Centrum Wiskunde & Informatica

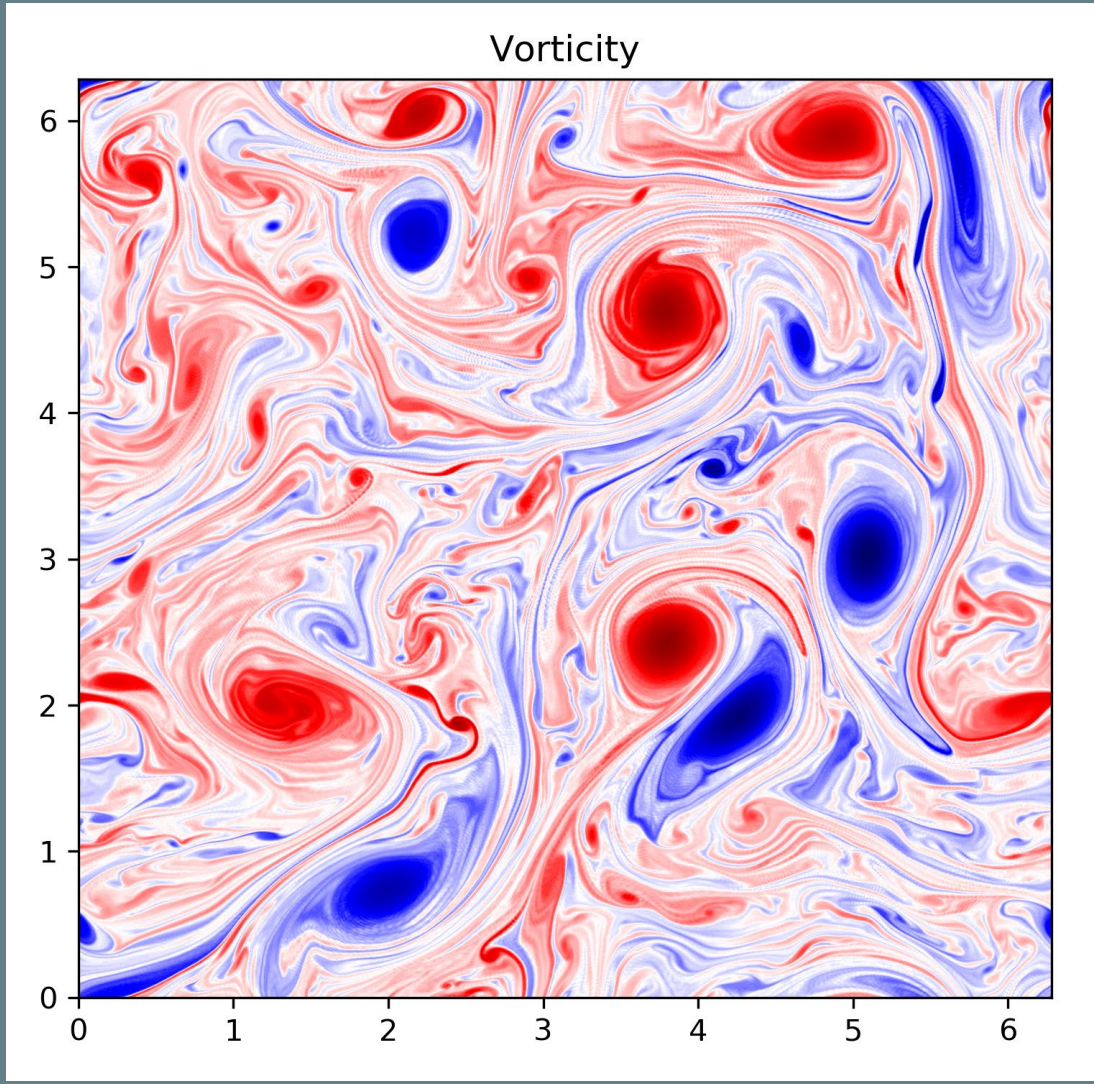
Model uncertainty in turbulent fluid dynamics

Daan Crommelin

Centrum Wiskunde & Informatica, Amsterdam
and KdV Institute for Mathematics, University of Amsterdam

Simulating fluid dynamics

Resolving all details of fluid flow in numerical simulations is computationally too expensive

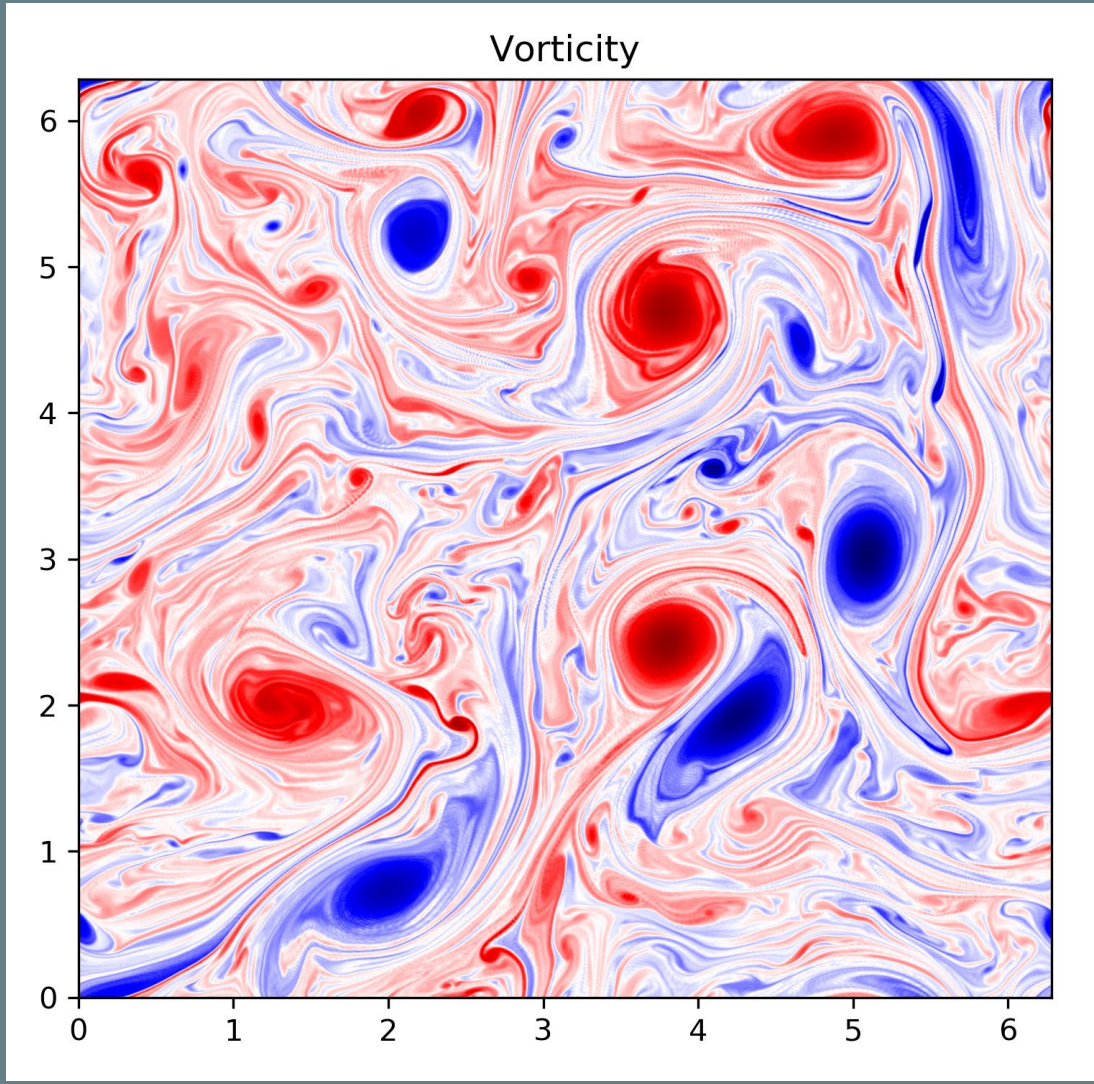


Simulating fluid dynamics

Resolving all details of fluid flow in numerical simulations is computationally too expensive

Numerical discretization of PDE (Navier-Stokes)
→ unresolved (subgrid scale) processes

Representing effects of unresolved processes:
Closure (or parameterization, turbulence model, …)



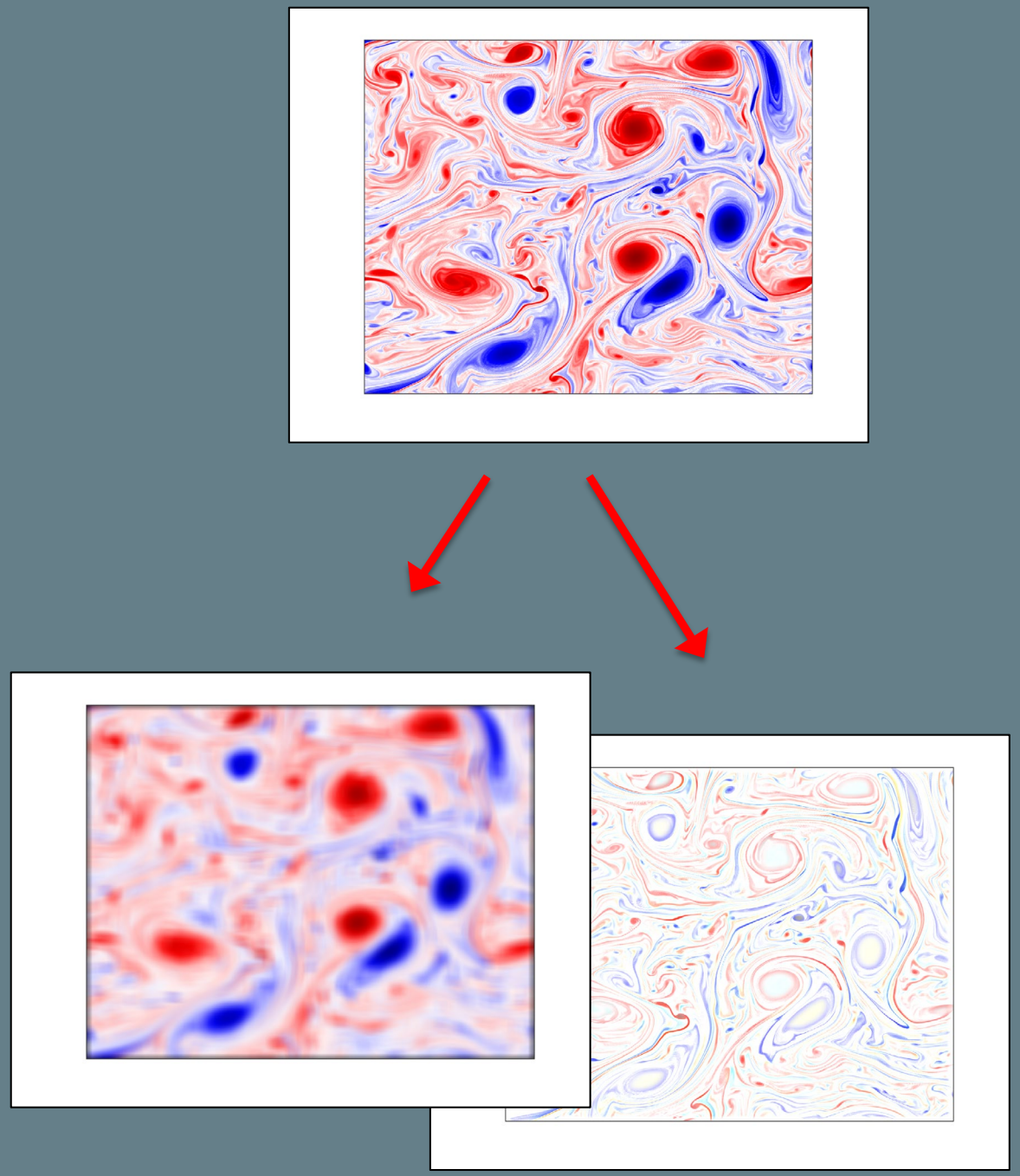
Simulating fluid dynamics

PDE for incompressible fluid velocity $u(x,t)$:

$$\partial_t u + u \cdot \nabla u = F - D$$

(forcing F, dissipation D)

Decompose: $u = \bar{u} + u'$ (large-scale + small-scale)



Simulating fluid dynamics

PDE for incompressible fluid velocity $u(x,t)$:

$$\partial_t u + u \cdot \nabla u = F - D$$

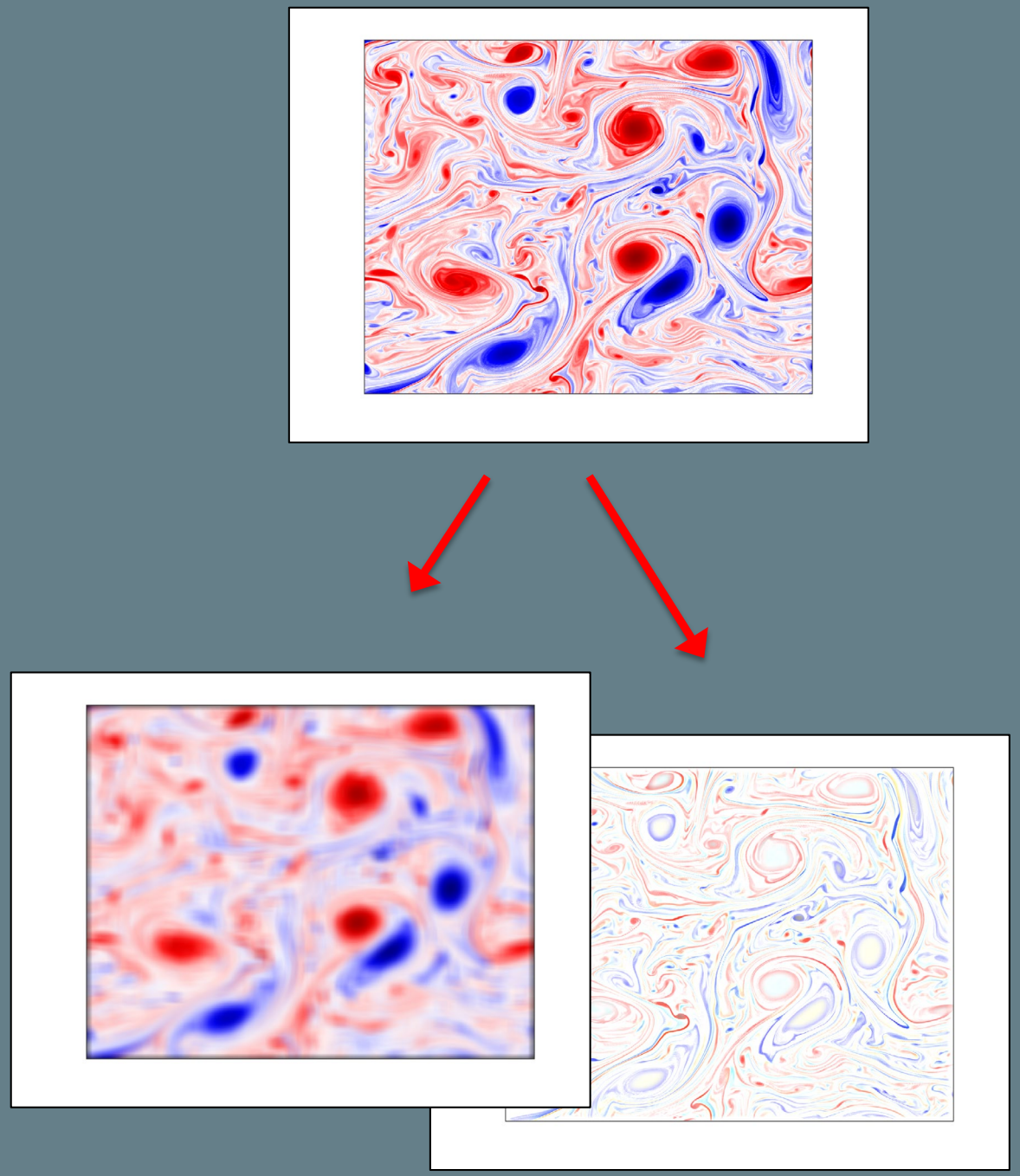
(forcing F, dissipation D)

Decompose: $u = \bar{u} + u'$ (large-scale + small-scale)

PDE for $\bar{u}$: $\partial_t \bar{u} + \bar{u} \cdot \nabla \bar{u} = \bar{F} - \bar{D} + B$

SGS term: $B = \bar{u} \cdot \nabla \bar{u} - \overline{u \cdot \nabla u}$ (unclosed)

Need to express B in terms of $\bar{u}$



Uncertainties, errors, choices

- Physical parameters
- Initial conditions
- Boundary conditions
- Model structural error / model form uncertainty
- Simulation choices:
  - numerical schemes
  - simulation parameters (e.g. time step, grid spacing)
  - closures / parameterizations

UQ in computational fluid dynamics

Extensive literature, see e.g.

- Najm, H. N., *Uncertainty quantification and polynomial chaos techniques in computational fluid dynamics*. Annual review of fluid mechanics, 2009
- Le Maître, O., & Knio, O. M., *Spectral methods for uncertainty quantification: with applications to computational fluid dynamics*. Springer, 2010

Emphasis on parameter uncertainty, IC, BC

Model uncertainty: still challenging

Model choices

Jansson et al., *Assessing uncertainties from physical parameters and modelling choices in an atmospheric large eddy simulation model,* Phil. Trans. R. Soc. A, 2021

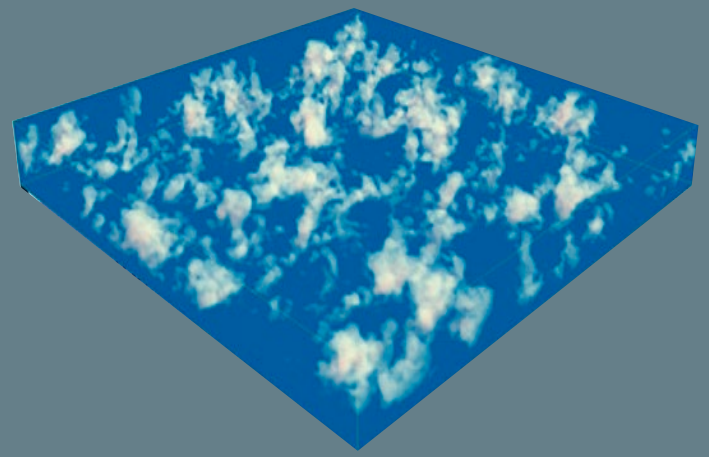
Parameter UQ and SA for model “switches” / choices:

Atmospheric LES model, 2 - 3 choices for:

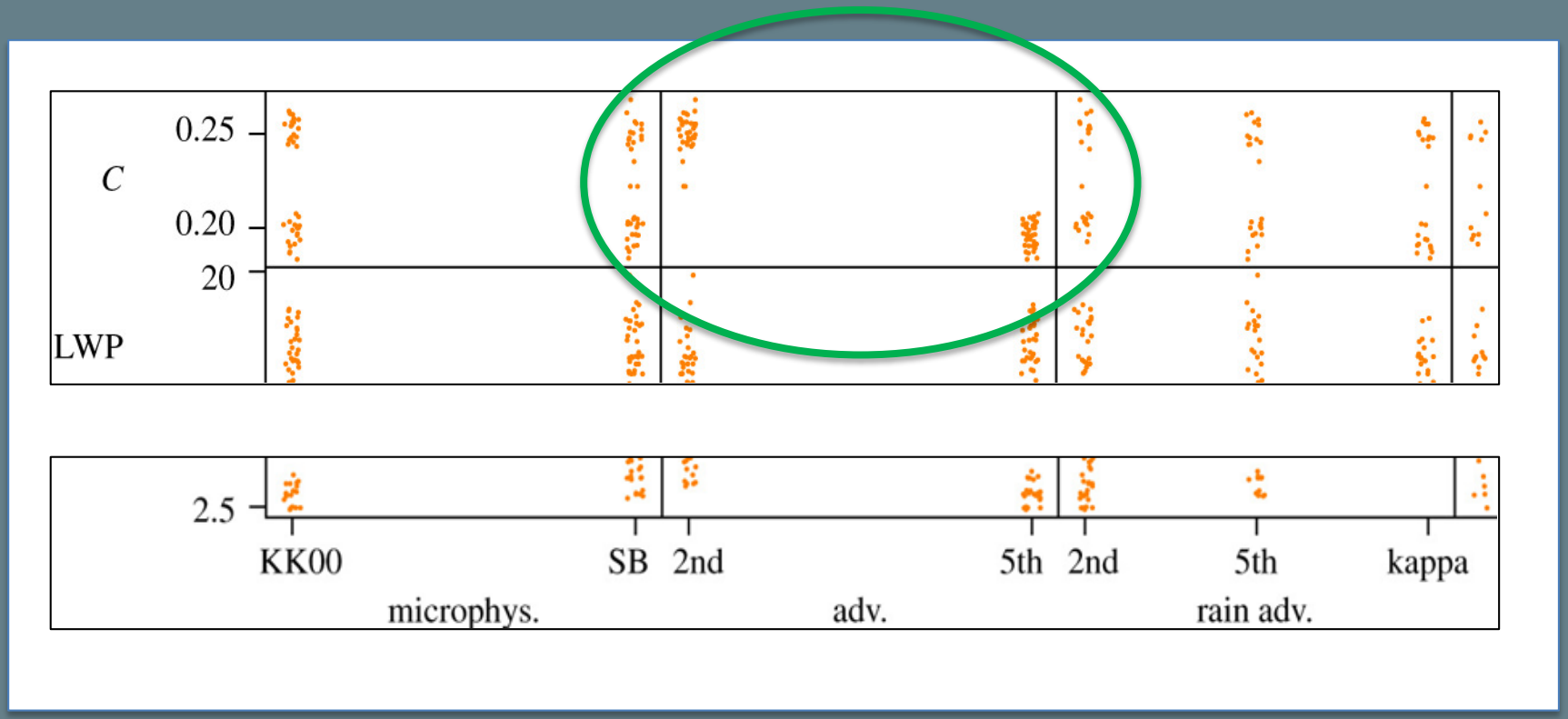
- Microphysics scheme
- Advection scheme
- Rain advection scheme

Uniform discrete distributions

Poisson solver tolerance $\epsilon = 10^{-d}, d \sim U[2,13]$



(Figure adapted from Jansson et al., JAMES, 2019)



Example: cloud cover (C) sensitive to choice of advection scheme but not to choice of (e.g.) cloud microphysics scheme

(Figure adapted from Jansson et al., Phil. Trans. R. Soc. A, 2021)

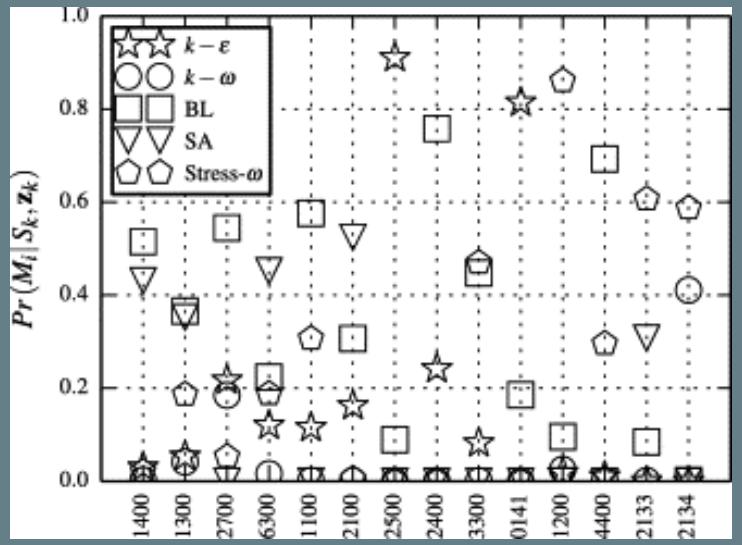
Choosing between different closures

Bayesian Model Averaging in context of fluid dynamics:

Ensemble of a single model outfitted with different closures

Edeling et al., *Predictive RANS simulations via Bayesian model-scenario averaging*. J. Comput. Phys., 2014

(BMA extended to include different scenarios)



(Figure from Edeling et al., J. Comput. Phys., 2014)

Stochastic modeling to represent model uncertainty

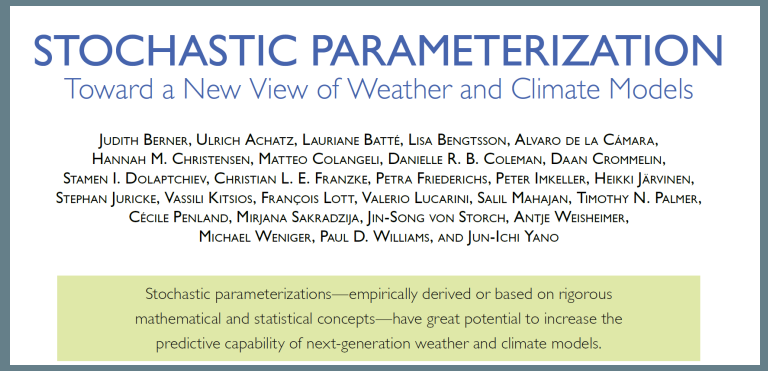
Inherent uncertainty of interactions between resolved and unresolved processes

Stochastic process as closure / parameterization

Pursued in weather & climate modeling for 20+ years, see e.g.:

Palmer, T. N., *A nonlinear dynamical perspective on model error: A proposal for non-local stochastic-dynamic parametrization in weather and climate prediction models*. QJRMS, 2001

Berner et al., 2017:


STOCHASTIC PARAMETERIZATION

Toward a New View of Weather and Climate Models

Judith Berner, Ulrich Achatz, Lauriane Batté, Lisa Bengtsson, Alvaro de la Cámara, Hannah M. Christensen, Matteo Colangeli, Danielle R. B. Coleman, Daan Crommelin, Stamen I. Dolaptchiev, Christian L. E. Franzke, Petra Friederichs, Peter Imkeller, Heikki Järvinen, Stephan Juricke, Vassili Kitsios, François Lott, Valerio Lucarini, Salil Mahajan, Timothy N. Palmer, Cécile Penland, Mirjana Sakradzija, Jin-Song von Storch, Antje Weisheimer, Michael Weniger, Paul D. Williams, and Jun-Ichi Yano

Stochastic parameterizations—empirically derived or based on rigorous mathematical and statistical concepts—have great potential to increase the predictive capability of next-generation weather and climate models.

Model reduction and Mori-Zwanzig formalism

Model reduction according to MZ formalism: noise and memory $\rightarrow$ Non-Markovian models

ODE: $\dot{z} := \frac{dz}{dt} = h(z)$, e.g. from discretizing PDE. Decomposing $z = (x, y)$ gives coupled ODEs:

$$\dot{x} = f(x, y)$$
$$\dot{y} = g(x, y)$$

Effective model for x only:

$$\dot{x} = \overline{f}(x) + \int_0^t K(x(t-s), s)ds + W'(t)$$

(memory kernel K, noise W')

(see e.g. Mori, 1965; Zwanzig 1973; Chorin et al. 2000; Gottwald et al., 2017)

Model reduction and Mori-Zwanzig formalism

Simple example: linear system

$$\dot{x} = L_{11}x + L_{12}y$$
$$\dot{y} = L_{21}x + L_{22}y$$

Integrating y leads to:

$$\dot{x} = L_{11}x + L_{12}\int_0^t e^{L_{22}(t-s)}\, L_{21}x(s)ds + L_{12}e^{L_{22}t}\, y(0)$$

IC $y(0)$: unknown / random

Model reduction and Mori-Zwanzig formalism

Effective model:

$$\dot{x} = \overline{f}(x) + \int_0^t K(x(t-s), s)ds + W'(t)$$

Numerical simulations with only x, not y

Model “error” due to omitting y includes memory and randomness

Learning from data

Learning closures / parameterizations with memory from data, inspired by MZ formalism

E.g.:

- Pan, S., & Duraisamy, K. (2018). *Data-driven discovery of closure models*. SIAM Journal on Applied Dynamical Systems, 17(4), 2381-2413.

- Wang, Q., Ripamonti, N., & Hesthaven, J. S. (2020). *Recurrent neural network closure of parametric POD-Galerkin reduced-order models based on the Mori-Zwanzig formalism*. Journal of Computational Physics, 410, 109402.

Learning from data

Crommelin, D., & Edeling, W. (2021). *Resampling with neural networks for stochastic parameterization in multiscale systems*. Physica D, 422, 132894.

Discrete time setting, time index $j \in \mathbb{N}$. System evolution: $x_{j+1} = F(x_j) + r_j$

Evolve r_j by sampling from conditional probability distribution

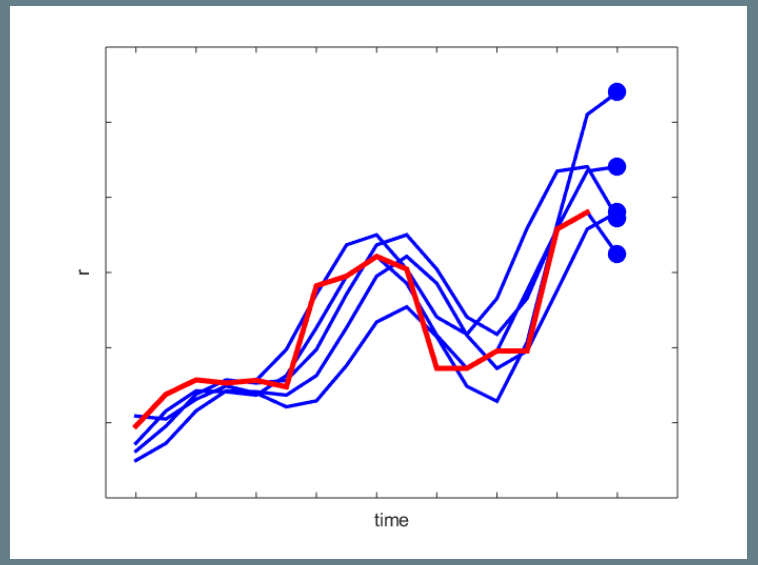
$r_{j+1} \mid r_j, r_{j-1}, r_{j-2}, \ldots, x_j, x_{j-1}, x_{j-2}, \ldots$

Learning from data

At each time step:
(i) Update $x_{j+1} = F(x_j) + r_j$
(ii) Sample from $r_{j+1} \mid r_j, r_{j-1}, r_{j-2}, \dots, x_j, x_{j-1}, x_{j-2}, \dots$

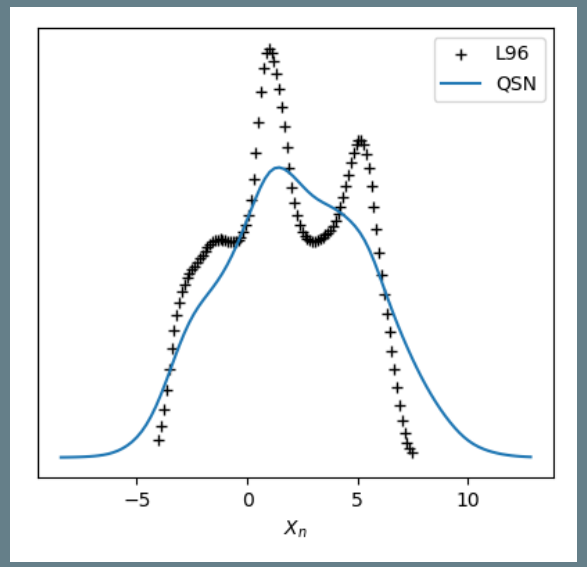
Distribution $r_{j+1} \mid r_j, r_{j-1}, r_{j-2}, \dots, x_j, x_{j-1}, x_{j-2}, \dots$ unknown

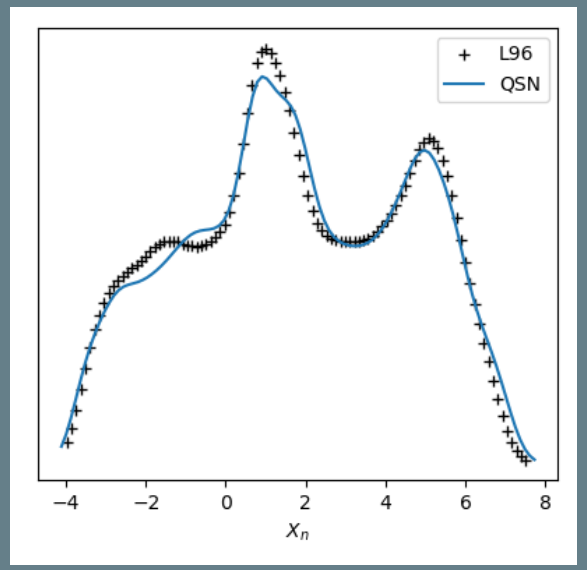
Sample by bootstrapping from observations
$\left(x_j^o, r_j^o\right)_{j=1}^{N}, \quad r_j^o := x_{j+1}^o - F\left(x_j^o\right)$



Learning from data

Numerical tests on L96 model, focus on long-term statistics





Left: memory depth J=10. Right: memory depth J=75

(Figures from Crommelin & Edeling , Phys. D, 2021)