Prediction and Data Assimilation for Nonlocal Diffusions, 4 – 5 June 2018

Abstracts

Ali Aydogdu and Alberto Carrassi
Some aspects of ensemble prediction and data assimilation using a Lagrangian model of sea-ice

In the first part of the talk, we present a sensitivity analysis of a novel sea ice model. neXtSIM is a continuous Lagrangian numerical model that uses an elasto-brittle rheology to simulate the ice response to external forces. The response of the model is evaluated in terms of simulated ice drift distances from its initial position and from the mean position of the ensemble, and compared to a free-drift model, i.e. when the ice rheology does not play any role. The large-scale response of neXtSIM is correlated to the ice thickness and the wind velocity fields while the free-drift model response is mostly correlated to the wind velocity pattern only. The seasonal variability of the model sensitivity shows the role of the ice compactness and rheology at both local and Arctic scales. In contrast of the free-drift model, neXtSIM reproduces the sea ice Lagrangian diffusion regimes as found from observed trajectories. The forecast capability of neXtSIM is also evaluated using a large set of real buoys trajectories, as well as in an idealized search-and-rescue operations exercise. Solving dynamical systems numerically on adaptive mesh raises interesting and challenging methodological issues for data assimilation, especially for ensemble-based techniques. The mesh being time-dependent implies that each ensemble member is represented on its own mesh and that, at the analysis times, the values of the physical variables on the mesh along with the mesh positions themselves have to be updated. In addition to the dynamical adaptivity, a remeshing process can be employed: mesh nodes can be added or removed at some point of the numerical integration, to avoid extreme distortion of the mesh. Remeshing implies that the mesh dimension is not conserved: the spatially discrete state-space dimension is time-dependent and different for each ensemble member. These aspects represent fundamental methodological challenges for classical data assimilation methods. Standard approaches for ensemble-based data assimilation rely on a fixed-in-time, and equal across members, mesh and are thus unsuitable in this case, for which even the computation of the ensemble-based error statistics is not straightforward. In the second part of the talk, we describe the specific challenges for classical EnKF in this context and present a method that relies upon the use of a reference fixed mesh thus allowing for evaluating the ensemble-based error statistics consistently. Numerical experiments are performed in a one- dimensional mesh using low-order. We finally discuss how to extend the method to a two- dimensional non-conservative adaptive mesh and its application to neXtSIM.

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Wietse Boon
Flow and Mechanics in Fractured Media as Mixed-Dimensional PDEs

In the mixed-dimensional representation of fractured media, the fractures are considered as lower-dimensional manifolds. This concept is successively applied to the lines and points at the intersections between fractures leading to a hierarchical geometry of manifolds of codimension one. By imposing these modelling assumptions a priori in the continuous setting, the basis is formed for the introduction of coupled PDEs on the mixed-dimensional geometry, which we refer to as mixed-dimensional PDEs.

In this work, we consider Darcy flow and linear elasticity on mixed-dimensional representations of fracture networks. Since the associated, governing equations are fully coupled, the systems of equations are presented using mixed-dimensional differential operators which map between the different dimensions. In turn, the resulting system of equations is considered as mixed-dimensional and is analysed as such, before the introduction of the discretization scheme. We present theoretical results related to the structure of mixed-dimensional elliptic partial differential equations from which multiple conforming discretization schemes arise using dimensionally hierarchical finite elements.

Keeping later purposes such as transport problems and fracture propagation in mind, our main interest lies in obtaining accurate flux fields and stress states which respect physical conservation laws. Therefore, we employ mixed finite elements which allow for a local preservation of such laws. The symmetry of the stress tensor is imposed in a weak sense, thus leading to the use of familiar, conforming, finite elements with relatively few degrees of freedom.

Jana de Wiljes (with Sahani Pathiraja, Sebastian Reich and Paul Rozdeba)
Linear ensemble transform filters and smoothers

A family of filters, the so called Linear Ensemble Transform Filters (LETFs), and their general extension to smoothers (LETSs) is presented [3]. This class of filters/smoothers is particularly valuable in the context of high dimensional state and parameter estimation since spatial as well as time-wise (in the smoothing case) localization can be implemented. Furthermore, the linear update of LETFs/LETSs enables hybrid formulations where various filters/smoothers with complementary beneficial properties can be combined (e.g., pairing a robust filter with underlying Gaussian assumptions with a consistent filter) [2, 3]. Another feature specifically developed for a particular subset of these families is the second order correction which helps to further improve estimation results and increase the correlation between prior and posterior ensembles [1, 3]. One member of the LETFs/LETSs, the Ensemble Transform Particle Filter/Smoother [4, 3], is particularly highlighted as it is consistent in the particle limit and does not require assumptions with respect to the posterior distribution. Further, an outlook on how these filters/smoothers can be beneficial in the context of Lagrangian-type data assimilation is given.

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Ahmed Elsheikh
Generation of stochastic fields using generative adversarial networks with applications to geological modelling

We investigate the use of generative adversarial networks (GANs) as a general samples-based parametrization tool for stochastic inputs of partial differential equations. We approach the parametrization as an emulation of a data generating process, instead of explicitly constructing a parametric form that preserves the statistics of the data. This is done by training a neural network to generate samples that mimics the data distribution. Neural networks are universal approximators and have the capacity to express complex relations far beyond linear and kernel based parametrization techniques. We present some applications of generating random fields representing geological models. We experiment with unconditional and conditional realizations of binary channelized geological models, and perform a number of uncertainty quantification and inverse modelling studies. Our results show that GANs based parametrization is very effective in preserving visual realism of the geological models as well as preserving the high order statistics of the flow responses.

Heiko Gimperlein
Adaptive finite element methods for nonlocal problems

Dan Goldberg
Ice shelf rifting: Constitutive modelling, satellite data assimilation, and connections to fracture mechanics

Ice shelves (not to be mistaken with sea ice!) comprise the floating extensions of meteoric ice from Glaciers that has flowed into the ocean. In the northern hemisphere they are usually not more than several kilometers long, whereas in Antarctica they can range from the size of Greater London to the size of France. But regardless of size these ice shelves play an important structural role in "buttressing" the flow of these glaciers against raised levels of ice loss and hence sea level rise. This structural integrity can be weakened, however, through the formation of deep crevasses (essentially, long cracks in the ice) or through calving of large icebergs through large-scale rifting. As such, understanding the development of large-scale crevassing and rifting in ice shelves is of great importance to predicting the future evolution of ice sheets.

Our understanding of large-scale ice shelf fracture remains limited, however, due in part to the scales involved. Rifts extend through the full thickness of the shelves (which are typically hundreds of meters) and extend for tens of kilometers. Moreover glacial ice is highly heterogeneous, often containing large deposits of accreted ocean water (marine ice), entrained clasts of sediment, and ice that has been reworked by surface melt and refreezing. Thus it is difficult to observe and measure large-scale fracture in a controlled laboratory environment. However, recent advances in airborne and satellite remote sensing has provided a rich set of data describing the phenomenology of ice shelf rifting and crevassing, in some cases with individual rifts being tracked on a daily or hourly basis. These observations are complemented by a well-developed framework of ice shelf stress modelling, which assimilates satellite observations of ice shelf geometry and velocity into a constitutive model for large-scale stresses. Recent work bringing together these methodologies suggests that these large-scale stresses do play a role in influencing and guiding the evolution of large-scale ice shelf rifts. However it remains to be seen whether progress can be made through combining these more "traditional" ice-sheet modelling and observational approaches, or whether an approach which considers fracture on unresolved scales in some statistical fashion is required.

A. D. Kirwan (with H. Huntley and H. Chang)
Prediction and Data Assimilation: Ocean vs. Arctic Sea Ice

Following prior developments in meteorology, predictions of the oceanic variables are now routine. Using standard meteorological skill metrics these predictions are generally regarded as reliable. However, there is a substantial user community in oceanography who require Lagrangian type forecasts. These are off-line products and are less reliable than Eulerian forecasts. Two reasons for this discrepancy are the lack of Lagrangian information in the assimilated data stream and inadequate parameterizations of submesoscale processes. Consequently, there is considerable research into methods to assimilate Lagrangian type data into ocean forecasts. Recent results show that assimilation of velocities from Lagrangian drifters substantially improves both Eulerian forecasts and Lagrangian products such as trajectories and associated transport properties. Based on this I offer some speculations on the implications of assimilation of Lagrangian data on forecasts of arctic sea ice.

Kody Law
Strategies for multilevel Monte Carlo

This talk will concern the problem of inference when the posterior measure involves continuous models which require approximation before inference can be performed. Typically one cannot sample from the posterior distribution directly, but can at best only evaluate it, up to a normalizing constant. Therfore one must resort to computationally-intensive inference algorithms in order to construct estimators. These algorithms are typically of Monte Carlo type, and include for example Markov chain Monte Carlo, importance samplers, and sequential Monte Carlo samplers. The multilevel Monte Carlo method provides a way of optimally balancing discretization and sampling error on a hierarchy of approximation levels, such that cost is optimized. Recently this method has been applied to computationally intensive inference. This highly non-trivial task can be achieved in a variety of ways. This talk will review 3 primary strategies which have been successfully employed to achieve optimal convergence rates – in other words faster convergence than i.i.d. sampling at the finest discretization level. Some of the specific resulting algorithms, and applications, will also be presented.

James Maddison
PDE constrained Hessian action information for time dependent finite element models

Recent developments in automated code generation have facilitated the derivation of discrete consistent adjoint models associated with finite element forward codes, enabling the calculation of partial differential equation constrained derivative information [1,2]. This derivative information may, for example, be used in the solution of partial differential equation constrained optimisation problems. Here the derivation of second order derivative information is presented, in particular for the calculation of partial differential equation constrained Hessian actions associated with forward models written using the FEniCS system [3]. This is used to compute an "optimality constrained derivative" – that is, a derivative which is constrained by the results of an optimisation, which is itself constrained by the partial differential equation. The approach is combined with the revolve algorithm [4,5] for optimal data checkpointing, which it is intended will facilitate the calculation of partial differential equation constrained Hessian information at scale.

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Erdogan Madenci *Peridynamics for paradigm shift in computational methods*

Although the idea of derivatives seems to be rather rudimentary, it has a profound impact on forming one of the building blocks in science and engineering. Over the years, scientists have tried to elaborate on it through different methods. Approximate solution of the governing differential equations of many physical fields requires the evaluation of derivatives at discrete points in the domain. Their solution becomes challenging due to the presence of higher order derivatives, abrupt change in behavior, nonlinearity and multi-scale resolution arising from characteristic parameters. In a quest to address these computational challenges, peridynamics enables the evaluation of derivatives of any order in a multi-dimensional space, and provides a unified approach to transfer information within a set of discrete data, and among data sets. It enables the computational solution of complex differential equations in the presence of jump discontinuities or singularities. This presentation will demonstrate the applicability of peridynamics for the solution of many fundamental and engineering problems as well as failure prediction in structural materials under complex loading conditions.

Erkan Oterkus
Peridynamics for Modelling Ice Fracture

Despite of its advantages, utilization of the Arctic region for sailing brings new challenges due to its harsh environment. Therefore, ship structures must be designed to withstand ice loads in case of a collision between a ship and ice takes place. Although experimental studies can give invaluable information about ship-ice interactions, full scale tests are very costly to perform. Therefore, computer simulations can be a good alternative. Ice-structure interaction modelling is a very challenging process. First of all, ice material response depends on many different factors including applied-stress, strain-rate, temperature, grain-size, salinity, porosity and confining pressure. Furthermore, macro-scale modeling may not be sufficient to capture the full physical behaviour because the micro-scale effects may have a significant effect on macroscopic material behaviour. Hence, it is necessary to utilize a multi-scale methodology. In order to capture the macro-scale behaviour of ice, well-known Finite Element Method (FEM) has been used in various previous studies. Within FEM framework, various techniques can be used to model crack propagation such as cohesive zone models (CZM) and extended finite element method (XFEM). However, a universally accepted CZM failure model is not currently available and the crack propagation may have mesh dependency. Although, the mesh dependency problem can be overcome by XFEM, enrichment process may lead to an algebraic system with billions of unknowns which is difficult to solve numerically. Furthermore, FEM is based on classical continuum mechanics which does not have a length scale parameter and is incapable of capturing phenomenon at the micro-scale. Hence, other techniques should be utilized at the micro-scale and linked to FEM simulation. However, it is not straightforward to obtain a smooth transition between different approaches at different scales. By taking into account all these challenging issues, a state-of-the-art technique, peridynamics can be utilized for ice fracture modelling. Peridynamics is a non-classical (non-local) continuum mechanics formulation which is very suitable for failure analysis of materials due its mathematical structure. Cracks can occur naturally in the formulation and there is no need to impose an external crack growth law. Furthermore, due to its non-local character, it can capture the phenomenon at multiple scales.

Abner Salgado
Optimization with respect to order in a fractional diffusion model: analysis and approximation

We consider an identification problem, where the state u is governed by a fractional elliptic equation and the unknown variable corresponds to the order $s \in (0,1)$ of the operator. We study the existence of an optimal pair (u,s) and provide sufficient conditions for its uniqueness. We develop semi-discrete and fully discrete algorithms to approximate the solution and provide an analysis of their convergence properties. We present numerical illustrations that confirm and extend our theory. This is joint work with E. Otarola and H. Antil.

Roland Potthast (with Jehan Alswaihli)
Data Assimilation and Kernel Reconstruction for Nonlocal Field Dynamics

Data assimilation is concerned with state estimation in dynamical systems. Methods such as three-dimensional or four-dimensional variational data assimilation have a long history and are used with large success in operational centers. Today, ensemble data assimilation and particle filters are methods which attract a lot of attention.

The reconstruction of unknown parts of some dynamical system such as structural functions or connectivity is a basic task of inverse problems, medical imaging and nondestructive testing. Here, we study the reconstruction of the neural connectivity kernel within a neural field given the full dynamical evolution. Kernels are non-local and model both short-range and long-range signal processing in living neural tissue.

We formulate an iterative data assimilation inversion method, where the activity fields of of some neural tissue is reconstructed from non-local measurements and the kernel is reconstructed given the reconstruction of the activity. This approach is iterated in the sense that the first guess for the state reconstruction can be improved based on the kernel reconstruction of step two.

We provide a description of the method, numerical examples and also the basic elements of a convergence proof of the iteration when the measurement error tends to zero.

Christian Sampson
Toward a metric for evaluating sea ice fracture forecast

Sea ice plays an important role in the Earths climate system and acts as a mediator of heat exchange between the ocean and the atmosphere in the polar regions. Important to modeling these heat fluxes is an accurate representation of sea ice fracture patterns, extent and size. Accurate fracture dynamics are also important to operational forecasting. Todays sea ice models use several different rheologies, each with their strengths and weaknesses. Of interest is the ability to determine which rheology and which parameter settings produce the best predictions of sea ice fractures, especially the correct geometries. In this talk I will describe ongoing work in the development of a suitable metric for this purpose. In particular, I will discuss a promising image warping technique found in Xie, Srivastava 2016 which utilizes the outer product of partial derivatives of functions in an image space to define a robust metric. The distance between two images is found after the application of an optimal, orientation preserving diffeomorphism which preserves the image boundary. I will highlight some of the challenges still faced in applying this technique, proposed solutions and show some initial results using code provided by Derek Tucker from Sandia National Labs.

Sergiy Zhuk
Geometry of data assimilation for non-linear differential equations

A new state estimation method for regular (in the sense of Oseledets) dynamical systems will be presented. The method is designed so that the Lyapunov exponents of the corresponding estimation error dynamics are negative, i.e. the estimation error decays to zero exponentially (but not uniformly!) fast. The latter is shown to be the case for generic regular flow maps if and only if the observation matrix H satisfies detectability conditions: the rank of H must be at least as great as the number of nonnegative Lyapunov exponents of the underlying attractor. Numerical experiments illustrate the exponential convergence of the method and the sharpness of the theory for the case of Lorenz 96 and Burgers equations with incomplete and noisy observations.