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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

Other Business Units
~ 2400 people

CEN « Simulation » (~ 70 people)

R&D and engineering

Expertise:
- Radar, optronics, sonar
- Geophysical fluid dyn.
- Mechanical and thermal

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

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

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

Resolved large scales

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

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

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

Resolved large scales

White-in-time small scales

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

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

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

Resolved large scales

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

White-in-time small scales

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 $\Theta$

\[
\frac{D\Theta}{Dt} = 0
\]
Advection of tracer \( \Theta \)

Large scales:
\( w \)

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

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

Large scales:
- $w$

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

Variance tensor:

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

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

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

Variance tensor:

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

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

Large scales:
- $w$

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

Variance tensor:
- $a = a(x, x) = \mathbb{E}\{\sigma dB (\sigma dB)^T\} dt$
Large scales: $w$
Small scales: $\sigma \dot{B}$
Variance tensor: $a = a(x, x) = \mathbb{E}\{\sigma dB (\sigma dB)^T\} / dt$

**Advection**

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

**Drift correction**

**Diffusion**

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

Multiplicative random forcing

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

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

Drift correction

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

Diffusion
Advection of tracer $\Theta$

Multiplicative random forcing

Large scales: $\omega$

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

Variance tensor:

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

Drift correction

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

Diffusion
Advection of tracer $\Theta$

Multiplicative random forcing

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

Variance tensor:

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

Drift correction

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

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

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

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

Multiplicative random forcing

Balanced energy exchanges

Drift correction
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

\[
\frac{Db}{Dt} = -\alpha_{HV} \Delta^4 b \\
u = \left( \text{cst.} \, \nabla^\perp \Delta^{-\frac{1}{2}} \right) b
\]

Reference flow:

deterministic

SQG

1024 x 1024

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

\[
\frac{D b}{D t} = -\alpha_{HV} \Delta^4 b \quad \text{Hyper-viscosity}
\]

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

**Reference flow:**
- deterministic
- SQG
- 1024 x 1024

\[t = 17 \text{ days}\]
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
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 x128

$t = 17$ days
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
Ensemble: uncertainty quantification

Bias LU

Estim. error LU

Estim. error RanIC

Spectrum of the errors and its estimation

Bias RanIC
Bias LU
Estim. error RanIC
Estim. error LU
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