

— PhD Thesis Defense —

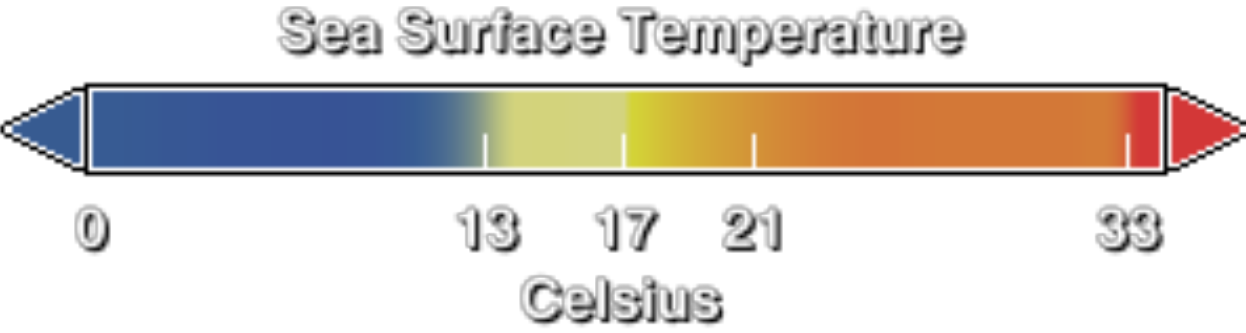
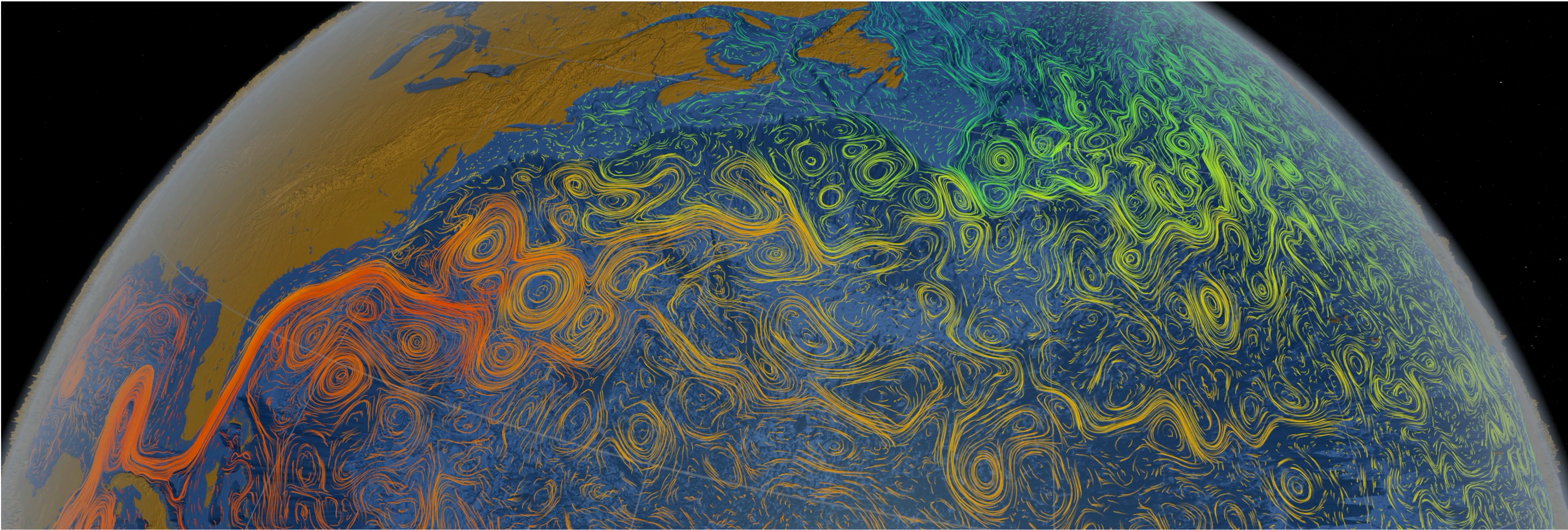
Stochastic modeling and numerical simulation of ocean dynamics

by **Long Li**

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Co-supervisor: Werner Bauer

Source: <https://svs.gsfc.nasa.gov/3913>



Methodologies

Eddy-induced advection

Gent & McWilliams
1990

Eddy-induced diffusion

Redi
1982



Ocean Modelling 2 (2000) 123–192

Ocean
Modelling

www.elsevier.com/locate/omodel

Developments in ocean climate modelling

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frontiers
in Marine Science

REVIEW
published: 26 February 2019
doi: 10.3389/fmars.2019.00065



Challenges and Prospects in Ocean Circulation Models

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Enrique Curchitser⁶, Gokhan Danabasoglu⁷, Carsten Eden⁸, Matthew H. England⁹,
Rüdiger Gerdes^{10,11}, Richard J. Greatbatch⁴, Stephen M. Griffies^{2,3}, Robert W. Hallberg^{2,3},
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Anne Marie Treguier²⁶, Hiroyuki Tsujino²⁷, Petteri Uotila²⁸ and Stephen G. Yeager⁷



Deterministic

Leith
1971

Griffies & Hallberg
2000

Fox-Kemper &
Menemenlis
2008

Stochastic

Berloff
2005

Jansen & Held
2014
Grooms & Majda
2014
Porta Mana & Zanna
2014

Grooms et al.
2015

Zanna et al.
2017

Bachman
2019
Jansen et al.
2019

Gugole & Franzke
2019, 2020

SALT

Holm
2015

Holm
2019
Cotter et al.
2019 a,b

Cotter et al.
2020

STUOD

LU

Mémin
2014

Resseguier et al.
2017 a,b,c

Bauer, Li et al.
2020 a,b
Resseguier, Li et al.
2021

Research goals

- I. Properly model small-scale dynamics effect on the large-scale circulation
- II. Develop flow-aware and resolution-aware parameterizations
- III. Application to uncertainty quantification & ensemble forecasts
- IV. Improve internal variability of ocean coarse-resolution models

Outline

I. Models under Location Uncertainty (LU)

- 1. LU principles**
- 2. LU parametrization**

III. Numerical applications of LU

- Ensemble forecasts
- Structuration and instability
- Low-frequency variability

Location Uncertainty (LU)

Stochastic flow

(Mémin, 2014)

$$d\mathbf{X}_t = \mathbf{v}(\mathbf{X}_t, t) dt + \sigma(\mathbf{X}_t, t) dB_t$$

Uncertainty / Noise

Integral operator

$$\sigma[f](\mathbf{x}, t) \triangleq \int_{\Omega} \check{\sigma}(\mathbf{x}, \mathbf{y}, t) f(\mathbf{y}) d\mathbf{y}, \quad f \in (L^2(\Omega))^d$$

Bounded kernel

Covariance operator

$$Q \triangleq \sigma \sigma^T \quad \rightarrow \quad \sigma dB_t \sim \mathcal{N}(\mathbf{0}, Q dt)$$

Lagrangian trajectory:

\mathbf{X}

Large-scale drift:

\mathbf{v}

Cylindrical Wiener process:

\mathbf{B}

Bounded domain:

$\Omega \subset \mathbb{R}^d$ ($d = 2, 3$)

Gaussian distribution:

\mathcal{N}

Location Uncertainty (LU)

(Mémin, 2014)

Spectral decomposition

$$\boldsymbol{\sigma}(\mathbf{x}, t) d\mathbf{B}_t = \sum_{n \in \mathbb{N}} \sqrt{\lambda_n(t)} \boldsymbol{\phi}_n(\mathbf{x}, t) d\beta_t^n$$

Eigenvalues problem:
 $Q\boldsymbol{\phi}_n = \lambda_n\boldsymbol{\phi}_n$
1D Brownian motions:
 $\{\beta_t^n\}_n$

Variance tensor

$$\mathbf{a}(\mathbf{x}, t) \triangleq \sum_{n \in \mathbb{N}} \lambda_n(t) \boldsymbol{\phi}_n(\mathbf{x}, t) \boldsymbol{\phi}_n^T(\mathbf{x}, t)$$

Transport under LU

(Resseguier et al., 2017a)

$$\Theta(\mathbf{X}_{t+\delta t}, t + \delta t) = \Theta(\mathbf{X}_t, t)$$

Stochastic transport operator

$$\mathbb{D}_t \Theta \triangleq d_t \Theta + (\mathbf{v}^* dt + \sigma d\mathbf{B}_t) \cdot \nabla \Theta - \frac{1}{2} \nabla \cdot (\mathbf{a} \nabla \Theta) dt = 0$$

Multiplicative
Advection Noise

Functional
Eddy Viscosity

Local time increment:
 $d_t \Theta = \Theta(x, t + \delta t) - \Theta(x, t)$

Effective advection velocity

$$\mathbf{v}^* \triangleq \mathbf{v} - \frac{1}{2} \nabla \cdot \mathbf{a} + \sigma^T (\nabla \cdot \sigma)$$

Noise
Inhomogeneity

\mathbf{v}_s – Itô-Stokes drift
(Bauer, Li et al., 2020a)

Noise
Compressibility

Proprieties of LU transport

Conservation of local moments *(Resseguier et al., 2017a)*

$$\mathbb{D}_t \left(\frac{1}{p} \Theta^p \right) = \Theta^{p-1} \mathbb{D}_t \Theta = 0, \quad p \geq 1$$

Conservation of global moments

$$\begin{aligned} \nabla \cdot \mathbf{v}^* &= \nabla \cdot \boldsymbol{\sigma} d\mathbf{B}_t = 0 \\ \mathbf{v}^* \cdot \mathbf{n} \Big|_{\partial\Omega} &= \boldsymbol{\sigma} d\mathbf{B}_t \cdot \mathbf{n} \Big|_{\partial\Omega} = 0 \end{aligned} \quad \Rightarrow \quad d_t \int_{\Omega} \frac{1}{p} \Theta^p d\mathbf{x} = 0, \quad p \geq 1$$

Normal vector:

\mathbf{n}

Domain boundary:

$\partial\Omega$

Control-volume:

$\mathcal{V}(t)$

Stochastic Reynolds transport theorem *(Mémin, 2014)*

(SRTT)

$$d_t \int_{\mathcal{V}(t)} \Theta d\mathbf{x} = \int_{\mathcal{V}(t)} \left(\mathbb{D}_t \Theta + \Theta \nabla \cdot (\mathbf{v}^* dt + \boldsymbol{\sigma} d\mathbf{B}_t) \right) d\mathbf{x}$$

Derived LU models

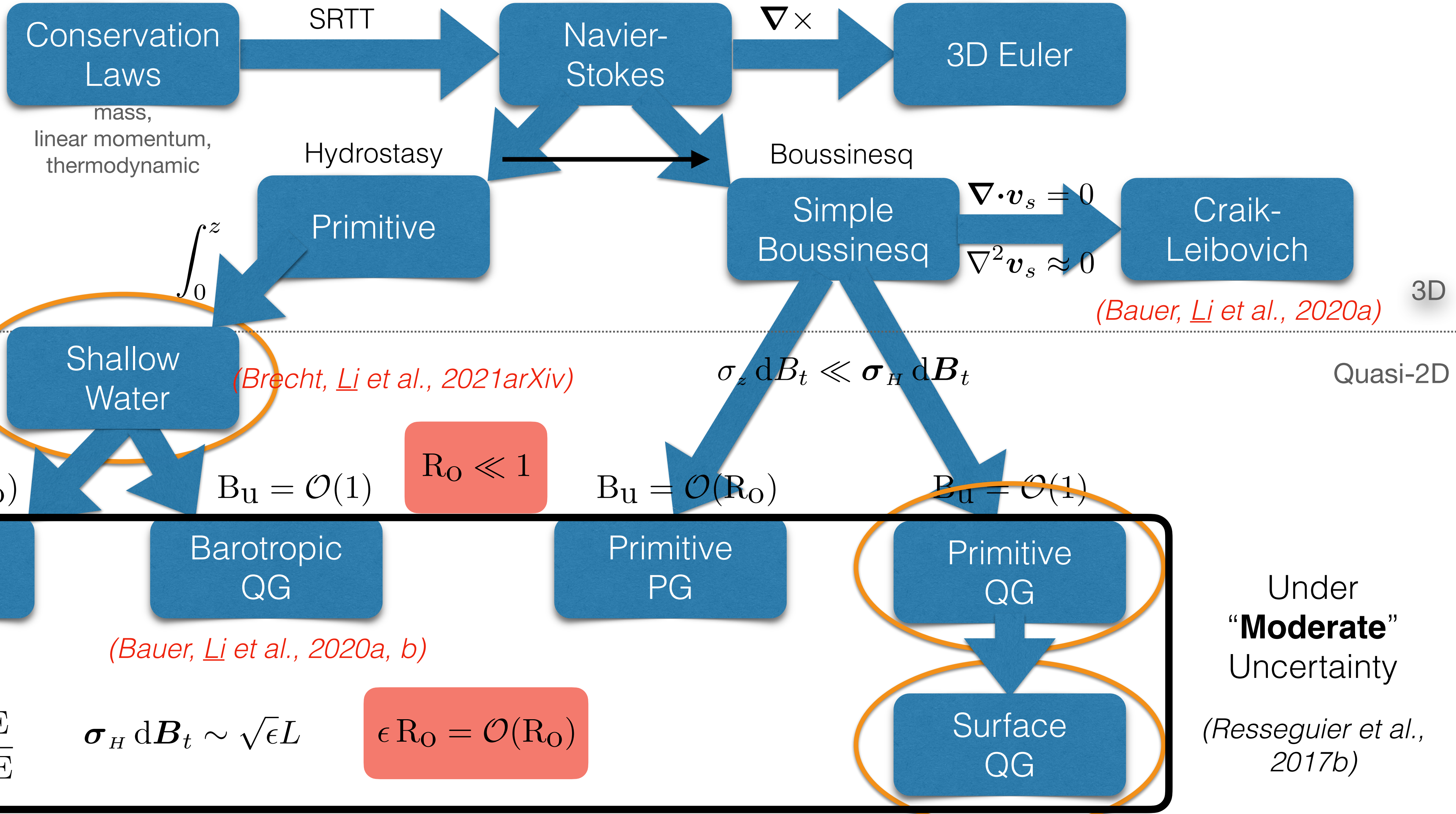
Rossby number:
 R_o

Burger number:
 B_u

Correlation time scale:
 T_σ

Advection time scale:
 T

Typical length:
 L



$$\epsilon \triangleq \frac{T_\sigma}{T} \frac{\text{EKE}}{\text{MKE}}$$

$$\sigma_H dB_t \sim \sqrt{\epsilon} L$$

$$\epsilon R_o = \mathcal{O}(R_o)$$

Under
"Moderate"
Uncertainty
(Resseguier et al.,
2017b)

LU parametrization

Data-driven

$$\begin{aligned}\sigma(\mathbf{x}, t) d\mathbf{B}_t &= \int_{\Omega} \check{\sigma}(\mathbf{x}, \mathbf{y}, t) d\mathbf{B}_t(\mathbf{y}) d\mathbf{y} \\ &= \sum_{n \in \mathbb{N}} \check{\phi}_n(\mathbf{x}, t) d\beta_t^n, \quad \check{\phi}_n \triangleq \sqrt{\lambda_n} \phi_n\end{aligned}$$

Parametrization

Homogeneous

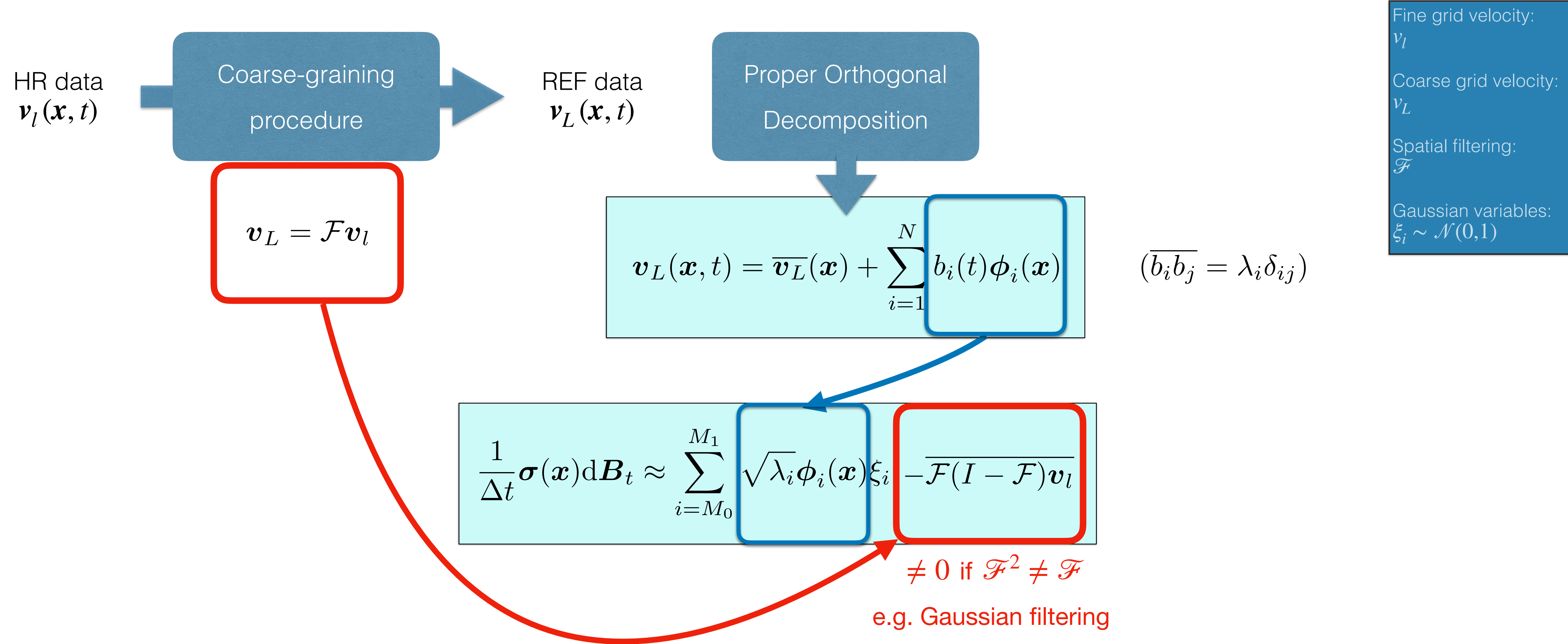
Heterogeneous

Stationary

Non-stationary

Method	Type	Sources
LU-FFT	Data-free, homogeneous, stationary	<i>Resseguier et al., 2017b</i>
LU-POD	Data-driven, heterogeneous, stationary	<i>Bauer, Li et al., 2020a, b; Brecht, Li et al., 2021arXiv</i>
LU-PSO	Data-free, heterogeneous, non-stationary	<i>Resseguier, Li et al., 2021; Brecht, Li et al., 2021arXiv</i>
LU-SGS	Data-free, heterogeneous, non-stationary	<i>Resseguier, Li et al., 2021</i>

Off-line learning from HR data (LU-POD)



Without data: On-line estimation of EOFs by sliding window on coarse resolution snapshots *(Resseguier, Li et al., 2021; Brecht, Li et al., 2021arXiv)*

Energy-budget based noise (LU-SGS)

$$\mathbb{D}_t \Theta = \mathbf{L}[\Theta] dt$$

Identification of diffusions

$$\frac{1}{2} \nabla \cdot (\mathbf{a} \nabla \Theta) = \gamma \mathbf{L}[\Theta], \quad \gamma > 0$$

Orthogonal basis:
 $\{e_n \in L^2(\Omega)\}_n$

1D Brownian motions:
 $\{\beta_t^n\}_n$

Inner product:
 $\langle f, g \rangle_\Omega = \int_\Omega f(x)g(x) dx$

Norm:
 $\|f\|_\Omega = \langle f, f \rangle_\Omega^{1/2}$

Random energy intake = $\gamma \times$ Dissipation

Simplified random equation
(Resseguier, Li et al., 2021)

$$d_t \Theta + \mathbf{v}^* \cdot \nabla \Theta dt = \mathbf{L}[\Theta] dt - \sqrt{2\gamma} \sum_n \lambda_n e_n d\beta_t^n$$

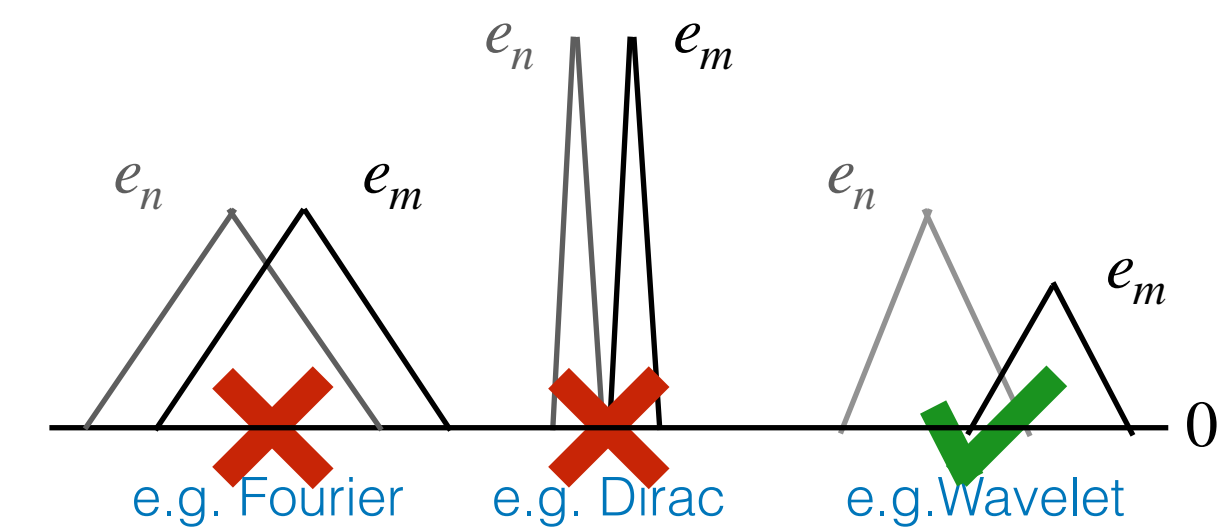
e.g.
 Inverse
 WT of
 $\{\lambda_n d\beta_t^n\}_n$

e.g.
 Wavelet
 Transform
 (WT) of
 $\sqrt{A_4} \nabla^2 \Theta$

$$\lambda_n = \langle \mathbf{H}[\Theta], e_n \rangle_\Omega, \quad \|\mathbf{H}[\Theta]\|_\Omega^2 = -\langle \Theta, \mathbf{L}[\Theta] \rangle_\Omega$$

e.g. $\{e_n\}_n$: Wavelets basis

e.g. $\mathbf{L}[\Theta] = -A_4 \nabla^4 \Theta$



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2. LU parametrization

III. Numerical applications of LU

- 1. Ensemble forecasts**
- 2. Structuration and instability**
- 3. Low-frequency variability**

Ensemble forecasts of SQG-LU

(Resseguier et al., 2017b;
Resseguier, Li et al., 2021)

SQG-LU

$$\mathbb{D}_t b = -A_8 \nabla^8 b dt$$

$$\mathbf{u} = -cst \nabla^\perp \Delta^{-1/2} b$$

$$\nabla \cdot \sigma dB_t = \nabla \cdot \mathbf{u}_s = 0$$

Stochastic transport:
 \mathbb{D}_t

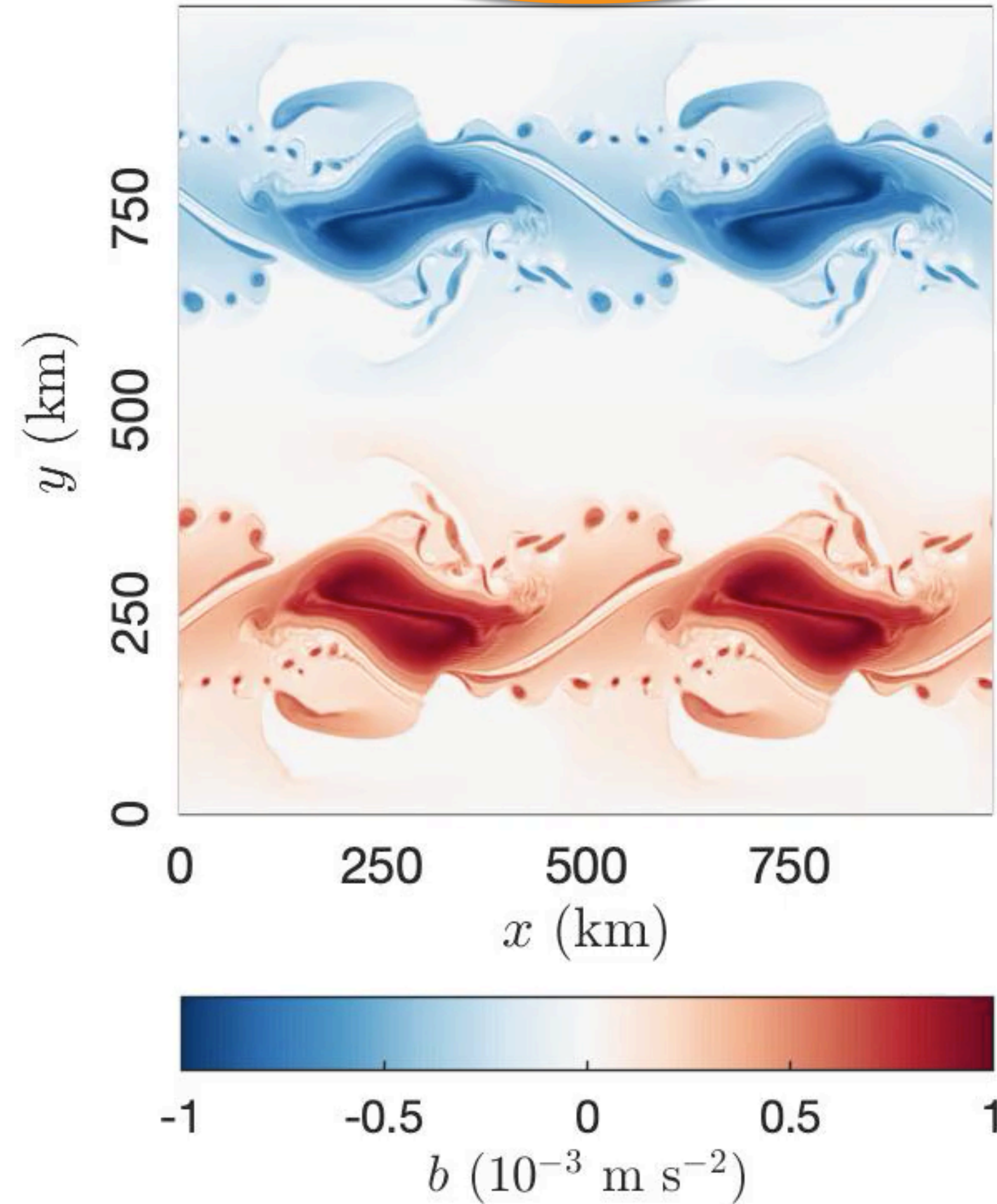
Surface buoyancy:
 b

Large-scale drift:
 \mathbf{u}

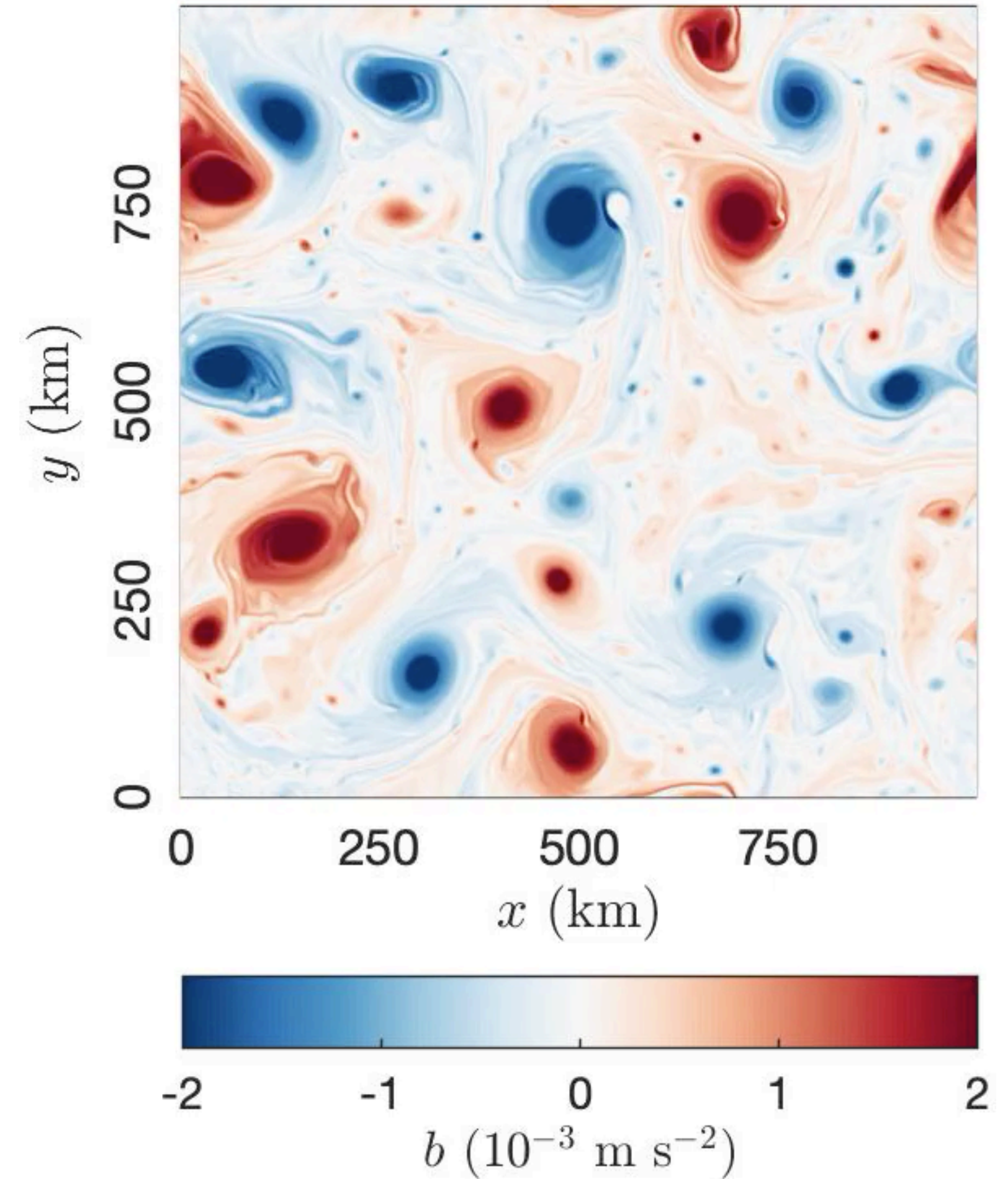
Small-scale noise:
 σdB_t

Ito-Stokes drift
 $\mathbf{u}_s = \frac{1}{2} \nabla \cdot \mathbf{a}$

Exp.1
Day = 17



Exp.2
Day = 17

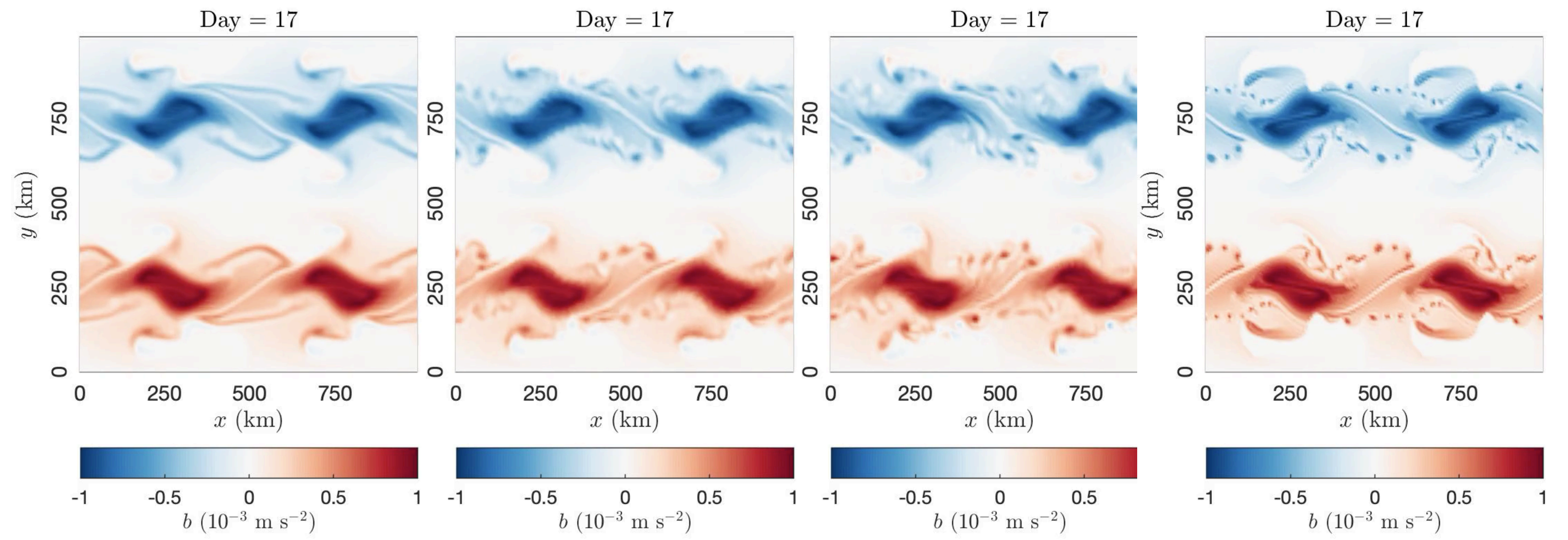


HR ($\Delta = 2$ km) deterministic simulations

Coarse-resolution simulations

($\Delta = 8$ km)

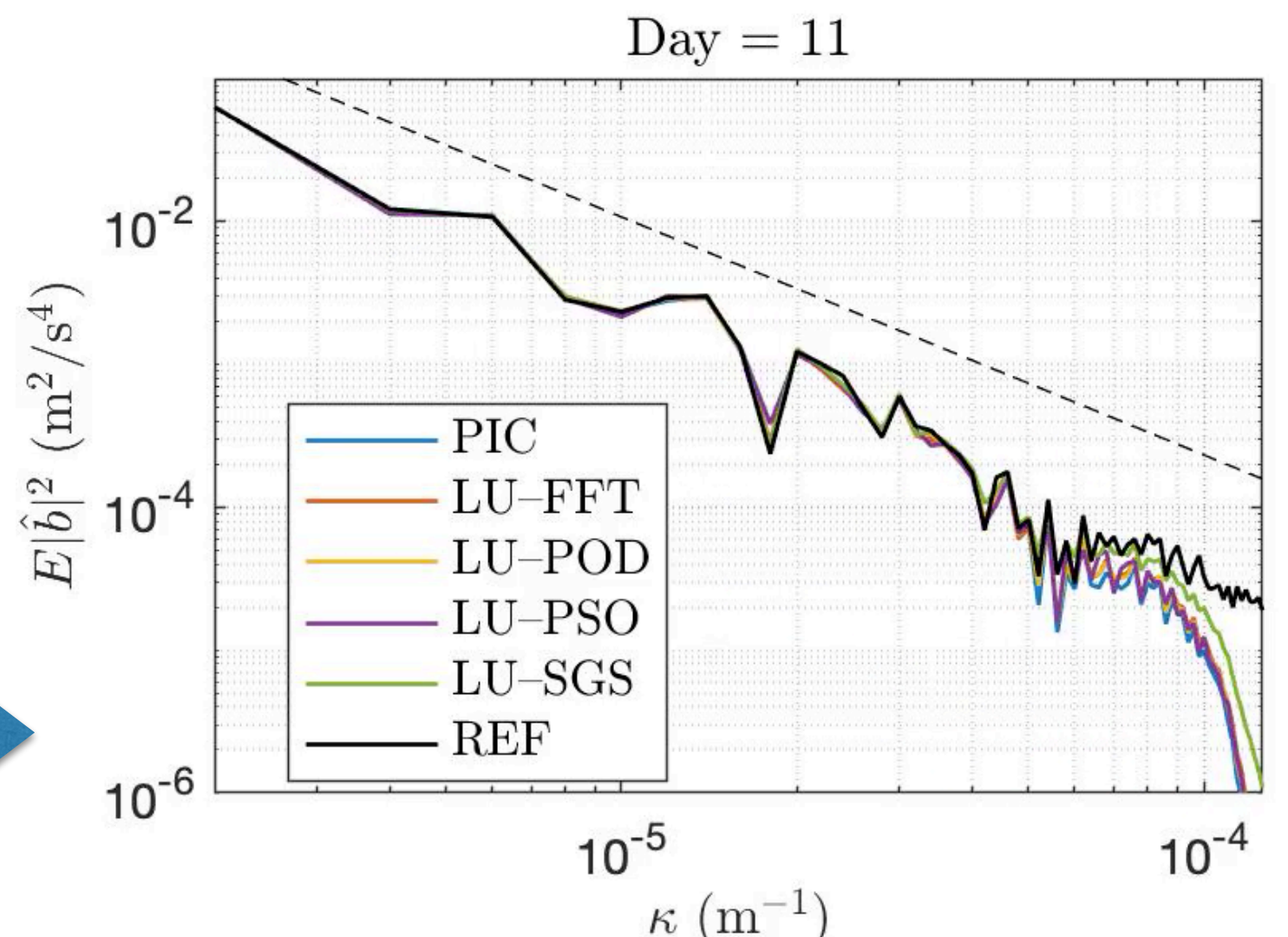
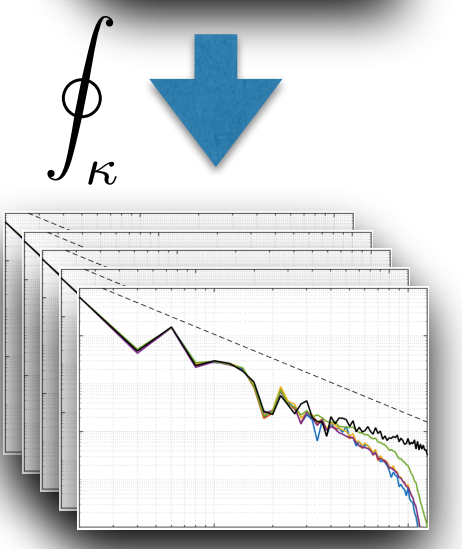
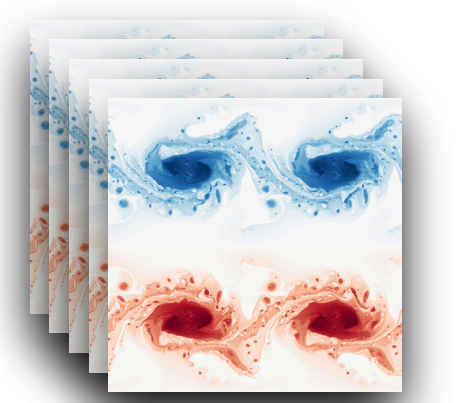
One realization



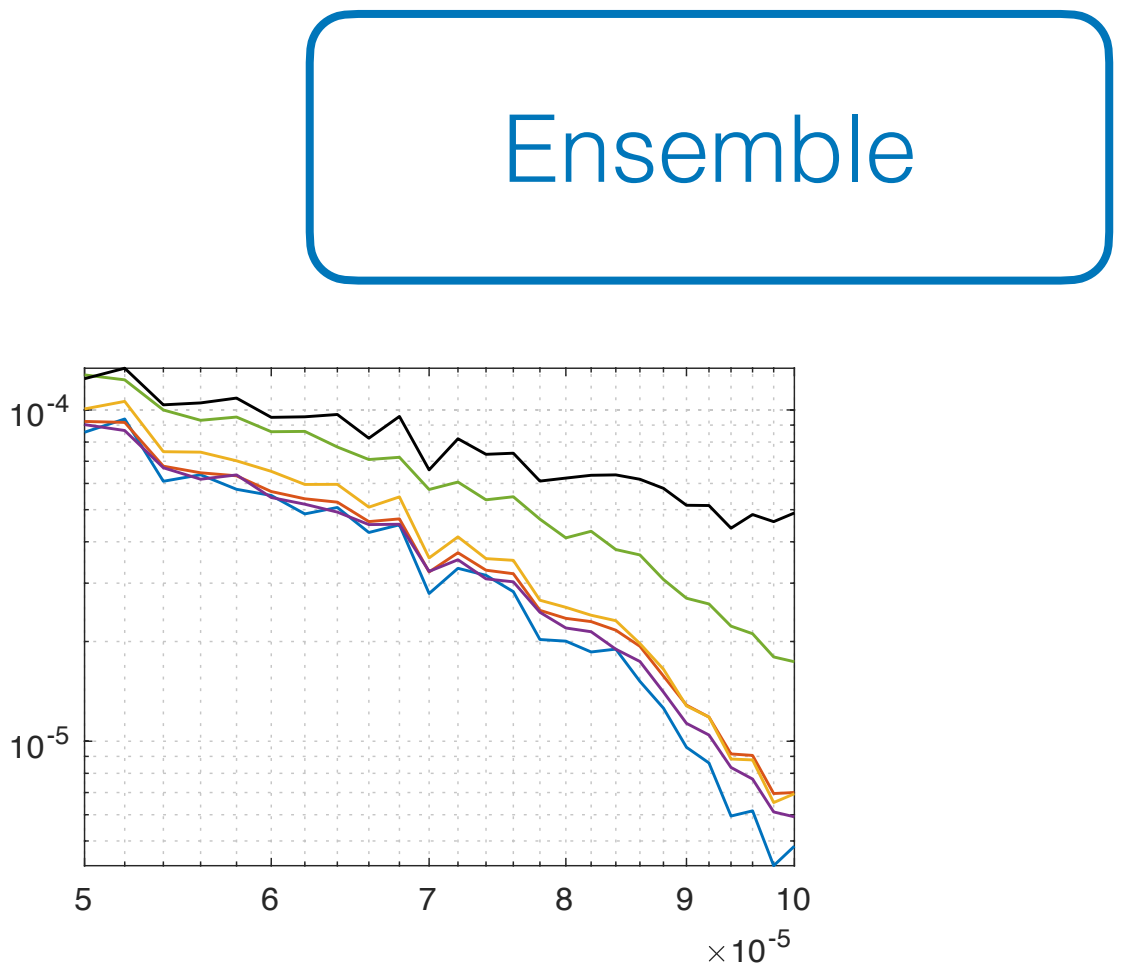
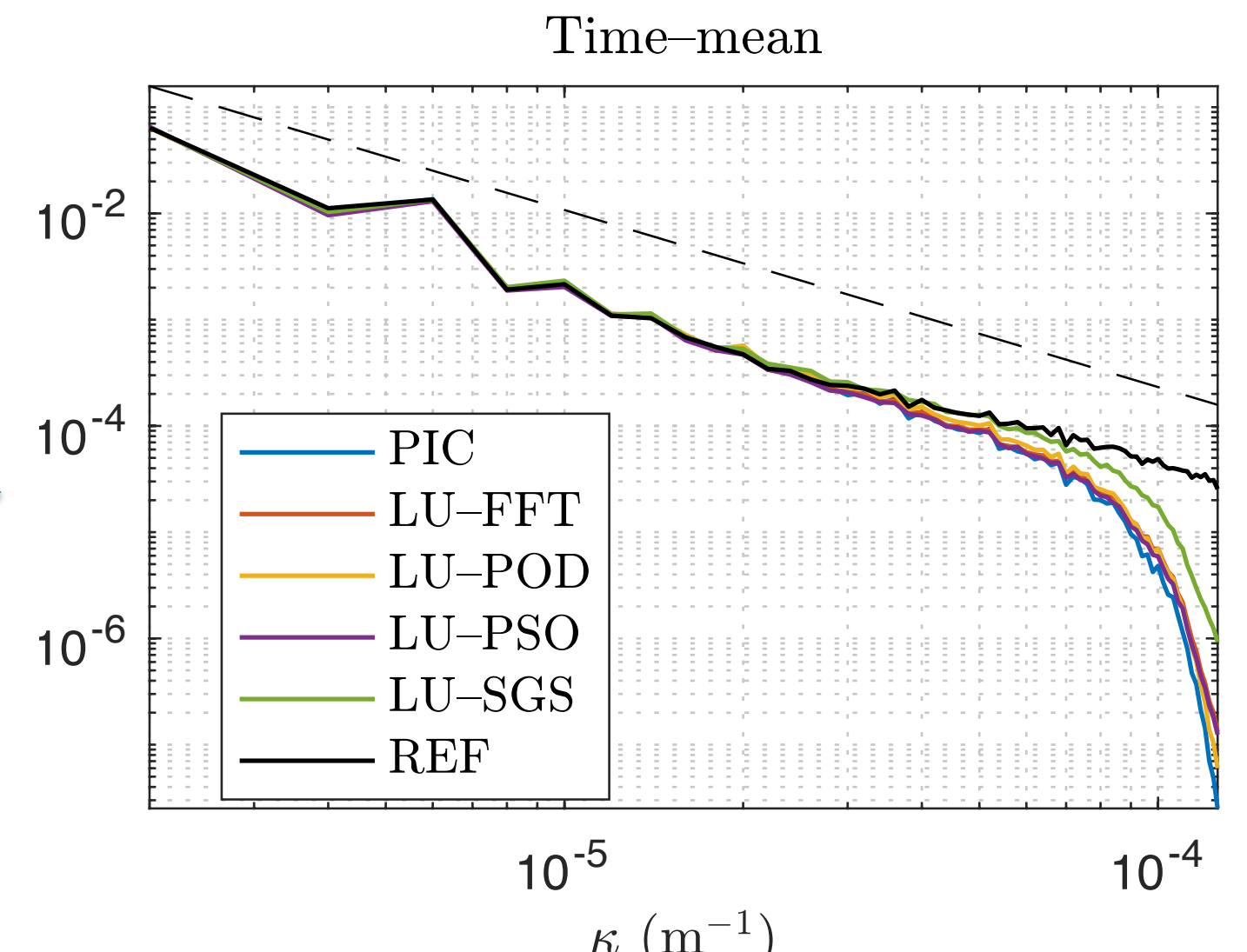
PIC $\xrightarrow{\text{(Resseguier et al., 2017b)}}$ LU-FFT $\xrightarrow{\text{(Resseguier, Li et al., 2021)}}$ LU-SGS REF

- Perturbed initial condition
PIC
- Homogeneous noise
LU-FFT
- Heterogeneous noises
LU-POD (data, off-line)
LU-PSO (no-data, on-line)
LU-SGS (energy-budget, wavelet basis, no-data, on-line)

Resolving small-scales: **LU better than PIC & LU-SGS better than other LUs**



\int_T

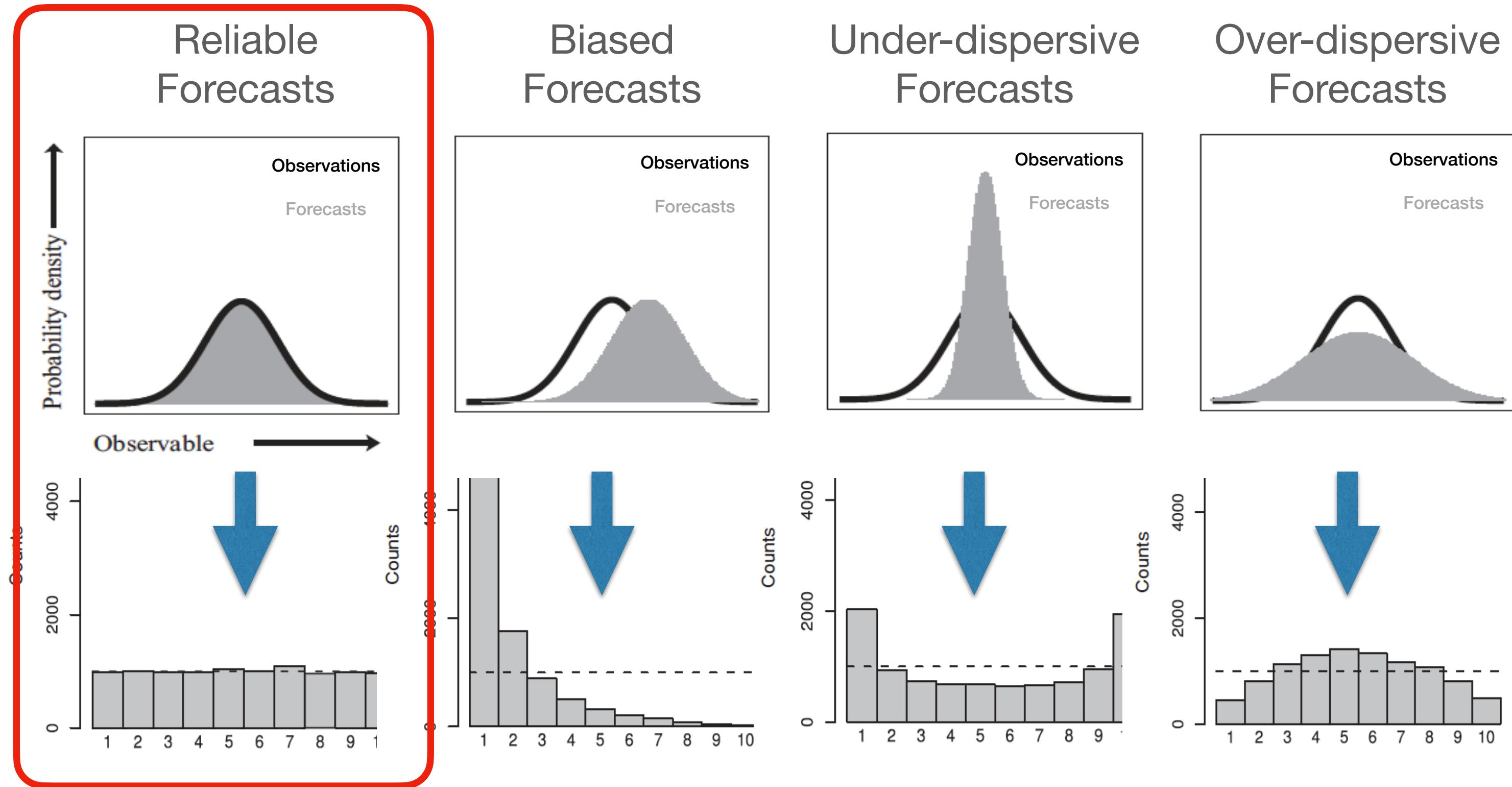


Ensemble

Metrics for ensemble forecasts

Rank Histogram

Capacity of the ensemble to explore all reference possible values



Continuous Ranked Proper Score

Distance between the cumulative probability distribution function of the forecasts and the observations

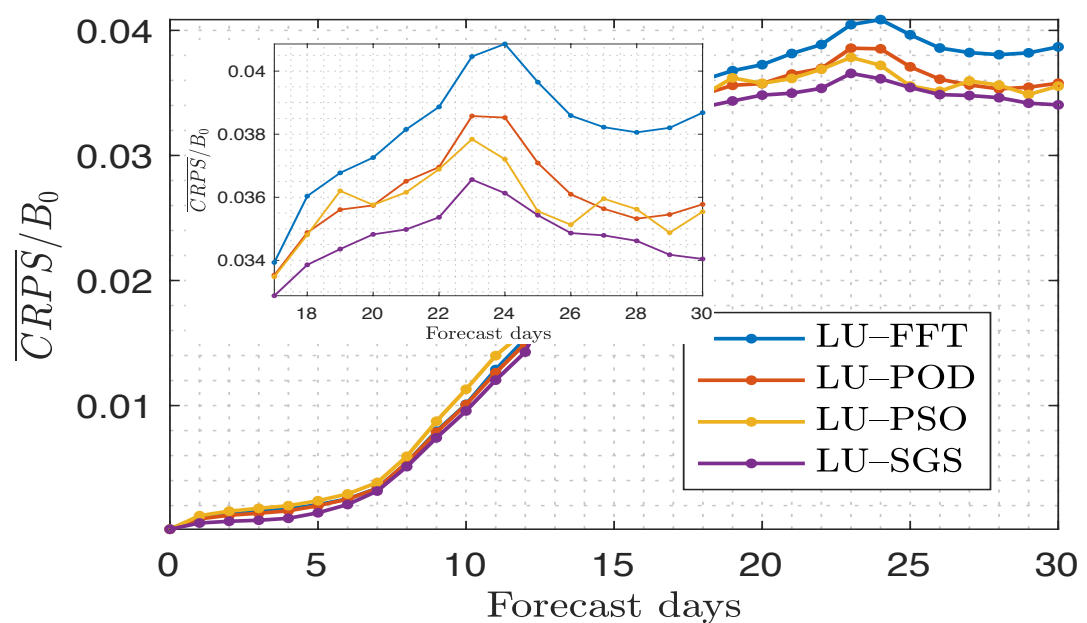
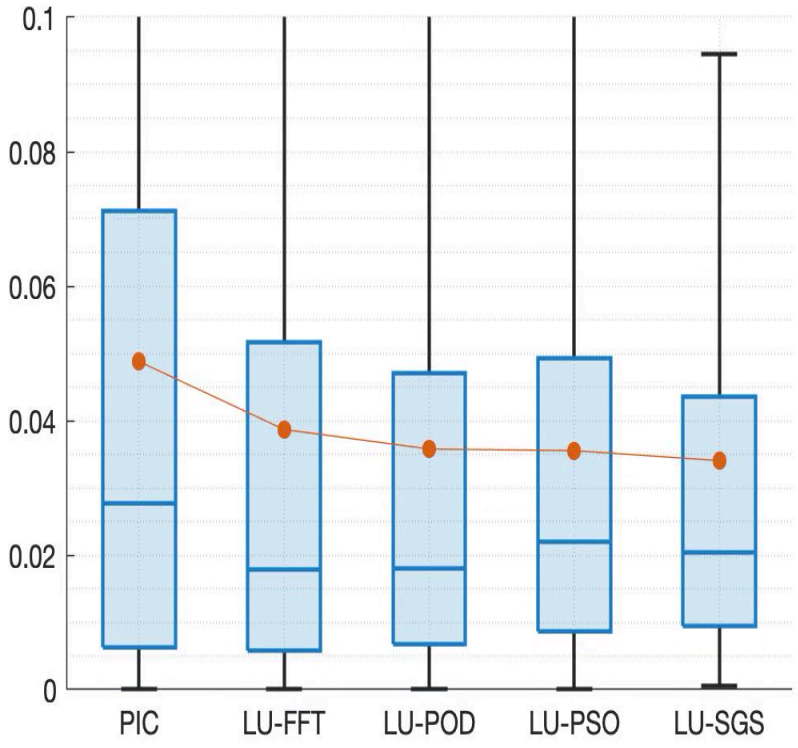
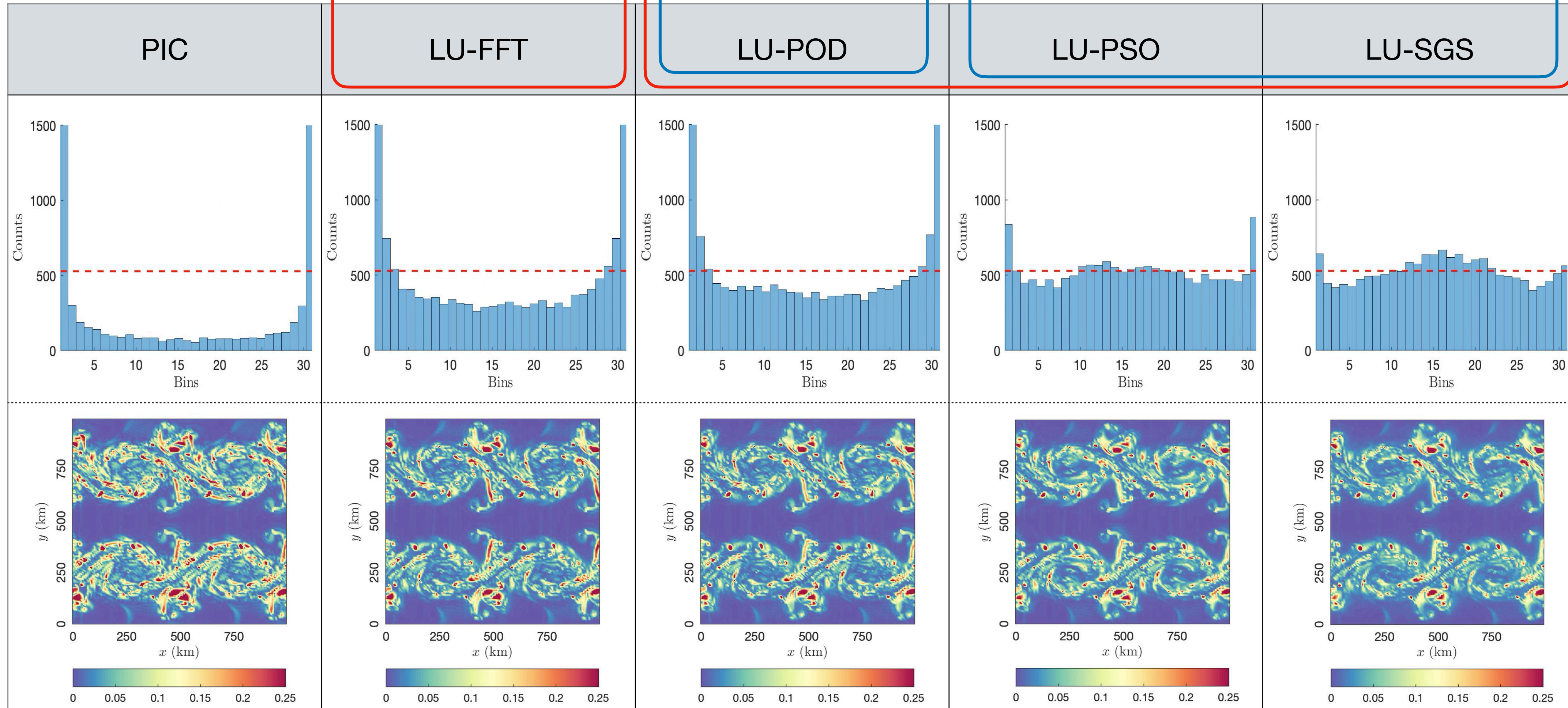
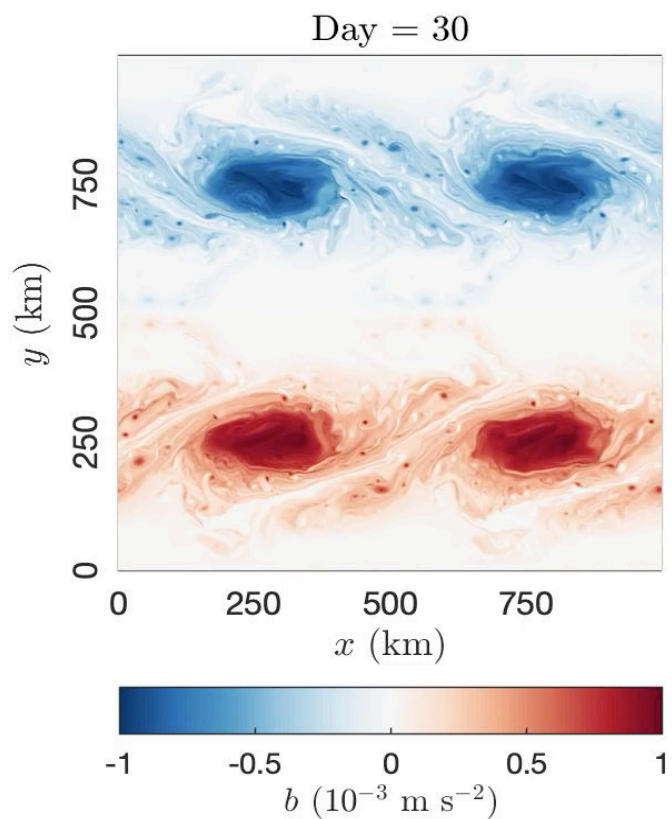
$$\text{CRPS}(F, q^o) = \int_{\mathbb{R}} (F(\mathcal{B}) - H(\mathcal{B} - q^o))^2 d\mathcal{B}$$



Observations:
 q^o
CDF of forecasts:
 F
Heaviside function:
 H

Ensemble forecasts of SQG-LU

(Resseguier, Li et al., 2021)



Reliability of ensemble forecasts **Better**

PIC v.s. LU	LU-SGS v.s. Others
Homogeneous v.s. Heterogeneous	Non-stationary v.s. Stationary

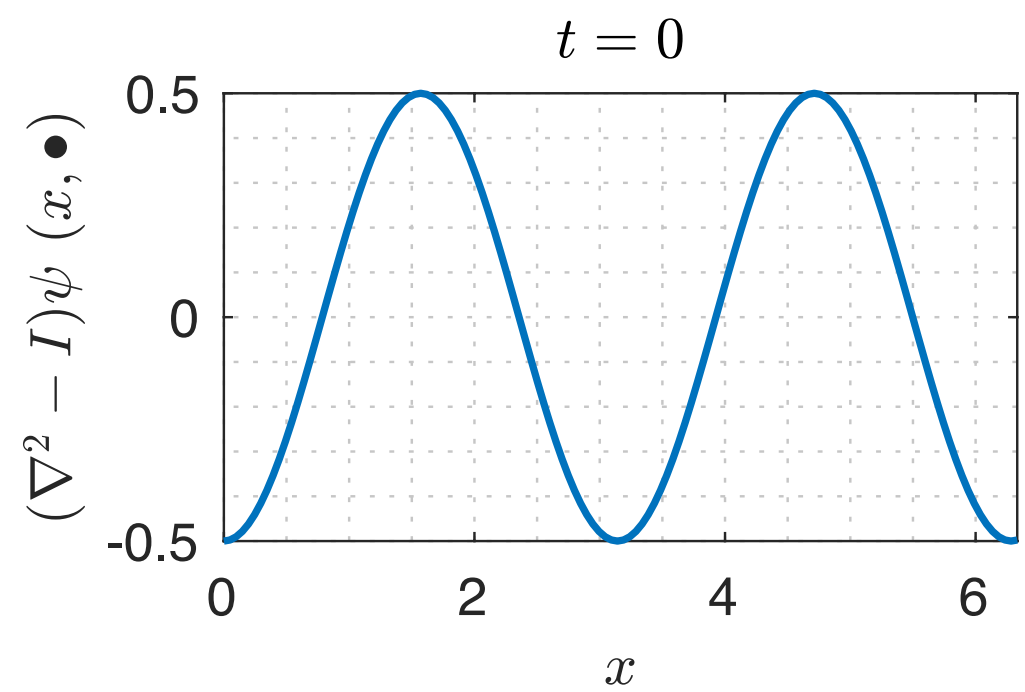
Effect of noise inhomogeneity

BQG-LU

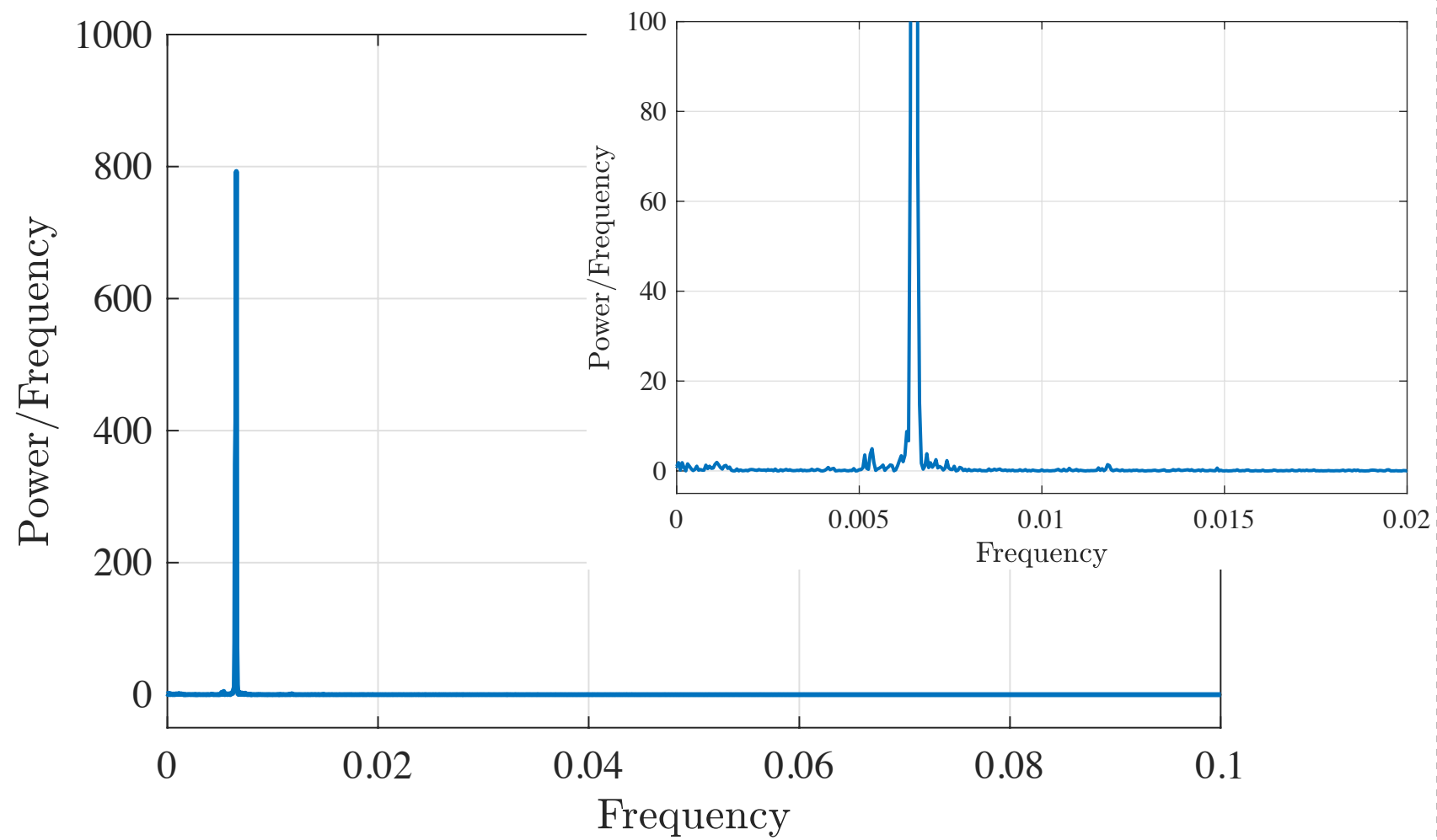
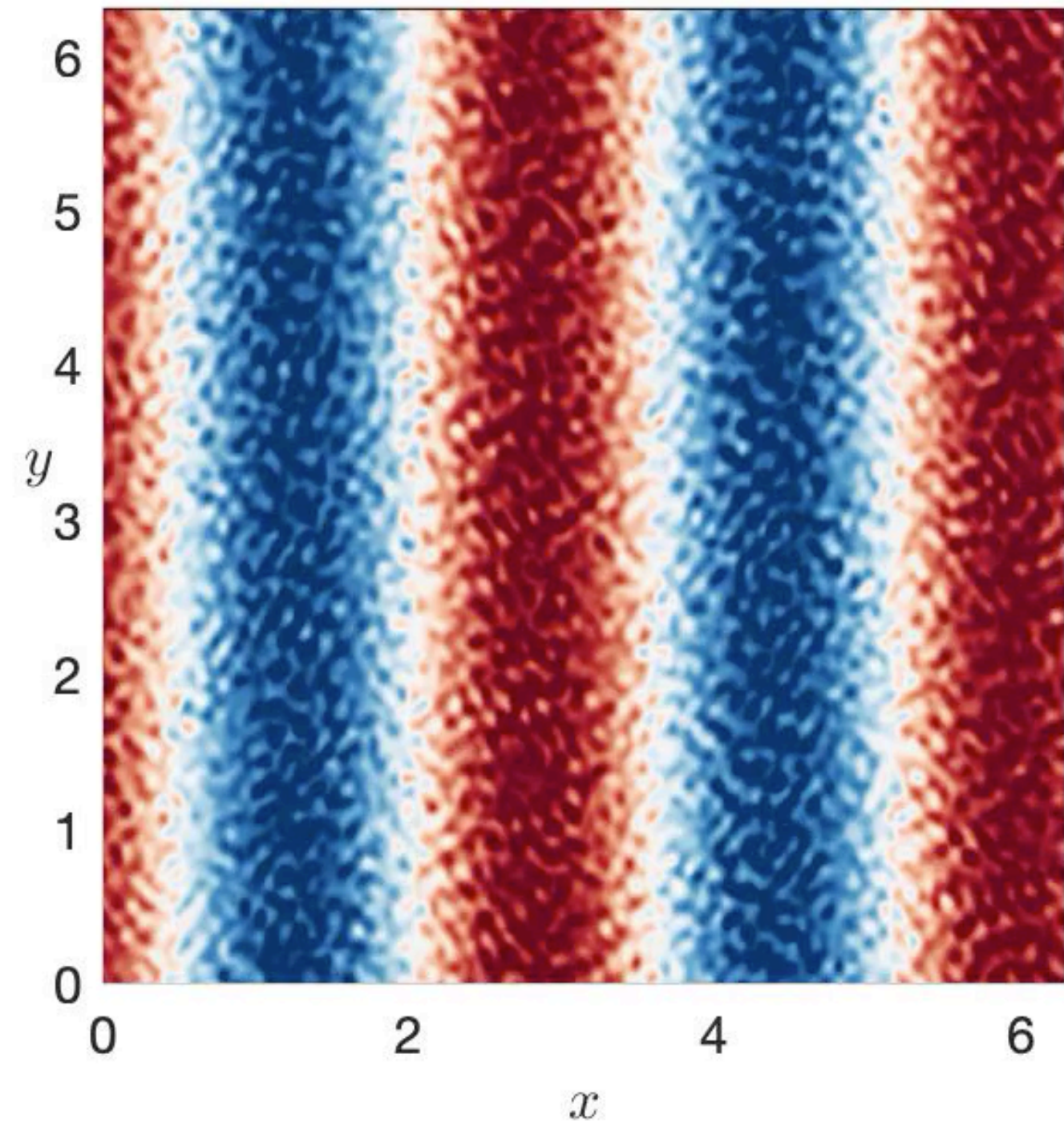
$$\mathbb{D}_t q = d\dot{Q}_t$$

$$q = (\nabla^2 - I)\psi + y$$

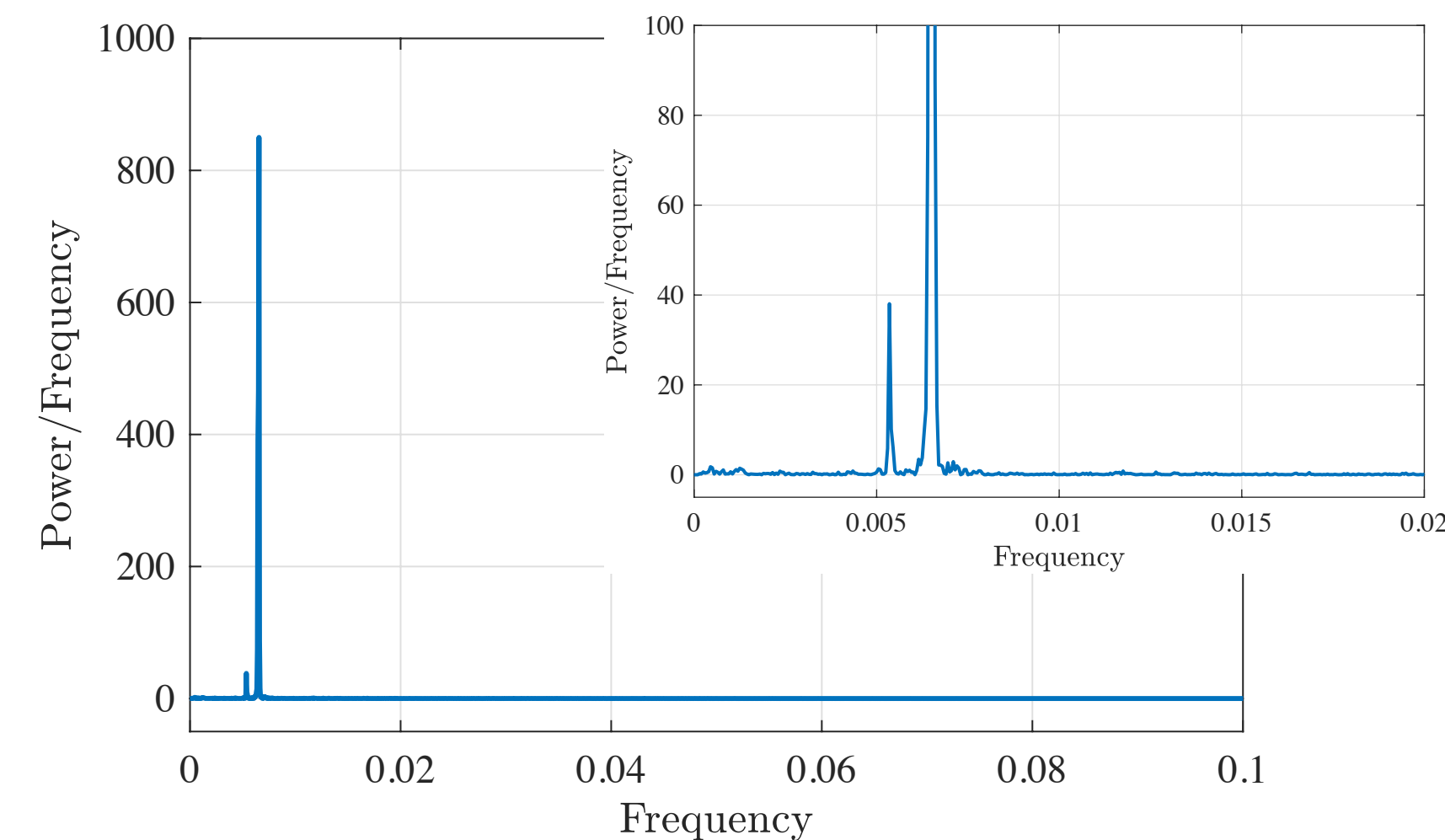
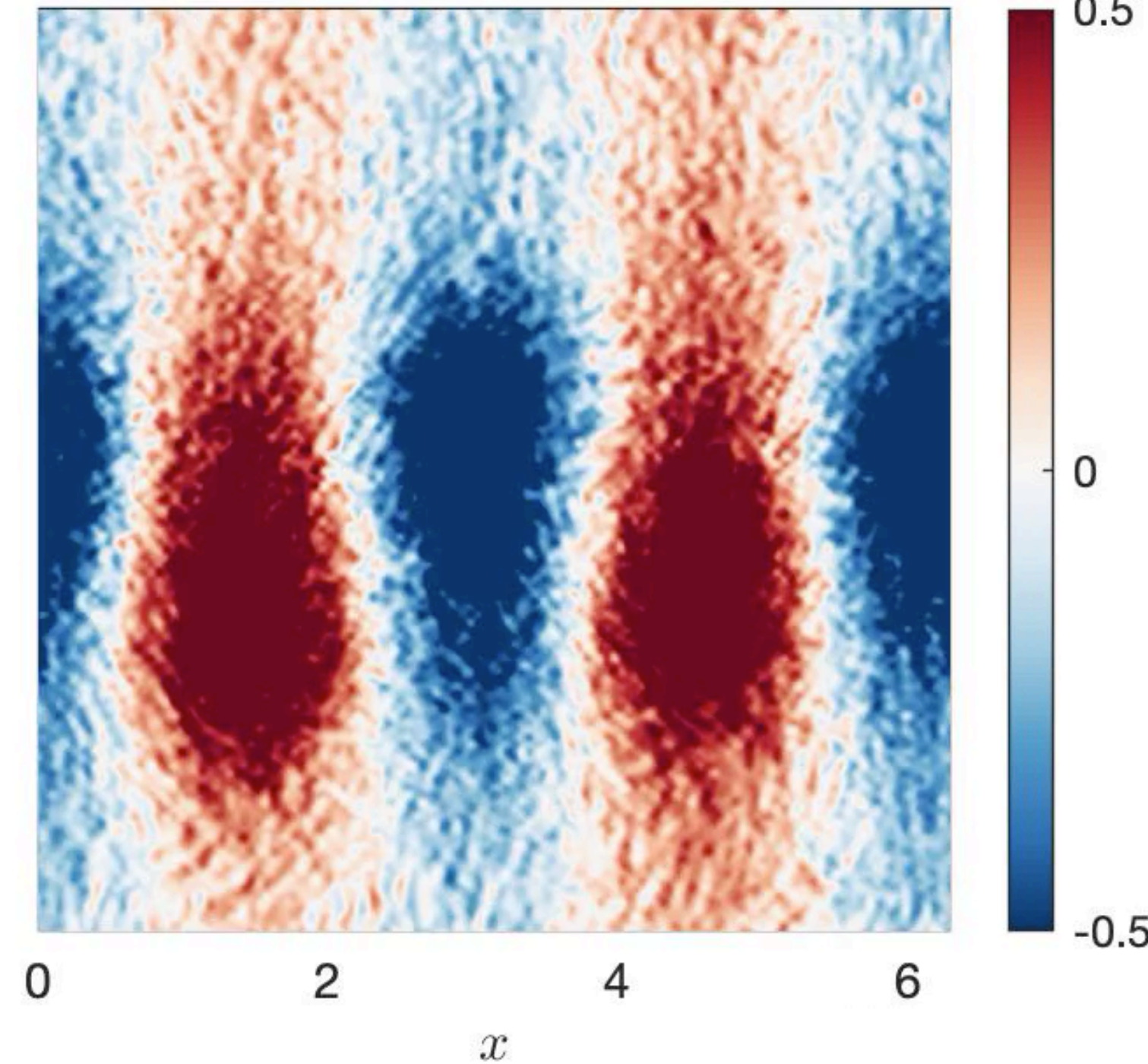
$$\mathbf{u} = \nabla^\perp \psi$$



(Homogeneous) LU-FFT



LU-PSO (Heterogeneous)



Small-scale inhomogeneity
 ↓
Large-scale structuration

(Bauer, Li et al., 2020a)

Potential vorticity (PV):
 q
 PV sources and sinks (LU):
 $d\dot{Q}_t$
 Stream function:
 ψ

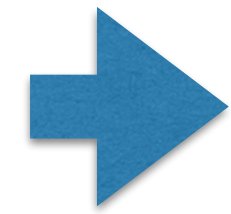
Prediction of barotropic instability

RSW-LU

$$\mathbb{D}_t \mathbf{u} + \mathbf{f} \times \mathbf{u} \, dt = -(g \nabla h + A_4 \nabla^4 \mathbf{u}) \, dt$$

$$\mathbb{D}_t h + h \nabla \cdot \mathbf{u} \, dt = 0$$

$$\nabla \cdot \boldsymbol{\sigma} \, dB_t = \nabla \cdot \mathbf{u}_s = 0$$



$(A_4 = 0)$

Energy conservation

$$d_t \int_{\Omega} \frac{\rho}{2} (h \|\mathbf{u}\|^2 + gh^2) \, d\mathbf{x} = 0$$

(Brecht, Li et al., 2021arXiv)

Day 6

Coriolis parameter:
 f

Water thickness:
 h

Water density:
 ρ

Gravity:
 g

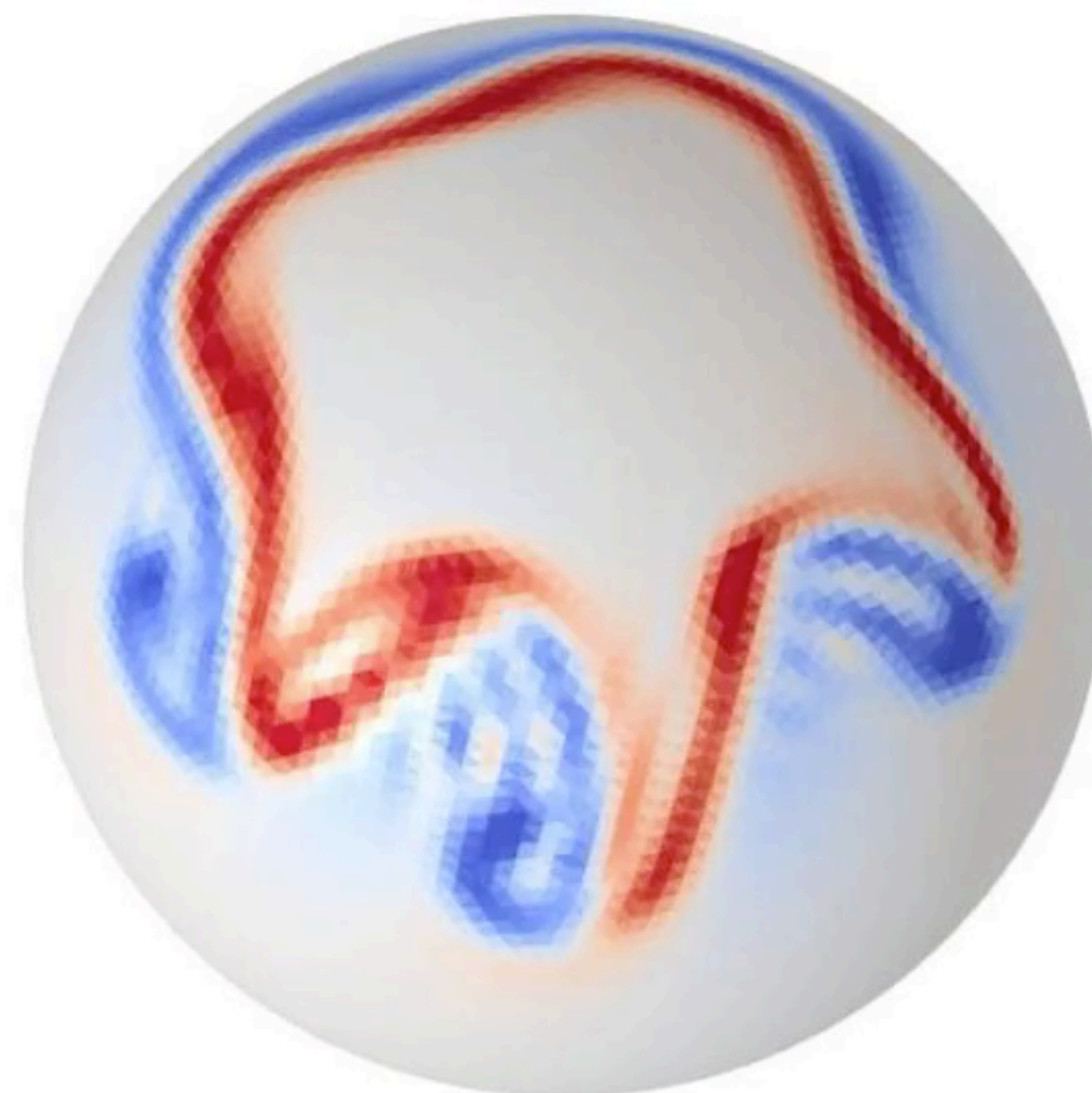
Relative vorticity:
 $q = \nabla \times \mathbf{u}$

**LU improves
in
triggering
instability**

REF



LU-PSO



LR



Resolution

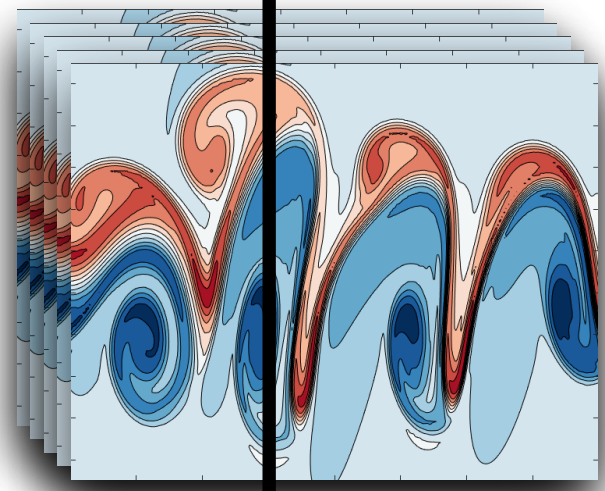
20408
triangles

20



(Brecht, Li et al.,
2021arXiv)

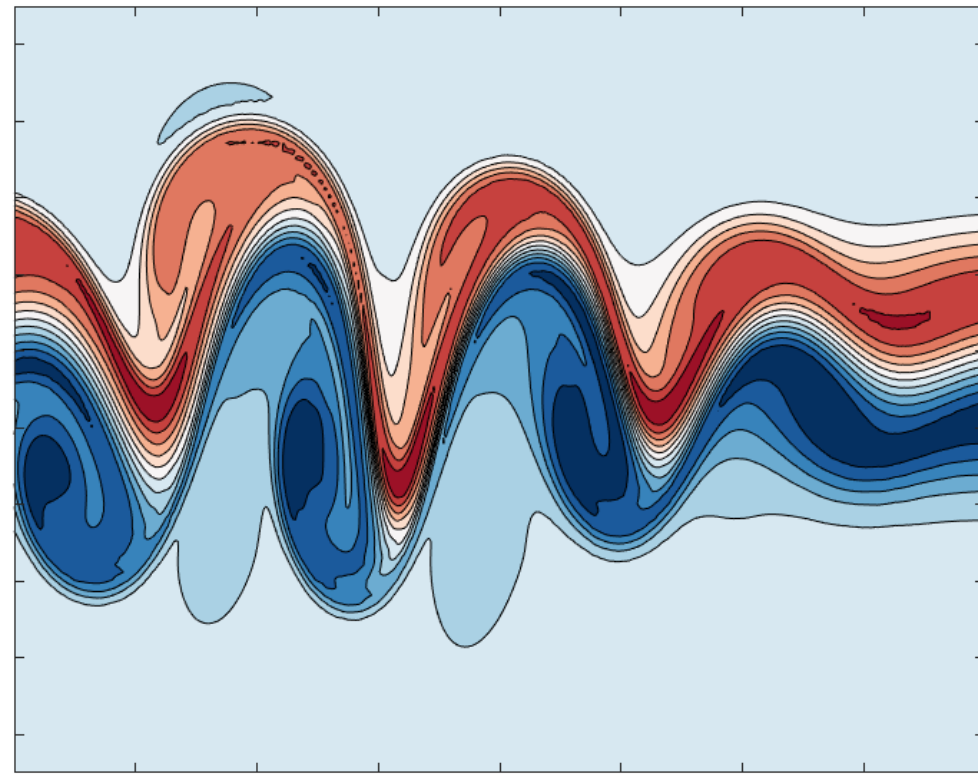
Ensemble mean
(Day 5)



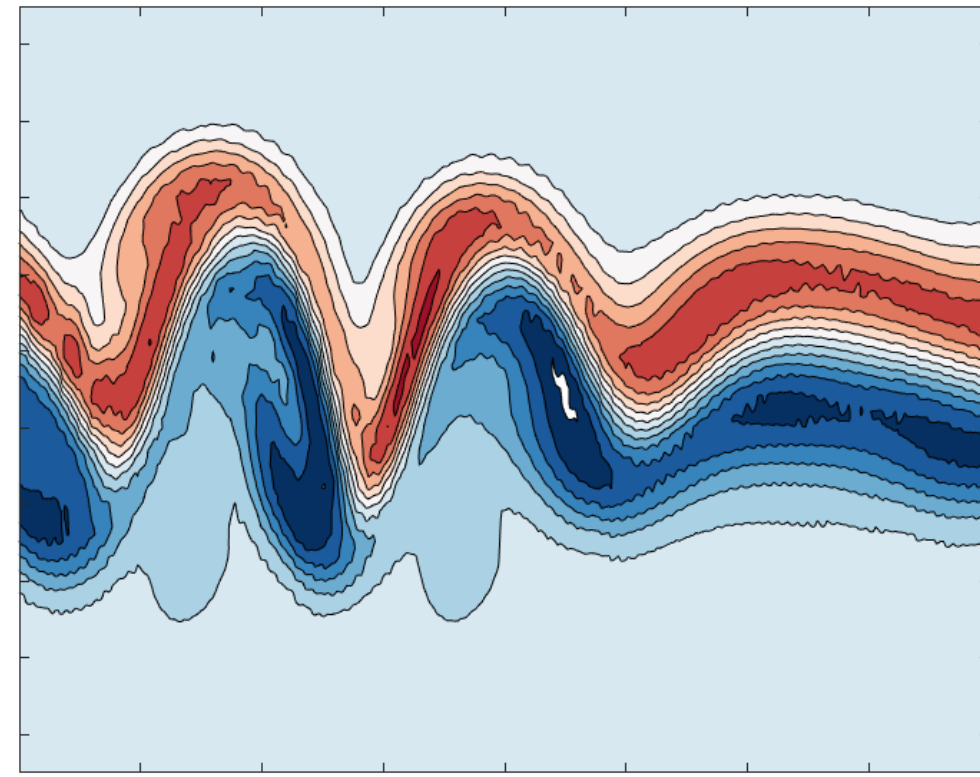
Evolution of
ensemble spread

— REF
■ PIC-PSO
■ LU-PSO

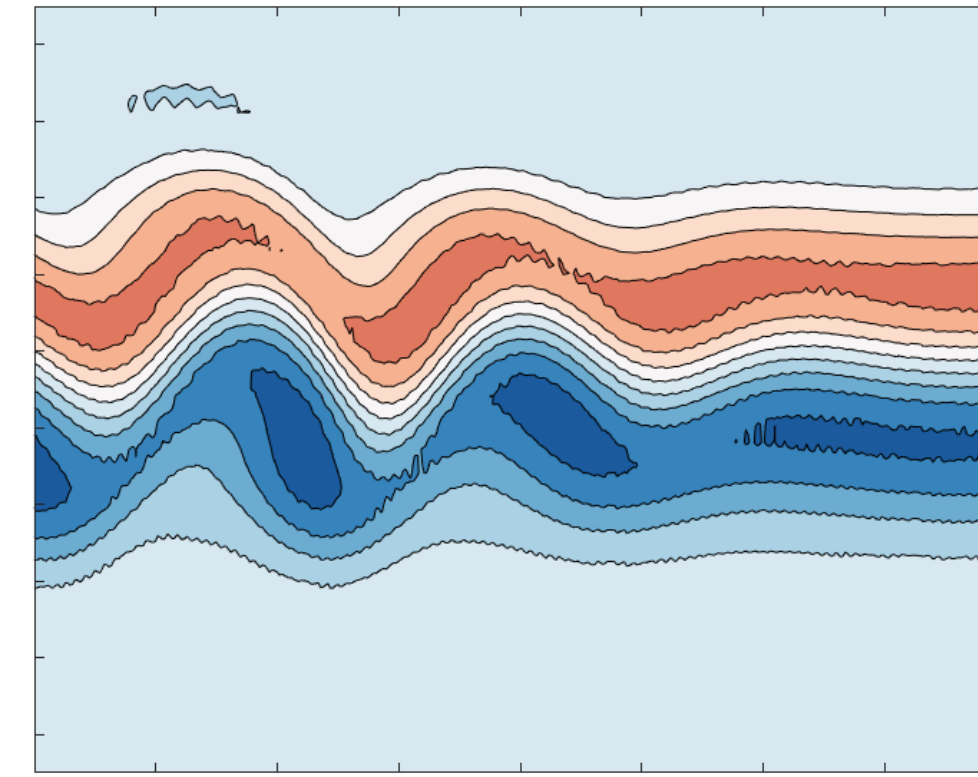
REF



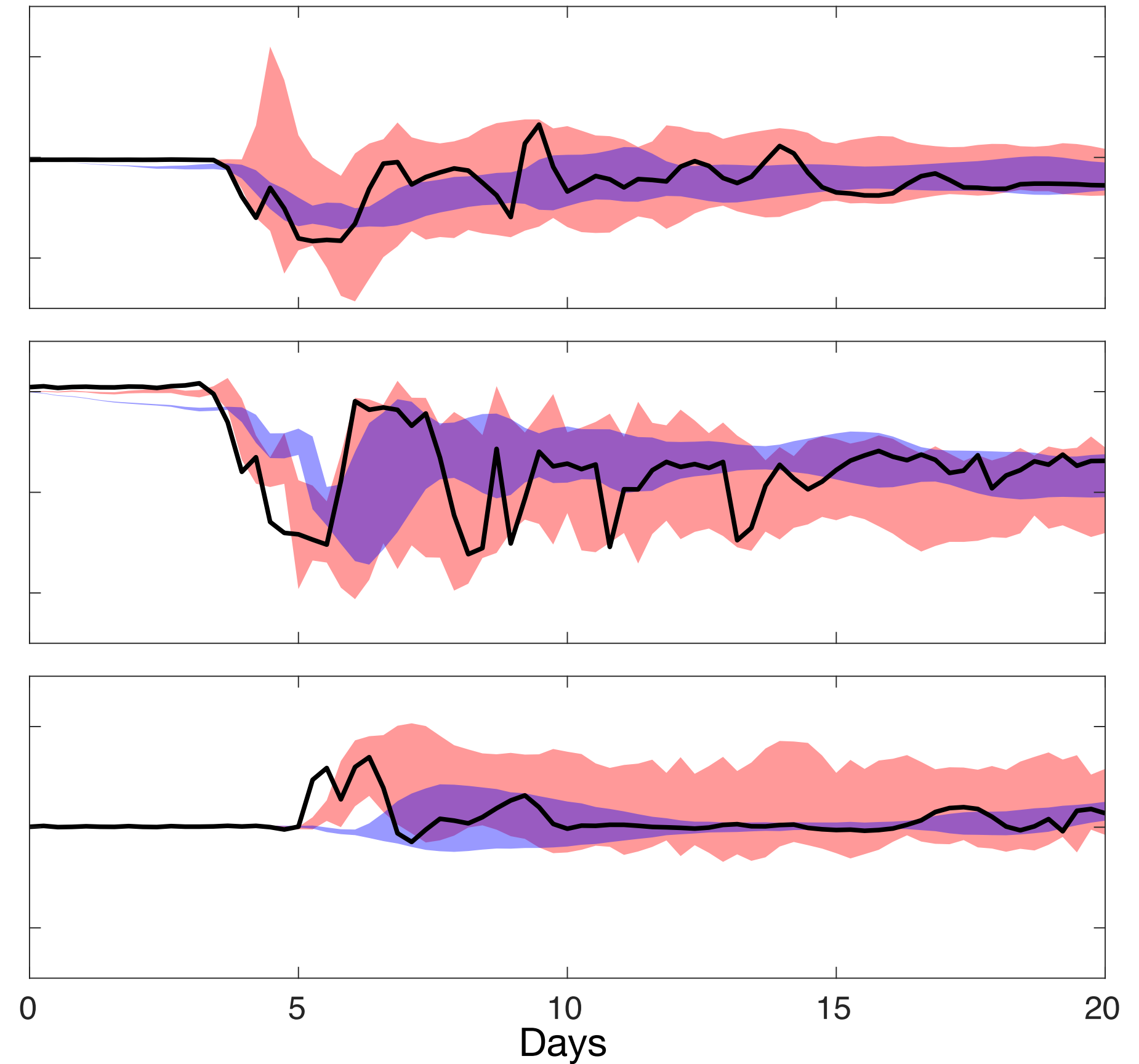
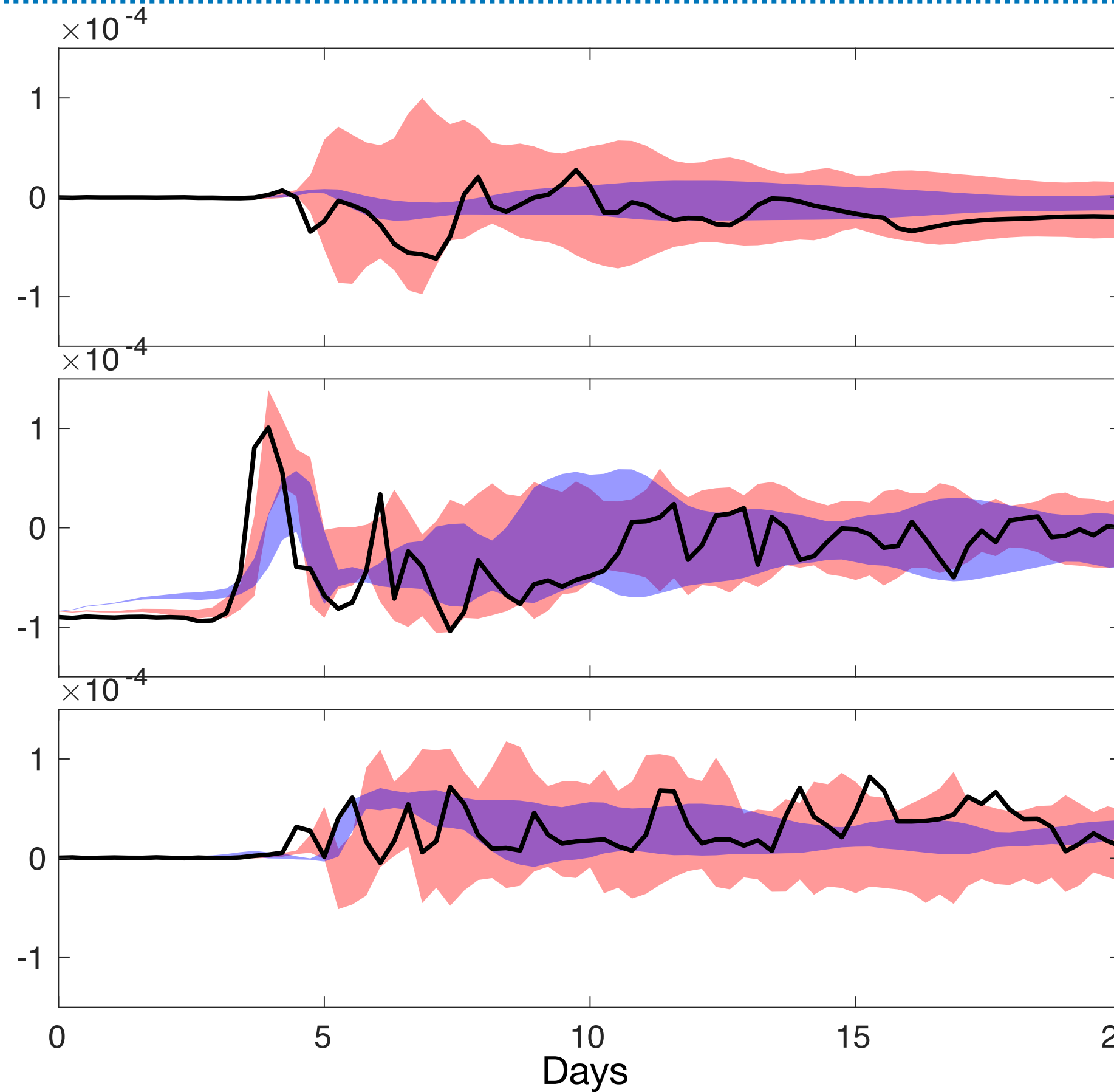
LU-PSO



PIC-PSO



**LU provides both
reliable mean
forecasts and
efficient spread**



QG-LU

$$\mathbb{D}_t \mathbf{q} = d\dot{\mathbf{Q}}_t + \mathbf{Be} - \frac{A_4}{f_0} \nabla^6 \mathbf{p}$$

$$\mathbf{q} = \frac{1}{f_0} \nabla^2 \mathbf{p} - f_0 \mathbf{A} \mathbf{p} + \beta \mathbf{y}$$

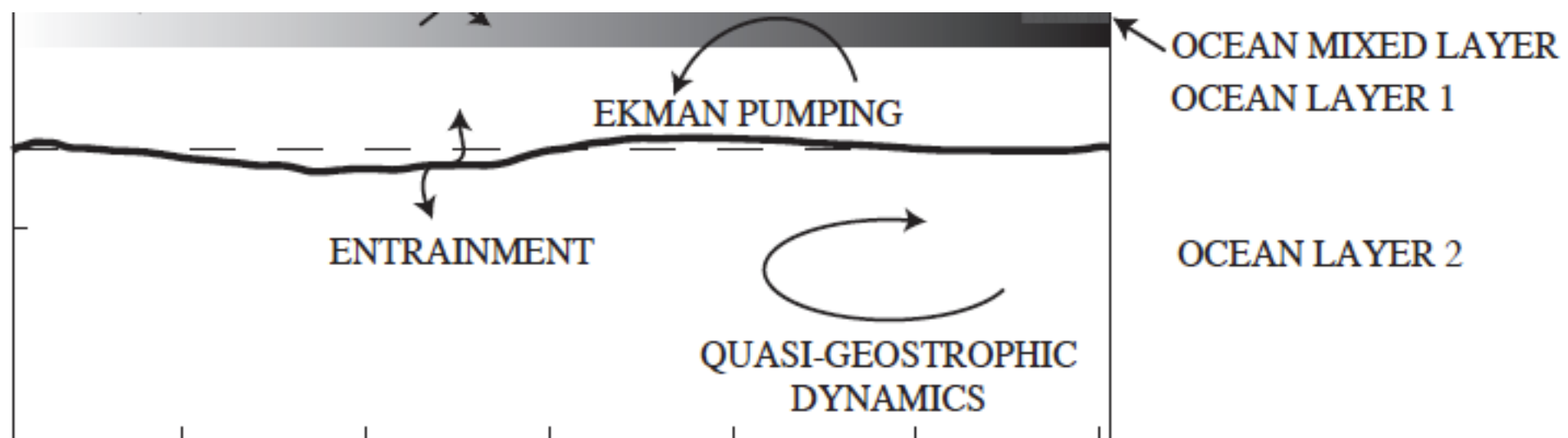
$$\mathbf{e} = \begin{bmatrix} w_{ek} \\ \frac{\delta_{ek}}{2f_0} \nabla^2 p_N \end{bmatrix}$$

Exp.2

Exp.1

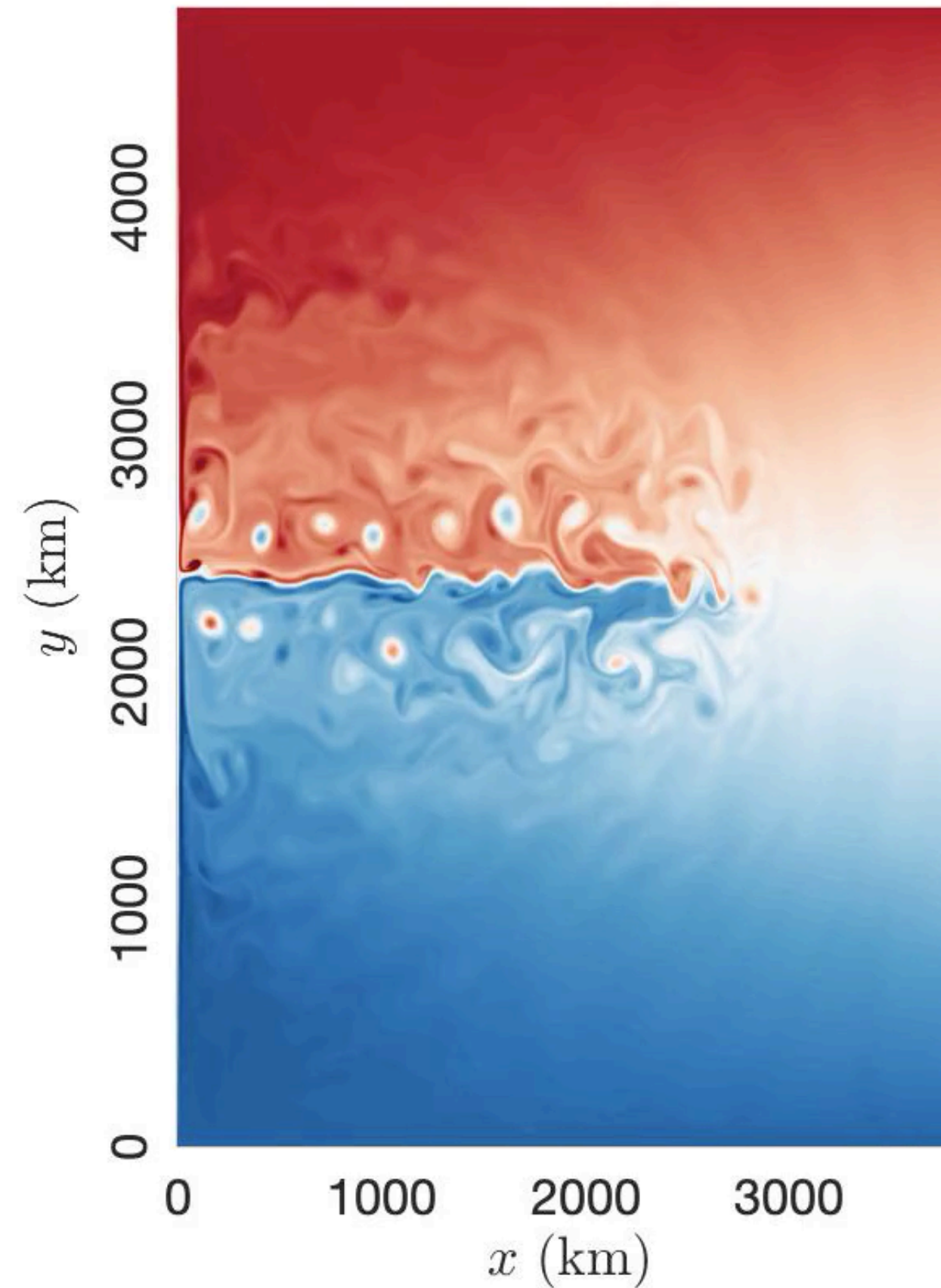
$$\mathbb{D}_t T_m = K_2 \nabla^2 T_m - K_4 \nabla^4 T_m + w_{ek} \frac{T_1 + T_m}{2H_m}$$

Source: <http://q-gcm.org>



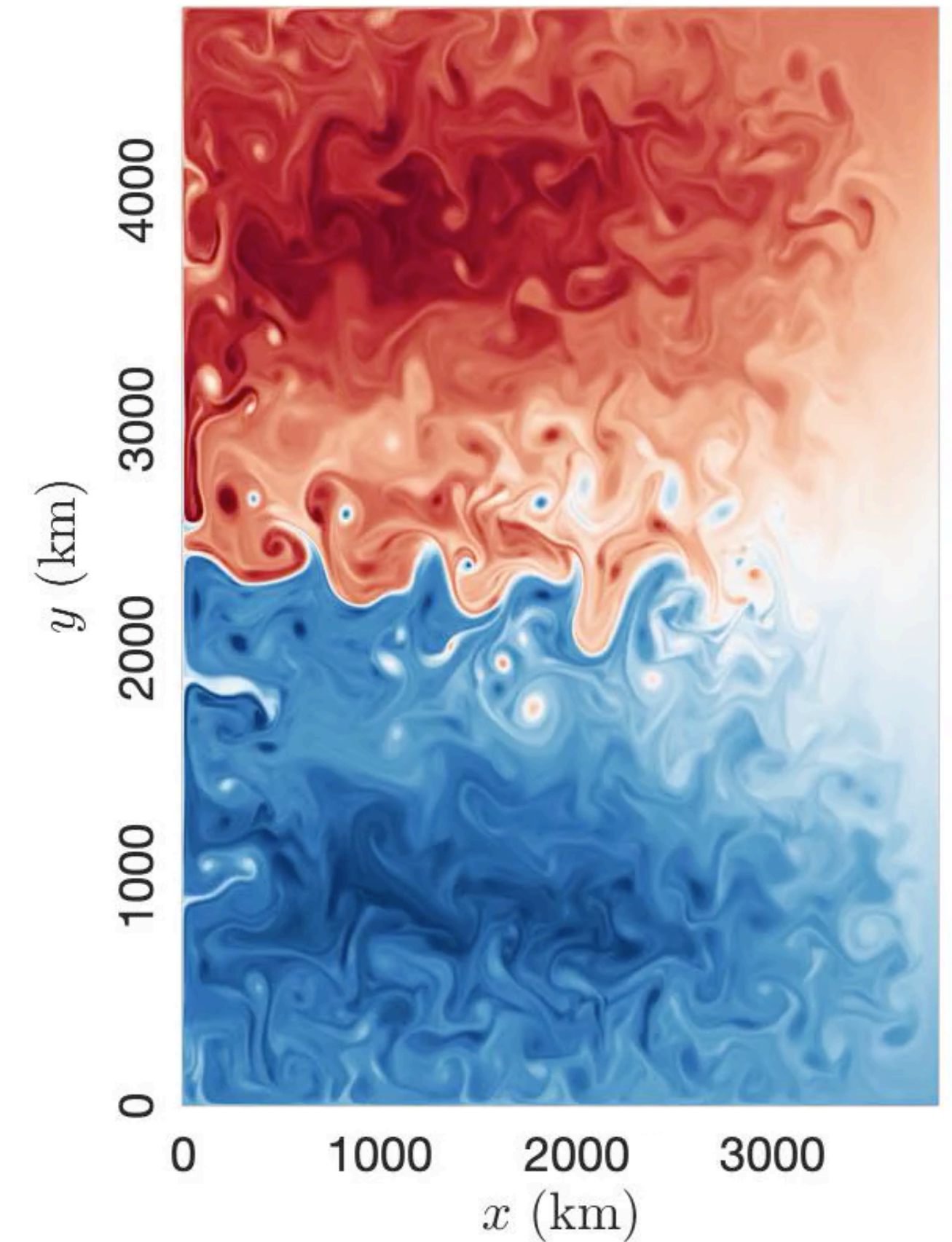
Exp.1

Year = 100.0



Exp.2

Year = 100.0



Upper-layer PV from eddy-resolving simulations ($\Delta = 5$ km, $L_d = 40$ km)

Coarse resolution simulations

LR (80 km)

LU-POD (80 km)

LU-POD-P (80 km)

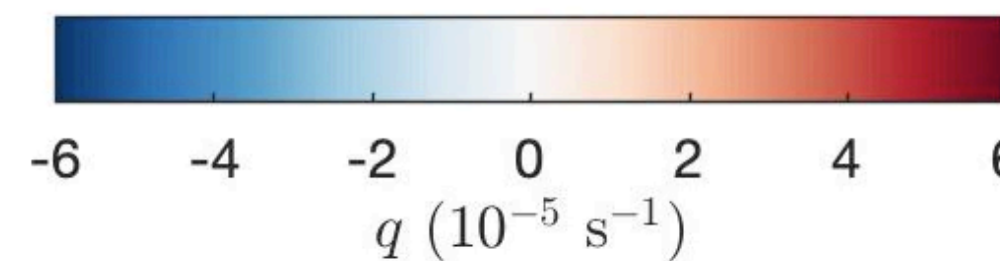
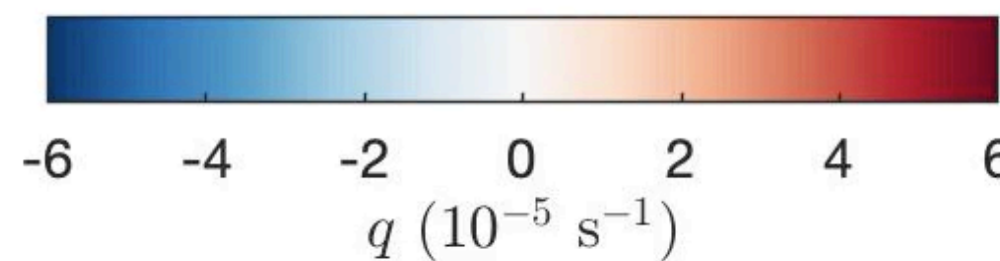
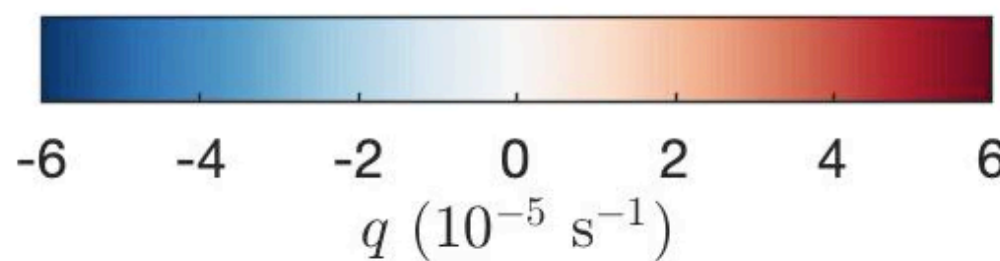
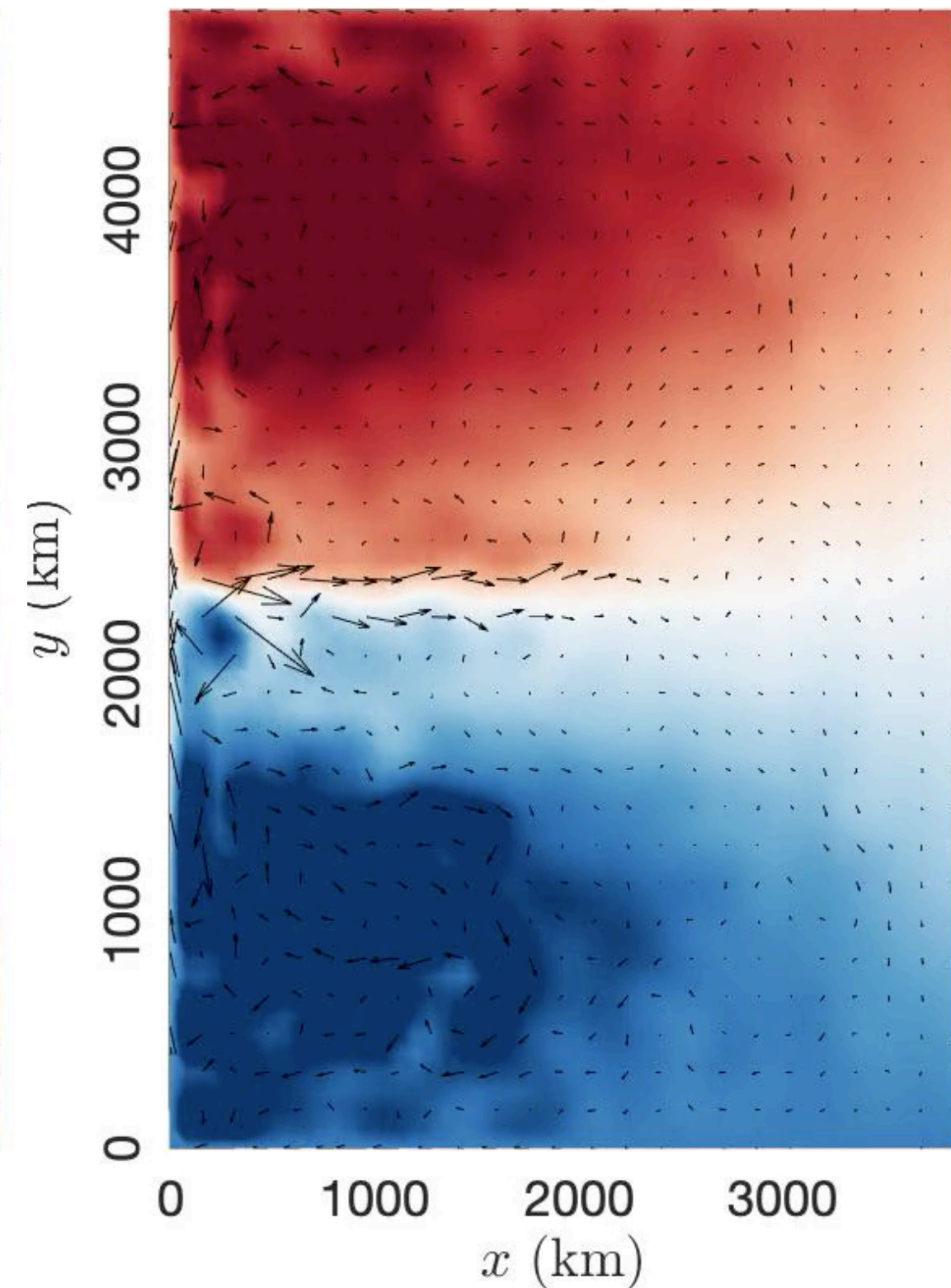
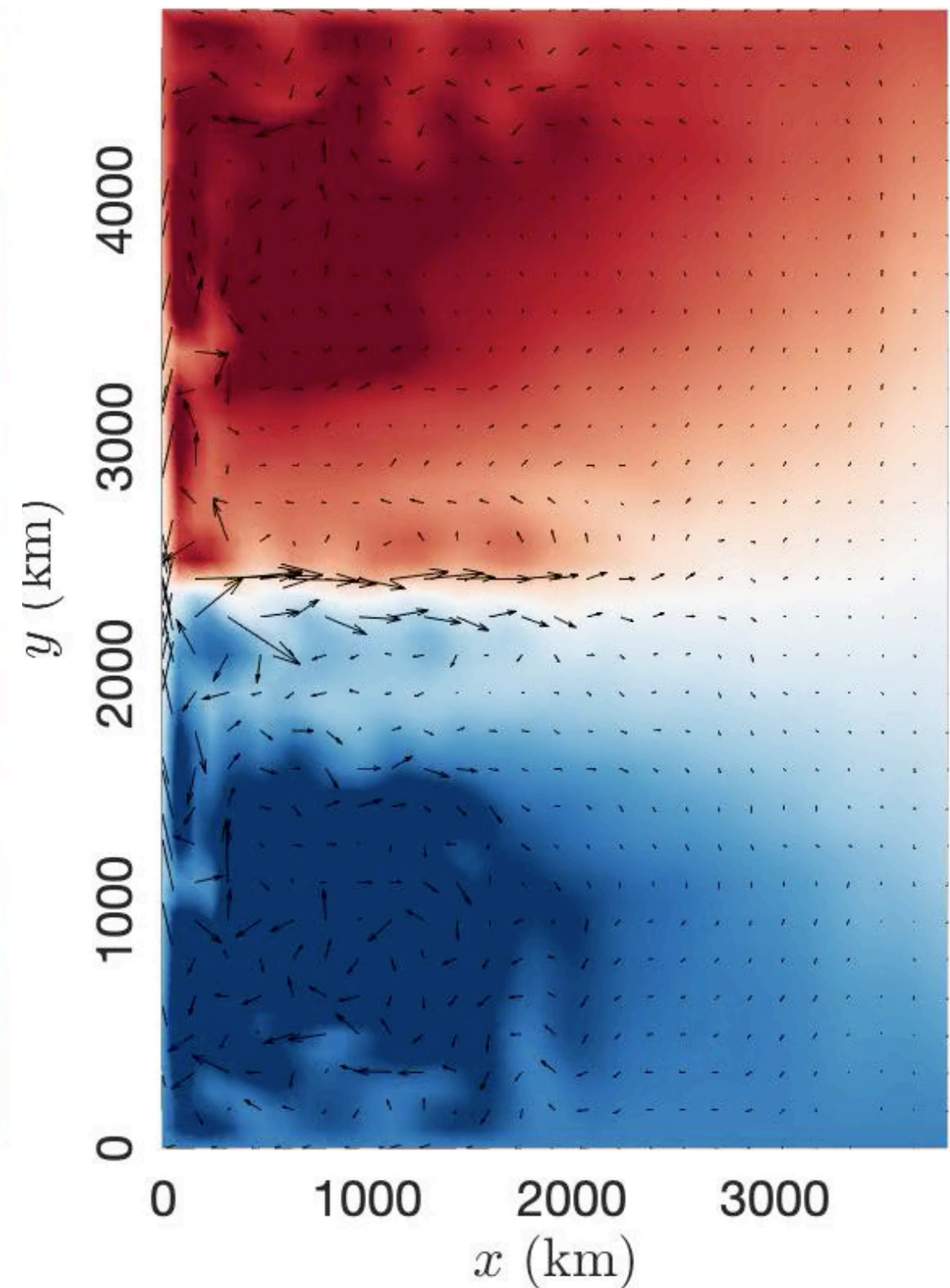
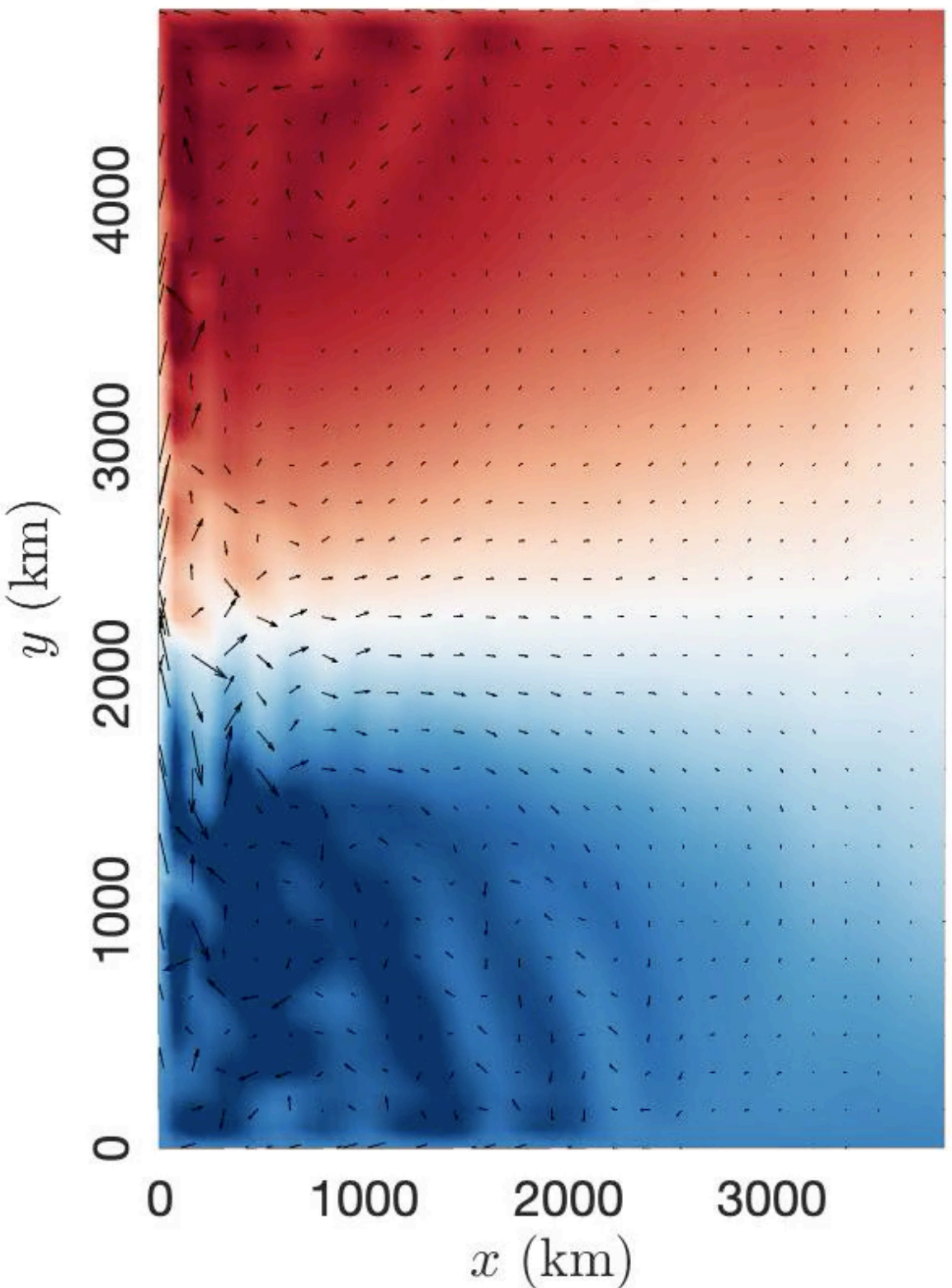
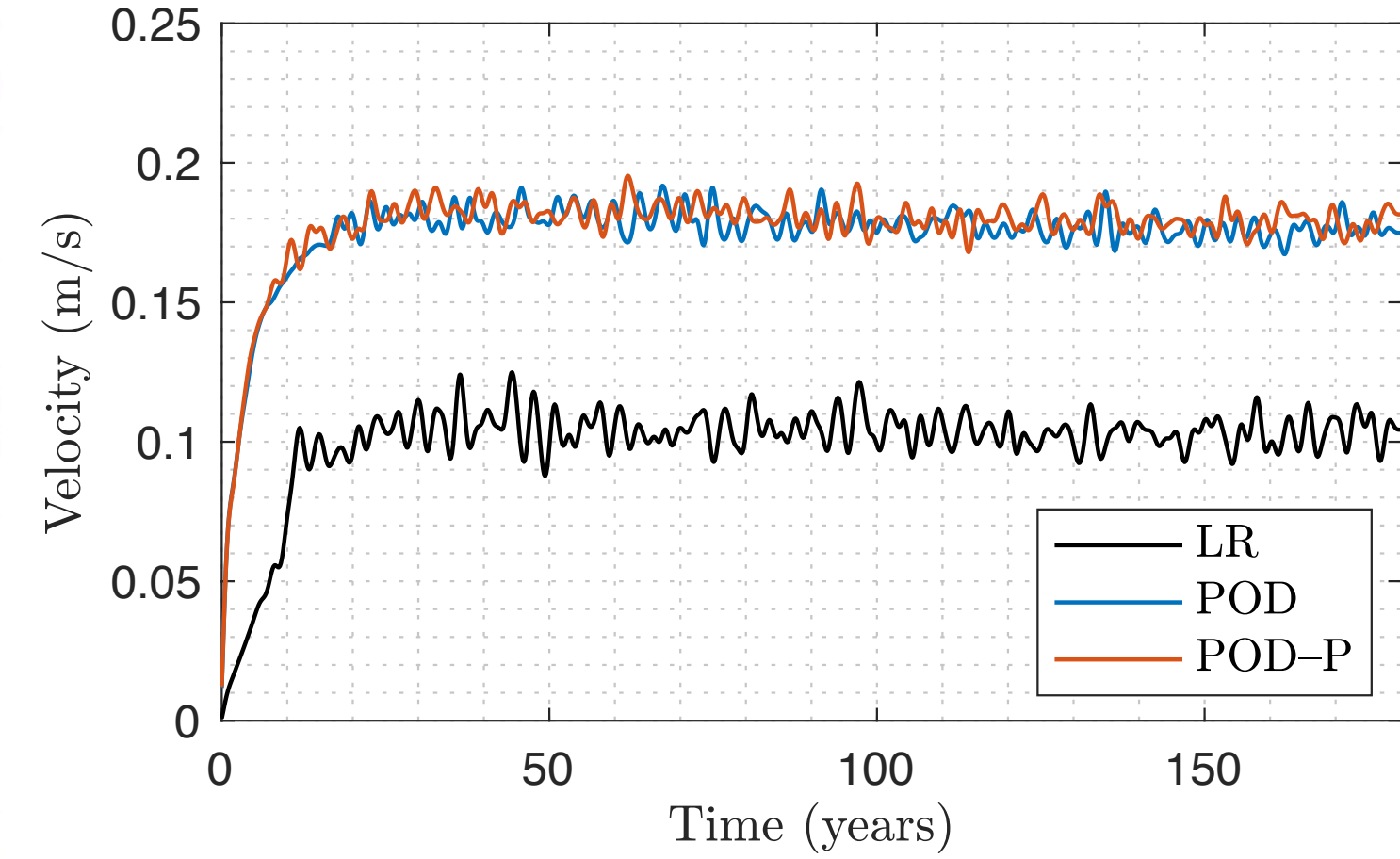
Year = 100.0

Year = 100.0

Year = 100.0

Time-series of jet velocity magnitude

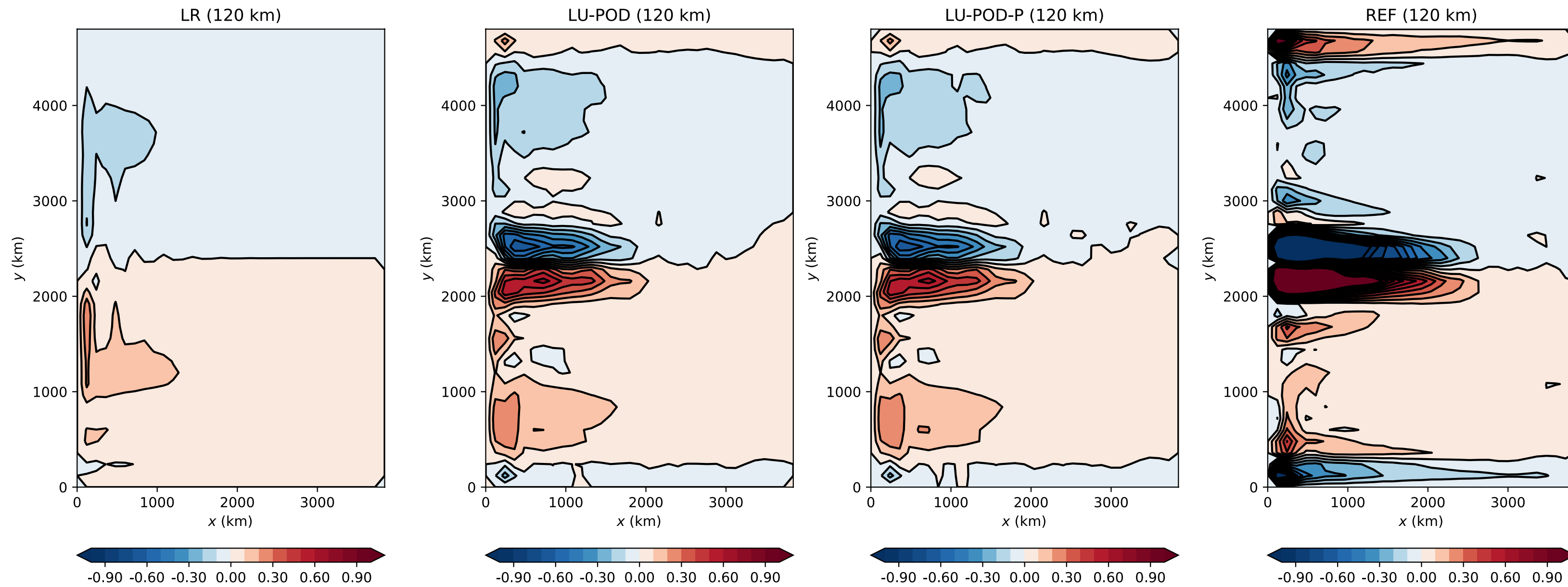
80 km



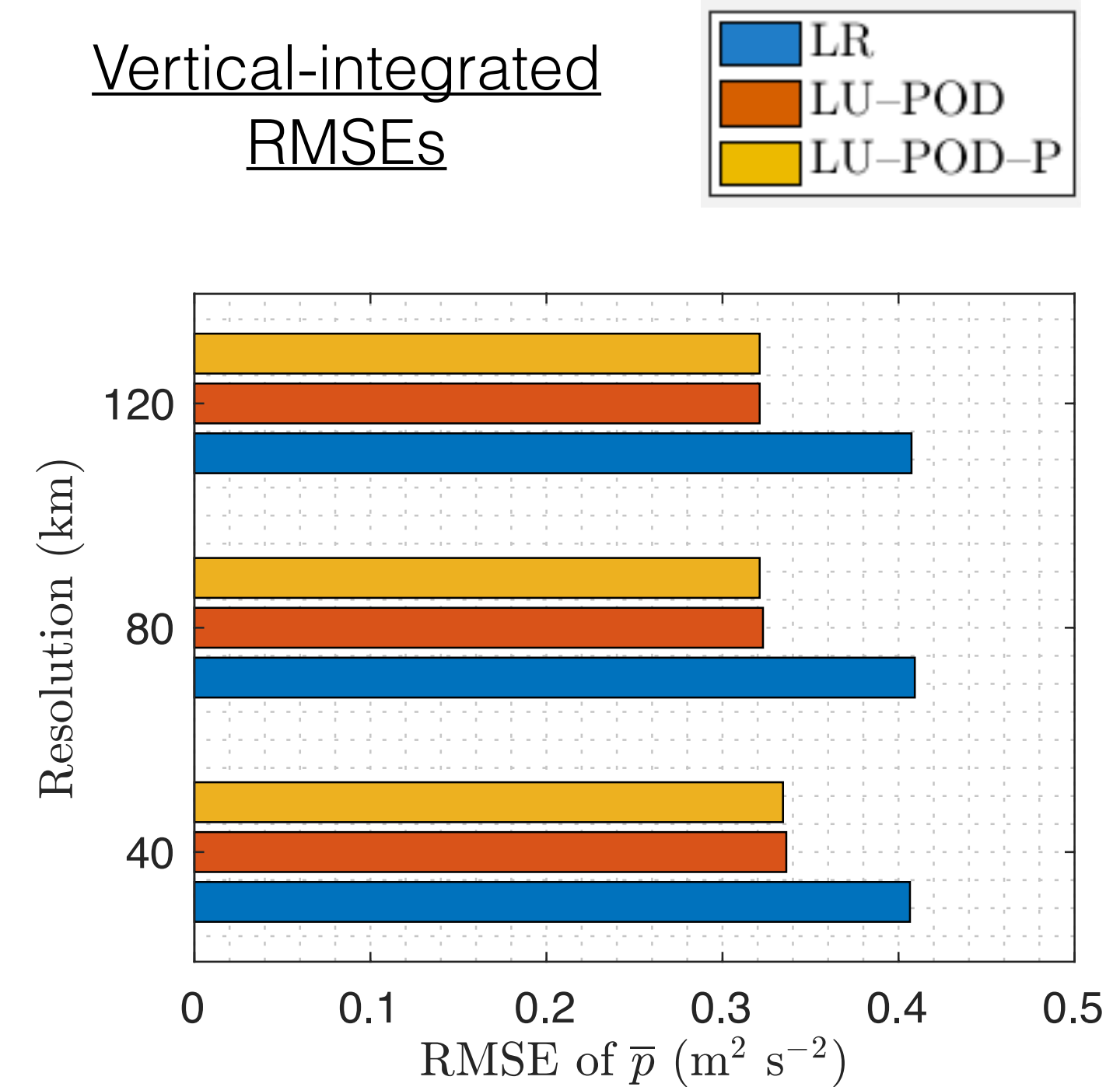
Upper-layer PV ($L_d = 40$ km)

Including the correction term, both LU coarse models can reproduce the eastward-jet

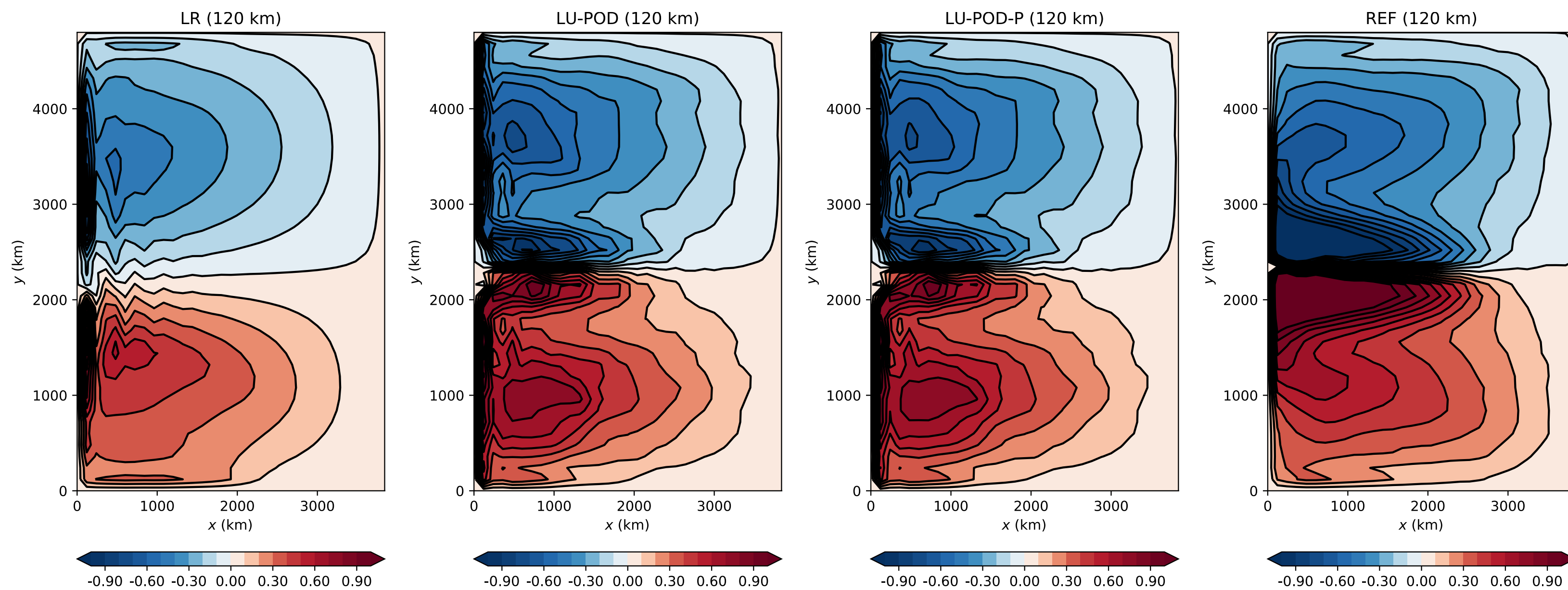
Time-mean of barotropic pressure ($\Delta = 120$ km)



Vertical-integrated RMSEs



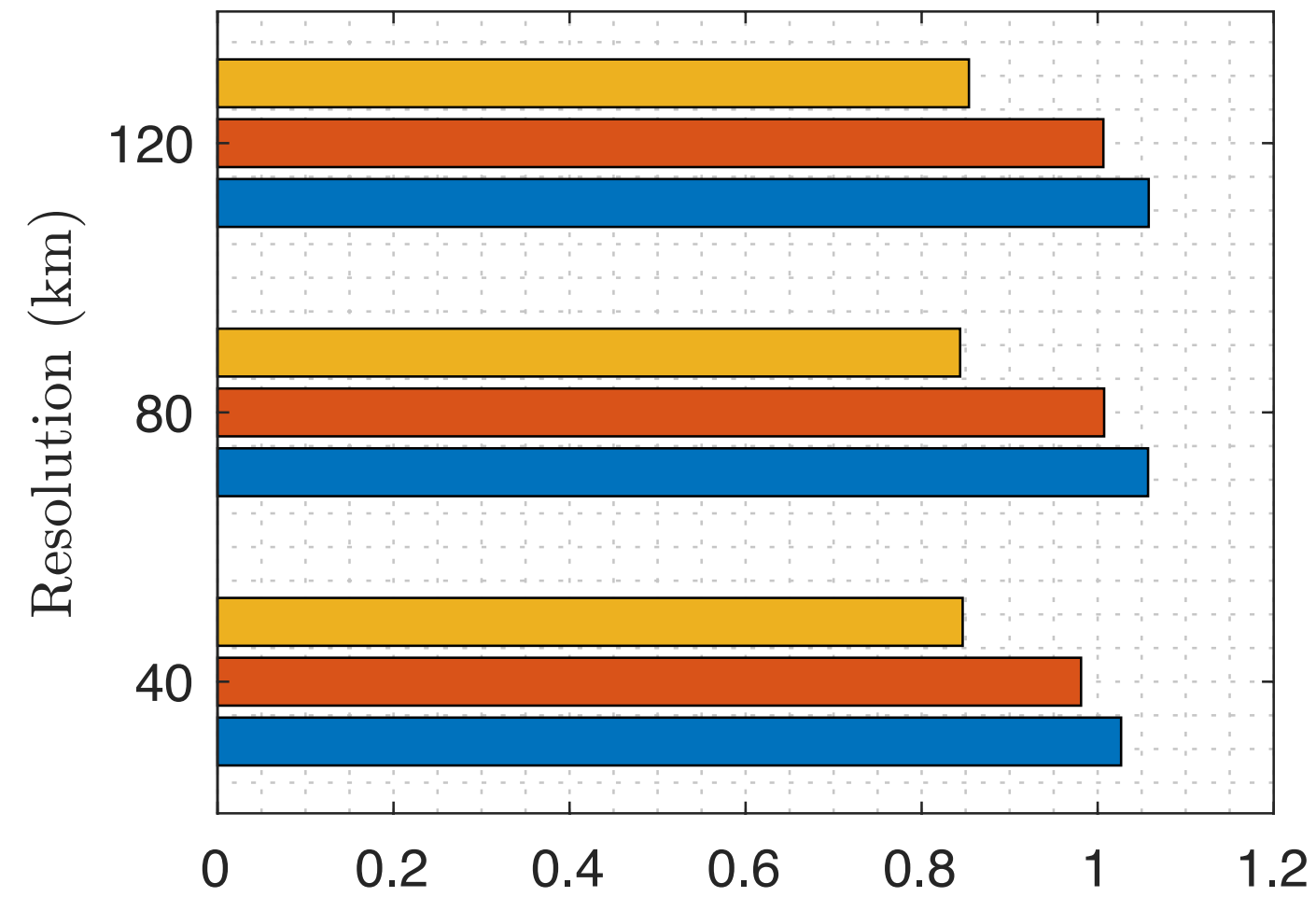
Time-mean of (1st) baroclinic pressure ($\Delta = 120$ km)



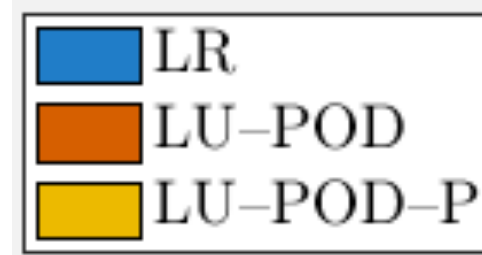
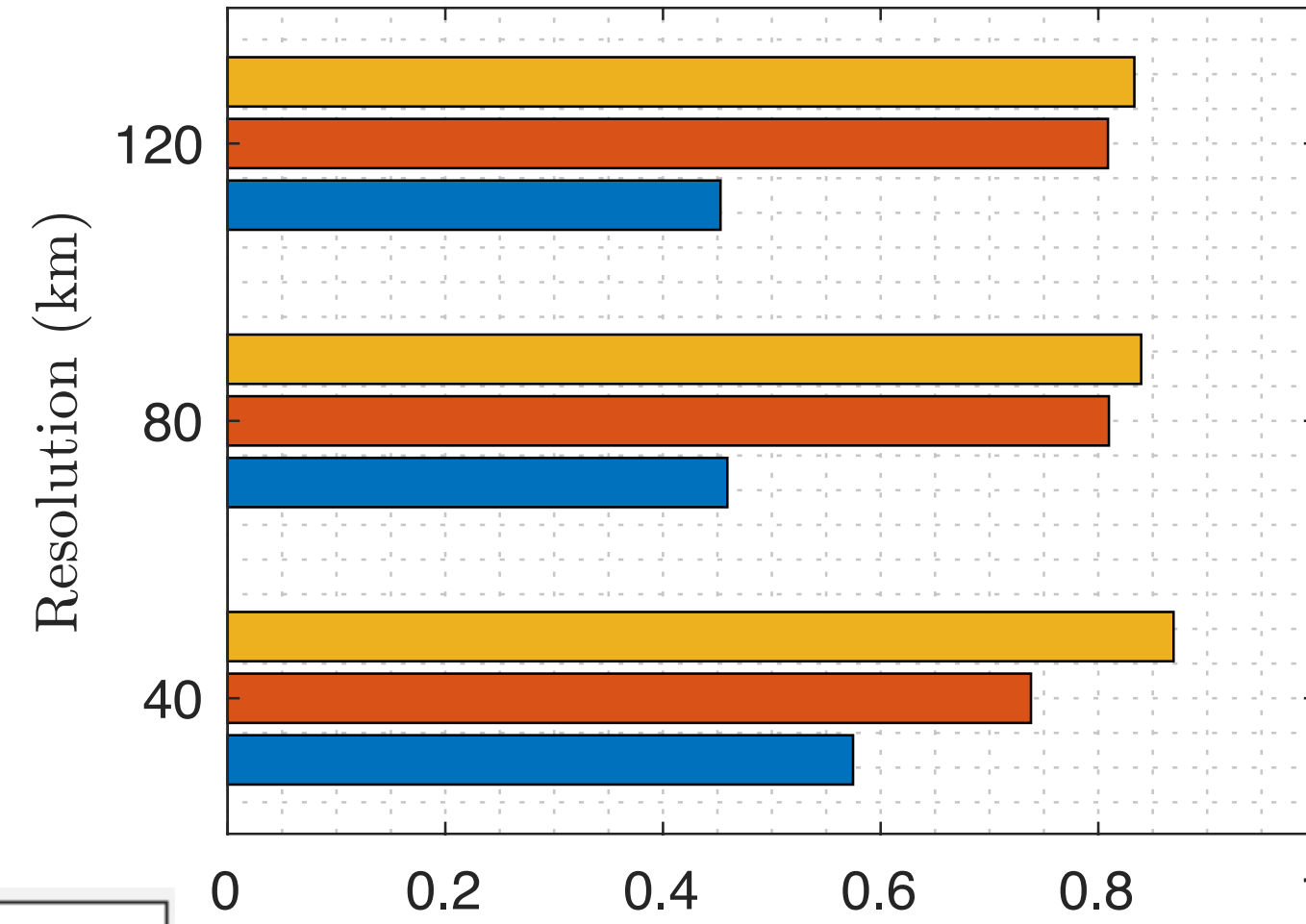
- **Both LU coarse models predict better the mean flow**
- **Results are not sensible to resolutions**

Diagnosis of variability

Vertical-integrated RMSEs of std (p)



Vertical-integrated PC of std (p)



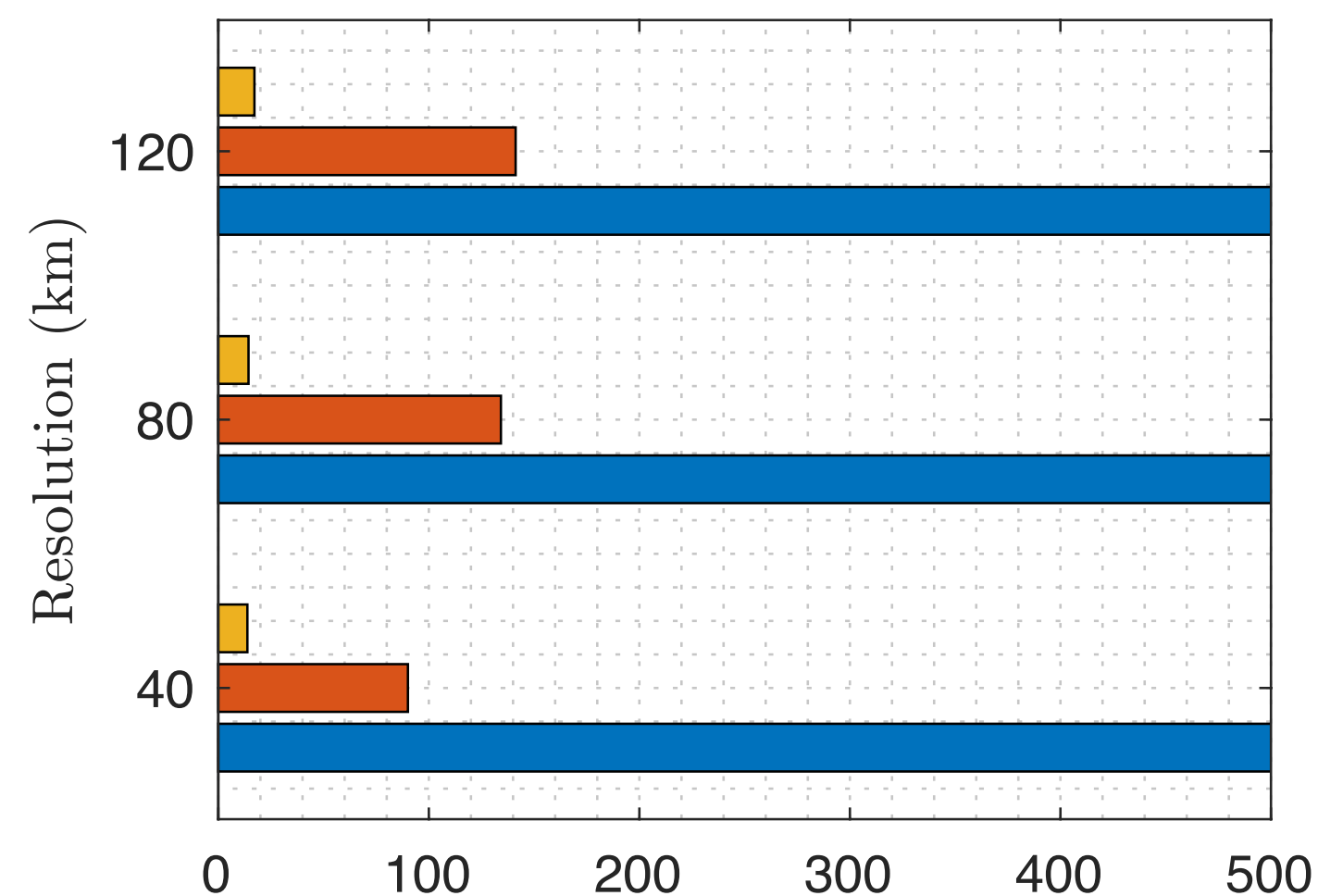
Metrics (*Grooms et al., 2015*)

$$PC = \frac{\|\sigma_{REF}\sigma_{MOD}\|_A^2}{\|\sigma_{REF}^2\|_A\|\sigma_{MOD}^2\|_A}$$

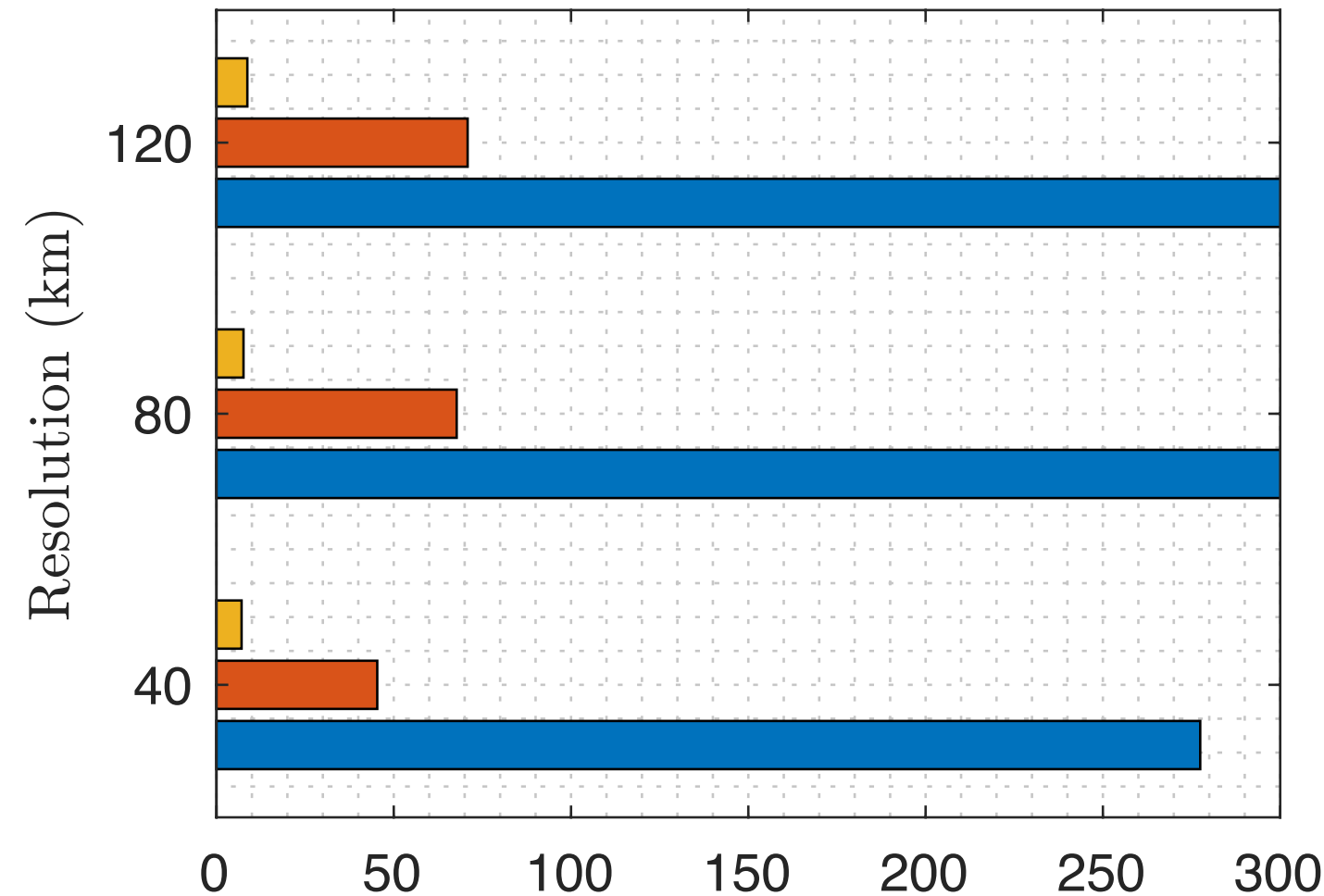
$$Dispersion = \frac{1}{|A|} \iint \left(\frac{\sigma_{REF}^2}{\sigma_{MOD}^2} - 1 - \log \left(\frac{\sigma_{REF}^2}{\sigma_{MOD}^2} \right) \right) dA$$

$$GRE = \frac{1}{2} \left\| \frac{\bar{p}_{REF} - \bar{p}_{MOD}}{\sigma_{REF}} \right\|_A^2 + \frac{1}{2} Dispersion$$

Vertical-integrated dispersion of std (p)

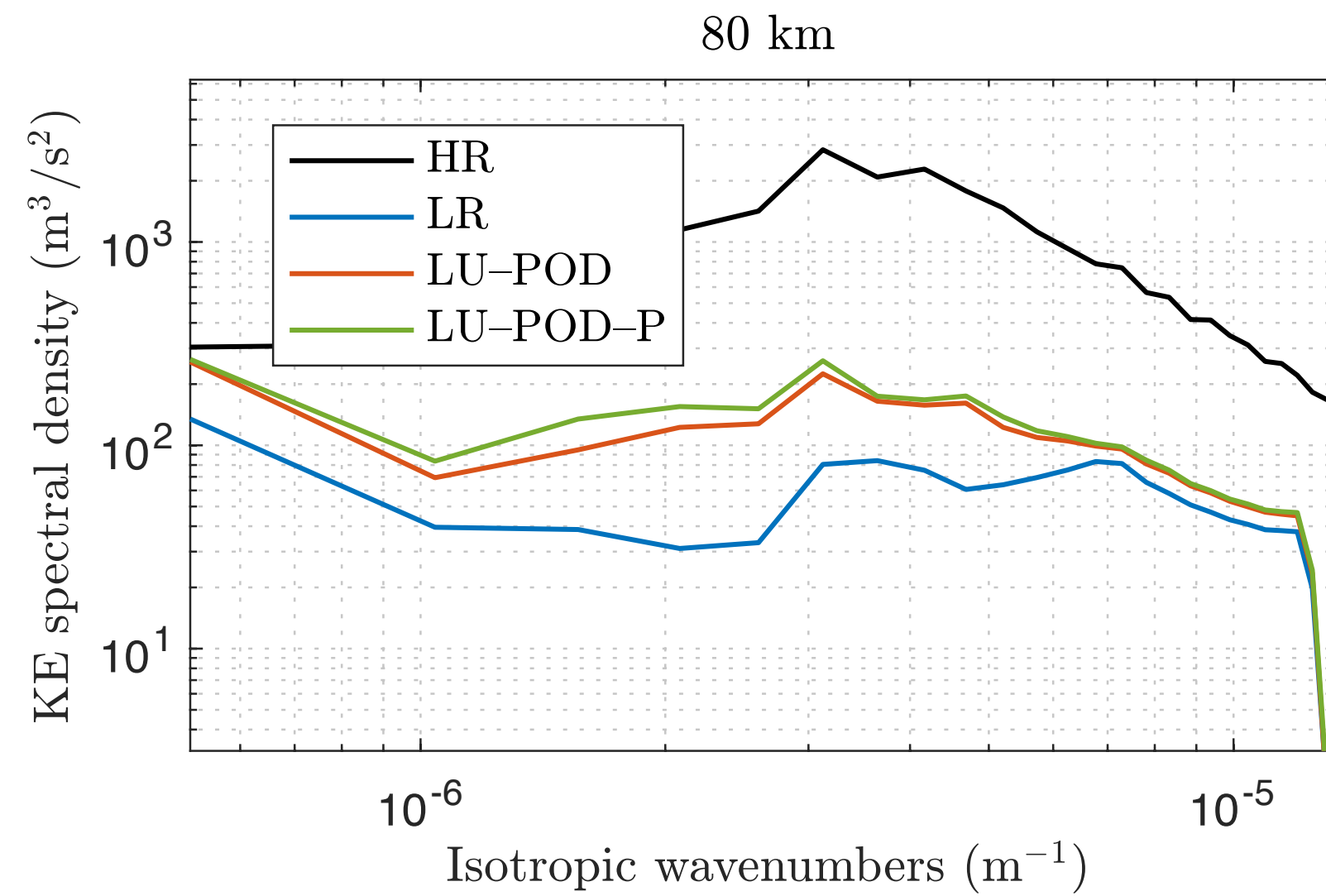
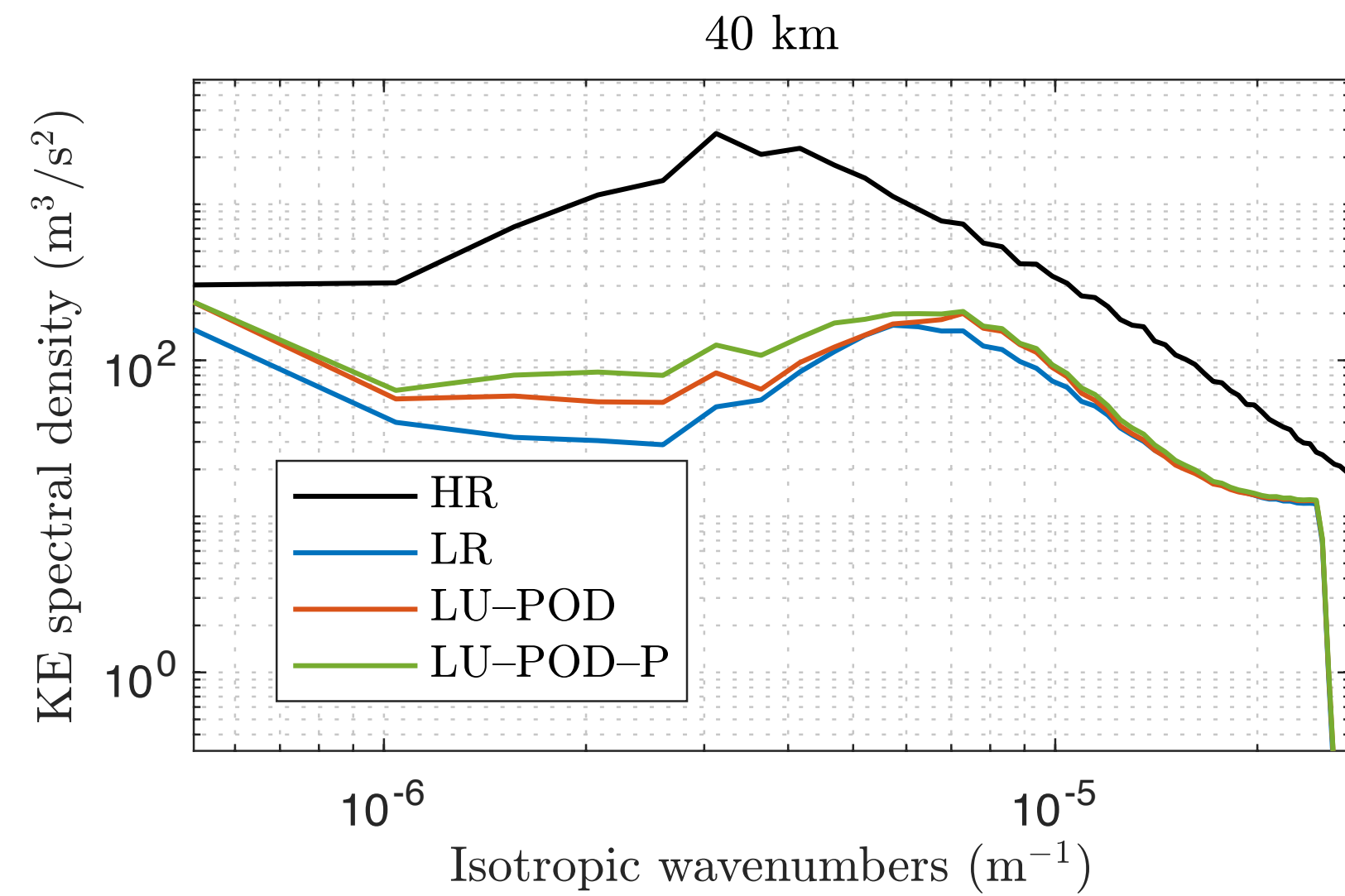


Vertical-integrated entropy of std (p)



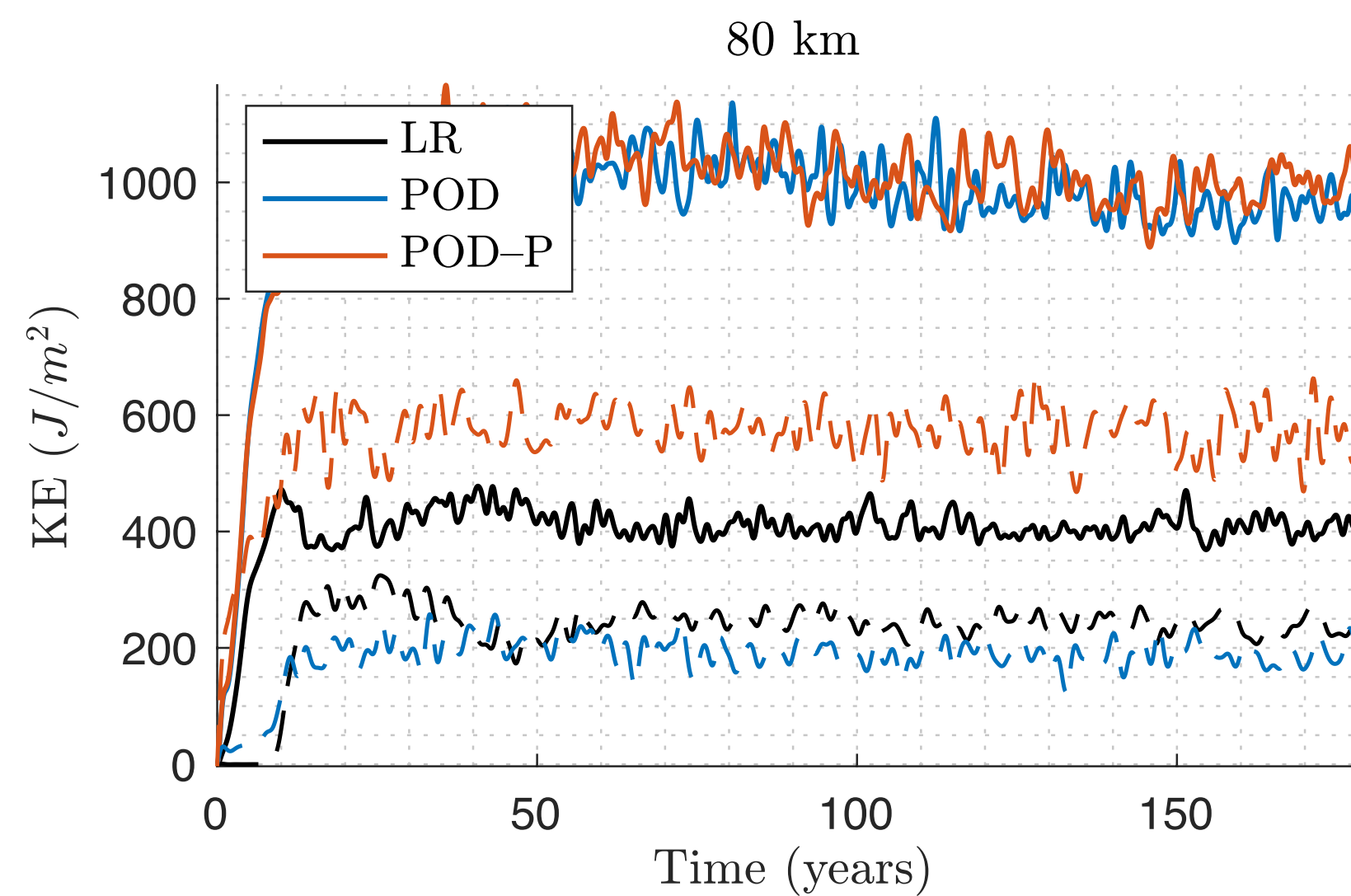
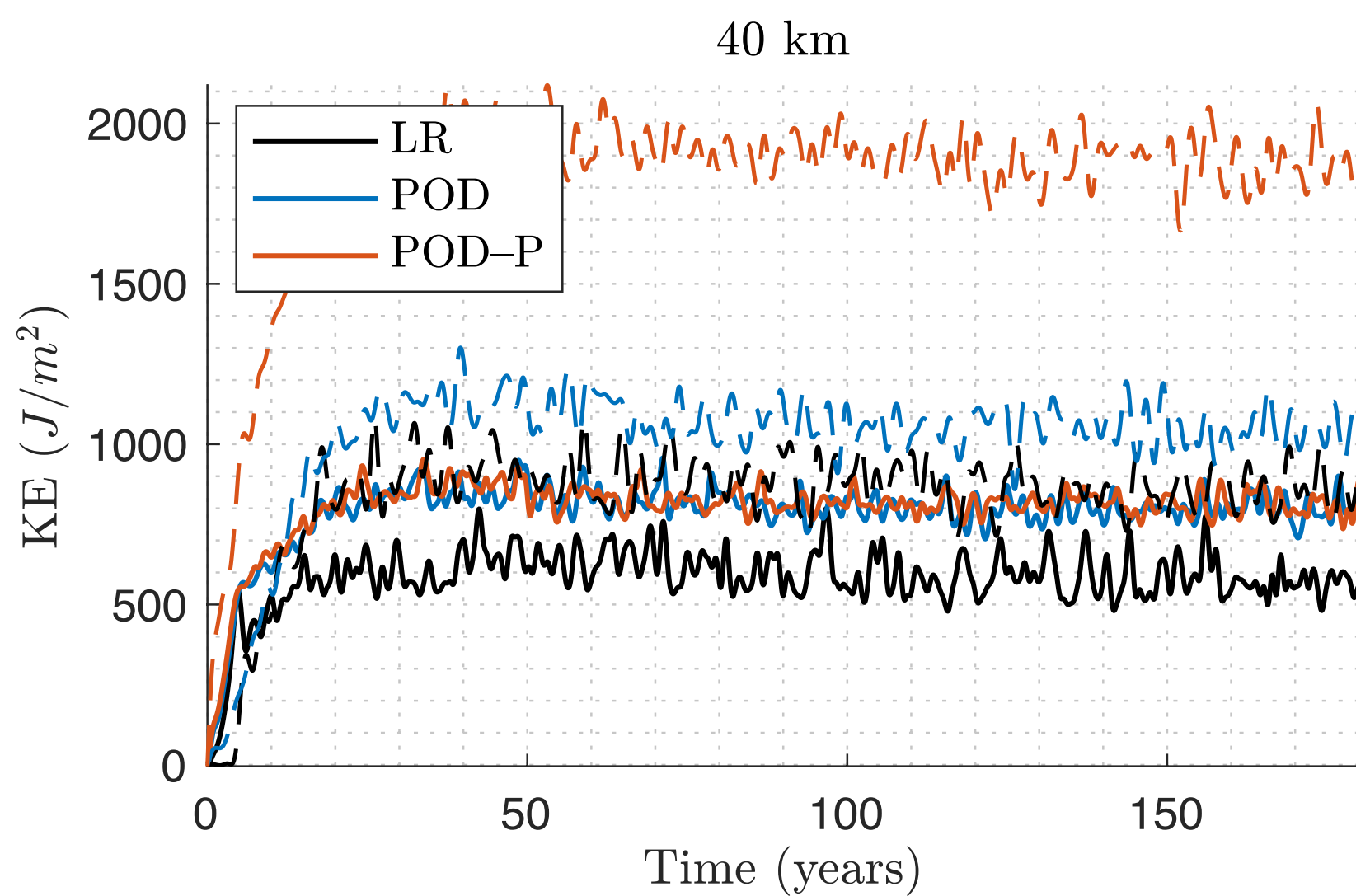
- **Non-stationary coarse model improves the prediction of variability**
- **Results are not sensible to the resolutions**

Energy analysis



Mean KE spectrum

- Both LU coarse models backscatter energy
- Non-stationary model produces more transient eddy energy



Low-pass filtering

EKE decomposition (Hogg et al., 2004)

$$u = \bar{u} + u'$$

$$\text{EKE} = \underbrace{\frac{\rho H}{2} \|\bar{u}\|_A^2}_{\text{Standing}} + \underbrace{\frac{\rho H}{2} \|u'\|_A^2}_{\text{Transient}}$$

Conclusion

- Expansion and applications of the LU models
- New parametrization of small-scale flow and tested for different flows
- Reliability of ensemble forecasts
- Effect of small-scale inhomogeneity on the large-scale flow structure
- Dynamical consistency on prediction of mean flow and low-frequency variability

Outlook

Model

- Atmosphere-Ocean coupled model
- Multi-scales coupled model
- Primitive model
- Compressible noise model

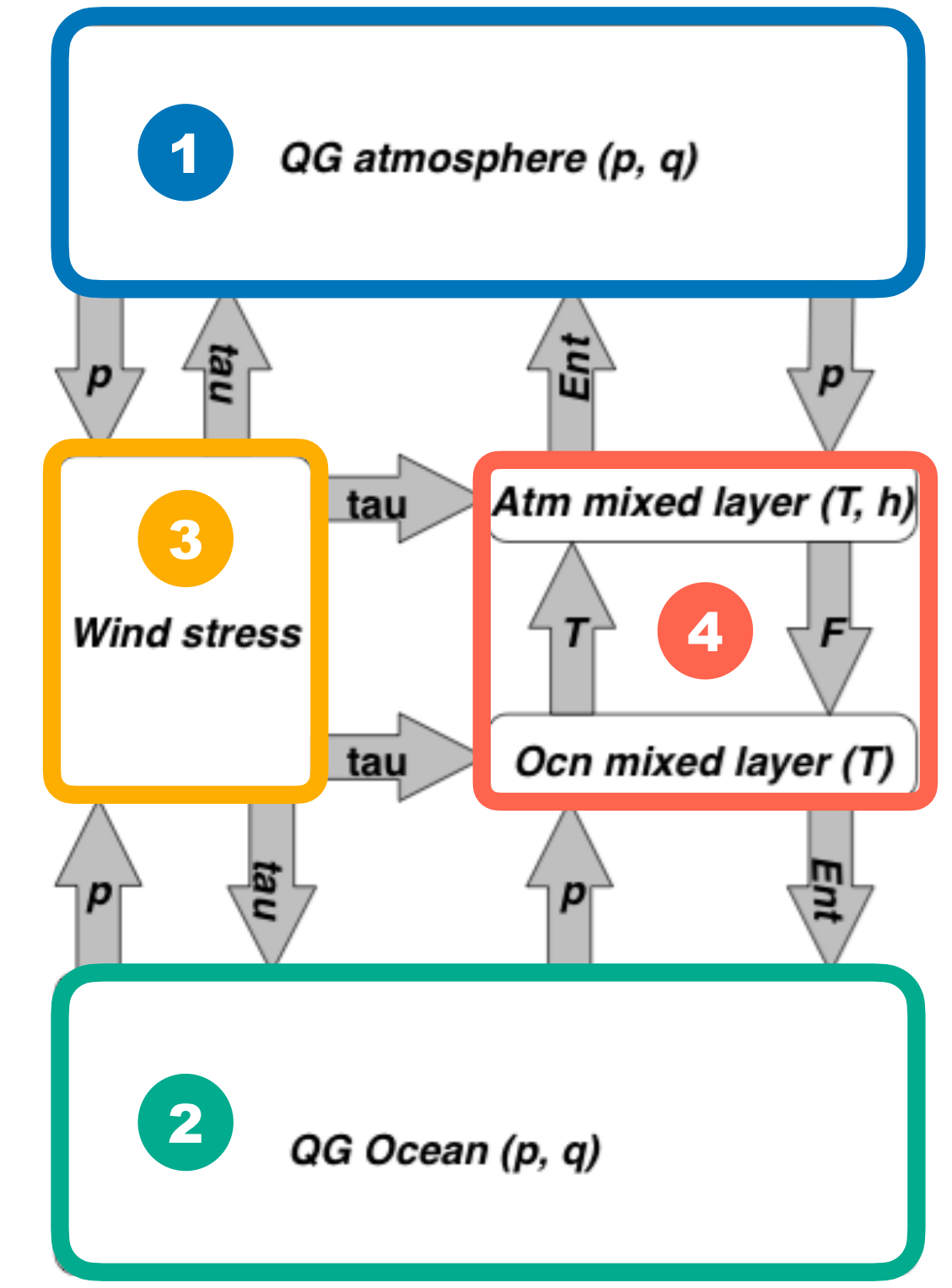
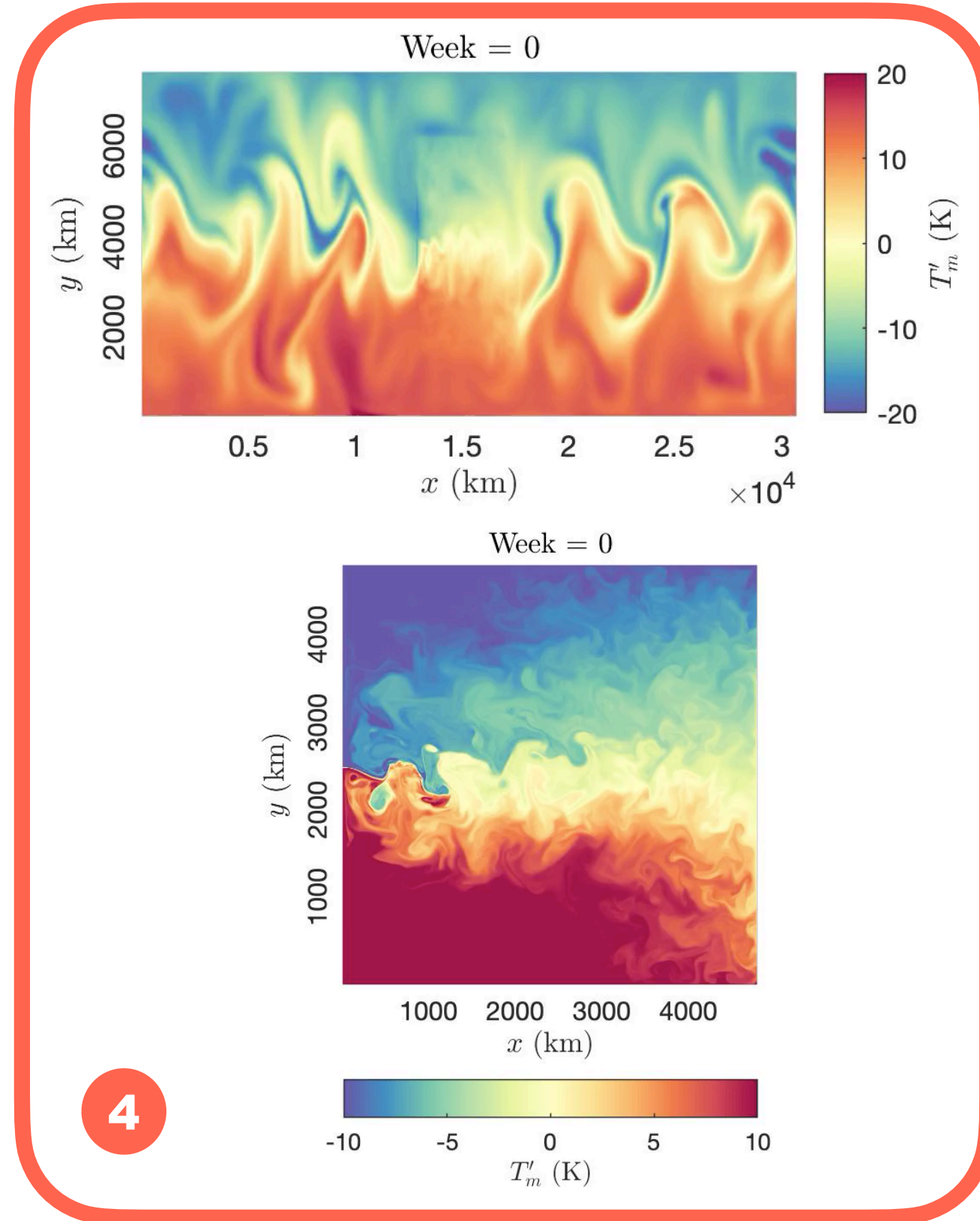
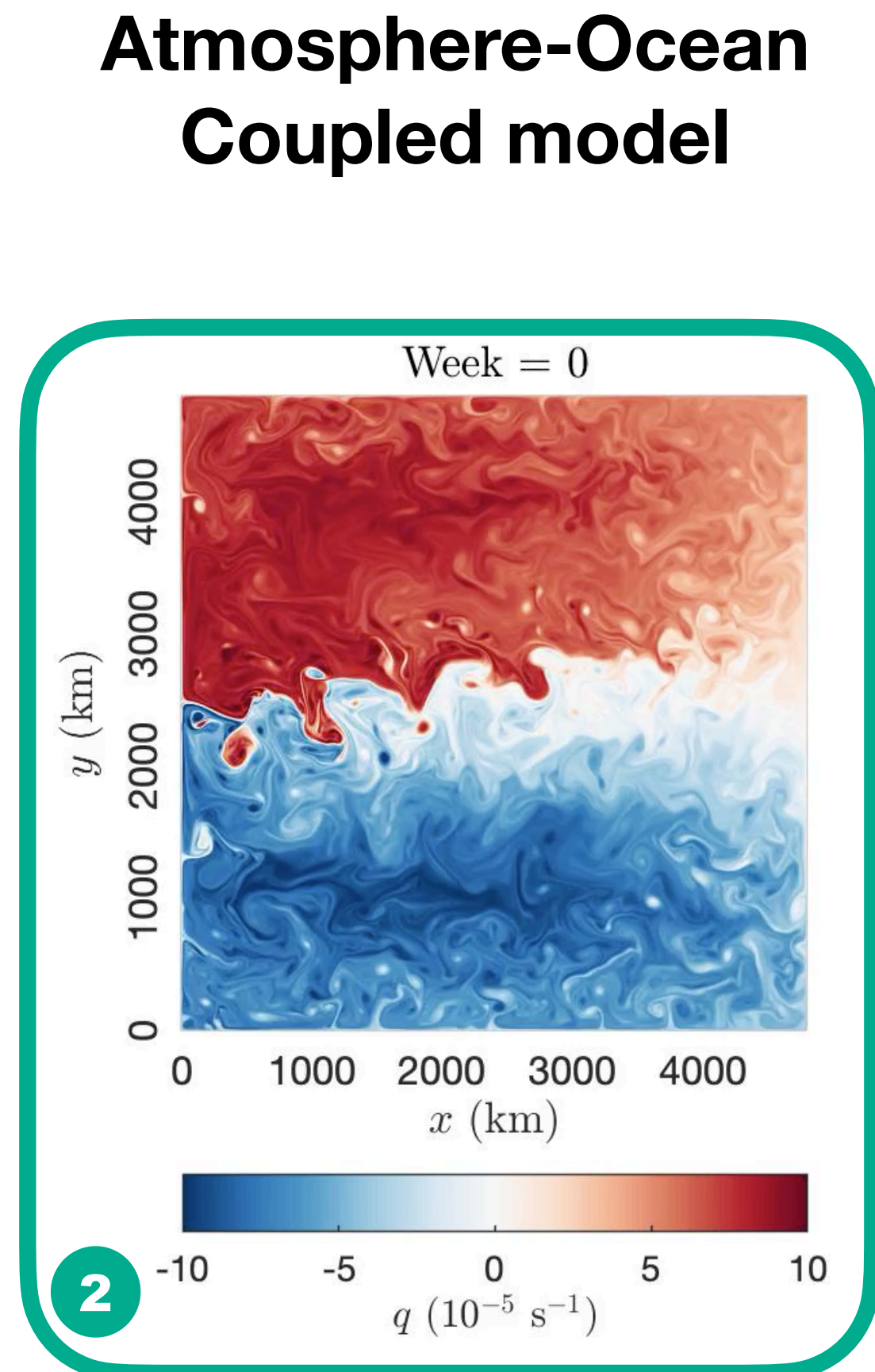
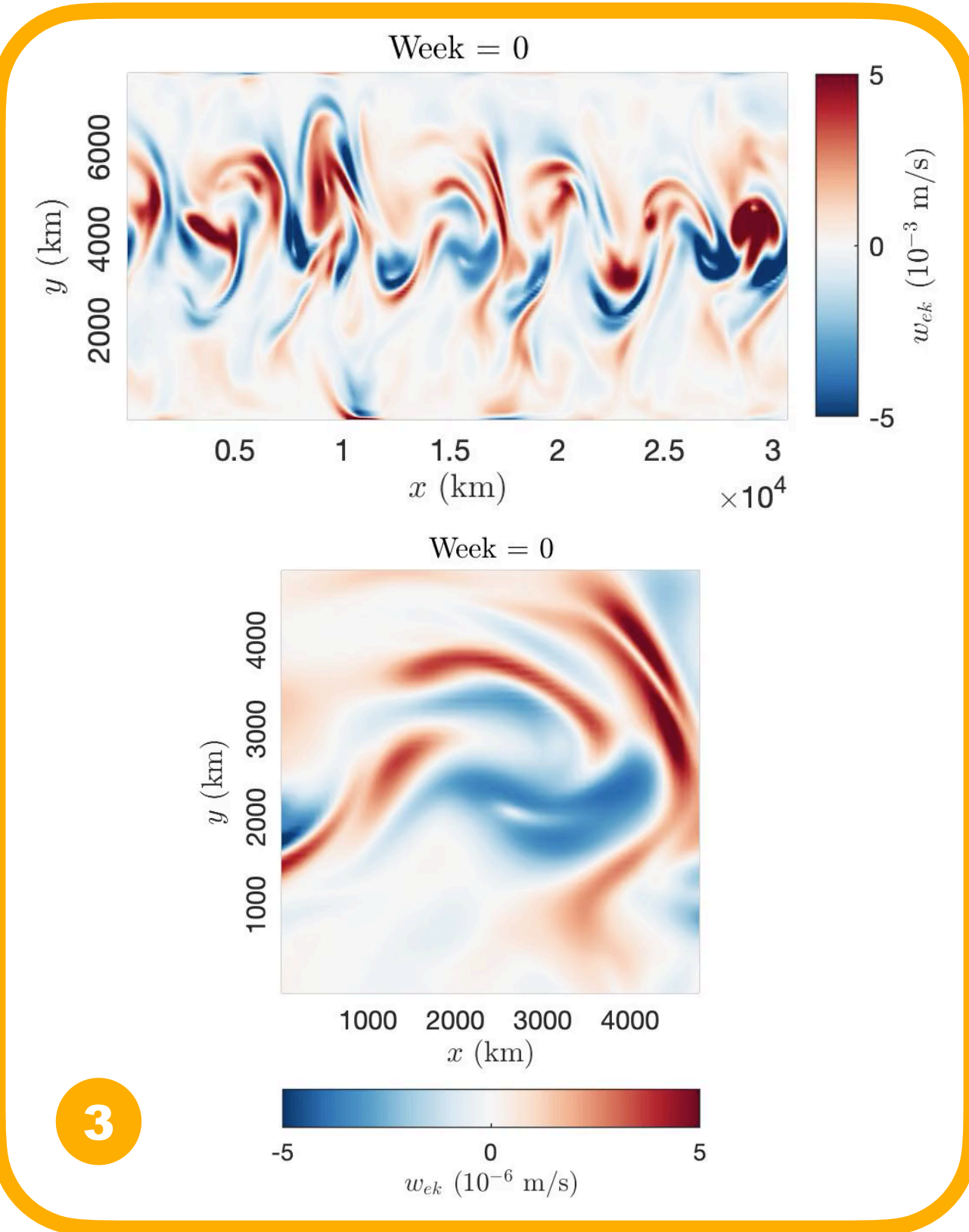
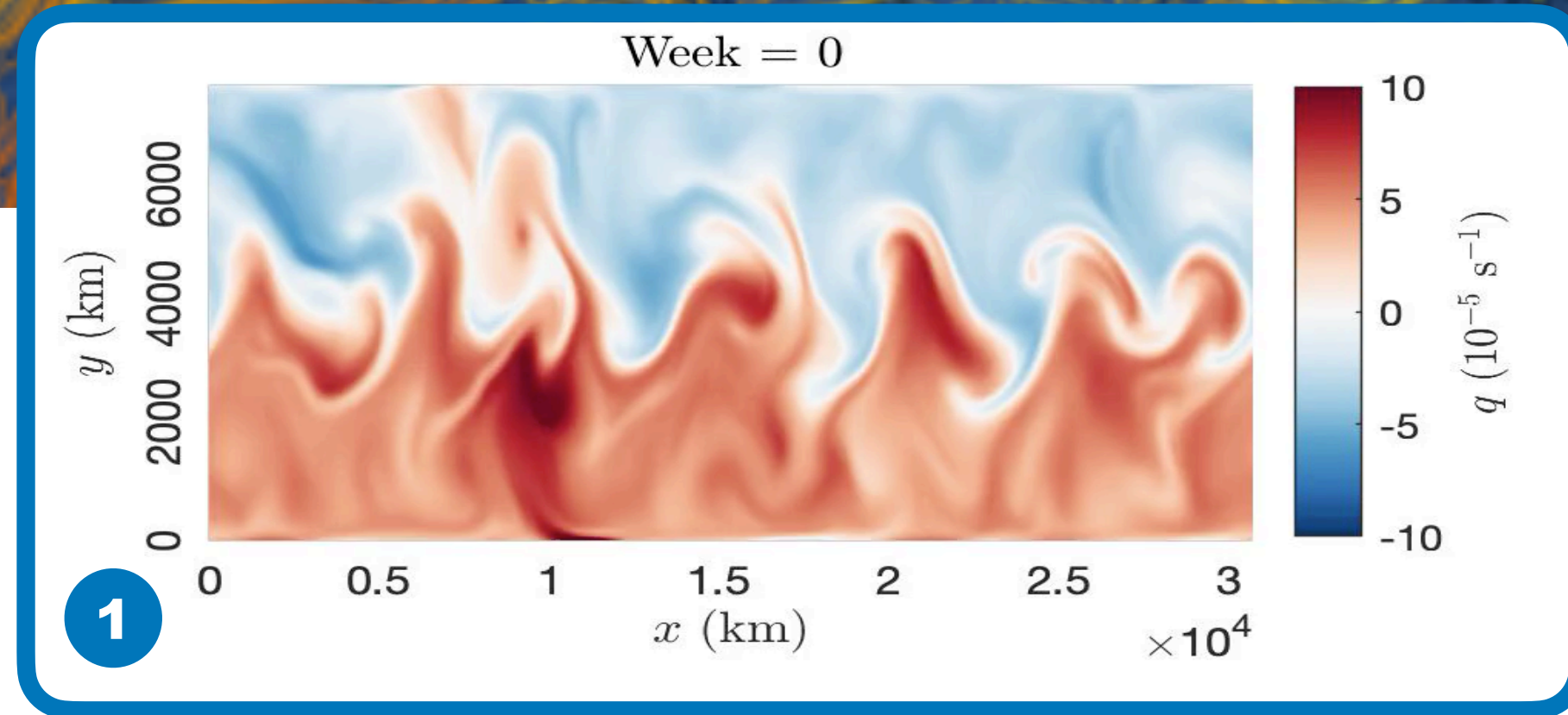
Noise

- Application of LU-SGS
- Linear stability analysis
- Koopman theory

Assimilation

- Particle filter
- Hierarchical

Working in process



Working in process

HR (5 km)

LR (80 km)

LU-POD (80 km)

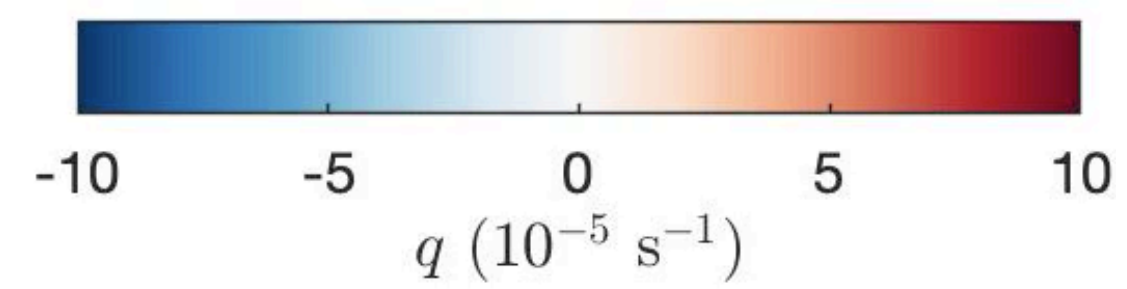
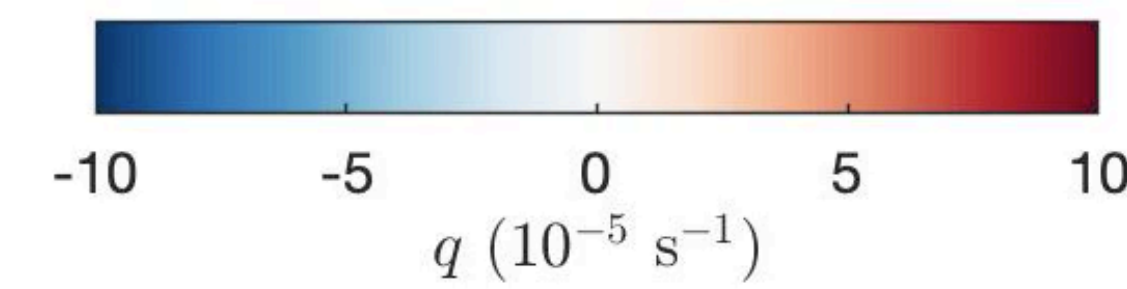
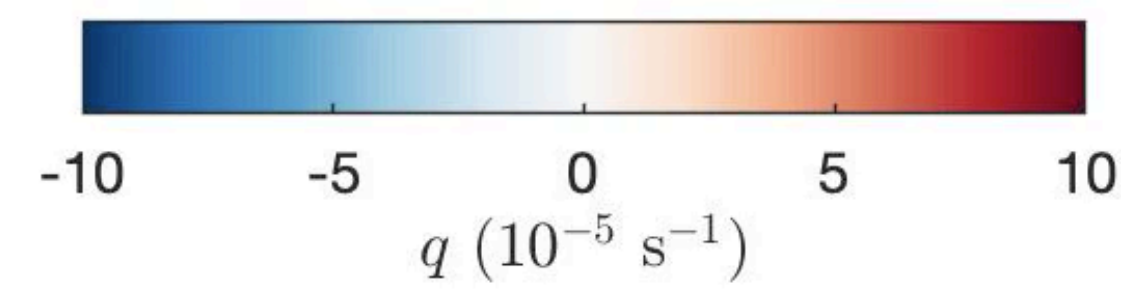
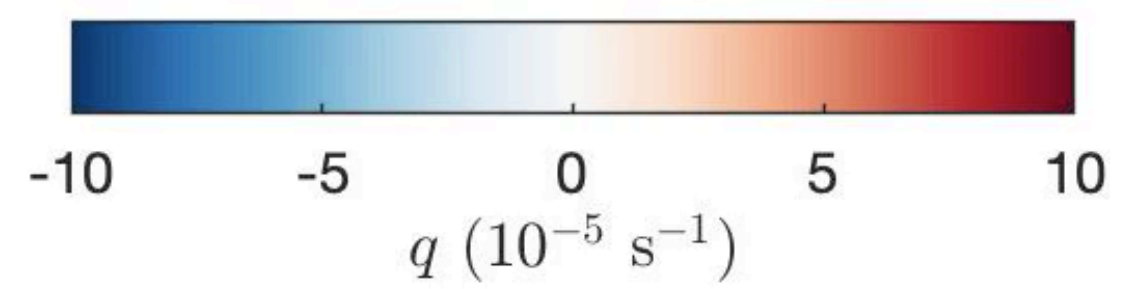
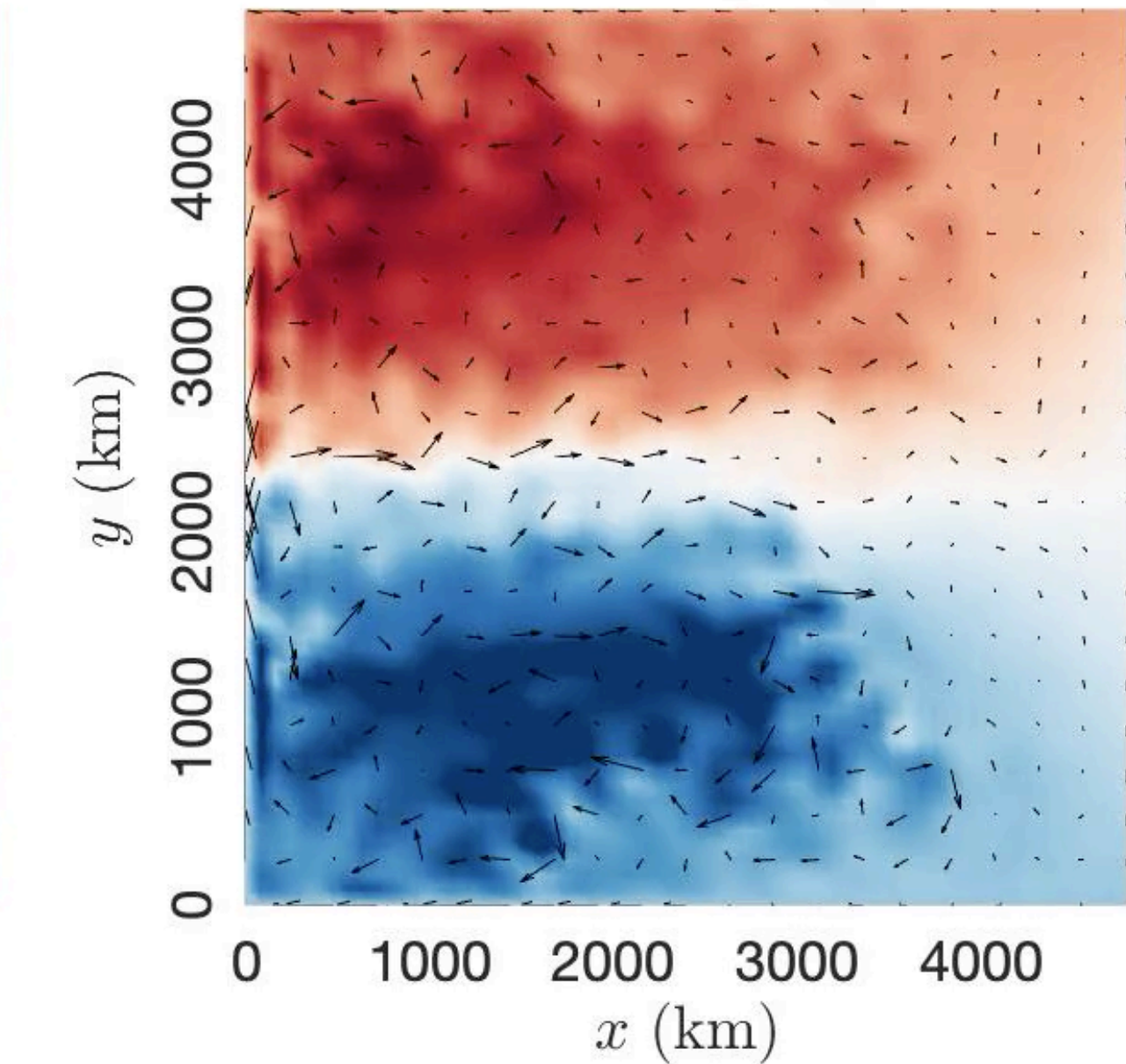
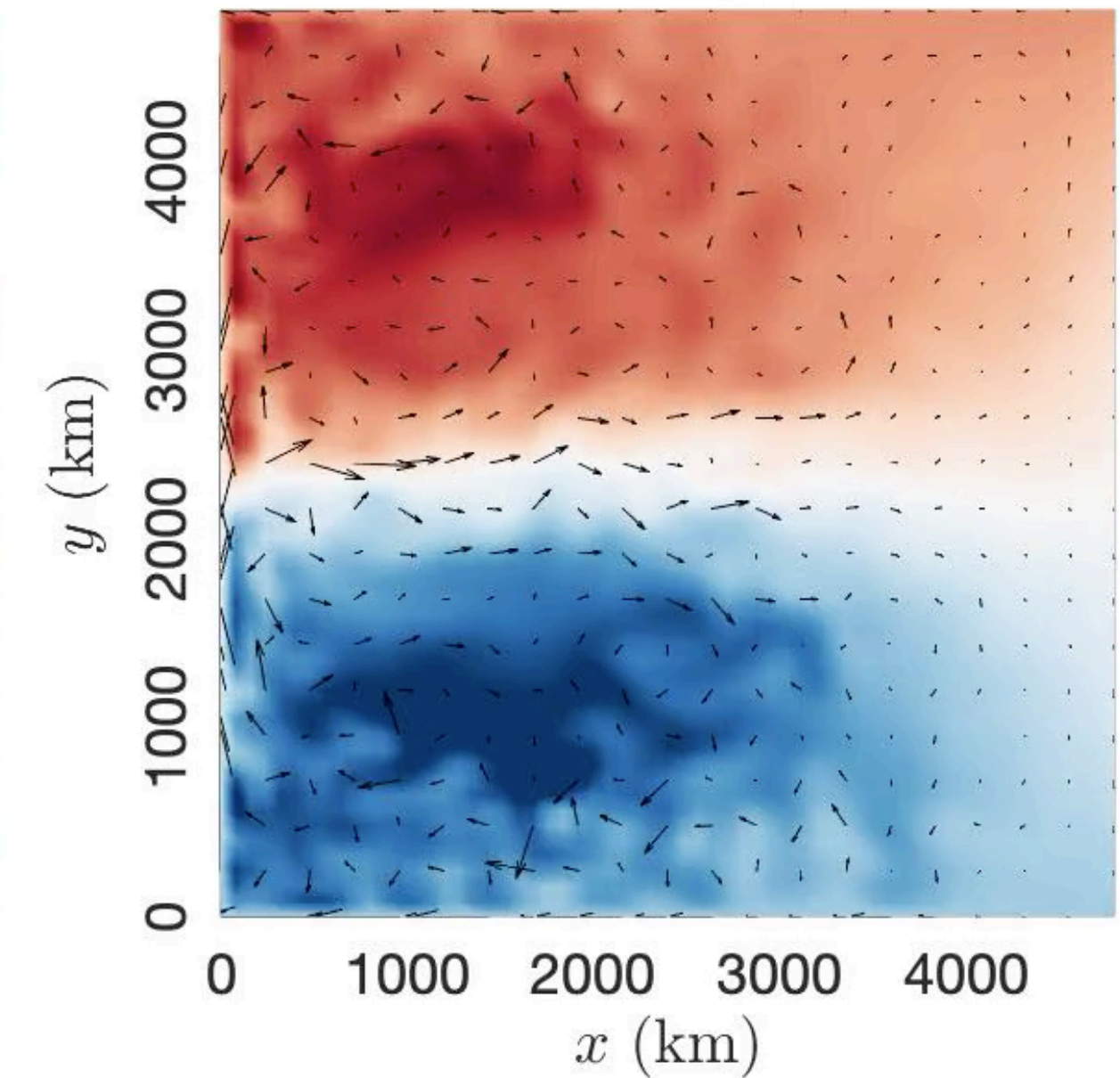
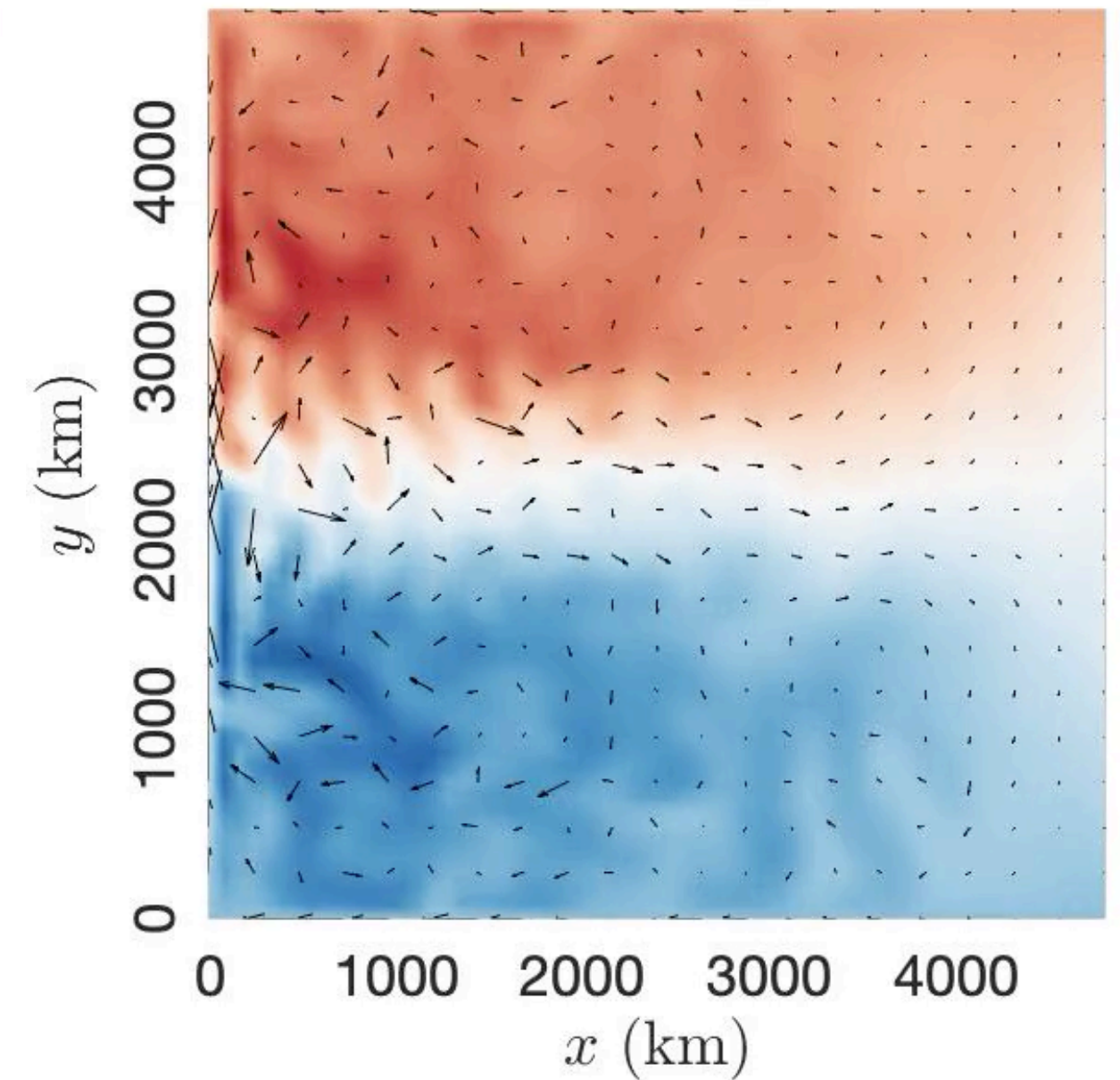
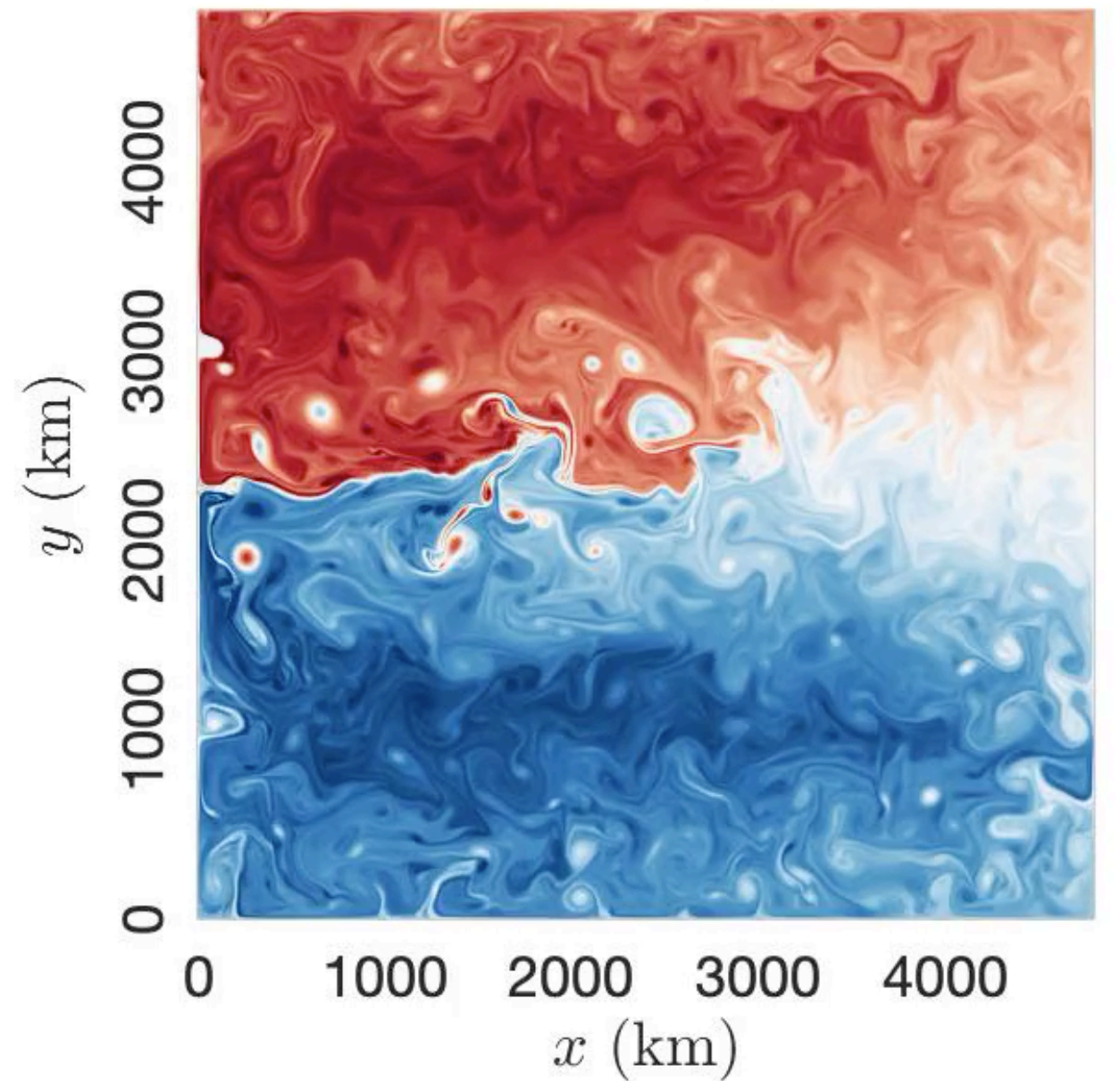
LU-POD-P (80 km)

Year = 104.0

Year = 100.0

Year = 100.0

Year = 100.0





Thanks for your attention !