FIELDS

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AARMS

THE 2015 BLUENOSE APPLIED & COMPUTATIONAL MATH DAYS *Workshop*

JULY 11 - 12, 2015

<u>The 2015 Bluenose Applied and Computational Math Days Workshop (July 11-12) is being held in association with the 2015 International Federation for Information Processing (IFIP) Working Group 2.5 on Numerical Software meeting (July 9-10, 2015) at St.Mary's University, Halifax, Nova Scotia.</u> The workshop is positioned to take place on the first weekend after the start of the 2015 AARMS Summer School Program on Differential Equations and Numerical Analysis, to be held at Dalhousie University, Halifax, Nova Scotia, July 6-31.

The Bluenose Workshop will be held over two days in order to expand the usual regional participation to include participants from the IFIP Working Group on Numerical Software and participants from the AARMS Summer School, as well as participants from outside the region. The primary form of participation in the workshop will be through presentations, but, in order to allow active participation by as many students as possible there will also be a poster session, giving students a featured forum in which to present their research.

Themes for the workshop include:

- Software and Tools for Reliable Mathematical Modelling in Scientific Computing
- Waves and Patterns in Nonlinear Systems Reaction-Diffusion Systems
- Structure Preserving Discretization of Differential Equations
- Numerical Analysis of Singularly Perturbed ODEs and PDES

Talks and posters in other areas of applied and computational mathematics and scientific computing are welcome.

Organizers:

PAUL MUIR
St. Mary's University

WAYNE ENRIGHT
University of Toronto

RICHARD KARSTEN
Acadia University

Bluenose II image: Nova Scotia Department of Tourism

For more information, please visit:
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Final Report on the Bluenose Applied and Computational Math Days Workshop/International Federation for Information Processing (IFIP) Working Group 2.5 on Numerical Software Meeting

Introduction

Research in many disciplines within science and engineering relies upon mathematical modelling as a key component of the investigative process. Examples of areas where mathematical modelling plays a significant role include mathematics of finance, weather forecasting, mathematical biology, computational geophysics, and computational astronomy. It is often expensive, impractical, or in many cases, e.g., analysis of financial markets, geophysics, or astronomy, impossible to set up and perform physical experiments and thus computational modelling must play a central role. While sophisticated applications-based models can lend substantial insight, it is usually the case that these models must be treated with a combination of classical applied mathematics techniques and software based approaches for the determination of accurate approximate solutions to these models.

In addition to many researchers in science and engineering who use computer models in their research, the Atlantic region also includes many researchers who specialize in the related areas of applied mathematics and numerical analysis. With the current trend by researchers towards increased specialization, a significant challenge in contemporary research efforts involving mathematical modelling is to encourage interaction between application-domain experts who develop the sophisticated mathematical models and applied mathematicians and numerical analysts who can provide expertise on available mathematical analytic techniques, numerical algorithms, and software.

ARRMS has already recognized the importance of this area of research; one of the current (2013-2015) AARMS Collaborative Research Groups is focused in Numerical Analysis and Scientific Computing (NA/SC). Furthermore a second Collaborative Research Group in Numerical Analysis and Scientific Computing was awarded by AARMS for 2015-2017. As well, the 2013 Annual Meeting of the Canadian Applied and Industrial Mathematics Society (CAIMS) featured the First Canadian Symposium in Numerical Analysis and Scientific Computing (CSNASC), an event that included more than 60 speakers; a second Symposium in Numerical Analysis and Scientific Computing took place at the CAIMS 2015 meeting.

In 2015, Halifax hosted what might be called "The Summer of Applied and Computational Mathematics":

- The AARMS Summer School in Differential Equations and Numerical Computing, organized by Theodore Kolokolnikov and Hermann Brunner, took place from July 6 – 31 at Dalhousie University. This summer school offered four graduate level courses: "Waves and Patterns in Nonlinear Systems", taught by Ricardo Carretero, "Topics in Reaction-Diffusion Systems: Theory and Applications", taught by Michael Ward and Juncheng Wei, "Structure-preserving Discretizations of Differential Equations", taught by Elena Celledoni and Brynjulf Owren, and "Numerical Analysis of Singularly Perturbed ODEs and PDES", taught by Martin Stynes.
- A Collaborative Workshop and Short Course on "Domain Decomposition Methods", organized by the AARMS CRG in NA/SC (Ronald Haynes, Hermann Brunner, Paul Muir) and featuring Martin Gander as the short course instructor, immediately followed the summer school (Aug. 3-8), and was also held at Dalhousie.
- A meeting of the IFIP Working Group 2.5 on Numerical Software with an associated workshop that followed the long running series of regional meetings in NA/SC known as the Bluenose Applied and Computational Mathematics Days was held at Saint Mary's on July 9-12. The meeting and the workshop were organized by Paul Muir, Wayne Enright, and Richard Karsten.

This report to AARMS is for the third activity: the joint Bluenose Applied and Computational Mathematics Days workshop/Working Group on Numerical Software meeting. Below we provide some background on the Working Group on Numerical Software, some background on the Bluenose Applied and Computational Mathematics Days series, a description of the event, and a final budget.

We also received support from the Fields Institute. The primary form of support received from the Fields Institute was the website they set up for the conference which was used to handle registration and submission of abstracts;

additional administration support was also provided by the Fields Institute. A small amount of funding was provided by the Fields Institute to cover travel expenses for two of the participants.

IFIP Working Group 2.5 on Numerical Software

IFIP was established under the auspices of UNESCO in 1960 to promote international cooperation in the field of information processing. IFIP does its work through a collection of 13 Technical Committees (TCs) and some 100 working groups. Working Group 2.5 on Numerical Software (WG 2.5), which is part of TC2 on Software Theory and Practice, works to improve the quality of scientific computation by promoting the development and availability of sound numerical software. WG 2.5 members come from all over the world and are elected both in recognition of the substantial contributions that they have already made to the field, but also for their commitment to actively participate in WG 2.5 projects. There are currently about 30 active members, along with a similar number of affiliated members.

WG 2.5 members take turns hosting the yearly meeting at their home institutions. At these meetings, members discuss the latest developments associated with topics that the group has decided to formally track, as well as crafting plans for joint projects. In addition, each WG 2.5 meeting is paired with a local workshop to foster exchange of information between the Working Group and local students and researchers with an interest in the design and effective use of numerical software. These workshops provide an excellent opportunity for local researchers involved in numerical analysis scientific computing to meet experts who are developing and implementing useful and reliable software tools that can be applied in a variety of application areas. As well, the members of the Working Group get a chance to find out about projects that are being undertaken by researchers who are local to the area where the WG 2.5 meeting is held.

In recent years these meetings have been held in Toronto, Canada, Raleigh, USA, Leuven, Belgium, Boulder, USA, Santander, Spain, Shanghai, China, and Vienna, Austria.

Bluenose Applied and Computational Math Days

The 2015 Bluenose Applied and Computation Math meeting represented the 12th such meeting in this series. The first meeting was held at Acadia University in 2000. Subsequent meetings have been held, in 2001 at Saint Mary's University, in 2002 at Dalhousie University, in 2003 at Saint Mary's University, in 2004 at Acadia University, in 2005 at Cape Breton University, in 2006 at St. Francis Xavier University, in 2007 at Saint Mary's University, in 2008 at Dalhousie University, in 2009 at Acadia University, and in 2011 at Saint Mary's University. This meeting series is well known to AARMS since many of the meetings have received financial support from AARMS.

Participants at these events have typically included a mix of researchers in application domains and researchers who specialize in numerical analysis and scientific computing, as well as many students who are working with these researchers. Participants typically come from academia but over the years there have also been a number of speakers from industry and government labs. As well, there have often been talks by students: typically graduate students or post-docs but occasionally undergraduate research students. All past meetings have been one day in length and have usually featured mostly regional participation, with at most one or two speakers from outside the region participating.

Description of 2015 Event

The IFIP Working Group 2.5 on Numerical Software meeting was held at Saint Mary's University July 9-10, 2015. The associated Bluenose Applied and Computational Math Days workshop was also hosted at Saint Mary's on July 11-12, 2015.

There was one regional participant in this year's WG 2.5 meeting; the remainder of the participants were from a number of countries from around the world. There were also two participants who participated by Skype – a first for the working group. (IFIP Participants: 2 from Canada, 5 from the US, 1 from Sweden, 1 from New Zealand, 1 from Belgium). A registration fee of $110 was charged to the IFIP members to cover an excursion and a dinner at the end of the second day of the meeting.

For the Bluenose workshop, as in the past, there were a number of participants (faculty and students) from the Atlantic region. However, since the workshop took place immediately after the Working Group meeting, we also drew a number of the members of the IFIP Working Group to the Bluenose workshop. Furthermore, because the workshop took place on a weekend during the AARMS Summer School, we had the participation of all the summer school instructors and many of the summer school students attended the workshop. There were 6 faculty participants from the Atlantic region and 12 faculty participants from outside the region (Canada, US, Norway, Sweden, India, New Zealand, UK). There were 4 student participants from the Atlantic region and 26 from elsewhere (Canada, US, Saudi Arabia, China, India, Italy).

A number of the faculty participants gave talks. All the summer school instructors give talks (5); there were 3 talks by IFIP members, and 4 talks by regional faculty. See Appendix A for talk titles and abstracts.

In order to allow active participation by students, we hosted a poster session that ran throughout the workshop, allowing students a forum in which to present their research. This was a first for the Bluenose workshop series. Eight students gave posters. Two of the poster presenters were from the region; the rest were from outside (AARMS summer school students). See Appendix B for poster titles and abstracts.

The program featured12 speakers and 8 student poster presentations, with additional participation from faculty and students who did not present, for a total of about 36 participants. We did not organize a conference proceedings for this event; thus there are no immediate publications resulting from this event. However this event did provide a unique opportunity to bring together a number of experts from the area of Numerical Software Development (members of the IFIP WG 2.5 on Numerical Software as well as local experts) with a number of experts in Applied Mathematics Application Areas (AARMS Summer School Instructors as well as local experts) where numerical software is widely used as a key component of the research process. The presentations by these experts gave insight into cutting-edge research results in a variety of important topics in numerical software and applied mathematics. The workshop featured talks by eight experts in numerical software or applied mathematics who were from various places around the world including Norway, China, New Zealand, the US, and other parts of Canada. The workshop gave these two groups the opportunity to hear about each other's work and to network on potential future collaborative research efforts. The workshop was also of substantial benefit to the many students who attended – both students from the AARMS Summer School as well as regional students. And the students who participated in the workshop's poster session had a chance to gain useful feedback on their work from the numerical software and applied mathematics experts who viewed their posters.

Final Budget for IFIP Meeting + Bluenose Workshop

We charged a modest registration fee to workshop participants, $70 for faculty, $60 for IFIP participants, and $50 for students. Expenses included coffee breaks, administrative support, printing costs, etc. Since the workshop was held over two days, we arranged a reception on the evening of the first night for all participants. We also provided some partial travel support for regional faculty and students who required assistance, and waived registration fees for the AARMS summer school participants.

Expenses:

- o **Coffee Breaks (7) = $853.55**
- o **Bluenose lunch for AARMS Summer Students (16) = $10.25 x 16 = $164.00**
- o **Student Assistants (61 hours @ $15.60/hour) = $951.60**
- o **Stationary/Printing = $241.55**
- Excursion for IFIP group (+ guests) = $627.90
- Dinner for IFIP group (+ guests) = $852.75
- Bluenose lunch for non-AARMS students = $235.61
- Bluenose reception = $1135.69

Total Expenses = **$5062.65**

Revenues:

- AARMS = $3570.70
    - o Coverage of selected expenses (**in red above**) = $2210.70
    - o **Registration Fee Waivers for AARMS Summer School Participants:**
        - **Grad Students (16 @ $50/student) = $800.00**
        - **Faculty (1 @ $70/faculty) = $70.00**
        - **Instructors (5 @ $70/instructor) = $350.00**
        - **Organizers (2 @ $70/organizer) = $140.00**
- Registration Fees (non-AARMS Sumer School participants) = $2774.20
- Mathematics and Computing Science Dept., Saint Mary's University = $11.30

Total Revenues = **$6356.2**

Revenues – Expenses = **$1293.55** (Surplus to be saved for future Bluenose workshop expenses.)

Bluenose Schedule

July 11th, Saturday: Saint Mary's University, Sobey Building, SB255

8:30 **Registration Opens**
With simple coffee and tea – Lobby area outside SB255

9:00-9:10 **Welcome/ Opening Remarks**

Session A: Chair – Richard Karsten

9:10-9:40 **Theodore Kolokolnikov** – Dalhousie University 14
Patterned vegetation, tipping points, and the rate of climate change

9:45-10:15 **Michael Ward** – University of British Columbia 16
The Slow Dynamics of Localized Spot Patterns for Reaction-Diffusion Systems on the Sphere

10:20-10:50 **Coffee/ Poster – Lobby area outside SB255**

Session B: Chair – Ronald Haynes

10:50-11:20 **Shaohua George Chen** – Cape Breton University 13
A Simple Moving Mesh Method for Blowup Problems

11:25-11:55 **Hermann Brunner** – Hong Kong Baptist University 11
Time-stepping for fractional evolution equations: recent developments and open problems

12:00-1:30 **Lunch – Dockside (Tickets provided)**

Session C: Chair – Wayne Enright

1:30-2:00 **Ronald F. Boisvert** – National Institute of Standards and Technology (USA) 11
Reproducibility in Computing: The Role of Professional Societies

2:05-2:35 **Elena Celledoni** – Norwegian University of Science and Technology 12
Analysis on Lie Groups with Applications in Computer Animation

2:40-3:10 **Coffee/ Posters – Lobby area outside SB255**

Session D: Chair – Shaohua Chen

3:10-3:40 **Brynjulf Owren** – NTNU, N-7491 Trondheim, Norway 15
Energy preserving methods for PDEs on moving meshes

3:45-4:15 **Paul Muir** – Saint Mary's University 14
B-spline Adaptive Gaussian Collocation Software for the Error Controlled Numerical Solution of ODEs and PDEs

4:20-6:00 **Reception – Lobby area outside SB255**

July 12th, Sunday: Saint Mary's University, Sobey Building, SB255

9:00	**Registration – Lobby area outside SB255** With simple coffee and tea	

Session E: Chair – Richard Karsten

9:30-10:00	**Martin Stynes** – Beijing Computation Science Research Center Some open problems in the numerical analysis of singularly perturbed differential equations	16
10:05-10:35	**Wayne Enright** – University of Toronto Accurate and Reliable Approximate Solution of ODEs and DDEs	13
10:40-11:10	**Coffee/ Posters – Lobby area outside SB255**	

Session F: Chair – Wayne Enright

11:10-11:40	**Ricardo Carretero** – San Diego State University Scattering and Leapfrogging of Vortex Rings in a Quantum Superfluid	12
11:45-12:15	**Philip Sharp –** University of Auckland A GPU-enabled Adams integrator for N-body simulations of the Solar System	15
12:20-12:30	**Closing/Goodbye**	

Appendix A:
Speakers

Reproducibility in Computing: The Role of Professional Societies

by

Ronald F. Boisvert

National Institute of Standards and Technology (USA)

A scientific result is not fully established until it has been independently reproduced. Unfortunately, much published research is not independently verified. And, in the rare cases when a systematic effort has been made to do so, the results have not been encouraging. This threatens to undermine public confidence in the enterprise, and has led to calls for improvements to the process of reporting and reviewing scientific research in, for example, the biomedical sciences. The record in computing is not much better. Changing this state of affairs is not easy. Reproducing the work of others can be quite challenging, and does not garner the same credit as performing the original research. Professional societies have an important role in developing and promoting an open science ecosystem. As part of their role of arbiters and curators of the research literature, they can play a key role in changing the incentive structure to promote higher standards of reproducibility. In this talk I will describe some of the grassroots efforts being undertaken to improve the scientific process within the Association for Computing Machinery (ACM), the world's largest professional society in computing research.

Time-stepping for fractional evolution equations: recent developments and open problems

by

Hermann Brunner

Hong Kong Baptist University

Following a brief review of some recent approaches to time-stepping for fractional evolution equations and related Volterra integral equations, the talk focuses on the convergence properties of time-stepping schemes based on the hp-versions of continuous and discontinuous Galerkin methods for problems with non-smooth solutions. It concludes by describing current work on hp-collocation time-stepping for such problems.

Scattering and Leapfrogging of Vortex Rings in a Quantum Superfluid

by
Ricardo Carretero
San Diego State University
Coauthors: Panayotis Kevrekdis and Ronald Caplan

In this talk we will explore the beautiful and complex world of vortex rings. A vortex ring is formed when a vortex line (a "twister") is looped back onto itself creating a close ring that carries vorticity. Vortex rings are commonplace in fluids. For example, in liquids, many species of marine mammals know how to create them, play with them and even use them to catch prey! Smoke rings in gases are also common. In fact not only people can make smoke rings, but volcanoes and chimneys are also at it!

We will focus on the occurrence of vortex rings in superfluids (fluids without viscosity) described by the nonlinear Schroedinger equation. We showcase some of their phenomenology including, internal excitation waves (Kelvin modes), their mutual interactions, collisions, and scattering scenarios. We also briefly discuss an efficient computational implementation for solving the ensuing partial differential equations using GPU accelerated codes that allow for numerical integration runs of vortex rings in real time!

Shape Analysis on Lie Groups with Applications in Computer Animation

by
Elena Celledoni
Department of Mathematical Sciences, Norwegian University of Science and Technology
Coauthors: Markus Eslitzbichler

Motion of virtual characters in video games is usually respresented using a skeletal animation. The underlying skeleton consits of bones connected by joints.
Animation of virtual characters relies on collections of data obtained by recording the movements of actors. The data consists of curves tracking the positions of the bones throughout the motion, and these curves can be processed by mathematical methods to produce new motions. The data consists of curves in SO(3)^N, where N is the number of bones in the skeleton. These curves are often represented using Euler angles and neglecting the underlying Lie group structure.

We will first discuss how techniques from shape analysis can be sucessfully applied to computer animation treating character animations as points in an infinite dimensional manifold. The main mathematical tools are gradient flows and the computation of geodesics with respect to appropriate Riemaniann metrics on the infinite dimensional manifold of curves in R^d. We will then extend the tools to the case of curves in SO(3)^N and show the advantages of the proposed approach for some problems in character animation.

A Simple Moving Mesh Method for Blowup Problems

by

Shaohua George Chen
Cape Breton University
Coauthors: Lauren DeDieu

We develop a simple and efficient adaptive mesh generator for time-dependent partial differential equations with singular solutions in two-dimensional spaces. The mesh generator is based on minimizing the sum of two diagonal lengths in each cell. We also add second order difference terms to obtain smoother and more orthogonal mesh. The method is successfully applied to the nonlinear heat equations with blowup solutions. We also discuss nonlinear heat equations whose solutions blow up at space infinity and whose blowup time is given.

Accurate and Reliable Approximate Solution of ODEs and DDEs

by

Wayne Enright
University of Toronto

Abstract

In recent years, advances in the development of adaptive and reliable numerical methods for initial value problems in ODEs has led to a new generation of numerical methods that can reliably deliver accurate approximate solutions at off-mesh points as well as at a standard underlying discrete mesh associated with the interval of interest. In this talk, I will describe how this new family of IVP methods has been extended to DDEs and how these methods can reliably and adaptively approximate systems of DDEs that may contain multiple state-dependent delays. For these methods, a user need only specify the DDE and a prescribed error tolerance. The method will generate a piecewise polynomial, defined on the interval of interest, which will satisfy the DDE everywhere to within a small multiple of the tolerance.

B-spline Adaptive Gaussian Collocation Software for the Error Controlled Numerical Solution of ODEs and PDEs

by

Paul Muir
Saint Mary's University

In this talk we discuss a number of software packages, based on B-spline adaptive Gaussian collocation, for the error controlled numerical solution of systems of nonlinear boundary value ODEs, systems of nonlinear parabolic 1D PDEs, and systems of nonlinear parabolic 2D PDEs. The talk with consider, in particular, our recent work in the development of software of this type for 1D PDEs and our progress to date for 2D PDEs.

Patterned vegetation, tipping points, and the rate of climate change

by

Theodore Kolokolnikov
Dalhousie
Coauthors: Yuxin Chen, Justin Tzou and Chunyi Gai

When faced with slowly depleting resources (such as decrease in precipitation due to climate change), complex ecological systems are prone to sudden irreversible changes (such as desertification) as the resource level dips below a tipping point of the system. A possible coping mechanism is the formation of spatial patterns, which allows for concentration of sparse resources and the survival of the species within "ecological niches" even below the tipping point of the homogeneous vegetation state. However, if the change in resource availability is too sudden, the system may not have time to transition to the patterned state and will pass through the tipping point instead, leading to extinction. We argue that the deciding factors are the speed of resource depletion and the amount of the background noise (seasonal climate changes) in the system. We illustrate this phenomenon on a model of patterned vegetation. Our analysis underscores the importance of, and the interplay between, the speed of climate change, heterogeneity of the environment, and the amount of seasonal variability.

Energy preserving methods for PDEs on moving meshes

by

Brynjulf Owren

Department of Mathematical Sciences, NTNU, N-7491 Trondheim, Norway

Coauthors: Sølve Eidnes and Torbjørn Ringholm

Recently, there has been a growing interest in designing integral preserving schemes for PDEs, which use well-known ideas from ordinary differential equations, such as discrete gradient methods and the averaged vector field method. Although adapting such schemes to simple finite difference or finite element methods on constant uniform grids is straightforward, the situation becomes much more challenging when the spatial mesh is non-uniform or even changing with time. In the latter case it is not even very clear what should be meant by an integral being preserved. In this talk we shall present a way of giving meaning to the concept of integral preservation of moving mesh PDEs and we provide some promising numerical results. The approach can be used both for finite difference schemes and finite element schemes, and by using ideas similar to the Partition of Unity method by Babuska and Melnik we can even adapt the approach to allow for h-p adaptivity.

A GPU-enabled Adams integrator for N-body simulations of the Solar System

by

Philip Sharp

University of Auckland

Coauthors: William Newman, Bruce Bills

N-body simulations with a small number of massive bodies representing the planets and a large number of small bodies are used extensively to study the dynamics of the Solar System. The simulations are of two general types, distinguished by whether the small bodies interact with one another. My talk considers simulations where the small bodies interact and form a disk centred on the Sun. For these simulations the cost of evaluating the acceleration of the N bodies is proportional to N^2, making long simulations very expensive computationally.

Graphical Processing Units (GPUs) are used extensively in modern (N-body) galactic simulations to permit simulations with an ever increasingly larger N. In contrast, GPUs have been used sparingly for Solar System simulations.

Grimm and Stadel [2014] developed the Solar System integrator GENGA for use on a GPU. GENGA is an implementation of the hybrid N-body symplectic integrator Mercury of Chambers [1999] with enhancements. Grimm and Stadel found GENGA was up to 30 times faster than Mercury. I recently implemented a variable-order, variable-order Adams method for accurate Solar System simulations on a GPU. I present this work in the talk.

I begin with a brief review of N-body simulations, the integration methods for them, and GPUs. I then describe the implementation of the Adams methods on a GPU and the efforts made to get the fastest implementation for a given error in the integration. I end with the results of some long simulations.

Some open problems in the numerical analysis of singularly perturbed differential equations

by

Martin Stynes

Beijing Computational Science Research Center

Coauthors: Hans-Goerg Roos

While much has been achieved in the numerical analysis of singularly perturbed differential equations during the last half-century, there are of course many open problems. Some of the more important ones (in the opinion of the speaker!) will be described and explored in this lecture.

The Slow Dynamics of Localized Spot Patterns for Reaction-Diffusion Systems on the Sphere

by

Michael Ward

Dept. of Mathematics, UBC

Coauthors: Phillipe Trinh, U. Oxford

In the singularly perturbed limit corresponding to large a diffusivity ratio between two components in a reaction-diffusion (RD) system, many such systems admit quasi-equilibrium spot patterns, where the solution concentrates at a discrete set of points in the domain. In this context, we derive and study the differential algebraic equation (DAE) that characterizes the slow dynamics for such spot patterns for the Brusselator RD model on the surface of a sphere. Asymptotic and numerical solutions are presented for the system governing the spot strengths, and we describe the complex bifurcation structure and demonstrate the occurrence of imperfection sensitivity due to higher order effects. Localized spot patterns can undergo a fast time instability and we derive the conditions for this phenomena, which depend on the spatial configuration of the spots and the parameters in the system. In the absence of these instabilities, our numerical solutions of the DAE system for N = 2 to N = 8 spots suggest a large basin of attraction to a small set of possible steady-state configurations. We discuss the connections between our results and the study of point vortices on the sphere, as well as the problem of determining a set of elliptic Fekete points, which correspond to globally minimizing the discrete logarithmic energy for N points on the sphere.

Appendix B:
Student Poster Presenters

Numerical Solutions of A Nonlinear Gas Transport Model in Unconventional Hydrocarbon Reservoirs

by

Iftikhar Ali

King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

Coauthors: Nadeem A. Malik

Mathematical modeling of gas transport through unconventional hydrocarbon reservoirs results into time-dependent advection-diffusion equations with highly nonlinear advection and diffusion coefficients. These coefficients involve many reservoir parameters such as, gas density, gas viscosity, rock permeability, rock porosity, etc. In this work, we present an algorithm for finding the numerical solutions of a nonlinear gas transport model, which is based on an iterative fully implicit finite volume scheme. The nonlinear coefficients are estimated at the previous time step (started by approximating at initial data) and then we use them to approximate solution at the next time level. The procedure is repeated until some tolerance level is achieved. We match the numerical results with the experimental data by adjusting the values of free constants so that the error between the numerical solutions and the data is minimized. We show the results by graphical illustrations. The current approach is more realistic and is more reliable for reservoir simulations than the previous approaches in the sense that we are estimating the values of nonlinear advection and diffusion coefficients at pressure values at all the grid points whereas in the past studies, advection and diffusion coefficients where estimated at some average pressure value.

Validating Tidal Models with ADCP and Drifter Data

by

Kody Crowell

Acadia University

In order to justify potential turbine sites in the Bay of Fundy, accurate models of the tides in that region are required. FVCOM produces tidal models with extremely high spatial and temporal resolution for the Digby Gut passage. In order to calibrate this model, the output is compared with observational data collected from ADCP and drifter measurements. More work is needed in order to fine tune the model so that it produces better agreements with observational data. Varying certain parameters in the model such as the bottom roughness alters the speed and elevation of the FVCOM output. One goal of this project is to find the optimal value of bottom roughness that fits best with the ADCP and drifter data.

Modeling Touchdown in MEMS

by

Kelsey DiPietro

University of Notre Dame

Coauthors: Dr. Alan Lindsay

Microelectromechanical systems (MEMS) combine electronics and micro-scale technology to create devices used in a variety of physical applications. A critical component of a MEMS device is the capacitor, consisting of an elastic plate situated above a fixed ground plate. When a voltage is applied to the plates, the top plate experiences deformation. Beyond a certain voltage, top plate will make contact with the fixed plate, a phenomenon known as touchdown. Deformation of the capacitor is modeled using a fourth order partial differential equation taken on various topologies. Our work focuses on establishing a geometric framework for predicting touchdown points on regular and irregular domains containing topological defects. Through numerical and analytical techniques, we focus on analyzing the pattern of touchdown points within these more physically realistic capacitor structures. By determining the behavior of touchdown points based on parameters in the partial differential equation, we can aid in the construction of optimal running MEMS devices.

Dynamical analysis of a coupled maps that is used for calculating environmental interface temperature

by

Dragana Draskovic

Lilike Bem 1/b, 21000 Novi Sad, Republic of Serbia

We might say that one of the key conditions for the functioning of the physical system is adequate inflow of energy. Dynamics of energy exchange is based on energy balance equation. In this paper, system that we are going to observe is ground surface, which is typical example of environmental interface in nature. We are going to give a general form of energy balance equation for the ground surface as an environmental interface, this equation is used for calculating the environmental interface temperature, and in addition we will consider prognostic equation for deeper soil layer temperature. This equation forms a system of two differential equation for which dynamical analysis will be conducted. Namely, the accent will be on stability of solution for given system.

Analytic Solution of Generalized Space Fractional Time Reaction Diffusion Equation

by
Sonal Jain
Malaviya National Institute of Technology, Jaipur-302017, Rajasthan, India

We investigate the solution of an generalized space-time fractional reaction-diffusion equation associated with Hilfer Prabhakar time fractional derivative and the fractional Laplace operators. The solution is derived by using the Laplace and Fourier transforms to obtain closed form in terms of the Mittag-Leffler function. A few applications and several special cases have also been discussed.

Solving A Brain Tumor Model with BACOLI

by
Alex MacKenzie
Saint Mary's University
Coauthors: Paul Muir

We consider mathematical models associated with the modeling of tumor growth in the brain. We will obtain numerical solutions to the models using sophisticated PDE software that features adaptive error control. Adaptive error controlled computations can provide the user with more confidence in the accuracy of the computed solution, and can also improve the efficiency of the computation. The original model we study employs a discontinuous diffusion coefficient to model different tumor diffusion rates in the grey and white matter regions of the brain. We argue, based on images of the transition between grey and white matter regions of the brain, that a continuous diffusion coefficient with steep layer regions representing the transition between grey and white matter regions provides a more realistic model. We apply BACOLI, a general purpose software package with adaptive error control to a model for tumor growth in the brain. The results show promise with BACOLI giving a numerical solution to the PDE that is comparable to previously published results.

Spectral Stability of Allen-Cahn reaction-diffusion equation with symmetric and asymmetric potential

by

Varatharajan

Indian Institute of Technology, Kharagpur, India - 721302

Coauthors: Anirvan Dasgupta (Indian Institute of Technology, Kharagpur, India-721302)

This paper describes the spectral stability of a class of solutions of the Allen-Cahn reaction-diffusion equation with spatial symmetry and asymmetry. The essential spectra of the perturbed differential operator at the equilibrium states are obtained. The Evans function is used to determine the point spectrum using Lie midpoint method and Magnus method over a large range of spatial distance. It is shown that for a symmetric potential, the stationary kink and antikink solutions connecting the stable equilibrium states are stable. The broken symmetry of the reaction term transforms the stable stationary solutions into stable traveling solutions. The advection in the Allen-Cahn equation results the both stable kink and antikink solutions are moving the same direction.

A multiscale implementation for the nonlocal peridynamics model in one dimension

by

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Peridynamics models for solid mechanics feature a horizon parameter delta that specifies the maximum extent of nonlocal interactions. In this paper, a multiscale implementation of peridynamics models is proposed. In regions where the displacement field is smooth, grid sizes are large relative to delta, leading to local behavior of the models, whereas in regions containing defects, e.g., cracks, delta is larger than the grid size. Discontinuous (continuous) Galerkin finite element discretizations are used in regions where defects (do not) occur. Moreover, in regions where no defects occur, the multiscale implementation seamlessly transitions to the use of standard finite element discretization of a corresponding PDE model. Here, we demonstrate the multiscale implementation in a simple one-dimensional setting. An adaptive strategy is incorporated to detect discontinuities and effect grid refinement, resulting in a highly accurate and efficient implementation of peridynamics.