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Uncertainty quantification and ensemble forecast in coarse-grid or dimensionally-reduced computational fluid dynamics

Valentin Resseguier, Etienne Mémin, Bertrand Chapron
Motivations

• Rigorously identified subgrid dynamics effects

• Injecting likely small-scale dynamics

• Studying bifurcations and attractors

  Climate projections

• Quantification of modeling errors

  Ensemble forecasts and data assimilation
Contents

- Scalian
- Location uncertainty
- SQG under moderate uncertainty
Part I: **SCALIAN**

- **L@b** (~ 15 peoples)
  - Research, R&T, R&D
  - Expertise:
    - Geophysical fluid dyn.
    - Signal, data assimilation
    - Machine Learning
    - Multi-agents systems
    - Drones

- **CEN « Simulation »** (~ 70 people)
  - R&D and engineering
  - Expertise:
    - Radar, optronics, sonar
    - Geophysical fluid dyn.
    - Mechanical and thermal

- **Other Business Units** ~ 2400 people
  - Business:
    - Scientific softwares
    - Simulations, HPC
    - VR & AR
Part II
Location uncertainty (LU)
Usual random CFD

- Random parameters, boundary conditions, forcing
- Random initial conditions
- Arbitrary Gaussian forcing
- Averaging, homogenization

Other (complementary) issues
Underdispersive + need large ensemble
Adding energy + wrong phase
Assumptions and energy issues
Usual random CFD

• Random parameters, boundary conditions, forcing

• Random initial conditions

• Arbitrary Gaussian forcing

• Averaging, homogenization

Other (complementary) issues

Underdispersive + need large ensemble

Adding energy + wrong phase

Assumptions and energy issues
LU : Adding random velocity

\[ v = w + \sigma \dot{B} \]
LU: Adding random velocity

Resolved large scales

\[ \nu = \omega + \sigma \dot{B} \]
LU: Adding random velocity

\[ v = w + \sigma \dot{B} \]

Resolved large scales

White-in-time small scales
LU : Adding random velocity

Large scales:
\( w \)

Small scales:
\( \sigma \dot{B} \)

Variance tensor:
\[
\alpha = a(x, x) = \frac{\mathbb{E}\{\sigma dB \sigma dB^T\}}{dt}
\]
LU : Adding random velocity

Large scales: $w$
Small scales: $\sigma \dot{B}$

Variance tensor:

$$a = a(x, x) = \mathbb{E}\{\sigma dB (\sigma dB)^T\} dt$$

Resolved large scales

White-in-time small scales

$$\nu = w + \sigma \dot{B}$$

References:

- Mikulevicius and Rozovskii, 2004
- Flandoli, 2011
- Memin, 2014
- Resseguier et al. 2017 a, b, c
- Chapron et al. 2017
- Cai et al. 2017
- Holm, 2015
- Holm and Tyranowski, 2016
- Arnaudon et al., 2017
- Cotter and al 2017
- Crisan et al., 2017
- Gay-Balmaz & Holm 2017
- Cotter and al 2018 a, b
Advection of tracer $\Theta$

\[
\frac{D\Theta}{Dt} = 0
\]

Large scales: $w$
Small scales: $\sigma \dot{B}$
Variance tensor:
\[
a = a(x, x) = \mathbb{E}\{\sigma dB (\sigma dB)^T\}
\]
Advection of tracer $\Theta$

Large scales: $w$
Small scales: $\sigma \dot{B}$

Variance tensor:

$$a = a(x, x) = \frac{\mathbb{E}\{\sigma dB (\sigma dB)^T\}}{dt}$$
Advection of tracer $\Theta$

\[ \partial_t \Theta + w^* \cdot \nabla \Theta + \sigma \dot{B} \cdot \nabla \Theta = \nabla \cdot \left( \frac{1}{2} \alpha \nabla \Theta \right) \]

Large scales: $w$
Small scales: $\sigma \dot{B}$
Variance tensor:
\[ a = a(x, x) = \frac{\mathbb{E}\{\sigma dB \sigma dB^T\}}{dt} \]
Advection of tracer $\Theta$

$$\partial_t \Theta + \mathbf{w}^* \cdot \nabla \Theta + \sigma \dot{\mathbf{B}} \cdot \nabla \Theta = \nabla \cdot \left( \frac{1}{2} \alpha \nabla \Theta \right)$$

Large scales:
\[ \mathbf{w} \]
Small scales:
\[ \sigma \dot{\mathbf{B}} \]
Variance tensor:
\[ a = a(x, x) = \mathbb{E}\{\sigma dB (\sigma dB)^T\} dt \]
Advection of tracer $\Theta$

Large scales: $w$
Small scales: $\sigma \dot{B}$

Variance tensor:
\[ a = a(x, x) = \frac{\mathbb{E}\{\sigma dB (\sigma dB)^T\}}{dt} \]

\[ \partial_t \Theta + w^* \cdot \nabla \Theta + \sigma \dot{B} \cdot \nabla \Theta = \nabla \cdot \left( \frac{1}{2} a \nabla \Theta \right) \]
Advection
of tracer $\Theta$

Large scales:
- $w$
Small scales:
- $\sigma \dot{B}$

Variance tensor:
- $a = a(x, x) = \mathbb{E}\{\sigma dB(\sigma dB)^T\} / dt$

Drift correction

$$
\partial_t \Theta + \mathbf{w}^* \cdot \nabla \Theta + \sigma \dot{B} \cdot \nabla \Theta = \nabla \cdot \left( \frac{1}{2} a \nabla \Theta \right)
$$

Diffusion
Advection of tracer $\Theta$

Large scales: $w$
Small scales: $\sigma \dot{B}$
Variance tensor:

$$a = a(x, x) = \frac{E\{\sigma dB \, (\sigma dB)^T\}}{dt}$$

Multiplicative random forcing

Drift correction

$$\partial_t \Theta + w^* \cdot \nabla \Theta + \sigma \dot{B} \cdot \nabla \Theta = \nabla \cdot \left( \frac{1}{2} a \nabla \Theta \right)$$

Diffusion
Advection of tracer $\Theta$

Large scales: $w$
Small scales: $\sigma \dot{B}$
Variance tensor:

$$a = a(x, x) = \mathbb{E}\{\sigma dB \sigma dB^T\}/dt$$

Multiplicative random forcing

Drift correction

$$\partial_t \Theta + w^* \cdot \nabla \Theta + \sigma \dot{B} \cdot \nabla \Theta$$

Diffusion

$$\nabla \cdot \left( \frac{1}{2} a \nabla \Theta \right)$$
Advection of tracer $\Theta$

Large scales: $\mathbf{w}$

Small scales: $\sigma \mathbf{\dot{B}}$

Variance tensor:

\[
a = a(x, x) = \mathbb{E}\{\sigma dB (\sigma dB)^T\}/dt
\]

Multiplicative random forcing

\[
\partial_t \Theta + \mathbf{w}^* \cdot \nabla \Theta + \sigma \mathbf{\dot{B}} \cdot \nabla \Theta = \nabla \cdot \left( \frac{1}{2} \alpha \nabla \Theta \right)
\]

Drift correction
Advection of tracer $\Theta$

\[
\partial_t \Theta + \mathbf{w}^* \cdot \nabla \Theta + \sigma \dot{\mathbf{B}} \cdot \nabla \Theta = \nabla \cdot \left( \frac{1}{2} \alpha \nabla \Theta \right)
\]

Multiplicative random forcing

Balanced energy exchanges

Drift correction

Large scales:
\[
\mathbf{w}
\]
Small scales:
\[
\sigma \dot{\mathbf{B}}
\]
Variance tensor:
\[
a = a(x', x) = \mathbb{E}\{\sigma dB(\sigma dB)^T\} dt
\]

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A word about reduced order models

- Very fast simulation of very complex system (e.g. for industrial application)
- Physical model (PDE) simplified using observations

**Reduced models under location uncertainty**
- Rigorous and low-cost estimators
- Stabilization of the unstable modes
- Maintain variability of stable modes
- Uncertainty quantification

**State of art**
- Possible parametrization with eddy viscosity
- Impossible to parametrize with additional dissipation
  Need ad hoc closure like MQG
  (Sapsis and Majda, 2013a,b,c)
Part III
SQG under Moderate Uncertainty

SQG MU

Code available online
SQG

\[ \frac{Db}{Dt} = -\alpha_{HV} \nabla^4 b \text{ Hyper-viscosity} \]

\[ u = \left( \text{cst.} \nabla^\perp \Delta^{-\frac{1}{2}} \right) b \]

Reference flow:

deterministic

SQG

1024 x 1024

\[ t = 17 \text{ days} \]
SQG

\[ \frac{Db}{Dt} = -\alpha_{HV} \Delta^4 b \text{ Hyper-viscosity} \]

\[ u = \left( \text{cst.} \nabla \Delta^{-\frac{1}{2}} \right) b \]

Reference flow:

deterministic

SQG

1024 x 1024

t = 17 days
One realization:
Stochastic destabilization

Deterministic 128 x 128

Deterministic 1024 x 1024

Location Uncertainty 128 x 128
One realization: Stochastic destabilization

Deterministic 128 x 128

Deterministic 1024 x 1024

Location Uncertainty 128 x 128

Spectrum
One realization: Stochastic destabilization

Deterministic 128 x 128

Deterministic 1024 x 1024

Location Uncertainty 128 x 128

Spectrum
One realization:
Stochastic destabilization

Deterministic 128 x 128

Deterministic 1024 x 1024

Location Uncertainty 128 x 128

Spectrum
One realization: Stochastic destabilization

Deterministic 128 x 128

Deterministic 1024 x 1024

Location Uncertainty 128 x 128
One realization:
Stochastic destabilization
One realization:
Stochastic destabilization

Deterministic 128 x 128

Deterministic 1024 x 1024

Location Uncertainty 128 x 128
One realization: Stochastic destabilization

- Deterministic 128 x 128
- Deterministic 1024 x 1024
- Location Uncertainty 128 x 128
Ensemble: random coherent structures
Ensemble: random coherent structures
Ensemble: uncertainty quantification

Bias LU

Estim. error LU

Estim. error RanIC

Spectrum of the errors and its estimation

$E(\kappa) (\text{rad.m}^{-1})$

$\kappa (\text{rad.m}^{-1})$

Bias RanIC

Bias LU

Estim. error RanIC

Estim. error LU
Ensemble: uncertainty quantification
Conclusion
Conclusion

LU models blindly describe unresolved triades

- Conserve energy
- Stabilization / destabilization in Reduced Order Model
- Instabilities triggered, possibly followed by extreme events
- Uncertainty quantification to address filter divergence
Related works, outlooks and application

• Bifurcations (SQG) and attractor (Lorenz 63) exploration

• Comparisons with data-driven parametrisation and SALT (Stochastic Advection by Lie Transport) (Holm and coauthors)

• Parametrization and tests based on higher-order statistics (curvature, energy flux through scales, bispectrum, …)

• (Surface gravity) wave / turbulence interaction

• **Data assimilation (DA)**:
  
  - Filtering / smoothing
  
    - EnKF with LU model as a R&D tool (for e.g. airplanes, drones)

    - **PF with reduced LU model for real-time monitoring and flow control**
      (for e.g. pollutant dispersion monitoring, drag and damage reduction in e.g. wind turbines)

  - Girsanov theorem for MLE and Bayesian estimations with e.g. satellite images