Programme & Abstracts



SANUM 2010

The 34th Annual South African Symposium on Numerical and Applied Mathematics

15, 16 and 17 March

Hosted by the Department of Mathematical Sciences Stellenbosch University South Africa

Welcome to SANUM!

Registration takes place on Monday 15 March from 08:15 to 08:50 in the foyer of the general engineering building, located on the corner of Banhoek and Joubert roads.



On the cover: Panoramic view of Stellenbosch from Papegaaiberg. Photo by Francois Malan.

Internet Access, Reception, Lunches

Internet access is available in room A308.

Automatic proxy configuration: <u>http://dip.sun.ac.za/local/proxy.pac</u>

Login: sanum Password: sanum

- Outgoing mail server: mail.sun.ac.za
- Wifi access point: "mrwifi"

Please join us for a **welcoming reception** on Monday evening, held at the botanical gardens. **Lunch** is served daily at "Die Bloukamer" restaurant on the top floor of the Neelsie student centre.



Conference Dinner (Tuesday evening)



Directions to Dieu Donné Restaurant
Uitkyk Street, Dieu Donne Vineyards, Franschhoek 7690, South Africa - 021
876 3384
30.7 km – about 33 mins

The conference dinner is held on Tuesday evening at the Dieu Donné restaurant. Come early to enjoy the breathtaking view!



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Joubert St, Stellenbosch, South Africa

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Programme for SANUM 2010

Time	Monday 15 March				l	Tuesday 16 March Wednesday 17 March			March				
08:15—09:00	Registration												
09:00—10:00	Plenary I Bernhard Schölkopf Learning and inference with positive definite kernels			opf e definite kernels	Chair: Weideman	Plenary I Peter Markowich The Numerical Solution of Semiclassical Schrödinger Equations	Chair: Mason	Plenary I Peter Clarkson Rogue Waves, Vortices and Rational Solutions of Soliton Equations					
10:00—10:30							Теа						
10:30—11:30	900 eman		Plenary II Iain Duff The solution of really large linear discretizations of three-dimer			r Iff ear sys mensio	stems arising from onal problems	erbst	Plenary II Uri Ascher Surprising computations	De Villiers	Ple Rob Polynomial Algebra	enary Cor	r II less lirkhoff Interpolants
11:30—12:00	Chair: Weid	Plenary III Mayya Tokman		u. Chair: He		Weideman	ombie	Smit	er Walt	Olivier			
12:00—12:30	Peri		rmance of exponential pro- ntegrators and their deriva	ators and their derivation using B-series.			Makinde	Schoo	Grieshaber	Van de	Fabris-Rotelli		
12:30—14:00	Lunch												
14:00—14:30	Se Ma	ssion on chine	De Pierro	atidar	Mason		SANUM General Meeting						
14:30—15:00	:00 Im		Van der Walt	Chair: P	Abelman	Schoombie	Laurie						
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16:00—16:30		Herbs	Reikeras		Patidar	belmá	Schoombie		information.				
16:30—17:00		hair:	Singels		Munyakazi	air: A	Ahmadinia						
17:00—17:30		0	Swanepoel	Chair	Mudzimbabwe	5							
18:00—	Welcoming Reception				on		Conference Dinner						

Monday 15 March

MONDAY PLENARY	6
Learning and inference with positive definite kernels	
Prof. Bernhard Schölkopf, Max Planck Institute for Biological Cybernetics	6
The solution of really large linear systems arising from discretizations of three-dimensional problems	
Prof. Iain Duff. RAL + CERFACS	6
Performance of exponential propagation iterative (EPI) integrators and their derivation using B-series	C
Proj. Mayya Tokman, OC Mercea	0 C
	0
New Optimization Models in Magnetic Resonance Imaging	7
A linear interpolation operator for super resolution imaging	1
A linear interpolation operator for super-resolution imaging Stefan Johann van der Walt University of Stellenhosch	7
Probabilistic image segmentation for volumetric silboutte based reconstruction	•
Dr Willie Brink. University of Stellenbosch	7
Variational Bayesian Inference Methods with Application to Audio-Visual Speech Recog-	
nition	
Helge Reikeras, Stellenbosch University	7
Real-time stereo reconstruction using hierarchical dynamic programming and LULU filter-	
ing	
Francois Singels, Stellenbosch University	8
Off-line Signature Verification using Flexible Grid Features and Classifier Fusion	_
Jacques Swanepoel, Stellenbosch University	8
MONDAY AFTERNOON	8
Two-dimensional turbulent wall jet	
Prof. David Mason, University of the Witwatersrand	8
On the Rayleigh problem for a Sisko fluid in a rotating frame	0
Prof. Snirley Abelman, University of the Witwatersrand, Johannesburg	8
Exact solutions of the two-dimensional steady in problem with temperature dependent	
Dr Loel Moitsbeki, University of the Witwatersrand	8
Higher order fitted operator methods for poplinear singular perturbation problems	0
Prof. Kailash C. Patidar. University of the Western Cape	8
A robust fitted operator method for singularly perturbed problems in higher dimension	
Dr Justin Bazimaziki Munyakazi, University of the Western Cape	9
A lower bound for pricing European basket options	
Walter Mudzimbabwe, University of the Western Cape	9

LEARNING AND INFERENCE WITH POSITIVE DEFINITE KER-NELS

Prof. Bernhard Schölkopf (Max Planck Institute for Biological Cybernetics)

Kernel methods have become one of the most widely used techniques in the field of machine learning. I will present my thoughts on what made them popular and where things are heading. I will discuss some recent developments for two-sample and independence testing as well as applications in different domains.

THE SOLUTION OF REALLY LARGE LINEAR SYSTEMS ARIS-ING FROM DISCRETIZATIONS OF THREE-DIMENSIONAL PROB-LEMS

Prof. Iain Duff (RAL + CERFACS)

The most challenging problems for numerical linear algebra arguably arise from the discretization of partial differential equations from three-dimensional modelling. The structure of the resulting equations causes problems for direct methods inasmuch the factors are much denser than the original system while their complexity causes major problems for the convergence of iterative methods.

In this talk we show how direct and iterative methods can be combined to solve problems that are intractable by one class of methods alone. Examples of these hybrid methods include using a direct method as a coarse grid solver in multigrid or to solve subproblems in domain decomposition. We show examples of these approaches and indicate how they can be used to solve very large problems. We also examine hybrid methods that use a fast but potentially inaccurate sparse factorization.

Researchers in the Parallel Algorithms Group at CERFACS in Toulouse have recently solved threedimensional Helmholtz problems in seismic modelling with over 65 billion unknowns. We briefly discuss how this has been done.

PERFORMANCE OF EXPONEN-TIAL PROPAGATION ITERATIVE (EPI) INTEGRATORS AND THEIR DERIVATION USING B-SERIES

Prof. Mayya Tokman (UC Merced)

Exponential integrators offer an efficient alternative to explicit and implicit schemes in integration of large stiff systems of ODEs. However, these methods have not yet attained wide popularity among practitioners. The limited use of exponential techniques is due in part to two reasons: lack of thorough performance comparisons with standard integrators and difficulties in derivation of these schemes. In this talk we address both of these questions. We will present analysis of the performance of exponential integration iterative (EPI) methods compared to widely-used implicit and explicit schemes on a suite of test problems. We will also discuss how the Butcher's theory of Bseries simplifies derivation of higher order exponential methods and demonstrate this point by presenting construction of new fifth- order EPI integrators.

NEW OPTIMIZATION MODELS IN MAGNETIC RESONANCE IMAG-ING

Prof. Alvaro Rodolfo De Pierro (University of Campinas)

Magnetic Resonance Imaging (MRI) is one of the most important tools for medical diagnosis. The main mathematical model for MRI is the Fourier Transform. This is a reasonable model for slow acquisition protocols that also assume a homogeneous magnetic field and complete data (the 'whole' kspace), essentially for what is called anatomic MRI. For faster acquisitions, the primary hipotheses, like magnetic field homogeneity and complete data, are no longer true. So, the inversion of the Fourier Transform produces distorted images with very strong artifacts and regularization is necessary. In this article we describe two new mathematical optimization models more adequate for solving the previously described problems. The first model introduces a variation of the magnetic field with higher resolution that leads to a nonconvex optimization problem. The second model is related to Compressed Sensing (CS). In CS applications to MRI, essentially for fast acquisitions with incomplete data, not only the magnetic field is considered homogeneous, but real and imaginary parts of the solution as well. This is also not true in practical applications for fast acquisitions, where the magnitude (image) can be considered sparse (at least approximately) and CS theories apply, but not the phase, that is smooth. So, our second model introduces a differentiated regularization for magnitude and phase that gives rise to another nonconvex optimization problem, and surprising results. References:

[1] M.W. Zibetti and A.R. De Pierro, A new distortion model for strong inhomogeneity problems in Echo- Planar MRI, IEEE Trans. Medical Imaging, 28, 11, 1736-1753.

[2] M.W. Zibetti and A.R. De Pierro, A regularization penalty for complex value signals and images with sparse magnitude and smooth phase, in preparation

A LINEAR INTERPOLATION OPERATOR FOR SUPER-RESOLUTION IMAGING

Stefan Johann van der Walt (University of Stellenbosch)

We discuss super-resolution imaging: the assumptions made, data requirements and the level of improvement that can be achieved practically. A linear interpolation operator, capable of modelling the underlying sensor process, is introduced. We conclude with a live reconstruction, performed using an open source software framework developed as part of this research.

PROBABILISTIC IMAGE SEG-MENTATION FOR VOLUMETRIC SILHOUETTE-BASED RECON-STRUCTION

Dr Willie Brink (University of Stellenbosch)

I will present a technique for incorporating probabilistic segmentations into the shape-from-silhouette (SFS) technique for 3D volumetric reconstruction from a set of images. In basic SFS points in 3D space are back-projected to all the images. Points for which any of the back-projections falls outside the contours of the object are disregarded so that, ultimately, a 3D model remains. By introducing probabilistic segmentations I will extend the concept to a more stochastic nature and show that high quality models can be obtained by thresholding final point probabilities. The segmentation method used is based upon maximum a posteriori estimates in a Bayesian framework. The proposed idea would, however, remain the same for any probabilistic image segmentation method.

VARIATIONAL BAYESIAN INFER-ENCE METHODS WITH APPLICA-TION TO AUDIO-VISUAL SPEECH RECOGNITION

Helge Reikeras (Stellenbosch University)

Motivated by the multi-modal manner humans perceive their environment, the field of Audio-Visual Automatic Speech Recognition (AVASR) focuses on the fusion of audio and video feature data to enhance automatic speech recognition systems. The technique is especially successful when the audio stream is contaminated by acoustic noise.

A core problem in AVASR research and the development of AVASR systems is the lack of labelled (transcribed) video data for learning audio- visual speech models. Videos featuring speech in itself is abundant on video sharing websites such as YouTube. However, this data is often noisy and lacks the necessary word labels to make it immediately useful for learning speech models. Existing audio-only speech recognition systems may be used to label the data, although unavoidably with some error. Noise and erroneous labels in the training data may easily lead to over-fitting of models when using standard learning methods such as Expectation Maximisation (EM).

Variational Bayesian inference is a framework for approximating posterior probability distributions using ideas borrowed from calculus of variations and mean field theory. We will show how this framework, without computational overhead, allows us to efficiently learn probabilistic models that are robust to the noise, singularities and over-fitting associated with standard learning methods. Furthermore, variational methods allow us to simultaneously perform model selection and parameter estimation without sorting to computationally expensive techniques such as cross-validation.

REAL-TIME STEREO RECON-STRUCTION USING HIERARCHI-CAL DYNAMIC PROGRAMMING AND LULU FILTERING

Francois Singels (Stellenbosch University)

We discuss some general topics relating to stereovision and the correspondence problem, where the aim is to reconstruct a dense 3D scene from images captured by two spatially related cameras. Our main focus is on speed and real-time implementation on a standard desktop PC, and we wish to use the CPU to solve the correspondence problem while reserving the GPU for model rendering. We discuss three fundamental types of algorithms and evaluate their suitability to this end, and eventually choose a hierarchical version of the dynamic programming algorithm because of the good balance between accuracy and speed. It becomes clear that the greatest weakness of the hierarchical dynamic programming algorithm is scanline inconsistency and we find that the onedimensional LULU-filter is computationally inexpensive and effective at removing outliers when applied across scanlines. We take advantage of the hierarchical structure of our algorithm and sub- pixel refinement to produce results at video rates (roughly 20 frames per second). A 3D model is also constructed at video rates in an on-line system, with only a small delay between obtaining input images and rendering the model. Not only is the quality of our results highly competitive with those of other state-of-theart algorithms, but the achievable speed is also considerably better.

OFF-LINE SIGNATURE VERIFICA-TION USING FLEXIBLE GRID FEA-TURES AND CLASSIFIER FUSION

Jacques Swanepoel (Stellenbosch University)

We present two novel off-line signature verification systems, constructed by combining an ensemble of eight base classifiers. Both score-based and decisionbased fusion strategies are investigated. Each base classifier utilises the novel flexible grid-based feature extraction technique.

We show that the flexible grid-based approach consistently outperforms the existing rigid grid-based approach. We also show that the combined classifiers outperform the most proficient base classifier. When evaluated on Dolfing's data set, a signature database containing 1530 genuine signatures and 3000 amateur skilled forgeries, an EER of 10.23% is obtained. We show that the combined classifiers outperform existing systems that were also evaluated on Dolfing's data set.

TWO-DIMENSIONAL TURBULENT WALL JET

Prof. David Mason (University of the Witwatersrand)

A two-dimensional turbulent wall jet described by eddy viscosity is formulated mathematically and it is demonstrated why a conserved quantity is needed to complete the formulation. Two models for the eddy viscosity are considered. In the first model the eddy viscosity is a power law of the distance along the jet and is constant across the jet. In the second model the eddy viscosity is a power law of the mean fluid velocity along the jet and therefore varies across the jet. Both models satisfy the conservation law. Analytical solutions in parametric form are presented for both models. The eddy viscosity increases the width of the wall jet. The second model provides only an inner solution which must be matched to the outer solution.

ON THE RAYLEIGH PROBLEM FOR A SISKO FLUID IN A ROTAT-ING FRAME

Prof. Shirley Abelman (University of the Witwatersrand, Johannesburg)

The unsteady rotating flow of a Sisko fluid bounded by a suddenly moved infinite flat plate is investigated. The fluid is electrically conducting in the presence of a transverse applied time-dependent magnetic field. A highly non-linear differential equation resulting from the balance of momentum and mass, coupled with appropriate boundary and initial conditions is solved numerically. The numerical solutions for different values of the parameters are compared and discussed.

EXACT SOLUTIONS OF THE TWO-DIMENSIONAL STEADY FIN PROBLEM WITH TEMPERATURE DEPENDENT THERMAL CONDUC-TIVITY AND HEAT TRANSFER COEFFICIENT

Dr Joel Moitsheki (University of the Witwatersrand)

This study investigates solutions of two-dimensional nonlinear fin problem with thermal conductivity, heat transfer coefficient and heat energy generating function being given as power laws of temperature. The resulting nonlinear problem is linearized by a point transformation when the exponents of the heat transfer coefficient and thermal conductivity are equal. Symmetry techniques are employed to the problem with distinct exponents. One dimensional optimal system of subalgebras is constructed and reductions are performed. Exact solutions satisfying the realistic boundary conditions are constructed. Heat flux, fin efficiency and the effects of the physical parameters such as extension factor and Biot number on temperature distribution through the fin are analyzed.

HIGHER ORDER FITTED OPER-ATOR METHODS FOR NONLIN-EAR SINGULAR PERTURBATION PROBLEMS

Prof. Kailash C. Patidar (University of the Western Cape)

For certain class of singularly perturbed nonlinear ordinary and partial differential equation models, we design and analyze some novel fitted operator methods. We then study how can we improve the accuracy of these numerical methods? Selected numerical results confirming the theoretical estimates will also be presented at the conference.

A ROBUST FITTED OPERATOR METHOD FOR SINGULARLY PER-TURBED PROBLEMS IN HIGHER DIMENSION

Dr Justin Bazimaziki Munyakazi (University of the Western Cape)

Singular perturbation problems (SPPs) have received tremendous attention in recent years. It is established that standard numerical methods fail to solve

these problems due to the presence of large gradients in their solution. In order to circumvent this difficulty several methods have been developed, including finite difference and finite elements methods. As far as finite difference methods are concerned, fitted mesh finite difference methods are well documented. However, to the best of our knowledge, very few fitted operator finite difference methods (FOFDM) for SPPs in higher dimensions exist. To close this gap, we develop a FOFDM for a singularly perturbed elliptic problem in two dimensions. A rigorous analysis shows that this method is second order in both variables. Moreover, a convergence acceleration technique for this method is analyzed and fourth order accuracy is achieved. Comparative numerical results supporting our theoretical findings will also be presented.

A LOWER BOUND FOR PRICING EUROPEAN BASKET OPTIONS

Walter Mudzimbabwe (University of the Western Cape)

We derive a lower bound for the price of a European Basket option under the Black and Scholes framework using the conditioning method. The results that we get are benchmarked using an adaptive Monte Carlo method. We also calculate the lower bound for various parameters involved. We finally compare these results with those obtained by the improved Monte Carlo method.

Tuesday 16 March

TUESDAY PLENARY	11
The Numerical Solution of Semiclassical Schrödinger Equations	
Prof. Peter Markowich, University of Cambridge	11
Surprising computations	
Prof. Uri Ascher, University of British Columbia	11
TUESDAY MORNING	11
High Accuracy Computation of the Free Propagator	
Prof. Andre Weideman, Stellenbosch University	11
Numerical investigation of thermal decomposition in a slab subjected to higher order oxi-	
dation chemical reaction	
Prof. Oluwole Daniel Makinde, Cape Peninsula University of Technology	11
TUESDAY AFTERNOON	11
Waves in a vibrating solid with boundary damping	
Prof. Nic Janse van Rensburg, University of Pretoria	12
Adaptive dynamics and Multiple scales: some thoughts	
Prof. Schalk Schoombie, University of the Free State	12
Approximate Solutions of Differential Equations with Boundary Conditions by Node Vari-	
able Linear Splines	
Dr Mehdi Ahmadinia, University of Qom	12

THE NUMERICAL SOLUTION OF SEMICLASSICAL SCHRÖDINGER EQUATIONS

Prof. Peter Markowich (University of Cambridge)

Linear (and nonlinear) Schrödinger equations in the semiclassical (small dispersion) regime pose a significant challenge to numerical analysis and scientific computing, mainly due to the fact that they propagate high frequency spatial and temporal oscillations. At first we prove using Wigner measure techniques that finite difference discretisations in general require a disproportionate amount of computational resources, since underlying numerical meshes need to be fine enough to resolve all oscillations of the solution accurately, even if only accurate observables are required. This can be migitated by using a spectral (in space) discretisation, combined with appropriate time splitting. Such discretisations are time-transverse invariant and allow for much coarser meshes than finite difference discretisations. In many physical applications highly oscillatory periodic potentials occur in Schrödinger equations, still aggravating the oscillatory solution structure. For such problems we present a numerical method based on the Bloch decomposition of the wave function.

SURPRISING COMPUTATIONS

Prof. Uri Ascher (University of British Columbia)

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, KdV and NLS, 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 problems.

HIGH ACCURACY COMPUTATION OF THE FREE PROPAGATOR

Prof. Andre Weideman (Stellenbosch University)

A new matrix approximation to the free propagator of quantum mechanics is proposed. It is a variant of the well-known Fourier pseudospectral approximation, but based on semi-discrete rather than fully discrete transforms. A computable error bound is derived and stability issues are discussed. Numerical comparisons involving the linear and nonlinear Schroedinger equations are presented.

NUMERICAL INVESTIGATION OF THERMAL DECOMPOSITION IN A SLAB SUBJECTED TO HIGHER OR-DER OXIDATION CHEMICAL RE-ACTION

Prof. Oluwole Daniel Makinde (Cape Peninsula University of Technology)

In this talk, we examine the transient heating of a slab subjected to a one-step irreversible chemical kinetics with reactant consumption and higher order oxidation exothermic reaction. It is assumed that the material surface exchanges oxygen and heat with its surroundings. The governing nonlinear partial differential equations are solved numerically by method of lines (MOL). Graphical results are presented and discussed quantitatively with respect to various embedded parameters controlling the systems. Our results reveal among others, that the internal heat generation in the system decreases while the oxygen concentration increases with an increase in the parameter values of reaction order index (n) and Biot number (Bi).

References:

O. D. Makinde, Exothermic explosions in a slab: A case study of series summation technique. International Communications in Heat and Mass Transfer, Vol. 31, No.8, 1227-1231, 2004.

O. D. Makinde, O. Anwar Beg: On inherent irreversibility in a reactive hydromagnetic channel flow, Journal of Thermal Science Vol.19, No.1, 72-79, 2010. R. J. Moitsheki, O. D. Makinde: Classical Lie point symmetry analysis of nonlinear diffusion equations describing thermal energy storage, Applied Mathematics and Computation 216, 251-260, 2010.

O. D. Makinde, M. Maserumule: Inherent irreversibility and thermal stability for steady flow of variable viscosity liquid film in a cylindrical pipe with convective cooling at the surface, Int. J. Num. Methods for Heat & Fluid Flow, vol. 20, No. 1, 5-16, 2010

WAVES IN A VIBRATING SOLID WITH BOUNDARY DAMPING

Prof. Nic Janse van Rensburg (University of Pretoria) The use of modal analysis for second order hyperbolic partial differential equations is well established. This is supported by a general theory when the associated eigenvalue problem is symmetric (or selfadjoint). The situation is different for the non-selfadjoint case and the usefulness of modal analysis is questioned. We show that modal analysis is useful for the wave equation with boundary damping but also show that sometimes more can be achieved by considering wave motion.

ADAPTIVE DYNAMICS AND MUL-TIPLE SCALES: SOME THOUGHTS

Prof. Schalk Schoombie (University of the Free State)

We discuss the mathematical modelling of evolution, using the adaptive dynamics approach. Besides describing an algorithm devised before to find a singular point, we also give a brief description of some work in progress, in which we aim to incorporate some ideas from multiple scales perturbation analysis.

APPROXIMATE SOLUTIONS OF DIFFERENTIAL EQUATIONS WITH BOUNDARY CONDITIONS BY NODE VARIABLE LINEAR SPLINES

Dr Mehdi Ahmadinia (University of Qom)

In the recent paper Loghmani used splines for solving arbitrary order differential equation with boundary conditions . He Proved the convergence of theory only for case of the first order differential equations. In this talk we present a method and proof for each order differential equations by linear splines. We consider node variable for decreasing of computations. We present some advantages of the method.

Wednesday 17 March

WEDNESDAY PLENARY	14
Rogue Waves, Vortices and Rational Solutions of Soliton Equations	
Prof. Peter Clarkson, University of Kent	14
Polynomial Algebra for Birkhoff Interpolants	
Prof. Rob Corless, University of Western Ontario	14
WEDNESDAY MORNING I	14
The use of Exponentially Fitted Runge-Kutta methods for Delay Differential Equations	
Jon Smit, University of the Free State	14
Discontinuous Galerkin finite element methods for elliptic equations	
Beverley Grieshaber, University of Cape Town	14
WEDNESDAY MORNING II	14
The numerical calculation of the discrete spectrum for the nonlinear Schrödinger equation	
Carel Olivier, UCT	15
LULU for Noise Removal in Signals - an investigation	
Inger Fabris-Rotelli, University of Pretoria	15

ROGUE WAVES, VORTICES AND POLYNOMIAL RATIONAL SOLUTIONS OF SOLI- BIRKHOFF IN TON EQUATIONS

Prof. Peter Clarkson (University of Kent)

In this talk I shall discuss special polynomials associated with rational solutions for the Painlevé equations and of the soliton equations which are solvable by the inverse scattering method, including the Korteweg- de Vries, Boussinesq and nonlinear Schrödinger equations.

The Painlevé equations are six nonlinear ordinary differential equations that have been the subject of much interest in the past thirty years, which have arisen in a variety of physical applications. Further they may be thought of as nonlinear special functions. Rational solutions of the Painlevé equations are expressible in terms of the logarithmic derivative of certain special polynomials. For the second Painlevé equation (PII) these polynomials are known as the Yablonskii-Vorob'ev polynomials, first derived in the 1960's by Yablonskii and Vorob'ev. The locations of the roots of these polynomials is shown to have a highly regular triangular structure in the complex plane. The analogous special polynomials associated with rational solutions of the fourth Painlevé equation (PIV), which are known as the *generalized* Hermite polynomials and generalized Okamoto polynomials, are described and it is shown that their roots also have a highly regular structure. The Yablonskii-Vorob'ev polynomials arise in string theory and the generalized Hermite polynomials in the theories of random matrices and orthogonal polynomials.

It is well known that soliton equations have symmetry reductions which reduce them to the Painlevé equations, e.g. scaling reductions of the Korteweg-de Vries equation is expressible in terms of PII and scaling reductions of the Boussinesq and de-focusing nonlinear Schrödinger equations are expressible in terms of PIV. Hence rational solutions of these soliton equations can be expressed in terms of the Yablonskii and Vorob'ev, generalized Hermite and generalized Okamoto polynomials. Further general rational solutions of equations for the Korteweg-de Vries, Boussinesq equations and de-focusing nonlinear Schrödinger equations, which involve arbitrary parameters, will also be described.

I shall also discuss applications of these special polynomials associated with rational solutions for the Painlevé and soliton equations to point vortex dynamics. Further I shall also describe some additional rational solutions of the Boussinesq equation and and rational-oscillatory solutions of the focusing Schrödinger equation which have applications to rogue waves.

POLYNOMIAL ALGEBRA FOR BIRKHOFF INTERPOLANTS

Prof. Rob Corless (University of Western Ontario)

We introduce a unifying formulation of a number of related problems which can all be solved using a contour integral formula. Each of these problems requires finding a non-trivial linear combination of some of the values of a function f, and its first and higher derivatives, at a number of data points. This linear combination is required to have zero value when f is a polynomial of up to a specific degree p. Examples of this type of problem include Lagrange, Hermite and Hermite-Birkhoff interpolation; fixed-denominator rational interpolation; and various numerical quadrature and dif- ferentiation formulae. Other applications include the estimation of missing data and root-finding.

THE USE OF EXPONENTIALLY FITTED RUNGE-KUTTA METH-ODS FOR DELAY DIFFERENTIAL EQUATIONS

Jon Smit (University of the Free State)

This article explores the construction of an Exponentially Fitted Runge-Kutta method based on the Bogacki-Shampine 3(2) pair for Delay Differential Equations with constant delays.

DISCONTINUOUS GALERKIN FI-NITE ELEMENT METHODS FOR ELLIPTIC EQUATIONS

Beverley Grieshaber (University of Cape Town)

There have been a number of discontinuous Galerkin (DG) finite element methods developed for solving PDEs numerically. Similarities amongst many of the DG formulations have prompted several authors to devise frameworks for developing and analysing classes of these formulations in a unified manner, for the purpose of understanding and comparison. In this context, I will discuss aspects of the development, analysis, and implementation of DG methods for elliptic problems.

THE NUMERICAL CALCULA-TION OF THE DISCRETE SPEC-TRUM FOR THE NONLINEAR SCHRÖDINGER EQUATION

Carel Olivier (UCT)

We present two algorithms for calculating the discrete spectrum associated with the scattering data that

arises in the solution of the nonlinear Schrödinger equation (NLS) by the inverse scattering method. The first algorithm is based on a spectral method and calculates the discrete spectrum directly. The second algorithm, based on Floquet theory, is more general and can be used to calculate both the discrete and continuous spectra. We apply both methods to analyze the homoclinic structure of the NLS subject to periodic boundary conditions. Examples of homoclinic chaos are presented. In addition, it is shown that the algorithms can be modified to investigate the soliton content of initial conditions on the infinite line.

LULU FOR NOISE REMOVAL IN SIGNALS - AN INVESTIGATION

Inger Fabris-Rotelli (University of Pretoria)

We shall show some experimentation done on the removal of various types of noise from a signal via the LULU smoothers L_n and U_n . The strength of the nonlinear LULU smoothers for this purpose will be demonstrated.

Participants

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