



**31st Annual Meeting
of the
Canadian Applied and Industrial
Mathematics Society
(CAIMS*SCMAI)**

hosted by
Memorial University of Newfoundland

July 17–20, 2010

Sheraton Hotel Newfoundland
St. John's, NL

Programme

Contents

| | | |
|-----------|-------------------------------------------------------|------------|
| 1 | Welcome | 1 |
| 2 | Local Organizing Committee | 2 |
| 3 | Patron of the meeting | 4 |
| 4 | Schedule Overview | 5 |
| 5 | Daily Schedules | 7 |
| 6 | Social Events | 9 |
| 6.1 | Welcome Reception | 9 |
| 6.2 | Banquet | 9 |
| 6.3 | NRC-IOT Events | 10 |
| 7 | AARMS Distinguished Lecture | 11 |
| 8 | Plenary lectures | 13 |
| 9 | Prize (Plenary) lectures | 18 |
| 10 | Invited Theme Sessions | 21 |
| 10.1 | Dynamical Systems | 21 |
| 10.2 | Fluid Dynamics | 30 |
| 10.3 | Mathematical Biology and Medicine | 46 |
| 10.4 | Mathematical and Theoretical Physics | 50 |
| 10.5 | Nonlinear Dynamics and Control | 58 |
| 10.6 | Ocean Modelling and Technology | 67 |
| 10.7 | Scientific Computing and Numerical Analysis | 73 |
| 10.8 | Statistical and Population Genetics | 81 |
| 11 | Minisymposia | 88 |
| 11.1 | Applied Combinatorics | 88 |
| 11.2 | Regulatory networks | 93 |
| 11.3 | Heart Simulation | 96 |
| 11.4 | Disease Modeling | 99 |
| 11.5 | Domain decomposition methods | 102 |
| 11.6 | Reaction–Diffusion Systems | 106 |
| 11.7 | Numerical solution of ODEs | 109 |
| 12 | Contributed Papers | 113 |

| | |
|--------------------------------|------------|
| 13 Posters | 121 |
| 14 Map of meeting rooms | 127 |

1 Welcome

On behalf of the Department of Mathematics and Statistics, Memorial University of Newfoundland, we would like to welcome you to CAIMS*SCMAI 2010, the annual meeting of the Canadian Applied and Industrial Mathematics Society (CAIMS)/ Société Canadienne de Mathématiques Appliquées et Industrielles (SCMAI) at the Sheraton Hotel Newfoundland in one of the world's most dramatic and captivating locations, St. John's, Newfoundland and Labrador, CANADA. A symbiotic mix of untouched landscape and world class tourist attractions – spectacular seascapes, impressive glacier carved fjords, pristine wilderness and magnificent waterfalls – the city of St. John's appeals to nature, culture and folklore enthusiasts alike (see www.acinl.ca/event/ for cultural events).

St. John's, the capital city of Newfoundland and Labrador, is Canada's oldest and, arguably, the most distinctive city in North America. The rich history and culture and affinity for “small town” quality of life make the city a pleasure in which to live, work, visit and play. A mosaic of fishing villages, cultural festivals and wildlife, St. John's is also an international centre for marine science and technology, and an active centre for investment and business activity in offshore oil development. While attending CAIMS*SCMAI 2010 take a break, explore the rocky shores, scenic walking trails, and rushing rivers; go whale and iceberg watching; browse the shops on Water Street, or take a stroll down George Street, understood to have the most pubs per square foot of any street in North America; visit the Newfoundland Museum, or the St. John's Fluvarium, the only public fluvarium in North America, or better still watch the sun rise on Signal Hill and set at Cape Spear, the most easterly port in North America. The options are endless and yours to explore while visiting St. John's.

Following upon a practice that began at Winnipeg in 1996, the 31st Annual Meeting of CAIMS*SCMAI 2010 will incorporate and be held simultaneously with the 19th Canadian Symposium on Fluid Dynamics (CSFD-2010). The programs for these two meetings have been constructed so that they are complementary and will provide maximum visibility for Canadian Applied Mathematics in general. The meetings will consist of invited plenary talks, the 2010 CAIMS*SCMAI prize plenary talks, invited session talks based on a set of themes from contemporary applied mathematics, mini-symposia, contributed papers and poster sessions. Two of the main themes for this conference are “Fluid Dynamics (CSFD-2010)” and “Ocean Modelling and Technology”, chosen to reflect our regional strengths in ocean-related research. In addition, a special invited lecture, the 2010 AARMS Distinguished Lecture, entitled “Ocean Space Centre - A centre of marine technology knowledge for the future” is planned to highlight the development of the most comprehensive and up-to-date marine technology knowledge center in the world by a group of Trondheim research organizations in Norway.

With Warm Regards,
Drs. Serpil Kocabiyik and Sharene Bungay,
Co-chairwomen of CAIMS*SCMAI 2010

2 Local Organizing Committee

Chairwomen:

| | |
|------------------|---------------------------------------------------------------------------------|
| Serpil Kocabiyik | Department of Mathematics and Statistics Memorial University of Newfoundland |
| Sharene Bungay | Department of Computer Science Memorial University of Newfoundland |

Committee Members:

| | |
|------------------|-----------------------------------------------------------------------------------|
| Jahrul Alam | Department of Mathematics and Statistics Memorial University of Newfoundland |
| Kelly Hawboldt | Faculty of Engineering and Applied Science Memorial University of Newfoundland |
| Ronald Haynes | Department of Mathematics and Statistics Memorial University of Newfoundland |
| Marco Merkli | Department of Mathematics and Statistics Memorial University of Newfoundland |
| F. Mary Williams | NRC Institute for Ocean Technology |

Local arrangements:

| | |
|------------------|---------------------------------------------------------------------------------|
| Rosalind English | Department of Mathematics and Statistics Memorial University of Newfoundland |
| Leonce Morrissey | Department of Mathematics and Statistics Memorial University of Newfoundland |
| Jennifer Bishop | Department of Mathematics and Statistics Memorial University of Newfoundland |

Contributed Papers and Poster Session Committee Members:

| | |
|------------------|---------------------------------------------------------------------------------|
| Canan Bozkaya | Department of Mathematics and Statistics Memorial University of Newfoundland |
| Shannon Sullivan | Department of Mathematics and Statistics Memorial University of Newfoundland |

CAIMS Board Members:

| | |
|----------------------------------|--------------------------------------------------------------------------|
| Jacques Bélair (President) | Département de Mathématiques et de Statistique Université de Montréal |
| Bob Russell (Past President) | Department of Mathematics Simon Fraser University |
| Jianhong Wu (President-Elect) | Department of Mathematics and Statistics York University |
| Abba Gumel (Secretary) | Department of Mathematics University of Manitoba |
| Paul Muir (Treasurer) | Department of Mathematics and Computing Science St. Mary's University |

Members at large:

| | |
|-------------------|-----------------------------------------------------------------------|
| Lucy Campbell | School of Mathematics and Statistics Carleton University |
| Sharene Bungay | Department of Computer Science Memorial University of Newfoundland |
| Rob Corless | Department of Applied Mathematics University of Western Ontario |
| Ian Frigaard | Department of Mathematics University of British Columbia |
| Nicholas Kevlahan | Department of Mathematics and Statistics McMaster University |
| Dhavide Aruliah | Faculty of Science University of Ontario Institute of Technology |

New members:

| | |
|----------------|------------------------------------------------------------------------------|
| Tony Humphries | Department of Mathematics and Statistics McGill University |
| Michael Y. Li | Department of Mathematical and Statistical Sciences University of Alberta |

3 Patron of the meeting

**Christopher W. Loomis, PhD (Queen's, 1983)
Vice-President (Research)
Memorial University of Newfoundland**



Dr. Loomis received his PhD in Pharmacology & Toxicology from Queen's University at Kingston in 1983. Until 1987, he was an Assistant Professor in the Faculty of Medicine at Queen's, holding joint appointments in the Departments of Pharmacology & Toxicology, Anaesthesia, and Pathology & Laboratory Medicine. In 1988, Dr. Loomis moved to Memorial University of Newfoundland as Associate Professor of Pharmacology in School of Pharmacy, with a joint appointment to Basic Medical Sciences (Neuroscience Group, Faculty of Medicine). He was promoted to Full Professor in 1996 and became the Director of the School of Pharmacy in 1998. In 2002, Dr. Loomis was appointed Vice-President (Research) of Memorial University. During his first term, total research income increased from approximately \$35M to more than \$90M per year, targeted largely in strategic areas. Memorial University ranked first among Canadian universities with medical/doctoral programs in the rate of growth in research income from 2002–2007 (RESEARCH Infosource Inc.) more than doubling the group average. Dr. Loomis was renewed for a second term as Vice-President (Research) in December 2006, was appointed Vice-President (Academic) pro tempore in October, 2008, and appointed as President and Vice-Chancellor, Pro Tempore from September 1, 2009 until June 30, 2009. He has published extensively on the spinal pharmacology of pain, with particular emphasis on neuropathic pain and signaling events early after nerve injury. Dr. Loomis was the recipient of a Medical Research Council (MRC) Development Grant at Memorial University, and held operating grants primarily from the Canadian Institutes of Health Research (formerly the MRC) from 1985 to 2004. He is a multiple recipient of the Dr. Albert R. Cox Award for outstanding medical research and the Bristol Myers-Squibb Award for excellence in pharmaceutical teaching. Dr. Loomis served as a member and officer of a number of MRC/CIHR peer-review committees, and was Memorial University's first MRC Regional Director. He is a member of the Science Advisory Board of Health Canada, the College of Reviewers for the Canada Research Chairs Program, and the Board of Directors of CANARIE (Canada's advanced network organization for research, industry and education). He also serves on a number of other Boards including Springboard Atlantic Inc.: the organization of Technology Transfer Offices in Atlantic Canada, Genesis Group Inc., and C-CORE. Dr. Loomis is a former member of the Board of Directors of Genome Atlantic, the Rx&D Health Research Foundation Advisory Council, and the Panel of Examiners of the Pharmacy Examining Board of Canada.

4 Schedule Overview

| | Sat., Jul.17 | Sun., Jul.18 | Mon., Jul.19 | Tues., Jul.20 | |
|-------------|---------------------------|-------------------------------------------|--------------------------------|--------------------------------------|-------------------------|
| 7:00–7:30 | | Breakfast | Breakfast | Breakfast | |
| 7:30–7:45 | | Welcome* | | | |
| 7:45–8:00 | | PL (Molin) | PL (Ward) | PL (Bloch) | |
| 8:00–9:00 | | DS, FD, MBM, MTP, SCNA, CT | DS, FD, MTP, NDC, OMT, SCNA | PL (Russell) | |
| 9:00–10:00 | | Coffee (Posters) | Coffee (Posters) | Coffee | |
| 10:00–10:30 | | DS, FD, MTP, SCNA, DM, CT | FD, NDC, OMT, SCNA, HS, CT | DS, FD, NDC, OMT, SPG, AC | |
| 10:30–12:00 | CAIMS Board Meeting | Lunch (Poster judging) | Lunch (CAIMS AGM) | Lunch | |
| 12:00–1:30 | | PR (Ascher) | PL (Braza) | PL (Nachtergaele), PR (Wetton) | |
| 1:30–2:30 | | PL (Miura) | PR (Berbeglia) | Coffee (IOT) | PL (Thompson) |
| 2:30–3:00 | | Coffee (Posters) | Coffee (Posters) | | Coffee (IOT) |
| 3:00–3:30 | | DS, FD, MBM, MTP, RN, DDM, NSODE | PR (Coombs) | Special lecture (Minsaas) | FD, NDC, SPG, AC, RD |
| 3:30–4:00 | | | | PL (Langford) | |
| 4:00–4:30 | | | | | |
| 4:30–5:00 | | | | | |
| 5:00–5:30 | | | | | |
| 5:30–6:00 | | | | | |
| 6:00–6:30 | Registration | | | | |
| 6:30–7:00 | | Reception | Banquet | | |
| 7:00–8:00 | | | | | |
| 8:00–9:00 | | | | | |
| 9:00–9:30 | | | | | |

* Dr. Serpil Kocabiyik (Memorial University)

Dr. Noreen Golfman, Dean of the School of Graduate Studies (Memorial University)

Dr. Kelly Hawboldt, Associate Dean of Engineering and Applied Sciences (Memorial University)

AC = Applied Combinatorics, **CT** = Contributed session, **DDM** = Domain Decomposition Methods, **DM** = Disease Modeling, **DS** = Dynamical Systems, **FD** = Fluid Dynamics, **HS** = Heart Simulation, **MBM** = Mathematical Biology and Medicine, **MTP** = Mathematical and Theoretical Physics, **NDC** = Nonlinear Dynamics and Control, **NSODE** = Numerical Solution of ODEs, **OMT** = Ocean Modelling and Technology, **PL** = Plenary lecture, **PR** = Prize lecture, **RD** = Reaction Diffusion Systems, **RN** = Regulatory Networks, **SCNA** = Scientific Computing and Numerical Analysis, **SPG** = Statistical and Population Genetics

5 Daily Schedules

Breakfast will be served in the **Court Garden and Avalon/Battery** (lower level) during the following times:

- Sunday, July 18 - 7:00–7:45am
- Monday, July 19 - 7:00–8:00am
- Tuesday, July 20 - 7:00–8:00am

Registration will take place in the **Pre-function area** during the following times:

- Saturday, July 17 - 6:00pm–9:00pm
- Sunday, July 18 - 8:00am–5:00pm
- Monday, July 19 - 8:00am–5:00pm
- Tuesday, July 20 - 8:00am–12:00pm

| Saturday, July 17 | | |
|-------------------|-------------------|---------------------|
| | Pre-function area | Amherst |
| 12:00–6:00 | | CAIMS Board meeting |
| 6:00–9:00 | Registration | |

| Sunday, July 18 | | | | | | | | |
|-----------------------|---------------------|---------|-------|-------|------|-------|------|------|
| | Pref | Sal.B | Sal.A | Sal.D | Ply. | Sig. | Vik. | Amh. |
| 7:45–8:00 | | Welcome | | | | | | |
| 8:00–9:00 | | Molin | | | | | | |
| 9:00–10:00 | | DS | FD | MBM | MTP | SCNA | CT | |
| 10:00–10:30 | Coffee (Posters) | | | | | | | |
| 10:30–12:00 | | DS | FD | DM | MTP | SCNA | CT | |
| 12:00–1:30 (Lunch) | Poster judging | | | | | | | |
| 1:30–2:30 | | Ascher | | | | | | |
| 2:30–3:30 | | Miura | | | | | | |
| 3:30–4:00 | Coffee (Posters) | | | | | | | |
| 4:00–6:00 | | DS | FD | MBM | MTP | NSODE | DDM | RN |

Pref = Pre-function area (main floor)
Sal.A = Salon A (main floor)
Sal.B = Salon B (main floor)
Sal.D = Salon D (main floor)
A/B = Avalon/Battery (lower level)

Ply = Plymouth (lower level)
Sig = Signal (main floor)
Vik = Viking (first floor)
Amh = Amherst (sixth floor)
IOT = NRC Institute for Ocean Technology

| Monday, July 19 | | | | | | | | |
|------------------------|---------------------|---------------|------------|--------------|-------------|-------------|-------------|------------|
| | Pref | Sal.B | A/B | Sal.D | Ply. | Sig. | Vik. | IOT |
| 8:00–9:00 | | Ward | | | | | | |
| 9:00–10:00 | | DS | FD | NDC | MTP | SCNA | OMT | |
| 10:00–10:30 | Coffee (Posters) | | | | | | | |
| 10:30–12:00 | | HS | FD | NDC | CT | SCNA | OMT | |
| 12:00–1:30 (Lunch) | | CAIMS AGM* | | | | | | |
| 1:30–2:30 | | Braza | | | | | | |
| 2:30–3:00 | | Berbeglia | | | | | | |
| 3:00–3:30 | | | | | | | | Coffee |
| 3:30–4:00 | Coffee (Posters) | | | | | | | Minsaas |
| 4:00–4:30 | | Coombs | | | | | | |
| 4:30–5:00 | | | | | | | | |
| 5:00–5:30 | | Langford | | | | | | Tours |
| 5:30–6:00 | | | | | | | | |

* CAIMS AGM lunch is open for CAIMS members only.

| Tuesday, July 20 | | | | | | | |
|-------------------------|-------------|--------------|------------|--------------|-------------|-------------|-------------|
| | Pref | Sal.B | A/B | Sal.D | Ply. | Sig. | Vik. |
| 8:00–9:00 | | Bloch | | | | | |
| 9:00–10:00 | | Russell | | | | | |
| 10:00–10:30 | Coffee | | | | | | |
| 10:30–12:00 | | DS | FD | NDC | AC | SPG | OMT |
| 12:00–1:30 (Lunch) | | | | | | | |
| 1:30–2:30 | | Nachtergaele | Wetton | | | | |
| 2:30–3:30 | | Thompson | | | | | |
| 3:30–4:00 | Coffee | | | | | | |
| 4:00–6:00 | | RD | FD | NDC | AC | SPG | |

6 Social Events

6.1 Welcome Reception

The Welcome Reception will take place at The Rooms (9 Bonaventure Ave.) on Sunday, July 18, 6:30–9:30pm. (See map below).

Reception Music: The Four Seasons String Quartet (7:00–8:30pm)

The 2010 CAIMS*SCMAI Awards Ceremony (8:30–9:10pm):

Dr. Sharene Bungay (Memorial University)

Dr. Jacques Bélair (Université de Montréal)

CAIMS*SCMAI 2010 Best Poster Awards Ceremony (9:10–9:20pm):

Dr. Chris Radford (Memorial University)

6.2 Banquet

The Banquet will take place at The Masonic Temple (6 Cathedral St.) on Monday, July 19, 6:30–9:10pm, in the form of a dinner theatre, with performance by the Spirit of Newfoundland. Dinner served at 7:00pm / Show: 8:15–9:10pm (See map below).

Google maps



6.3 NRC-IOT Events

The 2010 AARMS Distinguished Lecture by Dr. Atle Minsaas (MARINTEK, Norway) will take place at the National Research Council Institute for Ocean Technology (NRC-IOT) on Monday, July 19. The following is the schedule of events:

- The bus leaves from Sheraton Hotel at 2:40 pm for NRC-IOT
- Refreshments (Atlantic Foyer): 3:00–3:30pm
- Welcome by Dr. F. Mary Williams, Director General of NRC-IOT (Atlantic Room)
- Lecture by Dr. Atle Minsaas (Atlantic Room): 3:30–4:30pm
Introduction by Dr. Ray Gosine, Vice President (Research) Pro Tempore,
(Memorial University).
- Tour of IOT-NRC “See the tanks”, 4:30–5:30pm
- The bus leaves from NRC-IOT at 5:35 pm for Sheraton Hotel

Participants and organizers of the Fluid Dynamics, Ocean Modelling and Technology, and Nonlinear Dynamics and Control sessions, invited guests, and other participants working in ocean related research, are all invited to attend the NRC-IOT event as a part of CAIMS*SCMAI 2010.

7 Special Invited Lecture by Atle Minsaas

AARMS Distinguished Lecture

Ocean Space Centre – A centre of marine technology knowledge for the future

For generations, Norway has been a major maritime power, not least due to our dependence on the sea, combined with long-term thinking and a high level of knowledge and expertise in marine technology. MARINTEK and Norwegian University of Science and Technology have been essential for developing knowledge to keep Norway as a world leader in marine technology. It is by no means given that we can retain this position in the future. The Norwegian Government has in a series of white papers stated that there is a need for significant upgrades and new investments in research infrastructure to maintain our strong position in the maritime fields. This lies at the very core of the Ocean Space Centre, which is aimed at providing possibilities for the study of central problems related to the sea; problems of great importance for climate and the environment, for the balanced utilization of marine resources, for access to energy and for the development of the Arctic region. The pilot study of the Ocean Space Centre outlines the concept, and describes the gap between current laboratory facilities and future needs, in combination with numerical modelling.

Location: Atlantic Room – NRC-IOT

Date/Time: Monday, July 19, 2010, 3:30-4:30pm

Atle Minsaas, PhD (NTNU, 1990) **MARINTEK, Norway**

Dr. Atle Minsaas obtained his MSc within marine systems design from the Norwegian Institute of Science and Technology (NTNU), formerly NTH: Norwegian Institute of Technology (NTH) in 1977. He also holds a PhD from NTNU within the same field from 1990. Dr. Minsaas has been with MARINTEK since he graduated (Norwegian Marine Technology Research Institute; a research company within the SINTEF Group). MARINTEK is a versatile research company specializing in R&D in central areas of the maritime and offshore fields. He has been instrumental in building up logistics R&D as an important area of the MARINTEK services. He was also appointed the programme manager of the first 4 years national waterborne R&D programme funded by the Research Council of Norway. Dr Minsaas has more than 25 years experience working with logistics related R&D projects for the shipping and offshore industries, in Norway and abroad. Since 1995 he has also been heavily involved in many European Union (EU)-funded projects, also as a coordinator. Dr. Minsaas has held different positions in MARINTEK. He has been a vice president with responsibility of the Division of Logistics and Technical Operations, but is now a



special adviser in the staff. In December 2008 he was appointed as a project manager for the development of the next generation marine technology knowledge centre “The third Wave” in Norway, a truly visionary knowledge centre for all things maritime and most things marine, equipped with research facilities with content and a size capable of delivering state-of-the-art research and development well beyond 2050. The third Wave hints at the first wave, which was the initiation of the first ship model tank in 1939 and the second wave, which was the Marine Technology Centre including the ocean basin, opened in 1979.

8 Plenary lectures

| | | |
|-------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|------------------------------|
| Sunday, July 18 | | Location: Salon B |
| 8:00–9:00 | Bernard Molin Hydrodynamic modelling of perforated structures | Chair: Serpil Kocabiyik |
| 2:30–3:30 | Robert Miura Mathematical modeling with applications to biology and medicine | Chair: Sue Ann Campbell |
| Monday, July 19 | | Location: Salon B |
| 8:00–9:00 | Michael Ward Traps, Patches, and Spots: An asymptotic analysis of localized solutions to some diffusive and reaction-diffusion systems | Chair: David Iron |
| 1:30–2:30 | Marianna Braza Turbulence modelling for strongly detached unsteady high-Re flows, based on refined PIV experiments | Chair: Serpil Kocabiyik |
| 5:00–6:00 | William Langford Bifurcation and symmetry | Chair: Theodore Kolokolnikov |
| Tuesday, July 20 | | Location: Salon B |
| 8:00–9:00 | Anthony Bloch Nonholonomic mechanics and quantum dynamics | Chair: Jahrul Alam |
| 9:00–10:00 | Robert Russell Adaptive mesh generation and moving mesh methods | Chair: Ronald Haynes |
| 1:30–2:30 | Bruno Nachtergaele Propagation bounds for quantum dynamics and applications | Chair: Marco Merkli |
| 2:30–3:30 | Elizabeth Thompson The estimation of latent coancestry in pedigrees and populations | Chair: J.-C. Loredon-Osti |

Abstracts:

Nonholonomic mechanics and quantum dynamics

Anthony Bloch

University of Michigan

Email: abloch@umich.edu

In this talk I will discuss some connections between nonholonomic systems and quantum theory. Nonholonomic systems are mechanical systems subject to nonholonomic (non-integrable) constraints on system velocities and are a natural generalization of Hamiltonian systems. Nonholonomic systems conserve energy, but not necessarily volume or momentum. There is a natural bracket associated with such systems which does not

satisfy the Jacobi identity. We consider the question of quantization of such systems and also discuss an isomorphism between rolling on a surface and the dynamics of quantum spins.

Turbulence modelling for strongly detached unsteady high-Re flows, based on refined PIV experiments

Marianna Braza, Remi Bourguet, Rodolphe Perrin
CNRS - Institut de Mecanique des Fluides de Toulouse
Email: marianna.braza@imft.fr

The need of improvement for turbulence modelling strategies to capture strongly unsteady detached flows around bodies at high Reynolds numbers remains a crucial issue from a fundamental and applications point of view. In this conference, an appropriate turbulence macrosimulation approach will be presented, the OES, Organised Eddy Simulation, able to perform accurate prediction of the unsteady loads generated from strong flow detachment around bodies. This approach involves among other, a new tensorial eddy-viscosity concept, suitable for prediction of near-wall turbulence anisotropy. These aspects have been developed by means of well focused physical experiments in high-Reynolds flows around bodies, especially by using three-component - time resolved Particle Image Velocimetry. Applications for reference flows around fixed or moving bodies will be presented.

Bifurcation and symmetry

William Langford
University of Guelph
Email: wlangfor@uoguelph.ca

The inherent symmetries of a dynamical system play a fundamental role in determining the qualitative behaviour of its solutions. This talk begins with an overview of equivariant bifurcation theory and its applications to pattern formation and symmetry-breaking in dynamical systems. The theory is illustrated with concrete applications to problems of research interest. We begin with the classical problem of Huygens' clocks; that is, two symmetrically coupled identical oscillators. Here, the permutation symmetry implies periodic solutions that are phase-locked and either in-phase (identical motions) or anti-phase (opposite motions) as studied by P. Kitanov and first observed by C. Huygens. Other applications come from work with D. Rusu on annular electroconvection in a thin smectic film and atmospheric convection in the equatorial plane, and work with R. Akila on symmetric heat exchanger arrays that may undergo oscillations leading to metal fatigue and costly repairs. Recent work with G. Lewis idealizes the Earth's atmosphere in a simple PDE Boussinesq model with the symmetry of a rotating spherical shell and shows that the recently observed expansion of Hadley cells may be related to

enhanced polar warming.

Mathematical modeling with applications to biology and medicine

Robert M. Miura

New Jersey Institute of Technology

Email: miura@njit.edu

Complex phenomena in biology and medicine are a rich source of new, interesting, and difficult nonlinear mathematical problems. The translation from biomedical phenomena to mathematical equations is called “mathematical modeling”, and in this talk, the requirements for and the process of mathematical modeling will be outlined. Example problems from neuroscience will be given to illustrate some of the ideas described and to show the complexity involved in the resulting mathematical models. Mathematics can have an enormous impact on enriching and extending our understanding of these types of problems and how these complex systems work. Younger mathematical scientists are especially encouraged to explore and apply their quantitative skills to create and solve the mathematical problems in these fields.

Hydrodynamic modelling of perforated structures

Bernard Molin

Ecole Centrale Marseille

Email: bernard.molin@ec-marseille.fr

There are many cases of perforated structures in coastal and offshore engineering: Jarlan walls, mudmats, well-head covers, to name but a few. A hydrodynamic modelling of the wave-interaction of such bodies is proposed under the idealization that their wall thickness is negligible and the perforations are small and numerous to the point that they can be represented as a continuous porosity. The model is based upon potential theory and assumes that the perforations induce pressure losses that are quadratic with respect to the relative traversing velocities. Some simple geometries like a porous cylinder are shown to accept analytical expressions of their hydrodynamic coefficients (added mass and damping). Comparisons with experimental data show that the domain of validity of the proposed model is quite wide.

Propagation bounds for quantum dynamics and applications

Bruno Nachtergaele

University of California Davis

Email: bxn@math.ucdavis.edu

In recent years propagation estimates also known as Lieb-Robinson bounds have been obtained and refined for broad classes of quantum lattice systems. The bounds express

the locality of the dynamics of quantum systems with short range interactions. Simply stated, the dynamics up to time $t > 0$ of an observable involving the degrees of freedom in a bounded region of space depends in an essential way only on the degrees of freedom located at distance $d < vt$. The propagation estimates provide a bound for v , which is called the Lieb-Robinson velocity. This simple property has proven to be a key element in a number of important recent results on quantum dynamics, the low-lying spectrum, and the structure of ground states of quantum systems.

Adaptive mesh generation and moving mesh methods

Robert Russell, Weizhang Huang

Simon Fraser University

Email: rdr@cs.sfu.ca

Over the last several decades, many mesh generation methods and a plethora of adaptive methods for solving differential equations have been developed. In this talk, we take a general approach for describing the mesh generation problem, which can be considered as being in some sense equivalent to determining a coordinate transformation between physical space and a computational space. Some new theoretical results are given that provide insight into precisely what is accomplished using mesh equidistribution (which is a standard adaptivity tool used in practice). As well, we discuss two general types of moving mesh methods for solving time dependent PDEs, those based upon a variational formulation of the mesh generation problem and those which target mesh velocity. Among the methods in the latter class are those which solve the Monge-Ampere equation and the optimal mass transport problem, an area which has seen intense research activity of late.

The estimation of latent coancestry in pedigrees and populations

Elizabeth Thompson

University of Washington

Email: eathomp@uw.edu

Similarities among individuals derive from coancestry, or the descent of genome segments from common ancestors to extant individuals, leading to patterns of gene *identity by descent* (ibd) which vary along a chromosome. Modern genetic marker data permits imputation of these patterns of gene identity by descent among extant individuals, both in pedigrees and in populations. Realizations of ibd conditional on genetic marker data, inferred jointly among chromosomes and among individuals, can then be used in multiple trait analyses, providing, for example, Monte Carlo estimates of linkage test statistics or lod scores. This requires, first, a characterization of the ibd jointly among individuals and across chromosomes that can be compactly stored and efficiently accessed, and, second, methods of likelihood computation that works directly on this ibd, rather than

on more complex latent genotypes and descent patterns. With these tools, we can investigate not only patterns of lod score variation, but the distribution of contributions to a lod score deriving from alternate imputed ibd patterns.

Traps, Patches, and Spots: An asymptotic analysis of localized solutions to some diffusive and reaction-diffusion systems

Michael J. Ward, Wan Chen, Alexei Cheviakov, Alan Lindsay, Ronny Straube
University of British Columbia
Email: ward@math.ubc.ca

A survey of the development of a unified singular perturbation methodology to analyze some linear and nonlinear PDE diffusive-type models with localized solutions is presented. Results from this theory are given for three diverse applications.

The first problem is to determine the mean first passage time (MFPT) for diffusion from within a sphere to localized traps on its boundary. The results predict the time-scale for a diffusing molecule to arrive at localized signaling compartments on the boundary of a biological cell. The optimization of this MFPT is shown to be closely related to the classical problem of finding minimum energy configurations of repelling point charges on a spherical boundary.

Secondly, in the context of spatial ecology, a long-standing problem is to determine the persistence threshold for extinction of a species in a heterogeneous spatial landscape consisting of either favorable or unfavorable local habitats. For such a patch model, and in the context of the diffusive logistic model, specific results are given for the effect of both habitat fragmentation and location on the persistence threshold.

Finally, results for the dynamics, stability, and self-replication behavior of localized spot-type solutions to the Gray-Scott reaction-diffusion model of chemical physics are given. Phase diagrams in parameter space classifying the various spot instabilities are constructed.

9 Prize (Plenary) lectures

| | | |
|--------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|---------------------------------|
| Sunday, July 18 | | Location: Salon B |
| CAIMS*SCMAI-MITACS Research Prize | | |
| 1:30–2:30 | Uri Ascher The chaotic nature of faster gradient descent | |
| Monday, July 19 | | Location: Salon B |
| CAIMS*SCMAI Doctoral Dissertation Award | | |
| 2:30–3:30 | Gerardo Berbeglia Complexity analyses and algorithms for pickup and delivery problems | |
| CAIMS*SCMAI/PIMS Early Career Award | | |
| 4:00–5:00 | Daniel Coombs Understanding the dynamics of T cell surface receptor signaling with mathematical models | |
| Tuesday, July 20 | | Location: Avalon/Battery |
| CAIMS*SCMAI-MITACS Industrial Mathematics Prize | | |
| 1:30–2:30 | Brian Wetton Mathematical modelling of hydrogen fuel cells | |

Abstracts:

The chaotic nature of faster gradient descent

Uri Ascher, Kees van den Doel

University of British Columbia

Email: ascher@cs.ubc.ca

The integration to steady state of many initial value ODEs and PDEs using the forward Euler method can alternatively be considered as gradient descent for an associated minimization problem. Greedy algorithms such as steepest descent for determining the step size are as slow to reach steady state as is forward Euler integration with the best uniform step size. Yet other, much faster gradient descent methods using bolder step size selection exist. They can be preferable to conjugate gradients when matrix-vector multiplications are performed inaccurately. These faster gradient descent methods, however, yield chaotic dynamical systems for the iteration residuals.

The steepest descent method is also known for the regularizing or smoothing effect that the first few steps have for certain inverse problems, amounting to a finite time regularization. We further investigate using the faster gradient descent variants for this purpose in the context of denoising and deblurring of images and also of problems involving data inversion for elliptic PDEs. When the combination of regularization and accuracy requirements demands more than about a dozen steepest descent steps, the alternatives offer an advantage, even though (indeed because) the absolute stability limit

of forward Euler is carefully yet severely violated.

Complexity analyses and algorithms for pickup and delivery problems

Gerardo Berbeglia, Jean-Francois Cordeu, Gilbert Laporte

HEC Montréal

Email: gerardo.berbeglia@hec.ca

Pickup and Delivery Problems (PDPs) are a relevant class of vehicle routing problems in which objects or people need to be collected and distributed. These problems have many applications in logistics, ambulatory services and robotics. We analyze the complexity of counting the number of feasible solutions of a well known PDP, and of a related scheduling problem, and we show that both problems are hard, namely, $\#P$ -complete. We then introduce the Pickup and Delivery Problem with Fixed Partial Routes (PDP-FPR), in which certain fixed partial routes must be respected. We prove that determining whether an instance of the PDP-FPR is feasible is strongly NP-complete. The computational complexity of several relaxations of the PDP-FPR are also shown to be NP-complete, whereas for others relaxations the feasibility problem is shown to be polynomial time solvable. Based on some of these results, we then develop an exact algorithm for checking the feasibility of instances of the Dial-a-Ride Problem (DARP). Finally, we present a hybrid algorithm for the dynamic DARP in which service request arrive in real-time. The hybrid algorithm combines, in parallel, a modified version of an exact constraint programming algorithm and a tabu search heuristic.

Understanding the dynamics of T cell surface receptor signaling with mathematical models

Daniel Coombs

University of British Columbia

Email: coombs@math.ubc.ca

T cell activation is a crucial step in the adaptive immune response to infection. T cells can be activated by signals arising from binding between their surface T cell receptors (TCR) and peptide-major-histocompatibility-complex (pMHC) presented on the surfaces of antigen-presenting-cells. But so far as we can tell, the chemical bonds that form between TCR and pMHC are weak and transient. As part of a quantitative theory of immune cell activation, we would like to understand how bond kinetics control the T cell response. I will describe our evolving work on mathematical modelling and simulation of surface receptor dynamics and signaling. I will present joint work with Omer Dushek, Byron Goldstein, Raibatak Das and Anton van der Merwe, among others.

Mathematical modelling of hydrogen fuel cells**Brian Wetton**

University of British Columbia

Email: wetton@math.ubc.ca

Hydrogen Fuel Cells can efficiently convert Hydrogen fuel and air to electrical power with zero emissions. This talk concerns Polymer Electrolyte Membrane Fuel Cells (PEMFC). A general overview of how these devices are constructed and how they work is given. PEMFCs are fundamentally multi-scale. The central component of a PEMFC (the Membrane Electrode Assembly or MEA) has micron scale. The MEA is made of composite layers which must facilitate selective multiphase transport of reactants to and products from catalyst sites. The need for composite materials with these selective transport properties is a recurring theme in energy conversion and storage applications. MEAs are built into unit cells which are then arranged in stacks. The micro-components have behaviour determined by their structure on the nano-scale. Modelling stack level behaviour from component models and components from their nano-scale structure are both of interest and are illustrated with examples.

10 Invited Theme Sessions

10.1 Dynamical Systems

Organizer: Theodore Kolokolnikov

| Sunday, July 18 | | Location: Salon B |
|-------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|--------------------------|
| Chair: Theodore Kolokolnikov | | |
| 9:00–10:00 | Thomas Erneux Delay differential equations in action <i>(An introduction to delay differential equations)</i> | |
| Chair: Chritina Stoica | | |
| 10:30–10:50 | Rachel Kuske Sustained transients in systems with noise and delay | |
| 10:50–11:10 | Thomas Witelski Transient and self-similar dynamics in thin film coarsening | |
| 11:10–11:30 | Greg Lewis Mixed-mode solutions in an air-filled differentially heated rotating annulus | |
| 11:30–11:50 | Hui Sun A generalized Birkhoff-Rott equation for the 2D active scalar problems | |
| Chair: Greg Lewis & Yana Nec | | |
| 4:00–4:20 | Pietro-Luciano Buono Minimizing symmetric periodic orbits in Hamiltonian Systems: instability and bifurcations | |
| 4:20–4:40 | Christina Stoica Comet and Hill-type periodic orbits in restricted (N+1)-body problems | |
| 4:40–5:00 | Michael Ward Asymptotic analysis of biharmonic nonlinear eigenvalue problems of MEMS | |
| 5:00–5:20 | Alan Lindsay Optimization of the persistence threshold for the diffusive logistic model in spatial environments with localized patches | |
| 5:20–5:40 | Rebecca McKay Instability thresholds and dynamics of mesa patterns in reaction-diffusion systems | |
| 5:40–6:00 | Wan Chen Dynamics and instabilities of localized spot patterns in Gray-Scott model | |
| <i>continued on next page</i> | | |

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| Monday, July 19 | |
| Location: Salon B | |
| Chair: Michael Ward | |
| 9:00–9:20 | Maria D’Orsogna Two dimensional swarming patterns for interacting, self propelling particles |
| 9:20–9:40 | Ryan Lukeman Phase transitions in collective animal motion |
| 9:40–10:00 | Theodore Kolokolnikov Ring patterns in particle aggregation models |
| Tuesday, July 20 | |
| Location: Salon B | |
| Chair: Alan Lindsay | |
| 10:30–10:50 | Yana Nec Signal propagation in sub-diffusive media |
| 10:50–11:10 | Chunhua Ou Exponential and algebraical stability of traveling wavefronts in periodic spatial-temporal environments |
| 11:10–11:30 | Petko Kitanov Coupled oscillators with Huygens symmetry |

Abstracts:

Minimizing symmetric periodic orbits in Hamiltonian systems: instability and bifurcations

Pietro-Luciano Buono, Daniel Offin, Mitchell Kovacic
 University of Ontario Institute of Technology
 Email: luciano.buono@uoit.ca

Recently, many symmetric periodic orbits have been found in the N-body problem as minimizers of the Lagrangian action functional. In this talk, I will discuss a Maslov index based criterion for the instability of periodic orbits with spatio-temporal symmetries (but no time-reversal symmetries) obtained via minimization. The argument is geometric and is based on a result of Contreras and Iturriaga on the existence of stable and unstable invariant manifolds of minimizing trajectories. I will also discuss the case of the Hip-Hop periodic orbit (obtained via minimization) and show bifurcations occurring as the energy is varied.

Dynamics and instabilities of localized spot patterns in Gray-Scott model**Wan Chen**, Michael Ward

University of Oxford

Email: chenw1@maths.ox.ac.uk

Localized patterns including spots, stripes and labyrinths etc. have been observed in many physical and biological systems. In this talk, we analyze the dynamics and different instabilities of spot patterns, in different parameter regimes of two-dimensional Gray-Scott model, using a hybrid asymptotic and numerical methods. The three main types of fast instabilities for a multi-spot solution are spot self-replication, spot annihilation due to overcrowding, and an oscillatory instability in the spot amplitudes. These instability mechanisms are studied in detail and phase diagrams in parameter space where they occur are computed and illustrated for various spatial configurations of spots and several domain geometries.

Two dimensional swarming patterns for interacting, self propelling particles**Maria D'Orsogna**

California State University, Northridge

Email: dorsogna@csun.edu

Schools of fish, flocks of birds and swarms of insects arise in response to external stimuli or by direct interaction, and are able to fulfill tasks much more efficiently than single agents. How do these patterns arise? What are their properties? How are individual characteristics linked to collective behaviors? In this talk we discuss various aspects of biological swarming of discrete particles. We investigate a non-linear system of self propelled agents that interact via pairwise attractive and repulsive potentials. We are able to predict distinct aggregation morphologies, such as flocks and vortices, and by utilizing statistical mechanics tools, to relate the interaction potential to the collapsing or dispersing behavior of aggregates as the number of constituents increases. We also discuss passage to the continuum, devise an ad hoc kinetic theory and present possible applications to the development of artificial swarming teams.

Delay differential equations in action**Thomas Erneux**, Laurent Larger

Universite Libre de Bruxelles

Email: terneux@ulb.ac.be

In the first part of my presentation, I plan to review several applications modelled by delay differential equations (DDEs) starting from familiar examples to problems in physiology and industry. Delay differential equations have the reputation to be difficult mathematical problems but there is today a renewed interest for both old and new

problems modelled by DDEs. In the second part of my talk, I'll emphasize the need of developing asymptotic tools for DDEs in order to guide our numerical simulations or help our physical understanding. I illustrate these ideas by considering the response of optical optoelectronic oscillators that have recently been studied both experimentally and numerically.

Coupled oscillators with Huygens symmetry

Petko Kitanov, William Langford, Allan Willms

University of Guelph

Email: pkitanov@uoguelph.ca

We study two identical coupled oscillators modeled by a four-dimensional system of differential equations. The vector field possesses symmetry with respect to switching the two oscillators and with respect to switching left and right within both oscillators. An immediate consequence of this symmetry is the existence of flow invariant subspaces, which correspond to in-phase and anti-phase synchronization of the oscillators. In addition, the symmetry dictates that the Jacobian of the system is diagonalizable. Using Hilbert-Weyl theory, we derive the normal form for 1:1 resonance. For the truncated normal form, we show the existence of phase-locked mixed-mode solutions. Some typical phase portraits for these types of solutions are presented.

Ring patterns in particle aggregation models

Theodore Kolokolnikov, Hui Sun, David Uminski, Andrea Bertozzi

Dalhousie University

Email: tkolokol@gmail.com

We consider a two-dimensional kinematic model of pairwise particle interaction of the form

$$\frac{dx_j}{dt} = \frac{1}{N} \sum_{\substack{k=1 \dots N \\ k \neq j}} F(|x_k - x_j|) \frac{x_k - x_j}{|x_k - x_j|}, \quad j = 1 \dots N.$$

This general model was used recently by Topaz, Bernoff, Logan, and Toolson to model locust swarms; it also occurs in statistical mechanics.

Under certain general assumptions on $F(r)$, we show that a solution where all particles concentrate on a ring is possible. We also fully characterize the local stability of such a ring. We extend the concept of well-posedness to rings solutions, and show that necessary (but not sufficient) condition for stability of a ring is that $F(0) = 0$ and $F''(0) > 0$. When a ring is unstable, a rich variety of patterns is observed numerically, such as triangular curves, annulus solutions, and more intricate steady states. For the general case where solution concentrates on a closed curve, we also derive a set of integral evolution equations in the limit of large N .

Sustained transients in systems with noise and delay

Rachel Kuske, David Simpson
University of British Columbia
Email: rachel@math.ubc.ca

This talk will give an overview of the interaction of noise and delay in stochastic systems such as machine tools, diseases related to blood production, and models of balance. The common theme is the influence of random fluctuations in driving, sustaining, and amplifying seemingly deterministic complex dynamics in parameter regimes where the systems are expected to be quiescent. Analysing stochastic models with delay is challenging at best, so new approaches are developed to handle them. Several perspectives are borrowed from multiple scales analysis and from the ideas of coherence and stochastic resonance to allow progress in understanding the collusion of the noise, nonlinearities, and delay.

Mixed-mode solutions in an air-filled differentially heated rotating annulus

Greg Lewis
University of Ontario Institute of Technology
Email: greg.lewis@uoit.ca

We present an analysis of the Hopf bifurcations that occur in a mathematical model that uses the (three-dimensional) Navier-Stokes equations in the Boussinesq approximation to describe the flows of a near unity Prandtl number fluid (i.e. air) in the differentially heated rotating annulus. These bifurcations correspond to the transition from axisymmetric to nonaxisymmetric flow, where the axisymmetric flow loses stability to an azimuthal mode of integer wave number, and rotating waves may be observed. Of particular interest are the double Hopf (Hopf-Hopf) bifurcations that occur along the transition, where there is an interaction of two modes with azimuthal wave numbers differing by one.

Parameter-dependent centre manifold reduction and normal forms are used to predict the behaviour near the transition. The analysis shows that in certain regions in parameter space, stable quasiperiodic mixed-azimuthal mode solutions result from the mode-interaction. We also discuss the mode-interaction with 1:2 spatial resonance, which indicates another mechanism by which a mixed-mode solution may arise.

Optimization of the persistence threshold for the diffusive logistic model in spatial environments with localized patches.**Alan Lindsay**

University of British Columbia

Email: ael@math.ubc.ca

An indefinite weight eigenvalue problem characterizing the threshold condition for extinction of a population based on the single-species diffusive logistic model in a spatially heterogeneous environment is analyzed in a bounded two-dimensional domain with no-flux boundary conditions. In this eigenvalue problem, the spatial heterogeneity of the environment is reflected in the growth rate function, which is assumed to be concentrated in n small circular disks, or portions of small circular disks, that are contained inside the domain. The background growth rate is assumed to be spatially uniform. The disks, or patches, represent either strongly favorable or strongly unfavorable local habitats. For this class of piecewise constant growth rate function, an asymptotic expansion for the persistence threshold, representing the positive principal eigenvalue for this indefinite weight eigenvalue problem, is determined in the limit of small patch radii by using the method of matched asymptotic expansions. By analytically optimizing the coefficient of the leading-order term in the asymptotic expansion the persistence threshold, general qualitative principles regarding the effect of habitat fragmentation are derived. In certain degenerate situations, the optimum spatial arrangement of the favorable habit is determined by a higher-order coefficient in the asymptotic expansion of the persistence threshold.

Phase transitions in collective animal motion**Ryan Lukeman**

St. Francis Xavier University

Email: rlukeman@stfx.ca

Analogous to phase transitions in physical systems, animal groups (e.g., fish schools, bird flocks, locust swarms) can switch from disordered, low-alignment (zero net transport) groups to polarized (positive net transport) groups. Self-propelled particle models of collective motion have shown a number of pathways in which the system bifurcates from one phase to another, but comparison to real animal groups is limited due to a scarcity of data. In this talk, I describe work to connect the theoretical work on phase transitions with real animal groups; specifically, detailed trajectory data of flocking surf scoters, an aquatic duck.

Instability thresholds and dynamics of mesa patterns in reaction-diffusion systems

Rebecca McKay, Theodore Kolokolnikov
 Dalhousie University
 Email: wrebecca@mathstat.dal.ca

Consider the reaction-diffusion system

$$\begin{aligned} u_t &= \varepsilon^2 u_{xx} + f(u, w) \\ 0 &= Dw_{xx} + g(u, w). \end{aligned}$$

In the singular limit as $\varepsilon \rightarrow 0$, for some fixed D , the system has a steady state that consists of a periodic pattern of sharp interfaces and is stable in time. When $D = \infty$, this pattern is unstable. We examine the transition of a stable pattern to an unstable pattern as D is increased. We derive thresholds $D_1 \gg D_2 \gg D_3 \gg \dots$ such that the solution with $2K$ interfaces is stable for $D < D_K$ and unstable for $D > D_K$. As well, we consider the dynamics of the interfaces when D is exponentially large.

Signal propagation in sub-diffusive media

Yana Nec, Alexander Nepomnyashchy, Vladimir Volpert
 University of British Columbia
 Email: oulanka@math.ubc.ca

Molecules related to biological functions often perform sub-diffusion due to the properties of the embedding medium (obstructions, crowdedness) or the molecule itself (size, interactions). Biological signals are waves of information travelling through the living organism in the form of fronts or pulses by means of those sub-diffusing molecules.

Front solutions are analysed for two types of reaction – sub-diffusion models and different kinetics. One model is based on the diffusion PDE with a fractional time derivative. An exact solution of a travelling front is obtained for piecewise linear kinetics and an asymptotic solution is given in the case of a continuous kinetic function.

The second model is based on the integral master equation. Here one example of a front construction yields a reaction – diffusion equation with a time fractional diffusion coefficient. Again, exact and asymptotic solutions are presented for piecewise linear and continuous kinetics respectively.

Exponential and algebraical stability of traveling wavefronts in periodic spatial-temporal environments

Chunhua Ou, Ming Mei, Xiao-Qiang Zhao
 Memorial University of Newfoundland
 Email: ou@mun.ca

Global stability of traveling wavefronts in a periodic spatial-temporal environment in n -dimensions ($n \geq 1$) is studied. We begin with the case where the spatial dimension equals one. A new and easy to follow method is provided. The wavefront is proved to be exponentially stable in the form of $O(e^{-\mu t})$ for some $\mu > 0$, when the wave speed is greater than the minimal one, and algebraically stable in the form of $O(t^{-1/2})$ in the critical case. These results are extended to the cases of multiple spatial dimensions and time-periodic media. Finally, we illustrate how the stability result can be directly used to obtain the uniqueness of the wavefront with a given speed.

Comet and Hill-type periodic orbits in restricted (N+1)-body problems

Cristina Stoica
 Wilfrid Laurier University
 Email: cstoica@wlu.ca

Consider the motion of an infinitesimal particle in a rotationally invariant potential field associated to N point sources, called “primaries”. The interaction potential between the particle and the primaries is taken to be a finite sum of terms of the form $(distance)^{-\alpha}$, with $\alpha > 0$. The primaries are assumed to be in a relative equilibrium, that is, they form a uniformly rotating rigid configuration.

Using appropriate symplectic scalings, Poincaré’s continuation method and averaging, we show two results. First, if the infinitesimal particle is far from the primaries and the potential’s dominant term at infinity is attractive and such that $\alpha \neq 2$, then there exist two one-parameter families of large nearly circular periodic solutions. Second, if the infinitesimal particle is close to one of the primaries and the potential’s dominant term near collision is attractive and such that $\alpha < 2$, then there exist two one-parameter families of nearly circular periodic solutions that encircle the close-by primary.

This is joint work with Jaume Llibre (Universitat Autònoma de Barcelona).

A generalized Birkhoff-Rott equation for the 2D active scalar problems

Hui Sun, David Uminsky, Andrea Bertozzi
 University of California, Los Angeles
 Email: huiprobable@gmail.com

In this presentation we derive new evolution equations for the active scalar problem in 2D for the case when all scalars lie on a 1D curve, analogous to the Birkhoff-Rott

equation for 2D vorticity. The new equations are Lagrangian and valid for nonlocal kernels K that may include both a gradient and an incompressible term. We develop a numerical method for implementing the model which achieves second order convergence in space and fourth order in time. We simulate classic active scalar problems such as the vortex sheet problem (in the case of purely incompressible flow) and the collapse of delta ring solutions (in the case of pure aggregation) and find excellent agreement. We also include new examples that contain both incompressible and gradient flows.

Asymptotic analysis of biharmonic nonlinear eigenvalue problems of MEMS

Michael Ward, Alan Lindsay
 University of British Columbia
 Email: ward@math.ubc.ca

A class of Biharmonic nonlinear eigenvalue problem modeling the steady-state deflection of a deformable surface associated with a MEMS capacitor under a constant applied voltage is analyzed using formal asymptotic methods. In the limit of either a small or a large bending energy, an asymptotic expansion for the saddle-node bifurcation point at the end of the minimal solution branch is constructed in an arbitrary 2-D domain, and specific results are given for the case of the unit slab or disk. The determination of this bifurcation point is critical in device design as it determines the maximum steady-state voltage that can be safely imposed across the capacitor. In addition, a matched asymptotic analysis is used to construct nearly singular steady-state solutions describing the limiting behavior along the maximal solution branch for the Biharmonic nonlinear eigenvalue problem. Such nearly singular solutions, with localized concentration, are constructed in both the unit disk and in an arbitrary 2-D domain. The analysis requires the systematic use of switchback terms, which are notorious in low Reynolds number fluid flow problems, and certain detailed positivity properties of the Biharmonic Green's function.

Transient and self-similar dynamics in thin film coarsening

Thomas Witelski, Michael Gratton
 Duke University
 Email: witelski@math.duke.edu

The dynamics of arrays of droplets formed by the dewetting of viscous thin films on hydrophobic substrates can be reduced to a coarsening dynamical system (CDS) consisting of a set of coupled ODEs and deletion rules for when droplets vanish. We write a Lifshitz-Slyozov-Wagner-type (LSW) continuous mean-field model for the drop size distribution and compare it with simulations of discrete models derived from the CDS. Large transient deviations from self-similar LSW dynamics are shown to conform to bounds given by Kohn and Otto.

10.2 Fluid Dynamics

Organizers: Serpil Kocabiyik, Ian Frigaard, Richard Karsten, Bartosz Protas

| Sunday, July 18 | | Location: Salon A |
|-------------------------------|----------------------------------------------------------------------------------------------------------------------------|--------------------------|
| Chair: Bartosz Protas | | |
| 9:00–9:20 | Michael Renardy The mathematics of myth: Yield stress behavior as a limit of nonmonotone constitutive theories | |
| 9:20–9:40 | Brian Wetton Asymptotic Error Analysis of piecewise uniform grids | |
| 9:40–10:00 | Jahrul Alam A multiscale method for simulating geophysical flows | |
| Chair: Richard Karsten | | |
| 10:30–10:50 | Henry van Roessel Post-gelation behaviour for the coagulation equation with bilinear kernel | |
| 10:50–11:10 | Yuri Skrynnikov Solving an initial value problem for a parabolic equation by matching asymptotic expansions | |
| 11:10–11:30 | Serge D'Alessio Modelling gravity-driven flow over uneven surfaces | |
| 11:30–11:50 | Marek Stastna High order methods for simulating internal wave dynamics | |
| 11:50–12:10 | Lucy Campbell Exact expressions for transient forced waves in some geophysical flow configurations | |
| Chair: Yuriko Renardy | | |
| 4:00–4:20 | Ian Frigaard Stable multi-layer flows at all Re ; Visco-plastic lubrication of shear-thinning and viscoelastic fluids | |
| 4:20–4:40 | Jason Normore Efficient design and applications of fluid dynamics methods on graphics processing units | |
| 4:40–5:00 | Bartosz Protas The maximum enstrophy growth in Burgers equation | |
| 5:00–5:20 | Entcho Demirov Numerical modeling of interannual variability in the sub-polar North Atlantic and Arctic Oceans | |
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| 5:20–5:40 | Wenyuan Liao A higher-order finite difference method for solving 2D Burgers' equations |
| 5:40–6:00 | George M. (Bud) Homsy Some heat pipe problems |
| Monday, July 19 Location: Avalon/Battery | |
| Chair: John Bowman | |
| 9:00–9:20 | Iakov Afanassiev Jets in the ocean: laboratory experiment |
| 9:20–9:40 | Greg Lewis Flow transitions in a differentially heated rotating channel of fluid |
| 9:40–10:00 | John Stockie Coupled flow and reaction chemistry in porous concrete |
| Chair: Nicholas Kevlahan | |
| 10:30–10:50 | Rossitza Marinova Fully implicit time integration for incompressible Navier-Stokes equations |
| 10:50–11:10 | Nicholas Kevlahan The role of vortex wake dynamics in the flow-induced vibration of tube arrays |
| 11:10–11:30 | Miguel Moyers-Gonzalez Linear stability analysis of an elastoviscoplastic fluid with internal microstructure |
| Tuesday, July 20 Location: Avalon/Battery | |
| Chair: Ian Frigaard | |
| 10:30–10:50 | John Bowman Dealiased convolutions without the padding |
| 10:50–11:10 | Luca Cortelezzi Conceptual design of an optimal mixer |
| 11:10–11:30 | Marianna Carrasco-Teja Non-Newtonian fluid displacements in horizontal narrow eccentric annuli: Effects of slow motion of the inner cylinder |
| <i>continued on next page</i> | |

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| 11:30–11:50 | Michael Waite Simulating the energy cascade of stratified turbulence |
| Chair: Jahrul Alam | |
| 4:00–4:20 | Richard Karsten Assessment of tidal current energy in the Bay of Fundy |
| 4:20–4:40 | Yuriko Renardy Deformation of a hydrophobic ferrofluid droplet suspended in a viscous medium under uniform magnetic fields |
| 4:40–5:00 | Francis Poulin How barotropic instability can induce submesoscale motions |
| 5:00–5:20 | Georges Djoumna Sensitivity of the seasonal evolution of the stratification to the absorption of solar radiation and to the turbulent heat fluxes |
| 5:20–5:40 | Peter Berg Electrohydrodynamics of nano-pores in polymer electrolyte membranes |
| 5:40–6:00 | Yuri Muzychka Analytical and numerical modelling of slip flows in the hydrodynamic entrance region of channels |

Abstracts:

Jets in the ocean: laboratory experiment

Yakov Afanasyev, Sheilagh O’Leary
Memorial University of Newfoundland
Email: afanai@mun.ca

Nearly zonal jets recently discovered using satellite altimetry seem to originate at the eastern boundaries of oceans. Jets are generally interpreted in the context of small-scale turbulence. We show a mechanism whereby the jets result from the development of beta-plumes originated from the baroclinic meanders at the eastern boundary of the ocean. Eddies are intimately related and occur as a result of the instability of this process. This mechanism does not rely on the existence of the small-scale turbulence to sustain jets. The underlying dynamics include the propagation of Rossby waves. We demonstrate this mechanism using a rotating axisymmetric bowl of fluid with a paraboloidal free surface. The dynamical fields are measured by the laboratory analogue of the satellite altimetry.

A multiscale method for simulating geophysical flows**Jahrul Alam**

Memorial University

Email: alamj@mun.ca

Geophysical flows are often turbulent. This is especially true for the flows near the land-atmosphere interface, where large gradients of meteorological quantities are observed. This lower turbulent layer of the atmosphere is called the planetary boundary layer (PBL). Various complex physical processes in the PBL can be explained with high quality observational data, which is often difficult, expensive, and labor intensive. It is also difficult to agree on a general turbulence model so that observational data can be analysed to explain geophysical flows in the PBL. The numerical simulation approach seeks to compute the details of turbulence, and is enjoying an increasing popularity. In this talk, I will present a multiscale numerical method for simulating geophysical flows so that only the intermittent scales of turbulence are computed using an adaptive wavelet basis. Numerical results verifying the performance of the method will be presented.

Electrohydrodynamics of nano-pores in polymer electrolyte membranes**Peter Berg**, Kehinde Ladipo, Arian Novruzi

University of Ontario Institute of Technology

Email: peter.berg@uoit.ca

In this talk, we will explore continuum modelling approaches to investigate proton and water transport in nano-pores of polymer electrolyte membranes (PEM), and the limits to their applicability. Our focus will be on the Poisson-Nernst-Planck (PNP) equation, coupled to Navier-Stokes (NS) flow, which entails system parameters and boundary conditions that need to be chosen carefully.

We will discuss analytical solutions of simple geometries as well as numerical solutions pertaining to general geometries. The combination of both approaches highlights the modelling challenges of PNP-NS equations.

The applicability of such models would be of great advantage when considering PEM pore network models and their use in computing average (i.e. macroscopic) membrane properties, for example, conductivity or water drag. Their computational complexity is much reduced in comparison to discrete models such as Brownian dynamics or (ab initio) molecular dynamics.

Dealiased convolutions without the padding

John Bowman, Malcolm Roberts
University of Alberta
Email: bowman@math.ualberta.ca

An algorithm is described for calculating dealiased linear convolution sums without the expense of conventional zero-padding or phase-shift techniques. For one-dimensional in-place convolutions, the memory requirements are identical with the zero-padding technique, with the important distinction that the additional work memory need not be contiguous with the data. This decoupling of the data and work arrays dramatically reduces the memory and computation time required to evaluate higher-dimensional in-place convolutions. The technique also allows one to efficiently dealias the hyperconvolutions that arise on Fourier transforming cubic and higher powers. Implicitly dealiased convolutions can be built on top of state-of-the-art fast Fourier transform libraries: vectorized multidimensional implementations for the complex and centered Hermitian (pseudospectral) cases have now been implemented in the open-source software `fftw++`.

Exact expressions for transient forced waves in some geophysical flow configurations

Lucy Campbell, Martin Nadon, Nijimbere Victor
Carleton University
Email: campbell@math.carleton.ca

We discuss the derivation of exact solutions describing the propagation of transient forced internal gravity waves and Rossby waves in two-dimensional geophysical fluid flows. The configurations studied are simplified by the assumptions of zero aspect ratio and constant mean velocity. In each case, the solution consists of a part with steady amplitude and a transient part in the form of an infinite series that goes to zero in the limit of infinite time. Because of the exact nature of these solutions, they can be used as a starting point for further analytical and numerical studies of wave propagation.

Non-Newtonian fluid displacements in horizontal narrow eccentric annuli: Effects of slow motion of the inner cylinder

Mariana Carrasco-Teja, Ian A. Frigaard
University of British Columbia
Email: teja@math.ubc.ca

We study non-Newtonian fluid displacements in horizontal narrow eccentric annuli in the situation where the inner cylinder is moving slowly. We model the displacement using a Hele-Shaw approach. This represents a practically important extension of the model analysed by Carrasco-Teja et al., (2008: J. Fluid Mech. 605, pp. 293327). With

the inner cylinder moving, the Hele-Shaw model closure between the pressure gradient and the velocity field is highly complex and extremely costly to compute, except for Newtonian fluids. We consider the limit of large buoyancy number, in which the interface elongates along the annulus. We derive a lubrication-style model for this situation, showing that the leading order interface is symmetric. Rotation of the inner cylinder only affects the length of the leading order interface, and this occurs only for non-Newtonian fluids via shear-thinning effects. At first order, casing rotation manifests in an asymmetrical shift of the interface in the direction of the rotation. We also derive conditions on the eccentricity, fluid rheology and inner cylinder velocity, under which we are able to find steady traveling wave displacement solutions.

Conceptual design of an optimal mixer

Luca Cortelezzi, Oleg Gubanov

McGill University

Email: crtlz@cim.mcgill.ca

An optimal mixer can be defined as a mixing device able to deliver a uniformly optimal mixing performance over a wide range of operating and initial conditions. We conceptually design an optimal mixer starting from a reference mixing device, the sine flow. The time-periodic sine flow performs poorly and erratically over most operating and initial conditions. The optimal mixer is derived in steps modifying the design of the reference mixer and optimizing its operations. We first optimize the time-sequence of the stirring velocity fields. We obtain a mixer which performs substantially better than the sine flow, although its performance remains suboptimal due to a deficiency of the actuating system. Second, we improve the sine flow by implementing a new actuating system that allows optimized shifts of the stirring velocity fields in the cross-flow direction. The performance of the resulting mixer is suboptimal only at low operating conditions due to the use of a periodic stirring protocol. Finally, an optimal mixer is obtained by coupling the time and shift optimizations. The resulting optimal mixer is able to deliver a uniform optimal performance over the entire operating range and is quite insensitive to the geometry of the initial conditions.

Modelling gravity-driven flow over uneven surfaces

Serge D'Alessio

University of Waterloo

Email: sdalessio@uwaterloo.ca

This talk concerns the gravity-driven two-dimensional laminar flow of a thin layer of fluid down a wavy inclined surface. Three mathematical models describing the unsteady two-dimensional flow evolution will be presented and contrasted. The first is a shallow-water model while the other two are integral-boundary-layer models which

represent non-hydrostatic approximations to the two-dimensional Navier-Stokes equations for thin fluid layers. Various tests and simulations were conducted in order to assess the performance of these models. These include comparisons with theoretical and experimental data and also comparisons with direct numerical simulations using the computational fluid dynamics package CFX. The wavy surface considered in this study corresponds to that of a sinusoidal profile characterized by a wavelength and amplitude. The resulting interfacial wave structure along with the combined effect of bottom topography and surface tension will be presented and discussed.

This is joint work with J.P. Pascal (Ryerson University) and K.A. Ogden (University of Waterloo).

**Numerical modeling of interannual variability in the sub-polar North
Atlantic and Arctic Oceans**

Entcho Demirov, S. Graham, J. Zhu, Y. Zhang
Memorial University of Newfoundland
Email: entcho@mun.ca

The talk presents results from couple ice-ocean eddy permitting simulations of the circulation in the sub-polar North Atlantic and Arctic Oceans from 1948 to 2005. The ocean model is NEMO (Nucleus for European Modelling of the Ocean). The first part of the presentation will discuss the uncertainty in the ocean model solution related to unresolved subscale process. The model error is assessed through comparison of model and data. The second part of the talk discusses the major results from the model simulations of the interannual variability of regional atmospheric processes, sea-ice and ocean in the sub-polar region. The connections of the long term changes in the volume transport, the water masses properties and spreading with the atmospheric variability are discussed.

**Sensitivity of the seasonal evolution of the stratification to the absorption
of solar radiation and to the turbulent heat fluxes**

Georges Djournna, Kevin G. Lamb
University of Waterloo
Email: gdjournna@math.uwaterloo.ca

A sensitivity analysis of the seasonal evolution of the stratification in Lake Erie to the vertical fluxes of momentum, sensible and latent heat, and to radiative fluxes (short- and long-wave) is performed using the MITgcm model. The model is forced with observed winds, downward short-wave and long-wave radiation, air temperature, and specific humidity. The MITgcm (MIT General Circulation Model) is an efficiently parallelized non-hydrostatic model designed for studying of the atmosphere, ocean, and climate. Solar radiation is the primary source of energy that drives the atmospheric and oceanic

circulations. The absorption of solar energy and its transformation to heat has a profound effect on the thermal structure, and circulation pattern of lakes and oceans. The dynamics of a mixed layer is quite sensitive to the parametrization of downward short-wave radiation and the bulk transfer coefficients. Various parametrization schemes for bulk transfer coefficients, the absorption of penetrative solar radiation and long-wave radiation fluxes are compared. Model results are compared to available direct observations.

Stable multi-layer flows at all Re ; Visco-plastic lubrication of shear-thinning and viscoelastic fluids

Ian Frigaard, Miguel Moyers-Gonzalez, Cherif Nouar
University of British Columbia
Email: frigaard@math.ubc.ca

Multi-fluid flows are frequently thought of as being less stable than single phase flows and consideration of different non-Newtonian models can give rise to different types of hydrodynamic instability. Here we show that with careful choice of fluid rheologies and flow paradigm, one can achieve multi-layer flows that are linearly stable for $Re = \infty$. The basic methodology consists of 2 steps. First we eliminate interfacial instabilities by using a yield stress fluid in one fluid layer and ensuring that for the base flow configurations studied we maintain an unyielded plug region at the interface. Secondly we eliminate linear shear instabilities by ensuring a strong enough *Couette* component in the second fluid layer, imposed via the moving interface. We show that this technique can be applied to both shear-thinning and visco-elastic fluids.

Some heat pipe problems

George M. Homsy
University of British Columbia
Email: bud@math.ubc.ca

Heat pipes are engineering devices designed to transport energy at very high fluxes (power densities) without moving parts. They exploit evaporation/condensation cycles in which capillarity is used to pump liquid against a thermal gradient, moving it from colder regions where it condenses to hotter regions where it evaporates. With the advent of microfabrication techniques, so-called micro heat pipes, with their well-defined geometries, open the way for physically based and predictive modeling, and insight into mechanisms. This talk will cover our recent work based on lubrication theory and a class of contact line models that results in thin film equations that can be integrated semi-analytically. We follow with a discussion of optimal design of micro heat pipes, novel architectures, new physical mechanisms, and if time allows, a brief mention of some open problems in the field.

Assessment of tidal current energy in the Bay of Fundy**Richard Karsten**, Joel Culina, David Greenberg, Michael Tarbotten

Acadia Univeristy

Email: rkarsten@acadiu.ca

The Bay of Fundy, in particular the Minas Basin, has the worlds highest tides. The Minas Passage, which connects Minas Basin to the Bay of Fundy, has mean tidal currents of over 3 m/s making it an very promising location for tidal power. In this talk, we examine a variety of assessments of the potential power generation from these currents using in-stream tidal turbines. We discuss the initial assessments using idealized models have established that Giga Watts (GW) of power can be extracted from the currents in the passage with relatively small change in the tides in the Minas Basin and the Bay of Fundy. We then examine the potential power that could be extracted from Minas Passage with realistic arrays of 3D turbines. We show that as the size of a farm moves from a few turbines to large array of turbines the efficiency and impact of the turbines changes. Finally, we illustrate how the arrangement of a turbine farm could affect power and the design of the turbines.

The role of vortex wake dynamics in the flow-induced vibration of tube arrays**Nicholas Kevlahan**

McMaster University

Email: kevlahan@mcmaster.ca

Flow-induced vibration is now well understood for single cylinders, however the prediction of damaging flow induced vibration in tube arrays must still rely on incomplete ad hoc models with many experimentally measured parameters. Flow induced vibration in tube arrays is complicated because it involves the interaction of three distinct instability mechanisms: negative damping (involving one moving cylinder), stiffness controlled (involving more than one moving cylinder) and hysteresis (involving vortex shedding). Our goal is to untangle the relative roles of vortex induced vibration and fluidelastic instability in generating this instability. To address this question we use two numerical techniques: a pseudo-spectral computation of the full Navier-Stokes equations, and a Laurent series computation of the potential flow in multiply connected domains. We find that cylinder motion qualitatively changes the wake dynamics in inline arrays, and the vortex shedding is important even in the non-resonant case. We propose new methods for estimating the critical velocity for the onset of flow-induced vibration.

Flow transitions in a differentially heated rotating channel of fluid**Greg Lewis, Matt Hennessy**

University of Ontario Institute of Technology

Email: greg.lewis@uoit.ca

An investigation of the flow transitions that occur in an $O(2)$ -symmetric differentially heated rotating periodic channel is presented. The primary transition occurs when a time-independent flow that is uniform along the channel bifurcates to a stationary wave flow. We discuss the numerical bifurcation techniques used to trace out the transition in a two-dimensional space of parameters, and present an analysis of the mode-interactions that occur along the transition. The effects of the $O(2)$ symmetry are highlighted.

In addition, we search for the secondary transitions that occur from the stationary wave solution. We discuss a strategy for computing steady solutions of the three dimensional Navier-Stokes equations in the Boussinesq approximation and for determining the secondary transition. In particular, the Navier-Stokes equations are solved using a velocity-vorticity method in combination with a second-order centered finite-difference scheme on an unstaggered and nonuniform grid.

A higher-order finite difference method for solving 2D Burgers' equations**Wenyuan Liao**

University of Calgary

Email: wliao@ucalgary.ca

A fourth-order compact finite difference method is developed to solve the system of two-dimensional Burgers' equations. The new method is based on the two-dimensional Hopf-Cole transformation, which transforms the nonlinear system of two-dimensional Burgers' equations into a linear heat equation. The linear heat equation is then solved by an implicit fourth-order compact finite difference scheme. A compact fourth-order formula is also developed to approximate the boundary conditions of the heat equation, while the initial condition of the heat equation is approximated using Simpson's rule to maintain overall fourth-order accuracy. Numerical experiments have been conducted to demonstrate the efficiency and high-order accuracy of this method.

Fully implicit time integration for incompressible Navier-Stokes equations**Rossitza Marinova, Ray Spiteri, Eddy Essien**

Concordia University College of Alberta

Email: rossitza.marinova@concordia.ab.ca

Fluid flows with high Reynolds numbers or complex geometries are challenging to simulate and of great interest to industry; hence there is significant demand for robust and stable algorithms and software. Fully implicit time-stepping methods are generally more robust and stable than explicit and semi-explicit methods. Therefore, fully

implicit methods should be further investigated and developed. We will present a numerical method for the unsteady incompressible Navier–Stokes equations that is based on a fully implicit time integration and a conservative spatial discretization. The resulting discrete system is solved efficiently using vectorial operator splitting. The most important properties of the method are the overall stability due to the implicit treatment of the time-stepping and boundary conditions and the conservative spatial discretization.

Linear stability analysis of an elastoviscoplastic fluid with internal microstructure

Miguel Moyers-Gonzalez, Teodor Burghelea, Julian Mak
University of Canterbury
Email: miguel.moyersgonzalez@canterbury.ac.nz

We study the linear stability of Plane Poiseuille flow of an elastoviscoplastic fluid using a revised version of the model proposed by Putz and Burghelea (*Rheol. Acta* (2009)48:673–689). The behaviour of the microstructure is governed by a structural variable that switches on and off if τ , the second invariant of the deviatoric stress tensor, is below or above τ_Y , the yield stress. If $\tau \leq \tau_Y$ the material behaves as a viscoelastic solid, if $\tau > \tau_Y$ it behaves as a shear-thinning fluid. Stability results are in close conformity with the ones of a pseudo-plastic fluid.

Analytical and numerical modelling of slip flows in the hydrodynamic entrance region of channels

Yuri Muzychka, Ryan Enright
Memorial University of Newfoundland
Email: y.s.muzychka@gmail.com

A summary of work being undertaken on the numerical solution and modelling of slip flows in the entrance region of channels will be discussed. A review of recent work on the analytical modelling of such flows for circular tubes and parallel plate channels will be presented. A simple model based on these solutions is developed to bound the expected behaviour for other non-circular channels. Numerical simulations to validate the approximate solution of Sparrow are presented. Additional results on finite aspect ratio channels may also be considered.

Efficient design and applications of fluid dynamics methods on graphics processing units

Jason Normore, Simon Harding, Wolfgang Banzhaf
Memorial University of Newfoundland
Email: jnormore@mun.ca

Graphics Processing Units (GPUs) are a type of many-core processing units. They are also in nearly all modern computers, mainly used for graphics processing, such as with video games. The fact that they are so widespread and cost efficient make them ideal for scientific computing applications, such as computational fluid dynamics. We will present an efficient method for solving incompressible fluid flow, both transient flow and steady-state, on GPUs. The SIMPLE method is used for steady-state solver, and a PISO-like method for the transient solver, both efficiently mapped and optimized for the GPU architecture. We will show that these GPU solvers show significant speedup and scale very well with the size of the system. Reasons for the requirement of the design of these methods on GPUs will be discussed, such as optimized shape design with machine learning techniques on a cluster of GPUs, which required a more efficient solver than what is currently available.

How barotropic instability can induce submesoscale motions

Francis Poulin, Chris Subich
University of Waterloo
Email: fpoulin@uwaterloo.ca

The ocean contains a variety of motions over a vast range of length and time scales. The general circulation of the ocean is predominantly forced at the surface on synoptic length-scales, whereas the dissipation due to molecular viscosity is on length scales less than a centimeter. The mechanisms through which the ocean cascades energy have been intensely studied and at present the component of the oceanic energy budget that is least understood is the transfer of energy from the mesoscale to the submesoscale.

The generation of a submesoscale energy cascade can arise due to unbalanced motions, one important example of which is the instability of shear flows. In this work we investigate the barotropic instability with order one Rossby and Burger numbers with relatively weak stratification. We determine the effect of increasing vertical resolution has on resolving the 3D instability, both in the early onset and after the nonlinear adjustment. Furthermore, we compare the effect of the Non-Traditional Coriolis parameters versus making the Traditional Approximation.

The maximum enstrophy growth in Burgers equation

Bartosz Protas, Diego Ayala

McMaster University

Email: bprotas@mcmaster.ca

In this investigation we are interested in the largest enstrophy growth achievable in a hydrodynamic system with some fixed initial enstrophy \mathcal{E}_0 . This question is motivated by one of the “millennium problems” of the Clay Mathematics Institute, namely, whether the 3D Navier–Stokes equation with *smooth* initial condition at $t = 0$ admits smooth solutions for all times $t > 0$. While it is well known that the smoothness of the solution $\mathbf{u}(t)$ implies the finiteness of the enstrophy $\mathcal{E}(t) = \int_{\Omega} \mathbf{u}(t)^2 d\Omega$, the best estimate for the rate of growth of enstrophy is $d\mathcal{E}(t)/dt < C\mathcal{E}(t)^3$ for some constant $C > 0$.

The goal of our study was to establish whether the corresponding finite–time estimate for Burgers equation is sharp. Using computational methods of PDE–constrained optimization we determined a set of optimal initial conditions for Burgers equation which, for a broad range of initial enstrophies \mathcal{E}_0 and time windows $(0, T]$, resulted in the largest possible finite–time enstrophy growth. Our main finding is that while the maximum enstrophy exhibits a power–law behavior with respect to the initial enstrophy, i.e., $\max_{t \in [0, T]} \mathcal{E}(t) \sim \mathcal{E}_0^\alpha$, the exponent was found to be $\alpha \approx \frac{3}{2}$ which is significantly less than 3 predicted by theoretical estimate.

The mathematics of myth: Yield stress behavior as a limit of nonmonotone constitutive theories

Michael Renardy

Virginia Tech

Email: renardym@math.vt.edu

We formulate a model which can describe fluids with a nonmonotone shear stress / shear rate relationship. It is shown how yield stress fluids arise as a limiting case of such a model. Differences between critical stresses for “fast” and “slow” yielding, hysteresis phenomena and thixotropy are naturally explained by the model.

Deformation of a hydrophobic ferrofluid droplet suspended in a viscous medium under uniform magnetic fields

Yuriko Renardy

Virginia Tech

Email: renardy@vt.edu

This is joint work with J. S. Riffle (Chemistry, Virginia Tech), S. Afkhami (New Jersey Institute of Technology), T. G. St Pierre, A. J. Tyler, R. C. Woodward (U. Western Australia). The effect of applied magnetic fields on the deformation of a biocompatible

hydrophobic ferrofluid drop suspended in a viscous medium is investigated numerically and compared with experimental data. A numerical formulation for the time-dependent simulation of magnetohydrodynamics of two immiscible non-conducting fluids is used with a volume-of-fluid scheme for fully deformable interfaces. Analytical formulas for ellipsoidal drops and near-spheroidal drops are reviewed and developed for code validation. At low magnetic fields, both the experimental and numerical results follow the asymptotic small deformation theory. The value of interfacial tension is deduced from an optimal fit of a numerically simulated shape with the experimentally obtained drop shape, and appears to be a constant for low applied magnetic fields. At high magnetic fields, on the other hand, experimental measurements deviate from numerical results if a constant interfacial tension is implemented. The difference can be represented as a dependence of apparent interfacial tension on the magnetic field. This idea is investigated computationally by varying the interfacial tension as a function of the applied magnetic field, and by comparing the drop shapes with experimental data until a perfect match is found. This estimation method provides a consistent correlation for the variation in interfacial tension at high magnetic fields. A conclusion section provides a discussion of physical effects which may influence the microstructure and contribute to the reported observations.

Solving an initial value problem for a parabolic equation by matching asymptotic expansions

Yuri Skrynnikov

Medicine Hat College

Email: yskrynnikov@mhc.ab.ca

A parabolic equation describing fibre orientation in the turbulent flow along a paper machine headbox is considered. An initial value problem is posed to determine orientation distribution of fibres at the headbox exit when it is given at the headbox inlet. In the weak dispersion limit the solution to the initial value problem is sought in a form of an asymptotic expansion in powers of a small parameter. The regular expansion becomes nonuniform when the orientation angle $\phi \rightarrow 0$. Although the small parameter multiplies the second derivative with respect to ϕ , the regular way, by means of matching two asymptotic expansions obtained for small and larger values of ϕ respectively, does not lead to the uniform expansion. Applying the multiple scales method is also unsuccessful, although it yields the correct principal term. The uniform asymptotic solution is constructed by matching the asymptotic expansion solving the initial value problem in the vicinity of the headbox inlet with another asymptotic expansion that does not satisfy the initial condition but solves the equation at larger distances from the initial point.

High order methods for simulating internal wave dynamics**Marek Stastna**, C. Subich, D. Steinmoller

University of Waterloo

Email: mmstastn@uwaterloo.ca

Internal waves occupy a wide range of dynamically active length scales in lakes and the coastal ocean. They have been documented as influencing both mixing in the interior of the water column and resuspension from the bottom in field measurements, laboratory experiments and simulations. In this talk I will review two different spectral and pseudo-spectral approaches to the numerical modeling of internal waves: 1) two dimensional motions of continuously stratified fluids, 2) multi layer models. I will discuss the challenges this modeling presents, as well as the improvements on classical, inherently dissipative numerical models successful implementation yields. I will use boundary layer instability leading to sediment resuspension and the interaction of waves with simple models of plankton dynamics as illustrations. Time permitting I will discuss extensions of the present models to more complex geometries.

Coupled flow and reaction chemistry in porous concrete**John Stockie**, Michael Chapwanya

Simon Fraser University

Email: stockie@math.sfu.ca

We present a mathematical model for the flow of water in hardened concrete, in which the water also reacts with the calcium silicate compounds residing in the porous concrete matrix. The main reaction product – calcium silicate hydrate gel – clogs the pores in the concrete thereby hindering water transport. We use a finite volume method to solve the underlying partial differential equations, and compare our model results to experimental data available from the literature.

Post-gelation behaviour for the coagulation equation with bilinear kernel**Henry van Roessel**

University of Alberta

Email: henry.vanroessel@ualberta.ca

An important phenomenon in a wide variety of processes in physics, chemistry, biology, medicine and engineering is the coalescence or aggregation of small clusters of particles into larger ones. Examples include, but are not limited to, polymerization processes in polymer science, coagulation processes in aerosol and colloidal physics, planet and galaxy formation.

Coagulation processes are governed by integro-differential equations known as coagulation equations. These equations govern the evolution of the particle density as a

function of time. The evolution of the particle concentration depends on the particular coagulation kernel assumed in the model. For some coagulation kernels, there is a loss of mass due to a phase transition, commonly referred to as gelation. This talk discusses the post gelation behaviour for a general bilinear coagulation kernel.

Simulating the energy cascade of stratified turbulence

Michael Waite

University of Waterloo

Email: mwaite@uwaterloo.ca

Numerical simulations of turbulence in stably stratified fluids are sensitive to the relative sizes of the buoyancy and dissipation scales. When the buoyancy scale is smaller than the dissipation scale, downscale turbulent fluxes of energy are suppressed and a steep horizontal wavenumber spectrum develops. However, when the buoyancy scale is relatively free of dissipation, an energy cascade develops with a $-5/3$ spectrum. This regime has been proposed as a model for the atmospheric mesoscale cascade, yet large-scale atmospheric models rarely capture inviscid dynamics on the buoyancy scale. New high-resolution numerical experiments of stratified turbulence will be presented. The implications of using anisotropic numerical grids, which keep the buoyancy scale free of vertical dissipation but not horizontal, will be discussed. Finally, we will examine the extent to which stratified turbulence in these experiments resembles the dry dynamics in recent atmospheric mesoscale simulations.

Asymptotic error analysis of piecewise uniform grids

Brian Wetton

University of British Columbia

Email: wetton@math.ubc.ca

When computing approximations to PDE problems with smooth solutions using regular grids, the error has additional structure. For standard methods, an expansion for the error can be constructed that is regular in the grid spacing. This expansion can be used to justify why convergence with higher regularity is observed (a phenomenon sometimes called super-convergence in the FE community). For some methods, numerical artifacts (boundary layers and errors that alternate in sign between adjacent grid points) can also be present. Identifying the types of errors that are generated by a given scheme and the order at which they occur is called Asymptotic Error Analysis. Some simple cases of this analysis are shown followed by a new result, concerning a numerical artifact from an idealized adaptive grid with hanging nodes.

10.3 Mathematical Biology and Medicine

Organizers: Sharene Bungay and Sue Ann Campbell

| Sunday, July 18 | | Location: Salon D |
|-------------------------|----------------------------------------------------------------------------------------------------------------------|--------------------------|
| Chair: Sharene Bungay | | |
| 9:00–9:20 | Ronald Begg Brain biomechanics and poroelasticity | |
| 9:20–9:40 | Jacques Bélair Bistability and Hopf bifurcations in coupled FitzHugh-Nagumo oscillators | |
| 9:40–10:00 | Matthew Scott Approximating intrinsic noise in continuous multispecies models | |
| Chair: Sue Ann Campbell | | |
| 4:00–4:20 | Raluca Eftimie Mathematical modeling of cancer immunotherapy using a vesicular stomatitis virus and an adenovirus | |
| 4:20–4:40 | Abba Gumel Mathematics of HSV-2 transmission dynamics | |
| 4:40–5:00 | Rebecca Tyson A diffusion-based model to predict transgenic seed | |
| 5:00–5:20 | Jianhong Wu Spatiotemporal spread patterns of infectious diseases | |
| 5:20–5:40 | Hongmei Zhu Evolutionary spectral analysis and its application in studying brain functional networks | |

Abstracts:

Brain biomechanics and poroelasticity

Ronald Begg, Sivabal Sivaloganathan

University of Waterloo

Email: rbegg@uwaterloo.ca

In an attempt to gain a more mechanistic understanding of the pathogenesis and evolution of hydrocephalus, several authors have modelled the brain as a porous elastic medium. In the context of this clinical condition, the strain-rates are very low, so that the assumption of elasticity can be justified. However, experiments undertaken in order to measure brain elastic parameters usually have strain-rates much higher than those associated with hydrocephalus, so that there is a need to account for viscoelastic effects.

We propose an approach whereby the solid portion of the brain is modelled as a viscoelastic material. Using the elastic/viscoelastic analogy to derive overall governing

equations, and effective medium theory to relate the macroscopic parameters of the brain to the parameters of the solid portion, we can obtain theoretical consolidation curves which may be compared to experimental data as well as theoretical curves generated as output from other models.

Bistability and Hopf bifurcations in coupled FitzHugh-Nagumo oscillators

Jacques Bélair, Marcela Molini

Université de Montréal

Email: belair@crm.umontreal.ca

We consider a system of two identical FitzHugh-Nagumo oscillators, in the excitable regime, coupled in the slow variable. The ensuing four-dimensional system can have up to five equilibrium solutions. In a natural two-parameter space, their respective asymptotic stability can be investigated, along with the occurrence of Hopf bifurcations leading to the possible coexistence of multiple stable solutions. The particular role played by the symmetries in the system will be described.

Mathematical modeling of cancer immunotherapy using a vesicular stomatitis virus and an adenovirus

Raluca Eftimie, Jonathan L. Bramson, David J. D. Earn

McMaster University

Email: reftimie@math.mcmaster.ca

Many of the oncolytic viruses used in cancer therapies are rapidly eliminated by the immune response of the host (tumor-bearing hosts may have partially intact immune antiviral mechanisms). This diminishes their anti-tumor effect. However, recent experimental results have shown that the treatment of a particular type of murine melanoma with two viruses which express the same tumor-associated antigen, namely a replication-incompetent adenovirus and an oncolytic vesicular stomatitis virus, extends the survival rate of mice.

Here we derive a mathematical model to investigate the interactions among immune cells, cancer cells, and two viruses: the adenovirus and the vesicular stomatitis virus. We use experimental data from our lab to validate the model and estimate parameter values. This allows us to discuss conditions that lead to tumor growth and to propose hypotheses for tumor elimination which can be tested experimentally. We suggest that suppression of the immune response might improve viral oncolysis but cannot lead to a cure (i.e., no stable tumor-free steady states). However, complete elimination of cancer cells is possible in the presence of an immune response, and depends on the magnitude of this response as well as the parameters that control virus proliferation and tumor cell lysis.

Mathematics of HSV-2 transmission dynamics**Abba Gumel, C. N. Podder**

University of Manitoba

Email: gumelab@cc.umanitoba.ca

The talk focusses on the design and rigorous analysis of a deterministic model for the transmission dynamics of herpes simplex virus Type 2 in a population. Conditions for the effective control and/or persistence of the disease will be derived.

Approximating intrinsic noise in continuous multispecies models**Matthew Scott, Francis J. Poulin, Herbert Tang**

University of Waterloo

Email: mscott@math.uwaterloo.ca

In small-scale chemical reaction networks, the local density of molecules is changed by discrete jumps due to reactive collisions, and through transport. I will introduce a systematic perturbation scheme to analytically characterize these nonequilibrium intrinsic fluctuations in a multispecies spatially-varying system. The method is illustrated on a variety of model systems. In all cases, the continuous approximation method is corroborated with extensive stochastic simulation. In the case of a homogeneous steady-state, noise can lead to patterning in a subset of reactants. For a spatially-varying steady-state, I will demonstrate that embryonic patterning mediated by regulatory mRNA is surprisingly robust to intrinsic fluctuations. The connection to stochastic partial differential equations will be outlined, and I will indicate how most existing treatments of stochastic spatial models do not correctly accommodate intrinsic fluctuations.

**A diffusion-based model to predict transgenic seed contamination in
bee-pollinated crops****Rebecca Tyson, J. Ben Wilson, W. David Lane**

University of British Columbia Okanagan

Email: rebecca.tyson@ubc.ca

The adventitious presence of transgene containing seed in conventional crops is an issue of considerable interest; a model to predict levels will aid regulators and help to allay concerns of farmers and consumers. While outcrossing levels have been described in crops such as rape that are wind-pollinated, or both wind- and insect-pollinated, much less is known about pollen dispersal in exclusively insect-pollinated crops. In this talk, we report on experimental work measuring percent transgenic seed in an apple orchard with a row of 200 transgenic source trees and use this data to develop a mathematical model for pollen dispersal and subsequent transgenic seed distribution. The model is used to predict the percent transgenic seed in neighbouring conventional trees as a

function of the size of each orchard block and the distance between them. The model explicitly shows the effect of overlapping transgenic and nontransgenic pollen distributions in setting seed distributions, and also explains the value of buffer rows. The model may be useful for determining distributions on transgenic seed plantings needed to allow for an adventitious presence of, for example, 0.9%.

Spatiotemporal spread patterns of infectious diseases involving animal hosts

Jianhong Wu

York University

Email: wujh@mathstat.yorku.ca

Characterization of spatiotemporal patterns of diseases involving animal hosts such as West Nile virus, Lyme diseases and avian influenza requires incorporation of seasonality of a variety of biological activities and physiological structures of individuals into dynamical compartmental models. This gives rise to large scale systems of delay/partial differential equations with periodic coefficients and requires novel ideas and techniques of infinite dimensional dynamical systems, which will be briefly addressed in this talk.

Evolutionary spectral analysis and its application in studying brain functional networks

Hongmei Zhu, Cheng Liu, William Gaetz, T. P. L. Roberts

York University

Email: hmzhu@yorku.ca

The dynamics of brain functional activities make evolutionary spectral analysis a powerful tool in revealing the time-varying interactions among different brain regions. In this paper, we address ways of estimating evolutionary power spectrum and derive other statistical measures using the general Cohen's class distributions. A magnetoencephalography study using the developed evolutionary spectral analysis techniques reveals interesting temporal interaction between contralateral and ipsilateral motor cortices under the multi-source interference task.

10.4 Mathematical and Theoretical Physics

Organizer: Marco Merkli

| Sunday, July 18 | | Location: Plymouth |
|-------------------------------|------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|
| Chair: Marco Merkli | | |
| 9:00–9:20 | Frank Marsiglio The Dynamic Hubbard model: an introduction | |
| 9:20–9:40 | Robert Gooding A multi-site mean field theory of disordered cold atomic gases | |
| 9:40–10:00 | Malcolm Kennett Time dependent quantum phase transition in the Bose-Hubbard model | |
| Chair: Marco Merkli | | |
| 10:30–10:50 | Stephen Anco New conserved integrals of compressible fluid flow in $n > 1$ spatial dimensions | |
| 10:50–11:10 | Gustavo Carrero Studying receptor diffusion by interpreting SPT data with a correlated random walk and a first-passage time algorithm | |
| 11:10–11:30 | Vitali Vougalter On the solvability conditions for the diffusion equation with convection terms | |
| 11:30–11:50 | Brandon van Zyl The unitary Fermi gas and fractional exclusion statistics | |
| Chair: Chris Radford | | |
| 4:00–4:20 | Mohamed Azzouz Hidden order in high-temperature superconductors | |
| 4:20–4:40 | Duncan O'Dell Quantum catastrophes in the atomic Josephson junction | |
| 4:40–5:00 | Kirill Samokhin Goldstone modes in nonuniform superconductors | |
| 5:00–5:20 | Shannon Starr Graphical methods in quantum spin chains | |
| 5:20–5:40 | Mark Shegelski Quantum tunnelling of a molecule with a single bound state | |
| <i>continued on next page</i> | | |

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| <i>continued from previous page</i> | |
| Monday, July 19 | Location: Plymouth |
| Chair: Chris Radford | |
| 9:00–9:20 | Sheldon Opps Confinement effects on foraging efficiency in complex landscapes |
| 9:20–9:40 | Ben Fortescue Threshold quantum secret sharing using graph states of prime-dimensional systems |
| 9:40–10:00 | Marco Merkli Resonance theory for open quantum systems |

Abstracts:

New conserved integrals of compressible fluid flow in $n > 1$ spatial dimensions

Stephen Anco, Aman Dar
Brock University
Email: sanco@brocku.ca

I will present a summary of recent work on conservation laws of compressible fluid flow in $n > 1$ spatial dimensions. This work applies the general method of Euler operators and multipliers to give a complete classification of local conservation laws and conserved integrals for two primary cases of physical and mathematical interest in the study of fluid flow: (1) kinematic conservation laws, like entropy, mass, energy, momentum and angular momentum, for which the conserved density and flux depend only on the fluid velocity, pressure and density (but not their spatial derivatives), in addition to the time and space coordinates; (2) vorticity conservation laws, such as three-dimensional helicity and two-dimensional circulation, where the conserved density and flux have an essential dependence on the curl of the fluid velocity (in a form exhibiting odd parity under spatial reflections). As main results, the classification yields explicit conserved integrals describing in all even dimensions a generalized circulation and a circulatory entropy, and in all odd dimensions (greater than one) a generalized helicity.

Hidden order in high-temperature superconductors

Mohamed Azzouz
Laurentian University
Email: mazzouz@laurentian.ca

The so-called pseudogap (PG) phase of the high-critical temperature superconductors (HTSC) continues to challenge the current understanding of condensed-matter. The

HTSCs consist of CuO_2 planes, where holes are doped by chemically removing electrons from the Cu-O ligands. These materials show an antiferromagnetic phase below 2% doping. Between 5% and 30% doping the superconducting dome sets in below a transition temperature T_C that is optimal at 16% doping. The phase for doping above optimal is more or less a Fermi liquid. However, the PG phase for temperature above T_C and doping less than optimal is characterized by a depletion of the density of state, with no long-range conventional order. In 2003, I proposed the rotating antiferromagnetic (RAF) hidden order concept in order to interpret the experimental data of the PG phase. In this talk I will explain the RAF order, and present a comparison between the RAF hidden order in the HTSCs and the hidden order in other strongly-correlated fermions systems, like URu_2Si_2 .

Studying receptor diffusion by interpreting SPT data with a correlated random walk and a first-passage time algorithm

Gustavo Carrero, Vishaal Rajani, Gerda de Vries, Christopher Cairo
Athabasca University
Email: gustavoc@athabascau.ca

One of the most powerful and commonly used methods for studying molecular diffusion on the cell membrane is Single Particle Tracking (SPT). During an SPT experiment, the trajectory of a membrane-associated biomolecule, labeled with an optical bead or a fluorescent tag, is recorded. This trajectory or SPT data is used to quantify and characterize the motion of the individual particles being studied. In particular, one of the main problems in the analysis of SPT data of membrane receptors is to identify the presence of heterogeneity, which may be attributed to microdomains or receptor clusters. In this work, we apply a correlated random walk (CRW) model and adapt a first-passage time (FPT) algorithm originally developed for the interpretation of animal movement, to study the molecular diffusion of membrane receptors and provide a robust method for determining the presence and size of confined regions of diffusion. This SPT data analysis is used to identify heterogeneity for the lymphocyte receptor LFA-1 by determining the presence and size of receptor clusters.

Threshold quantum secret sharing using graph states of prime-dimensional systems

Ben Fortescue, Adrian Keet, Damian Markham, Barry C. Sanders
University of Calgary
Email: bfortesc@ucalgary.ca

Secret sharing schemes allow a classical or quantum secret to be divided among many parties such that it can be recovered only by some specified set of parties collaborating in order to do so. It is known that arbitrary secret sharing schemes may be constructed by

concatenating threshold schemes, in which the secret can be recovered by any sufficiently large number of parties, and the remainder are denied any knowledge of the secret

I will discuss a formalism within which, using entangled graph states of prime-dimensional systems, a variety of different threshold secret sharing schemes (involving both quantum and classical secrets and quantum and classical channels shared between parties) may be unified. I will give explicit protocols for three varieties of secret sharing within this formalism, including some for which the analogous formalism using graph states of two-dimensional systems is not sufficient.

A multi-site mean field theory of disordered cold atomic gases

Robert Gooding, Ryan Jones

Queen's University

Email: gooding@physics.queensu.ca

Mean field theories are often used as a first attempt when analyzing the properties of interacting systems. For cold atomic gases in the strong interaction limit (in and near the Mott Insulator regime), standard mean field theory is based on the sum of single-site Hamiltonians. The unusual behaviour of disordered systems, such as localization phenomena, requires that the spatial correlations introduced by the disorder be treated carefully. We will present new work associated with the development and implementation of a multi-site mean field theory for the disordered Bose Hubbard model, and demonstrate the changes of the Mott Insulator/Bose glass phase boundary that we have found.

Time dependent quantum phase transition in the Bose-Hubbard model

Malcolm Kennett

Simon Fraser University

Email: malcolmk@sfu.ca

Cold bosonic atoms confined in an optical lattice potential give a realization of the Bose Hubbard model, in which it is possible to study the phase transition between a superfluid and a Mott insulator as the depth of the optical lattice is varied. Cold atom systems are a particularly attractive setting in which to study the model due to ability to tune parameters in the model in real time. I will discuss the use of the Schwinger-Keldysh formalism to describe the effects of time dependent variations of the parameters in the Bose-Hubbard model, allowing for a description of a sweep across the quantum critical point associated with the superfluid insulator transition.

The Dynamic Hubbard model: an introduction**Frank Marsiglio**

University of Alberta

Email: fmars@phys.ualberta.ca

In condensed matter physics, especially in the sub-topic of high temperature superconductivity and strongly correlated electron systems, we almost never try to solve the difficult problem of the behaviour of many electrons in a solid state environment interacting with one another through the long-range Coulomb interaction. Instead we adopt ‘effective’ models, the most famous of which is perhaps the Hubbard model. The Hubbard model is not completely solved, but maybe the Hubbard model doesn’t have the ‘right stuff’ anyways. The Dynamic Hubbard model is a step in one particular direction to remedy this; the key ingredient is orbital relaxation. We provide an introduction to this model, and show some simple results obtained thus far through the dynamical mean field theory (DMFT) approximation. Connections with previous models used to describe the high temperature superconductors will be pointed out.

Resonance theory for open quantum systems**Marco Merkli**

Memorial University of Newfoundland

Email: merkli@mun.ca

We outline a rigorous theory for the reduced dynamics of open quantum systems interacting with heat reservoirs. The approach is based on a representation of the propagator in terms of the resonance data of the system. We present applications to a system of spins (qubits) coupled to reservoirs and estimate decoherence times and entanglement death and survival times.

Quantum catastrophes in the atomic Josephson junction**Duncan O’Dell**

McMaster University

Email: dodell@mcmaster.ca

I will discuss the application of Thoms catastrophe theory to the problem of a dilute gas Bose-Einstein condensate (BEC) in a double-well potential. A BEC in a double-well potential is a system closely related to the Josephson junction, i.e. two superconductors coupled via a tunneling junction. As is well known, this problem can be mapped onto the pendulum (or equivalently, a particle in a sinusoidal potential). For certain initial conditions, the dynamics of a pendulum leads to caustics which are regions of focusing where the probability for finding the pendulum at a particular angle diverges. Caustics are a well-studied phenomenon in geometrical optics and their natural description is

via catastrophe theory. Furthermore, catastrophe theory gives a prescription for taming the divergence at a caustic for optics this corresponds to upgrading the geometrical theory to a wave theory. For a BEC in a double-well, where the caustics correspond to Schrodinger cat states, catastrophe theory shows how divergences in the (mean-) field theory can be tamed by upgrading to a quantum field theory i.e. counting atoms.

Confinement effects on foraging efficiency in complex landscapes

Sheldon Opps, Todd Mackenzie
University of Prince Edward Island
Email: sopps@upei.ca

In fragmented landscapes that result from agricultural activities, portions of destroyed habitat are often replaced with novel habitats that may or may not be seen as hospitable habitats by animals. The responses of animals to these changes are influenced by their ability to move among patches, the population dynamics in habitat patches of different sizes, and the factors that control whether they remain in or disperse from suitable habitat. We have developed a computer simulation model to study the movement characteristics of a generic walker (animal) within spatially heterogeneous corridors of varying width. Each corridor was constructed with a certain percentage of good habitat having a characteristic fractal dimension, D , and containing randomly placed targets (resources). By varying a number of key parameters, such as the corridor width, the relative composition and complexity of the corridors, the target density, and the target regeneration time, we have been systematically studying confinement effects on movement within fragmented landscapes with edge habitat. The foraging efficiency of our composite walker was compared with other common walker models, including Lévy and Brownian walkers, each characterized by concatenated flights.

Goldstone modes in nonuniform superconductors

Kirill Samokhin
Brock University
Email: kirill.samokhin@brocku.ca

In addition to the $U(1)$ phase-rotation symmetry, the order parameter in nonuniform superconductors can also break translational symmetry, which leads to a rich spectrum of Goldstone modes. We present a microscopic derivation of the energy of these modes and calculate the superfluid phase stiffness and the elastic moduli of various nonuniform superconducting phases.

Quantum tunnelling of a molecule with a single bound state

Mark Shegelski, Jeremy Kavkay
University of Northern BC
Email: mras@unbc.ca

We discuss the quantum mechanical tunnelling of a diatomic, homo-nuclear molecule with a single bound state incident upon a delta potential barrier. We use a time-dependent formulation. The molecular wave function is modeled as a Gaussian wave packet. It is found that a molecule may transition between the bound state and an unbound state numerous times during the process of reflection from or transmission past the barrier. It is also found that, in addition to reflecting and transmitting, the molecule may also temporarily straddle the potential barrier in an unbound state.

Graphical methods in quantum spin chains

Shannon Starr, Bruno Nachtergaele, Stephen Ng
University of Rochester
Email: sstarr@math.rochester.edu

Some quantum spin chains may be studied using graphical methods. I will describe this for the one-dimensional spin-1/2 Heisenberg quantum spin chain using the Temperley-Lieb algebra. Then I will describe recent results we have made to extend this to higher spins. This talk describes work carried out by various people including Stephen Ng, Bruno Nachtergaele, Wolfgang Spitzer and myself.

The unitary Fermi gas and fractional exclusion statistics

Brandon van Zyl
St. Francis Xavier University
Email: bvanzyl@stfx.ca

Using the phenomenon of a Feshbach resonance, the two-body inter-particle interactions between the neutral ultra-cold fermions can be continuously tuned according to the magnitude of the magnetic field across the resonance region. Of particular interest is the so-called unitary regime, which occurs at the midpoint of this crossover, and is characterized by the divergence of the scattering length due to the existence of a zero-energy bound state for the two-body system. As the only relevant length scale in this regime is set by the Fermi momentum, the corresponding energy scale is the Fermi kinetic energy. It follows that in three-dimensions, the energy density should be proportional to that of a free Fermi gas, with the constant of proportionality being *a priori* unknown. The determination of this (universal) proportionality constant is a challenging problem for theorists owing to the fact that the usual perturbative techniques fail in the unitary regime.

In this talk, I will discuss the possibility of describing a gas of ultra-cold, neutral fermions in the unitary regime through the use of fractional exclusion statistics (FES). Within FES, the universal constant may be exactly determined.

On the solvability conditions for the diffusion equation with convection terms

Vitali Vougalter, Vitaly Volpert

University of Toronto

Email: vitali@math.toronto.edu

Linear second order elliptic equation describing heat or mass diffusion and convection on a given velocity field is considered in \mathbb{R}^3 . The corresponding operator L may not satisfy the Fredholm property. In this case, solvability conditions for the equation $Lu = f$ are not known. In this work, we derive solvability conditions in $H^2(\mathbb{R}^3)$ for the non self-adjoint problem by relating it to a self-adjoint Schrödinger type operator, for which solvability conditions are obtained in our previous work.

10.5 Nonlinear Dynamics and Control

Organizers: Jahrul Alam and Dong Eui Chang

| Monday July 19 | | Location: Salon D |
|-------------------------------|--------------------------------------------------------------------------------------------------------------------|--------------------------|
| Chair: Yasuhide Fukumoto | | |
| 9:00–9:20 | Cristina Stoica Some applications of genericity in dynamics and control | |
| 9:20–9:40 | Sue Ann Campbell Nonlinear analysis of a maglev system with time-delayed feedback control | |
| 9:40–10:00 | Dana Kulic Incremental learning of motion primitives for full body motions | |
| Chair: Dong Eui Chang | | |
| 10:30–10:50 | Razvan C. Fetecau A nonlocal hyperbolic model for self-organization of biological groups | |
| 10:50–11:10 | Abba Gumel Dynamically-consistent finite-difference methods for population biology models | |
| 11:10–11:30 | Shafiqul Islam Invariant measures of stochastic perturbations of dynamical systems using Fourier approximations | |
| 11:30–11:50 | Soo Jeon Global stability of controlled mechanical systems with static friction | |
| Tuesday July 20 | | Location: Salon D |
| Chair: Jahrul Alam | | |
| 10:30–10:50 | Scott David Kelly Idealized modeling of planar fishlike swimming for motion control | |
| 10:50–11:10 | Dong Eui Chang Application of differential algebra to LaSalle's invariance principle | |
| 11:10–11:30 | Melvin Leok Discrete Hamiltonian variational integrators | |
| 11:30–11:50 | Manfredi Maggiore Virtual holonomic constraints for Euler-Lagrange systems | |
| Chair: Dong Eui Chang | | |
| 4:00–4:20 | Abdol-Reza Mansouri Topological obstructions to transverse feedback linearization | |
| <i>continued on next page</i> | | |

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| 4:20–4:40 | Ilya Nemenman Adiabatic dynamics and control of nonlinear stochastic systems |
| 4:40–5:00 | David Siegel Persistence in chemical kinetics systems |
| 5:00–5:20 | Mireille Broucke Reach control problem on simplices |
| 5:20–5:40 | Yasuhide Fukumoto Energy, action and mean flow of waves on a vortex of a fluid flow, and their application to stability analysis |
| 5:40–6:00 | Dmitry Zenkov Quasivelocities in nonholonomic dynamics and control |

Abstracts:

Reach control problem on simplices

Mireille Broucke

University of Toronto

Email: broucke@control.utoronto.ca

This talk concerns the reach control problem, which is a subproblem within a family of problems concerning reachability specifications for control systems. The problem is formulated on polyhedra or simplices in the state space and has, so far, focused on the class of affine systems. Roughly speaking, the problem is for an affine system $x' = Ax + Bu + a$ defined on a simplex to reach a prespecified facet of the simplex in finite time without first exiting the simplex. The significance of the problem stems from its capturing the essential features of reachability problems for control systems: the presence of state constraints and the notion of trajectories reaching a goal in a guided and finite-time manner. I will give a brief overview of results on the reach control problem, especially concerning solvability by continuous state feedback. Then I will discuss recent results concerning the so-called reach control indices and how they can be used to construct discontinuous state feedbacks.

Nonlinear analysis of a maglev system with time-delayed feedback control

Sue Ann Campbell, Lingling Zhang, Lihong Huang

University of Waterloo

Email: sacampbell@uwaterloo.ca

We study a model for a maglev system with time-delayed feedback. Using linear analysis, we determine constraints on the feedback control gains and the time delay which

ensure stability of the maglev system. We then show that a Hopf bifurcation occurs at the linear stability boundary. To gain insight into the periodic motion which arises from the Hopf bifurcation, we use the method of multiple scales on the nonlinear model. This analysis shows that for practical operating ranges, the maglev system undergoes both subcritical and supercritical bifurcations, and which give rise to unstable and stable limit cycles respectively. Numerical simulations confirm the theoretical results and indicate that unstable limit cycles may coexist with the stable equilibrium state. This means that large enough perturbations may cause instability in the system even if the feedback gains are such that the linear theory predicts that the equilibrium state is stable.

Application of differential algebra to LaSalle's invariance principle

Dong Eui Chang

University of Waterloo

Email: dechang@math.uwaterloo.ca

LaSalle's invariance principle is one of the most powerful tools in Lyapunov stability theory. Despite its power, the application of LaSalle's invariance principle often involves complicated computations, which are not always easy to carry out. To overcome this difficulty, Jurdjevic and Quinn [1978] proposed a theorem that depends on the structure of a control-affine nonlinear system, being independent of the choice of a Lyapunov function. The Jurdjevic-Quinn method is a first-order condition, so it inherently gives limitations despite its simplicity. Lee and Arapostathis [1988] extended the Jurdjevic-Quinn method by adding higher-order conditions but the Lee-Arapostathis method depends on the choice of a Lyapunov function. Though both methods are useful, there is a gap between both the methods and LaSalle's invariance principle. In this talk, we take a different – perhaps better – approach. We interpret LaSalle's invariance principle in the context of differential algebra. Our formulation is very simple. Moreover, it is computationally powerful thanks to various symbolic computational tools in differential algebra that run on Maple or Mathematica.

A nonlocal hyperbolic model for self-organization of biological groups

Razvan Fetecau, Raluca Eftimie

Simon Fraser University

Email: van@math.sfu.ca

We introduce and study a new nonlocal hyperbolic model for the formation and movement of animal aggregations. The main modeling assumption is that the nonlocal attractive, repulsive, and alignment interactions between individuals can influence both the speed and the turning rates of group members. We establish the local existence and uniqueness and show that the nonlinear hyperbolic system does not develop shock

solutions (gradient blow-up). Depending on the relative magnitudes of attraction and repulsion, we show that the solutions of the model either exist globally in time or may exhibit finite-time amplitude blow-up. We illustrate numerically the various patterns displayed by the model: dispersive aggregations, finite-size groups and blow-up patterns, the latter corresponding to aggregations which may collapse to a point. Extensions to higher dimensions will be discussed briefly.

Energy, action and mean flow of waves on a vortex of a fluid flow, and their application to stability analysis

Yasuhide Fukumoto, Hirota Makoto

Kyushu University

Email: yasuhide@math.kyushu-u.ac.jp

A steady Euler flow of an inviscid incompressible fluid is characterized as an extremum of the total kinetic energy (= the Hamiltonian) with respect to perturbations constrained to an isovortical sheet (coadjoint orbits). An isovortical perturbation preserves vortex-line topology and is expressible only by the Lagrangian variables. The criticality in the Hamiltonian allows us to work out the energy and the mean flow, induced by nonlinear interaction of themselves, of three-dimensional waves on a steady vortical flow; these nonlinear quantities, of second order in amplitude, can be calculated solely from the linear Lagrangian displacement. By invoking Hamiltonian Noether's theorem, the wave-induced mean flow is shown to be the pseudomomentum, and therefore the both nonlinear quantities are deduced from the wave action. The stability of the motion of a strained vortex tube is put on the ground of Krein's Hamiltonian bifurcation theory. We demonstrate how the Lagrangian approach overcomes a difficulty in the Eulerian approach to weakly nonlinear stability analysis.

Dynamically-consistent finite-difference methods for population biology models

Abba Gumel, S.M. Garba, J.M. Lubuma

University of Manitoba

Email: gumelab@cc.umanitoba.ca

Population biology models, such as those associated with the transmission dynamics of human diseases, are often formulated in the form of systems of nonlinear differential equations. The (typically) large size and nonlinearity of these systems often make their analytical solutions difficult (or impossible) to obtain. Consequently, robust numerical methods have to be used to obtain their approximate solutions. This talk addresses the problem and challenges of designing discrete-time models (finite-difference methods) that are dynamically-consistent with the continuous-time disease transmission models they approximate (in particular in preserving some of the key properties of the

continuous-time models such as positivity and boundedness of solutions).

**Invariant measures of stochastic perturbations of dynamical systems using
Fourier approximations**

Shafiqul Islam, Pawel Gora

University of Prince Edward Island

Email: sislam@upei.ca

We consider dynamical system $\tau : [0, 1] \rightarrow [0, 1]$ and its stochastic perturbations $\bar{q}^N(\tau(x), \cdot)$, $N \geq 1$. Using Fourier approximation we construct a finite dimensional approximation P_N to a perturbed Perron-Frobenius operator. Let \hat{f} be an invariant density of τ and f_N^* be a fixed point of P_N . We show that $\{f_N^*\}$ converge in L^1 to \hat{f} .

Global stability of controlled mechanical systems with static friction

Soo Jeon

University of Waterloo

Email: soojeon@uwaterloo.ca

In servo control of mechanical systems, the Coulomb (or static) friction is an important nonlinearity not only as the source of tracking error but also as the cause of instability generating limit cycles. This talk focuses on the latter. As one of the simplest but unsolved nonlinear stability problems, it has a deep and long relationship with such classical theories as differential equations with discontinuities, relay feedback systems and sliding mode theories, and more recently with piecewise linear systems and hybrid systems. This talk will first discuss the existing theoretical results that have known to be applied (directly or indirectly) to this problem and then will introduce those that have been newly found to explicitly address this problem. This talk will specifically describe 1) the generalized characterization of controlled mechanical systems with nonlinear friction, 2) absolute stability for relay nonlinearity, 3) integral quadratic constraint (IQC) formalism, 4) piecewise quadratic Lyapunov function (PWQL) and 5) exact algebraic analysis of mechanical servo systems with first order controller.

Idealized modeling of planar fishlike swimming for motion control

Scott Kelly

University of North Carolina at Charlotte

Email: scott@kellyfish.net

Models for aquatic locomotion generally seek to balance fidelity and scope with analytical or computational tractability. When the goal in model development is a platform for model-based feedback control design, analytical structure is essential to provide a point of access for most current design techniques, but some fidelity may be sacrificed as

long as the scope of the model encompasses the range of situations under which control will be applied. This talk will describe a model for simplified fishlike swimming based on the Hamiltonian equations governing the interaction of a free deformable body with a system of point vortices in a planar ideal fluid. The use of this model in designing motion-control strategies for a biologically inspired robotic vehicle will be discussed, with a particular focus on the realization of energy-efficient gaits for solitary swimming and energy-harvesting methods for controlled schooling.

Incremental learning of motion primitives for full body motions

Dana Kulic

University of Waterloo

Email: dkulic@ece.uwaterloo.ca

As robots move to human environments, the ability to learn and imitate from observing human behaviour will become important. The talk will focus on our recent work on designing humanoid robots capable of continuous, on-line learning through observation of human movement. Learning behaviour and motion primitives from observation is a key skill for humanoid robots, enabling humanoids to take advantage of their similar body structure to humans. First, approaches for designing the appropriate motion representation and abstraction will be discussed. Next, an approach for on-line, incremental learning of whole body motion primitives and primitive sequencing from observation of human motion will be described. The second half of the talk will overview recent work on learning the appropriate robot controller in addition to the trajectory, based on incremental learning of the robot dynamics. The talk will conclude with an overview of preliminary experimental results and a discussion of future research directions.

Discrete Hamiltonian variational integrators

Melvin Leok, Jingjing Zhang

University of California, San Diego

Email: mleok@math.ucsd.edu

We consider the continuous and discrete-time Hamilton's variational principle on phase space, and characterize the exact discrete Hamiltonian which provides an exact correspondence between discrete and continuous Hamiltonian mechanics. The variational characterization of the exact discrete Hamiltonian naturally leads to a class of generalized Galerkin Hamiltonian variational integrators, which include the symplectic partitioned Runge-Kutta methods. We also characterize the group invariance properties of discrete Hamiltonians which lead to a discrete Noether's theorem.

Virtual holonomic constraints for Euler-Lagrange systems**Manfredi Maggiore**, Luca Consolini

University of Toronto

Email: maggiore@control.utoronto.ca

The notion of virtual holonomic constraint is a useful paradigm for the control of oscillations in mechanical systems. It is one of the underlying mechanisms in the technique developed by Grizzle and collaborators to stabilise walking motion in bipedal robots. This talk explores virtual holonomic constraints for Euler-Lagrange systems with n degrees-of-freedom and $n - 1$ controls. The constraints have the form $q_1 = \phi_1(q_n), \dots, q_{n-1} = \phi_{n-1}(q_n)$, where q_n is a cyclic configuration variable, so their enforcement corresponds to the stabilisation of a desired oscillatory motion. We will present conditions under which such a set of constraints is feasible, meaning that it can be made invariant by feedback. We will show that it is possible to systematically determine feasible virtual constraints as periodic solutions of a scalar differential equation. Further, under a symmetry assumption we will show that the motion on the constraint manifold is a Euler-Lagrange system with one degree-of-freedom, and use this fact to completely characterize its dynamical properties. Finally, we will show that if the constraint is feasible then the virtual constraint manifold is exponentially stabilisable.

Topological obstructions to transverse feedback linearization**Abdol-Reza Mansouri**

Queen's University

Email: mansouri@mast.queensu.ca

We consider the problem of transverse feedback linearization of a control affine system to a closed, connected, embedded submanifold of \mathbb{R}^n . This is a problem of importance in nonlinear control theory, with applications principally to set stabilization. We show that the requirement that, in a neighborhood of every point of the submanifold, the system be feedback-equivalent to a system whose dynamics transversal to the submanifold are linear and controllable imposes a number of topological conditions on the submanifold. These topological conditions manifest themselves as the vanishing of certain characteristic classes of the submanifold.

Adiabatic dynamics and control of nonlinear stochastic systems**Ilya Nemenman**

Emory University

Email: ilya.nemenman@emory.edu

Modern biochemical experiments can measure and perturb dynamics of thousands of molecular species at the same time. This provides data for and creates a need to build

computational models of large-scale stochastic dynamical systems, open to perturbations over long time scales. However, theoretical methods for analysis of such systems lag far behind. In this presentation, I will review our work on developing methods for coarse-graining nonlinear, stochastic dynamics with adiabatically slow external driving. I will show that the coarse-graining generally results in a geometric corrections to the moment generating functional of stochastic fluxes. The main property of such corrections is that they change their sign under time inversion of external driving. While generally small, such corrections become important in the presence of symmetries or of rare transitions. They have a variety of applications, including: reverse-engineering kinetic diagrams from experimental data; simulating complex, nonlinear, stochastic biochemical systems; or designing control strategies for stochastic processes. This work was done in collaboration with Nikolai Sinitsyn and Sorin Tanase Nicola and was supported in part by Los Alamos National Laboratory LDRD Program.

Persistence in chemical kinetics systems

David Siegel, Matthew Johnston

University of Waterloo

Email: dsiegel@math.uwaterloo.ca

It is known that a solution to a chemical kinetics system can only approach the boundary of the non-negative orthant at points belonging to a semi-locking set. We show that if every semi-locking set satisfies a conservation condition or is dynamically non-emptyable, the system is persistent. This generalizes results of Angeli, De Leenheer & Sontag (2007) and Anderson & Shiu (2010).

Some applications of genericity in dynamics and control

Cristina Stoica

Wilfrid Laurier University

Email: cstoica@wlu.ca

A property is generic within a space of functions if those functions with the given property form a residual subset of the space. We earlier showed that for any given smooth vector field, and generic smooth real-valued functions F , the vector field has no non-equilibrium solutions conserving F . An analogous statement holds for relative equilibria of symmetric vector fields, and symmetric functions F .

We present applications of the above results in two areas. First, we observe that the following generalization of Saari's conjecture in celestial mechanics is true for generic $SO(2)$ -invariant functions F : "In the planar Newtonian N -body problem, the only solutions along which F is conserved are the relative equilibria". Second, within the theory of nonlinear stabilization, we show that one generic control is sufficient to asymptotically stabilize an equilibrium.

This is joint work with Tanya Schmah (University of Toronto).

Quasivelocities in nonholonomic dynamics and control

Dmitry Zenkov, Anthony Bloch, Jerrold Marsden
North Carolina State University
Email: dvzenkov@ncsu.edu

Quasivelocities are the components of mechanical system's velocity relative to a set of vector fields that are not associated with configuration coordinates. This talk concentrates on the utilization of quasivelocities in the formulation of dynamics of systems with velocity constraints. Applications of quasivelocities to qualitative analysis of dynamics of systems with constraints and to stabilization of relative equilibria will be discussed.

10.6 Ocean Modelling and Technology

Organizers: Wei Qui, Christopher Williams, F. Mary Williams

| Monday, July 19 | | Location: Viking |
|-----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------|
| Chair: F. Mary Williams | | |
| 9:00–9:20 | Heather Peng Second-order shallow water long wave reproduction in a large wave basin | |
| 9:20–9:40 | Mahmoud Haddara Complete identification of the equation of motion of a single degree system in waves using its stationary random response | |
| 9:40–10:00 | Jeremy Dillon Velocity measurement in a turbulent jet: Observations with multi-frequency coherent Doppler sonar and particle image velocimetry | |
| Chair: Wei Qui | | |
| 10:30–10:50 | Qingyong Yang Computation of slamming loads on a catamaran | |
| 10:50–11:10 | Tim Rees Investigating near-resonant triad interactions in stratified flows | |
| 11:10–11:30 | Stéphane Etienne Some aspects of Vortex-Induced Vibrations of circular cylinders | |
| 11:30–11:50 | Don Bass Modeling using the ship motion code MOTSIM coupled to the CFD code Flow-3D | |
| Tuesday, July 20 | | Location: Viking |
| Chair: Christopher Williams | | |
| 10:30–10:50 | John Wang Numerical validation for ship performance in broken ice floes | |
| 10:50–11:10 | Wayne Raman-Nair Deployment of a freefall lifeboat into waves | |
| 11:10–11:30 | Christian Knapp Dynamics of ship towing in ice | |
| 11:30–11:50 | Dag Friis Fishing vessel energy efficiency projects at Ocean Engineering Research Centre of Memorial University | |

Abstracts:**Modeling using the ship motion code MOTSIM coupled to the CFD code
Flow-3D
Don Bass**

Memorial University of Newfoundland
Email: dbass@mun.ca

The presentation describes work carried out over a number of years in the field of Ocean Technology (and Naval Architecture) using a floating body motion simulation code (MOTSIM) coupled to a CFD code (Flow-3D). Examples include anti-roll tanks on fishing boats, water trapped on deck, flooding of decks on moving vessels, motions of water in moon pools, wave action in floating docks etc.

**Velocity measurement in a turbulent jet: Observations with
multi-frequency coherent Doppler sonar and particle image velocimetry**

Jeremy Dillon, Len Zedel, Alex Hay
Memorial University of Newfoundland
Email: jeremy.dillon@mun.ca

Coherent Doppler sonar is a useful tool for non-invasively measuring currents, sediment transport, and turbulence in coastal environments. However, measurement errors occur due to pulse-to-pulse backscatter decorrelation associated with: scatterer advection through the sample volume, velocity shear and turbulence within the sample volume, and receiver electronic noise. The use of multiple acoustic carrier frequencies achieves noise suppression by generating simultaneous measurements with uncorrelated errors. We present results from a laboratory turbulent jet experiment where velocity was measured simultaneously with multi-frequency coherent Doppler sonar and particle image velocimetry (PIV). Time series and turbulence spectra from PIV are compared to those obtained with conventional Doppler signal processing and a new technique called Maximum A Posteriori (MAP) velocity estimation. It is shown that optimally combining multi-frequency measurements results in improved velocity estimates in a highly turbulent flow with low signal-to-noise ratio, i.e. conditions in which coherent Doppler sonar does not normally perform well.

Some aspects of Vortex-Induced Vibrations of circular cylinders

Stéphane Etienne, Dominique Pelletier
Ecole Polytechnique de Montréal
Email: stephane.etienne@polymtl.ca

Three numerical simulation results about vibrations of isolated and aligned arrays of circular cylinders placed in a transverse flow are discussed. Considered ratios of structure

to fluid densities range from 0 to $4/\pi$. The first deals with the limit of Vortex-induced vibrations (VIV) for Reynolds number values below the first Hopf bifurcation ($Re < 47$). The second treats the effect on VIV of letting a circular cylinder roll freely about its axis. Finally, specific vibrational aspects of VIV and Wake instabilities for 2 and 3 cylinders arranged in-line and mounted on springs are addressed.

A monolithic fully-coupled and consistent Arbitrary Lagrangian-Eulerian Finite Element Method specifically designed to treat fluid-structure interactions is used. Proven third order space and time accuracies for the velocity (and second order for the pressure) are delivered thanks to the use of P2-P1 Taylor-hood elements and a third order implicit Runge Kutta scheme. Accuracy and consistency on deforming grids for the flow part result from the proper implementation of the Geometric Conservation Law (GCL).

**Fishing vessel energy efficiency projects at Ocean Engineering Research
Centre of Memorial University**

Dag Friis, Don Bass, Wei Qiu, Christian Knapp, Robert McGrath, Stephen Lane
Memorial University of Newfoundland
Email: dfriis@nl.rogers.com

The Ocean Engineering Research Centre is engaged in projects related to energy efficiency of fishing vessels. This work was used in establishing new vessel size restrictions for boats in the “Inshore Fleet” during the Fisheries Renewal deliberations. We started out by looking at the design and performance evaluation of two vessels for operation in a multi-species fishery, one restricted by the 65’ and cubic number restrictions, and the other without such restrictions. They both had the same quota to catch. There were tank tests and simulations carried out for resistance and seakeeping. The seakeeping simulations allowed one to establish the number of 5 day fishing trips by month. Further work was done investigating the influence of vessel length and vessel beam on energy efficiency. Monte Carlo simulations were run to evaluate the relative energy efficiency and vessel expected economic performances. A current project examines energy consumption patterns of 7 boats representative of the fleet. In addition a set of tank tests will be conducted on two fishing vessel models to establish the effectiveness of vessel lengthening and addition of bulbous bows in improving energy efficiency.

**Complete identification of the equation of motion of a single degree system
in waves using its stationary random response**

Mahmoud Haddara
Memorial University of Newfoundland
Email: mhaddara@mun.ca

The Fokker-Planck equation is used to derive the equations of motion for the mean and variance of the motion of a nonlinear, single degree of freedom system excited by random

waves. A neural network is developed to identify the parameters of the system. The parameters are used to predict the time series of the wave excitation per unit virtual mass moment of inertia using the stationary random response. The estimated variance and autocorrelation function of the excitation are compared with those obtained using numerically generated data. The agreement is excellent. The method was also applied to experimental data obtained using two ship models. The predicted autocorrelation function for the excitation was compared with the autocorrelation function of the wave height. The method predicts the form of the autocorrelation function accurately. The method lends itself for use aboard ships or offshore structures at sea or without interrupting the mission of the ship/offshore structure. Results of this analysis can help in planning optimum ship routing and damage occurring to the structure.

Dynamics of ship towing in ice

Christian Knapp, Bob McGrath, Wei Qiu, Claude Daley, Philip Hanbidge
Memorial University
Email: mcgrathknapp.nal@gmail.com

The dynamics involved in the towing of a small vessel by a large one is complex in nature and dependent on vessel dimensions and the environment. When a tow is conducted in ice filled waters, the degree of difficulty and uncertainty is greatly increased. This paper presents a preliminary model test program involving the investigation of the dynamics of a large vessel towing a comparatively small vessel in ice filled waters. The objective of the test program was to draw conclusions and make recommendations to the Canadian Coast Guard, regarding safe towing procedures for it's vessels while towing small vessels in ice covered regions. Tests were conducted in Memorials towing tank. Various force and inertial sensors were employed to determine vessel motions prior to and during a capsize event. Physical variables were limited to vessel metacentric height, vessel speed, hawser line length, and rudder angle of the towed vessel.

Second-order shallow water long wave reproduction in a large wave basin

Heather Peng, Hasanat Zaman, Emile Baddour, Don Spencer, Shane Mckay
Memorial University of Newfoundland
Email: hpeng@mun.ca

Accurate generation of the primary waves and the reproduction of the group-induced second-order low frequency waves in shallow water are investigated. For the design of floating platform, it is of great importance that the long waves in nature are correctly represented in model basin because of the dominant influence of the long waves on mooring forces and slow drift oscillations in shallow water. The occurrence of so-called "free" or parasitic Low frequency waves in addition to the second-order "bound" waves is a special challenge. It is desirable to eliminate free low frequency waves, or identify these

components for proper use of the model test results. In this paper, a second-order wave generation method for reduction/elimination for the free waves are described. Extensive experimental tests are carried out in the Offshore Engineering Basin (OEB) at the Institute for Ocean Technology of National Research Council Canada. In the experiments bi-chromatic waves are used. A wave splitting tool is developed to identify the primary waves, the bounded waves and the unwanted free waves from the measured data. The results show that the correction procedure works fairly well.

Deployment of a freefall lifeboat into waves

Wayne Raman-Nair

Institute for Ocean Technology
Email: wayne.raman-nair@nrc.ca

The equations of motion of a freefall lifeboat are formulated using Kane's method. Deployment from a moving ramp is assumed to occur in a known plane and a 2D model suffices. The contact forces with the ramp are modeled by stiff springs and applied to lifeboat segments. This automatically allows the simulation of the rotation phase at ramp exit. The results provide initial conditions for the water entry phase for which a separate 3D model is formulated. The hydrodynamic loads at water entry are also modeled using a segmented approach. To determine the appropriate added-mass coefficients, it is necessary to solve a boundary value problem for Laplace's equation for different immersion depths. This is accomplished via the boundary element method. The equations of motion are solved numerically using a standard Runge-Kutta MATLAB routine. Results are compared with available experimental data.

Investigating near-resonant triad interactions in stratified flows

Tim Rees, Francis Poulin, Kevin Lamb

University of Waterloo
Email: twrees@math.uwaterloo.ca

Resonant triad interactions among internal gravity waves provide a means for energy transfer across a wide range of time and length scales. This nonlinear mechanism plays an important role in mixing because it both transfers some energy to small scales and helps to establish a background wave field in which these waves may overturn. This is an important process throughout the atmosphere and oceans and, in particular, in the oceanic pycnocline. Previous oceanographic studies have focused primarily on wave interactions that exactly match resonance conditions for fluids with linear density stratifications. The oceans, however, do not generally possess a linear density profile, and the dispersion relation that results may not even permit triads of waves exactly meeting the resonance criteria. In this talk, I will demonstrate the importance of near-resonant triad interactions in fluids with nonconstant buoyancy frequencies. The intricacies of

numerically forcing waves in fluids of general stable stratification will also be highlighted. Direct numerical simulations of ocean-scale and lab-scale interactions will illustrate the role the interactions play in the transfer of energy across the spectrum.

Numerical validation for ship performance in broken ice floes

John Wang

Institute for Ocean Technology

Email: John.Wang@nrc.ca

Recently developed FE (Finite Element) Technology for ship performance in ice is presented. Hydrodynamic loads and ice interaction loads are numerically calculated based on the Fluid Structure Interaction (FSI) method by using commercial FE package (LS-DYNA). Model test data from ice tank are used to validate the code because model tests provided well-controlled data sets and most of the ice properties were identified. One of the IOTs standard icebreaker models is used and simulated with various ice conditions i.e., presawn ice and pack ice with three different concentrations (90%, 80%, and 60%). In this presentation, the simulations are limited to the broken ice condition, which means ice failure was not considered. All ice properties such as density and Youngs modulus used are the same as those measured from the ice tank. The challenge is to evaluate hydrodynamic loads because LS-DYNA is an explicit FE solver and FSI value is calculated by using a penalty method. Although the hydrodynamic loads directly affecting on the ship are small compared to the ice loads, interaction between water and ice could be important for simulating pack ice condition or ice floe management. Comparisons between numerical and experimental results are shown and discussed.

Computation of slamming loads on a catamaran

Qingyong Yang, Wei Qiu

Memorial University of Newfoundland

Email: qyang@mun.ca

A numerical method has been developed to compute the slamming loads on a catamaran. The highly nonlinear free surface problems governed by the Navier-Stokes equations are solved by a Constrained Interpolation Profile (CIP)-based finite difference method on a fixed Cartesian grid. The solid body and the free surface interfaces are identified by density functions in a multi-phase domain, and the CIP method is used to capture the free surface. The catamaran is treated as a rigid body and its motions are computed in six DOF. A cut-cell method is employed to represent the catamaran body surface. For the pressure calculation, a Poisson-type equation is solved at each time step by the Conjugate Gradient (CG) iterative method. The computed slamming forces and accelerations were compared with experimental data in the validation studies.

10.7 Scientific Computing and Numerical Analysis

Organizers: Ronald Haynes and Colin Macdonald

| Sunday July 18 | | Location: Signal |
|-------------------------------|-------------------------------------------------------------------------------------------------------------------|-------------------------|
| Chair: Ronald Haynes | | |
| 9:00–9:20 | Manfred Trummer Conditioning of differentiation matrices | |
| 9:20–9:40 | Weizhang Huang Mesh adaptation for the finite element solution of heterogeneous anisotropic diffusion problems | |
| 9:40–10:00 | Colin Macdonald Solving eigenvalue problems on surfaces with the Closest Point Method | |
| Chair: Colin Macdonald | | |
| 10:30–10:50 | Justin Wan A multigrid method for solving partial integro-differential equations | |
| 10:50–11:10 | George Miminis A numerically stable algorithm for allocating a new set of eigenvalues to a matrix | |
| 11:10–11:30 | Benjamin Ong Asymptotic preserving Maxwell solvers | |
| 11:30–11:50 | Steve Ruuth A method for phase separation patterns for diblock copolymers on general surfaces | |
| Monday July 19 | | Location: Signal |
| Chair: Colin Macdonald | | |
| 9:00–9:20 | Ray Spiteri Problem-solving environments for numerical analysis and scientific computing | |
| 9:20–9:40 | Lilia Krivodonova A numerical study of reflected waves using a discontinuous Galerkin method | |
| 9:40–10:00 | Uri Ascher Surprising computations | |
| <i>continued on next page</i> | | |

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|-------------------------------------|-----------------------------------------------------------------------------------------------------------------------|
| <i>continued from previous page</i> | |
| Chair: Ronald Haynes | |
| 10:30–10:50 | Brian Wetton Asymptotic error analysis for projection methods |
| 10:50–11:10 | Jose Urquiza Finite element implementations of the no-penetration boundary condition on curved boundaries |
| 11:10–11:30 | Peter Young Communications network analysis through numerical solution of computer-generated teletraffic equations |

Abstracts:**Surprising computations****Uri Ascher**

University of British Columbia

Email: ascher@cs.ubc.ca

Computer simulations for differential equations (DEs) often require complex numerical methods. It is important and often difficult to devise efficient methods for such purposes and to prove their properties. The resulting computations usually produce expected results, at least qualitatively, which in itself does not diminish the importance of the numerical methods.

Occasionally, however, one comes across a (correct) computation that yields surprising results. In the process of writing a textbook on numerical methods for time dependent DEs I have encountered some such, and this talk describes several instances including solving Hamiltonian systems, nonlinear Schroedinger, and applying WENO methods for nonlinear conservation laws. What can be qualified as “surprising” is of course a subjective matter; nonetheless, the combined effect of this talk hopefully sheds light on using marginally stable methods for solving marginally stable differential problems.

Mesh adaptation for the finite element solution of heterogeneous anisotropic diffusion problems

Weizhang Huang, Xianping Li

University of Kansas

Email: huang@math.ku.edu

Anisotropic diffusion problems arise in the various areas such as plasma physics, petroleum engineering, and image processing. For those problems standard numerical methods can

produce spurious oscillations in computational solutions. A common strategy to avoid the difficulty is to employ a scheme satisfying the discrete maximum principle (DMP). Numerical schemes of this type can be obtained by utilizing a special mesh or a special discretization of the underlying partial differential equation. For isotropic diffusion problems, a mesh satisfying the well-known non-obtuse angle condition guarantees the satisfaction of DMP by a linear finite element solution. Unfortunately, a mesh condition of this type is not available for anisotropic diffusion problems. In this talk we will show that a mesh satisfying a generalization of the non-obtuse condition will guarantee the satisfaction of DMP by the linear finite element solution for anisotropic diffusion problems. We will also present several variants of the new condition and discuss their use in developing metric tensors to account for DMP satisfaction and the combination of DMP satisfaction and mesh adaptivity. These metric tensors are needed in the practice of anisotropic generation and adaptation. Numerical examples are given to demonstrate the features of schemes based on DMP satisfaction and mesh adaptation.

A numerical study of reflected waves using a discontinuous Galerkin method

Lilia Krivodonova, Dale Connor

University of Waterloo

Email: lgk@math.uwaterloo.ca

We present numerical simulations of electromagnetic waves reflected from curved surfaces. For example, light rays reflected by a circular cup can produce a caustic, i.e. a region of bright light in the form of a nephroid. Bright regions are formed where reflected rays intersect and are characterized by a spike in energy. These regions are difficult to handle numerically due to steep gradients in the solutions. We investigate the use of the discontinuous Galerkin method for numerical simulation of such problems. As a high-order and a low dissipation method, the DGM can accurately resolve both the incoming waves and the high energy regions where they intersect. This is especially so at the cusp of a caustic, e.g. the point of the highest intensity, which is smoothed out by lower order schemes. The numerical results will be presented and the importance of the accurate representation of reflecting boundary conditions will be discussed.

Solving eigenvalue problems on surfaces with the Closest Point Method

Colin Macdonald, Jeremy Brandman, Steve Ruuth

University of Oxford

Email: macdonald@maths.ox.ac.uk

The Closest Point Method is a simple numerical technique for solving partial differential equations (PDEs) on curved surfaces and other general domains. The method works by embedding the surface in a higher-dimensional space and solving the PDE in that space.

Numerically, the method can make use of simple finite difference and interpolation schemes on uniform cartesian grids.

This presentation provides a brief overview of the Closest Point Method and outlines some current results on applying the method to surface eigenvalue problems. Computational examples include computing the spectra and eigenmodes of the Laplace–Beltrami operator on a variety of surfaces.

A numerically stable algorithm for allocating a new set of eigenvalues to a matrix

George Miminis

Memorial University of Newfoundland

Email: george@mun.ca

Given real $n \times n$ matrix A , real n -dimensional vector b and a self-conjugate set of n scalars Λ , an algorithm is given that computes an n -dimensional vector f such that the set of eigenvalues of $A - bf^T$ is equal to Λ . Therefore the algorithm can be seen as “allocating” eigenvalues to A .

A backward rounding error analysis of the algorithm has been developed in order to prove its numerical stability. The algorithm uses only real arithmetic even for the allocation of complex conjugate pairs of eigenvalues. The above are very important aspects for the efficient implementation of the algorithm on a computer.

The main use of this algorithm is in Control engineering where it solves the “Pole Placement problem” for single-input linear systems. However the algorithm is versatile enough and it can be used in other applications.

Asymptotic preserving Maxwell solvers

Benjamin Ong, Andrew Christlieb

Michigan State University

Email: bwo@math.msu.edu

We present ongoing research towards computing semi-implicit solutions to Maxwell’s equations. A desirable feature of our scheme, is that it recovers the asymptotic limit (i.e. Darwin limit) as $c \rightarrow \infty$. Our approach discretizes the time derivatives using finite difference approximations, and solves the resulting PDEs using boundary integral methods; i.e., a method of lines transpose methodology. We discuss our fast summation implementation of our 1D, 2D and 3D solver, and discuss various stability issues that arise when solving the canonical wave equations.

A method for phase separation patterns for diblock copolymers on general surfaces

Steven Ruuth, Bobak Shahriari, Rustum Choksi
Simon Fraser University
Email: sruuth@sfu.ca

There has been recent interest in understanding phase separation on general surfaces. A model of particular interest is the Cahn-Hilliard equation modified for diblock copolymers. A number of numerical methods are available for approximating such PDEs on surfaces. A particularly simple and general technique is the Closest Point Method [1,2]. In this talk we give a brief review of the Closest Point Method and consider its application to the problem of finding phase separation patterns for diblock copolymers on general smooth surfaces.

[1] S.J. Ruuth, B. Merriman: A simple embedding method for solving partial differential equations on surfaces, *J. Comput. Phys.*, 227(3): 1943-1961, 2008.

[2] C.B. Macdonald, S.J. Ruuth: The implicit Closest Point Method for the numerical solution of partial differential equations on surfaces, *SIAM J. Sci. Comput.*, 31(6): 4330-4350, 2009.

Problem-solving environments for numerical analysis and scientific computing

Raymond Spiteri, Jason Boisvert, Andrew Kroshko
University of Saskatchewan
Email: spiteri@cs.usask.ca

Problem-solving environments (PSEs) such as Matlab, Maple, and Mathematica have become the dominant mode for prototyping and experimenting with strategies for solving problems in numerical analysis and scientific computing. In keeping with their self-proclaimed mandate of being all things to all people, the usage of PSEs ranges from classroom instruction to substantive problems with applications in a number of diverse fields of science and engineering. However, in many cases the individual libraries are too coarse-grained for researchers in numerical analysis and scientific computing to easily modify and experiment with the finer points of the algorithms chosen. For example, a user working with the Matlab function `ode45` to solve an initial-value problem is likely to find it challenging to change the integration method, implement a new step-size controller, or investigate a different way to measure solution error. This is especially true for users who are averse to dirtying their hands by hacking into someone else's code. In this talk, I will describe some of our work on the development of PSEs for the numerical solution of nonlinear algebraic equations and ordinary differential equations, both initial- and boundary-value problems.

Conditioning of differentiation matrices**Manfred Trummer**

Simon Fraser University

Email: trummer@sfu.ca

It is well known that high-order differentiation techniques like spectral methods lead to very ill conditioned differentiation matrices. In practical calculations, computational accuracy is often achieved despite this ill-conditioning. We present some examples of solving boundary value problems with direct and iterative methods, and investigate the behaviour of time-stepping algorithms (method of lines) with these differentiation matrices.

Finite element implementations of the no-penetration boundary condition on curved boundaries**Jose M. Urquiza**, Ibrahima Dione, André Fortin, André Garon

Université Laval

Email: jose.urquiza@mat.ulaval.ca

In computational mechanics, the no-penetration boundary condition is just one part of some classical boundary conditions such as any kind of slip boundary conditions for fluids, or contact boundary conditions for solids. Nevertheless, when dealing with curved boundaries a naïve finite element implementation may lead to inaccurate approximations of the exact solution. In fact, the finite element approximations may converge towards the solution of another problem (with a different boundary condition). The definition or the approximation of the normal vector to boundary of the finite element mesh may be viewed as the source of these paradoxes.

In this presentation, for the case of fluids with slip boundary conditions and elastic solids with perfect contact boundary conditions, we present numerous numerical results that will show which are the bad and, most importantly, the best ways to impose the no-penetration boundary condition with the finite element method. Results will depend on the choice of the variational formulation which may results in a weak or a strong imposition of the no-penetration, on the approximation of the curved boundary as well as on the way to approximate the normal vector to the boundary.

A multigrid method for solving partial integro-differential equations**Justin Wan**

University of Waterloo

Email: jwlwan@uwaterloo.ca

Based on the Black-Scholes model, the option value of a contingent claim under a jump diffusion model such as the Levy process satisfies a partial integro-differential equation

(PIDE). An implicit discretization results in solving a full dense linear system due to the jump integral term in each time step. A fixed point iteration based on FFT has been proposed to solve the linear system without dense matrix computation. While it is proved to be convergent, the number of iterations can grow significantly in the case of infinite variation and when the mesh size decreases. In this talk, we present a multigrid method for solving the PIDE. The idea is to use the fixed point iteration as a smoother for multigrid, rather than a linear solver. To justify this analytically, we prove by Fourier analysis that the fixed point smoother effectively damps away high frequency errors. We demonstrate numerically the effectiveness of the multigrid method and show that the convergence rate is independent of the mesh size and insensitive to the singularity of the Levy measure.

Asymptotic error analysis for projection methods

Brian Wetton, Siyavash Towfighi

University of British Columbia

Email: wetton@math.ubc.ca

Implicit time stepping applied to discretized incompressible fluid flow problems results in discrete Stokes-like (saddle-point, KKT) problems. There is a class of so-called Projection Methods in which these Stokes-like problems are efficiently approximated by the solutions of standard, second order elliptic problems. Over the last 20 years, these methods have been increasingly well understood. In this talk, a review of the methods and the analytic results are given. Leading order errors (both character and order) from the methods can be precisely described using asymptotic techniques. This asymptotic error analysis is applied to a number of commonly used projection methods. The results are confirmed by careful numerical computations using a spectral method on a representative model problem.

Communications network analysis through numerical solution of computer-generated teletraffic equations

Peter Young

NATO C3 Agency

Email: Peter.Young@nc3a.nato.int

This paper discusses development of computational techniques for analysing generalised communications networks through application of classical teletraffic theory with validation through Monte Carlo simulation and study of the associated Markov System. The requirement to analyse large communications networks with high bandwidths but also high traffic loadings places a need for fast running computer models. Such a model was developed through application of classical teletraffic theory in which the parsing of a communications network leads to an automatic construction by a computer of the

teletraffic equations in symbolic form, these then being solved numerically for specified network parameters. The resulting model permits calculation of call blocking probabilities for given traffic loadings with ability to determine degradation effects on the network due to removal of nodes and/or links. Validation of the fast running model through Monte Carlo simulation and consideration of the corresponding Markov System, only permissible for small network configurations, has identified deficiencies in the approach based on classical teletraffic theory. Dynamics of how the Markov System evolves for increasing network configurations and varying traffic loads are now being analysed for refining the fast running model.

10.8 Statistical and Population Genetics

Organizer: JC Loredo–Osti

| Tuesday July 20 | | Location: Signal |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------|
| Chair: JC Loredo–Osti | | |
| 10:30–10:50 | Sabin Lessard Probability of fixation of a mutant and the ancestral selection graph | |
| 10:50–11:10 | Steven M. Carr Biodiversity Genomics: NextGen DNA sequencing biotechnology and bioinformatics for population and evolutionary mitogenomics | |
| 11:10–11:30 | David Hamilton Estimating disease penetrance odds ratios by genotype using discordant pairs | |
| 11:30–11:50 | Heather Dawn Marshall Near neutrality, rate heterogeneity, and linkage govern mitochondrial genome evolution in Atlantic cod (<i>Gadus morhua</i>) and other gadine fish | |
| 11:50–12:10 | JC Loredo–Osti The most likely path of descent of a genetic variant in a pedigree and related problems | |
| Chair: JC Loredo–Osti | | |
| 4:00–4:20 | Shelley Bull Addressing the Winner’s curse in genome-wide association studies | |
| 4:20–4:40 | Laurent Briollais A general statistical framework for Genome-Wide Association Studies (GWAS) based on Bayesian graphical modeling | |
| 4:40–5:00 | Joseph Beyene Methods and strategies for genomic data integration | |
| 5:00–5:20 | Karen Kopciuk Multi-state modelling approaches for estimating disease risk in gene mutation carriers from family data | |
| 5:20–5:40 | Jinko Graham On the use of haplotype-informed ancestries and fuzzy p-values for fine-mapping complex genetic traits | |
| 5:40–6:00 | Rafal Kustra Prediction error vs p -values in high throughput genomics | |
| 6:00–6:20 | Brad McNeney A statistical approach to high-throughput screening of predicted orthologs | |

Abstracts:**Methods and strategies for genomic data integration****Joseph Beyene**, Jemila Hamid, David Tritchler, Elena Parkhomenko

McMaster University

Email: beyene@mcmaster.ca

Due to rapid technological advances in recent years, various types of high-throughput genomic data with varying sizes, structures and complexities have become available. Among them are Single Nucleotide Polymorphisms (SNPs), Copy Number Variations (CNVs) and microarray gene expression measurements. Each of these distinct data types provides a different, partly independent and complementary view of the whole genome. However, understanding functions of genes and other aspects of the genome requires more information than provided by each of the data sets. We will present a conceptual integrative analysis framework and highlight novel methods we developed recently that can be used to integrate heterogeneous data types in order to answer different scientific questions. We will provide illustrative examples and discuss methodological issues.

A general statistical framework for Genome-Wide Association Studies (GWAS) based on Bayesian graphical modeling**Laurent Briollais**, Helene Massam, Adrian Dobra, Jinnan Liu

Samuel Lunenfeld Research Institute

Email: laurent@lunenfeld.ca

The actual paradigm to analyze GWAS is to perform an exhausting testing of all single SNP associations with the response variable with the major drawback that the selected subset of SNPs has in general a very low predictive value. As a shift to the usual approach, we propose here a general statistical framework for GWAS based on Bayesian graphical modeling and able to: 1) Assess the joint effect of multiple SNPs (linked or unlinked); 2) Explore the model space efficiently using the Mode Oriented Stochastic Search (MOSS) algorithm of Dobra (2008); 3) Incorporate expert prior knowledge in the model search in particular to enhance the detection of rare functional genetic variants. We illustrate this new methodology through a GWAS of 42 NCI cell lines classified as resistant ($n = 27$) or sensitive ($n = 15$) after exposure to estrogen using 25K SNPs. Our algorithm selected 17 SNPs embedded in multi-locus models with high posterior probabilities. Most of the selected SNPs have a biological interest and their predictive value is perfect in our sample. Interestingly, many of them would not have been detected in the single-SNP testing approach. Finally, we discuss the impact of informative priors in this statistical framework through simulations.

Addressing the Winner's curse in genome-wide association studies

Shelley Bull, Laura Faye, Lei Sun, Apostolos Dimitromanolakis

University of Toronto

Email: bull@lunenfeld.ca

Bias in genetic effect estimates, a phenomenon also known as the Winner's curse or the Beavis effect, can occur in both genome-wide linkage and genome-wide association studies (GWAS). Because the same sample is used for gene discovery and effect estimation, and the genetic effect is estimated only when the test for linkage or association is significant, the estimate is on average larger in magnitude than the true value. In GWAS the effect is exacerbated by use of stringent selection threshold and ranking over hundreds of thousands of genetic markers (SNPs). The available likelihood-based bias-reduced estimators for GWAS are limited to single-SNP analysis. Extending our previous work in linkage, we therefore develop a multi-locus bootstrap method that accounts for both ranking- and threshold-selection bias as well as for the complex correlation structure among SNPs in the GWAS setting. In simulation studies we demonstrate the adaptability of the bootstrap method to both ranking and threshold selection, with improved effect estimates that yield replication study sample size requirements with adequate power. We implement our methods in a user-friendly package for point and interval estimation of bias-reduced effect estimates for large-scale GWAS in an efficient and flexible manner.

Biodiversity Genomics: NextGen DNA sequencing biotechnology and bioinformatics for population and evolutionary mitogenomics

Steven M. Carr

Memorial University of Newfoundland

Email: scarr@mun.ca

Genome DNA sequencing projects are typically oriented toward single-species genomes that are of medical or commercial interest. "Next Gen Sequencing" technologies are now being developed to provide the massively-parallel capacity necessary to obtain whole-genome data as a matter of routine, e.g. the "\$1,000 genome" of several 109s bp for single humans. Rather than defining "the" sequence of particular species, biologists interested in population and evolutionary biodiversity seek to discern phylogeographic patterns (genetic relationships in geographic context) within species, and compare these patterns across species. Given NGS capacity to sequence 109 bp, we would deploy this to obtain 104 5 bps of homologous sequence data from each of 105 4 individuals. For such studies, the extranuclear mitochondrial DNA genome remains the molecule of choice. Despite its great success in human phylogeography, mitogenomics is only now being applied to other species (Carr et al. 2008 *Comp Biochem Physiol D* 3,11). For this goal, another NextGen technology, iterative DNA sequencing on microarrays, is a time- and cost effective alternative. We describe the design, bioinformatic evaluation, and

results from the “ArkChip” a multi-species iterative sequencing microarray for parallel sequencing of multiple mtDNA genomes from different animal species (Carr et al. 2009 Lab Focus 13,8).

On the use of haplotype-informed ancestries and fuzzy p -values for fine-mapping complex genetic traits

Jinko Graham

Simon Fraser University

Email: jgraham@sfu.ca

Shared ancestry underlies population associations between complex traits and haplotypes. This talk will review some basic ideas behind disequilibrium fine-mapping of complex trait loci and discuss the utility of coalescent ancestries and fuzzy p -values in this regard. I will present some preliminary results from ongoing experiments with these ideas on an example dataset of 125 cases and 125 controls defined by an immune marker predictive for type 1 diabetes. This is joint work with Kelly Burkett and Brad McNeney.

Estimating disease penetrance odds ratios by genotype using discordant pairs

David Hamilton, Vaneeta Mishra (Grover), David Cole

Dalhousie University

Email: hamilton@mathstat.dal.ca

Genotypic counts of paired subjects discordant for a disease are often used to test for association with a genetic locus. For a biallelic locus we show that the theoretical genotypic frequencies depend only on the penetrance odds ratios, conditional on the observed numbers of each type of discordant pair. A product binomial likelihood function can be used to estimate the odds ratios. This approach leads to a new test for association which uses two degrees of freedom. It may also provide insight into the mode of inheritance of the disease in question. The second degree of freedom should allow detection of some patterns of penetrance which are not as easily detected using current approaches. We illustrate our method using a data set on Alzheimer’s disease and the ApoE locus. Simulations are used to demonstrate the increased power of the test of association in comparison with McNemar’s test.

Multi-state modelling approaches for estimating disease risk in gene mutation carriers from family data

Karen Kopciuk, Yun-Hee Choi, Patrick Parfrey, Jane Green, Laurent Briollais
AHS - Cancer Care
Email: kakopciu@ucalgary.ca

Hereditary Nonpolyposis Colorectal Cancer (HNPCC) can cause different types of cancer within the same family, so understanding the patterns of various cancers among individuals can help dissect the genetic origin of the disease and predict future events in susceptible individuals. Some family members also experience successive primary HNPCC cancers. To model these types of data, we adopt progressive multi-state models to calculate age-specific penetrance estimates of experiencing multiple phenotypes in pedigree data. An EM algorithm is developed to estimate all regression model parameters by inferring missing genotypes. Our methods were applied to a retrolective cohort of 12 HNPCC families from Newfoundland who harbour a founder MSH2 mutation. We found the modulating time scale term unnecessary, lifetime penetrance for a second cancer high (70% for males, 50% for females) and hazard ratios of second to first cancer in carriers fell with age. Future directions will focus on assessing the impact of screening interventions, in particular, deriving adjusted estimates of penetrance.

Prediction error vs p -values in high-throughput genomics

Rafal Kustra

University of Toronto
Email: ProfKustra@gmail.com

In a typical high-throughput genomics experimental setup, large number of instances of molecular entity (e.g., gene) are interrogated in parallel, usually within a relatively simple experimental design. The classical and widely used statistical paradigm is to perform a corresponding set of parallel, and usually simple, analysis each of which is summarized by a p -value indicating a strength of evidence that the underlying entity is associated with the condition being studied. An enormous research effort in statistical methodology has been directed to invent most meaningful and rigorous summaries of the resulting “sea of p -values”, to address the challenge usually termed a “problem of multiple testing”. In this talk I will discuss whether looking at some of high-throughput genomics data as a problem in prediction rather than pure discover could be a more successful approach. During the talk I will show some simple simulation-based results that suggest both the dangers of single-entity p -value-based analysis, and some promising results of utilizing prediction-based machine-learning models. Some recent results from large-scale cancer-genetics data will also be presented.

Probability of fixation of a mutant and the ancestral selection graph**Sabin Lessard**

Université de Montréal

Email: lessards@dms.umontreal.ca

The ancestral selection graph can be used to study the probability of fixation of a mutant allele under weak selection and to get the n-th order approximation with respect to the scaled intensity of selection. The approach will be compared to classical diffusion approximations and direct methods of small perturbations away from neutrality.

The most likely path of descent of a genetic variant in a pedigree and related problems**J C. Loredano-Osti**, Qiong Li, Ken Morgan

Memorial University of Newfoundland

Email: jcloredanoosti@mun.ca

In population genetics, it has been a long interest in the study of the paths of descent of a genetic variant in the context of problems such as gene extinction, gene/allele origins, gene flow and its relationship with gene distribution. This is natural framework where the most likely path of descent problem arises but also it can be used as a dimension/complexity reduction procedure in the computation of likelihoods in large inbred pedigrees. In the hidden Markov models literature, there is a well known algorithm to find the most likely sequence of hidden states (the Viterbi algorithm); however, its implementation for large, but finite size, complex pedigrees is known to be computationally cumbersome. Nonetheless, for specific genetic modes of inheritance, the problem can be re-stated as a graph optimization task and use the arsenal of graph theory techniques in conjunction with Monte Carlo tools to tackle it. On this presentation we will discuss how this can be accomplished under a recessive model of inheritance.

Near neutrality, rate heterogeneity, and linkage govern mitochondrial genome evolution in Atlantic cod (*Gadus morhua*) and other gadine fish**Heather Dawn Marshall**, Mark Coulson, Steve Carr

Memorial University of Newfoundland

Email: dawnm@mun.ca

The mitochondrial DNA genome figures prominently in evolutionary investigations due to absence of Darwinian selection, high mutation rate, and inheritance as a single linkage unit. Given complete linkage and selective neutrality, mtDNA gene trees correspond to intraspecific phylogenies, and mtDNA diversity reflects population size, however the validity of these assumptions is rarely tested on a genome-wide scale. We analyzed patterns of molecular evolution among 32 Atlantic cod mitochondrial genomes and compared

them to the sister taxon, walleye pollock, and seven other gadines. We evaluated selection within Atlantic cod, between sister species, and among species, and intraspecific measures of recombination within cod. Strong rate heterogeneity occurs among sites and genes at all levels of hierarchical comparison, consistent with variation in mutation rates across the genome. Neutrality indices (dN/dS ratios) are significantly greater than unity among cod genomes and between sister species, suggesting that polymorphisms within species are slightly deleterious, as expected under “near neutrality”. Among species, dN/dS ratios are heterogeneous among genes, consistent with variation in functional constraint rather than positive selection. There is no evidence for recombination within cod. These patterns contrast those observed in humans, the only other species in which whole mtDNA genome population studies have been conducted.

A statistical approach to high-throughput screening of predicted orthologs

Brad McNeney

Simon Fraser University

Email: mcneney@stat.sfu.ca

Orthologs are genes in different species that have diverged from a common ancestral gene after speciation. In contrast, paralogs are genes that have diverged after a gene duplication event. Orthologs tend to have similar function and so their identification is important for prediction of gene function. In high-throughput settings, orthologs are commonly predicted by a method called Reciprocal-Best BLAST-hit (RBH). However, due to incomplete sequencing or gene loss in a species, RBH-predicted orthologs can sometimes be paralogs. To increase the specificity of ortholog prediction, Fulton et al. (2006, BMC Bioinformatics 7, 270) developed Ortholuge, a bioinformatics tool that identifies predicted orthologs with atypical genetic divergence. However, the cut-off values that Ortholuge generates for orthology classification can be too high, leading to decreased specificity of ortholog prediction. Therefore, we propose a complementary statistical approach and compare the two approaches by simulation. We find that the statistical approach improves the specificity of ortholog prediction for low-quality data sets. A benefit of the statistical approach is that it gives the user an estimated conditional probability that a predicted ortholog pair is unusually diverged. This is joint work with Jeong Eun Min, Matthew Whiteside, Fiona Brinkman and Jinko Graham.

11 Minisymposia

11.1 Applied Combinatorics

Organizers: Danny Dyer, Nabil Shalaby

| Tuesday, July 20 | | Location: Plymouth |
|-------------------------|----------------------------------------------------------------------------------------------------------------|---------------------------|
| Chair: Danny Dyer | | |
| 10:30–10:50 | Dariusz Dereniowski Multi-slot just-in-time scheduling on single and parallel machines | |
| 10:50–11:10 | Robert Gallant Finding discrete logarithms with a set orbit distinguisher | |
| 11:10–11:30 | David Pike A graph theoretic approach to ecological connectivity | |
| 11:30–11:50 | Danny Dyer Non-traditional edge searching | |
| Chair: Nabil Shalaby | | |
| 4:00–4:20 | Andrea Burgess Cycle decompositions of complete equipartite graphs | |
| 4:20–4:40 | Xiaoliang Qi G-decompositions of the complete graph K_n | |
| 4:40–5:00 | Nabil Shalaby Skolem-type sequences: applications and open questions | |
| 5:00–5:20 | Daniela Silvesan Extending Peltesohn-Skolem type constructions to the cyclic BIBD($v,4,1$) | |
| 5:20–5:40 | Asiyeh Sanaei Existential closure of block intersection graphs of infinite designs with infinite block size | |

Abstracts:

Cycle decompositions of complete equipartite graphs

Andrea Burgess

Memorial University of Newfoundland

Email: aburgess@mun.ca

Certain cycle decomposition problems have connections with experimental design. In this talk, we consider cycle decompositions of complete equipartite graphs. The complete equipartite graph $K_m * \overline{K_n}$ has mn vertices, partitioned into m parts, each of size n , such that two vertices are adjacent if and only if they are in different parts.

The determination of necessary and sufficient conditions for the existence of a decomposition of K_m or $K_{2m} - I$ into cycles of length k was completed by Alspach, Gavlas and Šajna. Since $K_m \cong K_m * \overline{K_1}$ and $K_{2m} - I \cong K_m * \overline{K_2}$, the question of cycle decomposition of $K_m * \overline{K_n}$ is a natural generalization of this result. We consider the problem of extending the Alspach-Gavlas-Šajna result to the case where $n = 3$. We discuss methods for constructing cycle decompositions of complete equipartite graphs, and show that the obvious necessary conditions for the existence of a k -cycle decomposition of $K_m * \overline{K_3}$ are sufficient in certain cases.

Multi-slot just-in-time scheduling on single and parallel machines

Dariusz Dereniowski, Wieslaw Kubiak

Gdansk University of Technology / Memorial University of Newfoundland

Email: deren@eti.pg.gda.pl

In the multi-slot just-in-time scheduling problem a set of jobs and an integer L are given. The time is divided into slots of length L . Each jobs has its processing time and its due-date. In a valid schedule each machine works on at most one job at a time, no preemptions are allowed, and each job ends exactly at its due-date in one of the slots.

In this talk we address the problem of minimizing the number of slots and makespan of multi-slot just-in-time schedules. We are interested in the latter (more general) optimization criterion. We present an efficient optimal algorithm for the single machine problem. For parallel machines we describe an optimal solution for the case when the processing time of each job does not exceed its due date and a polynomial-time approximation algorithm for general input instances.

We also present a possible application of the above scheduling model, namely a routing problem in a slotted ring network.

Non-traditional edge searching

Danny Dyer, Dariusz Dereniowski

Memorial University of Newfoundland

Email: dyer@mun.ca

Edge-clearing is a well established graph theoretic problem with links to graph parameters such as vertex separation and pathwidth. The traditional problem has been, given a graph, to determine the minimum number of searchers needed to successfully capture an intruder. We will instead consider some nontraditional measures of the efficiency of a search.

Finding discrete logarithms with a set orbit distinguisher**Robert Gallant**

Memorial University of Newfoundland SWGC

Email: gallant_rob@yahoo.com

The discrete logarithm problem in a finite group is fundamental to modern cryptography. We briefly motivate it and discuss algorithms for solving it. In particular we consider how one might find discrete logarithms when one has access to a certain helper function. This investigation leads to a connection between the discrete logarithm problem and certain error correcting codes.

A graph theoretic approach to ecological connectivity**David Pike**, Yubo Zou, Ian Bradbury, Paul Snelgrove, Paul Bentzen

Memorial University of Newfoundland

Email: dapike@mun.ca

We compare various applications of graph theory to ecological research (such as landscape connectivity models and population graph models). Further, we introduce two new models of connectivity measurement, one that entails an index of coincidence of genetic data collected from sample populations, and another that is based on pairwise comparisons of individuals.

We focus our analysis on a case study of rainbow smelt from Newfoundland coastal locations and evaluate the relative effectiveness of the graph theoretic techniques at discerning metapopulations and the degree of connectivity between population sampling sites.

 G -decompositions of the complete graph K_n **Xiaoliang Qi**

Memorial University of Newfoundland

Email: qi_tony@hotmail.com

A G -decomposition of a graph K is a set of edge disjoint subgraphs of K , where each subgraph is isomorphic to G , and the union of the subgraphs is equal to K . If a complete graph K_n has a G -decomposition, then we say we have a G -design of order n . The set $N(G)$ is a set of all positive integers n such that the complete graph K_n has a G -decomposition. Our goal is to study the problem for graphs G with four vertices or less. We present with examples some results of G -decompositions of K_n including results of Bermond and Sconheim.

Existential closure of block intersection graphs of infinite designs with infinite block size

Asiyeh Sanaei, David A. Pike, Daniel Horsley
Memorial University of Newfoundland
Email: asanaei@mun.ca

A graph G with vertex set V is said to be n -existentially closed, or n -e.c., if for each proper subset S of V with cardinality $|S| = n$ and each subset T of S , there exists some vertex x not in S that is adjacent to each vertex of T but to none of the vertices of $S - T$. The block intersection graph of a design is the graph having vertex set the set of blocks, and two vertices are adjacent if and only if their corresponding blocks share at least one point. We have extended the study of the n -existential closure property of block intersection graphs of designs to infinite designs. An infinite design is a design with an infinitely many points while k, t and λ can be either finite or infinite. We present a few examples of infinite designs with k infinite, and discuss the n -e.c. property of their block intersection graphs.

Skolem-type sequences: applications and open questions

Nabil Shalaby
Memorial University of Newfoundland
Email: nshalaby@mun.ca

A Skolem sequence of order n , $S = (s_1, s_2, \dots, s_{2n})$ is a sequence of $2n$ integers satisfying the conditions:

1. for every k in $1, 2, \dots, n$ there exists exactly two elements s_i, s_j in S such that $s_i = s_j = k$, and
2. if $s_i = s_j = k$ with $i < j$ then $j - i = k$.

For example, $(3, 4, 5, 3, 2, 4, 2, 5, 1, 1)$ is a Skolem sequence of order 5.

In this talk we discuss some applications of Skolem sequences and some open problems.

Extending Pelsesohn-Skolem type constructions to the cyclic BIBD($v, 4, 1$)

Daniela Silvesan, Nabil Shalaby
Memorial University of Newfoundland
Email: danielas@mun.ca

Very little is known about cyclic BIBDs(v, k, λ) with $k > 3$. In 1980, in her doctoral thesis Marlene Colbourn tried to construct cyclic designs with block size four using Pelsesohn's proof technique. She gave a description of a solution for Heffter problem in

the case $k = 4$. She also provided solutions for cyclic designs with block size three and $\lambda > 1$.

In this talk, we describe and give examples of a Skolem type solution for Heffter problem in the case $k = 4$.

This is joint work with my supervisor, Dr. Nabil Shalaby.

11.2 Regulatory networks: Horseshoes and Honeybees, Bacteria and Biomolecules

Organizer: Roderick Edwards

| Sunday, July 18 | | Location: Amherst |
|------------------------|------------------|---------------------------------------------------------------------------------------------------|
| Chair: Rod Edwards | | |
| 4:00–4:20 | Linghong Lu | Structural principles for complex dynamics in glass networks |
| 4:20–4:40 | Etienne Farcot | Horseshoes and chaos in glass networks |
| 4:40–5:00 | Theodore Perkins | Scaling laws for path probabilities in stochastic systems, with applications to cellular networks |
| 5:00–5:20 | Fang Yu | Continuous-time switching network for the hivebee to forager transition |
| 5:20–5:40 | Etienne Farcot | Qualitative control of periodic solutions in piecewise affine models of genetic networks |
| 5:40–6:00 | Rod Edwards | Control of oscillation in a two-gene regulatory network |

Abstracts:

Control of oscillation in a two-gene regulatory network

Rod Edwards, Sehjeong Kim, P. van den Driessche

University of Victoria

Email: edwards@uvic.ca

Control strategies for gene regulatory networks have begun to be explored, both experimentally and theoretically, with implications for control of disease as well as for synthetic biology. Recent work has focussed on controls designed to achieve desired stationary states. Another useful objective, however, is the initiation of sustained oscillations in systems where oscillations are normally damped, or even not present. Alternatively, it may be desired to suppress (by damping) oscillations that naturally occur in an uncontrolled network. We address these questions in the context of piecewise-affine models of gene regulatory networks with affine controls that match the qualitative nature of the model. In the case of two genes with a single relevant protein concentration threshold per gene, we find that control of production terms (constant control) is effective in generating or suppressing sustained oscillations, while control of decay terms (linear control) is not effective. We derive an easily calculated condition to determine an effective constant control. As an example, we apply our analysis to a model of the carbon

response network in *Escherichia coli*, reduced to the two genes that are essential in understanding its behavior.

Horseshoes and chaos in glass networks

Etienne Farcot, Roderick Edwards

Institut National de Recherche en Informatique et en Automatique

Email: etienne.farcot@sophia.inria.fr

Chaotic dynamics have been observed in example piecewise-affine models of gene regulatory networks. Here we show how the underlying Poincaré maps, of horseshoe type for example, can be explicitly constructed.

Qualitative control of periodic solutions in piecewise affine models of genetic networks

Etienne Farcot, Jean-Luc Gouzé

Institut National de Recherche en Informatique et en Automatique

Email: etienne.farcot@sophia.inria.fr

Piecewise affine (PWA) systems are often used to model gene regulatory networks. In this paper we elaborate on previous work about control problems for this class of models, using also some recent results guaranteeing the existence and uniqueness of limit cycles, based solely on a discrete abstraction of the system and its interaction structure. Our aim is to control the transition graph of the PWA system to obtain an oscillatory behaviour, which is indeed of primary functional importance in numerous biological networks; we show how it is possible to control the appearance or disappearance of a unique stable limit cycle by qualitative action on the degradation rates of the PWA system, both by static and dynamic feedback, i.e. the adequate coupling of a controlling subnetwork. This is illustrated on two classical gene network modules, having the structure of mixed feedback loops.

Structural principles for complex dynamics in glass networks

Linghong Lu, Roderick Edwards

University of Victoria

Email: lu_linghong@hotmail.com

Gene-regulatory networks are potentially capable of more complex behavior than convergence to a stationary state, or even cycling through a simple sequence of expression patterns. The analysis of qualitative dynamics for these networks is facilitated by using piecewise-linear equations and its state transition diagram (an n -dimensional hypercube, in the case of n genes with a single effective threshold for the protein product of each).

In this talk, we will first describe a few simple cycles of states in the state transition diagram that allow periodic solutions. Then we study a particular kind of figure-8 pattern in the state transition diagram and determine conditions that allow complex behavior. Previous studies of complex behavior, such as chaos, in such networks have dealt only with specific examples. Our approach allows an appreciation of the design principles that give rise to complex dynamics, which may have application in assessing the dynamical possibilities of gene networks with poorly known parameters, or for synthesis or control of gene networks with complex behavior.

Scaling laws for path probabilities in stochastic systems, with applications to cellular networks

Theodore Perkins, Roderick Edwards, Leon Glass
Ottawa Hospital Research Institute
Email: tperkins@ohri.ca

Markov chains are often used to model the dynamics of stochastic or complex systems, from the folding behavior of a protein to price fluctuations in the stock market. We study the asymptotic scaling of the probabilities of alternative paths back to a recurrent state. As observed by Mandelbrot over 50 years ago, for many chains, these probabilities follow a power law. However, other chains do not. We provide a criterion for discriminating between these two types of chains, and prove a more general scaling law that covers all chains. We demonstrate our theory on simple models drawn from the areas of nonlinear dynamics and molecular dynamics.

Continuous-time switching network for the hivebee to forager transition

Fang Yu, James Watmough
University of New Brunswick
Email: fang.yu@unb.ca

We present a neural-network switching model for the regulation of the transition from hive-worker to forager in a honey bee colony. For the simpler case of identical bees, the model has a unique globally stable equilibrium, up to permutation, and we obtain an expression for the equilibrium number of foragers. The transition from worker to forager is normally age-dependent, but is thought to be regulated through a feedback mechanism by which foragers produce a pheromone that delays the development of workers. However, foragers may also revert to workers. This feedback enables the colony to maintain a healthy balance of workers and foragers. We model the physiology of each bee by a single variable that increases at a rate dependent on the number of foragers. The transition from worker to forager occurs when this variable crosses a threshold. Thus the model is a system of differential equations with piecewise continuous right-hand-sides, referred to as a switching network.

11.3 Heart Simulation

Organizer: Raymond Spiteri

| Monday, July 19 | | Location: Salon B |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------|
| Chair: Raymond Spiteri | | |
| 10:30–10:50 | Mary MacLachlan Modeling age-related changes in the heart | |
| 10:50–11:10 | Alex Walter Numerical methods for a coupled multiphysics problem arising in heart modelling | |
| 11:10–11:30 | Kazi Haq Simulation of the time course of intracellular Ca^{2+} transients in a 2D model of Ca^{2+} release/ Ca^{2+} uptake in cardiac Purkinje cells | |
| 11:30–11:50 | Megan Lewis Improving the efficiency of heart simulations | |

Abstracts:

Simulation of the time course of intracellular Ca^{2+} transients in a 2D model of Ca^{2+} release/ Ca^{2+} uptake in cardiac Purkinje cells

Kazi Haq, Rebecca Daniels, Sharene Bungay, Bruno Stuyvers
Memorial University of Newfoundland
Email: b26kth@mun.ca

Intracellular Ca^{2+} abnormalities in cardiac purkinje cells are thought to be the source of ventricular arrhythmias after myocardial infarction (MI). Three types of Ca^{2+} events can be observed in cardiac purkinje cells: non-propagating Ca^{2+} spark, small Ca^{2+} wavelets and large cell wide waves. These phenomena have been observed using 1D and 2D confocal microscopy. Mathematical models are helpful to dissect the different functions involved in these cellular Ca^{2+} transients. The current study proposes 1D and 2D mathematical simulations of non-propagating Ca^{2+} release events (sparks) in normal purkinje cells. The partial differential equation used to describe the spatio-temporal changes in local Ca^{2+} concentrations includes the calcium release, uptake and leak functions. To mimic the phenomenon of Ca-induced Ca-release, a fixed threshold (determined from experiments) has been used to trigger the release function. The model parameters have been determined so that the predicted results match the experimental data. The parameters will be compared between normal and post-MI purkinje cells in order to detect alteration of Ca^{2+} transporters after MI. This work with 1D and 2D simulation provides the framework for development of a 3D model using the high computation facility of the Atlantic Computational Excellence network (ACEnet).

Improving the efficiency of heart simulations**Megan Lewis**, Raymond Spiteri

University of Saskatchewan

Email: mel864@mail.usask.ca

Heart disease accounts for over one third of all deaths in Canada. Heart simulation is a method for studying the heart that does not require invasive surgery. We are interested in developing numerical methods and software for real-time simulation of the electrical activity in the heart. The mathematical models describing the flow of electricity through the heart involve complicated differential equations that are impossible to solve analytically and difficult to solve numerically. The most commonly used model is known as the bidomain model and consists of two partial differential equations describing the flow of electricity across the heart tissue that are coupled with a cardiac cell model for the electrical flow across the cell membrane of a single cardiac cell. Ideally, a numerical simulation of a single heartbeat would take approximately the same amount of time as the actual time of a single heartbeat (approximately 500 milliseconds). However, billions of equations must be solved to obtain a realistic simulation, making the goal of real time simulations a challenge. We are interested in improving the efficiency of simulations of electrical activity in the heart by optimizing the numerical methods used to solve the bidomain model.

Modeling age-related changes in the heart**Mary MacLachlan**

CIGENE/Norwegian University of Life Sciences

Email: mama@umb.no

Age-related changes in cardiac structure and function are risk factors for cardiovascular disease. Incorporating these changes into multi-scale models of the heart will allow for “in silico” investigations aimed at a better understanding of aging and disease and the development of new treatment options. In this presentation we will discuss plans for modeling the aging heart and progress towards this goal.

Numerical methods for a coupled multiphysics problem arising in heart modelling**Alex Walter**, Kathryn Gillow, Simon Tavener, Jonathan Whiteley

University of Oxford

Email: walter@maths.ox.ac.uk

In many problems in biology and physiology the coupling between two models is such that the coupling between the models is assumed to be “strong” in one direction, and “weak” in the other direction. For example when modelling the coupling of cardiac

electrophysiology with tissue deformation, tissue deformation is strongly dependent on the electrophysiology. However, the electrophysiology is usually, but not always, only weakly dependent on the tissue deformation.

Often the quantity of interest is in the tissue deformation. Computational efficiency will be enhanced if (i) we can neglect the weak coupling and (ii) calculate the electrophysiology with on a low resolution mesh, whilst having negligible effect on the accuracy in the tissue deformation. For (i), we have developed an analytical result that allows automatic identification of when weak coupling can be ignored. For (ii), we have used “a posteriori” error estimation to develop an adaptive mesh refiner for the electrophysiology and tissue deformation.

11.4 Mathematical Techniques in Disease Modeling

Organizers: Jessica Conway, Rafael Meza

| Sunday, July 18 | | Location: Salon D |
|------------------------|--------------------------------------------------------------------------------------------------------------------------------|--------------------------|
| Chair: Rafael Meza | | |
| 10:30–10:50 | Jessica M. Conway Continuous-time branching processes to model ART-controlled viral load in HIV+ individuals | |
| 10:50–11:10 | Raluca Eftimie Investigating the complex cancer-immune interactions using simple mathematical models: a structural approach | |
| 11:10–11:30 | Rafael Meza Infectious diseases and cancer | |
| 11:30–11:50 | Timothy Reluga Equilibria and dynamics vaccination behaviors in response to annual epidemics on random networks | |

Abstracts:

Continuous-time branching processes to model ART-controlled viral load in HIV+ individuals

Jessica M. Conway, Daniel Coombs

University of British Columbia

Email: conway@math.ubc.ca

I will discuss continuous-time, multi-type branching processes that model aspects of HIV and T-cell dynamics in infected patients. While on anti-retroviral treatment (ART) for HIV, an infected individual's viral load remains non-zero, though it is very low and undetectable by routine testing. However, blood tests show occasional viral blips: very short periods of detectable viral load. I hypothesize that aspects of viral blips can be explained principally by the activation of cells latently infected by HIV before the initiation of treatment, which constitute a reservoir that has been observed to decay in time. Viral blips then represent large deviations from the mean. Modeling this system as a sub-critical 3-type branching process (latently infected cells, activated cells, virus), I derive equations for the probability generating function. Using a novel numerical approach I extract probability distributions for the viral load, yielding blip amplitudes consistent with patient data. This technique also allows us to calculate extinction probability distributions in time, which I relate to extinction of the latent cell reservoir.

Investigating the complex cancer-immune interactions using simple mathematical models: a structural approach

Raluca Eftimie, Jonathan L. Bramson, David J.D. Earn
McMaster University
Email: reftimie@math.mcmaster.ca

We briefly discuss non-spatial mechanistic models describing the interactions between a malignant tumor and the immune system. We begin with the simplest (single equation) models for tumor growth and proceed to consider greater immunological detail (and correspondingly more equations) in steps. This approach allows us to clarify the necessity for expanding the complexity of models in order to capture the biological mechanisms we wish to understand. We conclude by discussing two complex (five- and six-equation) models derived to explain a surprising experimental observation regarding the anti-tumor role of two types of immune cells (Th1 and Th2 cells). Adding complexity in steps allows us to identify immunological mechanisms that can explain the elimination of a particular type of skin cancer by the Th2 cells, and not the Th1 cells (typically, the Th1 cells are considered to be capable of eliminating the tumors).

Infectious diseases and cancer

Rafael Meza

UBC Centre for Disease Control
Email: Rafael.Meza@bccdc.ca

Infectious agents play a significant role in the etiology of several cancers. Notable examples are the increase of cervical cancer risk due to Human Papillomavirus infection (HPV), and the association of gastric cancer risk with the colonization of the gut by *Helicobacter pylori*. In many cases, although the association between an infectious disease and cancer is well established, the biological mechanisms are not completely understood. A new methodology designed to i) study the mechanisms by which infectious agents cause cancer and ii) predict the impact of infectious disease dynamics on future cancer trends will be presented. This framework couples traditional mathematical models of infectious disease dynamics with stochastic models of carcinogenesis, therefore capturing the time-scales of both disease processes adequately. Some examples will be discussed.

Equilibria and dynamics vaccination behaviors in response to annual epidemics on random networks

Timothy Reluga, Dan Cornforth, Eunha Shim, Chris Bauch, Alison Galvani, Lauren Ancel Meyer
Penn State
Email: treluga@math.psu.edu

While uniform-mixing assumptions have been very useful in recent years in development of various aspects of theoretical epidemiology, it is widely acknowledged that biases in contact patterns have important practical consequences for epidemic dynamics and management, and particularly for individuals. Theories of behavior in response to epidemics will have greater explanatory power if they can be conditioned on such heterogeneities in the population. In this talk, I'll describe the extension of epidemiological game theory to populations with random mixing conditional on degree distribution. The talk will emphasize proof techniques for the existence, uniqueness, and monotonicity of equilibria.

11.5 Parallelizing your Differential Equation Solver: A tutorial introduction to domain decomposition methods

Organizers: Martin Gander and Ronald Haynes

| Sunday July 18 | | Location: Viking |
|---------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------|
| Chairs: Ronald Haynes & Martin Gander | | |
| 4:00–4:20 | Martin Gander Domain decomposition methods for stationary and time dependent problems | |
| 4:20–4:40 | Ronald Haynes Domain decomposition for time dependent problems | |
| 4:40–5:00 | Felix Kwok Algebraic vs. continuous formulations of domain decomposition methods | |
| 5:00–5:20 | Sebastien Loisel Coarse grid correction for domain decomposition methods | |
| 5:20–5:40 | Loic Gouarin The Domain Decomposition Toolbox: a Python implementation of domain decomposition methods for steady and time dependent problems | |
| 5:40–6:00 | Loic Gouarin Continued | |

Abstracts:

Domain decomposition methods for stationary and time dependent problems

Martin Gander

University of Geneva

Email: martin.gander@unige.ch

It can be daunting for a newcomer to find a way through the jungle of domain decomposition methods, with all the Schwarz, primal and dual substructuring, FETI, Neumann-Dirichlet, Robin-Robin and waveform relaxation methods. I will give an overview of current domain decomposition methods, based on the following fundamental three classes of methods:

- Schwarz methods, traditionally based on an iterative process and overlap, but modern optimized Schwarz methods can be used without overlap,
- substructuring methods based on the elimination of interior unknowns, traditionally used without overlap,

- waveform relaxation methods, which solve evolution problems parallel in space and time.

In each case, I will describe the historical development of the methods, give their fundamental convergence behavior and illustrate it with numerical experiments. This introduction serves as a preparation for the later talks in the minisymposium.

The Domain Decomposition Toolbox: a Python implementation of domain decomposition methods for steady and time dependent problems

Loic Gouarin

Université Paris-Sud 11

Email: loic.gouarin@math.u-psud.fr

Python is a very simple and powerful programming language. In the last decade, this language has become very popular in scientific computing. Several scientific Python packages such as Numpy, Scipy and matplotlib allow us to develop scientific codes quickly and efficiently. The syntax is very similar to Matlab.

In this talk, I will present some basic elements to develop domain decomposition methods in Python with the packages mentioned above and the mpi4py package. I will begin with a very simple example solving the 1D heat equation with domain decomposition techniques:

- for explicit time discretization scheme: I will discuss some possible implementations with Python and then, I will do some comparisons of execution times with other implementations like Fortran or Matlab.
- for implicit time discretization scheme: I will show how to implement quickly the classical Schwarz method.

To conclude, I will talk about “optimism” which is a parallel finite element software for solving elliptic and parabolic problems with optimized Schwarz methods.

Domain decomposition for time dependent problems

Ronald D. Haynes

Memorial University of Newfoundland

Email: rhaynes@mun.ca

Domain decomposition (DD) methods were originally designed for elliptic problems. A natural way to extend the idea for time dependent problems is to discretize the problem in time and to solve the resulting elliptic PDEs using a standard DD approach. That is, we solve a sequence of elliptic problems. The solution at each time step may be obtained in parallel. An alternative approach is to decompose the space-time domain into subdomains which may or may not overlap in space. The time dependent PDE is

then solved independently on each subdomain with time dependent boundary data exchanged at the end of each iteration. This is known as the Schwarz waveform relaxation method. In this talk we will explain the pros and cons of each approach along with some numerical experiments. SWR methods allow flexibility with the solver used on individual subdomains. This presents the option of using specialized solvers – adaptive in space and time where needed.

Algebraic vs. continuous formulations of domain decomposition methods

Felix Kwok, Martin Gander

University of Geneva

Email: felix.kwok@unige.ch

In order to parallelize a PDE solver using domain decomposition (DD), one can choose to either start with the continuous DD method and discretize each continuous subproblem (the continuous approach), or start with the global discretized problem and use parallel DD preconditioners (the algebraic approach). The two approaches often lead to the same methods, especially when the decomposition does not contain points that belong to more than two subdomains (i.e., cross points). However, when cross points are present, the two approaches can lead to different methods with different convergence properties. In particular, we will show an example in which the continuous-based method converges whereas a seemingly equivalent algebraic method diverges; we will then show another example when the exact opposite happens. The discrepancy stems from the fact that even though both approaches end up having the same system matrices, the interface data being transmitted between subdomains can be extracted in many different ways, leading to different convergence behaviours.

Coarse grid correction for domain decomposition methods

Sebastien Loisel

University of Heriot-Watt

Email: sloisel@gmail.com

The main application for domain decomposition methods is for the purpose of solving a boundary value problem on a cluster of computers in parallel. The most interesting case is when there are many subdomains and where the grid of the discretization is very fine. In the limiting situation where the subdomains are of very small size, the amount of overlap is also forced to be small. One checks that the performance of classical Schwarz (and other) algorithms deteriorate as the amount of overlap decreases: a 1-level algorithm requires more and more iterations to obtain convergence as we increase the number of subdomains. In order to remedy this situation, a coarse grid is introduced. The coarse problem is a very rough approximation to the fine problem. The coarse problem is able to communicate low-frequency information rapidly over long

distances. The subdomain problems are able to resolve the high frequency information. Under some conditions, we will show that the number of iterations of a 2-level algorithm remains bounded as the number of subdomains increases.

11.6 Reaction–Diffusion Systems

Organizers: David Iron and Chun–Hua Ou

| Tuesday July 20 | | Location: Salon B |
|----------------------------------|----------------------------------------------------------------------------------------------------------------------|--------------------------|
| Chairs: David Iron & Chun–Hua Ou | | |
| 4:00–4:20 | Mohammadkheer Al–Jararha Population dynamics with age-dependent diffusion and death rates | |
| 4:20–4:40 | Shaohua Chen A new functional method in global and blowup problems | |
| 4:40–5:00 | David Iron Stability of patterns on lattices | |
| 5:00–5:20 | Chris Levy Model of cell signal transduction in a 3-dimensional domain | |
| 5:20–5:40 | Chun–Hua Ou Existence and nonexistence of monotone traveling waves for the delayed Fisher equation | |
| 5:40–6:00 | Paul Muir Collocation software with adaptive error control collocation software for 1D reaction-diffusion systems | |

Abstracts:

Population dynamics with age-dependent diffusion and death rates

Mohammadkheer AlJararha, Chun–Hua Ou

Memorial University of Newfoundland

Email: mmaj84@mun.ca

In this paper we investigate the population dynamics of a species with age structure in the case when the diffusion and death rates of the matured population are both age-dependent. A completely new model in terms of an integral equation is constructed. For unbounded spatial domain, we study the existence of traveling waves, while in bounded domain, we investigate the existence of positive steady-state solutions and their stability for different choices of birth function. As a by-product, we also prove rigorously the existence of real principle eigenvalue with positive eigenfunctions. Also, we present a numerical simulation.

A new functional method in global and blowup problems**Shaohua Chen**

Cape Breton University

Email: george_chen@cbu.ca

We use a new functional method to obtain lower and upper bounds for the solutions of the degenerate and quasilinear parabolic equations, as well as an activator-inhibitor model. In this method, we estimate the integral of a ratio of one solution to the other.

Stability of patterns on lattices**David Iron**, John Rumsey, Michael Ward

Dalhousie University

Email: iron@mathstat.dal.ca

We consider a system of reaction diffusion equations in the plane in which the solutions form localized structures. Equilibrium solutions will have all the localized structures arranged on a lattice. We fix the size of the lattice cell and then consider the relative stability of different types of lattices. In the talk I will discuss the spectra of periodic patterns in 1 and 2 dimensions. To determine the spectrum, I will need to find an appropriate Green's function. A large portion of the talk will be concerned with the construction of this Green's function.

Model of cell signal transduction in a 3-dimensional domain**Chris Levy**, Dalhousie University

Email: clevy@mathstat.dal.ca

Intracellular signaling molecules form pathways inside the cell. These pathways carry a signal to target proteins which results in cellular responses. We consider a spherical cell with two internal compartments containing localized activating enzymes where as deactivating enzymes are spread uniformly through out the cytosol. Two diffusible signaling molecules are activated at the compartments and later deactivated in the cytosol due to deactivating enzymes. The two signaling molecules are a single link in a cascade reaction and form a self regulated dynamical system involving positive and negative feedback. Using matched asymptotic expansions we obtain approximate solutions of the steady state diffusion equation with a linear decay rate. We obtain three dimensional concentration profiles for the signaling molecules which either decay exponentially or algebraically depending on the diffusion length of each molecule. We also investigate an extension of the above system which has multiple cascade reactions occurring between multiple signaling molecules. Numerically, we show that the speed of the signal is an increasing function of the number of links in the cascade.

Collocation software with adaptive error control collocation software for 1D reaction-diffusion systems

Paul Muir, Rong Wang, Pat Keast, Tom Arsenault, Tristan Smith
Saint Mary's University
Email: muir@smu.ca

In this talk, we discuss two recently developed software packages for the numerical solution of 1D Reaction-Diffusion Systems. These packages, called BACOL and BACOLR, have been shown to be more efficient, reliable and robust than other comparable packages, especially for problems with solutions exhibiting narrow spikes or boundary layers. These packages represent examples of the latest generation of method-of-lines (MOL) codes in that they feature adaptive control of an estimate of the spatial error (in addition to the standard temporal error estimate control provided by most MOL packages.) BACOL uses the time-stepping software called DASSL, while the time-stepping in BACOLR is based on the RADAU5 package.

While the BACOL/BACOLR spatial error estimation is generally reliable, the estimate is based on the expensive computation of two global collocation solutions, a higher order solution and a lower order solution. The second part of this talk will briefly consider our recent work on the development of two more efficient spatial error estimation algorithms based on (i) the use of a low cost, higher order (superconvergent) interpolant to replace the higher order collocation solution and, (ii) the use of low cost, lower order interpolant to replace the lower order collocation solution.

Existence and nonexistence of monotone traveling waves for the delayed Fisher equation

Chun–Hua Ou, Man Kam Kwong
Memorial University of Newfoundland
Email: ou@mun.ca

In this talk, a new approach based on a shooting method in a half line coupled with the technique of upper-lower solution pair is used to study the existence and nonexistence of monotone waves for one form of the delayed Fisher equation that does not have the quasimonotonicity property. A necessary and sufficient condition is provided. This new method can be extended to investigate many other nonlocal and non-monotone delayed reaction diffusion equations.

11.7 Recent Developments in Numerical Methods for the Solutions of ODEs

Organizers: Paul Muir and Ray Spiteri

| Sunday July 18 | | Location: Signal |
|-----------------------------------|-----------------------------------------------------------------------------------------------------|-------------------------|
| Chairs: Paul Muir and Ray Spiteri | | |
| 4:00–4:20 | George Corliss Propagating uncertainties in modeling nonlinear dynamic systems | |
| 4:20–4:40 | Andrew Kroshko Methods of solving ordinary differential equations using SIMD architectures | |
| 4:40–5:00 | Colin MacDonald RIDC: A multicore high-order time integrator | |
| 5:00–5:20 | Paul Muir A user-friendly Fortran 90/95 boundary value ODE solver | |
| 5:20–5:40 | Jason Boisvert A Hybrid global error and defect control schemes for boundary-Value problem codes | |
| 5:40–6:00 | Piers Lawrence Event handling with barycentric Hermite interpolation | |

Abstracts:

A hybrid global error and defect control schemes for boundary-value problem codes

Jason Boisvert, Paul Muir, Raymond Spiteri
University of Saskatchewan
Email: jjb701@mail.usask.ca

Some popular boundary value ordinary differential equations (BVODEs) codes, such as BVP_SOLVER, attempt to control a measurement of the defect, i.e., the amount by which the continuous numerical solution fails to satisfy the BVODE. Other BVODE codes, such as COLSYS, control a measurement of the global error, i.e., the amount by which the numerical and exact solution differ. Defect-control BVODE codes benefit from being able to estimate the defect even when a global-error estimation is unreliable. However, because the defect is only indirectly related to the global error, it is possible for these codes to return a solution that has a small defect norm and a relatively large global-error norm. In extreme cases, a defect-control code can return a solution to a BVODE that theoretically has none. Therefore, there is some advantage for these codes to control some measurement of the global error.

In this talk, we describe the implementation of two hybrid error-control strategies in BVP_SOLVER. These include a strategy that begins by controlling the defect and then controls the global error, and a strategy that simultaneously controls both error measurements. We also compare the accuracy and overall runtime of both error-control strategies.

Propagating uncertainties in modeling nonlinear dynamic systems

George Corliss, Elizabeth Untiedt, Weldon Lodwick, Joshua A. Enszer, Youdong Lin, Scott Ferson, Mark A. Stadtherr
Marquette University
Email: George.Corliss@Marquette.edu

In many practical applications of ordinary differential equations modeling physical phenomena, parameters and initial conditions are given with some uncertainties. How can we propagate these uncertainties rigorously through a solution approximation algorithm? We describe an approach that expands the solution in a Taylor model [Makino & Berz] in uncertain parameters and initial conditions. We evaluate the Taylor models using p-boxes [Ferson] and gradual numbers representing fuzzy numbers to represent the uncertainties in the state variables of the ODE. We give examples from reaction process dynamics to demonstrate the potential of this approach for studying the effect of uncertainties with imprecise probability distributions.

Methods of solving ordinary differential equations using SIMD architectures

Andrew Kroshko, Raymond Spiteri
University of Saskatchewan
Email: andrew.kroshko@usask.ca

The optimisation of physical processes often involves the solution of ordinary differential equations (ODEs) for each objective function evaluation. Particle swarm optimisation (PSO) is a promising recent global optimisation method because it can take advantage of objective function evaluations computed in parallel. Accordingly, the high floating-point throughput and parallelism of processors such as the Cell Broadband Engine (CBE) are ideal for these problems. In this talk I will describe an implementation on the CBE of the RODAS solver for stiff ODEs within the context of PSO. RODAS uses a fourth-order Rosenbrock method with a third-order embedded method for error and step-size control. We solve two ODE systems in parallel on each synergistic processing element (SPE) using SIMD for a total of 16 ODE systems solved in parallel using the 8 SPEs on each CBE chip; standard CBE code would only be able to solve 8 ODE systems in parallel. Using a variable step size for each problem we are able to achieve a speedup of 1.87 (a parallel efficiency of 93%) over the corresponding serial code.

Event handling with barycentric Hermite interpolation**Piers Lawrence**, Rob Corless, Ned Nedialkov

The University of Western Ontario

Email: plawren@uwo.ca

Physical systems modelled by ODE often have event functions to constrain the solution to some physical bounds. Thus accurate event location routines are needed to ensure that the solution correctly describes the dynamics of the system. Here we present an implementation of event location using barycentric Hermite interpolation. This form of Hermite interpolation is a convenient and stable procedure as it constructs the interpolant directly in the Hermite interpolation basis using Taylor series data. In this form the root-finding problem can be solved by constructing a companion matrix pencil without the need to express the interpolant in the monomial basis and hence is more stable. Events are located by finding eigenvalues of the companion matrix pencil and as all of the roots are found this ensures the first root and hence the event is located. Multiple roots are also dealt with via a clustering algorithm that takes into account the condition number of the roots. Examples of the event location procedure are presented for both simple and multiple events.

RIDC: A multicore high-order time integrator**Colin Macdonald**, Benjamin Ong, Andrew Christlieb

University of Oxford

Email: macdonald@maths.ox.ac.uk

RIDC (revisionist integral deferred correction) methods are a class of time integrators well-suited to parallel multicore computing. RIDC methods can achieve high-order accuracy in wall-clock time comparable to forward Euler. The methods use a predictor and multiple corrector steps. Each corrector is lagged by one time step; the predictor and each of the correctors can then be computed in parallel. This presentation introduces RIDC methods and demonstrates their effectiveness on some test problems.

A user-friendly Fortran 90/95 boundary value ODE solver**Paul Muir**

Saint Mary's University

Email: muir.smu@gmail.com

This talk will describe a recently developed user-friendly Fortran 90/95 software package for the numerical solution of boundary value ordinary differential equations (BVODEs) called BVP_SOLVER. This software was written by the author and Larry Shampine (Southern Methodist University) and was based on an earlier Fortran 77 package, MIKRDC, written by the author and Wayne Enright (University of Toronto). Both solvers are based on mono-implicit Runge-Kutta methods and on defect control.

Users often find it difficult to interact with standard Fortran 77 BVODE solvers; BVP_SOLVER has been written to address this issue; it takes advantage of a number of language features of Fortran 90/95 to provide a substantially simpler experience for the user, while at the same time employing the underlying robust, high quality algorithms of the original MIRKDC code. BVP_SOLVER also implements several numerical algorithms that represent improvements over those employed in MIRKDC. Examples are presented to demonstrate the capabilities of the new solver. Several current projects associated with enhancing the capabilities of BVP_SOLVER will also be mentioned.

12 Contributed Papers

Organizers: Canan Bozkaya and Shannon Sullivan

| Sunday July 18 | | Location: Viking |
|-------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|
| Chair: Gina Reid | | |
| 9:00–9:20 | Malcom Roberts The multispectral method | |
| 9:20–9:40 | Elizabeth Liverman Open-loop-controlled oscillations of a cylinder in a free-surface flow. Part 1: New vortex states | |
| 9:40–10:00 | Canan Bozkaya Open-loop-controlled oscillations of a cylinder in a free-surface flow. Part 2: Evaluation of fluid forces and pressure field | |
| Chair: Elizabeth Liverman | | |
| 10:30–10:50 | Donald Campbell The sigma-delta modulator as a chaotic nonlinear dynamical system | |
| 10:50–11:10 | Lennard Kamenski Anisotropic mesh adaptation for the finite element method using error estimates based on hierarchical bases | |
| 11:10–11:30 | Sven-Joachim Kimmerle An electrohydrodynamical problem for modelling polymer electrolyte membranes | |
| 11:30–11:50 | Allan Willms Near minimax continuous piecewise linear representations of discrete data | |
| 11:50–12:10 | Petro Babak A probabilistic model for forest fire spread | |
| Monday July 19 | | Location: Plymouth |
| Chair: Canan Bozkaya | | |
| 10:30–10:50 | Jared Penney A computational model of electro-osmotic flow | |
| 10:50–11:10 | Gina Reid Free surface flow past a cylinder under combined streamwise and transverse oscillations | |
| 11:10–11:30 | Kahinde Ladipo Tetrahedral elements in finite element models with continuous pressure approximation | |
| <i>continued on next page</i> | | |

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|-------------------------------------|--------------------------------------------------------------------------------------------------------|
| <i>continued from previous page</i> | |
| 11:30–11:50 | Nany Soontiens Hysteresis in supercritical trapped internal waves over topography |
| 11:50–12:10 | Vandad Talimi A numerical study on plug flow heat transfer between parallel plates and inside tubes |

Abstracts:**A probabilistic model for forest fire spread**

Petro Babak, Thomas Hillen

University of Alberta

Email: petro@math.ualberta.ca

Prediction of the spread of forest fires faces with a wide range of uncertainties caused by fuel complexity, spatial heterogeneity in environmental conditions, stochastic nature of atmospheric processes, etc. The aim of this presentation is to propose a novel methodology for incorporation of these uncertainties in forest fire spread simulations. In this talk we will derive a probabilistic model for forest fire propagation. This model contains coupled parabolic differential equation with an ordinary differential equation. The parabolic differential equation describes the probability density of fire, and contains diffusion, advection and reaction components. The diffusion component corresponds to different sort of uncertainties. The advection component represents, for example, the effects of wind and slope. And the reaction component describes the dynamics of change in the probability of fire without taking into account spatial interactions. The ordinary differential equation defines the cumulative probability of fire which is calculated as an integral of the probability density. Implementing the probabilistic model for forest fire spread allows estimation of fire propagation with any confidence level in much efficient way than simulation approaches for existing deterministic and stochastic models. Finally, numerical simulations of the probabilistic model for homogeneous and heterogeneous environments will be shown.

Open-loop-controlled oscillations of a cylinder in a free-surface flow.**Part 2: Evaluation of fluid forces and pressure field**

Canan Bozkaya, Elizabeth Liverman, Serpil Kocabiyik

Memorial University of Newfoundland

Email: canan@mun.ca

This study presents the results of a two-dimensional computational study of the free surface flow past a circular cylinder forced to perform rotational oscillations in the presence of an oncoming uniform flow. In Part 1, we have examined the effects of the inclusion

of the free surface on the vortex-shedding modes in the near wake region for the same problem at the Reynolds number of $R = 200$ for combinations of the maximum angular cylinder displacement and the forcing cylinder oscillation frequency-to-natural vortex shedding frequency ratio ($\theta_m = 15^\circ - 75^\circ$ and $f/f_0 = 0.5 - 4.0$). The numerical simulations are carried out using basically the same two-phase flow model and finite volume code as that used in Part 1 for solving the unsteady continuity and Navier-Stokes equations (when a solid body is present). The objective of this study is to examine the effect of the maximum angular displacement amplitude, θ_m , and the frequency ratio, f/f_0 , on fluid forces as well as the pressure field at a Froude number of $Fr = 0.2$ when $h = 0.75$.

The sigma-delta modulator as a chaotic nonlinear dynamical system

Donald Campbell

University of Waterloo

Email: doc11232003@yahoo.ca

Sigma-delta modulators (or noise shapers as they are also called) are extensively used for analogue-to-digital and digital-to-analogue data conversion (signal processing). Their dynamical behaviour can appear chaotic. I will explore this behaviour from the point of view of nonlinear dynamical systems analysis. To begin, the difference equation model of the sigma-delta modulator is introduced, and some basic results for bounded stability are obtained. The model is cast formally as a discrete dynamical system, and important continuity results allowing for a linear analysis are established. Drawing on this, I conduct a theoretical study of conditions for chaos or nonchaos using an adaptation of Devaney's definition of chaos. This study is extended to the dithered system, in the context of allowing stochastic aspects in the model. I then introduce a stochastic formulation of the long-run dynamics, which is applied to give conditions for uniformly distributed error behaviour — conditions under which important consequences arise when dither is used to control the error statistics.

Anisotropic mesh adaptation for the finite element method using error estimates based on hierarchical bases

Lennard Kamenski, Weizhang Huang, Jens Lang, Xianping Li

University of Kansas

Email: lkamenski@math.ku.edu

A common approach for generating an anisotropic mesh is based on generation of a quasi-uniform mesh in some metric space. A key component of the approach is the determination of an appropriate metric often based on some type of error estimate or post-processing of the obtained numerical solution. In this study, we consider an anisotropic mesh adaptation strategy for the finite element method and investigate the use of a global hierarchical basis error estimator for the development of an anisotropic

metric tensor. To avoid the expensive exact solution of the full error problem, a few iterations of the symmetric Gauss-Seidel method are employed to obtain a reasonably good approximation to the error for the use in anisotropic mesh adaptation. The new method is compared with several strategies using local error estimation or recovered Hessians. Numerical examples are presented for a selection of variational problems and boundary value problems of a second-order elliptic differential equation.

An electrohydrodynamical problem for modelling polymer electrolyte membranes

Sven-Joachim Kimmerle, Peter Berg, Arian Novruzi
University of Ottawa
Email: skimmerl@uottawa.ca

From a thermodynamic model for charged-fluid flow and the morphology of polymer electrolyte membranes (PEM) in hydrogen fuel cells, we derive a system of coupled partial differential equations. We model the velocity, pressure, electric field and proton concentration in a nano-scale channel that is filled with protonated water, and an equation for the mechanical displacement of the surrounding solid. The latter results in a free boundary between liquid and solid which is considered to be elastic. This is a generalization of the well-known Nernst-Planck-Poisson-Stokes system. The problem is important in order to understand better the behaviour of PEMs and improve material properties of the PEM. We solve the equations numerically and compare the results with those of similar situations.

Tetrahedral elements in finite element models with continuous pressure approximation

Kahinde Ladipo University of Ontario Institute of Technology
Email: kehinde.ladipo@uoit.ca

A method of discretizing a 3-D rectangular domain into brick-like macros consisting of six 4-node tetrahedral elements is presented. The space discretization is such that the pressure tetrahedral elements are macro-elements consisting of 8 velocity sub-tetrahedral elements. This method specifically considers splitting a brick-like macro into 6 tetrahedral elements when the same piecewise-linear approximations are employed for pressure and velocity, in 3-D numerical models involving Navier-Stokes equations, and the finite element method employs a mesh for velocity that is twice finer compared to the mesh for pressure. The tetrahedral elements are easily identified and the assembly of the discrete system of equations can be on the computer. Careful evaluation of the associated integrals is required for the inf-sup condition to be satisfied.

This spatial discretization technique is applied to simulate natural convection in a cubical box. Results obtained are in good agreement with published results in the literature.

Open-loop-controlled oscillations of a cylinder in a free-surface flow.**Part 1: New vortex states****Elizabeth Liverman**, Canan Bozkaya, Serpil Kocabiyik

Memorial University of Newfoundland

Email: eliverman@mun.ca

A computational study of a viscous incompressible two-fluid model with an oscillating cylinder is performed. Specifically, two-dimensional flow past a circular cylinder subject to forced rotational oscillations beneath a free surface is considered. Numerical method is based on the finite volume method for solving the two-dimensional continuity and unsteady Navier-Stokes equations (when a solid body is present). The numerical simulations are carried out at a Reynolds number of $R = 200$ and a Froude number $Fr = 0.2$, and the cylinder submergence depth $h = 0.75$. The flow characteristics are examined for combinations of the maximum angular cylinder displacement and the forcing cylinder oscillation frequency-to-natural vortex shedding frequency ratio ($\theta_m = 15^\circ - 75^\circ$ and $f/f_0 = 0.5 - 4.0$). The main objective of this study is to address the alterations of the near-wake region, in particular, the flow regimes and the locked-on vortex formation modes, due to the presence of the free surface. This investigation has shown that it is possible to generate distinctly different patterns of vortex formation than that of classical vortex shedding modes in the presence of the free surface depending on the values of the maximum angular cylinder displacement and the frequency ratio.

A computational model of electro-osmotic flow**Jared Penney**, Jahrul Alam

Memorial University of Newfoundland

Email: jmpenney@mun.ca

Electro-osmotic flow (EOF) is the bulk motion of a charged fluid due to the application of an electric field. EOF is of particular interest in science and engineering for various applications in analytical chemistry, protein separation, DNA sequencing, and lab-on-a-chip technology. When analyzing the nature and physics of EOF, computational fluid dynamics (CFD) can be used as a convenient and practical alternative to expensive and complex physical experimentation. In this work, a CFD approach for studying electro-osmotic flow in microchannels is examined. Using an existing CFD code, a mathematical model of incompressible EOF has been solved numerically on a collocated finite difference grid. It has been observed that a Lagrangian scheme is more appropriate than an Eulerian scheme for the numerical treatment of advection terms. The numerical results have been verified through mathematical analysis.

Free surface flow past a cylinder under combined streamwise and transverse oscillations**Gina Reid**, Serpil Kocabiyik

Memorial University of Newfoundland

Email: ginar@mun.ca

Combined wave motion and steady current past ocean structures can induce fluid excitation forces, which in turn cause structural vibrations due to asymmetric vortex shedding. Control of vortex shedding leads to reduction in the forces acting on the structure and can significantly reduce its vibrations. This study focuses on free surface flow past a circular cylinder based on a two fluid model at a Reynolds number of $R = 200$. Control is exerted to the fluid field by forcing the cylinder to perform combined transverse and streamwise oscillations in the presence of an oncoming uniform flow. The method is based on a finite volume discretization of the two-dimensional unsteady Navier-Stokes equations (when a solid body is present). The imposed streamwise and transverse displacements of the cylinder are assigned by $x(t) = y(t) = A \cos(2\pi ft)$. The study focuses on the laminar asymmetric flow structure transitions in the near wake region as well as evaluation of fluid forces and pressure field at a Froude number of $Fr = 0.2$ and cylinder submergence depth $h = 0.5$. Calculations are performed at fixed displacement amplitudes of $A = 0.13$ in forcing frequency-to-natural shedding frequency ratio range $1.25 \leq f/f_0 \leq 2.75$. The code validations in special cases show good comparisons with previous experimental and numerical results.

The multispectral method**Malcolm Roberts**, John Bowman, Bruno Eckhardt

University of Alberta

Email: mroberts@math.ualberta.ca

Spectral simulations of high Reynolds-number turbulence require a very large number of active modes, ranging from the largest scale of the system to the dissipation scale. Since there is no intermediate range of quiescent modes, numerical techniques cannot rely on a separation of scales to reduce the stiffness of the system. The *multispectral method* generalizes spectral reduction [Bowman, Shadwick, and Morrison, *Phys. Rev. Lett.* **83**, 5491 (1999)] to evolve time-dependent PDEs on a hierarchy of decimated grids in Fourier space. The grids can be decimated so that low-wavenumber modes are preserved. High-Reynolds number turbulence can then be simulated using far fewer degrees of freedom than required for a full pseudospectral simulation. In previous work [Roberts, *A Multi-Spectral Decimation Scheme for Turbulence Simulations*, Master's thesis, University of Alberta (2006)], the multispectral technique was demonstrated for shell models. Here, we apply the technique to the two-dimensional incompressible Navier-Stokes equation, taking care that the projection and prolongation operators between the grids conserve both energy and enstrophy. The nonlinear advection term is handled using efficient

algorithms that we have recently developed for computing implicitly dealiased convolutions (<http://fftwpp.sourceforge.net>).

Hysteresis in supercritical trapped internal waves over topography

Nancy Soontiens, Christopher Subich, Marek Stastna

University of Waterloo

Email: nksoonti@uwaterloo.ca

A model for steady flow of a stratified fluid over topography is examined using a pseudo-spectral, iterative numerical method. The results indicate that different size trapped internal waves can form depending on the strength of the background current. With a shear background current, multiple waves can be produced with the same current in the iterative solver. The result is a hysteresis loop based on wave amplitude and shear strength. For a constant background current, hysteresis is also found by varying the width of the topography. These results are confirmed by integrating the fully time-dependent Euler equations from rest with different rates of fluid acceleration.

A numerical study on plug flow heat transfer between parallel plates and inside tubes

Vandad Talimi, Yuri S. Muzychka, Serpil Kocabiyik

Memorial University of Newfoundland

Email: v.talimi@mun.ca

The heat transfer and flow pattern of a moving plug between two parallel plates and inside a circular tube are studied numerically. The problem is solved initially as a steady state problem for the velocity field and then the thermal conditions are applied. The fluid properties are assumed to be constant. The finite volume method is applied using the ANSYS Fluent software package. The results show good agreement with the published literature. The effect of different contact angles on the heat transfer is considered and a correction factor is suggested to correct this effect. The dimensionless heat transfer graphs are presented for both parallel plates and circular tubes.

Near minimax continuous piecewise linear representations of discrete data

Allan Willms, Emily Szusz

University of Guelph

Email: AWillms@uoguelph.ca

An algorithm that constructs a continuous piecewise linear representation of a given set of discrete data, subject to a novel constraint relating the segments' slopes and lengths, is described. The constraint is determined by a user-specified parameter, t_{\min} , which dictates the minimum length of segments whose slopes do not lie between the slopes

of their neighbours. For reasonable t_{\min} values, the resulting representation of the data captures the signal and both smooths the noise and provides a measure of it. The algorithm yields an optimal or near optimal representation, subject to this constraint, in the L^∞ norm and does so in at worst $O(nK)$ time, where n is the number of data points and K the number of segments. The algorithm is described, its capabilities demonstrated with several examples, and potential applications are discussed.

13 Posters

Organizers: Canan Bozkaya and Shannon Sullivan

The poster session will be held from

- Sunday July 18 10:00–10:30 during the coffee break
- Sunday July 18 12:00–1:30 during the lunch break
- Sunday July 18 3:30–4:00 during the coffee break
- Monday July 19 10:00–10:30 during the coffee break
- Monday July 19 3:30–4:00 during the coffee break

Judging will take place Sunday from 12:00–1:30. We ask that presenters try to be around during some of the above times to discuss their work. Participants should certainly make an effort to be around for the judging. Posters should be removed by 12:00pm Tuesday, July 20.

Abstracts:

Bifurcations of periodic solutions of functional differential equations with spatio-temporal symmetries

Juancho Collera

Queen's University

Email: 7jc1@queensu.ca

Functional Differential Equations (FDEs) are differential equations defined on a Banach space. We will only consider equations of retarded type or the so-called Retarded Functional Differential Equations (RFDEs). Periodic solutions with spatio-temporal symmetries of such class of FDE arise for example in Equivariant Hopf Theorem. Hale and Weedermann proved that under some perturbations these periodic orbits are continued, that is, they proved the existence of an integral manifold near the periodic orbit. They also showed that a centre manifold reduction is possible for the case when the periodic orbit is non-degenerate.

In this poster presentation, we examine how the spatio-temporal symmetries of the periodic solution affect the symmetry of the integral manifold. Furthermore, for the non-degenerate case, we show that the center manifold in the neighbourhood of the periodic orbit is invariant with respect to the spatio-temporal symmetry. This generalization of the result of Hale and Weedermann is used to develop a symmetry-breaking bifurcation of periodic solutions with spatio-temporal symmetry which generalize the results of Lamb and Melbourne to RFDEs. We also look at some examples on coupled cell systems.

Optimization of tidal turbine power

Amber Corkum and Amanda Swan, WeiWei Wang, Michael Deveau, Richard Karsten, Ronald Haynes, Hugh Chipman, Pritam Ranjan
Acadia University
Email: 088269c@acadiu.ca

Recent focus on green energy sources has placed a lot of emphasis on the energy potential in the tides. With the highest tides in the world, the Bay of Fundy offers an excellent location in which to implement in-stream tidal turbines. An important step is to find the best locations for turbine fences that will maximize the amount of extractable power. Mathematical models can be used in predicting energy generated by tidal turbines. They therefore allow for the power maximization to be carried out before placing real turbines. The computational cost of calculating the power for each turbine array however, can be high and the number of different arrangements of the turbines is very large. Our goal is to find a method that will find an accurate location of a turbine fence that provides maximum power using a minimum number of function evaluations.

Two different optimization techniques are considered, particle swarm optimization and Bayesian Additive Regression Trees. The models are tested by placing turbine fences sequentially and simultaneously.

Investigating ENSOs irregularity using a simple model for the thermoclines depth

Julia Davourie, Marek Stastna
University of Waterloo
Email: julia.davourie@gmail.com

ENSOs irregularity is investigated based on the work of Tziperman et al 1997, which considers a delayed oscillator model with a short Kelvin wave delay and a longer Rossby wave delay. The consistency and robustness of this nonlinear chaotic model is tested in three different ways:

1. The delay is distributed over time (up to seven days).
2. The period of the forcing is changed between one quarter to seven years.
3. Random noise in a range from 0 to 5% is added.

The output is studied in terms of the time series, the phase-space (Poincaré sections), and the spectrum. These allow for the identification of the timescales, amplitudes of the variation in thermocline depth. They also identify parameter regimes for which chaotic behavior is obtained. We find that:

1. Distributed delays results in a variation of the period and amplitude but does not affect the intensity of fluctuations.

2. Variation of the periodic forcing period shows that an annual forcing leads to powerful and chaotic variations, while long period forcing leads to phase-locking of the thermoclines depth variation.
 3. The addition of random forcing slightly affects the intensity and amplitude of fluctuations, and alters variations in phase space.
-

Shallow-water surface waves and bed ripples due to erosion

Matthew Emmett, T.B. Moodie
University of Alberta
Email: memmett@math.ualberta.ca

Deformations in the bed of a river or flume that are caused by erosion may eventually lead to the formation of ripples in the bed and surface roll-waves on the water. The complex interaction between the flow and bed that produces these phenomena is quite intriguing and we endeavour to understand the mechanisms behind it. To this end, we present a simple bulk model of sediment transport and erosion, and explore, using various analytic and asymptotic techniques, how the numerically observed roll-waves and bed ripples are formed.

Linear stability analysis of reactive convective mixing in porous media under gravity

S. Hossein Hejazi, J. Azaiez
University of Calgary
Email: shhejazi@ucalgary.ca

Density mismatch between two solutions laid on top of each other in a porous medium may result in an interfacial instability which is referred to as the Rayleigh-Taylor instability or convective mixing. Convective mixing may become further complicated as a result of a simple $A + B \rightarrow C$ chemical reaction at the interface of reactant solutions. Reactive convective mixing finds its interests in many underground reservoir flows such as in situ recovery of heavy oil recovery processes, the spreading of reactive pollutants in groundwater as well as geological CO_2 storage.

A linear stability analysis of a reactive interface under gravity is performed by solving a generalized eigenvalue differential equations and applying a quasi steady state approximation. The effect of various parameters including the densities of chemical species A, B and C and the viscosity of the chemical product C are studied in order to classify the unstable scenarios. Moreover, instability characteristics of the flow are examined to demonstrate how the presence of a transverse velocity which is common in many geological reservoirs may affect the fate of reactive convective mixing.

An adaptive wavelet collocation method for Fluid Dynamics

Mo Rokibul Islam, Md. Zahangir Hossain, Jahrul Alam, Nicholas Kevlahan, Oleg Vasilyev

Memorial University of Newfoundland

Email: mri305@mun.ca

The ability of wavelets for identifying localized structures such as coherent vortices made them attractive candidates for adaptive numerical simulation. As a result, there is a growing interest in the development of a wavelet methodology, which offers a relatively new technique for Computational Fluid Dynamics (CFD) applications. This paper presents an adaptive wavelet collocation method (AWCM) and its application to CFD. Numerical examples verifying the performance of the AWCM are presented. We show that if the time evolution of a smooth initial flow exhibits localized structures, the AWCM identifies the region of sharp change and adds new grid points so that the localized structures of the solution can be resolved.

Particle tracking through Minas Passage

Richard Karsten, Mitchell O'Flaherty-Sproul, Martin Tango

Acadia Univeristy

Email: rkarsten@acadiau.ca

In stream turbines are being placed in the Minas Passage to generate electricity from the strong tidal currents. These turbines will both have an impact on the environment and be impacted by the environment. To examine some of these impacts, Lagrange Particle Tracking code is used to predict the path of neutrally buoyant particles through Minas Passage. The code uses velocities output from a high resolution model of the tidal currents through Minas Passage, with and without modelled turbines present.

The particle tracking code is used to examine three problems of interest. First to determine which water is most likely to pass through a turbine. Second to examine where any material that is given off by a turbine would be carried by the flow. And thirdly, to estimate of the probability that material along the shore line of Minas Basin could be carried through Minas Passage and interact with a turbine.

Improving the efficiency of heart simulations

Megan Lewis, Raymond Spiteri

University of Saskatchewan

Email: mel864@mail.usask.ca

Heart disease accounts for over one third of all deaths in Canada. Heart simulation is a method for studying the heart that does not require invasive surgery. We are interested in developing numerical methods and software for real-time simulation of the electrical activity in the heart. The mathematical models describing the flow of electricity

through the heart involve complicated differential equations that are impossible to solve analytically and difficult to solve numerically. The most commonly used model is known as the bidomain model and consists of two partial differential equations describing the flow of electricity across the heart tissue that are coupled with a cardiac cell model for the electrical flow across the cell membrane of a single cardiac cell. Ideally, a numerical simulation of a single heartbeat would take approximately the same amount of time as the actual time of a single heartbeat (approximately 500 milliseconds). However, billions of equations must be solved to obtain a realistic simulation, making the goal of real time simulations a challenge. We are interested in improving the efficiency of simulations of electrical activity in the heart by optimizing the numerical methods used to solve the bidomain model.

Vortex wake transitions of an oscillating cylinder beneath a free surface

Elizabeth Liverman, Canan Bozkaya
Memorial University of Newfoundland
Email: eliverman@mun.ca

Free surface flow past a circular cylinder subject to forced rotary oscillations is investigated numerically. The numerical simulations are carried out at a Reynolds number of $R = 200$ and a Froude number $Fr = 0.2$, and the cylinder submergence depth, $h = 0.75$. The flow characteristics are examined for combinations of the maximum angular cylinder displacement and the forcing cylinder oscillation frequency-to-natural vortex shedding frequency ratio ($\theta_m = 15^\circ - 75^\circ$ and $f/f_0 = 0.5 - 4.0$). The imposed angular displacement of the cylinder is assigned by $a(t) = -\theta_m \cos(2\pi ft)$. The main objective of this study is to address the alterations of the near-wake region, in particular, the flow regimes and the locked-on vortex formation modes, due to the presence of the free surface. This investigation has shown that it is possible to generate distinctly different patterns of vortex formation than that of classical vortex shedding modes in the presence of the free surface depending on the values of the maximum angular cylinder displacement and the frequency ratio.

Control of free surface flow over a circular cylinder

Gina Reid, Canan Bozkaya
Memorial University
Email: ginar@mun.ca

The transformation between kinetic and potential energies and the coexistence of viscous and gravity forces at an unknown wavy boundary make free surface phenomena difficult to study. Understanding the physics of flow structures and the free surface interaction is fundamental to ocean engineering and undersea technology. This study focuses on free surface flow past combined streamwise and transverse oscillations of a circular cylinder

based on a two fluid model at a Reynolds number of $R = 200$. The method is based on a finite volume discretization of the two-dimensional unsteady Navier-Stokes equations (when a solid body is present). The imposed streamwise and transverse displacements of the cylinder are assigned by $x(t) = y(t) = A \cos(2\pi ft)$. The study focuses on the laminar asymmetric flow structure transitions in the near wake region and evaluation of fluid forces and the pressure field at a Froude number of $Fr = 0.2$ and the cylinder submergence depth, $h = 0.5$. Calculations are performed at a fixed displacement amplitude of $A = 0.13$ in forcing frequency-to-natural shedding frequency ratio range $1.25 \leq f/f_0 \leq 2.75$. The code validations in special cases show good comparisons with previous experimental and numerical results.

A generalized Birkhoff-Rott equation for the 2D active scalar problems

Hui Sun, David Uminsky, Andrea Bertozzi

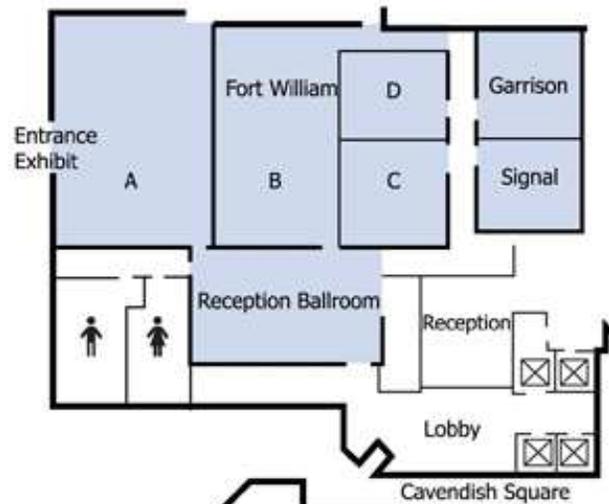
University of California, Los Angeles

Email: huiprobable@gmail.com

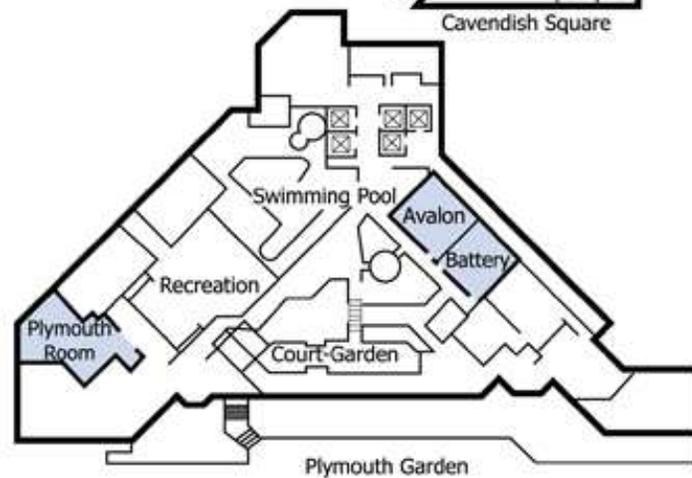
In this poster we derive new evolution equations for the active scalar problem in 2D for the case when all scalars lie on a 1D curve, analogous to the Birkhoff-Rott equation for 2D vorticity. The new equations are Lagrangian and valid for nonlocal kernels K that may include both a gradient and an incompressible term. We develop a numerical method for implementing the model which achieves second order convergence in space and fourth order in time. We simulate classic active scalar problems such as the vortex sheet problem (in the case of purely incompressible flow) and the collapse of delta ring solutions (in the case of pure aggregation) and find excellent agreement. We also include new examples that contain both incompressible and gradient flows.

14 Map of meeting rooms

Main Floor



Lower Floor



Pre-function area – main floor

Salon A – main floor

Salon B – main floor

Salon D – main floor

Avalon/Battery – lower level

Plymouth – lower level

Signal – main floor

Viking – first floor

Amherst – sixth floor

Speaker Index

- Afanasyev, 32
Alam, 33
AlJararha, 106
Anco, 51
Ascher, 18, 74
Azzouz, 51
- Babak, 114
Bass, 68
Begg, 46
Bélair, 47
Berbeglia, 19
Berg, 33
Beyene, 82
Bloch, 13
Boisvert, 109
Bowman, 34
Bozkaya, 114
Braza, 14
Briollais, 82
Broucke, 59
Bull, 83
Buono, 22
Burgess, 88
- Campbell, D., 115
Campbell, L., 34
Campbell, S.A., 59
Carr, 83
Carrasco-Teja, 34
Carrero, 52
Chang, 60
Chen, S., 107
Chen, W., 23
Collera, 121
Conway, 99
Coombs, 19
Corkum, 122
Corliss, 110
- Cortelezzi, 35
- D'Alessio, 35
D'Orsogna, 23
Davourie, 122
Demirov, 36
Dereniowski, 89
Dillon, 68
Djournna, 36
Dyer, 89
- Edwards, 93
Eftimie, 47, 100
Emmett, 123
Erneux, 23
Etienne, 68
- Farcot, 94
Fetecau, 60
Fortescue, 52
Frigaard, 37
Friis, 69
Fukumoto, 61
- Gallant, 90
Gander, 102
Gooding, 53
Gouarin, 103
Graham, 84
Gumel, 48, 61
- Haddara, 69
Hamilton, 84
Haq, 96
Haynes, 103
Hejazi, 123
Homsy, 37
Huang, 74
- Iron, 107
Islam, M.R., 124

- Islam, S., 62
Jeon, 62
Kamenski, 115
Karsten, 38, 124
Kelly, 62
Kennett, 53
Kevlahan, 38
Kimmerle, 116
Kitanov, 24
Knapp, 70
Kolokolnikov, 24
Kopciuk, 85
Krivodonova, 75
Kroshko, 110
Kulic, 63
Kuske, 25
Kustra, 85
Kwok, 104
Ladipo, 116
Langford, 14
Lawrence, 111
Leok, 63
Lessard, 86
Levy, 107
Lewis, G., 25, 39
Lewis, M., 97, 124
Liao, 39
Lindsay, 26
Liverman, 117, 125
Loisel, 104
Loredo-Osti, 86
Lu, 94
Lukeman, 26
Macdonald, 75, 111
MacLachlan, 97
Maggiore, 64
Mansouri, 64
Marinova, 39
Marshall, 86
Marsiglio, 54
McKay, 27
McNeney, 87
Merkli, 54
Meza, 100
Mimimis, 76
Minsaas, 11
Miura, 15
Molin, 15
Moyers-Gonzalez, 40
Muir, 108, 111
Muzychka, 40
Nachtergaele, 15
Nec, 27
Nemenman, 64
Normore, 41
O'Dell, 54
Ong, 76
Opps, 55
Ou, 28, 108
Peng, 70
Penney, 117
Perkins, 95
Pike, 90
Poulin, 41
Protas, 42
Qi, 90
Raman-Nair, 71
Rees, 71
Reid, 118, 125
Reluga, 101
Renardy, M., 42
Renardy, Y., 42
Roberts, 118
Russell, 16
Ruuth, 77
Samokhin, 55
Sanaei, 91

Scott, 48
Shalaby, 91
Shegelski, 56
Siegel, 65
Silvesan, 91
Skrynnikov, 43
Soontiens, 119
Spiteri, 77
Starr, 56
Stastna, 44
Stockie, 44
Stoica, 28, 65
Sun, 28, 126
Swan, 122

Talimi, 119
Thompson, 16
Trummer, 78
Tyson, 48

Urquiza, 78

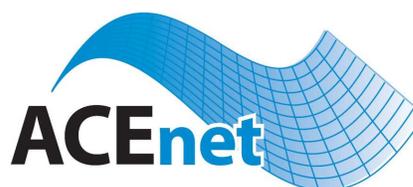
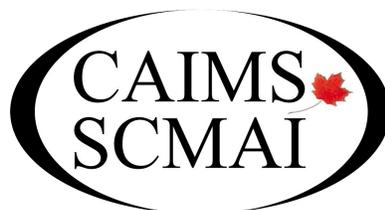
van Roessel, 44
van Zyl, 56
Vougalter, 57

Waite, 45
Walter, 97
Wan, 78
Wang, 72
Ward, 17, 29
Wetton, 20, 45, 79
Willms, 119
Witelski, 29
Wu, 49

Yang, 72
Young, 79
Yu, 95

Zenkov, 66
Zhu, 49

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