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.


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


(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:
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:

$$\begin{align*}
\dot{x} &= f(x, y) \\
\dot{y} &= g(x, y)
\end{align*}$$

Effective model for $x$ only:

$$\dot{x} = \bar{f}(x) + \int_{0}^{t} K(x(t - s), s) ds + W'(t)$$

(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.:


Learning from data


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

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

Sample by bootstrapping from observations
\[
\left(x_j^0, r_j^0\right)_{j=1}^N, \quad r_j^0 := x_{j+1}^0 - F(x_j^0)
\]
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)