

# VPAC NEWS

Issue 4 November 2004 Special e-Research Edition

## VPAC News Issue 4 November 2004: e-Research Special

Feature article: e-Research: The New Paradigm	1
Victorian Advanced Computing Association Keynote Speaker Program	3
News Updates	
Centre for Computational Prototyping: Declarative Design	4
Life Science: Bioterrorism	4
Computational Software Development: Snac Attack	5
For Sale: AlphaServer for Sale	5
Training Courses	6
Want to hear more?	7
Comic Relief: The Joy of Technology	7
Contact Information	8

# e-Research: The New Paradigm

## e-Research – the changing face of Research

Academic research has largely followed the same paradigm or process for hundreds of years: a cycle of discourse, discovery, peer-review and publication driven by individual researchers or small local teams. In this paradigm, each research project or publication is generally small and self-contained – an incremental advance on the prior art. Rapid advances in IT have made the traditional research process more efficient – email has replaced letters, terminals have replaced typewriters, and Google has replaced laborious literature searches. These IT advances, however, have not significantly changed the research process– just made it more efficient.

### e-Research: What is it?

Not all research can be undertaken by small, isolated teams. Sciences such as experimental High-Energy Physics and Astronomy rely on massive shared scientific instruments, and other sciences such as Genetics or Meteorology rely on access to vast shared historical databases of data gathered worldwide. In such fields, research is often driven by:

1. Global collaboration;
2. Large shared databases (data grids), and web portals;
3. Community-owned software, data, and models.

While researchers in such fields have their own specific projects and specialization, their research follows a fundamentally different paradigm than traditional research. The centerpiece of the paradigm is collaboration, as opposed to specialization and individualism in traditional research. We call this paradigm e-Research, or e-Science, when applied to traditional scientific disciplines. While e-Research sprang from traditional sciences, it is now finding increasing application in the Humanities and Social Sciences, with applications ranging from linguistic databases to health informatics. E-Research has close ties with trends to e-Government and e-Business. All of these have the same three themes: collaboration, data sharing and real-time online access to products and services.

### e-Research: What is it not?

As with any new paradigm or trend, there is some disagreement and misconception about what e-Research really means, and its impact. A common misconception is equating e-Research with grid computing. Grid computing is simply IT infrastructure that supports large-scale distributed data and computation. Grid computing provides IT technology that facilitates some, but by no means all, e-Research projects. VPAC, together with the Australian Partnership for Advanced Computing (APAC), has quite significant initiatives to provide better grid computing infrastructure to Victoria and Australia, but this effort has quite wisely focused on funding applications development (e-Research), as opposed to simply building infrastructure.

Furthermore, e-Research is not web candy such as glitzy websites and flashy graphics, nor is it simply using email and fancy PowerPoints to communicate. E-Research is a way of doing research, not the technology that enables it.

### What is fuelling e-Research?

The shift towards the e-Research paradigm will accelerate and researchers and institutions that stick to the traditional, individualistic research paradigm may be left behind and isolated. The reasons for the trend to e-Research are numerous, but include:

- A push by research funding agencies such as the ARC, the US NSF, and in particular the UK National e-Science Centre ([www.nesc.ac.uk](http://www.nesc.ac.uk)) to favor collaborative e-Research style projects and centres;
- The increasing complexity of research problems and projects. In a sense, all the "easy" problems have been solved. Remaining research problems are much harder and require much large diverse teams to tackle them – such as proteomics, climate modeling, or the evolutionary tree of all human languages.
- Increasing focus on applied and industry-funded research – where the outcomes are commercial products and processes, or have direct relevance to the economy or environment.

### Obstacles of e-Research

One obvious question is: what organizational factors act as inhibitors or accelerators to the uptake of e-Research? Departments or organizations that are able to accelerate their uptake of e-Research are likely to be more competitive and successful in the next five to 10 years. The key accelerators are:

1. Institutional support for larger collaborative e-Research projects;
2. Cross-disciplinary and cross-organizational collaboration;
3. IT infrastructure to support e-Research.

The successful uptake of e-Research requires fostering and nurturing collaborative cross-disciplinary research teams, and requires a shift of emphasis away from traditional specialist academic publications and grant proposals. Traditional academic promotion schemes can be disincentives to e-Research as they are often tied to recent individual peer reviewed publications and grants, as opposed to broader collaborative efforts that may take years to reach fruition.

## e-Research: The New Paradigm

Traditional academic departments can also hinder the uptake of e-Research as they are rarely set up to facilitate cross-disciplinary collaboration. Academic hiring and promotion focuses on specialization, and cross-departmental ties are often the exception rather than the norm.

Finally, IT infrastructure at many institutions is set up largely to support traditional ITS services: email, secure networks, corporate applications, and desktop office software. E-Research requires different types of IT support, ranging from scientific database design and deployment to dynamic web portals, application-specific research software, and experimental software.

### So what can organisations do?

E-research describes the method of practicing scientific research via distributed global and local collaborations that are generally cross-disciplinary and supported by specialized software. E-research requires, therefore, flexible and agile team organisation with a wider range of skills and expertise, including IT expertise in scientific computing.

E-research also calls for a different style of IT project management, involving closer interaction with clients (researchers) and iterative development and deployment of software based on feedback.

VPAC has been highly successful over the past four years, growing rapidly to the point where we are a commercially viable company with a strong balance sheet. One of the major factors in VPAC's success has been our ability to tap into the large and growing demand for e-Research services that VPAC provides. The growing demand for VPAC's services and support across its Members, Industry, and Government is a very clear indicator to us that Victoria is well placed to capitalize upon the e-Research trend.

To learn more about e-Research and how your organisation can move towards this new scientific research paradigm, please contact VPAC on +61 3 9925 4645 or email [info@vpac.org](mailto:info@vpac.org).

## 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).

## CfCP- Declarative Design

During the MSC.VPD2004 conference in October, CfCP presented groundbreaking software development achievements to leading manufacturing organizations.

Chris Seeling, Head of CfCP, introduced Declarative Design as the new software development principles for Virtual Integrated Design Environments (VIDE). He explored simulation technology created through the Declarative Design principles; a design space that removes the analyst from the functionality-cluttered engineering tool suites of today, by creating an environment that is based on engineering behaviour. Such a design environment will guide the analyst through the specific design process, intuitively adding only the necessary functions to carry out the desired behaviour.

Unlike today, where the analyst is required to carry out the design using a set process, Declarative Design principles in VIDE will enable the engineer to explore many paths to complete the design project. Behaviour driven Declarative Design will therefore enhance creativity, which in turn will foster innovative solutions.

Engineering environments developed using Declarative Design processes will reduce the knowledge barrier required to learn large tool chains and enable engineers to more efficiently carry out complex design projects.

The CfCP is currently using Declarative Design principles in the development of several new breakthrough VIDE prototypes. For enquires regarding VIDE and Declarative Design please contact Chris Seeling on (03) 9647 5432 or email [chs@vpac.org](mailto:chs@vpac.org).

## Geospatial Sciences: Countering Terrorism and Ensuring Public Safety

The VPAC Geospatial Sciences team have been working with the Victorian Police and RMIT's Interactive Information Institute to develop a range of simulated events that can be used for training and emergency response planning in the event of a major disaster or potential terrorist attack at a major event or facility.

This has incorporated the use of multi faceted technologies involving Global Positioning Systems, (GPS); satellite and aerial spatial information and 3D advanced visualization to simulate events. These events have been created using a range of situations based on international terrorist and major disasters including the release of a toxic gas within a public transport environment, a serious fire within an underground train station, a potential bomb threat within a public place and a hostage situation within a sports arena or theatre.

The positive outcomes from the creation of this type of technology simulated environment, is that it can assist in the training and integration of real time visualization tools that can assist multi faceted emergency services from Fire, Ambulance, Police and government agencies in dealing with serious events through a simulated 3D visual experience.

For further information on the work of the Geospatial Sciences team at VPAC, please contact Bill Yeadon on +61 3 9925 4719 or [b.yeadon@vpac.org](mailto:b.yeadon@vpac.org).

### CSD- Snac Attack

The Computational Software Development (CSD) group held a weeklong coding-fest on October 18th to 22nd. Entitled the "Snac Attack", it is the second in the likely long running bi-annual series of "StGermain retreats". StGermain is the core computational infrastructure developed by the CSD group. It provides explorative computational researchers a reliable basis for computational codes (e.g. meshes, debugging, regression testing and so on) as well as promoting contemporary software development practices (such as extensibility and re-use). Snac is a crustal-deformation modelling code being co-developed with the Californian Institute of Technology (Caltech), USA. The last event was entitled the *Snark Offensive*, after the Snark project aimed at developing numerical techniques for mantle convection problems.

Present at the *Snac Attack* were Professor Michael Gurnis and two other members of the Caltech Snac team, Associate Professor Louis Moresi and the Underworld/Snark team of Monash, Matt Knepley of the PETSc project at Argonne, Senior Researcher Mike Sandiford of the Cascade/SPModel project at the University of Melbourne, Lutz Gross of eScript project at the University of Queensland/ACcESS, and the VPAC CSD crew. It was a productive week of collaborative, algorithmic and coding development, spanning researchers across Australia and the United States.

If you would like to learn more about Snac or St Germain, please contact Steve Quenette, VPAC R&D Manager and Head of CSD on +61 3 9925 4726 or email at [steve@vpac.org](mailto:steve@vpac.org).

### Refurbished Training and Videoconferencing Room

The VPAC Training and Videoconferencing room, housing the Access Grid advanced videoconferencing facility, has recently been re-decorated to give a highly professional and intimate environment for videoconferencing, training and workshops.

The room is available for hire free of charge to VPAC Members and can also be hired by industry and other organisations for company training and workshops as well as advanced videoconferencing meetings, lectures or seminars. Simply call the Access Grid Administrator on +61 3 9925 4947 to check for room availability.



### AlphaServer for Sale

VPAC is replacing its AlphaServer SC Supercomputer over Christmas. Its very unlikely that anyone would be in a position to continue running it as a Supercomputer because of the very high cost of software licenses involved. However, the individual ES40 boxes that make up this machine are still a very viable computer and capable of doing significant work. They can be used with the free Alpha Debian release of Linux or, if you have site licenses for Tru64 from HP they be even more attractive. With four CPUs and their excellent 64 bit floating point performance, each is a very useful machine for engineering or scientific applications. Just what you need under your desk! We're likely to want to sell 28 of them, each one configured like this:

4 x 833MHz Alpha Chips.  
2Gig Ram  
3 x 18Gig SCSI disks  
CD drive, Floppy, serial, printer, keyboard and mouse ports.

Note: graphics card not included.

For further info, please contact David Bannon, [D.Bannon@vpac.org](mailto:D.Bannon@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.

A list of up and coming training courses is provided below. 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.

**When:** Thursday 25th November 2004 at 1:30pm at the VPAC Offices

## Parallel Programming Workshop

Many users find that although they have the necessary programming skills, making the transition to parallel programming is not easy. This course will explore the many factors that can come into play in a parallel application and provide the student with the information necessary to design a new application or convert an existing serial application to parallel.

It should be noted that this course does not concentrate on code or syntax; instead it looks at design issues and high-level parallel techniques.

**When:** Wednesday 1st December 2004 at 1.30pm at the VPAC Offices. **NOTE: Change of date**

## MPI Courses

This course will concentrate on the syntax and coding using MPI, the popular and VPAC recommended method of communication between parallel applications. It will be of great interest to programmers who already have a reasonable grasp of Fortran, C or C++. Over all design issues are not covered, instead this course is very much at the code level.

**When:** Thursday 2nd December 2004 at 1.30pm at the VPAC Offices. **NOTE: Change of time**

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).

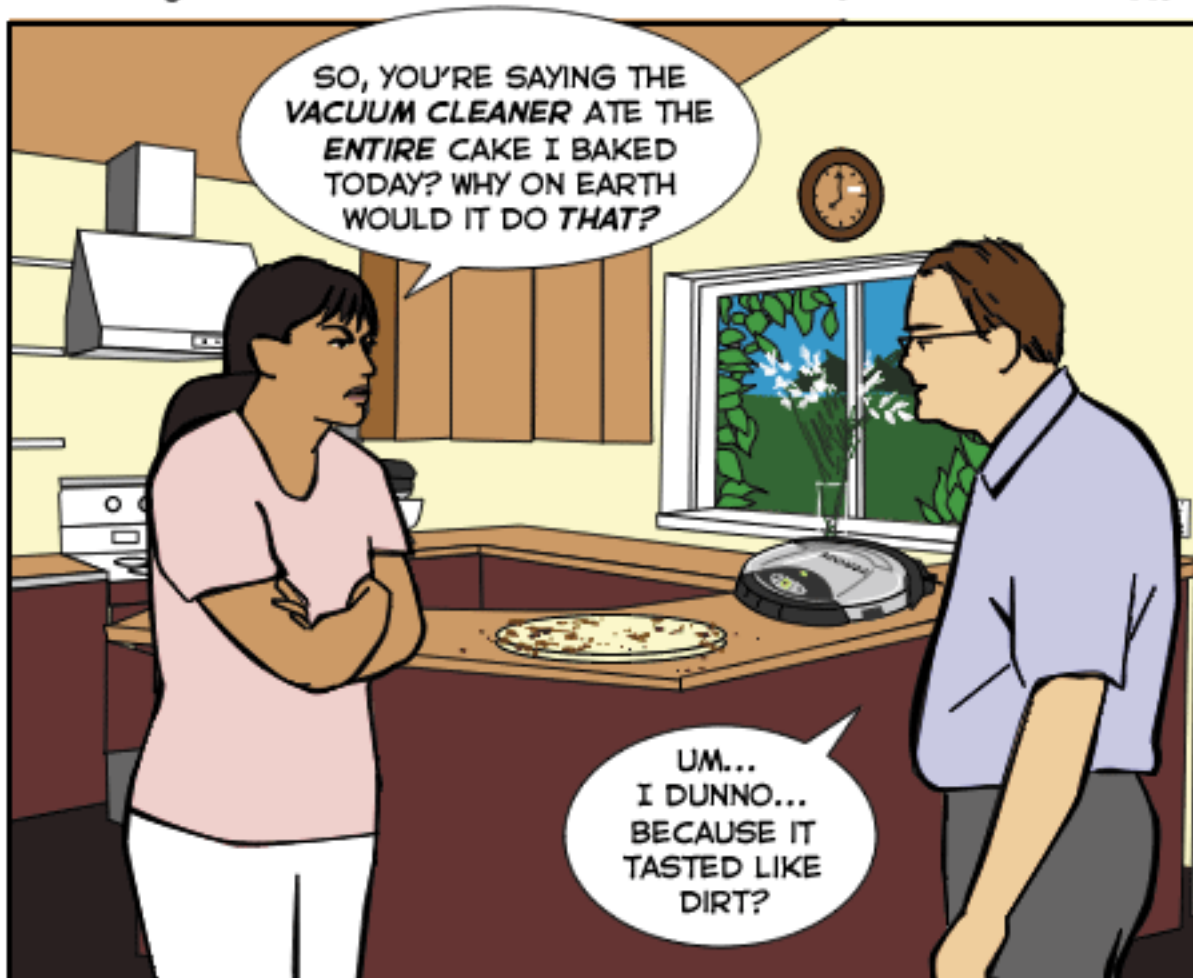
For enquiries regarding VPAC's e-Research Program grant schemes or training in advanced computing please visit our webpage at [www.vpac.org](http://www.vpac.org) or contact Cammie Lazzaro at +61 3 9925 4645 or by email at [cammie@vpac.org](mailto:cammie@vpac.org).

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).

## The Joy of Tech™

by Nitrozac & Snaggy

Indulge. Get the Joy of Tech book!



©2004 Geek Culture®

joyoftech.com

That wasn't the right answer.



Victorian Partnership for Advanced Computing Ltd

Innovation Powered by Advanced Computing

110 Victoria Street PO BOX 201 Carlton South VIC 3053

t. +61 3 9925 4645

f. +61 3 9925 4647

info@vpac.org

www.vpac.org