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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

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

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

Resolved large scales

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

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

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

Variance tensor:

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

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

Resolved large scales
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 $\Theta$

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

Large scales:
$\mathbf{w}$

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

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

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

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

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

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

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

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

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

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

Drift correction
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

Drift correction

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

Multiplicative random forcing

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

Variance tensor:

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

Drift correction

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

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

Multiplicative random forcing

Drift correction

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

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

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

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

Drift correction

Multiplicative random forcing

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

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

Reference flow:
- deterministic
- SQG
- 1024 x 1024

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

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

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

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
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

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Location Uncertainty 128 x 128
One realization: Stochastic destabilization

Deterministic 128 x 128

Deterministic 1024 x 1024

Location Uncertainty 128 x 128
One realization: Stochastic destabilization

\[ \hat{b}(\kappa) \]

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

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

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

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