MITACS Environment and Natural Resources Theme Meeting
December 2–4, 2005

MEETING OBJECTIVES

Some of the most challenging problems being studied today involve coupling between various nonlinear physical phenomena which occur on a wide range of spatial and temporal scales. The primary tool for studying such complex problems is numerical simulation. A plethora of new methods have been developed in recent years which aim to deal with problems of stiffness inherent in multiscale problems. However, more research is needed in order to develop more efficient algorithms which are specially tailored for individual problems.

The projects within the MITACS Environment and Natural Resources Theme span a diverse range of application areas, involving fuel cells, seismic imaging, spatio-temporal population dynamics, and computational fluid dynamics. However, these projects are connected by their common need for numerical methods that solve differential and integro-differential equations. Several projects within this theme are leading the development of such methods, and so we plan to provide a forum for discussing these recent advances in numerical methods, and to share expertise between the participants. There is also a recognized need for development of more expertise in parameter sensitivity analysis, which is an essential technique for understanding the dependence of such complex models on important system parameters.

The purpose of this workshop is to bring together the projects participating in this theme for the first time, and to explore common interests related to recent advances in numerical methods for differential (and integro-differential) equations.

MEALS

Breakfast (Continental): 7:00 - 9:00 am, 2nd floor lounge, Corbett Hall, Friday & Saturday
* Lunch (Buffet): 11:30 am - 1:30 pm, Donald Cameron Hall, Friday & Saturday
* Dinner (Buffet): 5:30 - 7:30 pm, Donald Cameron Hall, Thursday & Friday
Coffee breaks: As per daily schedule, 2nd floor lounge, Corbett Hall

** Please remember to scan your meal card at the host/hostess station in the dining room for each lunch and dinner.*

MEETING ROOMS

All lectures are held in Max Bell 159. Hours: 6 am - 12 midnight. LCD projector, overhead projectors and blackboards are available for presentations

Please note that the meeting space designated for BIRS is the lower level of Max Bell, Rooms 155-159. Please respect that all other space has been contracted to other Banff Centre guests, including any food and beverages in those areas.

SCHEDULE

Thursday December 2

16:00	Check-in begins (Front Desk, Professional Development Centre - open 24 hours)
	Lecture rooms available after 16:00
17:30–19:30	Dinner (Donald Cameron Hall)
19:30	Informal gathering (2nd floor lounge, Corbett Hall)
	Beverages and an assortment of snacks are available on a cash honour-system basis

Friday December 3

7:00–9:00	Breakfast (2nd floor lounge, Corbett Hall)
9:00–9:15	John Stockie: *Introductory remarks*
9:15–10:15	Linda Petzold: *Sensitivity analysis of differential-algebraic equations and partial differential equations*
10:15–11:00	Coffee break (2nd floor lounge, Corbett Hall)
11:00-11:30	Tyson Josey: *Numerical modelling capabilities and the need for efficient timestepping algorithms*
11:30-12:00	Rong Wang: *Preliminary tests for Zephyr*
12:00–13:30	Lunch (Donald Cameron Hall)
13:30–14:30	Linda Petzold: *Sensitivity analysis in condition and error estimation*
14:30-15:00	Discussion
15:00–15:30	Coffee break (2nd floor lounge, Corbett Hall)
15:30-16:00	Xiaoqiang Zhao: *An epidemic model in a patchy environment*
16:00-17:00	Brock Nyquist: *Modelling tree squirrel population growth in a managed forest*
17:30–19:30	Dinner (Donald Cameron Hall)
evening	Free

Saturday December 4

7:00–9:00	Breakfast (2nd floor lounge, Corbett Hall)
9:00–9:30	Jiri Patera: *Applications of an n-dimensional generalization of the cosine transform, based on any compact semi simple Lie group of rank n*
9:30–10:00	Gary Margrave: *Seismic imaging in theory and practice*
10:00–10:30	Coffee break (2nd floor lounge, Corbett Hall)
10:30–11:00	Paul Chang: *Electrical and thermal coupling in proton exchange membrane fuel cells*
11:00–11:30	Lloyd Bridge: *Some ideas for capturing a moving two-phase/vapour interface in a porous medium*
12:00	Check-out time

*** You are welcome to use the BIRS facilities (2nd Floor Lounge, Max Bell Meeting Rooms, Reading Room) until 16:00 on Saturday, although participants are still required to check out of the guest rooms by 12:00 noon. There is no coffee break on Saturday afternoon, but self-serve coffee and tea are always available in the 2nd floor lounge, Corbett Hall. ***

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ABSTRACTS

Speaker: **Lloyd Bridge** (Institute of Applied Mathematics, University of British Columbia)

Title: *Some ideas for capturing a moving two-phase/vapour interface in a porous medium*

Abstract: We describe a model problem of water transport and phase change in a finite porous layer, which is of interest to our PEM fuel cell modelling group. In preference to trying to track the two-phase/vapour interface explicitly, we consider two methods for capturing the interface, which both simply require finite difference solutions to a fixed domain problem. However, the inherent singularity and degeneracy in the problem make computations anything but simple. In this talk, I'll discuss unsuccessful smoothing strategies, the enthalpy method, degenerate diffusion, and our ongoing battles with this problem.

Speaker: **Paul Chang** (Department of Mathematics, University of British Columbia)

Title: *Electrical and thermal coupling in proton exchange membrane fuel cells*

Abstract: A mathematical model describing the effects of electrical and thermal coupling of proton exchange membrane unit fuel cells through shared bipolar plates is developed. The unit cell model, developed by Berg et al. (2004), couples the consumption of reactants in the flow field channels to the current density and water content in the polymer membrane. Differing current density profiles in neighboring cells leads to in-plane currents in the bipolar plates, and the redistribution of current is governed by the nonlocal voltage equations. Thermal transport is decoupled into the in-plane and cross-plane directions; this is reasonable because of the large aspect ratio of the typical fuel cell geometry and the large in-plane to cross-plane conductivity ratio. Numerical results showing the effects on stack voltage and current density due to anomalous oxidant and coolant flow rates in the center cell are shown. It is shown that both electrical and thermal coupling have a significant effect on fuel cell performance.

Speaker: **Tyson Josey** (Martec Ltd.)

Title: *Numerical modelling capabilities and the need for efficient timestepping algorithms*

Speaker: **Gary Margrave** (Department of Geology and Geophysics, University of Calgary)

Title: *Seismic imaging in theory and practice*

Abstract: I will present an overview of the seismic imaging problem with an emphasis upon the problems of shot-record depth migration and nonstationary deconvolution. The common link between these topics is that both can be formulated as requiring the inversion of nonstationary filters that specifically are either Fourier integral operators or pseudodifferential operators. I will pose these problems and outline some of the possible solutions being explored by our MITACS research team.

Speaker: **Brock Nyquist** (Department of Mathematics and Statistics, Okanagan University College)

Title: *Modelling tree squirrel population growth in a managed forest*

Abstract: While many population models exist which examine the growth of a populace with regards to spatial distributions, we have worked to design a model that takes into account changes within the environment which impact the modeled species. In this case, the aim is to examine the effects of clear-cut logging, or other regular removal of habitat, upon forest tree squirrel populations. We have developed a coupled system of ordinary differential equations to model the system, and we present salient results.

Speaker: **Jiri Patera** (Centre de recherches mathématiques, Université de Montréal)

Title: *Applications of an n-dimensional generalization of the cosine transform, based on any compact semi simple Lie group of rank n*

Abstract: New discrete and continuous group transforms are used to process n-dimensional digital data. Features: (i) New expansion functions are discretized in a very versatile way on Abelian subgroups of the maximal torus of the Lie group. (ii) Continuous extension of the transforms between digital points is very smooth, first and second derivatives of the extension can be used.

Applications to be shown involve image enhancements and data compression in the context of 2-dimensional images from FLIR (forward looking ifrared radar), medical X-ray data, and enhancing resolution of remote sensing images. Cryptographic application of the same method, based on non-crystallographic Coxeter groups, are to be shown.

Speaker: **Linda Petzold** (Departments of Computer Science, and Mechanical & Environmental Engineering, University of California, Santa Barbara)

Title: *Sensitivity analysis of differential-algebraic equations and partial differential equations*

Abstract: Sensitivity analysis of differential-algebraic equation (DAE) systems generates essential information for design optimization, parameter estimation, optimal control, model reduction, process sensitivity and experimental design. Recent work on methods and software for sensitivity analysis of DAE systems has demonstrated that forward sensitivities can be computed reliably and efficiently. However, for problems that require the sensitivities with respect to a large number of parameters, the forward sensitivity approach is intractable and the adjoint (reverse) method is advantageous. In this talk we introduce the forward and adjoint sensitivity methods for DAEs. We give the adjoint system for general DAEs and investigate some of its fundamental analytical and numerical properties. We describe our forward and adjoint DAE software.

Defining the adjoint sensitivity system and writing the appropriate software to describe it can be a very challenging problem for large-scale engineering systems, particularly when it comes to finding appropriate boundary conditions for the adjoint partial differential equation (PDE) system. Therefore our goal for both DAE and PDE systems has been the development of methods and software in which generation and solution of the sensitivity system are transparent to the user. This has been largely achieved for DAE systems. We propose a solution to this problem for PDE systems solved with adaptive mesh refinement.

Speaker: **Linda Petzold** (Departments of Computer Science, and Mechanical & Environmental Engineering, University of California, Santa Barbara)

Title: *Sensitivity analysis in condition and error estimation*

Abstract: The forward and adjoint methods for sensitivity analysis are powerful tools for an amazing range of applications. In this lecture we show how to use sensitivity analysis, in combination with the small sample statistical condition estimation method, to estimate condition and error in the solution of linear systems, to estimate and control the global error in the numerical solution of ordinary differential equations, and to estimate errors and regions of validity for reduced order models of dynamical systems. Numerical examples illustrate the effectiveness of this approach.

Speaker: **Rong Wang** (Department of Mathematics and Statistics, Dalhousie University)

Title: *Preliminary tests for Zephyr*

Abstract: Zephyr is a software package developed by Martec, Ltd. that is designed to solve the Euler equations for an ideal (or perfect) gas. The software employs a Godunov-type scheme, where the Godunov flux is computed by solving the corresponding Riemann problem with an approximate Riemann solver, HLLC. Instead of applying the traditional Godunov scheme, Zephyr performs the time integration with certain Runge-Kutta (RK) schemes. In this talk we first describe the schemes in Zephyr for both spatial and time discretization. We then describe results for the classical shocktube problem, using both the RK methods originally in Zephyr and the other RK methods that we have added. Computational results show that the stability restriction is the major barrier in terms of efficiency of the time stepping. That is, the stability requirement forces the software to use tiny timesteps that lead to unecessarily small temporal errors.

Speaker: **Xiaoqiang Zhao** (Department of Mathematics, Memorial University of Newfoundland)

Title: *An epidemic model in a patchy environment*

Abstract: In this talk, we will present an epidemic model with population dispersal in a patchy environment. The global dynamics of this model will be discussed in terms of reproduction number, and two examples will be provided to illustrate the effect of population dispersal on the spread of a disease.