



# VPACNews

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Innovation Powered by Advanced Computing

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Many projects in Victoria are showing strong collaborations emerging between **libraries** and **HPC facilities**, which is rather ironic...

# Data Repositories and Data Federation

by Professor Bill Appelbe

The focus of high performance computing (HPC) has traditionally been on computation, and over the past five years there has been significant investment both nationally and internationally on large HPC computational facilities. This investment is culminating in the APAC Computational Grid, headquartered at VPAC, which supports a federation of HPC facilities to provide seamless access to HPC across Australia.

While this investment in HPC has been going on, there has been a growing investment in data storage, and national and international data repositories. The requirement for such repositories has been driven by several needs, including:

1. Access to archival data from previous observations and experiments (e.g., Astronomy);
2. Sharing data internationally online in near real-time (e.g. Genetics);
3. Improved “quality” of data and data access.

Quality of data access has many dimensions beyond just speed of access, including freedom from data errors, annotation and organisation of the data, as well as curation (long-term preservation of the data). As data repositories become more widespread, and researchers rely on them ever more increasingly, the need for reliability and accessibility is increasing. A recent major crash in a US climate data repository, for example, caused Victorian researchers relying on the database delays of many weeks in their research.

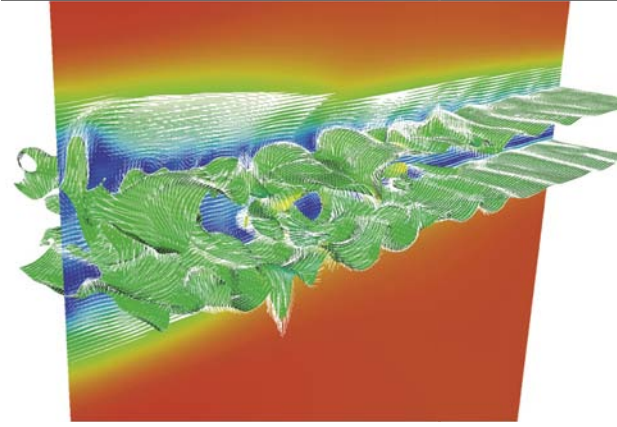
Maintaining very high reliability and availability in large-scale international data archives is very costly. Arguably, the only institutions that can guarantee to curate large data sets for decades, are major museums and libraries. There is an interesting convergence at present between libraries (traditional curators of books and other artifacts), who are moving into digitisation of their collections, and research institutes, who are moving into curation of digital data. In Victoria, projects such as Arrow and Dart are showing strong collaborations emerging between Libraries and HPC Facilities. Such collaboration is ironic, given that the emergence of the internet at first seemed to be making libraries irrelevant (everything is online). Of course, putting everything online begs the question of who should curate the online repositories, and one logical answer is libraries.

Another major problem in digital repositories is how to organise and access the data. Google is, alas, not the answer to everything, and certainly not the highly structured data repositories such as are common in the sciences. The traditional way to organise data has always been based on physical directories and file systems, with permissions simply based on “read, write, or execute” access for user groups. Such a simple system does not scale well to global data repositories, where access to data should be based on logical data attributes, not physical location, and access permissions might be dynamic on a per project basis. There are active efforts to develop solutions and standards for digital repositories, such as SRB and Shibboleth, but these efforts are moving targets at present.

“The **Bio21:MMIM** project is an example of a very successful Victorian project to federate medical research databases.”

Finally, digital repositories bring up the issue of whether it is better to “centralise” or “federate” databases. Both approaches have their merits, and the decision as to whether to centralise or federate has to be made on a case-by-case basis. The Bio21:MMIM project is an example of a very successful Victorian project to federate medical research databases. The decision to federate was driven by the research institutes’ needs to maintain their own private research data locally, but allow access to other researchers on a project-by-project basis, with the involvement of medical ethics boards. DEST has funded scaling the successful Bio21:MMIM project up to a much larger scale, which introduces all the problems of curation, data validation, and mapping between different data formats in different local databases. But the ability to run large scale statistical analysis and case studies across large medical research data sets is well worth the effort and cost of scaling up the Bio21:MMIM project.

For further information, please contact Professor Bill Appelbe, VPAC CEO, [bill@vpac.org](mailto:bill@vpac.org).



# Centre for Computational Prototyping (CfCP)

VPAC's Centre for Computational Prototyping (CfCP) is one of Australia's leading R&D centres focused on developing virtual product development strategies that harness the power of current and emerging process technologies.

The Centre combines automotive industry expertise with development process and supporting technology expertise in order to deliver the required solutions. CfCP is a trusted collaborator and strategic partner to engineering and research organisations Australia-wide and delivers client-focused, tailored solutions and services, linking the expertise of the world's best of breed software and hardware suppliers with VPAC's state of the art high performance computing infrastructure.

Currently, CfCP is working on a number of projects with a local design house, a not for profit commercial centre and other companies within the Automotive and Aerospace sectors. Current projects include:

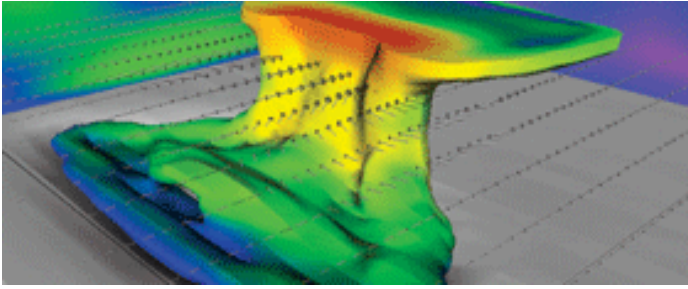
1. Development of a 3D stereo visualisation facility for a large automotive client for the purpose of exploring and developing the use of this technology for automotive engineering design and manufacturing. The technology is intended to improve the efficiency and quality of the design process and the end-product.
2. Development of an advanced version of a Calibration Management Tool currently in use by a large automotive client. The Calibration Management Tool is used to support the management of the release of new calibrations for various vehicle platforms and their variants. The advanced version will allow for improved management capabilities and quality assurance support across the calibration cycle, reducing the amount of manual data entry and manual handling of data. This reduces the time required to

manage a vehicle calibration while improving the quality of the data in the calibration. The advanced tool will allow for improved quality of the calibration, in turn allowing designers to optimise vehicle performance while balancing fuel efficiency and emissions.

3. Engineering support to a large automotive client, specifically the development of a working application Demonstrator of C-SAW, a software program that rapidly prepares concept-phase designs of cars for analysis. C-SAW is a CfCP-developed program that allows for analysis of important design factors such as vehicle strength, weight and stiffness. The program allows vehicle developers to finalise designs in less time by doing more work up-front in the concept phase, thereby eliminating much of the re-work of the vehicle in the later stages. Not only does this allow vehicle manufacturers to get their product to market faster, it saves money.

Recently commenced structural simulation of water tanks for a fast growing SME domestic and agricultural water tank manufacturer as part of the Australian Institute for Commercialisation's Techfast Program. VPAC is working with the manufacturing organisation to develop a structural simulation report on the tanks using Virtual Engineering (CAD & CAE).

For more information on any of these projects, please feel free to contact Thomas Ting on +61 3 9647 5437 or [thomas@vpac.org](mailto:thomas@vpac.org).



## Computational Software Development - GALE Force Winds

The past few months have seen StGermain's multigrid component near completion, now being used to enhance several existing simulations. Essentially, Multigrid is a method used to counter poor scalability in certain problems, allowing exploration of greater resolutions. For example, now complex 3D mantle convection models are feasible, whereas previously only the 2D equivalents were possible. The StGermain software framework provides infrastructure to create sustainable, collaborative computational development environments. It aims to provide the efficiency and style of coding near that of traditional HPC, whilst also aiming to foster the techniques and OO methods in scientific computing. From a computational science perspective, StGermain is the application of strategic software engineering for the facilitation of effective phenomena modelling. This means the "ease of ability" in creating computational models of new science problems. Computational researchers can "grow" their capabilities whilst maintaining the integrity of the pieces of code they already rely on, and those they are creating. StGermain goes beyond this; it is multi-disciplinary, able to be used to build software in a wide variety of sciences.

In other news, CSD held a miniature version of last year's 'Snark retreat' at the VPAC head office, the primary goal of which was to discuss the path forward for a new and exciting project, named GALE. GALE, an ALE (Arbitrary Lagrangian-Eulerian) formulation for finite-element problems, is to be developed as a collaboration between Caltech and VPAC.

For further information, please feel free to contact Steve Quenette at [steve@vpac.org](mailto:steve@vpac.org).

Contributed by Luke Hodkinson, CSD Computational Scientist.  
Deakin Sonar Project



## Geospatial Science

The data acquisition phase of the Deakin University co-ordinated Marine Habitat Mapping project commenced early November, with quality assessment of source data being carried out onboard the research vessel. The project aims to improve knowledge about the location and condition of coastal fringe marine habitats and associated biodiversity in Victorian state waters, and thus to help guide informed decision making in natural resource management. VPAC participant Shoab Burq provided expertise gained from his recent time spent with world leaders in the field of multi-beam SONAR, University of New Brunswick Ocean mapping group.

### Summer Internships

2004-2005 VPAC interns Chee Yin Lee and Carly Lambert both exceeded expectations with their final year Major projects, both scoring a High Distinction. Yin's project investigated photogrammetric techniques to identify snow pack thickness in alpine regions using snow covered and bare earth digital air photographs. Carly investigated experimental field and airborne spectroscopic techniques for the discrimination and spatial mapping of noxious weeds in Victoria. Both projects have generated considerable interest, and are being pursued in ongoing research.

2005-2006 internships projects are focused on GIS support of Emergency Services Organisations, with projects are as follows:

1. Wildfire Threat Modelling
2. Surf Life Saving Hazard & Incident Web Mapping
3. An Investigation of Real-time Visualisation Technologies for Collaborative Decision Making

For more information on these internship projects and others, please see page 9, Summer Internships: Surf, Sand and Science or visit [www.vpac.org](http://www.vpac.org).

# Life Science - Molecular Modelling, Bioinformatics, Health Informatics

## Bioinformatics

Over the past few months, with the welcoming of Dr Robert Flegg as VPAC's new Bioinformatics Manager, VPAC has been growing its Bioinformatics services and support capabilities to meet the ever growing needs and demands of bioinformaticians and life scientists around Victoria.

As part of a long term strategic objective to offer intensive support to the bioinformatics field throughout Victoria and Australia, VPAC has recently developed a comprehensive plan for training in bioinformatics. The training will include an intensive introduction to the theory and methods of bioinformatics, sessions detailing how to use various popular web-based resources, and short courses on particular topics such as molecular modelling and proteomics. Sessions are scheduled to commence early 2006 and will run throughout the entire year. For further information, contact Robert Flegg on 9925 4645 or keep an eye on our website at [www.vpac.org](http://www.vpac.org).

VPAC has also identified a set of bioinformatics analysis programs and databases for use by our Members, Industry and other organisations and has added these resources to the VPAC BioPlatform.

Other Bioinformatics news:

-VPAC has participated in the creation of a video defining and describing the Human Variome Project.

-The company recently participated in the development of mutation/phenotype data submission and database resources through the Genomic Disorders Research Centre and the Human Genome Variation Society

For further information on the BioPlatform or for details on future bioinformatics training, please feel free to contact Dr Robert Flegg, VPAC Bioinformatics Manager, [r.flegg@vpac.org](mailto:r.flegg@vpac.org).

## Molecular Modelling

Michael Kuiper, VPAC's resident molecular modelling scientist has been working with Dr Richard Wilson of the Royal Children's Hospital to model one of the genetic causes of a particular form of Dwarfism known as Schmidt metaphyseal chondrodysplasia. By modelling the wildtype and mutant forms of Collagen X, the gene thought to be responsible for this form of dwarfism, Dr Richard Wilson has been able to ascertain the likely mechanism of the folding mutation leading to stunted bone growth.

Work has also been conducted with Dr Angeline Bartholomeusz from the Victorian Infectious Disease Reference Laboratory (VIDRL) and others,

investigating the role of the hepatitis B virus precore protein in modulating the human immune response. VPAC and Dr Bartholomeusz have also been working on a large scale solvated molecular model of the hepatitis B polymerase. Taking advantage of the interactive Molecular Dynamics feature of NAMD, a molecular modelling program from the University of Illinois, Angeline and her team have been able to dock various drugs interactively.

## Health Informatics

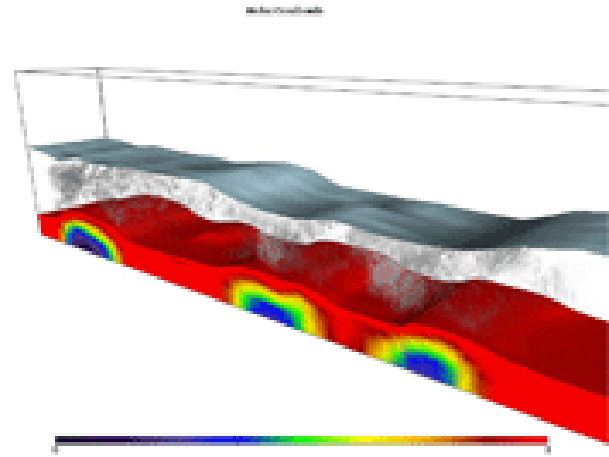
VPAC is a lead technology partner in a project led by Melbourne Health and in conjunction with Bio21 to establish the Bio21 Molecular Medicine Informatics Model (Bio21:MMIM), a resource of data sets physically located at various organisations, that are able to be integrated, search and queried seamlessly via a federated data integrator. The project was established as a pilot project with a \$1.6m STI grant from the Victorian Government and is now to be expanded after receiving Department of Education, Science and Technology (DEST) funding of \$4.3m to increase the number of participating sites and diseases and to provide access to new clinical specialty groups, new data types (e.g. images) and different styles and areas of research.

As lead technology partner, VPAC will be providing the advanced computational infrastructure necessary to complete the project and VPAC's systems management and life sciences teams will provide programming expertise to support the development and implementation of the critical IT requirements of this project. VPAC will also offer its advanced visualisation capabilities to enable the analysis of large complex data sets and the communication of this information into a 2D or 3D visual form enabling enhanced understanding.

VPAC is also involved in a project to implement a Victorian Nosocomial Infection Surveillance System (VICNISS). The proposed VICNIS system will significantly improve collection and reporting of infections in Victorian Hospitals. The purpose of the system is to provide Infection Control staff at approximately 30 large Victorian hospitals an enabling and common method for collection of Nosocomial infection surveillance data. The system will enable Victorian hospitals to extract information about their surveillance data to help them improve their processes and to better manage Nosocomial infection in their own environments.

Again, VPAC will be providing the advanced computational infrastructure necessary for the completion of the project.

For further information on any of these projects please feel free to contact Dr Marianne Hibbert at [mhibbert@vpac.org](mailto:mhibbert@vpac.org).



## St Germain Test Run on IBM's Blue Gene a Success

The Computational Software Development (CSD) team at VPAC has demonstrated its St Germain Finite Element Method (StgFEM) framework can adapt to suite small footprint and constrained system designs by scaling linearly to 128 CPUs during a test run on IBM's Blue Gene computer in preparation for the APAC05 conference in September.

The success of this test run demonstrates that CSD have established the ground work for potentially scaling StgFEM up to as many as 10,000 CPUs in the future. For researchers, this means the possibility to look at larger multi-scaled problems, for example, mantle-convection coupled to lithospheric deformation and erosional models. With this capability we can begin to really understand the Australian plate to unprecedented levels of detail, with potential impact on resources and safety for Australia and its neighbours.

The Blue Gene, labelled as the world's fastest computer, is optimised for scalability and the ability to handle large amounts of data while consuming a fraction of the electrical power and floor space required by other systems. Compared to a standard cluster, the Blue Gene achieves this scalability by reducing the speed of each processor, restricting the amount of memory per processor, and utilising a high-speed, but restrictive, processor communication network. The result is that less space is required and less heat is generated per processor, both of which form the fundamental physical constraints on the scalability of cluster based systems. Software for the Blue Gene has to adjust accordingly. The two critical facets are dealing with the reduced memory footprint per processor (which is about one quarter of the size considered normal for HPC systems), and complying with a single-object (no shared libraries) / single-threaded operating system.

The StgFEM framework facilitates a novel way to define finite element problems. The user's model is created by declaratively composing both the linear system to be solved and the finite element discretisation of the problem domain in a manner that can be described in the input file.

This level of granularity is chosen as it provides numerical mathematicians, material scientists and applied scientists with the right level of building blocks to develop their own algorithms and models, and to actively share them, whilst maintaining computational efficiency required for supercomputing. Moreover, researchers can develop their modules in 2D on an Apple iBook, knowing that they can they have proven scalability to deploy their problem in 3D on VPAC's own computational resources, or on possible future resources such as a Blue Gene.

For further information please feel free to contact Steve Quenette, Research & Development Manager CSD, [steve@vpac.org](mailto:steve@vpac.org).

# Summer Internships: Surf, Sand and Science

VPAC has recently announced the students and projects that will be forming the 2005/2006 Summer Internship Program. This year, the program will see the participation of 13 students working on 13 projects in fields including Computational Science, Computational Prototyping, Geospatial Science, Life Science and Grid Computing, making this round the largest to date.

The Summer Program employs high quality, niche-skilled students from Member Institutions including Deakin University, La Trobe University, Monash University, Swinburne University of Technology, RMIT University, The University of Melbourne and University of Ballarat, who are interested in science and advanced computing. VPAC, Member Institutions and students have the opportunity to participate in pilot projects, thereby promoting specific research areas and providing a basis for further research work. The program provides support for innovative research projects, and the results from these projects seed potential collaborative agreements between VPAC, Member Institutions and industry partners.

The Summer Internship Program is widely recognised for providing students with the opportunity to adopt new skills and industry experience prior to entering the workforce. The program also provides students with the opportunity to evaluate further study and provides excellent opportunities for students to continue ongoing employment with VPAC following completion of the internship.

This year, VPAC received over 180 applications from university students from across all Member Institutions. Out of these applications, forty students were short listed and interviewed with 13 students being selected for placements.

For further information regarding VPAC's Summer Internship Program or to view case studies from previous rounds, please visit [www.vpac.org](http://www.vpac.org) or email [info@vpac.org](mailto:info@vpac.org).

Project Title	Summer Intern	Project Overview
Multilevel and Longitudinal Statistical Analysis	Belinda May	<p>The project is basically to implement a fast C encoding of published algorithms for multilevel and longitudinal statistical analysis as a “plug-in” for the open source statistics package R. Ideally, the implementation would be parallel, and an extensible library. There are standard statistical benchmarks that the plug-in can be tested against. Multilevel statistical analysis applies when the data samples taken come from a hierarchy of distributions (e.g., a two-level hierarchy of State, and Hospital within state). There is an existing implementation of such statistical models, e.g., in the package gllamm for stata, but these are proprietary and slow.</p>
The Kidneyome project	Fransisca Kurnia	<p>The project is to develop an XML-based language (RenalML) to represent kidney physiology for the Kidneyome Project group’s commonwealth funded project, a project concerned with the development of an interactive, distributed web-based model of the mammalian kidney.</p>
Grid Enabled Life Science Applications	Lei Xing	<p>The project will involve grid enabling at least one Life Science application, NAMD. If time permits, another, possibly GAMESS or Amber will also be so treated. The underlying technology will be Java, Swing, Globus Toolkit and a reliance on the existing APAC Grid infrastructure which will provide NG2, certificates and gateways.</p>
The Grid Project	Panu Phinjaroenphan	<p>The Grid project will be focused on providing a useful tool in managing the APACGrid system. The APACGrid is an Australia wide project to provide user friendly compute and data facilities to a range of sciences while minimising the required computer skills from the end user.</p>
LSDb-in-a-box: Adding an XML import/export capability	Paras Jethawani	<p>The Genomic Disorders Research Centre and its collaborators within the Human Genome Variation Society are developing software and databases for the collection and dissemination of information about human mutation and disease. Crucial to the success of the system as a whole, is an ability to transfer information from one database resource to another. One component of this development is the Leiden Open-Source Variation Database software created by Johan den Dunnen in The Netherlands (<a href="http://www.dmd.nl/LOVD/">http://www.dmd.nl/LOVD/</a>).</p> <p>Other research communities have solved the data transfer problem by developing XML-DTD schema. This summer intern project involves two parts. The first is the extension of an existing markup language for biological sequence variation to satisfy the requirements of the GDRC. The second is to implement an import/export module for the LOVD software that uses this DTD.</p> <p>This project will add an important functionality to existing open-source software for single gene mutation databases.</p>

Project Title	Summer Intern	Project Overview
<p>ACCORD v2.0 Upgrade</p>	<p>Ujjavaal Suthar</p>	<p>Established in 1993, Cancer Trials Australia (CTA) is recognised as a leader in cancer clinical trial practice. The core business of CTA is to secure and administer cancer clinical trials for its member institutions. These clinical trials provide Victorian patients with access to cutting-edge cancer therapies. In order to remain competitive, CTA must have the ability to conduct clinical trials that maintain a high standard of quality, are carried out in a timely fashion, and at a competitive cost.</p> <p>The project will aim to upgrade ACCORD to v2.0 by implementing:</p> <ul style="list-style-type: none"> <li>- Revised data items and data types.</li> <li>- A comprehensive brain cancer data set.</li> <li>- A new front-end with improved functionality, user-friendliness, appearance; and searching, querying and reporting capabilities.</li> <li>- An improved interface with hospitals' PAS to more effectively identify new and returning patients.</li> <li>- The capacity to add or modify database fields.</li> <li>- Migrate existing Breast Disease Clinical Database (BDCCD) data into ACCORD and build appropriate front-end forms.</li> </ul>
<p>Surf Life Saving Hazard &amp; Incident Web Mapping</p>	<p>Angus MacAuly</p>	<p>This project is being developed in partnership with the Life Saving Victoria, and aims to develop a "proof of concept" Internet distributed mapping application to collect and report of spatialised hazard and incident information for Surf Life Saving organisations. The core emphasis of the project is to provide basic mapping &amp; GIS functionality to Life Saving Club volunteers using commodity computer hardware and services. The application service package will be developed using Open Source Software services for a low cost server-side solution with users accessing the service using generic web browser tools.</p>
<p>Wildfire Threat Modelling</p>	<p>Simon Flannery</p>	<p>This project is supported by the Country Fire Authority (CFA), and looks to increase the spatial resolution of current model generation from a 1km grid to a 20m grid. Computational resources to complete such an exercise are a principal limitation. The focus of this project, therefore, is the robust deployment of this modelling tool in a HPC environment. Supplementary to this, a feasibility study for the parallel deployment of CFA stochastic fire propagation model for each 20m cell in the whole state.</p>
<p>Multi-scale Metal Forming</p>	<p>Mitzi McCarthy</p>	<p>Peter Hodgson's advanced materials research group is actively researching in multi scale phenomena of metals to better understand the influences of manufacture on structures, such as automotive parts. Material point methods, for example the PIC integration scheme, to finite elements are a popular method for discretising simulations in this field. More recent efforts has begun to perform the constitutive update at critical areas in the simulation, with a representative volume. This project is to leverage on the StGermain? to PICellator developments of VPAC's CSD and of Monash's MC2, to provide the Deakin group with their own representative volume development framework.</p>

Project Title	Summer Intern	Project Overview
StgFEM-Composer	Kent Humphries	<p>The VPAC StgFEM software facilitates a framework for building finite element applications by means of a component-based architecture. What makes StgFEM novel is in the chosen abstractions for these components; a user (developer) composes the discretisation, the systems of equations and fields required for the model. This can presently be done by explicitly coding, scripting or describing in XML how these components interact to create the numerical basis for a model. What is missing is the ability to compose via a user-friendly tool and to take existing compositions and view them. Such a tool would be similar to OpenDX's network map and the Common Component Architecture's Ccaffeine GUI. This capability would provide for users at the "scientist / engineer" end of the spectrum an adequate representation of models such that they can also readily partake in "model changes".</p> <p>This project aims to develop the ability for any StGermain component to partake in a network diagram Component maps for existing models (benchmarks and production codes).</p>
Service Oriented Architecture for Multi-Disciplinary Optimisation	Rohan Borse	<p>Multi-disciplinary optimisation is an advanced use of CAE for exploring the functional performance space of parametric models of components or assemblies. Typically, a large number of points in the parameter space are evaluated for two or more disciplines per point. CfCP-VPAC has developed an end-to-end MDO capability. The purpose of this project is to explore the feasibility of using a SOA to enable the creation of flexible, maintainable and rapidly configurable MDO based services.</p>
Parametric Modelling using Open Source Geometry Engine (Open Cascade)	Chris Zeng	<p>The ability to build and manage the structure of parametric models is critical in advanced CAE applications. Building a parametric model is not just like building a software function with parameters. A better analogy is building a software API. The architecture of the API is critical and clear interfaces hide implementation of lower level functions. The same principles need to be applied to building a parametric model for advanced CAE or MDO.</p> <p>Current approaches have shown to be non-robust. This is due to inadequate management of when and how detailed dependencies are introduced. This project aims to show that Open Cascade can be used as a foundation for building robust parametric models. The results of this project can be directly linked with the MDO work at the CfCP.</p>
An Investigation of Real-time Visualisation Technologies for Collaborative Decision Making	Binh Nguyen	<p>This project will explore commodity based collaborative visualisation, comparing the "distributed model" and "remote rendering" paradigms. It will utilise two demonstrator projects in the fields of Automotive Design and Emergency Services Decision Support to highlight the benefits and shortcomings of these contemporary methodologies.</p>



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. Courses are held at the VPAC Training Room.

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)

## On-Site Training

VPAC also runs a number of on-site training courses throughout the year, on request by Member Institutions. Members are welcome to request an onsite-training course by contacting Leena on +61 3 9925 4645 or [leena@vpac.org](mailto:leena@vpac.org).

### 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.

### 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 Annual Report 2004/2005

The VPAC 2004/2005 Annual Report is now available online at [www.vpac.org](http://www.vpac.org). The report outlines VPAC's strategic objectives over the past financial year and the year to come and covers VPAC's projects and systems operations for the 2004/2005 financial year.

The report is also available in hard copy or on an interactive CD, where some of VPAC's major projects are showcased as animations and movies, such as a simulation of the Immersive Visualisation of Smoke Plume Dispersion in the Melbourne Docklands Area or a simulation of the Hepatitis B Core Viral Capsid Protein modelled in conjunction with VIDRL. To request a free copy, please contact Maria on +61 3 9925 4645 or [maria@vpac.org](mailto:maria@vpac.org).

### e-Research Brochure

VPAC has released a new e-Research brochure, highlighting some of the dozens of the major e-Research projects currently in progress at VPAC and its Member Institutions. The brochure showcases work done in collaboration with Bio21, for example, developing and implementing the Bio21 Molecular Medicine Informatics Model and the work conducted on Deakin University's Victorian Marine Habitat Mapping project. To view the brochure and learn more about these and other e-Research projects, visit [www.vpac.org](http://www.vpac.org) or contact Maria on +61 3 9925 4645 or [maria@vpac.org](mailto:maria@vpac.org) to order a copy.



## Want to Hear More?

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 utilising advanced computing tools. For article submissions or comments please contact Maria Kambourakis on +61 3 9925 4630 or email [maria@vpac.org](mailto:maria@vpac.org).

If you are a Member of VPAC and would like to have your project promoted through the VPAC News Magazine as part of VPAC's Project Promotion Scheme, please contact Maria on +61 3 9925 4630 or [maria@vpac.org](mailto:maria@vpac.org).

# Victorian Advanced Computing Association

Promoting Advanced Computing throughout Victoria free lecture series

## THE VACA KEYNOTE SPEAKER PROGRAM

VACA is association proudly sponsored by VPAC and 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.

Some of this year's events have included a seminar on Multi-scale Models and Emergence of Function in the Kidney Medulla: Difficulties Technical and Conceptual, by the world renowned researcher, Dr S. Randall Thomas, Director of Research, CNRS and a workshop and subsequent seminar on Nimrod and Applications Development for Computational Grid by Monash University's Professor David Abramson.

Visit [www.vpac.org/vaca](http://www.vpac.org/vaca) for more information on past events and to keep up to date with future seminars.

## FREE 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 click 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.

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