2017 SOCAMS Poster List

Name:

Jason Dark

Institution:

UC Irvine

Title:

A Chemical Master Equation Toolkit

Abstract:

The direct solution of the chemical master equation (CME), when paired with approximation techniques like the finite state projection algorithm, is known to provide orders-of-magnitude speed-up over stochastic simulations when characterizing probability trajectories over the state-space of a biochemical reaction network (BRN). The problem of automatically and efficiently constructing the CME from a BRN is considered with the goal of reducing the storage requirements of the solution, which consists of 3 fundamental computations:

1. Enumeration. I provide an algorithm to enumerate the high-dimensional state-space of the CME without explicit storage of any integer tuples, instead exploiting the conservation laws of the BRN to generate these states on the fly.
2. Indexing. I detail a method for the computation of a state's enumerative index, again without explicit storage of the states or their indices.
3. Matrix-free operation. In addition to the construction of a matrix-free Markov operator, I present preliminary observations on the development of optimal preconditioners for use in the solution of the associated linear problem.

Taken together, this work both provides a complimentary approach to the finite state projection methods for the solution of large BRNs and significantly reduces the logistical burden in formulating and evaluating the CME.

Name:

Ben Gross

Institution:

UC Santa Barbara

Title:

Numerical Exterior Calculus Methods for Fluctuating Hydrodynamics Within Curved Fluid Interfaces

Abstract:

We use exterior calculus of differential geometry to formulate fluctuating hydrodynamic equations to account phenomena within curved fluid interfaces. For manifolds of spherical topology, we present spectral methods that provide a discrete approximation of exterior calculus operators such as the exterior derivative, Hodge star, co-differential, or Hodge Laplacian. Our numerical approximation of the exterior calculus for surfaces of spherical topology is based on hyperinterpolation and Lebedev quadratures. We show how our methods can be used to formulate fluctuating hydrodynamic descriptions to investigate phenomena within curved fluid interfaces.

Enter the names of your co-authors

Paul Atzberger

Name:

Eleni Panagiotou

Institution:

University of California Santa Barbara

Title:

Topological analysis and fluctuating hydrodynamics simulation of the roles of polymer entanglements in the viscoelastic responses of complex fluids

Abstract:

We explore how the microscopic interactions link to bulk macroscopic properties of materials. We study systems of polymer chains in a solvent and examine the effect of hydrodynamic and of bonded and excluded volume interactions. First, we investigate how the entanglement of polymeric chains relates to bulk viscoelastic responses in polymeric materials. We show how the structure of the material can be analyzed using results from topology to develop new tools for entanglements. Next, we investigate the hydrodynamic effect of thermal fluctuations to the macroscopic properties of the material using the Stochastic Eulerian Lagrangian Method. Our studies will lead to a better understanding of the viscoelastic properties of materials which involve different length

scales and complex microscopic interactions, like the cytoskeleton.

Enter the names of your co-authors

K. C. Millett and P. J. Atzberger

Name:

Christian Bueno

Institution:

University of California, Santa Barbara

Title:

Methods for Data-Driven Dimension Reduction of Stochastic Systems using Diffusion Maps

Abstract:

Many stochastic dynamical systems arising in scientific and engineering applications exhibit significant variations in associated time-scales. A central challenge in dimensionality reduction of these systems is to obtain simplified descriptions more amenable to analysis and simulation and to identify a splitting between the "fast" degrees of freedom to be averaged and the "slow" degrees of freedom to be retained. We develop practical computational methods based on recent manifold learning techniques such as Diffusion Maps. This allows us to develop a data-driven descriptions of the stochastic system based on learning a manifold for the slow temporal dynamics. In practice, a number of challenges arise which we are working to address with our methods. This includes cases where the system state may have a small number of samples or the manifold may be obscured by noise or numerical artifacts. We introduce approaches to grapple with these challenges and illustrate our approach on a few example stochastic dynamical systems to obtain effective drift-diffusion coefficients for a reduced SDE describing the system.

Enter the names of your co-authors

Paul J. Atzberger

Name:

Hyun-Jung Kim

Institution:

University of Southern California

Title:

Time-homogeneous parabolic Wick-Anderson model in one space dimension: regularity of solution

Abstract:

We consider the stochastic parabolic Anderson model driven by time-independent random potential with Wick product on a bounded interval (a,b) or the whole line R.

Our aim is to define an L_p-bounded (chaos) solution by means of chaos expansion in a probability space and to establish the optimal space-time regularity of the solution under a minimal assumption on
the initial condition u_0.

Two main noticeable features of our model in the paper are
1) time-independent white noise,
2) special multiplication called Wick product between u and white noise.
Even though time-dependent models have been well-studied thanks to
the It\^o theory, time-independent models like our model still need more improvement.
Instead of using the usual point-wise product, the model
is interpreted in the renormalized sense by using the Wick product.
This allows us to reduce the stochastic model into countably many deterministic propagators. With the help of the Malliavin Calculus,
we achieve the same optimal space-time regularity results either on a bounded interval (a,b) or the whole line R.

Enter the names of your co-authors

Sergey Lototsky

Name:

Ka Chun Lam

Institution:

Caltech

Title:

Energy Decomposition With Applications to Matrix Compression And Multiresolution Decomposition

Abstract:

In this paper, we introduce the notion of {\bf Energy decomposition} for self-adjoint, positive definite matrix A using the representation of {\bf energy elements}. The interaction between these energy elements depicts the underlying topological structure of the operator. This concept of decomposition naturally reflects the hidden geometric structure of the operator which inherits the localities of the structure. By utilizing the intrinsic geometric information under this Energy framework, we propose a systematic operator compression scheme for the inverse operator A^{-1}. In particular, with an {\it appropriate partitioning} of the underlying geometric structure, we can construct localized basis by using the concept of {\bf interior} and
{\bf closed energy}. Meanwhile, two important localized quantities are introduced, namely the {\bf error factor} and the {\bf condition factor}. Our error analysis results show that these two factors will be the guidelines for finding the appropriate partition of the basis functions such that prescribed compression error and acceptable condition number can be achieved. By virtue of this insight, we proposed the {\bf Patch Pairing} algorithm to realize our energy partition framework for operator compression with controllable compression error and condition number. From the perspective of linear system solver, we also extend our compression scheme into a multi-resolution matrix factorization algorithm which achieves nearly optimal performance on both complexity and well-posedness.

Enter the names of your co-authors

Yizhao Hou, De Huang

Name:

Shay Deutsch

Institution:

University of California Los Angeles

Title:

Zero Shot Learning via Multi-Scale Manifold Regularization

Abstract:

We address zero-shot learning using a new manifold alignment framework based on a localized multi-scale transform on graphs. Our inference approach includes a smoothness criterion for a function mapping nodes on a graph (visual representation) onto a linear space (semantic representation), which we optimize using multi-scale graph wavelets. The robustness of the ensuing scheme allows us to operate with automatically generated semantic annotations, resulting in an algorithm that is entirely

free of manual supervision, and yet improves the state-of-the-art as measured on benchmark datasets.

Enter the names of your co-authors

Soheil Kolouri, Kyungnam Kim, Yuri Owechko, Stefano Soatto