Tenth Annual Front Range Applied Mathematics Student Conference March 1, 2014

Registration: 8:30 - 9:00

Morning Session I - Room NC1323 9:00 - 11:35

9:00 - 9:20	Thomas Cabell-Kluch Colorado School of Mines	Reconstruction of refractive index for a class of heterogeneous medium in atmospheric sciences
9:25 - 9:45	David Nieves University of Colorado, Boulder	Statistical classification of flow morphology in rapidly rotating Rayleigh-Benard convection
9:50 - 10:10	Tony E. Wong University of Colorado, Boulder	A model-based evaluation of the efficacy of evapotranspiration partitioning from stable water isotopes
10:10 - 10:25	15 Minute Break	
10:25 - 10:45	Brent Davis Colorado State University	New Computational Tools for Analyzing Models of Phylogenetic Trees
10:50 - 11:10	George Borleske Colorado State University	Comparing Roughness Metrics with Morphometric Roughness Lengths for a Snowpack Surface
11:15 - 11:35	Volodymyr Kondratenko University of Colorado, Denver	Assimilation of the fire perimeter data using the fire spread model SFIRE coupled with the WRF model

Morning Session II - Room NC1324 9:00 - 11:35

9:00 - 9:20	Deborah Shutt Colorado School of Mines	Models of in-host Population Dynamics of the HIV-1 Virus and $CD4^+T$ cells
9:25 - 9:45	Farrah Sadre-Marandi Colorado State University	Geometric Aspects of Viral Capsids
9:50 - 10:10	Inom Mirzaev University of Colorado, Boulder	Laplacian Dynamics of Biochemical Synthesis and Degradation
10:10 - 10:25	15 Minute Break	

10:25 - 10:45	Stephen Kissler University of Colorado, Boulder	Determination of personalized diabetes treatment plans using a two-delay model
10:50 - 11:10	Victoria Gershuny University of Colorado, Boulder	Changes in the lateral diffusion of surface molecules
11:15 - 11:35	Mike Mikucki Colorado State University	Modeling membrane dynamics with surface harmonics

Morning Session III - Room NC1325 9:00 - 11:35

9:00 - 9:20	Ruth A. Martin University of Colorado, Boulder	Three-wave resonant interactions
9:25 - 9:45	Ahmad Alyoubi Colorado School of Mines	Parallel-in-Time HPC Algorithms for Fractional Space-Time Models
9:50 - 10:10	Brad Dworzak Colorado School of Mines	A non-polynomial FEM for simulation of scattering from multiple particle configurations
10:10 - 10:25	15 Minute Break	
10:25 - 10:45	Justin Praast Colorado School of Mines	A finite-difference time-domain method for first-order Maxwell systems
10:50 - 11:10	Nathan D. Monnig University of Colorado, Boulder	Inverting Non-Linear Dimensionality Reduction with Scale-Free Radial Basis Interpolation
11:15 - 11:35	Bradley Martin University of Colorado, Boulder	Accurate seismic wave simulation through radial basis function-derived finite differences (RBF-FD): preliminary results from a new 3rd-order numerical method

Lunch: 11:45 - 12:25

Plenary Address: 12:30 - 1:30, Room NC1539

Dr. Stephan Sain, Computational and Information Systems Laboratory, Geophysical Statistics Program - NCAR, Boulder

Solving the Earth's Equations: Mathematics and Statistics at the National Center for Atmospheric Research

Group Photographs at 1:30

Afternoon Session I - Room NC1323 1:45 - 3:50

1:45 - 2:05	Melody Dodd Colorado State University	A fast implementation of the D-bar algorithm for electrical impedance tomography
2:10 - 2:30	Yan Chen University of Colorado, Boulder	Convergent Series Solution to 1D Schrodinger Equation
2:35 - 2:55	Tim Hodges Colorado State University	Computing Syzygies of Homogeneous Polynomials Using Linear Algebra
3:00 - 3:20	Rees McNally University of Colorado, Boulder	Gravity Gradiometry: A Novel Application for Compressed Sensing
3:25 - 3:45	Charles Morgenstern Colorado School of Mines	Coupled Finite and Boundary Element Methods for Wave Propagation in Inhomogeneous Media

Afternoon Session II - Room NC1324 1:45 - 3:50

1:45 - 2:05	Axel Brandt University of Colorado, Denver	Turan Numbers of Expanded Hypergraphs
2:10 - 2:30	Rachel Neville Colorado State University	A Pattern in Chaos: Persistent Homology of the Logistic Map
2:35 - 2:55	Warren M. Lord University of Colorado, Boulder	A singular value decomposition approach to connecting topology and dynamics on complex networks
3:00 - 3:20	Yogesh S. Virkar University of Colorado, Boulder	Hamiltonian Mean Field Model: Effect of network structure on synchronization dynamics
3:25 - 3:45	Tim Marrinan Colorado State University	Detecting Dampened Signals in Image Subspaces Using the Flag Mean

Afternoon Session III - Room NC1325 1:45 - 3:50

1:45 - 2:05	Prosper Torsu University of Wyoming	A Truncation Method for Elliptic Boundary Value Problems: An Application to Monte Carlo Simulations
2:10 - 2:30	Evan Kwiatkowski University of Colorado, Denver	Convergence of the Unbiased Square Root Kalman Filter in the Large Ensemble Limit
2:35 - 2:55	Jennifer Diemunsch University of Colorado, Denver	Robber Locating Strategy for Trees
3:00 - 3:20	V. Ganesh Karapakula Colorado College	Optimizing Class Schedules on the Block Plan
3:25 - 3:45	James Syme University of Colorado, Denver	A Mathematical Model of Political Borders

Plenary Speaker 12:30 - 1:30, NC1539

Solving the Earth's Equations: Mathematics and Statistics at the National Center for Atmospheric Research

Dr. Stephan Sain

Computational and Information Systems Laboratory, Geophysical Statistics Program NCAR, Boulder

The Institute for Mathematics Applied to Geosciences (IMAGe) plays an integral role in the scientific mission of the Computational and Information Systems Laboratory (CISL) at the National Center for Atmospheric Research (NCAR). IMAGe and CISL research activities support scientific computation, numerical methods, geophysical modeling, and the analysis of geophysical data and model experiments. In this talk, I will discuss a number of different mathematics and statistics projects from our research groups (e.g., computational mathematics, data assimilation, regional integrated science, and statistics) and show how this research enables and supports the scientific mission of the center.

About the Speaker

Stephan Sain is a Scientist with IMAGe at NCAR in Boulder, CO. He is also head of the Geophysical Statistics Project, one of five sections that comprise IMAGe. His research focuses on developing statistical methodology for analyzing the complex, multivariate data that arise in the atmospheric sciences, and, in particular, that capitalize on multicore or high performance computing environments to address big data challenges. Current work centers on the analysis of climate model ensembles, assessment of the impacts of climate change, and the design and analysis of computer experiments. This research brings together a broad range of statistical areas: spatial and spatial-temporal methods, hierarchical models, statistical computing, and extremes. Steve has been active in organizing conferences and workshops highlighting the connections between statistics, big data, and the geosciences, for example serving on the organizing committee for the 2012-13 Statistical and Applied Mathematical Sciences Institute (SAMSI) Program on Statistical and Computational Methodology for Massive Datasets and the organizing committee for the 2012 SIAM Conference on Uncertainty Quantification. Finally, Steve was recognized for his work at the intersection of statistics and the atmospheric sciences by receiving the ASA Section on Statistics Environment Distinguished Achievement Medal in 2012.

MORNING SESSION I

RECONSTRUCTION OF REFRACTIVE INDEX FOR A CLASS OF HETEROGENEOUS MEDIUM IN ATMOSPHERIC SCIENCES Thomas Cabell-Kluch Colorado School of Mines

The ability to accurately correct for the effects of strong atmospheric turbulence on light has been a major area of research in astronomy and adaptive optics. Atmospheric turbulence induces an optical region with inhomogeneous refractive index. This research's main focus is to efficiently reconstruct the refractive index using observed/simulated optical phase aberrations. A standard reconstruction method is based on the tomography associated with these aberrations. In this work, assuming the turbulent atmosphere is of Kolmogorov type, we extend the range of this reconstruction. We demonstrate the approach for simulated data from an astronomy model.

STATISTICAL CLASSIFICATION OF FLOW MORPHOLOGY IN RAPIDLY ROTATING RAYLEIGH-BÉNARD CONVECTION David Nieves Collaborators: Antonio Rubio and Keith Julien University of Colorado, Boulder

In rapidly rotating convection four flow regimes with distinct characteristics have been identified as a function of the asymptotically reduced Rayleigh number $RaE^{4/3}$ (where E is the non-dimensional Ekman number) and Prandtl number σ . In each regime the flow organizes, with varying intensity, into coherent vertical structures. The identified morphologies, in order of increasing $RaE^{4/3}$, consist of the cellular regime, the convective Taylor column (CTC) regime, the plume regime, and a regime characterized by geostrophic turbulence. We use experimentally accessible statistical measures to distinguish between flow morphologies in rapidly rotating Rayleigh-Bénard convection (RRBC). Namely, the utilization of auto- and cross-correlations of

temporal and spatial signals that synthesize experimental data obtained form thermistor measurements or particle image velocimetry (PIV). We show how these statistics can be employed for laboratory experiments to (i) identify transitions in the flow morphology, (ii) capture the radial profiles of coherent structures, and (iii) extract transport properties of these structures.

A MODEL-BASED EVALUATION OF THE EFFICACY OF EVAPOTRANSPIRATION PARTITIONING FROM STABLE WATER ISOTOPES Tony E. Wong¹ Collaborators: Max Berkelhammer² and David Noone¹ University of Colorado, Boulder¹ University of Illinois²

The partitioning of evapotranspiration (ET) into ground evaporation and plant transpiration in land surface models is crucial for understanding the surface energy balance and a key feature of any hydrological scheme, but notoriously difficult to resolve. We present results for the partitioning of ET from an isotopically-enabled land surface model (ISOLSM), driven by data collected at the Manitou Experimental Forest during the summer and autumn of 2011. From an ensemble of 18341 simulations, 219 produced physically plausible realizations. Even when three flux constraints are met, the transpiration fraction is not well-constrained and the estimate of ET partitioning from isotopic data does not adequately represent the modeled partitioning. The ensemble mean partitioning is $F_T=49\%$ (max. 73, min. 19%), whereas the isotope ratios of $H_2^{18}O$ and HDO yielded an estimate of 56% (max. 69, min. 50%). We find that while the simple isotopic budget method produces ET partitioning results with significant errors, relative humidity is the strongest driver of this estimate of transpiration fraction. These model experiments show that previous work using isotopic observations to partition ET likely have significant uncertainty in their estimates. While the isotopic method for ET partitioning has shortcomings, we find strong correlation between transpiration fraction

and surface and soil water isotope ratios, showing that soil water isotopic information holds the most promise for further constraining ecosystem process models.

NEW COMPUTATIONAL TOOLS FOR ANALYZING MODELS OF PHYLOGENETIC TREES Brent Davis¹ Collaborator: Joseph Rusinko² Colorado State University¹ Winthrop University²

Computational Phylogenetics studies computational methods to analyze and construct phylogenetic (evolutionary) trees. The larger goal may be to construct the tree of life or find better treatments for diseases from gene sequence databases. Given a finite collection of unrooted evolutionary tree of modest size, we develop and implement a euclidean distance-based criterion, based on the methods of numerical algebraic geometry, to accept or reject statistical models from simulated data and, in addition, approximate the evolutionary rates or tree lengths.

COMPARING ROUGHNESS METRICS WITH MORPHOMETRIC ROUGHNESS LENGTHS FOR A SNOWPACK SURFACE George Borleske Collaborators: Iuliana Oprea, Steven R. Fassnacht and David Kamin Colorado State University

The snow surface is the interface between the atmosphere and the earth. It is very dynamic, and varies spatially and temporally. Its roughness influences turbulence and is used to estimate the sensible and latent heat fluxes to and/or from the snow surface to the atmosphere. We use airborne lidar-derived snow surface measurements from the NASA Cold Land Process Experiment Fraser Alpine intensive study area collected in March 2003. Meteorological data were used to determine the dominant wind direction. The raw surface elevation data were rotated to yield a 100 by 100m, that was square (parallel/perpendicular) to the wind. The data were interpolated to a 1-m resolution. Roughness metrics, including the random roughness, autocorrelation, and fractal dimension were computed, and compared to the geometric-based roughness (z0).

ASSIMILATION OF THE FIRE PERIMETER DATA USING THE FIRE SPREAD MODEL SFIRE COUPLED WITH THE WRF MODEL Volodymyr Kondratenko Collaborators: Jan Mandel and Adam Kochanski University of Colorado, Denver

Fire simulation starts from an ignition point, and when fire perimeter data are assimilated, the state of the fire spread model is changed to become closer to the data. This, however, presents a difficulty in coupled fire-atmosphere The fire has a very strong effect on models. the atmosphere and changes in atmospheric state due to the fire take time to develop, so the existing atmospheric circulation is no longer compatible with the modified fire. Moreover, linearized changes to the atmospheric state have no hope of establishing the properly changed circulation in a physical balance. We have recently developed a technique for fire ignition from perimeter data, which goes back in time and replays an approximate fire history to allow the proper atmospheric circulation patterns to develop. Here, we extend this technique to the assimilation of a fire perimeter into a developed fire state with an established atmospheric state. The SFIRE model uses the level set method to simulate the fire spread. Our data assimilation approach takes advantage of the manipulation of the fire state through level set functions, which is much easier than manipulating the fire areas directly. The new method is applied to a real fire case study.

MORNING SESSION II

MODELS OF IN-HOST POPULATION DYNAMICS OF THE HIV-1 VIRUS AND CD4⁺T CELLS Deborah Shutt Colorado School of Mines

We will describe and analyze a mathematical model capable of predicting the time course of HIV infection within the human body. Upon entering a host, HIV infects CD4⁺T cells, a key component of the immune system, in order to replicate. Thus, the virus will inhibit the immunological function of the T cell. During the replication process, mistakes can occur and a new mutated strain of HIV can develop. This mutated strain will then posses a new structure which may allow it to escape the body's immune response or resist the effects of anti-retroviral drugs. Uninfected CD4⁺T cells are left to work against the infection but the presence of HIV in the body will eventually lead to a depletion of these cells and finally the development of Acquired Immune Deficiency Syndrome (AIDS). Using biological data such as infection rates, production rates of virions from infected T-cells, and mutation rates, we construct a model which examines the in-host population dynamics of the virus. The result is a nonlinear seven component ODE model and we examine the qualitative behavior of the various populations through mathematical analysis and computational approximations.

GEOMETRIC ASPECTS OF VIRAL CAPSIDS Farrah Sadre-Marandi Colorado State University

The assembly of proteins on a virus shell, called the capsid, are marvels of molecular architecture. We can observe symmetry at various levels and the important roles of hexagons and pentagons in viral capsid structures. This talk starts from icosahedral virus but focuses on the features of the HIV-1 conical core. We examine the critical role of pentamers in the HIV-1 core and present noval results of curvature calculations.

LAPLACIAN DYNAMICS OF BIOCHEMICAL SYNTHESIS AND DEGRADATION Inom Mirzaev University of Colorado, Boulder

In recent years, many researchers have devoted their efforts to developing a systems-level understanding of biochemical reaction networks. In particular, the study of these chemical reaction networks (CRNs) using their associated graph structure has attracted considerable attention. In our previous work, we have developed a framework for finding steady states of a biochemical reactions. Specifically, we associated each biochemical network with a labeled, directed graph, G, and with the corresponding Laplacian matrix. If there is an edge from vertex j to vertex i, we label it with $e_{ij} > 0$, and with $e_{ij} = 0$ if there is no such edge. The Laplacian matrix of given digraph G is then defined as

$$(\mathcal{L}(G))_{ij} = \begin{cases} e_{ij} & \text{if } i \neq j \\ -\sum_{m \neq j} e_{mj} & \text{if } i = j \end{cases}$$

The corresponding Laplacian dynamics are then defined as

$$\frac{dx}{dt} = \mathcal{L}(G)x,$$

where $\mathcal{L}(G)$ is Laplacian matrix of G,

 $\mathbf{x} = (x_1(t), \dots, x_n(t))^T$ is column vector of concentrations at each vertex, $1, \dots, n$. For Laplacian dynamics we have shown that, for any graph and any initial condition, the dynamics always reaches a steady state which can be algorithmically calculated.

Here we investigate behaviors of Laplacian dynamics when synthesis and degradation are added to the system. We consider additional edges to the core digraph, G,

$$\stackrel{s_i}{\rightarrow} i \text{ or } i \stackrel{d_i}{\rightarrow}$$

corresponding to zero-order synthesis or first-order degradation, respectively. Each vertex can have any combination of synthesis and degradation edges. The dynamics can now be described by the following system of linear ordinary differential equations (ODEs):

$$\frac{d\mathbf{x}}{dt} = \mathcal{L}(G)\mathbf{x} - D\mathbf{x} + S$$

where D is diagonal matrix with degradation edges, and S is column matrix with synthesis edges. We provide necessary and sufficient conditions for the system to possess non-negative, stable, steady state solution. As in the case of Laplacian dynamics, we again provide an algorithm for finding steady state solutions using underlying digraph structure. The algorithm utilizes the Matrix-Tree Theorem (also known as Kirchhoff's theorem) to construct steady state solutions using the underlying digraph structure. To illustrate our results, we apply the algorithm to a kinetic model for insulin metabolism and secretion in pancreatic β -cells. Finally, we conclude with a discussion of the implications of these results.

DETERMINATION OF PERSONALIZED DIABETES TREATMENT PLANS USING A TWO-DELAY MODEL Stephen Kissler Collaborators: C. Cichowitz, S. Sankaranarayanan and D.M. Bortz University of Colorado, Boulder

Diabetes cases worldwide have risen steadily over the past decades, lending urgency to the search for more efficient, effective, and personalized ways to treat the disease. Current treatment strategies, however, may fail to maintain ultradian oscillations in blood glucose concentration, an important element of a healthy alimentary system. Building upon recent successes in mathematical modeling of the human glucoseinsulin system, we show that both food intake and insulin therapy demand increasingly precise control over insulin sensitivity if oscillations at a healthy average glucose concentration are to be maintained. We then suggest guidelines for how a clinician can develop personalized treatment options for diabetic patients that maintain these oscillations. Lastly, we note that all suggested strategies rely on existing clinical techniques and established treatment measures, and so could potentially be of immediate use in the design of an artificial pancreas.

CHANGES IN THE LATERAL DIFFUSION OF SURFACE MOLECULES Victoria Gershuny University of Colorado, Boulder

In this research, the lateral diffusion of molecules in the cell membrane is studied with the goal of being able to detect lipid-protein interactions on the cell surface. Protein-lipid binding changes the overall mass of the lipid structure and thus the rate at which particles laterally diffuse along the membrane. We model the diffusion of the lipids using a discrete-time stochastic process and the change in mass by changes in the rate of diffusion. Then, through the fitting of lipid trajectories using Rayleigh and Gaussian probability distributions, it is possible to detect five-fold, three-fold, and even two-fold changes in the rate of diffusion.

MODELING MEMBRANE DYNAMICS WITH SURFACE HARMONICS Mike Mikucki Colorado State University

Lipid membranes appear in every known form of life. The shape and deformation of lipid membranes play a critical role in many cellular processes, including ion transport, budding, binding, fusion, endocytosis, exocytosis, etc. The fluid-like properties of the membrane allow it to undergo large deformations, producing both axisymmetric shapes, such as the shape of red blood cells, and non-axisymmetric shapes, such as the tubules of the endoplasmic reticulum. Deriving and solving a mathematical model of membrane mechanics that can account for large deformations is important to understanding these processes better. From first principles in thermodynamics, equilibrium conformations of the membrane are determined by minimizing the total mechanical energy of the membrane. Solutions to this energy minimization problem have been obtained in various ways. Solving the Euler-Lagrange equations directly over the entire membrane surface has yielded only axisymmetric conformations. For nonaxisymmetric conformations, the solution can be found by minimizing the energy over a smaller subspace. A triangulated approximation of the membrane surface, as used by finite element methods, can be computationally costly, since it requires the minimization at thousands of triangular vertices. In this presentation, surface harmonics are used to parameterize the membrane surface, drastically reducing the degrees of freedom to less than 100 modes. Some equilibrium shapes will be presented, including conformations exhibited by red blood cells and conformations which are non-axisymmetric. Finally, the numerical results are verified against previous work from the literature.

MORNING SESSION III

THREE-WAVE RESONANT Ruth A. Martin University of Colorado, Boulder

The resonant interaction of three wavetrains is one of the simplest forms of nonlinear interaction for dispersive waves of small amplitude. This behavior arises frequently in applications ranging from nonlinear optics to internal waves through the study of the weakly nonlinear limit of a dispersive system. The slowly varying amplitudes of the three waves satisfy a set of coupled, nonlinear PDEs known as the three-wave equations. These equations were shown to be completely integrable by Zakharov & Manakov (1973), and solutions for the problem with spatially localized wave packets were given by Zakharov & Manakov (1976), Kaup (1976), and others. Numerical simulations of the three wave resonance problem typically impose periodic boundary conditions, although the known methods of analytic solution fail in this case. We present an alternative way to study this problem. In particular, we consider a convergent Laurent series solution (in time), which contains five real-valued functions (in space). These functions must satisfy some differentiability constraints, but are

otherwise arbitrary; as a result, our method allows for any type of boundary conditions and for any number of spatial dimensions. A general solution of the problem would involve six such functions, so our current work stops just short of a general solution.

PARALLEL-IN-TIME HPC ALGORITHMS FOR FRACTIONAL SPACE-TIME MODELS Ahmad Alyoubi Colorado School of Mines

Space-time models that require long-time simulation and resolving fine structures occur in many physical processes. Classical Brownian motion based standard modeling techniques lead to integer derivatives in the time variable. Consequently, one obtains classical parabolic diffusion or wave partial differential equations (PDEs) modeling various quantities of interest (QoI). However, some class of processes in biological applications are best modeled using anomalous subdiffusion and in viscoelastic applications as fractional wave equations. These can be represented using fractional time derivatives. Fractional derivative PDEs (FPDEs) are a generalization of the classical PDE models and such models are well known in the literature. In this talk, we discuss and demonstrate efficient parallel-in-time algorithms for long-time simulation for a class of FPDEs with millions of spatial degrees of freedom to resolve multiscale structures in the model.

A NON-POLYNOMIAL FEM FOR SIMULATION OF SCATTERING FROM MULTIPLE PARTICLE CONFIGURATIONS Brad Dworzak Colorado School of Mines

In this presentation we consider an efficient simulation of scattering quantities of interest (such as far-field pattern) from a class of two dimensional acoustic configurations comprising several smooth and non-smooth particles with random attributes. The random aspect includes the location, material properties, shape, and size of particles in the configuration. The main focus of this preliminary research is on efficient and accurate simulation of large number of realizations of the model arising from sampling of the random attributes. In particular, we apply a high-order non-polynomial finite element method (FEM) for each realization. We demonstrate the approach for a class of model configurations.

A FINITE-DIFFERENCE TIME-DOMAIN METHOD FOR FIRST ORDER MAXWELL SYSTEMS Justin Praast Colorado School of Mines

We consider a finite-difference method in space and time for efficiently simulating non-timeharmonic first-order Maxwell systems in \mathbb{R}^n , n =1,2,3. An industrial standard approach to approximate the time-dependent system for unknown electric and magnetic fields is the explicit finitedifference time-domain (FDTD) method on the Yee cell grid. The Yell cell facilitates the expression of essential physical relationships of electromagnetic fields and the approach is based on the idea of staggered grid evaluation.

In this presentation, we discuss the Yee cell based algorithm, its stability constraints given by the CFL condition, dispersion and dissipation relations and its relation to the CFL condition, material boundary conditions, and artificial domain boundary conditions. We demonstrate preliminary FDTD simulation results of a monochromatic and a broadband pulse input in one and two dimensions and consider a parallel computing implementation of the FDTD algorithm.

INVERTING NON-LINEAR DIMENSIONALITY REDUCTION WITH SCALE-FREE RADIAL BASIS FUNCTIONS Nathan D. Monnig University of Colorado, Boulder

A numerical method is proposed to approximate the inverse of a general bi-Lipschitz nonlinear dimensionality reduction mapping, where the forward and consequently the inverse mappings are only explicitly defined on a discrete dataset. A radial basis function (RBF) interpolant is used to independently interpolate each component of the high-dimensional representation of the data as a function of its low-dimensional representation. The scale-free cubic RBF kernel is shown to perform better than the Gaussian kernel, as it does not require the difficult-to-choose scale parameter as an input, and does not suffer from ill-conditioning.

ACCURATE SEISMIC WAVE SIMULATION THROUGH RADIAL BASIS FUNCTION-DERIVED FINITE DIFFERENCES (RBF-FD): PRELIMINARY RESULTS FROM A NEW 3RD-ORDER NUMERICAL METHOD Bradley Martin University of Colorado, Boulder

Numerically solving hyperbolic partial differential equations (PDEs) within domains featuring discontinuous PDE parameters is an important process in a number of scientific fields. Here, we discuss a new RBF-FD-based approach to accurately simulate elastic waves in 2D. Finite difference weights are constructed using a traditional RBF basis (continuous across interfaces) along with specially modified support polynomials (possibly kinked and even discontinuous across the interface). The combined RBF and polynomial bases are designed to enforce physically correct continuity conditions across the interface. Convergence of the method currently appears to be 3rd-order which agrees with heuristics on how the implementation was designed but near-future refinements may allow a straightforward extension to a higher order of accuracy (depending on stability issues).

AFTERNOON SESSION I

A FAST IMPLEMENTATION OF THE D-BAR ALGORITHM FOR ELECTRICAL IMPEDANCE TOMOGRAPHY Melody Dodd Colorado State University

Electrical impedance tomography is an imaging technique in which applied boundary currents and resulting boundary voltages are used to reconstruct the conductivity distribution within a body. D-bar methods are a class of direct (noniterative) reconstruction algorithms that make use of complex geometrical optics (CGO) solutions to PDEs known as D-bar, or $\bar{\partial}$, equations. D-bar equations are of the form $\bar{\partial} u = f$, where f may depend on u, and the $\bar{\partial}$ operator is defined by $\partial = 0.5 (\partial_x + i \partial_y)$. The common threads in these methods are (1) a direct relationship between the CGO solutions and the unknown conductivity, (2) a nonlinear Fourier transform, also known as the scattering transform, providing a link between the data and the CGO solution, and (3) a D-bar equation to be solved for the CGO solutions with respect to a complex-frequency variable.

CONVERGENT SERIES SOLUTION TO 1D SCHRODINGER EQUATION Yan Chen University of Colorado, Boulder

The N^{th} partial sum of an infinite power series has the form $\sum_{n=1}^{N} c_n x^n$, where x is a parameter and $\{c_n\}$ are known numbers. The infinite series is *convergent* if this sum has a finite limit as $N \to \infty$, with x fixed. The series is *asymptotic* if the error incurred by truncating the series after N terms is $O(x^{-(N+1)})$ as $x \to 0$. The two concepts, which involve two different limits, are independent - a given series might have both properties, or one, or neither.

Divergent asymptotic series can be quite useful: the well known formula of Stirling (1730) for $\ln(m!)$ for large m is a divergent series (in powers of $\frac{1}{m}$) for all finite m, but Stirling calculated $\log_{10}(1000!)$ to ten decimal places using only a few terms in his series. (see Copson, 1967).

Divergent asymptotic series are most useful when the parameter x is small but not zero. In this situation, with x fixed, one finds that the error gets smaller as one keeps more terms in the series until a specific point, after which the error begins to grow. In this way, a divergent asymptotic series can approximate a function for small, fixed x up to some optimal accuracy, but no better. Dingle (1973) began development of a method to create a follow-on series, which begins at the point of optimal accuracy of the original series, and can be used to improve the accuracy further, but again with a minimal error that cannot be reduced by further use of the two series. Berry & Howls (1990) developed Dingle's idea further, using a sequence of divergent series, with each series improving on the accuracy of the preceding one. Again, they eventually came to a (much smaller) minimal error that they could not reduce. They named this sequence of increasingly accurate asymptotic series hyperasymptotics. They demonstrated their approach by developing hyperasymptotic series, valid for large positive z, for the Airy function, Ai(z), and showed that they could evaluate Ai(z)with 20 decimal places of accuracy, even down to z = 5.241.

COMPUTING SYZYGIES OF HOMOGENEOUS POLYNOMIALS USING LINEAR ALGEBRA Tim Hodges Colorado State University

Polyonomial systems arise in science and engineering frequently. Using Algebraic Geometry we can solve these polynomial systems and find relations for the polynomials. In particular, given a ideal generated by polynomials $f_1, ..., f_n$ in $\mathbb{C}[x_1, ..., x_m]$ a syzygy is a n-tuple $(\alpha_1, ..., \alpha_n)$, $\alpha_i \in \mathbb{C}[x_1, ..., x_m]$ such that $\sum_{i=1}^n \alpha_i \cdot f_i = 0$. That is, that a syzygy has the orthogonality property with the generating set for the ideal. Syzygies can be computed by Buchberger's algorithm for computing Gröbner Bases. Unfortunately with time Gröbner bases have been computationally impractical as the number of variables and number of polynomials increase. The aim of this research is to give a way to compute syzygies without the need for Gröbner bases and possibly still give the same information as Gröbner bases. The approach is to use the monomial structure of each polynomial in our generating set to build syzygies using nullspace computations.

GRAVITY GRADIOMETRY: A NOVEL APPLICATION FOR COMPRESSED SENSING

Rees McNally¹ Collaborators: Stephen Libby² and David Chambers² University of Colorado, Boulder¹ Lawrence Livermore National Lab²

During the past decade, compressed sensing (CS) has proven to be extremely useful for sparse signal reconstruction. For this work the method of CS is applied to fast mass distribution determination based on cold atom gravity gradiometer measurements. Specifically we consider an array of M gradiometers placed around a 2D target area in order to determine the interior mass distribution in cases where the set of (M) sensor measurements undersamples the distribution. This was done by assuming that the system's sparsity comes from the mass distributions only having K non-zero masses, which led to a non-orthogonal basis dictionary. This lack of orthogonality caused interesting behaviors, including weakened noise performance, and breaking of the typical CS motivated logarithmic scaling of required M values for larger K values. However, for low K values M scaled as expected. Modifications to the gravity sensor model to promote orthogonality and test its impact on signal recovery postponed the onset of anomalous scaling, suggesting that lack of orthogonality is the primary cause. While CS works for this sparse, but intrinsically ill-posed problem, this sensor system displayed increased noise sensitivity and a smaller upper bound on the size of recoverable K sets. However, while these limitations decrease CS performance, significant improvements over traditional sensing approaches are still possible.

COUPLED FINITE AND BOUNDARY ELEMENT METHODS FOR WAVE PROPAGATION IN INHOMOGENEOUS MEDIA Charles Morgenstern Colorado School of Mines

This research is concerned with simulation of time-harmonic acoustic wave propagation exterior to and interior of a bounded inhomogeneous configuration in \mathbb{R}^n , n = 2, 3. Standard numerical approaches for simulation of mathematical models are finite element or boundary element methods.

Finite element methods (FEMs) are well suited for general shape inhomogeneous media. However, FEMs require bounded regions for triangulation of the media. Hence, for a wave propagation model described in unbounded media, standard FEMs require artificial truncation of the unbounded region. Further the truncation requires approximation of the radiation condition.

Boundary element methods (BEMs) do not require such artificial truncations, and the BEM solution ansatz automatically satisfies the radiation condition in the model. However, BEMs require the fundamental solution of the wave propagation models, and hence BEMs are restricted to constant coefficient, homogenous media, models.

In this work, for simulation of wave propagation in the inhomogeneous media, we get the best of both FEM and BEM worlds by combining a low-order FEM with a high-order BEM. This is achieved through an unknown function that couples the interior FEM and exterior BEM solutions. We demonstrate the approach and its parallel performance for a class of two dimensional smooth and non-smooth configurations.

AFTERNOON SESSION

TURAN NUMBERS OF EXPANDED HYPERGRAPHS Axel Brandt¹ Collaborator: Tao Jiang² University of Colorado, Denver¹ Miami University²

A graph G is defined as a set of vertices and a set of edges, which are pairs of vertices. A classic problem in extremal graph theory is the forbidden subgraph question: for a given graph F, what is the maximum number of edges that can be arranged on n vertices without creating a copy of F? This maximum number of edges is called the Turán number and is known for graphs.

A hypergraph H is defined as a set of vertices and a set of edges, which are subsets of the vertex set. Finding the Turán number for hypergraphs has proven to be a notoriously difficult problem. For example, although the Turán number for complete graphs (graphs in which all edges appear) has been known since 1941, the Turán number is not known for the complete hypergraph on four vertices with edges of size three.

This talk will present recent progress in this area and discuss the challenges of extending proof techniques from graphs to hypergraphs.

A PATTERN IN CHAOS: PERSISTENT HOMOLOGY OF THE LOGISTIC MAP Rachel Neville Colorado State University

Given a discrete sampling of points, how can one reconstruct the underlying geometric object? Further, the question arises how can one discern between noise and sampling distortion and important topological features. In recent years, persistent homology had been explored as a computational way to capture information regarding the longevity of topological features of discrete data sets. In this project, the persistent homology of functions is explored specifically as a way of examining features of functions. Persistent homology tracks the longevity of connected components of level sets in a persistence diagram. By connecting points generated by a discrete time dynamical system with line segments, this data can be viewed as a (piecewise linear) function, persistent homology is used to track features of the data. This provides a novel and interesting tool for computationally examining dynamical systems.

The logistic map is one of the simplest examples of a nonlinear map that displays periodic behavior for some parameter values, but for others, displays chaotic behavior. When the persistence diagram is generated for an orbit of the logistic map, all of the points surprisingly lie approximately on a line. This is not true for a general sequence. This pattern arises not only after stability has been reached in the periodic case, but also as points approach stability for parameters in the periodic regime but also perhaps more surprisingly, for parameter values that lie in the chaotic regime as well. In fact, the slope of this line is fairly similar as the parameter values are varied. This arises from the order in which the points pair to form the persistence diagram and a scaling factor seen in the periodic regime of a class of maps (including the logistic map). It is interesting that the effects of this scaling are still seen in the chaotic regime. This pattern not only arises for the logistic map, but for other unimodal maps and other higher dimensional systems that are "close" to these maps such as the Lorenz system.

A SINGULAR VALUE DECOMPOSITION APPROACH TO CONNECTING TOPOLOGY AND DYNAMICS ON COMPLEX NETWORKS Warren M. Lord Collaborator: Juan G. Restrepo University of Colorado, Boulder

Researchers in many scientific disciplines are interested in how network topology influences dynamics that occur on networks. The largest eigenvalue of the adjacency matrix of a network is a topological description that has proven useful in describing dynamics. Largest eigenvalue methods work well for a wide variety of degree distributions on random networks, but do not perform as well when structures that are common to real world networks, such as communities, are introduced. Motivated by the fact that truncated singular value decompositions often capture the essential structure of complicated matrices, we combine previous approaches based on the largest eigenvalue with the more detailed description of the network topology given by the singular value decomposition of the adjacency matrix. This approach captures the essential aspects of very high dimensional network dynamics with a low dimensional system. We use this method to predict steady states of both networks of oscillators in continuous time and networks of excitable elements in discrete time, and to predict the rate of convergence to steady state in networks of oscillators. The predictions are tested on both random networks and networks derived from real world datasets.

HAMILTONIAN MEAN FIELD MODEL: EFFECT OF NETWORK STRUCTURE ON SYNCHRONIZATION DYNAMICS Yogesh S. Virkar Collaborators: Juan G. Restrepo and James D. Meiss University of Colorado, Boulder

In the past, synchronization processes have been the focus of immense research in many diverse fields such as physics, biology, chemistry, social science, etc. Examples include simple pendulums suspended from a common beam locking to a common frequency, epileptic seizures in the brain, the mutual synchronization of menstrual cycles in groups of women, swarms of fireflies flashing synchronously, and the chirping of crickets in unison. Efforts have been made to quantify these processes using simple mathematical models.

One of the earliest models was the Kuramoto model that provided a link between synchronization dynamics and phase transitions. In its simplest form, each oscillator interacts with every other oscillator with equal coupling strength and this interaction depends sinusoidally on the phase difference between the two oscillators. A phase transition occurs from the incoherent to the coherent state at a critical value of the coupling strength. In the more general case, this model can be put on a network where each oscillator is a node and coupling depends on the adjacency matrix. Hence, the phase transition now depends on the structural properties of the network. More recently, analyzing such synchronization dynamics as a function of network structure has gained significant attention.

A similar model which has been less studied is the Hamiltonian Mean Field (HMF) model, a version of the Kuramoto model that conserves energy. We study the HMF model on different types of network structures. Preliminary results for the Erdös-Renyi network indicate that the critical coupling constant K_c is inversely proportional to the principal eigenvalue λ of the adjacency matrix.

DETECTING DAMPENED SIGNALS IN IMAGE SUBSPACES USING THE FLAG MEAN Tim Marrinan Colorado State University

Given a finite set of linear subspaces perhaps of differing dimensions, we describe a flag of vector spaces (i.e. a nested sequence of vector spaces) that best represents the collection based on a natural optimization criterion and we present an algorithm for its computation. The utility of this flag representation lies in its ability to represent subspaces of differing dimensions, and in the ordering of the nested subspaces it contains. As the output subspaces are arranged from best fit to worst, it is possible to observe weak signals common to the collection of input subspaces that may be washed out by noise in other representations.

There are numerous ways to describe sets of images in terms of linear subspaces. These representations naturally lend themselves to analysis on Grassmann manifolds. Depending on how the subspaces are chosen, the data may live on a collection of Grassmannians rather than a single one. The flag representation that we describe allows subspaces of different dimensions to be represented with a single geometric object, and forces common information to the front of the flag. This property acts like a subspace median, and can be beneficial for identifying weak or dampened signals common to the the collections of images. We present preliminary results on how these image signals can be detected and classified using a flag representation for a collection of these subspaces.

AFTERNOON SESSION

A TRUNCATION METHOD FOR ELLIPTIC BOUNDARY VALUE PROBLEMS: AN APPLICATION TO MONTE CARLO SIMULATIONS Prosper Torsu University of Wyoming

Truncation methods have been used widely to estimate solutions of complicated mathematical problems. One particular type that has been implemented represents the elliptic coefficient as an infinite series of some bounded function. The approximate solution is represented as a truncation of an infinite series. The structure of the method is such that these solutions are obtained successively. They are then summed up to approximate the true solution. A consequence of this method is that a higher-order solution depends on all lower-order ones. Hence, creating data for a fixed higher-order problem forces us to invert a system as many times as the order of the problem.

In this study, we propose a alternative method that minimizes the computational burden. The most important advantage of the proposed method is that irrespective of the order of approximation, we only need to invert the system twice making the whole calculation much more efficient. A convergence analysis of the perturbation method will be given.

The proposed method is directly applicable in the framework Monte-Carlo simulation. Monte-Carlo simulation can be very expensive especially when the coefficients relatively complicated. With the proposed method, the system inversion is

very much minimized thereby making the simulation more efficient. The performance of the method within the Monte-Carlo simulation will be shown, in particular as it compares to traditional Monte-Carlo simulation.

CONVERGENCE OF THE UNBIASED SQUARE ROOT KALMAN FILTER IN THE LARGE ENSEMBLE LIMIT Evan Kwiatkowski Collaborator: Jan Mandel University of Colorado, Denver

Ensemble filters implement sequential Bayesian estimation by representing the probability distribution by an ensemble mean and covariance. Unbiased square root ensemble filters use deterministic algorithms to produce an analysis (posterior) ensemble with prescribed mean and covariance, consistent with the Kalman update. This includes several filters used in practice, such as the Ensemble Transform Kalman Filter (ETKF), the Ensemble Adjustment Kalman Filter (EAKF), and a filter by Whitaker and Hamill. We show that at every time index, as the number of ensemble members increases to infinity, the mean and covariance of an unbiased ensemble square root filter converge to those of the Kalman filter, in the case a linear model and an initial distribution of which all moments exist. The convergence is in L^p and the convergence rate does not depend on the model dimension.

ROBBER LOCATING STRATEGY FOR TREES Jennifer Diemunsch Collaborators: Axel Brandt, Catherine Erbes and Casey Moffatt University of Colorado, Denver

We consider the robber locating game introduced by Seager, a variation of the classic cops and robbers game. This is a turn-based game between a cop and robber, played on a graph G. The robber starts at any vertex in G, and may move to a vertex neighboring his current position on his turn. The cop meanwhile knows the graph, but does not know where the robber is located; instead the cop probes any vertex of G on her turn, and is told the distance to the robber. The cop wins when she can determine the location of the robber, and the robber wins if the cop can never determine the robber's location. This talk discusses an algorithm that meets the known bound for the number of turns needed to locate a robber on a tree.

OPTIMIZING CLASS SCHEDULES ON THE BLOCK PLAN V. Ganesh Karapakula Colorado College

Colorado College operates on the Block Plan, which is an academic schedule consisting of eight blocks per academic year. A block lasts for three and a half weeks; the students take one class at a time every block. Every academic department at the college makes an annual schedule of classes under various department-wide and

professor-specific constraints. Department-wide constraints include limitations on the conjunction of some courses and on the number and the timings of offerings of each kind of course. Professor-specific constraints include restrictions on the number and the sorts of courses and the blocks in which a professor can teach. Literature dealing with optimization of class schedules does not adequately consider Block Plan-type systems. This talk tackles optimization of class schedules in settings such as the Block Plan using binary integer linear programming; solutions to similar optimization problems will also be explored in this talk.

A MATHEMATICAL MODEL OF POLITICAL BORDERS James Syme University of Colorado, Denver

Cities and metropolitan areas act as the centers of national cultural, linguistic, governmental, and economic exchange, while also acting as portals for international immigration and foreign relations. I hypothesize that, due to relative cultural dispersion from city centers, preeminent world and primate cities can act as generating nodes for the geographic expanse of nation states. I present a 3 phase model of the geographic territorial expanse of nation states: (1) use bounded Voronoi tessellations generated with longitude/latitude coordinates of cities as central nodes to create regions of urban influence (RUIs); (2) generate countries using RUIs, an alliance matrix, and simulated border segments; and (3) use dynamics to update the alliance matrix and generate new states. A dynamical model is presented to demonstrate the ability of the model with the intent of encouraging social scientists to apply their own models.