Classic and Stochastic Approaches to Mathematical Fluid Dynamics

Imperial College London, Mathematics of Planet Earth, EPSRC Centre for Doctoral Training Suite[1]

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Monday

Valerio Lucarini

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Title Response, Fluctuations, and Critical Transitions in the Climate System

Abstract The climate is a nonequilibrium system characterised by variability of a vast range of spatial and temporal scales. The complexity of climate dynamics results from a very nontrivial interplay of feedbacks, instabilities, and re-equilibrating processes. The understanding of climate variability and climate response to forcings is one of the great challenges of contemporary science. We will show how statistical mechanics and the theory of dynamical systems provide a powerful framework for advancing our understanding of the climate system. We will explore the smooth regime of climate response to forcings, the conditions under which high sensitivity is observed, and provide a general framework for critical transitions.

References:

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Manuel de León

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Title Material Distributions

[1] http://mpecdt.org/

Abstract The concept of material distribution is introduced as describing the geometric material structure of a general non-uniform body. Any smooth constitutive law is shown to give rise to a unique smooth integrable singular distribution. Ultimately, the material distribution and its associated singular foliation result in a rigorous and unique subdivision of the material body into strictly smoothly uniform components. Thus, the constitutive law induces a unique partition of the body into smoothly uniform sub-bodies, laminates, filaments and isolated points. These results arise in a very natural way when one considers the material groupoid given by the constitutive law.

Freddy Bouchet

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Title Extreme heat waves sampled through large deviation algorithms

Authors Freddy Bouchet, Francesco Ragone, and Jeroen Wouters. ENS de Lyon and CNRS

Abstract For some aspects of climate dynamics, rare dynamical events may play a key role, for instance when they have a huge impact. We will study the paradigmatic example of extreme heat waves. In the recent past, new theoretical and numerical tools have been developed in the statistical mechanics community, in order to specifically study such rare events. Some of those approaches are based on large deviation theory for complex dynamical systems. We will study the probability of extreme heat waves in a comprehensive GCM. At a fixed numerical cost, several hundreds more heat waves are observed than in a control run. The thousands of sampled extreme heat waves open the door to their dynamical studies, precursor, and fluctuation paths, in a way that can not be foreseen using conventional tools based on direct numerical simulations. Moreover extreme events that can not be observed in a GCM at a reasonable cost can now be studied. This new tool open new perspectives for the study of climate extremes. As an example we discuss teleconnection patterns for extremes. The relation with statistical mechanics tools in general, and especially large deviation theory, will be emphasized.

Tuesday

James Maddison

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Title Quasi-geostrophic eddy fluxes: Interpretation and applications

Abstract The eddy forcing in the mean quasi-geostrophic equations can be conveniently expressed in terms of the double-divergence of an Eliassen-Palm flux tensor, whose magnitude can be related to eddy energetics. This viewpoint provides a way to parameterise for geostrophic turbulence while preserving key conservation principles, including constraints imposed by energetics.

The Eliassen-Palm flux tensor can be derived by first constructing an equation for a quantity termed the "potential vorticity induction", whose divergence is the quasi-geostrophic potential vorticity. The structure of the potential vorticity induction equation can be described in terms of a weighted Helmholtz decomposition. Implications for the testing and development of geostrophic eddy parameterisations will be discussed, including the diagnosis of parameterisation coefficients via variational optimisation. The implementation of an energetically constrained variant of the Gent and McWilliams parameterisation will also be described.

Mike Cullen

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Title Stochastic solutions to (apparently) deterministic atmospheric models.

Co-authors Misha Feldman and Jingrui Cheng (Wisconsin), Miles Caddick (Oxford)

Abstract Atmospheric behaviour can be described accurately by simple models in particular asymptotic regimes. This requires a proof that the simple models are well-posed and so can be solved. I will show three cases where simple models can be solved, but only in a measure-valued sense. This means that the solution is probabilistic, rather than deterministic. In the first two examples, this behaviour comes from the degeneracy of solutions in a Lagrangian frame where the fluid is well-mixed. There is then no way of deterministically identifying the positions of fluid particles in terms of their initial positions. The third example comes from non-monotonicity of the diffusion operator used to represent boundary layer transport.

François-Xavier Vialard

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Title TBA

Abstract TBA

Sebastian Reich

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Title Data Assimilation as Interacting Particle Systems

Abstract I will review recent results on interacting particle systems for estimating the state of a dynamical system using partial and noisy observations. I will start from the ensemble Kalman filter (EnKF) and discuss its generalisation to the continuous-time filtering problems. It will be revealed that the general filtering problem still allows for an interacting particle approximation in the form of a generalised Kalman gain formulation. I will also review recent results on the stability and accuracy of the EnKF and links to optimal transportation.

Anthony Bloch

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Title Reduction and Control for Cellular Reprogramming.

Abstract In this talk we discuss data-guided frameworks for the problem of cellular reprogramming. We discuss reduced models of dynamical systems that can be applied to problems in various areas including fluids. In particular we describe how to describe a reduced model of moderate complexity for the reprogramming problem based on data sampling of the cell cycle and the notion of topologically associating domains. We then discuss a model of data-guided control using notions of optimality and with control inputs being suitable transcription factors. This is work with I. Rajapakse, R. Brockett. S. Ronquist, G. Patterson and others.

François Gay-Balmaz

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Title A Lagrangian variational formulation for nonequilibrium thermodynamics

Abstract We present a Lagrangian variational formulation for nonequilibrium thermodynamics. This formulation extends the Hamilton principle of classical mechanics to include irreversible processes in both discrete and continuum systems. The irreversibility is encoded into a nonlinear nonholonomic constraint given by the expression of entropy production associated to the irreversible processes involved. The introduction of the concept of thermodynamic displacement allows the definition of a corresponding variational constraint. We show that the evolution equations for nonequilibrium thermodynamics admit an intrinsic formulation in terms of Dirac structures. Finally, we illustrate our theory with both finite and infinite dimensional examples, including mechanical systems with friction, chemical reactions, electric circuits, the Navier-Stokes-Fourier equations, and moist atmospheric modelling.

Wednesday

David Martín de Diego

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Title Discrete Lie-Poisson equations

Abstract Classical integrators are mainly focused on solving nonlinear ordinary differential equations (ODEs) or partial differential equations (PDEs) for which is not easy or possible to derive analytic solutions. In many cases of interest, without solving explicitly the equations, we known some important qualitative and geometric features of the solutions of the equations of motion. For instance, preservation of the energy or other conservation laws, preservation of geometric structures like symplectic forms, volume forms, Poisson structures... or even, preservation of the manifold structure of the configuration space where the system evolves (for example, a Lie group structure). Standard finite difference schemes often cannot preserves these geometrical quantities which can result in qualitatively incorrect behavior.

As a consequence, in the last years, the subject of structure preservation has emerged in numerical analysis with important ramifications in differential geometry, theoretical mechanics and engineering applications. The idea is to design numerical methods preserving one or more of these geometric or qualitative properties exactly. These methods are called geometric integrators. In this talk, we will focus on geometric integrators for Lie-Poisson equations. These equations play a fundamental role in the description of rigid bodies, fluids, plasma… Moreover, we will discuss the error between an exact trajectory and the discrete trajectory derived by a family Lie-Poisson integrators.

Tudor Ratiu

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Title Multisymplectic variational integrators for nonsmooth Lagrangians

Abstract I will present a numerical algorithm used in elasticity. Starting with field theory and nonsmooth analysis combined with constraints, a general model for a large classes of continuum mechanical systems is formulated. Discretizing this model, leads to variational integrators for which the Noether conserved quantitities are preserved. As illustration, the impact of two colliding beams will be presented.

Cesare Tronci

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Title Hydrodynamic vorticity and helicity of liquid crystal flows

Abstract After a brief review of liquid crystal dynamics, this talk presents explicit expressions of the helicity conservation in nematic liquid crystal flows, for both the Ericksen-Leslie and Landau-de Gennes theories. This is done by using a minimal coupling argument that leads to an Euler-like equation for a modified vorticity involving both velocity and structure fields (e.g. director and alignment tensor). This equation for the modified vorticity shares many relevant properties with ideal fluid dynamics and it allows

for vortex filament configurations as well as point vortices in planar configurations. The interplay of noise with the orientational order will be also discussed.

Martins Bruveris

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Title Riemannian geometry on spaces of submanifolds induces by the diffeomorphism group

Abstract The space of embedded submanifolds plays an important role in applications such as computational anatomy and shape analysis. We can define two different classes on Riemannian metrics on this space: so-called 'outer metrics' are metrics that measure shape changes using deformations of the ambient space and they are used mostly in computational anatomy; the second class, so-called 'inner metrics' are defined directly on the space of embeddings using intrinsic differential operations and they are used in shape analysis. In this talk I want to compare relate these two classes of metrics and show how the topologies induces by the geodesic distance function relate to each other.

Benedict Leimkuhler

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Title Numerical methods for stochastic differential equations: from molecules to data science

Abstract In this talk I will describe our efforts to establish a systematic framework for the design of numerical methods for stochastic models based on Langevin dynamics, generalized Langevin, and alternative thermostats, discussing their ergodic properties, accuracy, and flexible application. I will then consider several case studies relevant in different contexts (molecular dynamics, sheared polymer melts, data analytics) to demonstrate how the design of the numerical methods can dramatically effect the efficiency and reliability of simulation.

Thursday

Wei Pan & Igor Shevchenko

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Title Numerically Modelling Stochastic Lie Transport in Fluid Dynamics (Euler and Quasi-Geostrophic Dynamics)

Abstract There are two main types of uncertainty in the prediction of weather and its variability. The first is the transport uncertainty of where the ow takes the thermodynamics. The second is the uncertainty in what the thermodynamics does when it gets there. We address the first type of uncertainty in our models, due to what we call "stochastic Lie transport". The framework for introducing cylindrical stochastic noise is based on the well known Hamilton's variational principle. This was first developed in D. Holm's 2015 paper. The result is the Eulerian representation of ideal fluid dynamics in the form of stochastic partial differential equations, or SPDEs for short, where the stochastic perturbation is in the form of Stratonovich stochastic integrals of vector fields that depend on the gradients of the solution. This previously unseen form of noise is what we call transport noise. For application purposes, e.g. data assimilation, the spatial correlation structure (SCS) of the transport noise is crucial and must be specified apriori. This leads to many important theoretical and practical questions regarding the determination of SCS as it is not possible to directly observe such quantity in practise. Thus, determining SCS would introduce its own uncertainty, but not even trying to determine them will mean neglecting the effects of transport uncertainty on weather prediction. As this form of noise is new, we propose the SCS components are to be supplied as spatial correlation EOFs of the data. We describe our estimation methodology, and how we benchmark the validity of the estimation. We aim to answer important questions such as the interpretation of SCS, the choice on the number of SCS and the implications of these choices on the Eulerian distributional properties of the velocity and vorticity, and the impact on practical computations. This is the first step of a larger data assimilation project which we are embarking on.

In this talk, we will demonstrate our methodology using a stochastic Euler model and a stochastic QG model. This is joint work with C. Cotter, D. Crisan and D. Holm

Alexis Arnaudon

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Title Statistical mechanics with coadjoint orbits

Abstract In this talk and I will show how to implement classical statistical mechanics (canonical ensemble only) on coadjoint orbits. With the example of the free rigid body, I will show numerical simulations and phase transitions in a lattice of coadjoint orbits.

Ana Bela Cruzeiro

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Title An entropic interpolation problem for incompressible viscid fluids

Abstract A natural analogue of Brenier's problem for viscous fluids is introduced, where generalized flows are no more supported by absolutely continuous paths, but by Brownian sample paths. This stochastic variational problem turns out to correspond to an entropy minimization problem with marginal constraints. The talk will explore the connection between this variational problem and Brenier's original one. The dual problem is derived and the general shape of its solution is described. Under the restrictive assumption that the pressure is a nice function, the kinematics of its solution is made explicit and the connection with Navier-Stokes equation is established.

This is joint work with M. Arnaudon, C. Léonard and J.C. Zambrini.

Edriss Titi

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Title Global Well-posedness of an Inviscid Three-dimensional Pseudo-Hasegawa-Mima-Charney-Obukhov Model

Abstract The 3D inviscid Hasegawa-Mima model is one of the fundamental models that describe plasma turbulence. The same model is known as the Charney-Obukhov model for stratified ocean dynamics, and also appears in literature as a simplified reduced Rayleigh-B\'enard convection model. The mathematical analysis of the Hasegawa-Mima and of the Charney-Obukhov equations is challenging due to the their resemblance with the Euler equations. In this talk, we introduce and show the global regularity of a model which is inspired by the inviscid Hasegawa-Mima and Charney-Obukhov models, named a pseudo-Hasegawa-Mima model. The introduced model is easier to investigate analytically than the original inviscid Hasegawa-Mima model, as it has a nicer mathematical structure. To establish our global regularity result we implement a new logarithmic inequality, generalizing the Brezis-Gallouet-Berzis-Wainger inequalities. (This is a joint work with C. Cao and A. Farhat.)

Beth Wingate

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Title Think Globally, Act Locally: Numerical analysis with finite time scale separation in oscillatory PDEs

Abstract It has long been understood that accuracy and stability of discrete representa- tions of PDEs is intimately connected to its mathematical structure. One such PDE that governs many physical applications, including weather and climate, plasma physics, etc, has the following mathematical form:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\varepsilon} L(\mathbf{u}) + N(\mathbf{u},\mathbf{u}) = D(\mathbf{u}), \quad \mathbf{u}(\mathbf{0}) = \mathbf{u_0} \tag{1}$$

where the linear operator L has pure imaginary eigenvalues, the nonlinear term $N(\mathbf{u},\mathbf{u})$ is of polynomial type, the operator D encodes a form of dissipation, and ε is a small non-dimensional parameter. We let $\mathbf{u}(\mathbf{t})$ denote the spatial (vector-valued) function $\mathbf{u}(\mathbf{t},\cdot) = (\mathbf{u}_1(\mathbf{t},\cdot), \mathbf{u}_2(\mathbf{t},\cdot), \ldots)$. The operator $\varepsilon^{-1}L$ results in time oscillations on an order $\mathscr{O}(\varepsilon)$ time scale, and small time steps are required if standard explicit numerical integrators are used. Even implicit integrators need to use small time steps if accuracy is required.

For next generation computer architectures, we wish to find algorithms that allow for more parallelism while reducing the wall clock time. The time-step and its connection to accuracy and stability are one possible path of investigation to push past current limitations.

Therefore, examining the low-frequency content of the PDEs and understanding its role in in numerical algorithm development is essential if we are to make best use of the new computer architectures. The type of equation (1) is known as a fast singular limit, and we therefore expect small scale oscillations will remain a part of the solution even when the nonlinearity, or 'phase scrambler' creates low frequency dynamics. We are called to see if we can use the long-time, low-frequency dynamics (think globally) to advance an accurate solution (act locally) for PDEs of the type (1).

In this talk I discuss a parareal-type method [3, 1] for equations of the form (1), where we have used the above strategy of using the long-time, low frequency dynamics to drive a locally accurate solution. I show that under certain regularity constraints this method has superlinear convergence [2] as $\varepsilon \to 0$ and sketch the ideas behind a new proof of convergence, one that relies on the role of near-resonances inherent in the PDEs, for the case when ε is finite[4].

References

[1] M. J. Gander, 50 years of time parallel time integration, in Multiple Shoot- ing and Time Domain Decomposition, T. Carraro, M. Geiger, S. Korkel, and R. Rannacher, eds., Springer-Verlag, 2015.

[2] T. Haut and B. Wingate, An asymptotic parallel-in-time method for highly oscillatory pdes, SIAM Journal of Scientific Computing, 36 (2014), pp. A693– A736. arXiv:1303.6615.

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