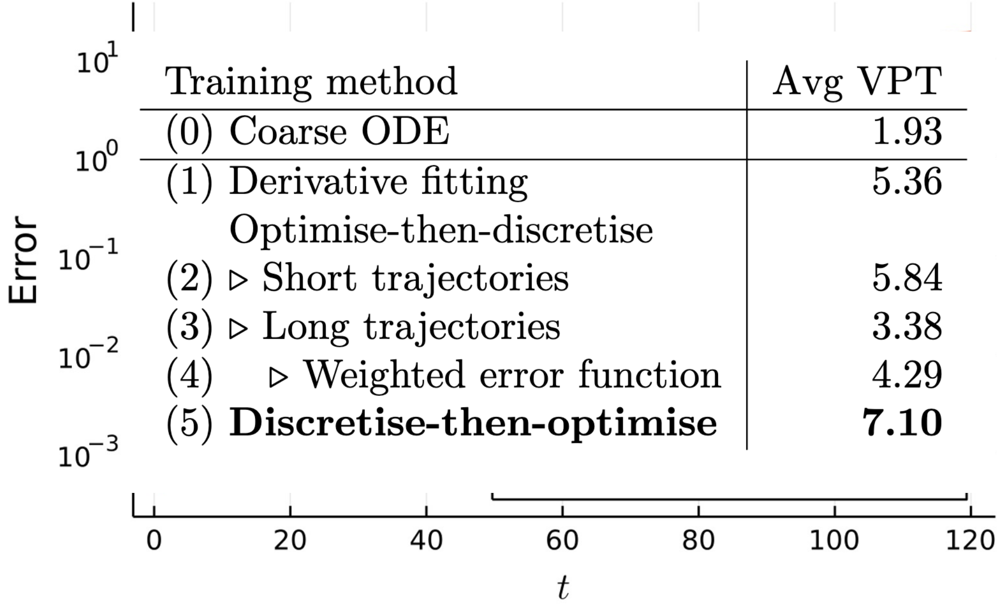
Effect of trajectory length, discretise-then-optimise

- Discretise-then-optimise higher VPT than optimise-then-discretise
- In both cases: **trajectories should not be 'too long'**



Comparison of training approaches

- **Discretise-then-optimise overall best performance**
- Optimise-then-discretise sensitive to training interval; longer interval less accurate
- Derivative fitting reasonable but diverges (for Burgers: unstable)



Training method	Avg VPT
(0) Coarse ODE	1.93
(1) Derivative fitting	5.36
Optimise-then-discretise	
(2) ▷ Short trajectories	5.84
(3) ▷ Long trajectories	3.38
(4) ▷ Weighted error function	4.29
(5) Discretise-then-optimise	**7.10**

Conclusions

- **“Discretize first”**
  - Tailor-made closure models
  - Useful framework when using neural networks, eases analysis
- **“Preserve structure”**
  - Accuracy improves by adding physics knowledge
  - Non-linear stability possible with energy conserving methods
- **“Embedded learning”** with **trajectory fitting**
  - Discretise-then-optimise with **differentiable solvers** preferred
  - Promising but with strings attached: problem-dependent, comparison not easy

Julia is great for differentiable programming

- Neural closure models
  - https://github.com/HugoMelchers/neural-closure-models
- Incompressible, energy-conserving Navier-Stokes code
  - https://github.com/agdestein/IncompressibleNavierStokes.jl
- DifferentialEquations.jl by Rackauckas et al.
  - https://sciml.ai