2020 SIAM Student Mini-Symposium in Applied Mathematics

University of Michigan

29th May 2020

Event schedule

Keynote talk

10:00 – 10:35am Professor Silas Alben:
Dynamics of active elastic sheets

Student talks

10:35 – 11:00am Christiana Mavroyiakoumou:
Simulations of large-amplitude membrane motions in inviscid flow

11:00 – 11:25am Saibal De:
Large scale simulation of non-smooth dynamics in granular media

11:25 – 11:50am Hai Zhu:
Panel-based high order Nyström schemes for Laplace layer potentials

11:50am – 1:00pm *Lunch break*

1:00 – 1:25pm Rishi Sonthalia:
Tree! I am no Tree! I am a Low Dimensional Hyperbolic Embedding

1:25 – 1:50pm Nathan Vaughn:
Integral equation electronic structure calculations

1:50 – 2:15pm Leighton Wilson:
GPU-Accelerated Particle-Cluster and Cluster-Cluster Barycentric Lagrange Treecode

2:15 – 2:45pm *Coffee break*

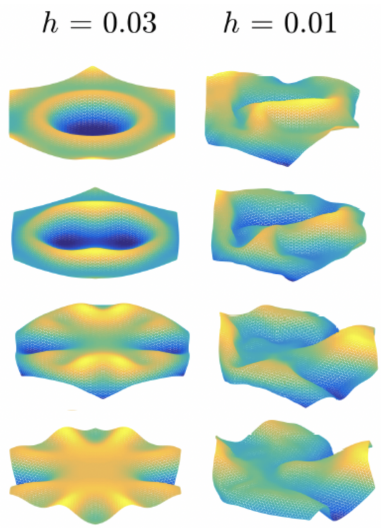
2:45 – 3:10pm Christina Athanasouli:
Dynamics of a flip-flop sleep-wake model

3:10 – 3:35pm Andrew McMillan:
Sum of squares optimization in non-autonomous differential equations

Abstracts

Dynamics of active elastic sheets

Keynote speaker: Professor Silas Alben



Recent applications (e.g. active gels and self-assembly of elastic sheets) motivate the need to efficiently simulate the dynamics of thin elastic sheets. We present semi-implicit time stepping algorithms to improve the time step constraints that arise in explicit methods while avoiding much of the complexity of fully-implicit approaches. For a triangular lattice discretization, our semi-implicit approach is stable for all time steps. For a more general finite-difference formulation the analogous approach is stable for time steps two to three orders of magnitude greater than for an explicit scheme. We study a model problem with a radial traveling wave form of the sheet's reference metric, and find transitions from quasi-periodic to chaotic dynamics as the sheet thickness is reduced, wave amplitude is increased, and a damping constant is reduced.

Simulations of large-amplitude membrane motions in inviscid flow

Speaker: Christiana Mavroyiakoumou

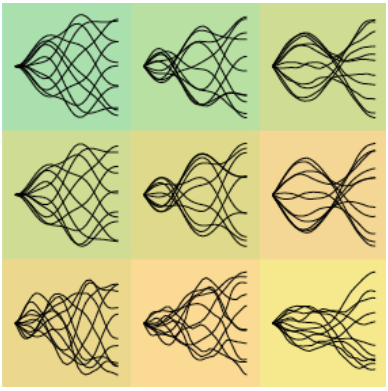
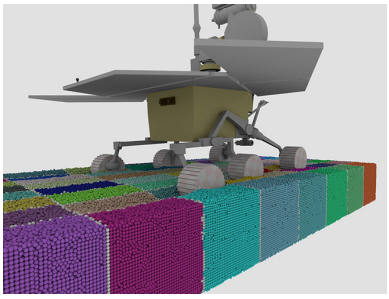


Figure 1: Fixed-free membrane snapshots with different mass, stretching rigidity, and pretension.

We study the dynamics of thin membranes—extensible sheets with negligible bending stiffness—initially aligned with a uniform inviscid background flow. This is a benchmark fluid-structure interaction that has previously been studied mainly in the small-deflection limit, where the flat state may be unstable. Related work includes the shape-morphing of airfoils and bat wings. We investigate the initial instability and large-amplitude dynamics with respect to three key parameters: membrane mass density, stretching rigidity, and pretension. When both membrane ends are fixed, the membranes become unstable by a divergence instability and converge to steady deflected shapes. With the leading edge fixed and trailing edge free, divergence and/or flutter occurs, and a variety of periodic and aperiodic oscillations are found. With both edges free, the membrane may also translate transverse to the flow, with steady, periodic, or aperiodic trajectories.

Large scale simulation of non-smooth dynamics in granular media

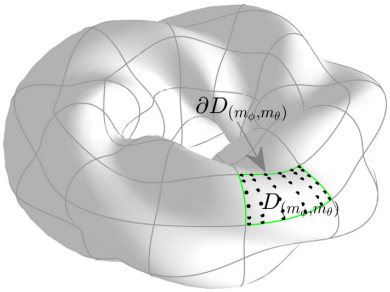
Speaker: Saibal De



Granular media is a common form of material in many physical and industrial applications. However, since it does not conform to a standard state of matter, there is no single constitutive law that describes all aspects of its behavior. In this talk, we discuss a physics based model for simulating granular media, and discuss some of the challenges in implementing it. We present an efficient framework for detecting and resolving rigid body collisions in large scale granular media simulations. We demonstrate strong and weak scalability of our framework for up to 128 million bodies and 256 processors.

Panel-based high order Nyström schemes for Laplace layer potentials

Speaker: Hai Zhu



There are two major games researchers are competing in developing numerical schemes for solving physical problems using boundary integral formulation, speed and accuracy. While the speed game is partially settled with the developments on fast algorithms, like FMM and treecode, for applying discretized integral operators. It is still debatable which singular quadrature scheme performs better for near-field interaction, at least in three dimensions. In this talk, we are proposing a new approach of close evaluation scheme for 3D Laplace double and single layer potential, which we think could be extended to various other kernels.

Integral equation electronic structure calculations

Speaker: Nathan Vaughn

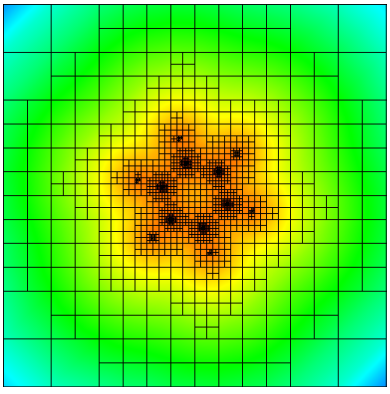


Figure 2: 2D slices of the electron density computed with TAGI for the benzene molecule C_6H_6 on adaptively refined meshes.

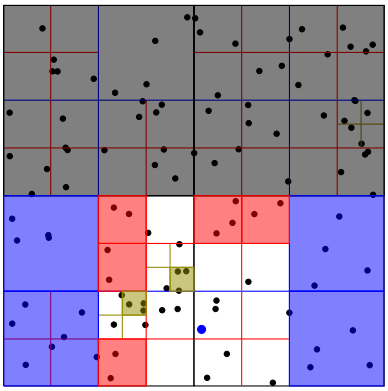
Electronic structure calculations are an integral part of materials design and engineering, allowing scientists to screen many candidate materials for advantageous properties prior to synthesis. Density Functional Theory is a formulation of electronic structure based on the electron density that is well suited for computation. I present a real-space method for Kohn-Sham Density Functional Theory based on an integral equation formulation of the Kohn-Sham equations, called Treecode-Accelerated Green's Iteration (TAGI). In this approach, the standard eigenvalue problem for the Kohn-Sham differential operator is converted to a fixed point problem for an integral operator by the method of Green's functions, then the fixed points

are computed using Green's iteration. Essential to this method is the accurate and efficient evaluation of the convolution integrals arising in the iteration.

TAGI achieves accuracy and efficiency through the use of adaptive mesh refinement to represent the fields, singularity subtraction schemes to reduce the quadrature error due to the singular Green's functions, and a GPU-accelerated treecode to reduce the computational complexity of the convolution integrals. We have performed all-electron and pseudopotential calculations with TAGI for non-periodic systems and demonstrated systematic convergence to chemical accuracy.

GPU-Accelerated Particle-Cluster and Cluster-Cluster Barycentric Lagrange Treecode

Speaker: Leighton Wilson

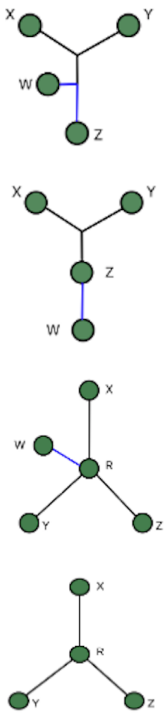


We present an MPI + OpenACC implementation of particle-cluster (PC) and cluster-cluster (CC) kernel-independent barycentric Lagrange treecodes (BLTC) for $\mathcal{O}(N \log N)$ summation of particle interactions on GPUs. The distributed memory parallelization uses recursive coordinate bisection for domain decomposition and MPI remote memory access to build locally essential trees on each rank. The particle interactions are organized into target batch/source cluster interactions in the PC approach, or target cluster/source cluster interactions in the CC approach, which efficiently map onto the GPU; target batching or clustering provide an outer level of parallelism, while the direct sum form of the barycentric treecode approximation provides an inner level of parallelism. The GPU-accelerated BLTC performance is demonstrated on several test cases for uniform, Gaussian, and exponential particle distributions interacting via the Coulomb potential or Yukawa potential.

Tree! I am no Tree! I am a Low Dimensional Hyperbolic Embedding

Speaker: Rishi Sonthalia

Given data, finding a faithful low-dimensional hyperbolic embedding of the data is a key method by which we can extract hierarchical information or learn representative geometric features of the data. In this paper, we explore a new method for learning hyperbolic representations that takes a metric-first approach. Rather than determining the low-dimensional hyperbolic embedding directly, we learn a tree structure on the data as an intermediate step. This tree structure can then be used directly to extract hierarchical information, embedded into a hyperbolic manifold using Sarkar's construction[1], or used as a tree approximation of the original metric. To this end, we present a novel fast algorithm TreeRep such that, given a δ-hyperbolic metric (for any $\delta \geq 0$), the algorithm learns a tree structure that approximates the original metric. In the case when $\delta = 0$, we show analytically that TreeRep exactly recovers the original tree structure. We show empirically that TreeRep is not only many orders of magnitude faster than previous known algorithms, but also produces metrics with lower average distortion and higher mean average precision than most previous algorithms for learning hyperbolic embeddings, extracting hierarchical information, and approximating metrics via tree metrics.



[1] Sarkar, Rik. "Low distortion delaunay embedding of trees in hyperbolic plane." International Symposium on Graph Drawing. Springer, Berlin, Heidelberg, 2011.

Dynamics of a flip-flop sleep-wake model

Speaker: Christina Athanasouli

Humans spend about a third of their lives sleeping. Despite the fact that sleep plays a big role in many bodily functions, such as supporting learning processes and clearing out toxins in the brain accumulated throughout periods of activity, scientists still don't know its ultimate purpose. Therefore, mathematical modeling can be useful in studying features of sleep-wake regulation. The timing of sleep is affected by two main factors: 1) the circadian system, i.e. our internal biological clock, and 2) the sleep homeostasis which operates as a timer reminding the body to sleep. I will present a sleep-wake model and fundamental tools that we use to analyze the dynamics of sleep-wake regulation. I will also talk about the bifurcations that emerge in this model when we change some of the physiological parameters that dictate the homeostatic sleep drive and the circadian waveform.

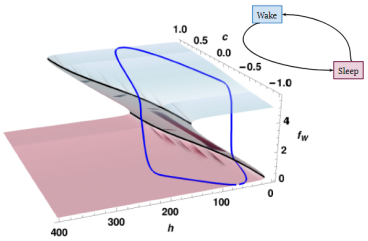


Figure 3: A stable orbit on a fast-slow surface in the c–h–f_W space.

Sum of squares optimization in non-autonomous differential equations

Speaker: Andrew McMillan

For nonlinear, ordinary differential equations whose solutions are unknown or computationally intractable, rigorous bounds on time averages can be proved using variational methods and auxiliary functions, for which optimal auxiliary functions can be recovered by solving a convex optimization problem. In fact, finding extremal trajectories and optimal auxiliary functions are strongly dual problems, so that the method is capable of producing arbitrarily sharp bounds. For polynomial dynamical systems, optimal or near optimal bounds can be computed via sum of squares technology, realized as a semidefinite program. Here, this method is extended to dynamics with autonomous and non-autonomous trigonometric dependence.

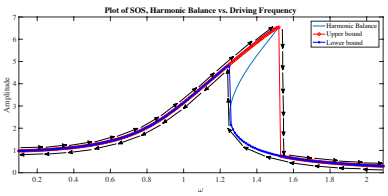


Figure 4: Plot of SOS, Harmonic Balance vs. Driving Frequency