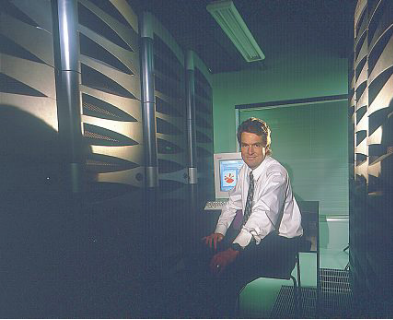


# VPAC NEWS

January 2005 Edition

## VPAC News January 2005

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Dear VPAC Members and Partners

The past year has been a very successful year for VPAC. We have experienced significant growth across all areas of the organisation. Highlights of the year include:

- The success of the AutoCRC proposal;
- Successful projects with two aerospace companies;
- The initiation of the APAC grid projects and APAC funding to Members;
- VPAC's engagement in the contracts to support computing at the Victorian state departments DPI and DSE;
- VPAC's support for e-Research;
- VPAC's election to a position on a major US National Science Foundation executive;
- A diversification of VPAC's Member support to faculties outside the traditional users of HPC (Science and Engineering).

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2005 is already shaping up to be another year of growth, as there is growing demand for Advanced Computing R&D support in areas as diverse as counter-terrorism and life sciences, and new projects such as the AutoCRC

will come onstream. We are forging new interstate and overseas collaboration as well.

All of these achievements would not have been possible without the collaboration and support of countless individuals outside VPAC. In many respects, the success of VPAC is due in large part to your willingness to work with us. Our thanks for your support, and we look forward to new opportunities to work together in the coming year.

Professor Bill Appelbe, VPAC CEO

# Software Quality Assurance

Software projects are notorious for budget and schedule overruns and failures of one type or another - whether it is software developed by industry, universities, or government. VPAC is increasingly involved in large scale commercial software development in areas as diverse as computational engineering, life sciences, and geospatial science. The risks in these projects can be quite high, as most VPAC software projects are research and development - not off-the-shelf applications such as websites or financial reporting packages.

To date, VPAC has been quite successful in software development. As we continue to engage in ever larger and more complex software projects, we are refining and improving our processes and undertaking training to minimise the risk of software project failures and maximise the quality of the software we develop. The modern definition of quality includes not just the quality of the product (functionality, reliability, cost), but also project and process quality (productivity, developer satisfaction, schedules and budgets met, etc.).

There are several complementary ways to maximise software quality that we are addressing.

1. Adoption of an appropriate Software Development Life Cycle (SDLC) including how project scoping, requirements analysis, design, coding and testing are done; documentation; version control, and so on.
2. Development of a Risk Management Strategy
3. Application of Software Quality Assurance techniques

Different groups within VPAC use somewhat different SDLC processes and procedures - as the client needs for production engineering software versus research software for geophysics are quite distinct. However, almost all our software projects are based on a version of the SDLC called "agile software development" ([www.agilealliance.org](http://www.agilealliance.org)). Agile development has many facets, but key aspects of agile development include: continuous engagement of the client, early delivery of initial versions, and continuous focus on software quality.

Having a good SDLC is no guarantee of a successful project, as external risks such as loss of key staff or other unanticipated events can cause failure. To mitigate against this requires a risk management strategy - an ongoing process of identifying risks, prioritizing them, and developing action plans to address key risks (such as a succession plan to mitigate against loss of key staff).

VPAC is now moving to a more formal and adaptive risk management strategy - beyond the current process of documenting risks and the mitigation strategy annually in our business plan.

Finally, Software Quality Assurance (SQA) is gradually being introduced more formally into VPAC. SQA consists of a set of policies and procedures for measuring and improving software product, project, and process quality on an ongoing basis. Measurement techniques bug tracking, and regression testing (running each new software version over the same test code). Improvement techniques include adopting new tools and technology as they become available, such a twiki sites for managing collaborative development and documentation ([www.twiki.org](http://www.twiki.org)).

(contributed by Professor Bill Appelbe)

To learn more about software quality assurance and how your organisation can move towards adopting SQA best practices, please contact VPAC on +61 3 9925 4645 or email [info@vpac.org](mailto:info@vpac.org).

## VPAC CRC COLLABORATION SUCCESSFUL

The Australian Government announced yesterday the successful selection of the CRC for Advanced Automotive Technology, Manufacturing Technology Sector (Victoria). VPAC is a major partner in the CRC, that will provide the automotive industry with the opportunity to work with research providers in design, engineering and manufacturing research to enhance the industry's international competitiveness. The CRC will receive programme funding of \$38.35 million and will help the automotive industry to reduce concept-to-concept cycle times through the introduction of paradigm shifts in process and production methodologies, improved manufacturing flexibility and efficiency and the development of new material systems to meet the challenges of weight reduction, increased safety and greater functionality. The CRC will also improve vehicle safety through delivering improvements in the crash worthiness of vehicles and new intelligent products/systems that provide increased comfort, performance and entertainment.

For more information on the CRC for Advanced Automotive Technology, contact Dr Laurence Sparke on +61 3 9647 1111 or Laurie.Sparke@holden.com.au.

## IBM POWER5 SERIES NEW ADDITION TO VPAC SYSTEM

In mid January 2005, VPAC will be installing a new machine based on Linux and IBM Power5 and consisting of 36 four-way boxes with a total of 432Gig ram and fast local disks.

The new system will replace the now extinct Grendel. Users of the existing VPAC systems (ie Brecca and Wexstan) will automatically have access to the new machine as it comes on line.

## SUMMER 2005 INTERNSHIPS

The VPAC 2005 Summer Internship Program has recently commenced, with participants selected from a wide range of disciplines, including software engineering, biotechnology, computational engineering and software development. From over 250 applications received, twelve students were accepted into the program, representing VPAC's largest summer internship intake to date. The Summer Internship program is a three-month program widely recognised for its employment of final year students to work with both industry and academia on upstream industry-inspired projects utilising advanced computing techniques. The projects apply advanced computing to practical applications in engineering, life sciences, bioinformatics and

geosciences. 2002 Summer Internship students redesigned the B14 Racing Boat Center-board and created a geological mantle-convection proof of concept code. Last year, VPAC Summer Internship students set a new record in the field of combinatoric mathematics, parallelised an internationally renowned hydrodynamics code, and parallelised a code now used by the minerals industry.

The Summer Program provides students with the opportunity to adopt new skills and industry experience prior to entering the workforce. VPAC attracts talented computer scientists from a theoretical science or engineering background. The program also provides students with the opportunity to evaluate future studies including honours and PhD.

Training is provided to students in parallelization and computational methods such as Finite Element, Finite Difference and Discrete Elements. Student induction is over a period of two days and involves project leaders and collaborators for each project to mirror real-life work environments. Students work in a collaborative-style environment to ensure that all experiences are shared.

This year's projects are some of the Internship program's most exciting and innovative yet. They include:

- Computational Grid Portals and their Applications in Virtual Engineering and Design
- Real-time Visualisation of Engineering Models, Analysis and Results
- Snark Modelling of Venusian Mantle Dynamics and Tessera Formation
- Implementing Message Passing Interface (MPI) into the Australian Air Quality Forecasting System-Chemical Transport Model (AAQFS-CTM)
- Health Informatics/Data Mining and Tools Development
- Hyper-spectral Remote Sensing
- Weeds Sensing from Remote Images.

For more information on the VPAC Summer Internship Program visit [www.vpac.org](http://www.vpac.org) or contact the Grants Coordinator on +61 3 9925 4645.

# e-Research Grants Round 7 Announcements

VPAC recently announced the recipients of the latest round of funding (Round 7) under the VPAC e-Research Grants program. Grant recipients received a total of more than \$330,000 of funding to support research projects in the fields of Geoscience, Biotechnology, Virtual Engineering and Computational Software Development. The e-Research Grants program provides seed funding for short-to-medium term research projects that effectively utilise Advanced Computing and generate significant research outcomes.

The program has been running for over four years and has provided funding of more than \$3.9M to more than 100 projects. The program has resulted in hundreds of publications and been instrumental in raising ARC and industry funding of more than \$8M.

## ROUND 7 PROJECT OVERVIEWS:

### Deakin University

**Project Number:** EPPNDE125.2005

**Project Title:** Reliable methods of data approximation and forecasting

**Project Chief Investigator:** Gleb Beliakov

**Funding Obtained:** \$21,000

**Project Summary:**

Even though we may not fully understand many complex systems, like weather patterns, we can predict their behaviour based on past observations. Automatic prediction tools have delivered great benefits in banking, insurance, information technology, biochemistry, medicine and other sciences. This project is about development of a new generic tool for reliable prediction, based on recent theoretical advances in approximation theory. Mathematical theory will be converted into fast and reliable algorithms.

**Project Number:** EPPNDE126.2005

**Project Title:** New methods for predicting molecular structures

**Project Chief Investigator:** Kieren Lim

**Funding Obtained:** \$23,000

**Project Summary:**

The molecular geometry, the 3-dimensional arrangement of atoms in space, is a major factor determining the properties and reactivity of molecules, biomolecules and macromolecules. Molecular geometry prediction has specific application to protein structure elucidation, drug design, modelling of host-guest interactions, and the identification of transition states. In spite of much

world-wide research concentrated on this problem, it remains one of the (USA) National Academy of Science's grand challenges in the 21st century. The researchers will build on their recent mathematical advances to develop and verify new reliable computational techniques for molecular structure prediction tasks (such as protein folding problems, molecular shape description). In this project the researchers will use a new global optimization method termed Cutting Angle, and apply it to predicting geometry of molecules using the MM3/MM4 force field.

**Project Number:** EPPNDE127.2005

**Project Title:** Simulating the Process of Knife Stabbing

**Project Chief Investigator:** Lijing Wang

**Funding Obtained:** \$21,000

**Project Summary:**

Soft protective articles are required by police, soldiers, security personnel and corrections officers who are exposed to stab threats in various operational situations. The process of material selection, engineering and assessing these articles is costly and time consuming. Mathematical simulation of the effect of various attacks on different substrates is therefore vital for product development and applications. The aim of this project is to model and compute a knife stabbing process on the stab-resistant materials using ANSYS computing facilities under the simulated end-use conditions. This program is a significant first step towards developing specialised protective garments for local and export markets. Results from this study will produce fundamental knowledge on stab resistant fabrics and body armours, and will provide practical information on the preparation of commercially acceptable protective products. The success of this project will accelerate the design and development phases of stab-resistant fabrics, and strengthen the competitiveness of the Australian protective apparel industry in the global market.

# e-Research Grants Round 7 Announcements

**Project Number:** EPPNDE128.2005

**Project Title:** A Novel Computational Approach for Identifying Transcription Factor Binding Sites in Gene Promoters

**Project Chief Investigator:** Wanlei Zhou

**Funding Obtained:** \$23,000

**Project Summary:**

Transcription Factor Binding Sites (TFBS) play a key role in the regulation of the gene expression. The discovery of unknown TFBS will help to find out unknown transcription factors and acquire better understanding of gene regulation network. Currently there are many approaches proposed for finding the TFBS in the gene promoters of various organisms, but most of these approaches are designed to find longer or more general motifs than are required for identifying transcription factor binding sites. The price paid for this generality is that many of the existing approaches are not guaranteed to find globally optimal solutions, since they employ some form of local search, such as Gibbs sampling, expectation maximization or greedy algorithms, that may terminate in a locally optimal solution.

The aim of this project is to propose a novel computational approach that identifies good candidates for transcription factor binding sites. Specifically, our approach will enumerate all motifs in the search space and is guaranteed to produce the motifs with greatest motif factors (MF) and the smallest chance of being random. All the gene promoters of Homo sapiens will be analysed to try to find those DNA sequences with greatest motif factors. We will determine the statistical significance of DNA sequences with various lengths ranging from 5 to 10 bp. Random data sets of gene promoters are generated to determine the non-random probability of DNA sequences appearing in the original gene promoters. The DNA sequences with the maximal statistical significance and non-random probability will be compared with known TFBS in the TRANSFAC database to verify our approach.

## La Trobe University

**Project Number:** EPPNLA129.2005

**Project Title:** Calculation of the 3-dimensional structure of drugs in solvents emulating biological environments.

**Project Chief Investigator:** Bob Brownlee

**Funding Obtained:** \$21,000

**Project Summary:**

Many drug molecules adopt different 3-dimensional structures during transport, adsorption and in binding to a receptor where it acts therapeutically. Information about these structures is required to enhance the drug design

process.

This project will calculate structures of antibiotics, antifungal and anticancer drugs in a range of solvents using AMBER, GAMESS and NAMD software packages and the computational power of the VPAC cluster. The significance of this project is that detailed information on the drug structures and drug flexibility is required to optimise drug design and the results can be validated against experimentally determined structures by our group.

**Project Number:** EPPNLA130.2005

**Project Title:** Computer Molecular Models for Catalytic Brown Coal Gasification and the Study of Fell-Fell Structures

**Project Chief Investigator:** George Domazetis

**Funding Obtained:** \$19,000

**Project Summary:**

The project aims to develop computational expertise on structures of macromolecules for application in catalytic gasification of brown coals; use VPAC HPC computational molecular modelling capabilities to enhance our understanding of macromolecular structures of brown coal and interactions with inorganic species; and undertake modelling studies of the transformation of coal molecules and inorganic species during pyrolysis and gasification of brown coals.

This project will enhance La Trobe University's output from post-graduate research that has produced a number of publications in international journals and a local conference. The project will improve linkages between La Trobe University and the brown coal industry, as evidenced by the on-going collaborative project with Clean Coal Technology Pty Ltd (CCT). It will promote the effective use of VPAC's Computing Facility for the development of effective catalysts in brown coals and make fundamental contributions in research to improve the utilisation of Victorian brown coals with a reduction in emissions of Greenhouse gases. This will significantly extend the HPC molecular capabilities developed at La Trobe University over the past three years.

# e-Research Grants Round 7 Announcements

**Project Number:** EPPNLA131.2005

**Project Title:** Inversion of Over-The-Horizon Radar (OTHR) data to obtain 3-D maps of ionospheric electron density

**Project Chief Investigator:** Peter Dyson

**Funding Obtained:** \$19,000

**Project Summary:**

This project aims to:

1. Develop a 2-D HPC grid point model of the ionosphere in the region of the Tasman International Geospace Environment Radar (TIGER) coverage area. The grid point model will be 2-D in ground range and height, and each grid point will specify ionospheric layer parameters determined from real TIGER ground scatter data using a new inversion technique we have developed. This modelling effort will help to improve our understanding of ionospheric structure on global scales, including gradients in electron density, the occurrence of high-latitude ionospheric troughs and sporadic E, and the associated generation of ionospheric irregularities.
2. To extend the 2-D grid point model to a 3-D grid point model of the ionosphere within the footprint of TIGER. TIGER routinely records echoes on 16 different beam directions so by applying the 2-D grid point approach to each of the beams a 3-D description of the ionosphere may be achieved. We have also developed a 3-D analytic ray tracing technique (not yet published) that can be applied to the 3-D grid point ionospheric model to further test the integrity of the inversion results.
3. To apply the 3-D inversion technique to data recorded with the new TIGER OTHR currently being installed near Invercargill, New Zealand.

**Project Number:** EPPNLA132.2005

**Project Title:** A Real-time Emotion based e-Sales Recruitment and Benchmarking System

**Project Chief Investigator:** Rajiv Khosla

**Funding Obtained:** \$18,000

**Project Summary:**

There are many situations in business involving the use of computer, internet and mobile communication devices in which emotions of a user play an important role. Consumer behaviour, selling behaviour, education, health care, travel, entertainment or Internet based information retrieval are instances of such situations. The existing work on computer-based analysis of human emotions has primarily centred around embodiment of emotional or affective characteristics like happiness, anger, fear, etc. in robots or software agents. However, there is very little research done in processing emotions and integrating the emotional (affective) states of user for e-decision support

and e-commerce systems.

**Project Number:** EPPNLA133.2005

**Project Title:** Medical Information Systems Interoperability and Retrieval

**Project Chief Investigator:** Wenny Rahayu

**Funding Obtained:** \$19,000

**Project Summary:**

The integration of different documents and resources in health information systems into a standardised knowledge representation has created a key area in health informatics e-research in the last few years. The establishment of an ontology in medical domains such as the UMLS (Unified Medical Language Systems) forms the conceptual standard that can be used to support data and knowledge interoperability and sharing.

**Project Number:** EPPNLA134.2005

**Project Title:** Band structures and electron scattering in conducting solids.

**Project Chief Investigator:** John Riley

**Funding Obtained:** \$18,000

**Project Summary:**

Funds are requested to enable the work funded last year to continue on VPAC's HPC system. The Chief Investigators are active researchers with local and international collaborative research projects and have proven excellence in their areas of research.

The previously funded program aimed to determine electronic structures using the first principles density functional theory quantum mechanical computing packages Wien 2K and abinit. It studied materials including Cu<sub>3</sub>Au, the shape memory alloy Ni<sub>2</sub>MnGa, which has two-phase transitions, and important magnetic alloys such as Permalloy. This present work will continue the successful comparison of photoemission experimental results with the theoretical calculations.

This project supports a successful, long term experimental program in electronic structure determination based at La Trobe University. Electronic band structures are of fundamental importance as they determine the electrical, magnetic and optical properties of metals and semiconductors and are critical in the design and understanding of modern semiconductor devices. The present project will concentrate on the calculation of surface electronic states, which are more computationally intensive than the previously calculated bulk states. Access to an HPC environment greatly enhances this process.

# e-Research Grants Round 7 Announcements

## R.M.I.T.

**Project Number:** EPPNRM135.2005

**Project Title:** Development of a Fast, Robust Explicit Finite Element Tool for Design and Evaluation of Impact-Resistant Aerospace Composite Structures in a High-powered Computing Environment

**Project Chief Investigator:** Javid Bayandor

**Funding Obtained:** \$17,500

**Project Summary:**

The highly competitive nature of both civil and military aviation requires that aircraft performance should continue to increase, while costs decrease. Composite materials have been used to improve aircraft performance, however their application has been restrained due to uncertainties surrounding their damage tolerance, in particular with respect to impact events. This has resulted in an overly-conservative design philosophy for aerospace composite structures.

**Project Number:** EPPNRM136.2005

**Project Title:** Molecular simulation of the rheology of nanocomposite polymer materials

**Project Chief Investigator:** Peter Daviss

**Funding Obtained:** \$12,500

**Project Summary:**

The major aims of this project are:

- to make some crucial performance and usability improvements to a new non-equilibrium molecular dynamics program recently developed in Applied Physics at RMIT University so that it can be applied to the prediction of the rheological properties of practical polymer nanocomposite materials
- to extend the preliminary results that we have already obtained for low molecular weight polymer nanocomposite materials to a practically useful range of polymer molecular weights, filler particle shapes and flow conditions.

**Project Number:** EPPNRM137.2005

**Project Title:** Investigation of protein molecular structures using dihedral angles and quantum mechanical ab initio calculations.

**Project Chief Investigator:** Margaret Hamilton

**Funding Obtained:** \$12,500

**Project Summary:**

The researchers plan to model the Rosetta method, which is currently one of the best ab initio methods available. As the researchers investigate this method, and parallelise it, the researchers also hope to find areas for further optimisation of the algorithm.

This is a collaborative project between Swinburne

University and RMIT. When the researchers have parallelised and improved this ab initio method successfully, the results will be compared with experimental results obtained from Flinders University and La Trobe University, both of which have the chemical instrumentation necessary to perform some complicated experiments, and which have been involved in collaboration previously.

**Project Number:** EPPNRM138.2005

**Project Title:** A molecular approach to the development of nanoscale diagnostic platforms for Hepatitis C

**Project Chief Investigator:** David Mainwaring

**Funding Obtained:** \$17,500

**Project Summary:**

Since its first medical identification in 1989, the blood based viral infection - Hepatitis C (HCV) is now estimated to affect 170 million people worldwide. As such HCV now represents a significant and serious health threat in most countries including Australia, since it is difficult to track, has few initial symptoms, is hard to detect clinically, and can result in severe outcomes that can take up to ten years to develop. Most of those infected are chronic and might not be aware of their infection because they are asymptomatic (not clinically ill). When untreated, infected people are a source of transmission to others and are at risk of eventual chronic liver disease, hepatic fibrosis, and hepatocellular carcinoma. It is well recognised that improved treatment outcomes are dependant on pre-treatment viral load, ie early and effective diagnosis.

**Project Number:** EPPNRM139.2005

**Project Title:** Developing an e-Platform for Testing Drug Delivery System through the Human Respiratory Airway System

**Project Chief Investigator:** Jiyuan Tu

**Funding Obtained:** \$12,500

**Project Summary:**

The need to develop new and innovative drug delivery systems is becoming more crucial for the improvement of patient compliance, overcoming delivery problems with difficult drug molecules, increasing cost-effectiveness, extending the patent life of drug compounds and reducing systemic side effects. Recent years have shown that the inhaled/pulmonary drug delivery system for the human respiratory system still is a long standing challenge due to the complexity of the geometry and material properties, which lead to the difficulties by experimental study, and expected to be explored deeply by numerical study due to increased capabilities of computers and computational fluid dynamics (CFD) techniques.

# e-Research Grants Round 7 Announcements

**Project Number:** EPPNRM140.2005

**Project Title:** Computational Analysis of Aerodynamic Interactions Between Passenger Cars

**Project Chief Investigator:** Simon Watkins

**Funding Obtained:** \$17,500

**Project Summary:**

Aerodynamic development of road vehicles is performed in wind tunnels and/or computational domains with smooth and uniform flows and thus with negligible temporal and spatial variations. However, in the real world, vehicles spend much driving time in a flow environment that is far from ideal (i.e. under the influence of atmospheric winds and traffic) and all indications are that this will increase. A major technological shift in the automotive world is the adoption of Intelligent Transport Systems that offer considerable reductions in inter-vehicle spacing (via fly-by-wire and associated sensing systems) which can result in greater highway "throughput" and significant drag reductions. However for these advantages to be gained there is a need for understanding of this new aerodynamic domain and the significant influences it will have on vehicle design and testing. Currently all major vehicle wind tunnels around the world are faced with having test sections that are too short to enable this to occur. Computationally this is generally not the case – CFD offers the ability to extend the domain to encompass upstream, downstream and cross stream influences of other vehicles. The primary focus of this work is to investigate the simulation techniques and the possibilities offered by extending the testing domain via CFD.

**Project Number:** EPPNRM141.2005

**Project Title:** An investigation of future global navigation satellite systems in support of research and development of positioning technology in Australia

**Project Chief Investigator:** Kefei Zhang

**Funding Obtained:** \$24,000

**Project Summary:**

Global Navigation Satellite Systems (GNSS) have been identified as the primary positioning technology for a large number of critical industry sectors such as location based services, maritime, aviation, agriculture, mining, surveying, military, road transport, and personal mobility. GNSS is well on its way to becoming an essential element of personal, commercial and public infrastructure and consequently part of our daily lives. Current generation GNSS is dominated by the United States Global Positioning System (GPS). However, in the near future, additional satellite infrastructures will become available, and are presently in development in Europe, Japan and China. In addition, innovative techniques are being developed to enhance the performance of GPS with complementary

ground-based systems. There is no doubt that the combined use of different satellite systems (e.g. GPS and its European equivalent – "Galileo") will improve the integrity, accuracy, reliability and availability of the position solution. However, no investigation has been carried out to accurately quantify and reliably evaluate these improvements, in Australia and Asia.

## The University of Ballarat

**Project Number:** EPPNBA124.2005

**Project Title:** Development of data mining tools for the prediction of genomic linked clinical outcomes in a genetic disease state Cystic Fibrosis

**Project Chief Investigator:** John Yearwood

**Funding Obtained:** \$20,000

**Project Summary:**

This project is an E-Research based proof of concept to develop data mining tools for the prediction of genomic linked clinical evidence based outcomes within a genetic based disease, Cystic Fibrosis. Current research into Genomic Disorders does not apply data management and data mining principles to the linkage of genomic and clinical prognosis of a disease state in a way that can predict and visualise the clinical outcomes.

The objective of this study is to build an e-Research network within which specialist collaborators in genomics (Deakin); Clinical based medicine (La Trobe), Mathematical based data mining tools (Ballarat) and the advanced visualisation of complex scientific data (RMIT I-Cube) can develop predictive models using longitudinal clinical and genomic data collected by the Royal Childrens Hospital since 1974.

The main objective of mining clinical data is to assist public health agencies and clinicians, who rely on timely and accurate information, about any emerging trends in disease, treatment records and history, to guide decision making.

# Computational Software Development News

The last six months have, as usual, been busy for VPAC's Computational Software Development group. Here is a summary of the main happenings, achievements, and upcoming events:

## Education and Outreach:

CSD's Steve Quenette and Patrick Sunter hosted training courses in August and December for researchers from our member institutions on HPC hardware, MPI Programming and developing HPC applications. We will be running further courses in 2005, so if interested check the VPAC website for details on course dates and registration.

We have continued work on our parallel HPC modelling framework **StGermain**, which we hope to formally release early next year. StGermain and course material on how to use it will be made available to members of both VPAC and APAC as part of APAC's Computational Tools & Techniques program. For more information, check out StGermain's homepage on our wiki at <http://csd.vpac.org/twiki/bin/view/Stgermain/WebHome>.

## Geodynamics Research Collaborations:

Research continues steadily on our collaborations with the University of Melbourne, Monash University and CalTech on various HPC Geodynamics modelling research projects. Some of this work was presented at the American Geophysics Union's annual conference recently, including coupled mantle-crust simulations using [Snac](#) and [CitCom](#), the [GLucifer](#) visualisation framework and work on modelling subduction using [Snark](#) and [UnderWorld](#).

## Super Computing 2004 Conference:

VPAC made its way to the SC (Super Computing) 2004 conference, as a regular exhibitor once again. Held in

Pittsburgh USA, VPAC showcased the results of our latest achievements amongst the other players in the industry including IBM, CalTech, Argonne National Lab and NASA to name a few. The conference is a gathering of manufacturers, research and high performance computing facilities in the computing industry which gives VPAC the opportunity to learn from and strengthen collaborations with teams in the United States.

For more details on any of the above, head to the CSD homepage at <http://csd.vpac.org>.

(contributed by Patrick Sunter and Alan Lo.)

## VACA: PROMOTING ADVANCED COMPUTING THROUGHOUT VICTORIA

The Victorian Advanced Computing Association (VACA) is an association sponsored by the Victorian Partnership for Advanced Computing (VPAC); a company whose mission is to improve the international competitiveness of Australian industry and organisations through the provision and support of Advanced Computing technologies. VACA is supported by the Victorian State Government and is the first association of its kind to be formed in Victoria.

### THE VACA KEYNOTE SPEAKER PROGRAM

VACA is committed to actively promoting the use of High Performance Computing (HPC) within Victoria, ensuring the smooth transition of new tools and technology to both Academia and Industry, by providing regular free lectures, seminars, workshops and events on Advanced Computing from recognised world leaders in HPC through the VACA Keynote Speaker Program.

### MEMBERSHIP

VACA welcomes new academic, commercial or industry members with an interest in Advanced Computing. As a member of VACA, you will automatically receive updates on lectures, seminars, workshops and events and will also receive the free online VPAC HPC News Magazine, issued quarterly.

To apply for your free VACA membership, simply complete the online form provided here and press the 'submit' button. Upon registering, you will receive a member number that will make it easy for you to register for future VACA seminars and events.

VACA will not provide membership lists to any commercial organisation for advertising or any other purpose. Any material sent to you from VACA will come directly from the VACA offices, currently housed at VPAC.

### KEYNOTE SPEAKER PROGRAM SPEAKER REGISTRATION

The VACA Keynote Speaker Program offers Industry and Academic organisations and researchers the opportunity to communicate with the Victorian research and Advanced Computing communities in an intimate and flexible environment. Organisations who register speakers are able to choose their target audience and the style and scale of the seminar, lecture, workshop or event. As a sponsored association, VACA does not charge for venues and catering or publicity and communications (email and web-based only).

If you would like more information on VACA and the VACA Keynote Speaker program or to register a Speaker visit [www.vpac.org/vaca](http://www.vpac.org/vaca) or contact Maria on +61 3 9925 4630 or [maria@vpac.org](mailto:maria@vpac.org).



VPAC holds a variety of training courses and workshops throughout the year aimed at helping VPAC Members and Users get the most out of our Advanced Computing Facility.

An overview of VPAC training courses is provided below. Visit [www.vpac.org](http://www.vpac.org) for schedule details. If you would like to register for any of these courses or workshops simply complete the online registration form by following the link below:

[http://www.vpac.org/content/services\\_and\\_support/training/registration.php](http://www.vpac.org/content/services_and_support/training/registration.php)

### **Introduction Course- A 'Hands on' Introduction to VPAC Facilities**

This course is designed as a quick start to get users going as quickly as possible by concentrating on basic skills and highlighting the areas that often confuse those new to this sort of technology.

This course is a 'hands on' course. Most of the material presented is supported by exercises that the students are strongly encouraged to do and discuss the results with the presenter and other students. It is suggested that this course is suitable for people who:

- Have limited experience with UNIX.
- Have little or no experience in parallel computers.
- Intend to attend one of the more advanced courses or will be using precompiled applications only.

### **Introduction to HPC and Parallel Programming Basics (Previously Parallel Programming)**

This course provides an introduction to both high performance computing hardware and theory, and the MPI parallel programming library. We suggest it is appropriate for those who are relatively new to HPC, and would like a general introduction to the field, information to help choose which hardware and software to use, and skills for developing parallel codes. The afternoon session requires at least a basic knowledge of C or Fortran.

The morning session will introduce the various HPC platforms, architectures, & programming approaches: allowing you to make an informed decision about what is appropriate for your needs. Topics covered will include:

- What is HPC?
- Taxonomy of computer architectures
- VPAC's facilities & approach to hardware
- Parallel Programming styles & libraries.

The afternoon session will provide a hands-on introduction to the widely-used MPI parallel programming language. By the end of the session you should understand the structure and thinking-model required to write MPI programs, and be able to write & debug basic MPI applications.

- Introduction to the Message Passing philosophy
  - Hands on walkthrough of the core MPI communication functions
  - Tutorial on working with multi-use clusters, including VPAC's Brecca
  - Tutorial on debugging MPI programs
- If you intend to do a significant amount of parallel programming, we strongly suggest you also attend the Intermediate MPI Programming & Parallel Application Development Workshop, to consolidate your skills

### **Intermediate MPI Programming and Parallel Application Development Workshop (Previously MPI)**

This course combines an overview of how to solve the design issues you'll face when writing large-scale parallel programs, and a hands-on workshop on using the MPI parallel communication library to implement these solutions. It is suitable for those who have some knowledge of parallel programming, but would like to improve their skills and effectiveness. We strongly suggest you attend the previous day's "Introduction to HPC & Parallel Programming Basics", unless you already have experience of using MPI and its core functions.

Topics covered will include:

- Domain Decomposition
- MPI Derived datatypes
- Latency hiding for improved performance
- Profiling parallel programs
- Discussing attendees' parallel programming applications.

VPAC is a leading Advanced Computing R&D service provider. VPAC is an independent, not for profit registered research agency established in 2000 by a consortium of Victorian Member Universities. VPAC's mission is to provide expert services, training and support in Advanced Computing to VPAC Members, Industry and other organisations.

If you would like to be updated with regular newsletters and workshops on various Advanced Computing tools and technologies, register your details with the Victorian Advanced Computing Association (VACA), an association sponsored by VPAC whose objectives are to lift the awareness of High Performance Computing within Victoria by providing regular lectures and seminars on Advanced Computing from recognised world leaders in HPC. All subscriptions to VACA are free so please visit [www.vpac.org/vaca](http://www.vpac.org/vaca).

For enquiries regarding VPAC's e-Research Program grant schemes or training in advanced computing please visit our webpage at [www.vpac.org](http://www.vpac.org) or contact the Grants Coordinator at +61 3 9925 4645 or by email at [karen@vpac.org](mailto:karen@vpac.org).

VPAC News is distributed quarterly and is intended to provide readers with a broad outlook of the Victorian Advanced Computing industry as well as inform VPAC Members, Industry and other organisations of VPAC news and events. We are always open to suggestions as to how to improve our newsletter and welcome VPAC Members to submit articles or case studies about research projects utilizing advanced computing tools. For article submissions or comments please contact Maria Kambourakis on +61 03 9925 4630 or email [maria@vpac.org](mailto:maria@vpac.org).

## Up & Coming Events

### **January 19-22, 2005**

[Cast](#)

Orlando, Florida USA

### **February 3, 2005**

[Lorne Cancer & Genome Conference 2005](#)

Lorne, Victoria

### **February 9-10, 2005**

[Hybrid Vehicle Technologies](#)

Hilton Costa Mesa, Costa Mesa, CA

### **March 5-12, 2005**

[2005 IEEE Aerospace Conference \(international\)](#)

Big Sky, MT, USA

### **April 11-14, 2005**

[SAE2005](#)

Detroit, Michigan, USA

### **April 18-23, 2005**

[Linux Australia](#)

Canberra, ACT

### **April 25, 2005**

[Access Grid](#)

Berkeley, California USA

### **May 9-12, 2005**

[CC Grid](#)

Cardiff, UK

### **July 31-4 August, 2005**

[ACM Siggraph](#)

Los Angeles, California, USA

### **August 21-25, 2005**

[APCO \(national\)](#)

Denver, Colorado, USA



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