SCALA 2015 : SCIENTIFIC COMPUTING AROUND LOUISIANA

GOLDRING/WOLDENBERG HALL I (Building 39)
Room GWH-110

Friday, March 20

1:10 – 1:55	Lisette, De Pillis (Mathematics, Harvey Mudd College) **Modeling Cancer-Immune System Dynamics**
2:00 – 2:15	Jacek Wrobel (Mathematics, Tulane Univ.) **Regularized Image System Formulation for Stokes Flow Outside a Solid Sphere**
2:15 – 3:00	***Coffee Break***
3:00 – 3:15	Ataollah Mesgarnejad (Center for Computation and Technology, LSU) **Validation Simulation for Variational Approach to Fracture Mechanics**
3:15 – 3:30	Rosalyn Rael (Tulane/Xavier Center for Bioenvironmental Research, Tulane Univ.) **Evolution of Dynamic Ecological Food Web Networks**
3:30 – 3:45	Tchavdar Marinov (Natural Science, SUNO) **MVI for Coefficient Identification Problem in SIR Epidemic Models**
4:00 – 5:30	***Posters and Refreshments***

Saturday, March 21

9:00 – 9:45	Michele Benzi (Mathematics and Computer Science, Emory Univ.) **Some Mathematical and Computational Challenges in Network Science**
9:45 – 10:00	Fei Xue (Mathematics, University of Louisiana Lafayette) **Efficient Solution of Large-scale Nonlinear Hermitian Eigenproblems With a Variational Characterization**
10:00 – 10:15	Brad Burkman (Mathematics, Louisiana School for Math, Science and the Arts) **Preparing the Next Generation in Scientific Computing**
10:15 - 10:45	***Coffee Break***
10:45 – 11:00	Joscha Gedicke (Mathematics and Center of Computation and Technology, LSU) **Massive Parallel Computation of a Biharmonic Obstacle Problem**
11:00 – 11:15	Zachary Byerly (Center for Computation and Technology, LSU) **STORM: a Scalable Toolkit for an Open Community Supporting Near Realtime High Resolution Coastal Modeling**
11:15 – 11:30	Tong Wu (Mathematics, Tulane Univ.) **Well-Balanced Positivity Preserving Central-Upwind Scheme for the Shallow Water System with Friction Terms**
11:30 – 11:45	Agnimitro Chakrabarti (Civil and Environmental Engineering, LSU) **Numerical Modeling of Wave Hydrodynamics Near the Marsh Edge With and Without a Breakwater**
11:45 – 1:00	***Lunch (Provided)***
1:00 – 1:45	Greg Forest (Mathematics, University of North Carolina - Chapel Hill) **Computational Challenges in Complex Biological Fluids**
1:45 – 2:00	Scott Hymel (Biomedical Engineering,Tulane Univ.) **Three-Dimensional Modeling of Circulating Cell Separation in a Bifurcating Microchannel**
2:00 – 2:15	***Coffee Break***
2:15 – 2:30	Yuanzhen Cheng (Mathmetics, Tulane Univ.) **Moving-water Equilibria Preserving Central-Upwind Schemes for the Shallow Water Equations**
2:30 – 2:45	Shawn Walker (Mathematics, LSU) **A Finite Element Method For Nematic Liquid Crystals With Variable Degree Of Orientation**
2:45 – 3:00	Julie Simons (Mathematics, Tulane Univ.) **Sperm Motility in Three Dimensions**

Poster Presentations

Jordan Adam (Earth and Environmental Sciences, Tulane)
Comparative analysis of steady and non-steady flow routing and their impacts on erosion in the Landlab modeling framework

Vanya Cherneva (ECE, LSU)
Distributed Algorithms for wireless networks

Farren Curtis (Physics , Tulane)
Many-Body Dispersion Interactions of Molecular Crystals

Christina Hamlet (Mathematics, Tulane)
Sensory feedback in lamprey locomotion

Yue Hu (Center for Computation and Technology, LSU)
Model-Driven Auto-Tuning of Stencil Computations on GPU's

Sam Karhbet (Mathematics, University of Louisiana Lafayette)
Experimental study of approximate inverse preconditioners for symmetric indefinite matrices

Gerald Knapp (Mechanical Engineering, LSU)
Use of Provenance Data Management Systems for K-Edge Analysis of Flame Retardant X-Ray Tomography

Joe Knight (Physics, Tulane)
Benchmark of GW methods of electron acceptors

Sanjaya Lohani (Physics, Tulane)
Scaling of FHI-aims on Sphynx and Cypress

Forest Mannan (Mathematics, Tulane)
Singly-Periodic Stokes Flow with a Wall

Zhuolin Qu (Mathematics, Tulane)
A Fast and Stable Explicit Operator Splitting Method for Phase-Field Models

Owen Richfield (Mathematics, Tulane)
Cooperation and Efficiency in Sperm Motility Patterns

Zhongyi Sheng (Biomedical Engineering, Tulane)
Cell deformation in a cross-flow channel: integration of computational modeling with experiment

Xiaopeng Wang (Physics and Engineering Physics, Tulane)
Formation and Annealing behaviors of qubit centers in 4H-SiC from first principles

Zhuo Wang (Center for Computation and Technology, LSU)
One Dimensional Prescribed Curvature Equation

Poster Abstracts

Jordan Adam (Earth and Environmental Sciences, Tulane)

Comparative analysis of steady and non-steady flow routing and their impacts on erosion in the Landlab modeling framework

Traditional landscape evolution models calculate flow in a simplified way, assuming steady-state flow throughout an entire precipitation event, which, in turn, drives steady incision of channels throughout a landscape. This method routes flow throughout a landscape, but only in one downstream direction. In contrast, non-steady approaches calculate flow and channel incision rate as variable through time, and allows for flow to move in multiple directions into and out of a given cell. Because flow is not forced to move in just one direction, the direction of steepest descent, overland or sheet flow can occur, allowing smaller channels to form upstream on hillslopes and near zero-order tributaries. Due to these differences, steady-state, single direction flow routing models is likely to overestimate calculated peak discharge, incision rate and total eroded depth when compared to the non-steady “hydrograph” method. In both cases, the integrated, or total, discharge should be approximately the same. In short storms, discharge events will likely last longer in the hydrograph method, but because peak discharge will be less than in the steady-state method, total eroded depths will be less. A sensitivity analysis will be run using the Landlab modeling framework to quantify the relationship between these two models as well as investigate how each model method drives long-term landform morphology through increased erosion. Landlab is an interdisciplinary, open-source 2-D modeling environment that evolves topography using surface process components over time in response to climatic, tectonic and other geomorphic drivers. In this analysis, Landlab will be used to build a structured raster grid, and then couple flow and erosional processes across that grid. Precipitation intensity and duration data is input into or generated by Landlab, and the model uses these parameters to calculate water depths and discharge at each time step, which drive channel erosion. For each precipitation event, the steady-state method outputs peak discharge and a single incision rate, while the hydrograph method outputs discharge and incision rate throughout a discharge event. Preliminary analysis suggests that, for a 90-minute storm across a 27-square kilometer watershed, the steady-state method overestimates peak discharge by an order of magnitude when compared to the hydrograph method. When compared to the hydrograph method of erosion calculations, the steady-state erosion method overestimated incision rate by three orders of magnitude. These results indicate that when calculating flow and erosion over longer time scales, the choice of flow routing and erosion method could affect long-term evolution of landscapes through differences in erosion rates. This work explores these two flow routing and erosion methods using different precipitation events (duration and intensity), as well as exploring landscape response across centennial and millennial time scales in an effort to understand the significance of flow routing methodologies in landscape evolution modeling.

Vanya Cherneva (ECE, LSU)

Distributed Algorithms for wireless networks

Our current work is directed towards channel models in which the channel feedback can indicate the number of writers to it. More specifically, we are considering channels that can provide this feedback fairly reliably for a small number of writers, but not so reliably for larger numbers. Our focus is on fast leader election or, more generally, ordering a subset of active users.Our approach is to trying to leverage the more detailed channel feedback to better estimate the number of writers, which, in turn, leads to a faster a randomized leader election algorithm.

An application of our research is in the coordination and scheduling of packets in wireless networks. The approaches we consider use a lean protocol (requiring each writer to write only one bit at a time). therefore, it may also prove useful a bridge across communication protocol, such as those needed across first responder agencies.

Farren Curtis (Physics , Tulane)

Many-Body Dispersion Interactions of Molecular Crystals

Polymorphism in molecular crystals is a physical phenomenon where crystals of the same molecular composition can have more than one form or crystalline structure. Different polymorphs of the same crystal may be close in energy but may possess vastly different physical properties. Understanding polymorphism in crystals is therefore crucial for a wide range of applications, from pharmaceuticals to organic solar cells.

Alanine is a chiral amino acid that may form enantiomeric (L-alanine) or racemic (DL-alanine) crystals. Depending on the method used, recent studies have shown conflicting results as to which form of alanine is more stable [1,2]. Density functional theory (DFT) with the many-body dispersion (MBD) [3] method has yielded highly accurate results for the structure and energetic of glycine polymorphs [4]. The present research aims to investigate the relative stability of racemic and chiral alanine using the revised

DFT+MBD method, which employs range-separation (rs) of the self-consistent screening (SCS) of polarizabilities and the calculation of the long-range correlation energy (MBD@rsSCS) [5]. Furthermore, this research investigates the role of many-body dispersion interactions in the elastic properties of L-alanine and DL-alanine.

Christina Hamlet (Mathematics, Tulane)

Sensory feedback in lamprey locomotion

The lamprey is considered a model organism for neurophysiology and locomotion studies. A 2D, integrative, multi-scale model of the lamprey's anguilliform (eel-like) swimming driven by neural activation and muscle kinematics coupled to body interactions with fluid surroundings and implemented using the immersed boundary method is presented. The effects of sensory feedback on muscle activation and swimming are examined.

Yue Hu (Center for Computation and Technology, LSU)

Model-Driven Auto-Tuning of Stencil Computations on GPU's

Stencil computations are a class of algorithms which perform nearest-neighbor computation, often on a multi-dimensional grid. This type of calculation forms the basis for computer simulations across almost every field of science. The increasing computational speed of graphics processing units (GPUs) make their use for stencil computations an interesting goal. However, achieving highly efficient implementations is often nontrivial, as numerous publications attest. In this work, we propose an analytic performance model for stencil codes on GPUs, which both delivers close-to optimal performance, but at the same time does not require extensive tuning at compile or run time. We evaluate the effectiveness of our performance model using different stencil benchmarks and with various stencil radii.

Sam Karhbet (Mathematics, University of Louisiana Lafayette)

Experimental study of approximate inverse preconditioners for symmetric indefinite matrices

We propose a new algorithm for the construction of approximate inverse preconditioners for a symmetric indefinite matrix A. The method is based on the idea of the Bunch-Kaufman LDL^* decomposition. It generates a matrix M such that $M^*AM \approx D$ where D is a block diagonal matrix with 1x1 or 2x2 blocks on the diagonal. The preconditioned operator is therefore $MD^{-1}M^*$. Drop tolerance is applied to control the density of M and the quality of the preconditioner. Numerical experiments are given to illustrate the efficiency of this approach.

Gerald Knapp (Mechanical Engineering, LSU)

Use of Provenance Data Management Systems for K-Edge Analysis of Flame Retardant X-Ray Tomography

The quantitative measurement of 3D elemental composition at near micron resolution is possible with K-edge X-ray tomography, however the workflow is extremely demanding when using conventional software resources, hence the motivation for a provenance data management system. Provenance systems have been used for multispectral 2D image processing; this is one of the first applications to 3D multispectral data.

K-edge X-ray tomography is based on the image contrast due to the energy-dependent X-ray absorption of the elements. At X-ray energies below a K-edge, the element is relatively transparent, but above the K-edge, the element is more opaque to X-rays. The K-edge is determined by the energy required to eject an electron from the element's 1s atomic orbital, ranging from 7.112 keV for Fe (Z=26) to 13.47 keV for Br (Z=35) to 30.49 keV for Sb (Z=51).

The data processing of the raw absorption data in Mathematica and MATLAB generates over 200 GB of data for eleven samples so the data provenance management system VisTrails, developed at New York University, is used to help manage the processing of the data. VisTrails allows for the storage of data processing history to observe what results were obtained by processing with varying parameters. Steps taken during processing are compiled into a single pipeline that is easily transferable, increasing the transparency and repeatability of data processing. Currently, both Mathematica and MATLAB code have been embedded in our workflow, and execute on an interactive HPC cluster Melete. The use of the workflow and data management system VisTrails to produce results X-ray tomography data should allow for shorter data processing time in future experiments and easier sharing of data within the tomography community.

Joe Knight (Physics, Tulane)

Benchmark of GW methods of electron acceptors

This work benchmarks the performance of methods based on many-body perturbation theory within the Green's function with screened Coulomb interaction (GW) approximation in calculating the electronic properties of 24 electron-accepting molecules. We test non-self-consistent GW (G_0W_0), using several mean-field starting points, as well as partially and fully self-consistent GW ($scGW_0$ and scGW). The results are compared to experiment and to results from coupled cluster singles, doubles, and perturbative triples (CCSD(T)) calculations. The G_0W_0 plus a second-order screened exchange (SOSEX) correction to the self-energy, and G_0W_0 based on an optimally tuned long-range corrected (LRC) hybrid functional perform best.

Sanjaya Lohani (Physics, Tulane)

Scaling of FHI-aims on Sphynx and Cypress

In the present work we demonstrate the scaling of FHI-aims on Tulane University's two Super Computers, Sphynx and Cypress, using the generalized gradient approximation technique of Perdew-Berke_Ernzerfof (PBE). We plotted CPU time for Single Self-Consistent Field (SCF) iteration as a function of the number of CPU cores. The benchmarking systems consisted of a broad range of molecular crystal (Glycin, Alanin and Paracetamol) and dye sensitized TiO2 clusters (Ti3INA3, Ti2cat2, and Ti17INA4). Benchmark results were obtained for up to 128 CPU cores on Sphynx and 240 CPU cores on Cypress. For large molecules on Sphynx, our experiments showed that computational speed was dependent upon choice of node. On both systems we observed linear scaling of iteration time as a function of the number of cores.

Forest Mannan (Mathematics, Tulane)

Singly-Periodic Stokes Flow with a Wall

A closed formula for the 2D singly-periodic laminar velocity field near a solid straight boundary is derived using the method of images. The flow is induced by regularized periodic forces. This result provides a model, for instance, for the modeling of cilia.

Zhuolin Qu (Mathematics, Tulane)

A Fast and Stable Explicit Operator Splitting Method for Phase-Field Models

Numerical simulations of the phase-field models require long time computations, and therefore it is necessary to apply stable large time-stepping methods. In this paper, we propose a fast explicit operator splitting method for both one- and two-dimensional nonlinear diffusion equations for thin film epitaxy with slope selection and Cahn-Hillard equation. The equations are split into the nonlinear and linear parts. The nonlinear part is solved using the method of lines approach together with an efficient large stability domain ODE solver. The linear part is solved by a pseudo-spectral method, which is based on the exact solution and thus has no stability restriction on the size of time step. We demonstrate the performance of the proposed method on a number of one- and two-dimensional numerical examples, where different stages of coarsening such as the initial preparation and the alternating rapid structural transition and slow motion can be clearly observed.

Owen Richfield (Mathematics, Tulane)

Cooperation and Efficiency in Sperm Motility Patterns

In order to fertilize the egg, sperm of certain species engage in co-operative swimming behaviors. These cooperative motility patterns result in differences in velocity and efficiency of swimming. In order to understand the empirical effects on the swimming of sperm as a result of various cooperative swimming behaviors, we employ a simple preferred curvature model for a single-flagellum or multi-flagellum system. Flagella are simulated using a two-dimensional mass-spring model, and regularized Stokeslets are employed to simulate the viscous environment these flagella swim through.

Zhongyi Sheng (Biomedical Engineering, Tulane)

Cell deformation in a cross-flow channel: integration of computational modeling with experiment

Using the three-dimensional computational algorithm for multiphase viscoelastic flow, this study focuses upon modeling the deformation of living cells in channels with a cross junction (cross-flow channel). Several flow conditions, channel configurations, and cells including cancer cells, leukocytes and red blood cells are investigated. This research is done in collaboration with Dr. Dino Di Carlo’s laboratory at UCLA, who has patented the use of a cross-flow channel for measurements of the deformability of living cells (cross-channel microfluidic flow cytometry). The goal of this study is to use our computational algorithm to extract the mechanical properties of the cells from the experimental data from Dr. Di Carlo’s laboratory. By doing so, we will be able to accurately measure, for example, differences in the mechanical properties of tumor cells with different metastatic potential or predict how the activation of leukocytes during inflammation changes their mechanical properties. Such measurements are very important for understanding of cancer metastasis and inflammatory disease development. The computational algorithm is the finite difference method for the solution of the Navier-Stokes equations and the Giesekus model for cell viscoelasticity, where the interfaces are tracked by the Volume of Fluid Method.

Xiaopeng Wang (Physics and Engineering Physics, Tulane)

Formation and Annealing behaviors of qubit centers in 4H-SiC from first principles

Inspired by finding that the nitrogen-vacancy center in diamond is a qubit candidate, similar defects in silicon carbide (SiC) have drawn considerable interest. However, the generation and annealing behaviors of these defects remain unclear. Using first-principles calculations, we describe their equilibrium concentrations and annealing mechanisms based on the diffusion of silicon vacancies. The formation energies and energy barriers along different migration paths, which are responsible for the formation rates, stability, and concentrations of these defects, are investigated. The effects of charge states, annealing temperature, and crystal orientation are also discussed. These theoretical results are expected to be useful in achieving controllable generation of these defects in experiments to advance the implementation of quantum computers.

Zhuo Wang (Center for Computation and Technology, LSU)

One Dimensional Prescribed Curvature Equation

In this talk we will present theoretical and numerical results for the Dirichlet boundary value problem of the one dimensional prescribed curvature equation.