Background	Bayesian Inference for Diffusivities	Applications to simulated ocean drifters	Summary	Extra slides
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### Y.K. Ying, James R. Maddison, Jacques Vanneste

School of Mathematics The University of Edinburgh

Scales and scaling cascades in geophysical systems, 4th April, 2018

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## Outline

### Background

### Modelling the Turbulent Ocean

### Bayesian Inference for Diffusivities

Formulation Computations Sampling

### Applications to simulated ocean drifters

Specifications Results

### Summary

### Extra slides

Convergence Extra Examples

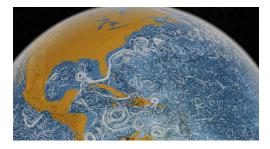
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Summary

Extra slides

### Background The turbulent ocean



### Eddies in the highly turbulent ocean. Image courtesy: NASA.

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What is turbulent diffusion/eddy diffusion?

Simple models for transport in the ocean: With a 'turbulent' velocity field  $\mathbf{u} = \mathbf{u}(x, t), x \in \mathbb{R}^2$ :

Passive scalar $c(x, t)$ :	Particle position $X_t$ :
$\partial_t \boldsymbol{c} + \boldsymbol{u}(\boldsymbol{x}, \boldsymbol{t}) \cdot \nabla \boldsymbol{c} = \kappa_m \nabla^2 \boldsymbol{c},$	$dX_t = \mathbf{u}(X_t, t)dt + \sqrt{2\kappa_m}dW_t,$

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 $\Box \kappa_m$ : small-scale diffusivity.

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 $\Box \kappa_m$ : small-scale diffusivity.

'Averaging'/'Homogenization':

Decompose  $\mathbf{u}(x, t) = \mathbf{v}(x) + \mathbf{u}'(x, t)$ :

Averaged scalar $\bar{c}(x, t)$ :	Particle position $\bar{X}_t$ :
$\partial_t \bar{c} + \mathbf{v}(x) \cdot \nabla \bar{c} = \nabla \cdot (\kappa_e(x) \nabla \bar{c}),$	$dar{X}_t =  ilde{oldsymbol{v}}(ar{X}_t)dt + \sqrt{2\kappa_e(ar{X}_t)}dW_t,$

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 $\Box \kappa_e(x): \text{ turbulent/eddy diffusivity tensor field.} \\ \Box \tilde{\mathbf{v}}(x) = \mathbf{v}(x) + \nabla \cdot \kappa_e(x): \text{ 'effective' drift.}$ 

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Relation between stochastic processes and the advection-diffusion equation

Stochastic Differential Equations

Consider the trajectory of a passive particle  $X_t$  at time t:

$$dX_t = \left[\mathbf{v}(X_t) + \nabla \cdot \kappa_e(X_t)\right] dt + \sqrt{2\kappa_e(X_t)} dW_t,$$

### Fokker-Planck Equations

The transition probability density  $p(x, t|x_0)$  of a passive particle:

$$\partial_t p + \mathbf{v}(x) \cdot \nabla p = \nabla \cdot (\kappa_e \nabla p),$$
  
 $p(x, 0|x_0) = \delta(x - x_0).$  (Initial condition)

### Interpretation:

The transition density of an SDE is a passive scalar with an initial Dirac-Delta profile

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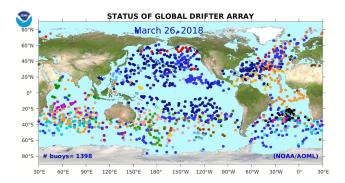
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### Description

#### How to estimate the turbulent diffusivity $\kappa(x)$ in the ocean?



#### Figure: Some available drifters across the globe.

[Image retrieved from website of The Global Drifter Program]

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## Description

How to estimate the turbulent diffusivity  $\kappa(x)$  in the ocean?

### Inference

В

Given the position data  $\{X_t\}$ , at discrete time  $t = t_n$  from the ocean drifters:

1. Seek  $\mathbf{u}(x)$  and  $\kappa(x)$  of

$$dX_t = \mathbf{u}(X_t)dt + \sqrt{2\kappa(X_t)}dW_t$$

that 'fits' with the observation data.

2. Quantify the **uncertainty** of the inferred  $\mathbf{u}(x)$  and  $\kappa(x)$ 

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## Methodology: How to diagnose eddy diffusivity?

### Conventional Approach:

Given the eddy velocities  $\{u'(t)\}$  of drifters, integrate the velocity autocorrelation function

$$\kappa = \int_0^\infty ig\langle u'(t) u'(t+ au) ig
angle \, d au$$

 $\Rightarrow$  Obtain one estimate for  $\kappa$ 

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## Methodology: How to diagnose eddy diffusivity?

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### Bayesian SDE Inference Approach:

Given sequences of positions  $\{X_t\}$  at  $t = t_n, n = 0, 1, ..., N$ , formulate the posterior distribution

$$p(\mathbf{u},\kappa|\{X_t\})$$

 $\Rightarrow$  Obtain a probability distribution on **u** and  $\kappa$ , conditioned on the available data  $\{X_t\}$ 

Bayesian Inference for Diffusivities ○● ○○○ Applications to simulated ocean drifters

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# Bayesian Inference

Bayes' Theorem **RECALL:** Probability 101:

> P(A|B)P(B) = P(B|A)P(A) $\Rightarrow P(A|B) \propto P(B|A)P(A)$

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## Bayesian Inference

Bayes' Theorem **RECALL:** Probability 101:

> P(A|B)P(B) = P(B|A)P(A) $\Rightarrow P(A|B) \propto P(B|A)P(A)$

**TARGET:** Posterior distribution density  $p(\mathbf{u}, \kappa | \{X_t\})$ :

 $p(\mathbf{u},\kappa|\{X_t\}) \propto p(\{X_t\}|\mathbf{u},\kappa)p(\mathbf{u},\kappa)$ 

Fill in the gaps:

- 1. Proportional factor  $\Rightarrow$  normalisation constant for a p.d.f.
- 2. Likelihood  $p({X_t} | \mathbf{u}, \kappa) \Rightarrow$  needs to be computed
- 3. Prior  $p(\mathbf{u},\kappa) \Rightarrow$  subjectively chosen

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## Bayesian Inference

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### Bayesian Inference Computational Aspects

1. How to construct the likelihood  $p({X_t} | \mathbf{u}, \kappa)$ ?

= Probability of reproducing the data  $\{X_t\}$ , given  $(\mathbf{u}, \kappa)$ **Evaluation:** 

1. Pair up the observed positions  $\{X_t\}$  consecutively

$$\{X_0, X_1\}, \{X_1, X_2\}, \ldots, \{X_{n-1}, X_n\},\$$

where  $h = t_{i+1} - t_i$  is the duration between observation

- 2. Evaluate transition density  $p(X_{i+1}, h|X_i)$
- 3. Likelihood  $p({X_t} | (\mathbf{u}, \kappa)) = \prod_i p(X_{i+1}, h | X_i)$

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### Bayesian Inference Computational Aspects

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## Bayesian Inference

Bayes' Theorem **RECALL:** Probability 101:

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**TARGET:** Posterior distribution density  $p(\mathbf{u}, \kappa | \{X_t\})$ :  $p(\mathbf{u}, \kappa | \{X_t\}) \propto p(\{X_t\} | \mathbf{u}, \kappa) p(\mathbf{u}, \kappa)$ 

Fill in the gaps:

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Bayesian Inference for Diffusivities  $\circ \circ$   $\circ \circ \bullet$ 

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### Bayesian Inference Computational Aspects

- 2. How to take Prior  $p(\mathbf{u}, \kappa)$ ?
- = Preference for  $(\mathbf{u}, \kappa)$  from experts' opinion **Choice of prior:** 
  - $(\mathbf{u},\kappa) \sim \text{Uniform distribution on a given range}$  $\Rightarrow \text{No preference}$



Extra slides

### Bayesian Inference Machinery Sampling

What to do with the posterior density  $p(\mathbf{u}, \kappa | \{X_t\})$ ?

Sampling by Metropolis-Hasting Algorithm

 $\iff$  produce a histogram

Inference from the posterior density  $p(\mathbf{u}, \kappa | \{X_t\})$ 

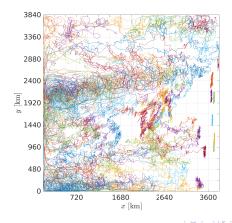
- 1. Estimate  $(\mathbf{u}, \kappa)$  via
  - Posterior mean
  - Maximum a posteriori (MAP) estimates
- 2. Quantify uncertainties via
  - Posterior variance
  - Local modes

[Lost? Examples coming up in a few slides!]

Background	
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## Particles in an Ideal Ocean Model

- *Data input:* Daily positions of 1024 passive particles over 10 years using the quasi-geostrophic equations (similar to *Karabasov et al*, *Ocean Modelling 2009*)
- 'Spaghetti' plot of trajectories of 64 particles: Click me



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### Particles in an Ideal Ocean Model

### Inference model

- 1. Resolution: Partition the domain into bins of size 240km  $\times$  240km
- 2. Fields: For each bin, impose a velocity and diffusivity field

$$\mathbf{u}(x, y) = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & -A_{11} \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},$$
$$\kappa(x, y) = \begin{bmatrix} \kappa_{11} & \kappa_{12} \\ \kappa_{21} & \kappa_{22} \end{bmatrix}.$$

3. Locality: Group the consecutive positions of particles {X<sub>i</sub>, X<sub>i+1</sub>} into bins based on their starting points {X<sub>i</sub>}

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Applications to simulated ocean drifters

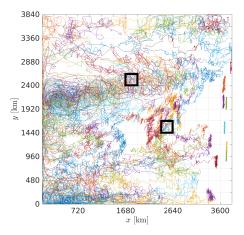
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### Passive Particles in an Ideal Ocean Model

#### Focus on two cells: jet vs not on jet

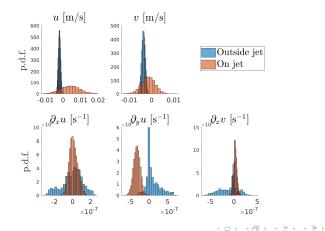
 $\Box$  Boxes: the chosen two cells:



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## Passive Particles in an Ideal Ocean Model

Posterior Distributions in two selected cells, sampling interval h = 64 days Velocity fields u(x, y), v(x, y) at cell centres  $\Rightarrow$  faster flow, but more uncertain, on the jet.

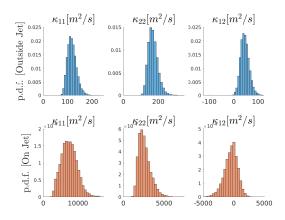


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## Particles in an Ideal Ocean Model

Posterior Distributions in two selected cells, sampling interval h = 64 days Diffusivity  $\kappa = \begin{bmatrix} \kappa_{11} & \kappa_{12} \\ \kappa_{21} & \kappa_{22} \end{bmatrix}$  at cell centres  $\Rightarrow$  much larger and much more uncertain diffusivity on the jet.



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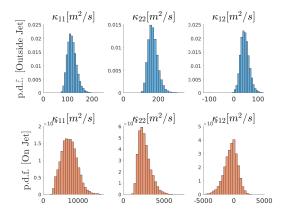
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### Particles in an Ideal Ocean Model

### A representative number to simplify the analysis?

Locate the mode of the probability distribution  $\Rightarrow$  MAP estimates



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## Particles in an Ideal Ocean Model

### MAP estimates for diffusivity field (Sampling interval h = 64 days)

Diagonal components of the diffusivity tensor  $\kappa_{11}$  and  $\kappa_{22}$ :

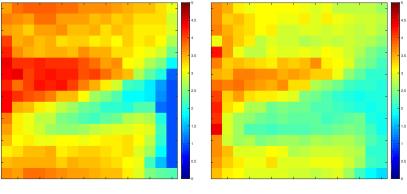


Figure:  $\kappa_{11}$  [m<sup>2</sup>/s] on a log10-scale Figure:  $\kappa_{22}$  [m<sup>2</sup>/s] on a log10-scale

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## Take Home Messages

- A Bayesian Inference for Ocean Diffusivities
  - A probabilistic inference for  ${\bf u}$  and  $\kappa$
  - Uncertainty quantification with ease
  - No a priori decomposition of velocity fields required
  - Capable of inferring an anisotropic diffusivity tensor  $\boldsymbol{\kappa}$
- A physically meaningful diffusivity  $\kappa$ 
  - Robust inference: Convergence over sampling interval h
- Importance in resolving the spatial variation in velocity field  $\mathbf{u}(x, y)$ 
  - Robust inference: Convergence requires sufficient resolution of velocity fields

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## Future work

- Comparisons with existing diffusivity diagnostics
  - Lagrangian methods
  - Passive tracer methods
- Relax the locality assumptions
  - Ensure globally smooth fields are inferred
  - Make diffusivity diagnosis possible in the fast regions

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• Inference using real drifters!

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## Particles in an Ideal Ocean Model

### MAP estimates for diffusivity field (Sampling interval h = 64 days)

Diagonal components of the diffusivity tensor  $\kappa_{11}$  and  $\kappa_{22}$ :

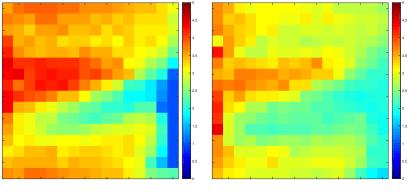


Figure:  $\kappa_{11}$  [m<sup>2</sup>/s] on a log10-scale Figure:  $\kappa_{22}$  [m<sup>2</sup>/s] on a log10-scale

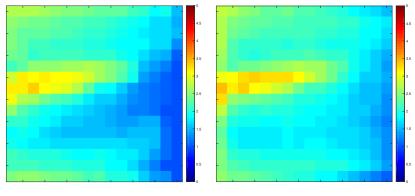
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## Particles in an Ideal Ocean Model

### MAP estimates for diffusivity field (Sampling interval h = 1 days)

Diagonal components of the diffusivity tensor  $\kappa_{11}$  and  $\kappa_{22}$ :



### Figure: $\kappa_{11}$ [m<sup>2</sup>/s] on a log10-scale Figure: $\kappa_{22}$ [m<sup>2</sup>/s] on a log10-scale

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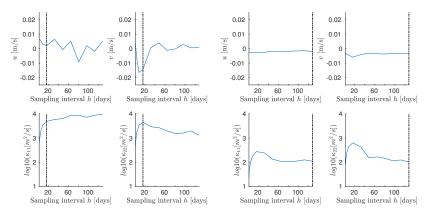
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## Particles in an Ideal Ocean Model

#### What sampling interval h to use?

MAP Fields at cell centres vs sampling interval *h* [Left: On the jet; Right: outside the jet]



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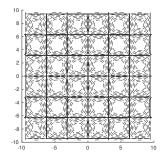
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## Test Case - Taylor-Green Vortex

Particle advection:

$$dX_t = \mathbf{u}^{TG}(X_t)dt + \sqrt{2\kappa_m}dW_t, \quad \text{where } \mathbf{u}^{TG}(x,y) = \begin{pmatrix} \sin(x)\cos(y) \\ -\cos(x)\sin(y) \end{pmatrix},$$

Figure: Streamlines of Taylor-Green Vortex; Video at [Click me]



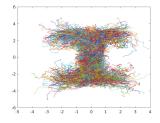
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### Test Case - Taylor-Green Vortex

• For t sufficiently large, coarse-graining the SDE

$$dX_t = \mathbf{u}^{TG}(X_t)dt + \sqrt{2\kappa_m}dW_t \to dX_t^c = \sqrt{2\kappa}dW_t.$$

- Simulated Trajectories
  - 1. Number of Particles: 1024
  - 2. Initial conditions: Located at the origin
  - 3.  $\kappa_m = 0.1 \rightarrow \kappa \approx 0.342I$



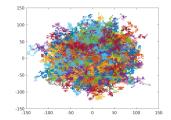


Figure: Simulated Trajectories, up to t = 50

Figure: Simulated Trajectories, up to t = 2500

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### Test Case - Taylor-Green Vortex

Bayesian Inference: Impose the coarse-grained model

$$dX_t = \begin{pmatrix} u \\ v \end{pmatrix} dt + \sqrt{2 \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix}} dW_t$$

• Plots of mean quantities over sampling interval h

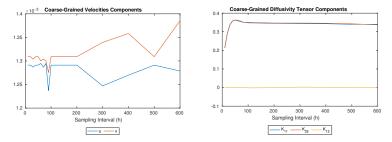


Figure: Mean velocity (u, v) against sampling interval h

Figure: Mean diffusivity *K* against sampling interval *h* 

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