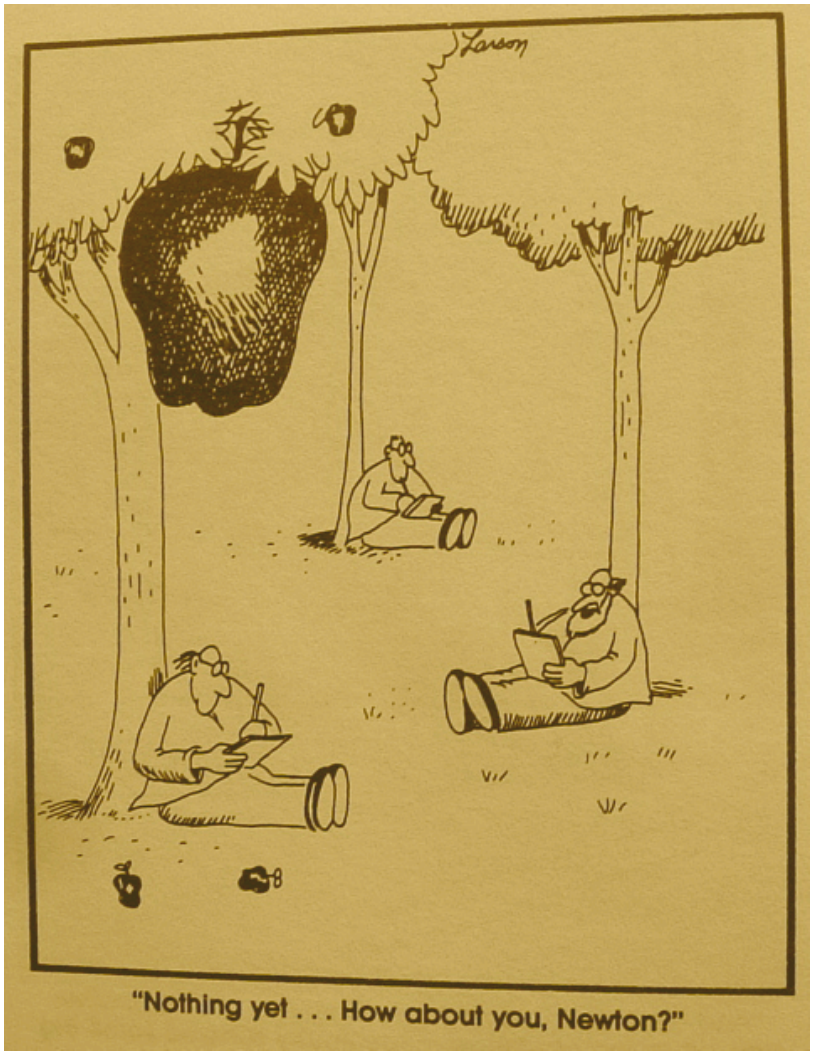
THE EIGHTH MANAWATU-WELLINGTON APPLIED MATHEMATICS CONFERENCE

The McDiarmid Centre, Industrial Research Ltd, Gracefield Research Centre

PROGRAMME



Friday 1 July 2005

Mark McGuinness

programme

10:00am **Kit Withers**: Relations between multivariate moments and cumulants via multivariate Bell polynomials.

10:30 **Philip Zhang** and Robert McLachlan: Well-posedness and blowup for a modified Camassa-Holm equation

11:00 **Morning Tea - McDiarmid Centre**

11:30 **Brett Ryland:** Geometric Methods for PDEs

12:00 **Igor Boglaev**: Domain Decomposition Algorithms on Serial and Parallel Computers

12:30pm **LUNCH** - at staff cafeteria, pay for yourselves.

2:15 **Shaun Hendy** and Dmitri Schebarchov: Phase coexistence in metal nanoparticles

2:45 **Stephen White:** Pitting of stainless steel

3:15 **Afternoon Tea - McDiarmid Centre**

3:45 **Warwick Kissling:** Modelling the Taupo Volcanic Zone

4:15 **John F. Harper and D. Lynden-Bell:** Minding one's P's and Q's on the cut

4:45 **Recovery Drinks and a Meal**

abstracts

in alphabetical order of presenting author

Igor Boglaev

Institute of Fundamental Sciences, Massey University

Domain Decomposition Algorithms on Serial and Parallel Computers

We are interested in solving nonlinear singularly perturbed reaction-diffusion problems of a parabolic type. On each time level, a domain decomposition algorithm is applied to computing a nonlinear difference scheme. From an arbitrary initial mesh function satisfying the boundary conditions, the algorithm generates a sequence of mesh functions which converges monotonically to the exact solution of the nonlinear scheme. Each iterate arises from the solution of only linear difference problems on the various subdomains. This talk describes sequential and parallel implementations of the algorithm. For a model problem we report execution times on serial and parallel computers.

J. F. Harper and D. Lynden-Bell

School of Mathematics, Statistics and Computer Science, Victoria University of Wellington, NZ, and

Institute of Astronomy, University of Cambridge, UK

Minding one's P's and Q's on the cut.

The sum $\sum_{n=0}^{n=\infty}(2n+1)P_n(x)P_n(y)P_n(z)$ has a known closed form in elementary functions except at points where a certain polynomial in x, y, z vanishes. The sum converges pointwise only if all three of x, y, z are in $(-1, 1)$, and not at all points there. We show that it converges distributionally throughout that region, that its sum may also involve the Dirac delta function, but only in certain well-known special cases, and we find closed forms for the corresponding series with one or two of the Legendre polynomials P_n replaced by the Legendre function Q_n, which also converge distributionally in the same region.

Certain traps for young players were found and had to be avoided in the course of the exercise.

The authors' previous work on this subject, reported to the ANZIAM conference in Napier in February 2005, dealt with these functions for values of x, y, z where they are analytic: various subsets of the complex plane with the cut $[-1, 1]$ removed.

Shaun Hendy and Dmitri Schebarchov

Industrial Research Ltd

Phase coexistence in metal nanoparticles

We have recently used microcanonical critical droplet (MCD) theory to show that the coexistence of solid and liquid phases in metal nanoparticles becomes unstable in sufficiently small particles. Although in the last year, electron beam excitation has been used to map coexistence between solid and liquid phases in metal nanoparticles as a function of particle energy, it may be some time before a definitive test of the theory is conducted. Thus in order to test the theory we have been using molecular dynamics simulations to construct microcanonical caloric curves for a variety of metal particles to determine the limits of stability of phase coexistence. Here we will review our recent results for aluminium, copper, nickel, palladium, platinum and silver.

Brett Ryland

Massey University, New Zealand

Geometric Methods for PDEs

Multisymplectic integrators are geometric numerical integrators for PDEs of the form $Kz_t + Lz_x = \nabla_Z S(z)$ that preserve a discrete version of the multisymplectic conservation law $\omega_t + \kappa_x = 0$. Except under special conditions, applying a Gaussian Runge-Kutta discretisation to certain PDEs leads to a method that, despite formally having a multisymplectic conservation law, in fact fails to be well-defined. For some of these PDEs, the form of the K and L matrices are such that it is possible to obtain a well-defined multisymplectic method using the Lobatto IIIA-IIIB class of partitioned Runge-Kutta discretisations.

Stephen White

Industrial Research Ltd., Lower Hutt

Pitting of stainless steel

NUMERICAL SIMULATION OF PITTING CORROSION IN STAINLESS STEELS UNDER GALVANOSTATIC AND OPEN-CIRCUIT CONDITIONS

Stephen White†, Donal Krouse† and Nick Laycock††

†Industrial Research Limited, PO Box 31-310, Lower Hutt, New Zealand
††MPT-Solutions, PO Box 31-310, Lower Hutt, New Zealand

We have previously presented a model of pit propagation in stainless steel under potentiostatic conditions, and numerical simulations of single pit growth have reproduced many of the experimentally observed characteristics of pitting [1,2]. Furthermore, this deterministic model of single pit growth has been combined with a purely stochastic model of pit nucleation, and Monte Carlo simulations were used to compare the predictions of this combined model with potentiodynamic experimental measurements of the pitting potential [3,4]. Here we report the extension of this model to include pit growth under galvanostatic and open-circuit conditions.

Firstly, for single pits, it is found that there is a distinct difference between pit shapes formed under different growth regimes. Pits grown under galvanostatic regimes have a much higher aspect ratio than the-dish shaped pits resulting from growth under a constant potential. The pit shapes resulting from open-circuit corrosion lie between the two extremes. Secondly, we have again used the Monte Carlo method to compare model simulations against experimental results – see Figure 1.

However, the simulation of Figure 1 does not include any interactions between different pitting sites, whilst such coupling is considered by some to be a critical factor in formation of stable pits [5,6]. In potentiostatic conditions, pits are coupled mainly by changes in local chemistry near a pit mouth, although relatively small IR effects are also present. Under galvanostatic and open-circuit conditions, pits are also coupled via their competition for a limited supply of current and variations in potential are much more significant. During the lifetime of any given pit, these factors will affect the nucleation and growth processes at nearby pitting sites – see Figure 2.

REFERENCES

1. N.J. Laycock, S.P. White, J.S. Noh, P.T. Wilson and R.C. Newman, *J. Electrochem. Soc.*, **145**, 1101 (1998).
2. N.J. Laycock and S.P. White, *J. Electrochem. Soc.*, **148**, B264 (2001).
3. N.J. Laycock, S.P. White and D.P. Krouse, in *Pits and Pores II: Formation, Properties and Significance for Advanced Materials*, p 100, PV 2000-25, ECS, Pennington NJ (2000).
4. N.J. Laycock, J.R. Mackay, S.P. White and D.P. Krouse, in *Critical Factors in Localized Corrosion IV*, p 490, PV 2002-24, ECS, Pennington NJ (2002).
5. B. Wu, J.R. Scully, J.L. Hudson and A.S. Mikhailov, *J. Electrochem. Soc.*, **144**, 1614 (1997).
6. C. Punckt, M. Bolscher, H.H. Rotermund, A.S. Mikhailov, L. Organ, N. Budiansky, J.R. Scully and J.R. Hudson, *Science*, **305**, 1133 (2004).

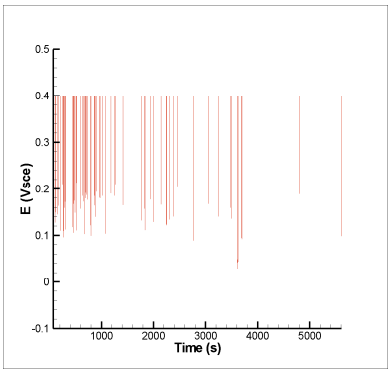


Figure 1: Long–term simulation results for a macroscopic sample, with multiple possible pit initiation sites, under open-circuit conditions

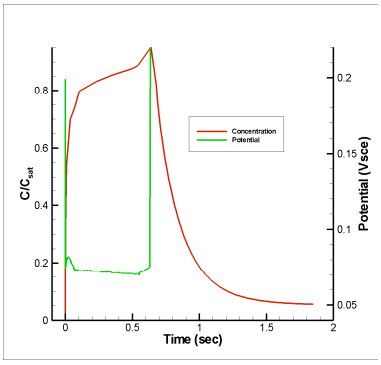


Figure 2: The potential and the normalized concentration of dissolved corrosion products at a point on the passive surface close to a single pit in open-circuit conditions, during and just after the lifetime of that pit.

Kit Withers

Industrial Research Ltd., Lower Hutt

Relations between multivariate moments and cumulants via multivariate Bell polynomials

The Bell polynomials give a natural way to express central and non-central moments in terms of cumulants and vice versa. We give these relations and show how they extend to vectors and matrices. Bell polynomials are also the natural way to calculate moments of means and sums. Bell polynomials are also the building blocks for the chain rule for composite functions.

Philip Zhang and Robert McLachlan

Massey University, Palmerston North

Well-posedness and blowup for a modified Camassa-Holm equation

Geodesics on Lie groups, known as Euler equations, play a fundamental role in mathematical physics. Examples include the Euler fluid equations, the Landau-Lifshitz equation of micromagnetics, and the template matching equation used in image processing. One well-studied example is the Camassa-Holm equation describing shallow water waves in 1D, being geodesics with respect to an H^1 metric. It is completely integrable and supports special peaked soliton solutions. To determine how the dynamics depends on the metric, we have taken an H^2 metric and find that, although the equation is now non-integrable, much of its behaviour persists, including existence and uniqueness of solutions, existence of N-solitary wave solutions, and blow-up of bump-like initial data to solitary waves.

attendees

Igor Boglaev	I.Boglaev@massey.ac.nz
Shaun Hendy	s.hendy@irl.cri.nz
Warwick Kissling	W.Kissling@irl.cri.nz
Mark McGuinness	Mark.McGuinness@vuw.ac.nz
Robert McLachlan	r.mclachlan@massey.ac.nz
Brett Ryland	b.n.ryland@massey.ac.nz
Dmitri Schebarchov	Industrial Research Ltd
Stephen White	S.White@irl.cri.nz
Kit Withers	C.Withers@irl.cri.nz
Philip Zhang	X.Y.Zhang@massey.ac.nz

with thanks to:

IRL Applied Math: sponsor

ANZIAM NZ: sponsor

Victoria University of WN: sponsor