Estimation of multiplicative noise operator statistics for reduced data assimilation in fluid mechanics



V. Resseguier, M. Ladvig, A. M. Picard & D. Heitz

INRAO SCALIAN

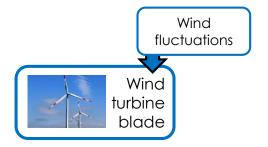




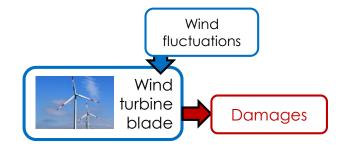
## Context Observer for wind turbine application



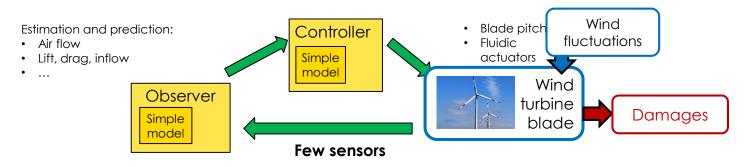
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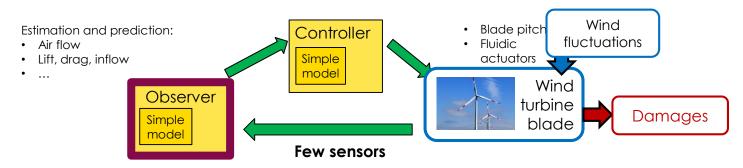
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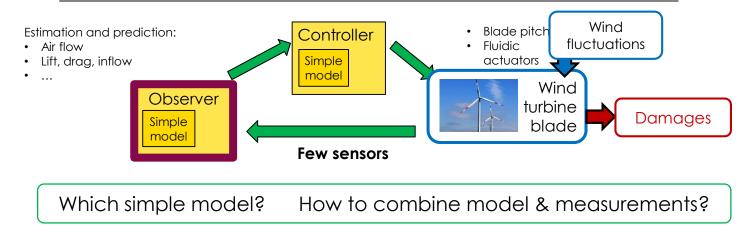
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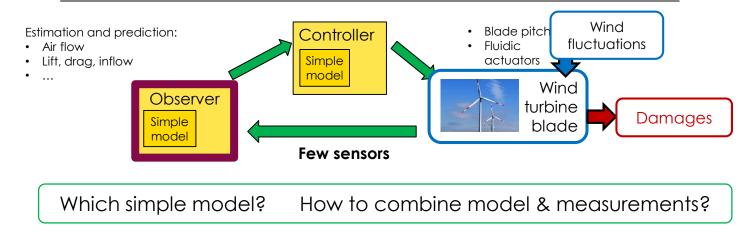


## Context Observer for wind turbine application



## Context Observer for wind turbine application

### Application: Real-time estimation and prediction of 3D fluid flow using strongly-limited computational resources & few sensors



Scientific problem : Simulation & data assimilation under severe dimensional reduction typically,  $10^7 \rightarrow O(10)$  degrees of freedom

# Content

- I. State of the art
  - a. Intrusive reduced order model (ROM)
  - b. Data assimilation
- II. Reduced location uncertainty models
  - a. Multiscale modeling
  - b. Location uncertainty models (LUM)
  - c. Reduced LUM
- III. Numerical results

# PARTI

## STATE OF THE ART

- a. Intrusive reduced order model (ROM)
- b. Data assimilation

# Reduced order model (ROM)

Solution of an PDE with the form:

$$v(x,t) \approx \sum_{i=0}^{n} b_i(t) \phi_i(x)$$



# Reduced order model (ROM)

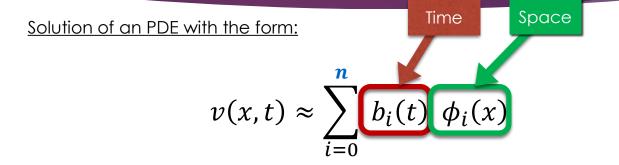
Solution of an PDE with the form:

$$v(x,t) \approx \sum_{i=0}^{n} b_i(t) \phi_i(x)$$

Time



# Reduced order model (ROM)



# Reduced order model (ROM)

Solution of an PDE with the form:

$$v(x,t) \approx \sum_{i=0}^{n} b_i(t) \phi_i(x)$$

Time

<u>Order of</u> <u>magnitude</u> <u>examples in</u> <u>CFD</u>

Full spaceReduced  
spaceSolution  
coordinates
$$(v_q(x_i,t))_{q,i}$$
 $(b_i(t))_i$ Dimension $M \times d \sim 10^7$  $n \sim 10 - 100$ 

Space

• <u>Principal Component Analysis (PCA)</u> on a *dataset* to reduce the dimensionality:

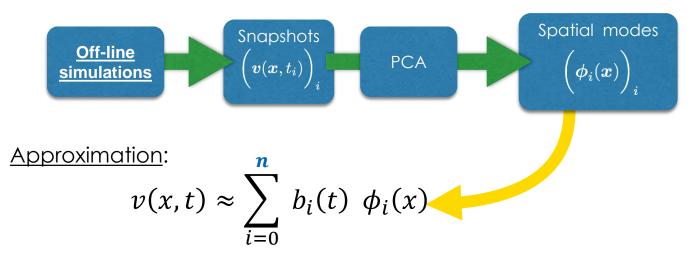
Off-line  
simulationsSnapshots  
$$(v(x,t_i))_i$$
Spatial modes  
 $(\phi_i(x))_i$ 

• Approximation:

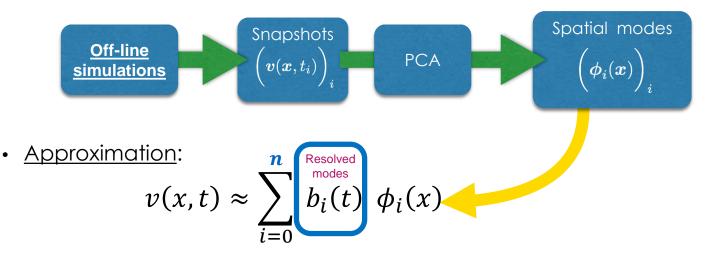
$$v(x,t)\approx \sum_{i=0} \ b_i(t) \ \phi_i(x)$$

n

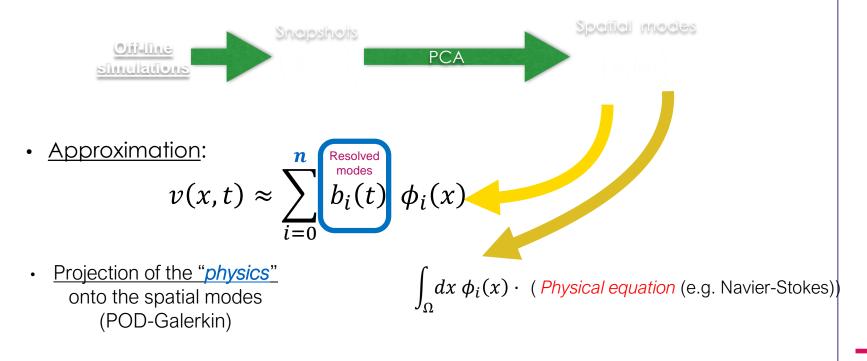
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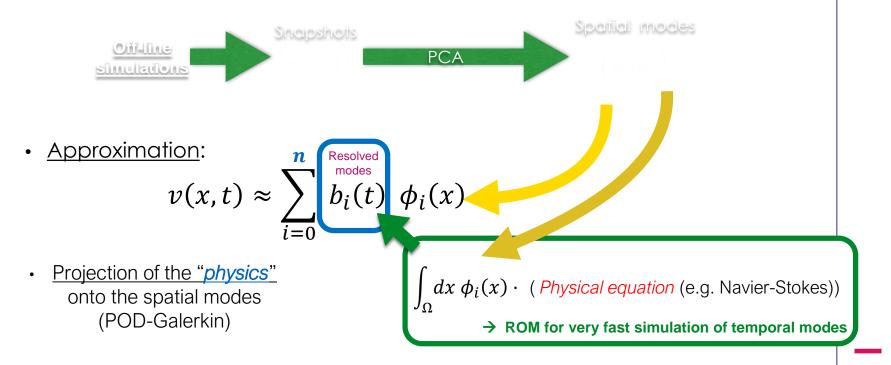
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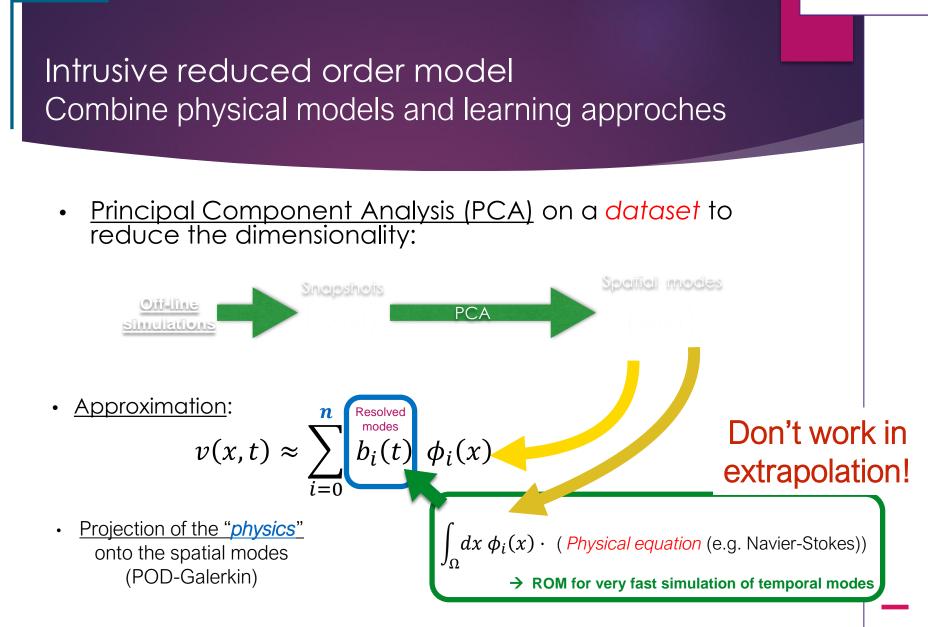


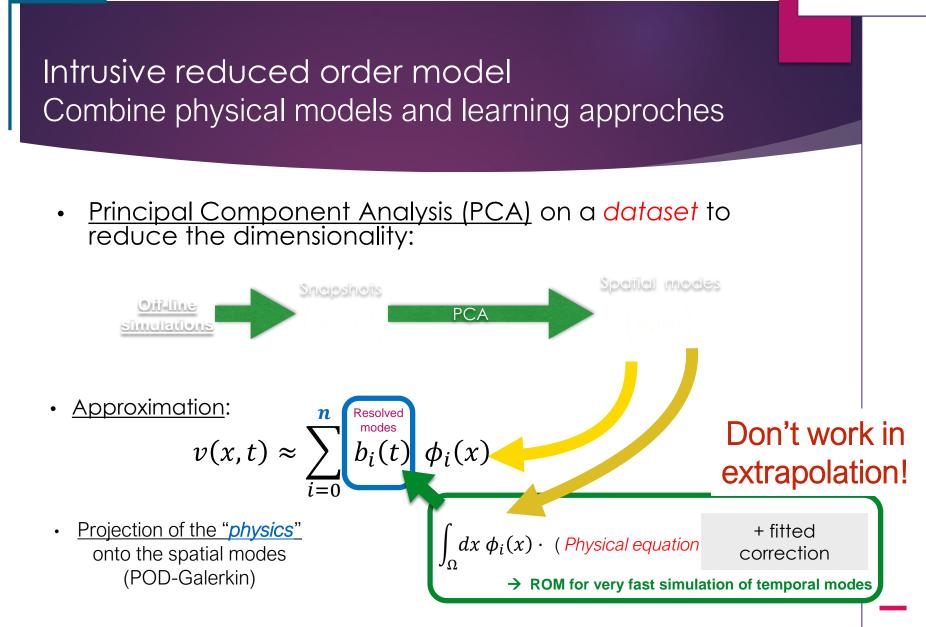
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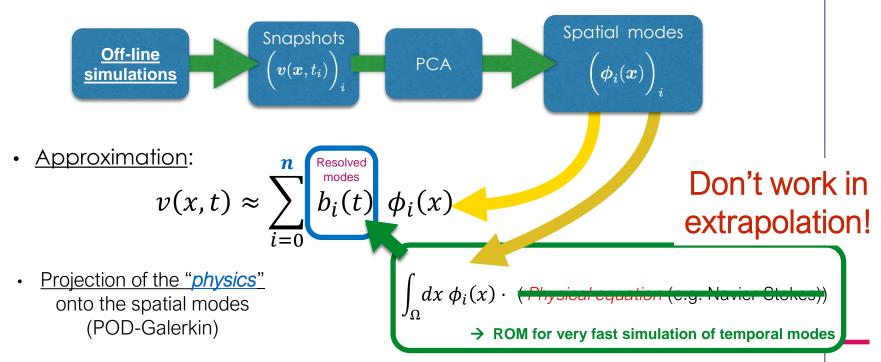




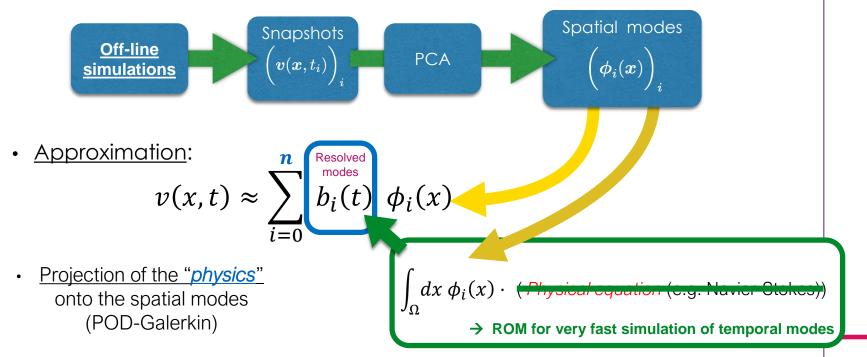


#### Intrusive reduced order model Combine physical models and learning approches <u>Principal Component Analysis (PCA)</u> on a dataset to reduce the dimensionality: Spatial modes Snapshois Oiii-Iline PCA simulations Approximation: ٠ lesolved modes Don't work in $v(x,t) \approx$ $b_i(t)$ $\phi_i(x)$ extrapolation! + fitted $\int_\Omega dx \, \phi_i(x) \cdot \, ($ Physical equation Projection of the "physics" correction onto the spatial modes + additive noise (POD-Galerkin) $\rightarrow$ ROM for very fast simulation of temporal modes

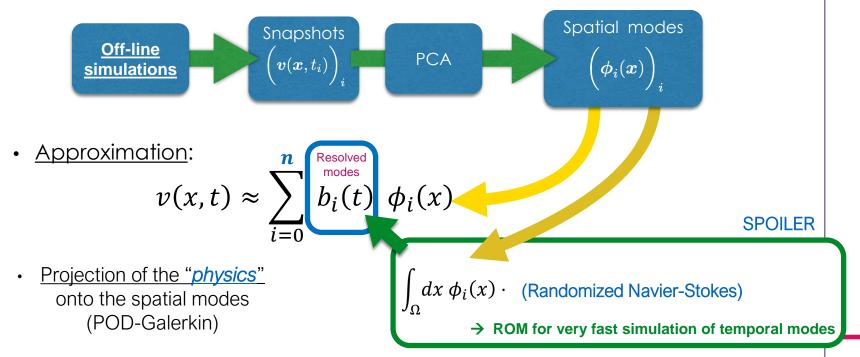
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 <u>Principal Component Analysis (PCA)</u> on a <u>dataset</u> to reduce the dimensionality:



 <u>Principal Component Analysis (PCA)</u> on a <u>dataset</u> to reduce the dimensionality:



## Data assimilation = Coupling simulations and measurements y

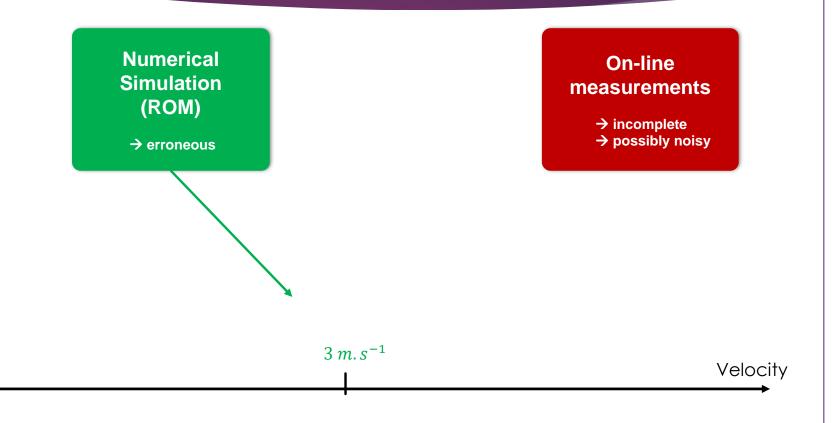
Numerical Simulation (ROM)

 $\rightarrow$  erroneous

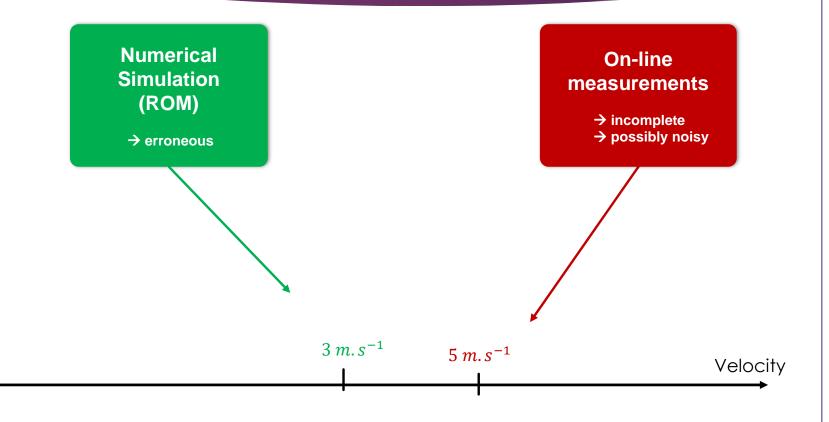
#### On-line measurements

→ incomplete
 → possibly noisy

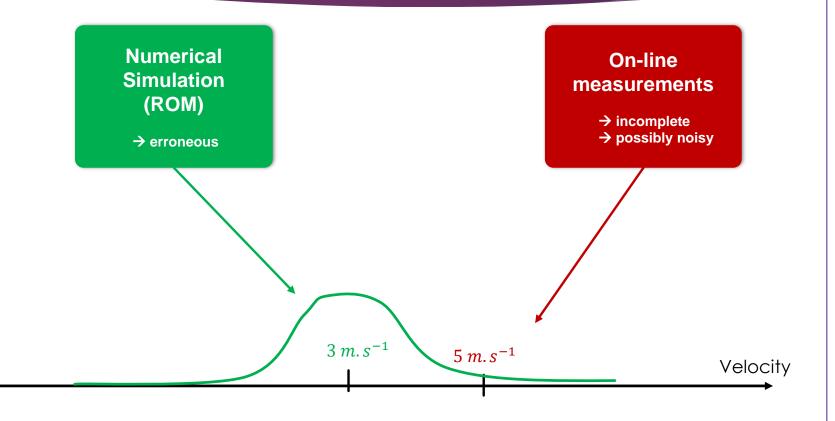
Velocity



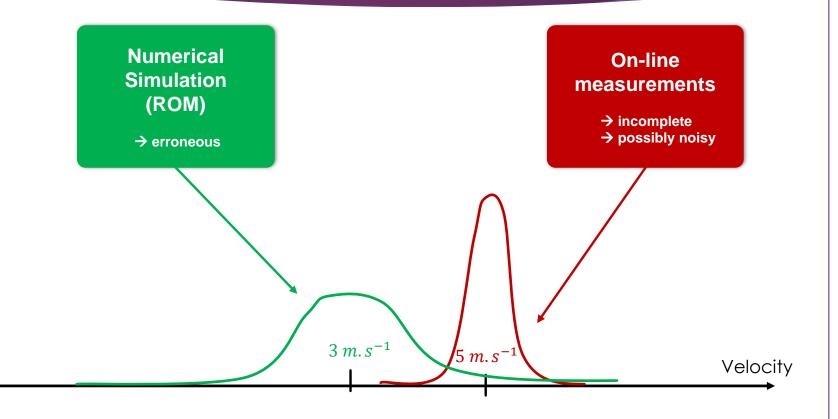
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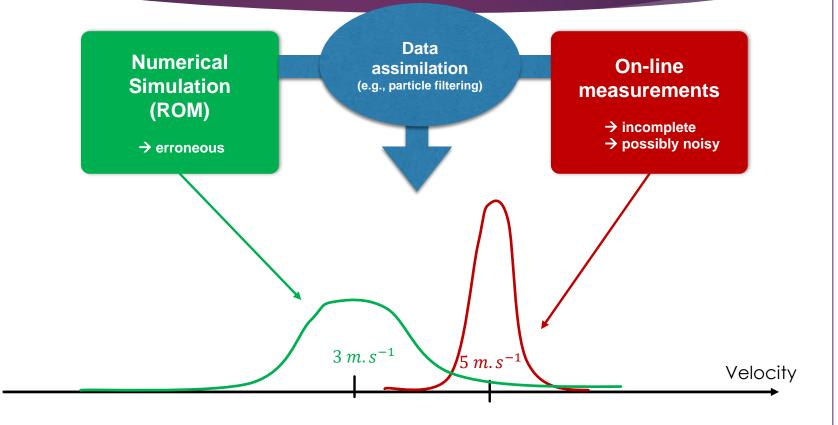
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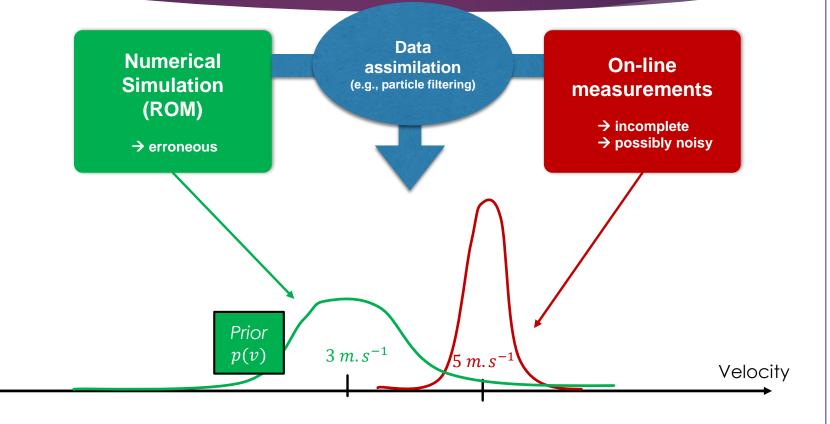
# Data assimilation <u>= Coupling simulations and measurements y</u>

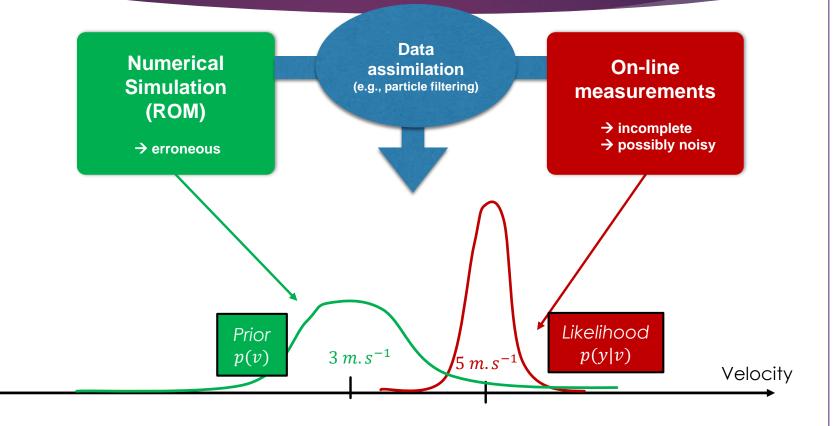


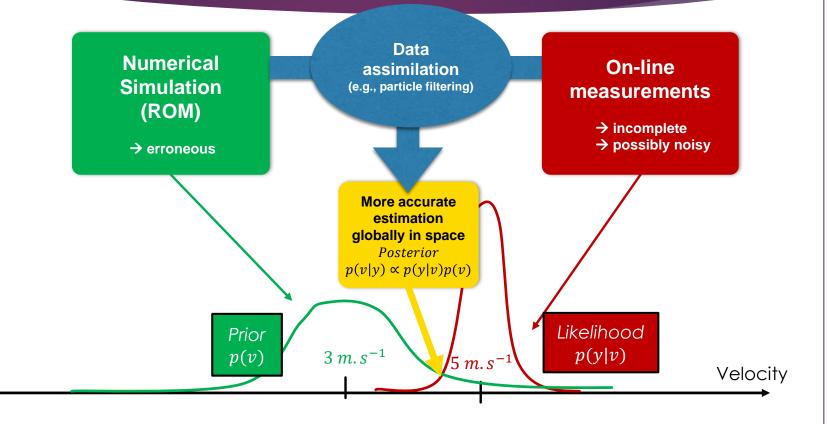
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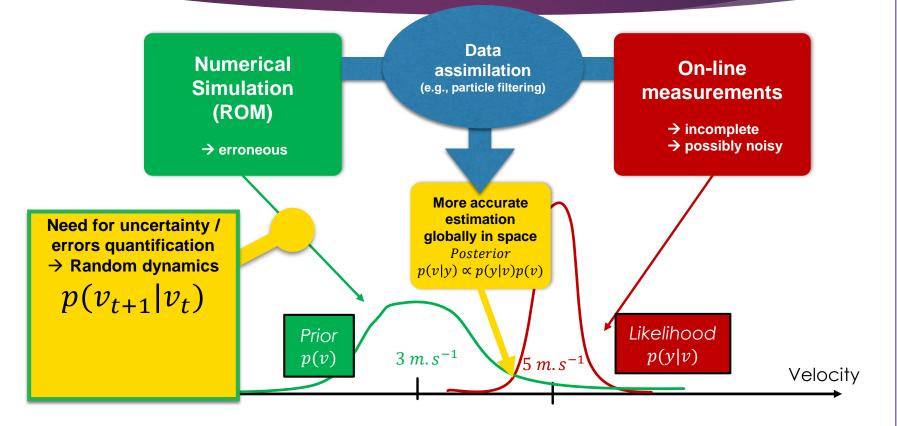
# Data assimilation

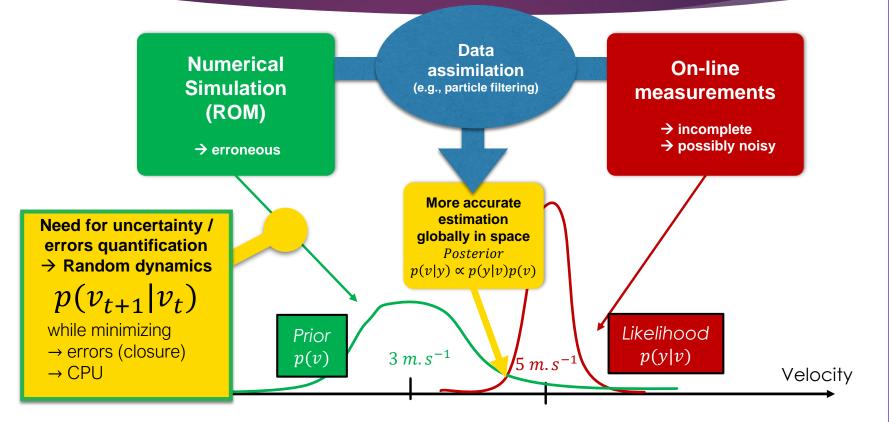
## = Coupling simulations and measurements y









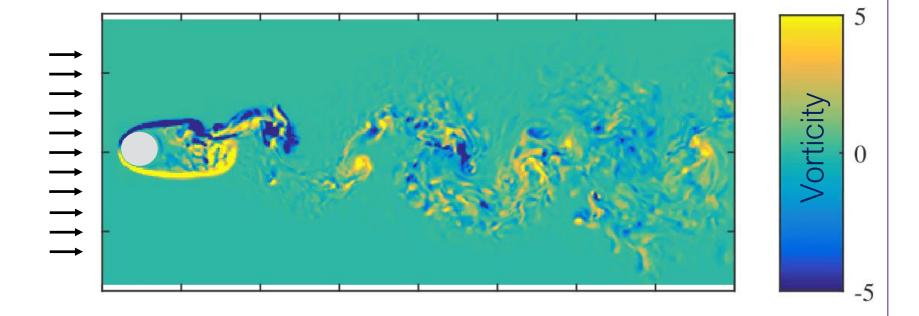


## Part II

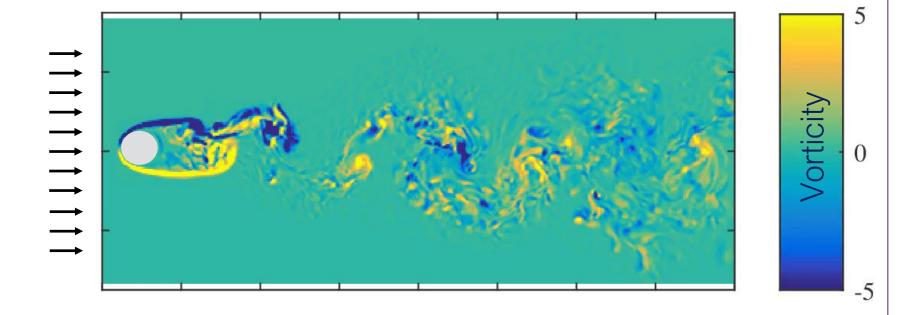
#### REDUCED LOCATION UNCERTAINTY MODELS

- a. Multiscale modeling
- b. Location uncertainty models (LUM)
- c. Reduced LUM (Red LUM)

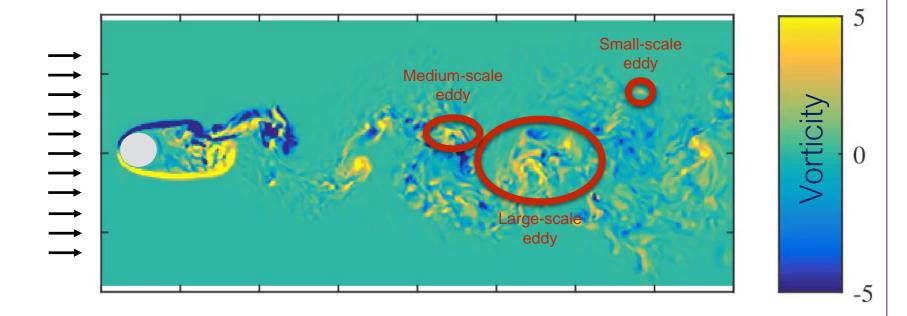
## Multiscale modeling



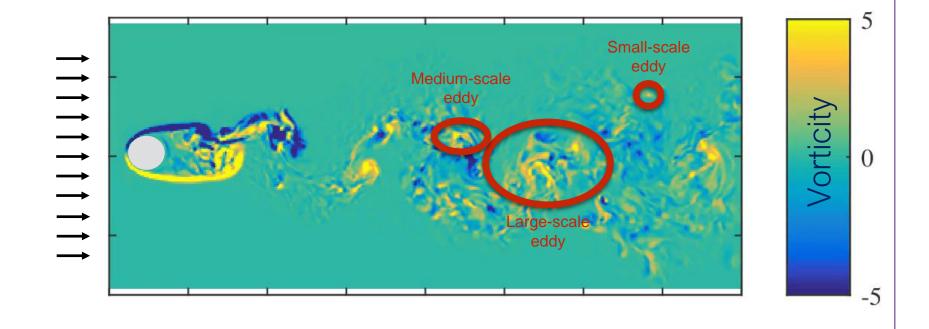
## Multiscale modeling



## Multiscale modeling



## Multiscale modeling



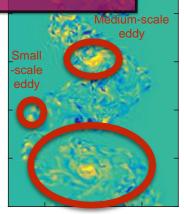
Fluids are multiscale — Many coupled degrees of freedom





Resolved fluid velocity:  $w = \sum_{i=0}^{n} b_i \phi_i$ 

Unresolved fluid velocity: v'



Large-scale eddy

## Multiscale modeling

Fluids are multiscale



Many coupled degrees of freedom

We cannot simulate (or observe) every scales.

Generally, authors

- simulate large scales w,
- model the effect of small scales v' in the equations (closure).

#### Here, we

- model the small scales v' through stochastic processes,
   <u>calibrated from data and/or from physical scale symmetries.</u>
- inject those in *physical* equations

for physical understanding, simulations & data assimilation.

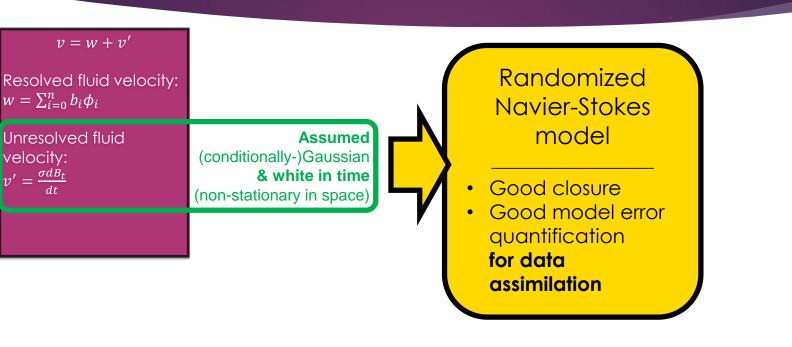


## location uncertainty models (LUM)

v = w + v' Resolved fluid velocity: $w = \sum_{i=0}^{n} b_i \phi_i$	
Unresolved fluid velocity: $v' = \frac{\sigma dB_t}{dt}$	Assumed (conditionally-)Gaussian & white in time (non-stationary in space)



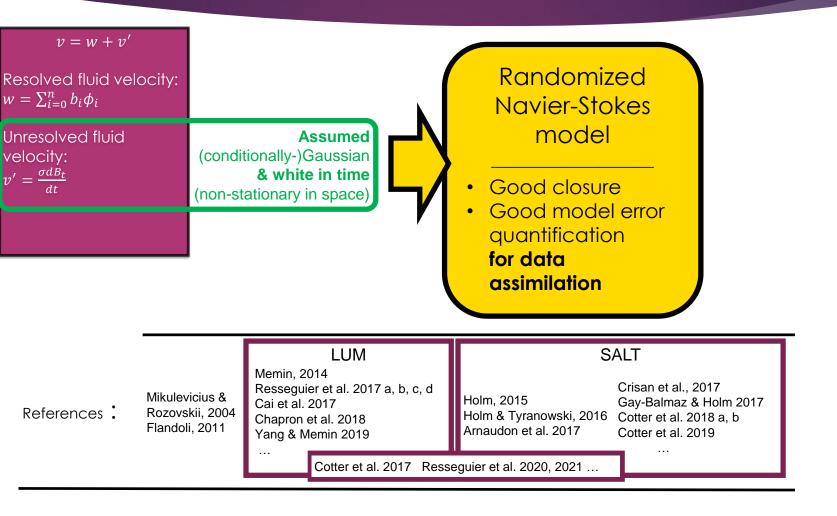
## location uncertainty models (LUM)



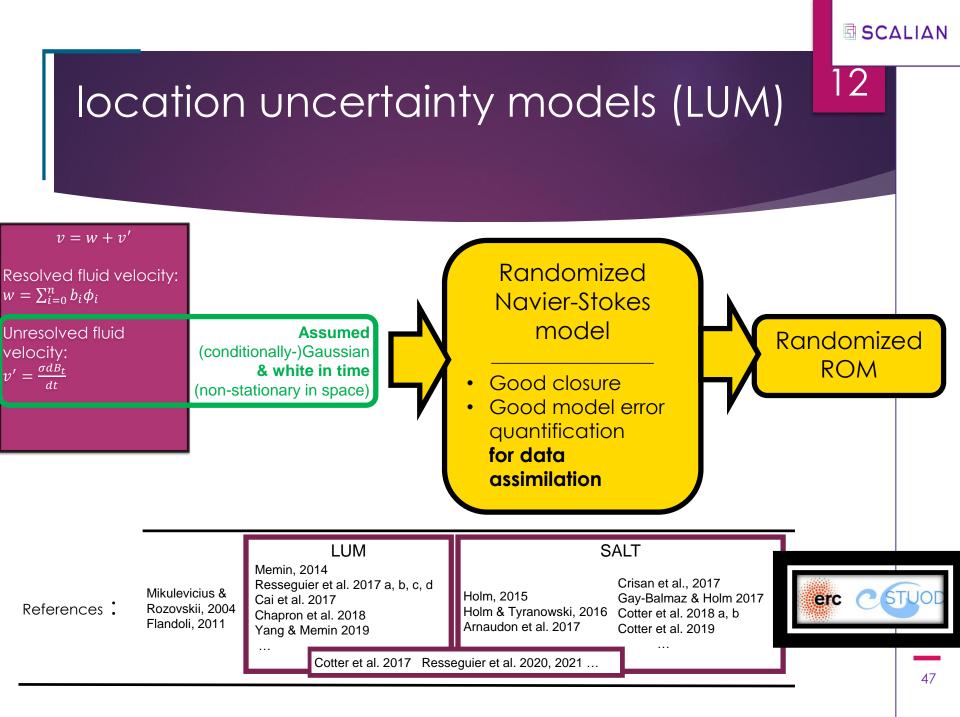
#### SCALIAN



## location uncertainty models (LUM)



#### location uncertainty models (LUM) v = w + v'Randomized Resolved fluid velocity: $w = \sum_{i=0}^{n} b_i \phi_i$ Navier-Stokes model Unresolved fluid Assumed (conditionally-)Gaussian velocity: $v' = \frac{\sigma dB_t}{dt}$ & white in time Good closure (non-stationary in space) Good model error quantification for data assimilation LUM SALT Memin. 2014 Crisan et al., 2017 Resseguier et al. 2017 a, b, c, d Mikulevicius & STUOL Holm, 2015 Gay-Balmaz & Holm 2017 erc Cai et al. 2017 References: Rozovskii, 2004 Holm & Tyranowski, 2016 Cotter et al. 2018 a, b Chapron et al. 2018 Flandoli, 2011 Arnaudon et al. 2017 Cotter et al. 2019 Yang & Memin 2019 Cotter et al. 2017 Resseguier et al. 2020, 2021 ... 46



## location uncertainty models (LUM), Randomized Navier-Stokes

v = w + v'

Resolved fluid velocity: *w* 

```
Unresolved fluid
velocity:
v' = \frac{\sigma dB_t}{dt} (Gaussian, white
wrt t)
(assuming \nabla \cdot w = 0 and \nabla \cdot v' =
```

# Momentum conservation $d(w(t, X_t)) = dF$ (Forces)

Positions of fluid parcels  $X_t$ :  $dX_t = w(t, X_t)dt + \underbrace{\sigma(t, X_t)dB_t}$ 

> Gaussian process white in time

#### SCALIAN

From Ito-Wentzell

formula (Kunita

with Ito notations

1990)

## location uncertainty models (LUM), Randomized Navier-Stokes

#### v = w + v'

Resolved fluid velocity: w

Unresolved fluid velocity:  $v' = \frac{\sigma dB_t}{dt}$  (Gaussian, white wrt t)

(assuming  $\nabla \cdot w = 0$  and  $\nabla \cdot v' = 0$ )

Variance tensor:  $a(x,x) = \frac{\mathbb{E}\{(\sigma dB_t)(\sigma dB_t)^T\}}{dt}$ 

$$d_t w + w^* dt \cdot \nabla w + \sigma dB_t \cdot \nabla w - \nabla \cdot \left(\frac{1}{2}a\nabla w\right) dt = dF$$

Resseguier V. & al. (2017). Part I. Geophys. Astro. Fluid. hal-01391420

SCALIAN

## location uncertainty models (LUM), Randomized Navier-Stokes

From Ito-Wentzell formula (Kunita 1990) with Ito notations

Advection  
$$d_t w + w^* dt \cdot \nabla w + \sigma dB_t \cdot \nabla w - \nabla \cdot \left(\frac{1}{2} a \nabla w\right) dt = dF$$

Variance tensor:  $a(x, x) = \frac{\mathbb{E}\{(\sigma dB_t)(\sigma dB_t)^T\}}{dt}$ 

(assuming  $\nabla \cdot w = 0$  and  $\nabla \cdot$ 

v = w + v'

Resolved fluid velocity:

(Gaussian, white

Unresolved fluid

velocity:  $v' = \frac{\sigma dB_t}{dt}$ 

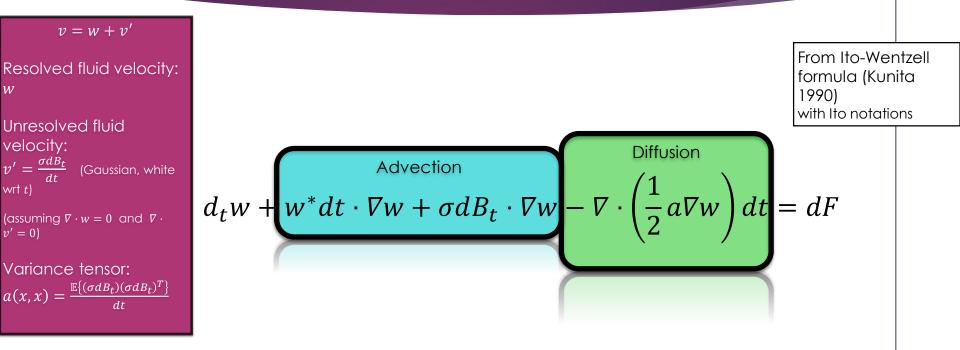
wrt t)

v'=0)

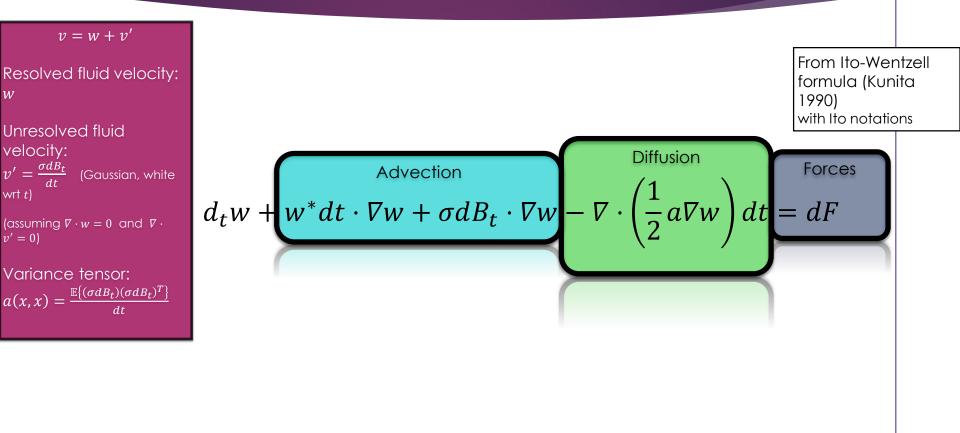
W

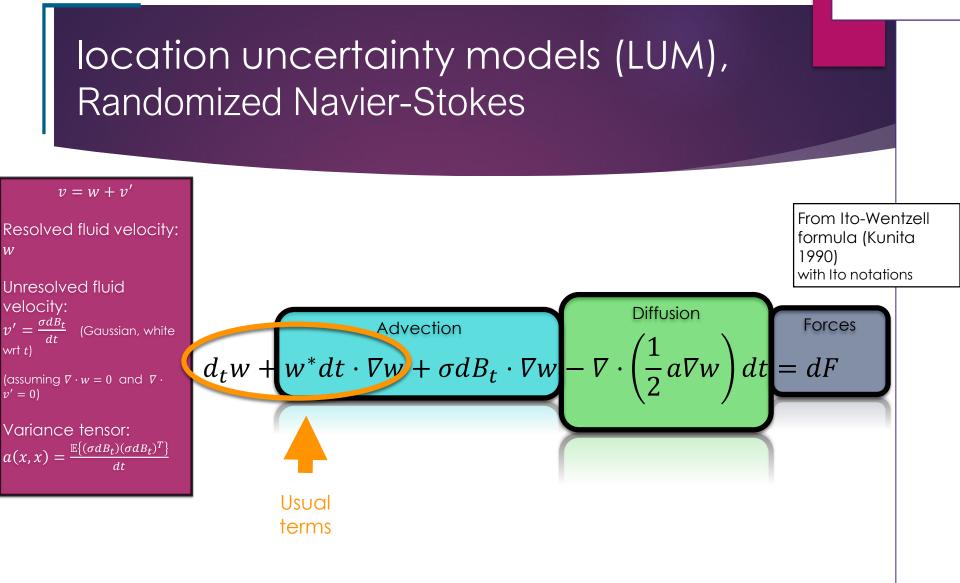




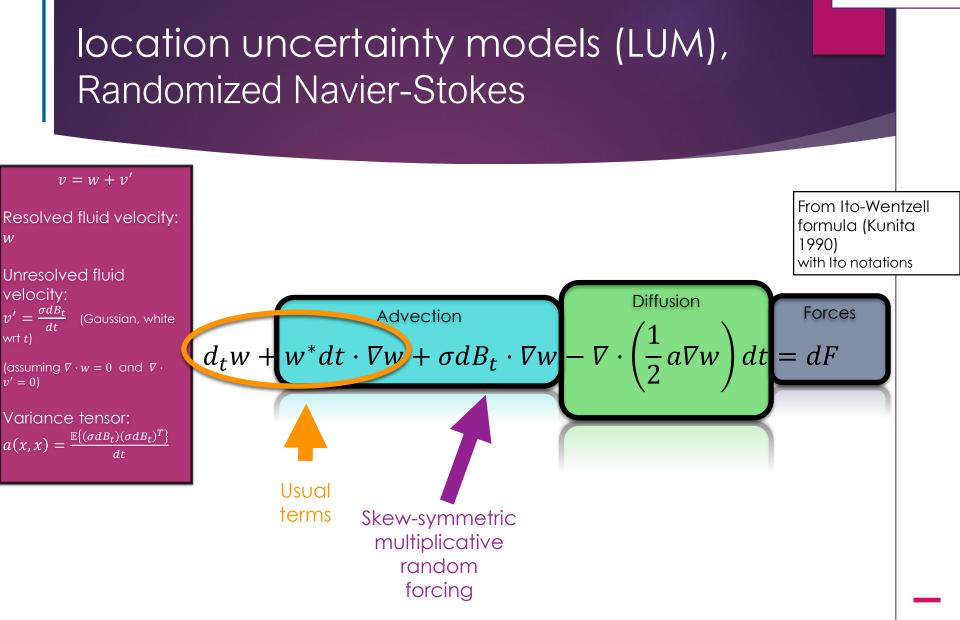




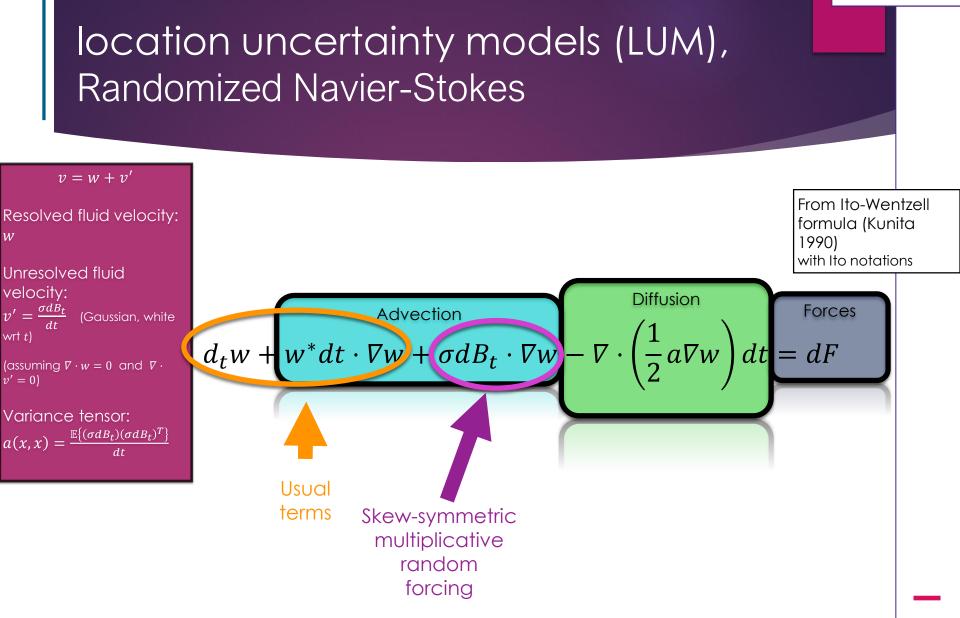




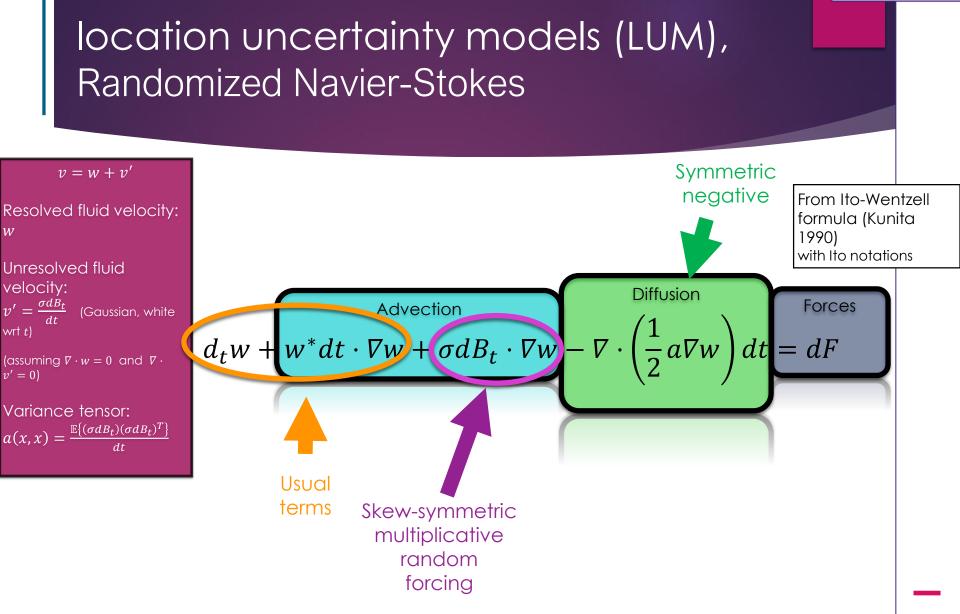
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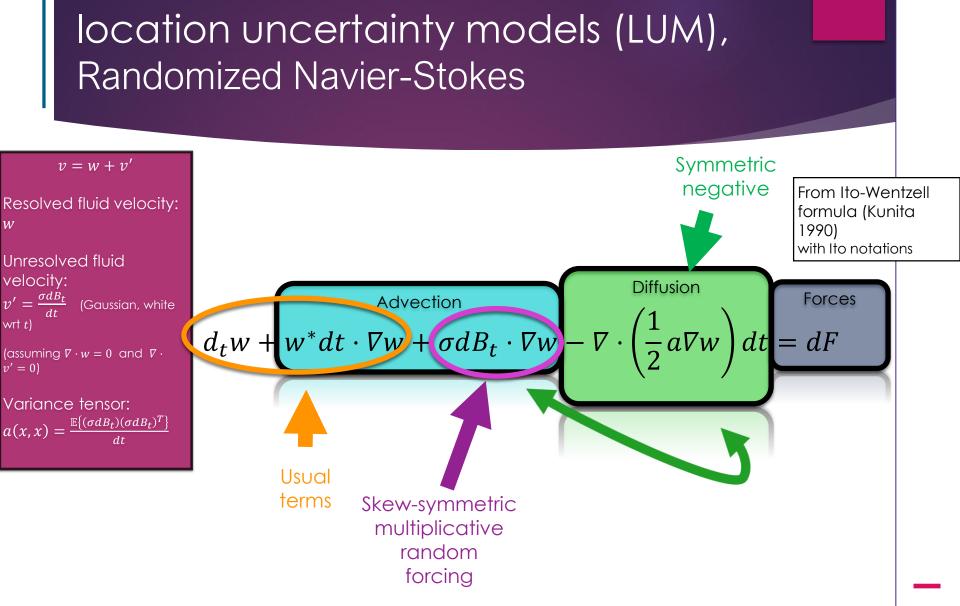


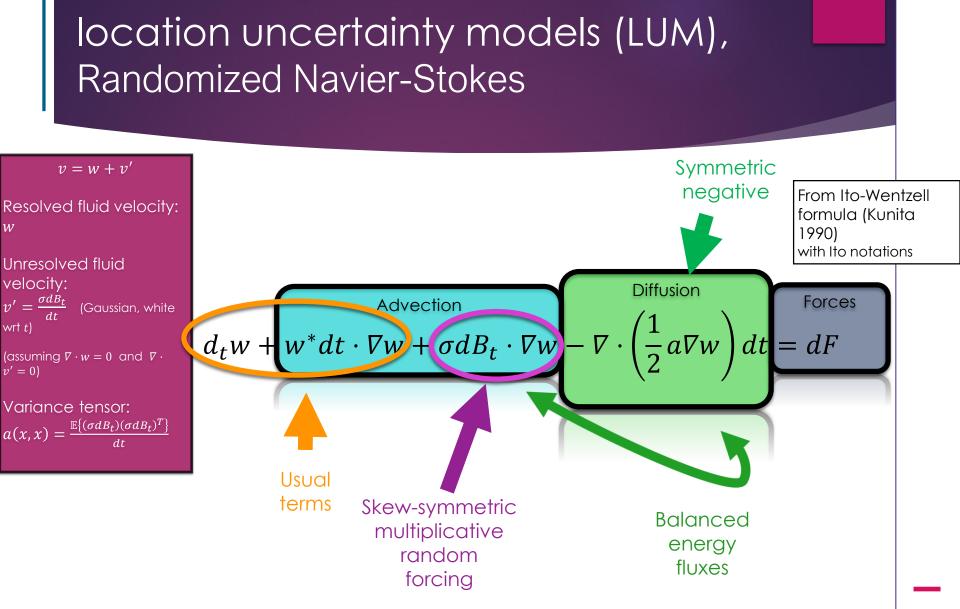
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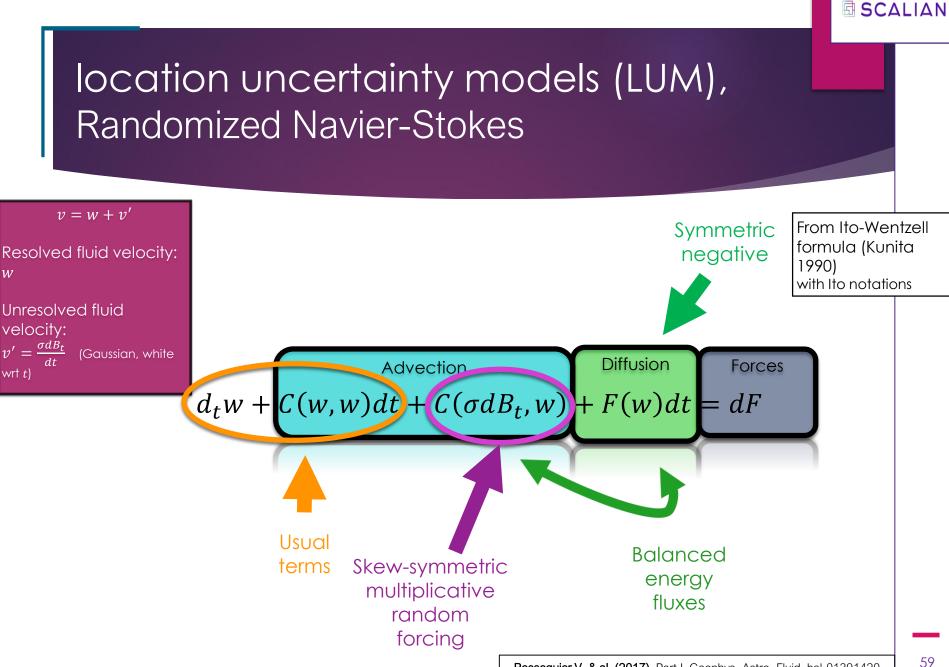












Full order :  $M \sim 10^7$ 

Reduced order :  $n \sim 10$ 

## Reduced Lum (Red LUM) POD-Galerkin gives SDEs for resolved modes

v = w + v'

Resolved fluid velocity:  $w(x,t) = \sum_{i=0}^{n} b_i(t)\phi_i(x)$ 

ſ

Unresolved fluid velocity:  $v' = \frac{\sigma dB_t}{dt}$  (Gaussian, white wrt t)

$$\int_{\Omega} \phi_i(x) \cdot (d_t w + C(w, w)dt + F(w)dt + C(\sigma dB_t, w) = dF) dx$$

Full order :  $M \sim 10^7$ 

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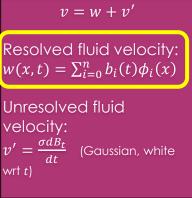
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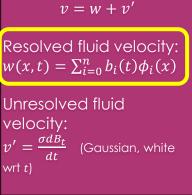
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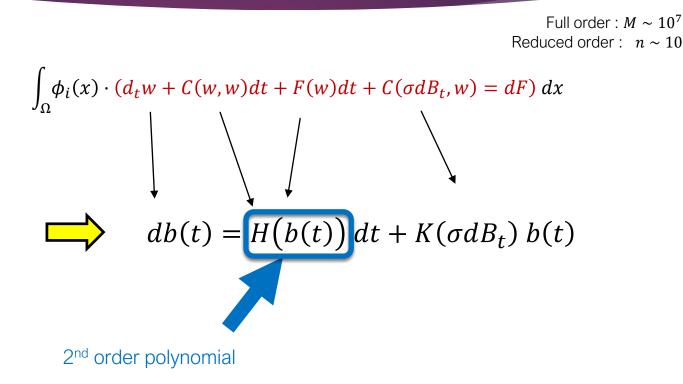
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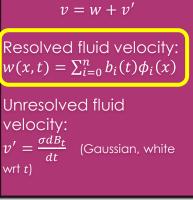
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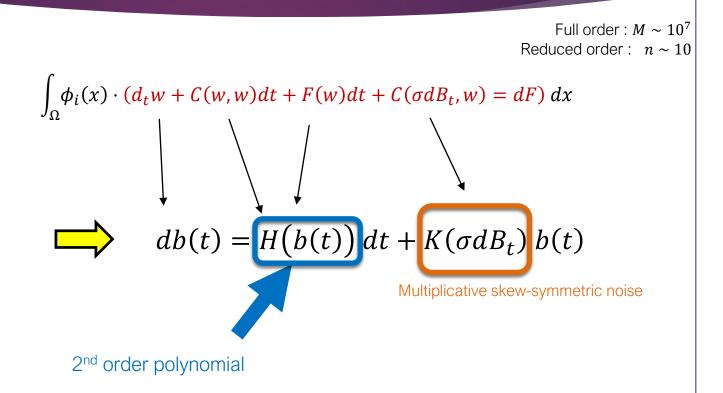


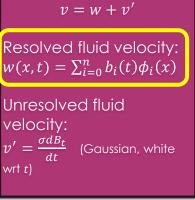
Resseguier et al. (2021). SIAM-ASA J Uncertain . hal- 03169957

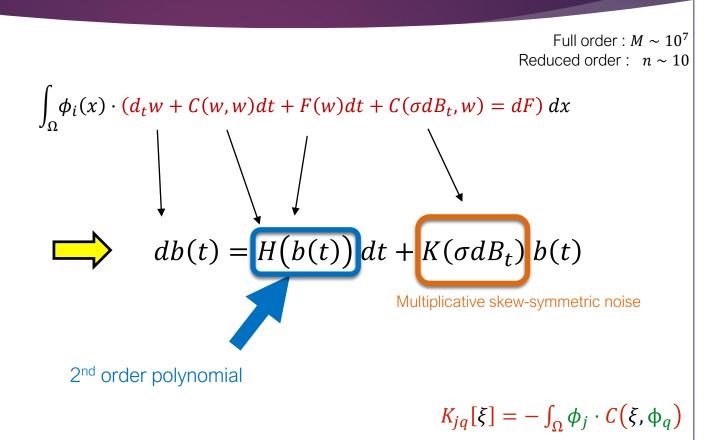












v = w + v'

Resolved fluid velocity:  $w(x,t) = \sum_{i=0}^{n} b_i(t)\phi_i(x)$ 

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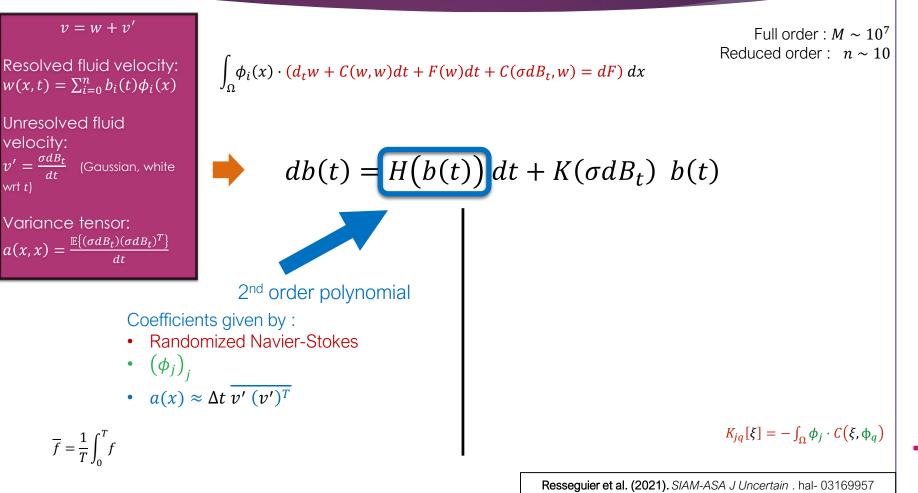
Variance tensor:  $a(x,x) = \frac{\mathbb{E}\{(\sigma dB_t)(\sigma dB_t)^T\}}{dt}$   $\int_{\Omega} \phi_i(x) \cdot (d_t w + C(w, w)dt + F(w)dt + C(\sigma dB_t, w) = dF) dx$ 

$$db(t) = H(b(t)) dt + K(\sigma dB_t) b(t)$$

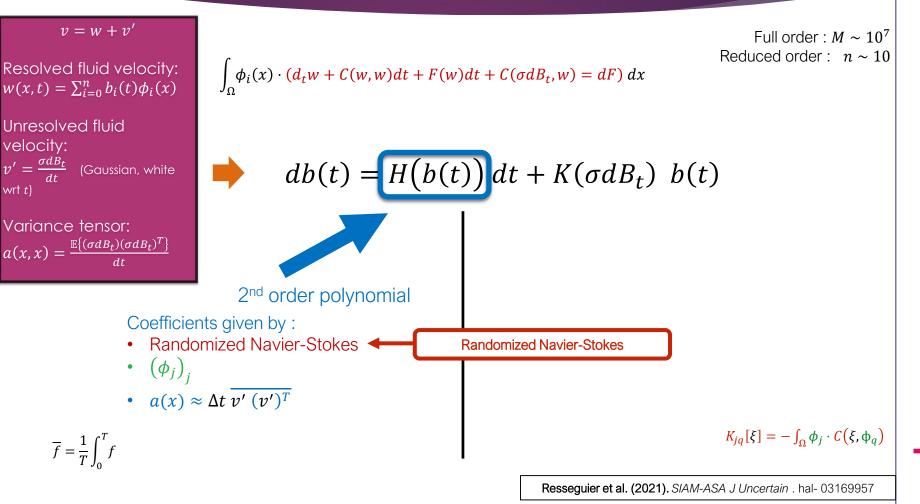
$$K_{jq}[\xi] = -\int_{\Omega} \phi_j \cdot C(\xi, \phi_q)$$

Full order :  $M \sim 10^7$ Reduced order :  $n \sim 10$ 

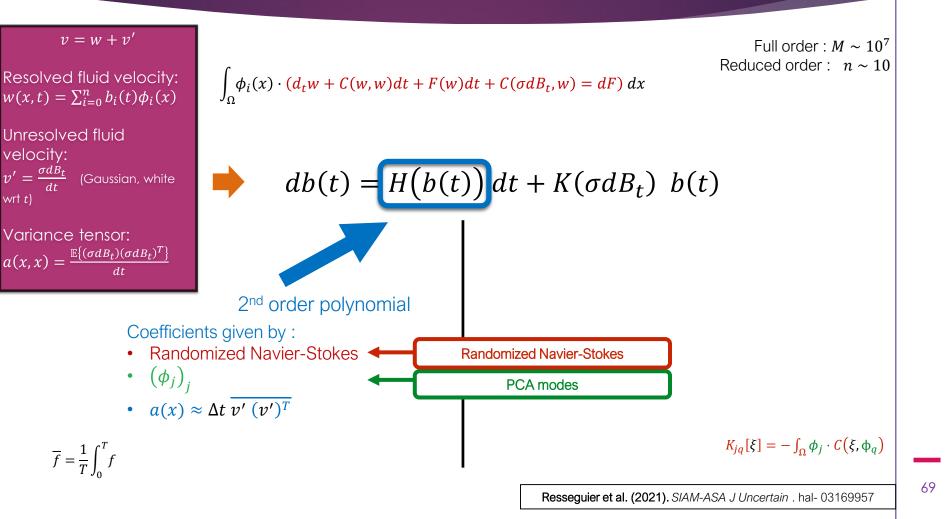




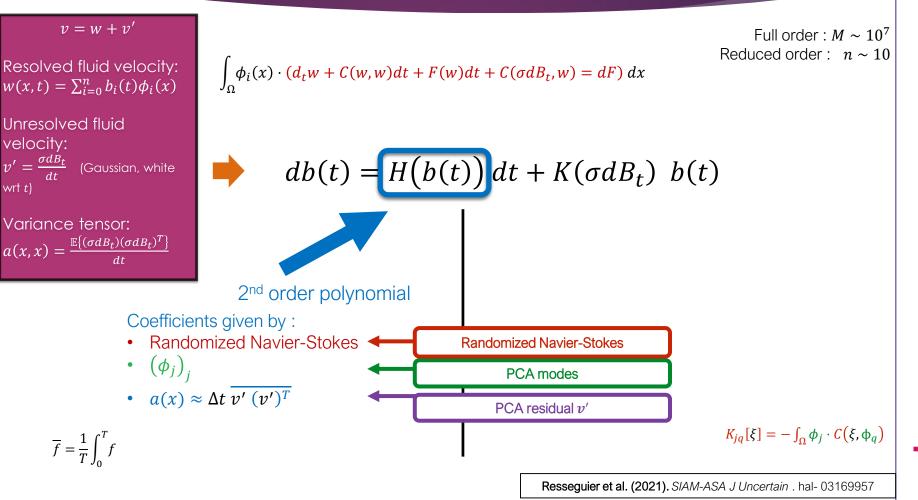




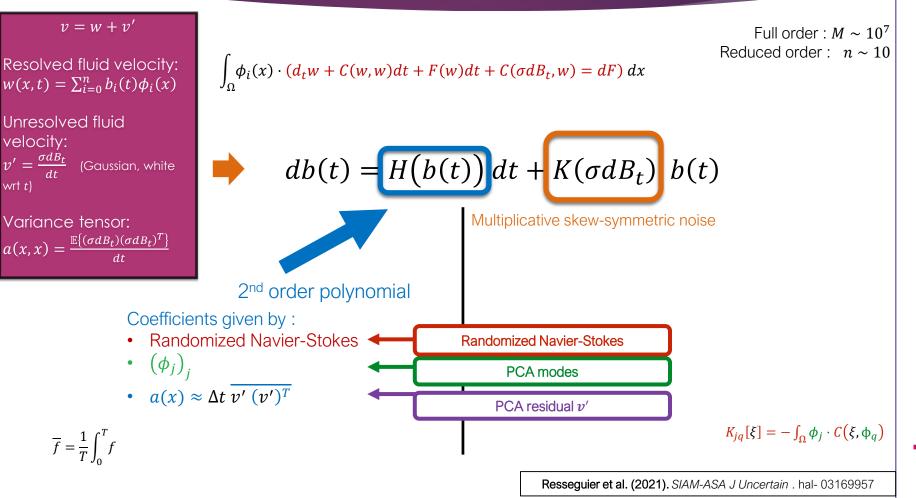




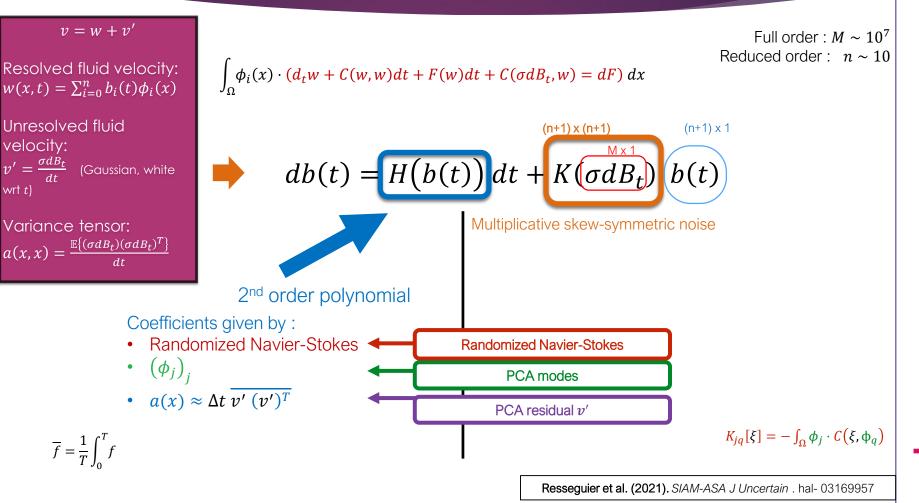




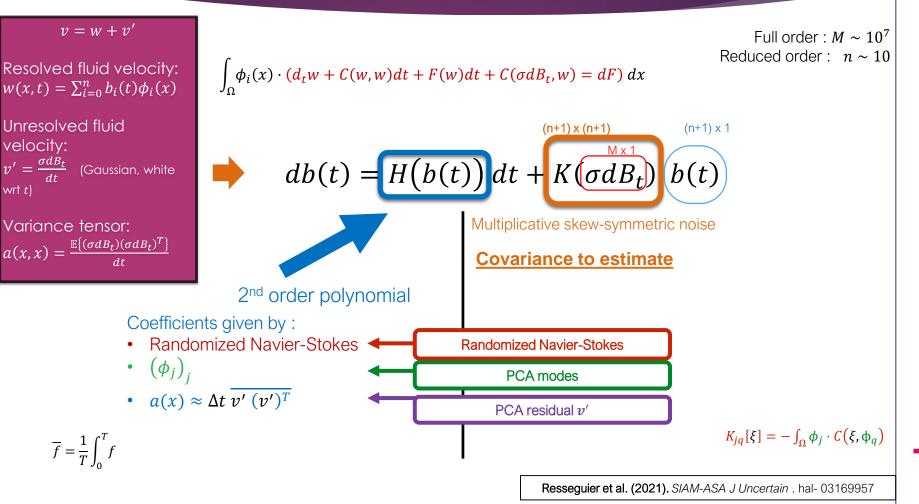




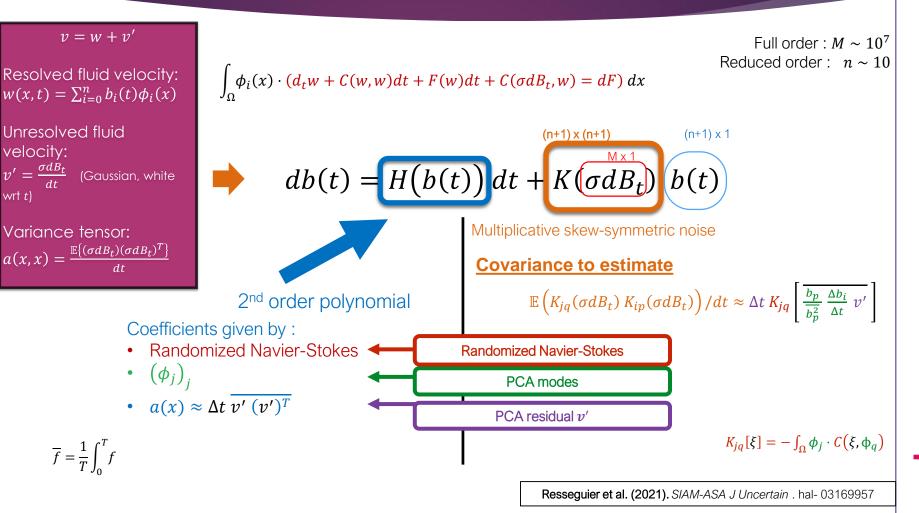




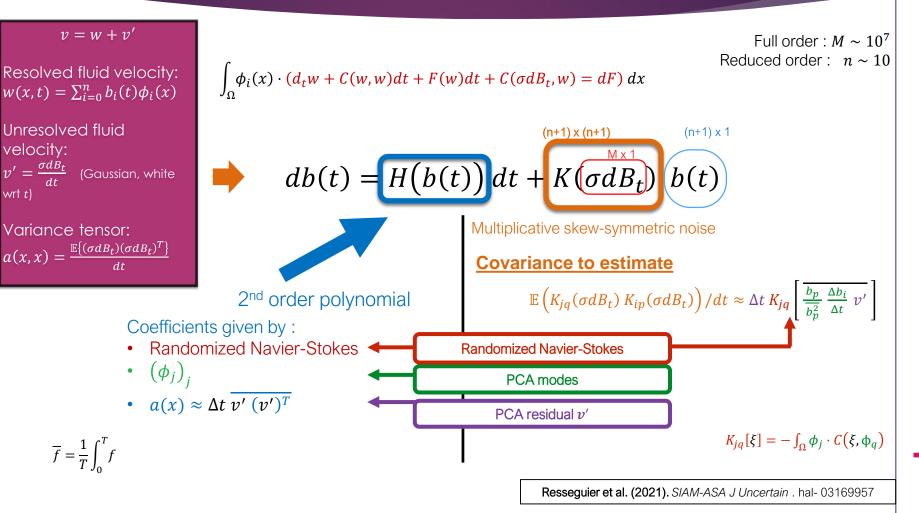




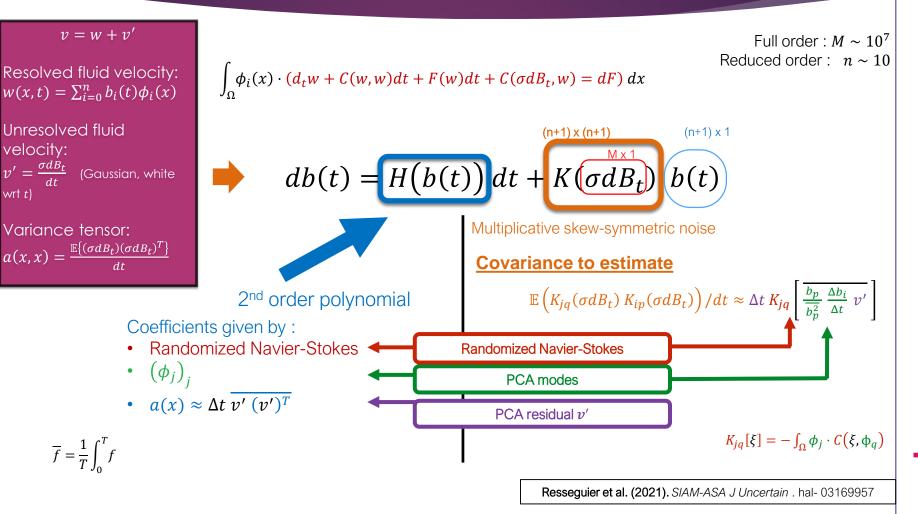




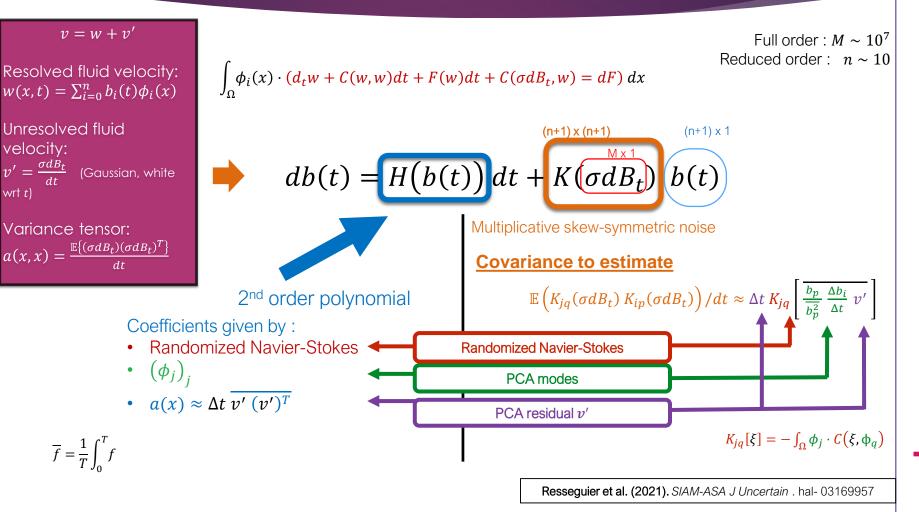




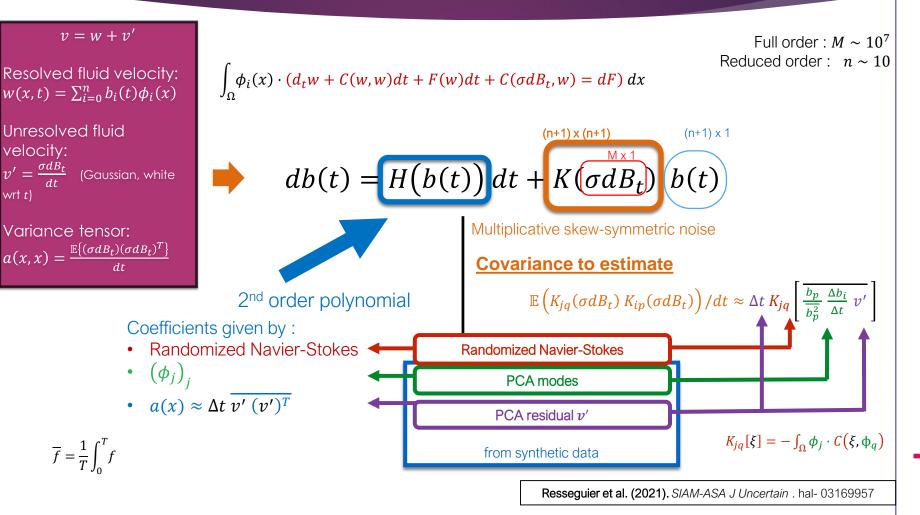




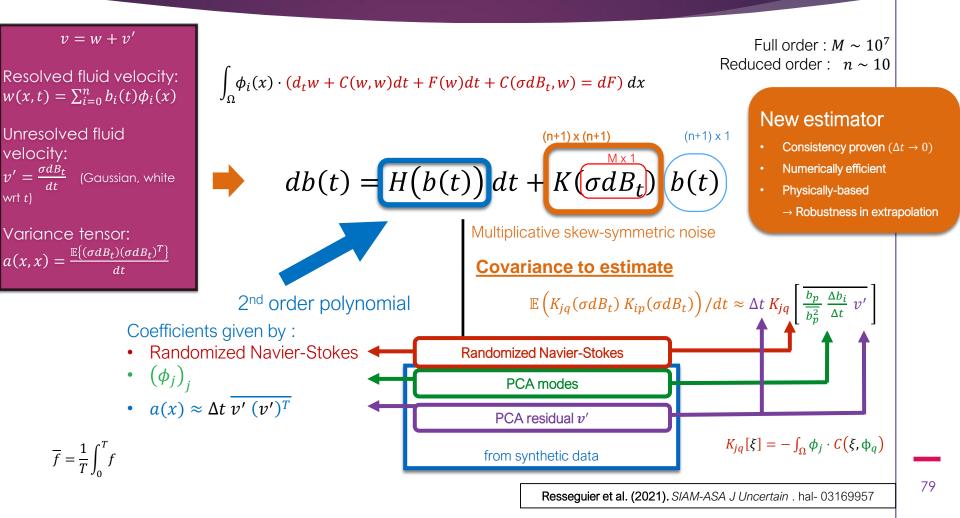












## Reduced Lum (Red LUM) Multiplicative noise covariance

v = w + v'

Resolved fluid velocity:  $w(x,t) = \sum_{i=0}^{n} b_i(t)\phi_i(x)$ 

Unresolved fluid velocity:  $v' = \frac{\sigma dB_t}{dt}$  (Gaussian, white wrt t)

Randomized Navier-Stokes
PCA modes
PCA residual $v'$
from synthetic data

 $\overline{f} = \frac{1}{T} \int_{0}^{T} f$ 

$$db(t) = H(b(t)) dt + K(\sigma dB_t) b(t) \text{ with } K_{jq}[\xi] = -\int_{\Omega} \phi_j \cdot C(\xi, \phi_q)$$

- Since  $\sigma dB_t$  is white in time,  $\Sigma_{jq,ip} = \mathbb{E} \left( K_{jq} (\sigma dB_t) K_{ip} (\sigma dB_t) \right) / dt \approx \Delta t \ \overline{K_{jq}(v') K_{ip}(v')}$
- K is a matrix of integro-differential operators  $\rightarrow$  cannot be evaluated on v'(x,t) at every time t
- Covariance of  $\sigma dB_t \approx \Delta t^2 \overline{(v'(x,t))(v'(y,t))}^T : M \times M \sim 10^{13} \text{ coefficients} \rightarrow \text{intractable}$

### New estimator

- Consistency proven  $(\Delta t \rightarrow 0)$
- Numerically efficient
- Physically-based

Reduced order :  $n \sim 10$ 

Number of time steps :  $N \sim 10^4$ 

Full order (~ nb spatial grid points):  $M \sim 10^7$ 

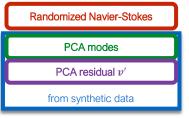
 $\rightarrow$  Robustness in extrapolation

## Reduced Lum (Red LUM) Multiplicative noise covariance

v = w + v'

Resolved fluid velocity:  $w(x,t) = \sum_{i=0}^{n} b_i(t)\phi_i(x)$ 

Unresolved fluid velocity:  $v' = \frac{\sigma dB_t}{dt}$  (Gaussian, white wrt t)



 $\overline{f} = \frac{1}{T} \int_{0}^{T} f$ 

$$db(t) = H(b(t)) dt + K(\sigma dB_t) b(t) \text{ with } K_{jq}[\xi] = -\int_{\Omega} \phi_j \cdot C(\xi, \phi_q)$$

- Curse of dimensionality
  - Since  $\sigma dB_t$  is white in time,  $\Sigma_{jq,ip} = \mathbb{E} \left( K_{jq} (\sigma dB_t) K_{ip} (\sigma dB_t) \right) / dt \approx \Delta t \ \overline{K_{jq}(v') K_{ip}(v')}$ 
    - K is a matrix of integro-differential operators  $\rightarrow$  cannot be evaluated on v'(x,t) at every time t
    - Covariance of  $\sigma dB_t \approx \Delta t^2 \overline{(v'(x,t))(v'(y,t))^T}$ :  $M \times M \sim 10^{13}$  coefficients  $\rightarrow$  intractable
  - **Efficient estimator**  $\Sigma_{jq,ip} \approx \Delta t K_{jq} \left[ \frac{b_p}{b_p^2} \frac{\Delta b_i}{\Delta t} v' \right]$  (hybrid fitting & physics-based) requires only  $O(n^2 M)$  correlation estimations and  $O(n^2)$  evaluations of K

- New estimator
- Consistency proven  $(\Delta t \rightarrow 0)$
- Numerically efficient
- Physically-based

Reduced order :  $n \sim 10$ 

Number of time steps :  $N \sim 10^4$ 

Full order (~ nb spatial grid points):  $M \sim 10^7$ 

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PCA modes
PCA residual $v'$
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$$\Delta t \, K_{jq} \left[ \overline{b_p \frac{\Delta b_i}{\Delta t} \, v'} \right] = \Delta t \, \overline{b_p \frac{\Delta b_i}{\Delta t} \, K_{jq}[v']} \approx \frac{1}{r} \int_0^T b_p \, d < b_i, \\ K_{jq}(\sigma B) > = \frac{1}{r} \int_0^T b_p \sum_{r=0}^n b_r d < K_{ir}(\sigma B), \\ K_{jq}(\sigma B) > = \sum_{r=0}^n \sum_{jq,ir} \overline{b_p b_r} = \sum_{jq,ir} \overline{b_p b_r} = \sum_{r=0}^n \sum_{jq,ir} \sum_{jq,ir} \sum_{jq,ir} \sum_{jq,ir} \sum_{jq,ir} \sum_{jq,ir}$$

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• Optimal time subsampling at Δ*t* needed to meet the white assumption

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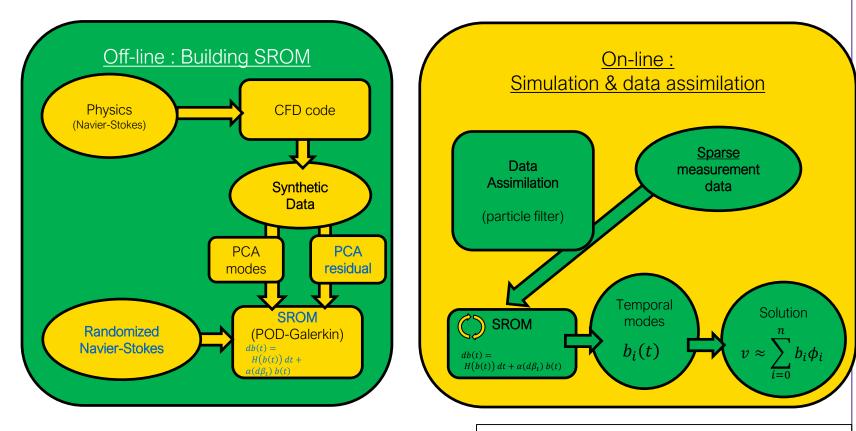
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- Optimal time subsampling at  $\Delta t$  needed to meet the white assumption
- Additional reduction for efficient sampling : diagonalization of  $\Sigma \rightarrow K(\sigma dB_t) \approx \alpha(d\beta_t)$  with a n-dimensional (instead of (n+1)<sup>2</sup>-dimensional) Brownian motion  $\beta$

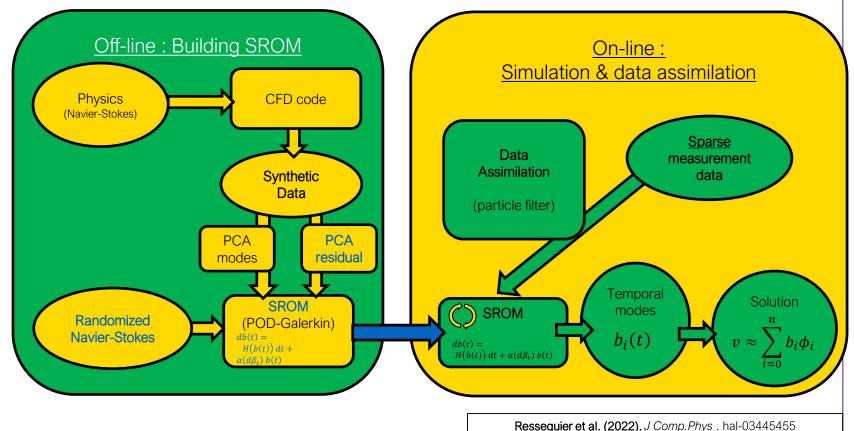
Resseguier et al. (2021). SIAM-ASA J Uncertain . hal- 03169957

## Summary Stochastic ROM + Data assimilation

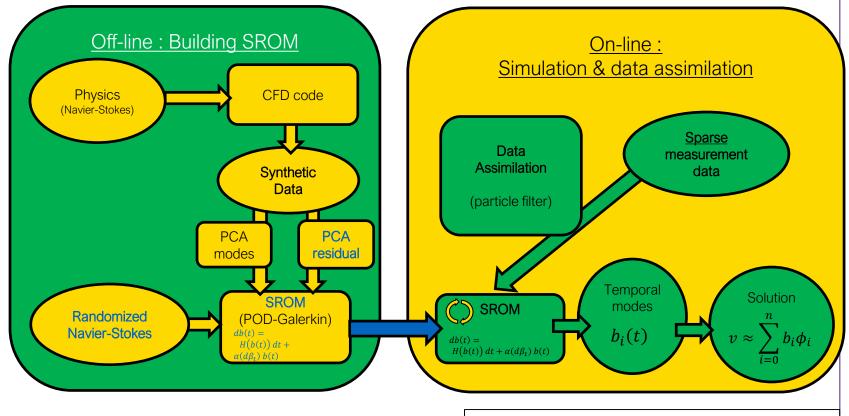


Resseguier et al. (2022). J Comp. Phys . hal-03445455

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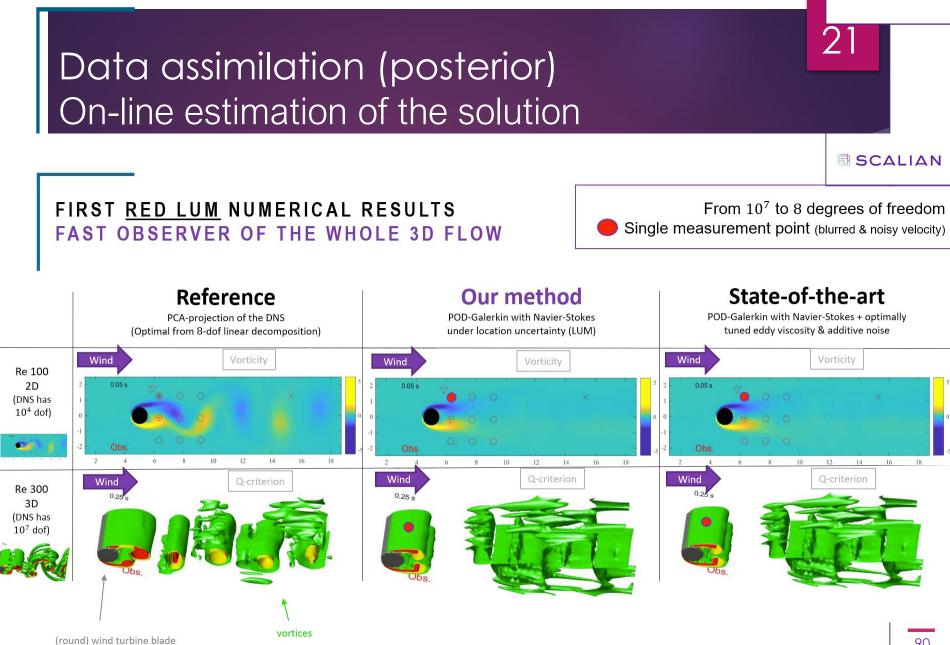
## Part III

## NUMERICAL RESULTS

SCALIAN

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## Data assimilation (posterior) On-line estimation of the solution



## CONCLUSION

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## Conclusion

- Reduced order model (ROM) : for very fast and robust CFD  $(10^7 \rightarrow 8 \text{ degrees of freedom.})$ 
  - Combine data & physics (built off-line)
  - Closure problem handled by LUM
  - Efficient estimator for the multiplicative noise
  - ▶ Efficient generation of prior / Model error quantification
- Data assimilation (Bayesian inverse problem) : to correct the fast simulation on-line by incomplete/noisy measurements
- First results
  - Optimal <u>unsteady</u> flow estimation/prediction in the whole spatial domain (large-scale structures)
  - Robust far outside the training set

### NEXT STEPS

- Real measurements
- Better stochastic closure
- Parametric ROM (unknown inflow)

More turbulent flows



### THANK YOU

- Resseguier, V., Mémin, E., & Chapron, B. (2017). Geophysical flows under location uncertainty, Part I Random transport and general models. Geophysical & Astrophysical Fluid Dynamics, 111(3), 149-176.
- Resseguier, V., Picard, A. M., Mémin, E., & Chapron, B. (2021). Quantifying truncation-related uncertainties in unsteady fluid dynamics reduced order models. SIAM/ASA Journal on Uncertainty Quantification, 9(3), 1152-1183.
- Resseguier, V., Ladvig, M., & Heitz, D. (2022). Real-time estimation and prediction of unsteady flows using reduced-order models coupled with few measurements. *Journal of Computational Physics*, 471, 111631.

valentin.resseguier@scalian.com

## Bonus slides

## 26

### Data assimilation Example : the Particle Filter (PF) generates an ensemble $\sim p(v|y)$

- Initialization  $v_{t=0}^{(j)} \sim \mathcal{N}(0, \Sigma)$
- Loop over time t

Importance sampling

► 
$$v_t^{(j)} = M\left(v_{t-1}^{(j)}, noise(t-1)\right)$$
 Forecast ("Prior" or "background")

- If an observation  $y_t$  is available at the current time t
  - $\blacktriangleright \quad W_j(t) \propto p\left(y_t \middle| v_t^{(j)}\right)$

 $\blacktriangleright \quad \mathbf{W}_j(t) = \frac{W_j(t)}{\sum_{k=1}^{N_p} W_k(t)}$ 

Normalization

Resampling

• Each new  $v_t^{(j)}$  is replaced by one of the old particles  $v_t^{(1)}, ..., v_t^{(N_p)}$  with probability  $\mathbf{W}_1(t), ..., \mathbf{W}_{N_p}(t)$ , respectively.

Likelihood evaluation, up to a constant

Final posterior distribution

 $p(v_t|y_{t_1}, \dots, y_{t_K}) \approx \sum_{k=1}^{N_p} \frac{1}{N_p} \delta\left(v_t - v_t^{(k)}\right)$ 

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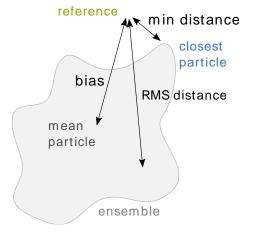
### UNCERTAINTY QUANTIFICATION (Prior) Known initial conditions b(t = 0)

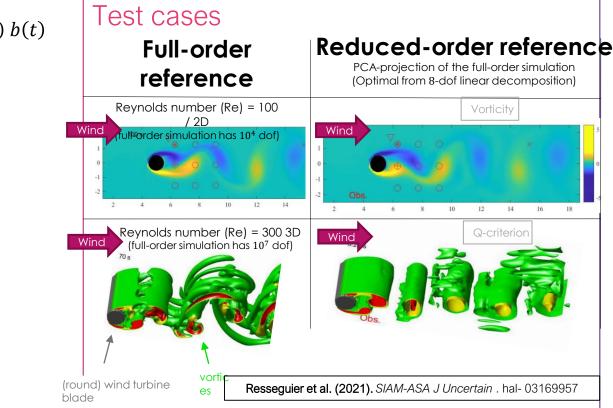
From  $10^7$  to 8 degrees of freedom No data assimilation Known initial conditions b(t = 0)

### $db(t) = H(b(t)) dt + \alpha(d\beta_t) b(t)$

### Metrics choice

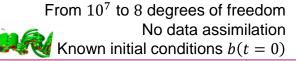
- $b_i(t)$  VS reference
- Error metrics

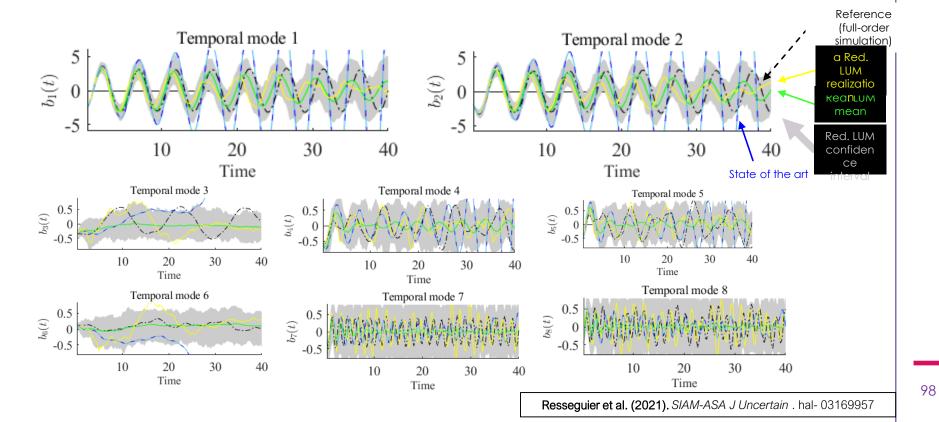






# UNCERTAINTY QUANTIFICATION (Prior) $b_i(t)$ VS reference

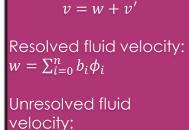


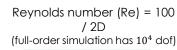


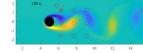


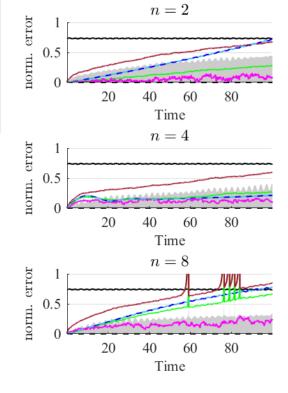
### UNCERTAINTY QUANTIFICATION (Prior) Error on the reduced solution *w*

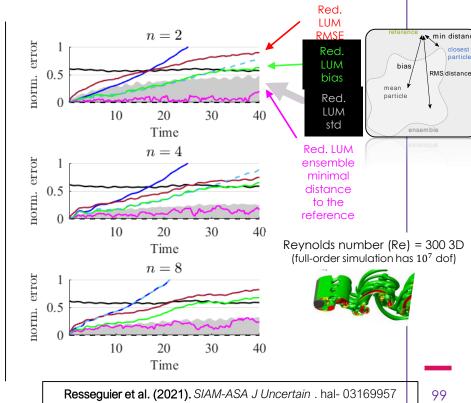
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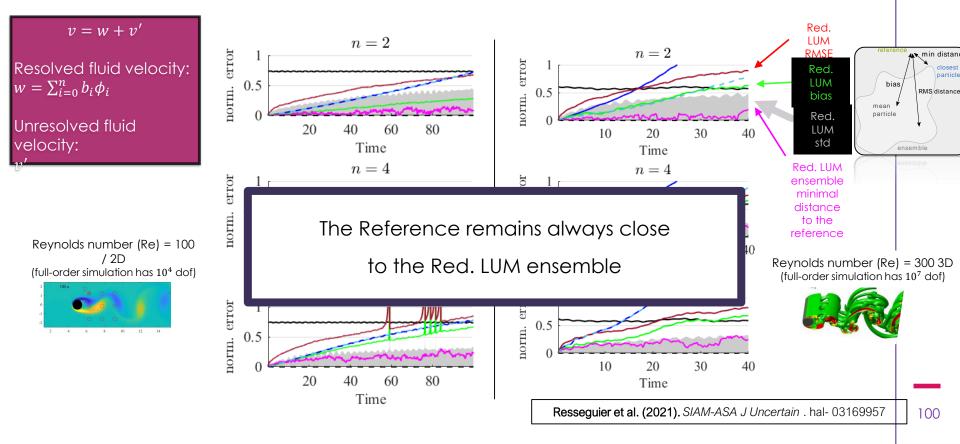






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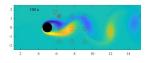
## Data assimilation (posterior) Error on the solution estimation

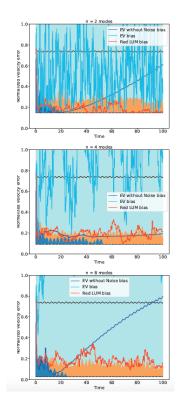
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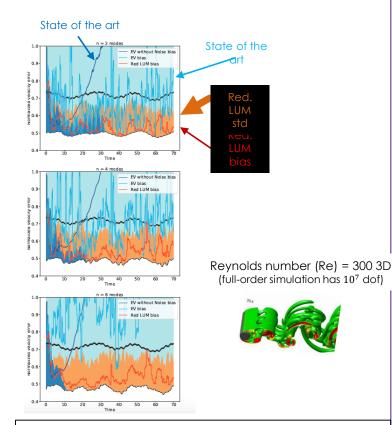
Resolved fluid velocity:  $w = \sum_{i=0}^{n} b_i \phi_i$ 

Unresolved fluid velocity:

> Reynolds number (Re) = 100 / 2D (full-order simulation has  $10^4$  dof)







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