36th Annual SANUM Conference

Programme Schedule

Venues:

All Contributed and Plenary talks will take place in Room 211, Professional Development Hub.

All talks that are a part of one of the Special Sessions will take place in Room G14, Professional Development Hub.

The Opening and Closing addresses will take place in Room 211, Professional Development Hub.

The Break-Away rooms available as work areas or for further discussions are G05 and G09.

Monday, 2 April 2012

08:00 - 09:00	**Registration**
	Chair: E. Momoniat
09:00 - 09:30	**Opening address: A. Crouch,** *Dean of the Faculty of Science, University of the Witwatersrand*
09:30 - 10:30	**Plenary: J. C. Butcher,** *Faithful Forever: Long term integration using general linear methods*
10:30 - 11:00	**Tea Break**
	Chair: R. J. Moitsheki
11:00 - 11:25	M. Molati, *Lie Symmetry Classification of the BBM equation with time-dependent coefficients*
11:25 - 11:50	R. Morris, *Double reductions for a class of nonlinear partial differential equations*
11:50 - 12:15	F. M. Mahomed, *Boundary Value Problems for a Fourth-Order Dynamic Euler-Bernoulli Beam Equation*
12:15 - 12:40	R. Klein, *Domain mapping using harmonic functions in non-convex domains of genus non-zero*
12:40 - 13:30	**Lunch Break**
13:30 - 14:30	*Plenary Chair: R. J. Moitsheki* **Plenary: J. A. C. Weideman,** *Efficient Contours for the Numerical Computation of the Bromwich Integral*
	Chair: B. A. Jacobs
14:30 - 14:55	K. Colville, *Introduction to the Systems and Research at the Centre for High Performance Computing*
15:00 - 16:30	K. Colville, *Centre for High Performance Computing: mini-course for scientists who wish to use the CHPC computers*
16:30 - 17:00	**Tea Break**
17:30 - 20:30	**Welcoming Braai: Hofmeyer House**

Monday, 2 April 2012

Special Session: Numerical Aspects of Dynamical Systems, Partial Differential Equations and Inequalities, Arising in Applications

08:00 - 09:00	**Registration**
	Chair: E. Momoniat
09:00 - 09:30	**Opening address: A. Crouch,** *Dean of the Faculty of Science, University of the Witwatersrand*
09:30 - 10:30	**Plenary: J. C. Butcher,** *Faithful Forever: Long term integration using general linear methods*
10:30 - 11:00	**Tea Break**
	Chair: J. Djoko Kamdem
11:00 - 11:25	D. Reddy , *Algorithms for the solution of non-smooth problems arising in elasto-plasticity*
11:25 - 11:50	M. Basson, *Large Finite element analysis of a vibrating Timoshenko beam with damping*
11:50 - 12:15	A. Chama, *Stable mixed finite element approximations for problems in elasticity*
12:15 - 12:40	A. Adebayo, *On the Numerical solution of Kuramoto-Sivashinky equation*
12:40 - 13:30	**Lunch Break**
13:30 - 14:30	*Plenary Chair: R. J. Moitsheki* **Plenary: J. A. C. Weideman,** *Efficient Contours for the Numerical Computation of the Bromwich Integral*
	Chair: D. Reddy
14:30 - 14:55	J. Djoko Kamdem, *Discontinuous Galerkin Finite element discretization for steady Stokes flows with threshold slip boundary condition*
14:55 - 15:20	M. Mbehou, *Finite element analysis for power law Stokes equations*
15:20 - 15:45	N. F. Janse van Rensburg, *Using energy methods to compare models*
15:45 - 16:05	B. J. Grieshaber, *Three-field discontinuous Galerkin methods for elasticity problems*
16:30 - 17:00	**Tea Break**
17:30 - 20:30	**Welcoming Braai: Hofmeyer House**

Tuesday, 3 April 2012

	Plenary Chair: C. Harley
08:00 - 09:00	**Plenary: M. Sears,** *The Real Dimension of Hyperspectral Data*
	Chair: D. Fanucchi
09:00 - 09:25	S. Abelman, *Oscillatory Couette flow of a Sisko fluid in a rotating system*
09:25 - 09:50	J. C. Butcher, *Variable order and stepsize for numerical integrators*
09:50 - 10:15	H. Abelman, *Matrix diagonalization and clinical measurements in Optometry*
10:15 - 10:45	**Tea Break**
	Chair: S. Abelman
10:45 - 11:10	H. K. Voruganti, *A novel geometric criterion for prediction of protein interactions*
11:10 - 11:35	P. Kumar, *Image processing and analysis to investigate the morphological design parameters for nanofibrous and macroporous polymeric scaffolds*
11:35-12:00	A. Traore, *On the numerical solution of nonlinear age-dependent sis epidemics*
12:00 - 12:45	**Lunch Break**
13:00 - 17:30	**Excursion: Maropeng, Cradle of Humankind**
18:00 - 21:00	**Conference Dinner: Hofmeyer House**

Tuesday, 3 April 2012

Special Session: Image Processing

	Plenary Chair: C. Harley
08:00 - 09:00	**Plenary: M. Sears,** *The Real Dimension of Hyperspectral Data*
	Chair: I. Fabris-Rotelli
09:00 - 09:25	D. Laurie, *LULU: a personal view*
09:25 - 09:50	B. A. Jacobs, *On the Application of the fractional Cattaneo equation to Image Processing*
09:50 - 10:15	A. R. De Pierro, *Filtering and Regularization in Image Reconstruction*
10:15 - 10:45	**Tea Break**
	Chair: B. A. Jacobs
10:45 - 11:10	J. Drijer , *Conditional Random Fields and Cardiac MRI Segmentation*
11:10 - 11:35	I. Fabris-Rotelli, *LULU Operators: the Discrete Pulse Transform and Applications in Image Analysis*
11:35 - 12:00	G. G. Stoltz, *Objects as perceived by a machine*
12:00 - 12:45	**Lunch Break**
13:00 - 17:30	**Excursion: Maropeng, Cradle of Humankind**
18:00 - 21:00	**Conference Dinner: Hofmeyer House**

Wednesday, 4 April 2012

08:00 - 09:00	*Plenary Chair: R. J. Moitsheki* **Plenary: J.E. Sader,** *The Dynamics of Nanoscale Mechanical Devices in Fluid*
	Chair: M. K. Banda
09:00 - 09:25	D. P. Mason, *Coal mine pillar extraction*
09:25 - 09:50	R. Kgatle , *Effects of fluid tortuosity on a two-dimensional hydraulic fracture*
09:50 - 10:15	D. Fanucchi, *An efficient numerical scheme for capturing correlation effects in ab-initio Quantum Chemistry*
10:15 - 10:45	**Tea Break**
	Chair: D. P. Mason
10:45 - 11:10	M. K. Banda, *A finite volume scheme application in fluid structure interaction for gas dynamics*
11:10 - 11:35	Z. Adegboyega, *Error analysis in Runge-Kutta Methods for the case of Linear Multistep Methods*
11:35 - 12:00	R. S. Herbst, *Radiation from a Relativistically Rotating Neutron Star: The Effects of Mass*
12:00 - 12:30	**Closing address: E. Momoniat,** *Head of the School of Computational and Applied Mathematics*
12:30 - 14:00	**Lunch Break**

Additional abstracts

Oscillatory Couette flow of a Sisko fluid in a rotating system

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The normal motion of sinovial fluid (a clear viscous fluid that lubricates the linings of joints and the sheaths of tendons) can be viewed as oscillating Couette flow in a finite domain. We present a study of rotating oscillatory Couette flow of an incompressible and electrically conducting Sisko fluid between two non-conducting plates. The upper plate is oscillating in its own plane, while the lower plate is kept stationary. The resulting nonlinear problem is solved numerically. The effects of emerging parameters on the velocity are studied.

An efficient numerical scheme for capturing correlation effects in ab-initio Quantum Chemistry

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The majority of ab-initio quantum chemistry is concerned with the time independent Schrödinger Equation acting over antisymmetrized multi-electron (Fock) space. It has proven notoriously difficult to obtain analytical solutions to the many-body Schrödinger equation in all but the simplest of cases. Early attempts to find solutions numerically also yielded little fruit. In the 1930's, Dirac famously stated that the equations of quantum chemistry were "far too complicated to be soluble".

We present a concise review of the progress in numerical solutions to the ab-initio problem of Quantum Chemistry over the last century. The main landmarks - the introduction of the Hartree-Fock Integro Differential Equation, the advent of Density Functional theory and the development of Valence Bond Theory - are presented as ideas in numerical analysis.

Many of the current approaches begin with an uncorrelated estimate to the solution wave-function, and add corrections via the Variational Principle. We discuss A new method obtained by beginning with a very specific set of configurations produced by Goddard's GVB method, instead of the uncorrelated Hartree Fock reference configuration. This captures some of the dynamic correlation up-front,

and leaves less work for the higher order corrections. A very rich structure emerges which allows us to perform correlation corrections far more efficiently than in the general multi-reference case.

The improved algorithms are implemented in parallel on NVIDIA's CUDA architecture, and some results are shown for medium sized molecules.