Stochastic Variational Principles for GFD: Modelling the unknown unknowns

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So far today we have raised these “Primary Questions”

How to develop a data-driven model? Model driven error? Which comes first? The data or the model?

The model may give sufficient conditions to match the data, but to what extent are these conditions at all necessary, or even unique?


How to use data assimilation to model the model error?
Our strategy: learn the models by blending data with numerics in **two data assimilation steps**
Fundamental ideas and goals of this work

- Develop an approach to SPDEs in which noise terms have data driven coefficients, linked to a stochastic variational principle.

- Combine geometric mechanics with probabilistic analysis, in a variational hierarchy of data driven GFD approximations which preserve the invariance properties of the original system.

- Specifically, combine different rapidly developing methods (particle filters, stochastic calculus of variations, regularisation methods for singular SPDEs) with new ideas from geometric mechanics exploiting “stochastic advection” (Lie-derivative transport of advected quantities by a stochastic vector field, indexed by the Eulerian spatial position).

- Contribute to both applications and foundations of stochastic fluid dynamics and other complex nonlinear systems, to enhance numerical methods and statistical modelling.
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What is our task?

Our task: *Learn from stochastic assimilation* of observed data (tracers) how to produce stochastic fluid motion equations whose numerics will yield the observed statistics and variability of the data.
Numerical simulations show this sea surface elevation
Observations of tracers in the Ocean show this.
What *fluid equations* produce this scalar turbulence?

Figure: Here are all surface drifter trajectories since 1980 to have passed between Eastern Australia & New Zealand, courtesy Eric van Sebille [2014].
Claim: Stochastic terms for the motion equation can be derived via Hamilton’s variational principle, by constraining its variations to agree with the spatial correlations seen in the tracer data.

How? Our strategy is to impose stochastic transport of advected quantities as a constraint in Hamilton’s principle \( \delta S(u, p, q) = 0 \) with,

\[
S(u, p, q) = \int \left( \ell(u, q) dt + \left< p, dq + L_{dx_t} q \right>_V \right)
\]

Here \( \ell(u, q) \) is the unperturbed deterministic fluid Lagrangian, written as a functional of velocity vector \( u \), tracers \( q \) and . . . we’ll get to \( dx_t \) later.
How would these observations guide the modelling?

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we’ll get to $dx_t$ later.
Our strategy: learn the models by blending data with numerics in two data assimilation steps.
What would we get?

**What?** New stochastic GFD models for climate & weather variability.

New motion equations contain stochastic perturbations which multiply both the solution and its spatial gradient *(in a certain transport way)*.

Remarkably, these stochastic GFD models *still preserve* fundamental properties such as Kelvin’s circulation theorem and PV conservation.

Example. *Stochastic QG.*
In the **Kraichnan model**, advection of passive scalar $\theta$ is governed by

\[
\partial_t \theta + \mathbf{v} \cdot \nabla \theta = \kappa \Delta \theta + F, \quad \nabla \cdot \mathbf{v} = 0,
\]

where $\theta(t, \mathbf{r})$ is the scalar (temperature), $F(t, \mathbf{r})$ is the external source, $\mathbf{v}(t, \mathbf{r})$ is the advecting velocity, and $\kappa$ is diffusivity.

Both $F(t, \mathbf{r})$ and $\mathbf{v}(t, \mathbf{r})$ are independent Gaussian *random* functions of $t$ and $\mathbf{r}$, which are $\delta$-correlated in time, e.g., $\mathbf{v}(t, \mathbf{r}) = \sum_k \xi_k(\mathbf{r}) \circ dW_k(t)$.

The $dW_k(t)$ are independent 1D Brownian motions, with $\nabla \cdot \xi_k = 0$ and with bounded $\sum_k \xi_k^T \xi_k$.

Typical numerical solutions show the *patchiness* in $\theta$ associated with intermittency (anomalous scaling). **Very non-Gaussian!**
How to derive stochastic GFD motion equations?

**How?** Our strategy is to impose stochastic transport of advected quantities (a lá Kraichnan) as a constraint in Hamilton’s principle,

$$0 = \delta S(u, p, q) = \delta \int \left( \ell(u, q) dt + \langle p, dq + \mathcal{L}_{dx_t} q \rangle_V \right).$$

Physics + Tracer data

Here $\ell(u, q)$ is the unperturbed deterministic fluid Lagrangian, written as a functional of velocity vector field $u$, and . . .

\[ \mathcal{L}_{dx_t} \] is the transport operator (Lie derivative) for any advected quantity $q \in V$ by a stochastic vector field, $dx_t$, at fixed Eulerian position $y$ as

$$dx_t(y) = u(y, t) dt + \sum_k \xi_k(y) \circ dW_k(t).$$

Flow + Noise

The stochastic vector field $dx_t(y)$ contains cylindrical Stratonovich noise whose spatial correlations are given by $\xi_k(y)$ (a lá Kraichnan).
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Here \( \ell(u, q) \) is the unperturbed *deterministic* fluid Lagrangian, written as a functional of velocity vector field \( u \), and \ldots

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Deterministic QG is basically PV transport:

\[
\frac{\partial Q}{\partial t} = - \mathbf{u} \cdot \nabla Q ,
\]

where PV (Potential Vorticity) is defined

\[
Q := \Delta \psi - \mathcal{F}\psi + f ,
\]

in terms of the stream function \( \psi \) of the geostrophic fluid velocity, \( \mathbf{u} := \nabla^\perp \psi = \left( - \frac{\partial \psi}{\partial x_2} , \frac{\partial \psi}{\partial x_1} \right) \).
In Stochastic QG, Hamilton’s principle $\Rightarrow$ stochastic PV transport,

$$dQ = -d\mathbf{x}_t \cdot \nabla Q,$$

with

$$d\mathbf{x}_t := \nabla^\perp d\psi = u dt + \sum_k \xi_k(\mathbf{x}) \circ dW_k(t).$$

Two further properties of Stochastic QG

1.) Itô form. The Itô form of stochastic QG is,

\[ dQ = - \left( u \, dt + \sum_k \xi_k(x) \, dW_k(t) \right) \cdot \nabla Q \]
\[ + \frac{1}{2} \text{div} \left( \sum_k \xi_k^T \xi_k \right) \text{grad} \, Q \, dt \quad \text{⇒ \ (Itô drift)} . \]

Itô drift is how the noise contributes to the mean flow velocity.

2.) PV enstrophies. Both the Stratonovich and Itô stochastic QG equations preserve the infinite family of potential enstrophies,

\[ C_\Phi = \int_{\mathbb{R}^2} \Phi(Q) , \]

for any smooth function \( \Phi \). Proof: \( dC_\Phi = - \int_{\mathbb{R}^2} dx_t \cdot \nabla \Phi(Q) = 0 \).
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Why? We needed to learn from stochastic assimilation of tracer data how to produce stochastic fluid motion equations which would reproduce the observed statistics and variability of the data.

We asked, How would observed stochastic tracer transport data guide us in modifying the deterministic GFD motion equations?

How? Stochastic terms for the motion equation were derived via Hamilton’s variational principle, by constraining its variations to agree with the spatial correlations seen in tracer transport data.

What? New methods of finding GFD models for climate and weather. New motion equations contained stochastic perturbations multiplying both the solution and its spatial gradient (in a certain transport way). Remarkably, these stochastic GFD models preserved fundamental properties such as Kelvin’s circulation theorem and PV conservation.

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Example. Stochastic QG.
Conclusion: This is just the beginning of the work!

1. The fundamental mathematical structure of fluids is preserved by (1) injecting stochasticity via Hamilton’s principle, using (2) a stochastic transport constraint for advected quantities.

2. E.g., deterministic transport became stochastic transport for QG.

3. And, for QG, stochastic transport still preserved PV enstrophies.

4. The theory applies to all fluid models derived from Hamilton’s principle. (The spatial correlations $\sum_k \xi_k^T \xi_k$ derive from data.)

5. The theory includes stochastic versions of the usual GFD Euler-Boussinesq equations, primitive equations, etc.

6. There’s so much more to do, e.g., in analysing and applying these new stochastic GFD equations!

7. Until recently, the existence and uniqueness for our example of stochastic 2D QG flows were still open! Now they are solved.

8. Recently, we have shown finite time existence, uniqueness and regularity of 3D stochastic Euler equations derived this way!
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3D stochastic Euler equations are derived this way

The Itô vorticity equation for incompressible stochastic Euler flow is

\[
d\omega + [u,\omega] \, dt - \frac{1}{2} \sum_i \left[\xi_i(x), [\xi_i(x),\omega]\right] \, dt + \sum_k [\xi_k(x),\omega] \, dW_k(t) = 0,\]

with Lie bracket \([u,\omega] = u \cdot \nabla \omega - \omega \cdot \nabla u =: B_u \omega\) with \(B_u^\dagger = -B_u\),

and \(\omega := \text{curl } u\). Equivalently,

\[
d\omega + (B_u + \sum B_{\xi_i}^\dagger B_{\xi_i}) \omega \, dt + \sum_k B_{\xi_k} \omega \, dW_k(t) = 0 .
\]

The operator formed by the sum

\[
B_u + \sum B_{\xi_i}^\dagger B_{\xi_i}
\]

is hypo-coercive [Villani, 2012], which greatly facilitates the analysis of these eqns, in showing finite time existence, uniqueness and regularity!
The issues at the heart of this project relate to Stochastic Partial Differential Equations (SPDEs), Stochastic Variational Principles (SVPs) and Numerical Modelling, in connection with Complex Nonlinear Systems, Applied Analysis, Numerical Analysis, Stochastic Geophysical Fluid Dynamics (SGFD) and Turbulence.
The new stochastic methodology fits together
Objectives of the new stochastic methodology

- Create new parameterisation approaches in SGFD for mathematics of climate change and weather variability
- Quantify variability in SGFD models due to stochastic transport, by determining the Fokker-Planck evolution of the probability density
- Apply to quantify variability for each member of the new SGFD hierarchy, first for the lowest level approximation, later for more realistic SGFD models at higher orders in the GFD asymptotic expansion
- Use PV preservation and the dissipative double-bracket operators in the Itô interpretation of these SGFD models as input for obtaining finite-horizon parameterising manifolds [Chekroun & Liu, 2015]
Machine learning & the new stochastic methodology

- In our *Input Step*, we could use methods of belief propagation, message passing, statistical inference and particle image velocimetry; all of which are standard in tracking fluid particle paths in turbulence.

- Can we regard our data assimilation and data-driven modelling steps as a form of machine learning? How is our approach different from usual machine learning problems?

- Our approach imposes a probabilistic structure on the “outside model”, and propagates it from the tracer equations to the motion equation via Hamilton’s principle and then to a numerical solver.

- How to compare our approach with standard methods in machine learning, which focus on a stochastic representation of the uncertainty in *individual terms* within the model, and then draw from that ensemble and propagate the results through a numerical solver?
Variational principles for stochastic fluid dynamics

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This paper derives stochastic partial differential equations (SPDEs) for fluid dynamics from a stochastic variational principle (SVP). The paper proceeds by taking variations in the SVP to derive stochastic Stratonovich fluid equations; writing their Itô representation; and then investigating the properties of these stochastic fluid models in comparison with each other, and with the corresponding deterministic fluid models. The circulation properties of the stochastic Stratonovich fluid equations are found to closely mimic those of the deterministic ideal fluid models. As with deterministic ideal flows, motion along the stochastic Stratonovich paths also preserves the helicity of the vortex field lines in incompressible stochastic flows. However, these Stratonovich properties are not apparent in the equivalent Itô representation, because they are disguised by the quadratic covariation drift term arising in the Stratonovich to Itô transformation. This term is a geometric generalization of the quadratic covariation drift term already found for scalar densities in Stratonovich’s famous 1966 paper. The paper also derives motion equations for two examples of stochastic geophysical fluid dynamics; namely, the Euler–Boussinesq and quasi-geostrophic approximations.

1. Introduction

In this paper, we propose an approach for including stochastic processes as cylindrical noise in systems of evolutionary partial differential equations (PDEs) that derive from variational principles which are invariant under a Lie group action. Such dynamical systems are called Euler–Poincaré equations [1,2]. The main objective of the paper is the inclusion of stochastic processes in ideal fluid dynamics, in which case the variational principle is invariant under the Lie group of smooth invertible maps acting to relabel the reference state.

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