

WHAT'S HAPPENING IN  
HPC IN VICTORIA  
No4 AUGUST 2004

# VPAC NEWS



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# Message from the CEO

## New Corporate Structure

VPAC is a unique organization, having few parallels in Australia or even internationally. Over the past year, there have been some changes made to the organisation that will enable VPAC to deliver our company objectives, better support our Member Universities and industry and remain one of Australia's leading advanced computing organisations.

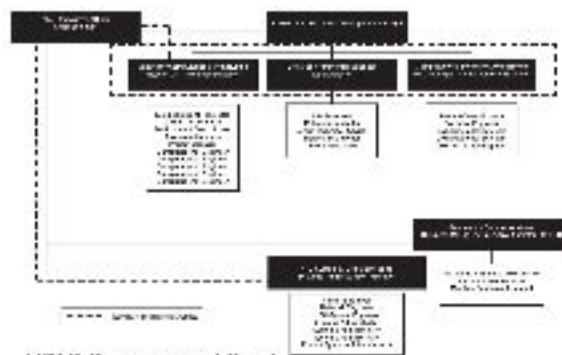
Since its founding four years ago, VPAC has grown to over forty staff and an annual budget of over \$5M from industry, Member subscriptions, and government grants. That growth is projected to continue, calling for an organizational restructure to avoid running into common risks associated with a rapid corporate growth rate. VPAC has been broken up into independent strategic business units, each of which has its own budget and business plan. The three corporate business units are:

- The Center for Computational Prototyping (CfCP);
- Computational Software Development (CSD) and;
- Life and Environmental Sciences (LES), incorporating both the Life Science team and the Environmental Science and Geographic Information Systems (EGIS) Team.

In addition, the HPC Facility is run as another formal business unit. Each business unit is an accountable/self-sufficient/independent operation, with the exception of the HPC Facility, which primarily provides "cycles and support" for Member University researchers. Since VPAC is not a public company, its profits are not paid back directly as dividends to its Member Universities (shareholders). Instead, VPAC's "profits" are used to improve the HPC Facility and to fund R&D support programs for Members, such as the VPAC Expertise program.

On the operational side of things, VPAC is gradually growing its commercial business to diversify our funding base and staff expertise. Such diversity improves VPAC's long-term sustainability, but more importantly, improves the level of service and support that VPAC can provide to Member university staff, companies, government, and other organizations.

VPAC is also focusing on maintaining a staff base that is comprised of some of the industry's most highly regarded experts in their fields. Having in-house staff who are expert computational scientists does set up the potential for competition with Member universities and others. VPAC recognizes this potential and is managing the risk in two ways. Firstly, VPAC will continue to build partnerships and collaborative ventures with Member staff and research centres, turning any potential competition into collaboration. Secondly, VPAC does not undertake any independent or pure research, unlike Member Universities. Instead, VPAC remains an R&D service provider for Member Universities and other organizations.



Professor Bill Appelbe, VPAC CEO

# Special News Flash

## Registered Research Agency Approval

### RRA Approval Granted

It is with great pleasure that VPAC announce our recent approval as an official registered Research Agency (Reg No. 40150). Currently, the following classes of research and development activities have been approved, however, VPAC are endeavoring to obtain approval for a further four classification areas.

#### Approved Classes of Research:

Genetics, Molecular Biology and Biotechnology  
Geophysics  
Computer Software  
Aerospace Technologies and Engineering  
Manufacturing and Process Technologies and Engineering  
Mechanical and Industrial Engineering

#### What is a Registered Research Agency?

A Registered Research Agency (RRA) is an organisation approved by the Industry Research and Development Board that is capable of carrying out contracted Australian R&D, in one or more classes of activity, on behalf of eligible companies, or through collaborative arrangements for a group of companies.

#### What are the advantages for VPAC Members?

The advantages that VPAC can now offer to companies as an RRA is:

-Expenditure for Australian R&D work contracted to an RRA (now VPAC), within approved classes of activity (see above), is eligible for the full 150% tax deduction in the year of income, irrespective of the annual R&D expenditure of the claimant. The normal annual expenditure threshold of \$20K does not apply, and prepayments for contracted Australian R&D may be claimed by companies up to 12 months in advance of the work being carried out. Obviously clients will need to be Taxpaying bodies.

-VPAC will need to ensure that client companies are aware of the eligibility, registration and contractual requirements described in guidelines that will be distributed to each Department Manager governing the operation of the RRA. The contractual arrangements specify the requirement to maintain, and make available, records of contract work undertaken through the program. Failure to comply may result in the ATO disallowing claims for the 125% tax concession made by client companies.

For more information regarding VPAC's approval as a Registered Research Agency and the effect on your organisation contact Karen Iatrou on 03 9925 4734 or email at karen@vpac.org.

# Press Release

## VPAC Partners with plm

### VPAC Forms Collaboration with Software Provider plm

VPAC's Centre for Computational Prototyping (CfCP) and Product Life Cycle Management (Australasia) Pty Ltd (plm) are pleased to announce a formal collaboration to bring leading-edge engineering solutions to academia and industry.

plm will contribute the latest in engineering software which will enable the collaboration to drive advanced research and development and industry solutions using the world class NX software range (including CAD, visualisation and CAE technology). The CfCP will bring software application and integration experience as well as HPC and visualisation infrastructure. Together CfCP and plm will be able to bring joint services to the engineering industry based on the strengths of each organisation.

*Chris Seeling – Head of CfCP said, "The relationship with plm brings the CfCP a key step closer to realising our Virtual Integrated Design Environments (VIDE™) vision. We are very excited at the prospect of working closer with PLM as well as our other technology partners to help the Australian industry compete on a global level."*

*Dennis Colusso – Director of Marketing and Consulting at plm, added "the relation between plm and CfCP leverages complementary skills to provide comprehensive CAE modelling and simulation capabilities on an advanced computing platform."*

For more information regarding the VPAC plm collaboration please contact Jon Carroll – Associate Manager CfCP on 03 9647 5434 or email at [jon@vpac.org](mailto:jon@vpac.org).



# APAC Partnership and the Grid

VPAC is a partner of the Australian Partnership for Advanced Computing (APAC). Through APAC, VPAC has access to and contributes to the APAC National Facility, are involved in building the APAC Grid and participates in the APAC education, outreach and training activities.

APAC is a national partnership committed to providing an advanced computing and grid infrastructure for the Australian research community. APAC is supported by a grant from the Australian Government through the Department of Education, Science and Training.

VPAC will be receiving \$2.565M over 3 years from APAC for its continued participation in the following programs:

-Computational Tools and Techniques, aimed at improving the software development environments for users of advanced computational systems. The kinds of projects anticipated include:

- Tools to improve the performance and parallelization of codes.
- Mechanisms for checkpoint/restart and increased robustness of codes.
- Management of large scale parallel jobs.
- Porting and optimising heavily used applications with algorithm development where appropriate.
- Libraries for mesh generation and solvers.
- Tools for computational steering and visualisation.

-Education, Outreach and Training aimed at significantly increasing the skills of users and potential users of advanced computing and grid facilities. The program will cover three areas:

- Education and Training Courses in Computational Engineering and Life Sciences available both online and through face-to-face delivery, including over the Access-grid, and

- on-line, interactive learning materials for these courses and,
- on-line case studies for these courses to be built up into an organized online website or repository.

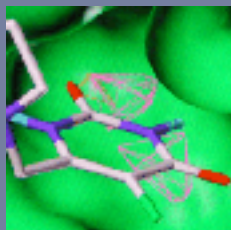
-APAC Grid Projects

- To build specific infrastructure and application tools related to Grid Computing; and
- To develop grid architecture, software and services to support users of the APAC and partner (VPAC) facilities.

The APAC Grid is an Australia-wide project that aims to establish an efficient working Grid servicing, initially, Australian Researchers. VPAC is a leading player in this major project and is responsible for delivering the Compute Infrastructure component. This project is initially concentrating on academic users but will ultimately offer massive advantages to all technical computing users around the country.

The APAC Grid will provide seamless infrastructure to link computing facilities at APAC members' sites to provide researchers with access to compute capacity, storage and related systems without needing an extensive knowledge of the underlying technology.

To learn more about the APAC Grid contact David Bannon on 03 9925 4733 or email [david@vpac.org](mailto:david@vpac.org). To learn about the Education, Outreach and Training programs contact Bill Appelbe on 03 9925 4648 or email [bill@vpac.org](mailto:bill@vpac.org). To get more information on the Computational Tools and Techniques projects contact Steve Quenette on 03 9925 4726 or email [steve@vpac.org](mailto:steve@vpac.org).



### Advanced Scientific Software Tools for the Australian Life Science Research Community

VPAC, in partnership with the Victorian Bioinformatics Consortium (VBC) and in collaboration with best of breed software vendors such as Tripos, Accelrys and LionBioscience and hardware vendors IBM and HP, has developed an advanced life science research resource aimed at bringing the Australian Life Science Community to the forefront of R&D advancements. The resource, called the "BioPlatform", is a collection of advanced, high performance and cutting-edge software and hardware life science tools designed by the world's leading vendors. The BioPlatform places advanced research capabilities into the hands of Australian research organisations and aims to enhance the international competitiveness of the Australian research industry.

The BioPlatform supports the VBC and other partner organisations and has been developed to provide small to medium Australian research organisations easy and cost effective access to advanced life science research tools.

The Australian life science community benefits from lower research development costs and shorter R&D time frames and cycles, VPAC facilitated training and support and technology diffusion enhancing the international competitiveness of our research organisations.

Some of the advanced software research tools available through the VPAC BioPlatform include:

- Tripos Discovery Software
- Lion Bioscience Software
- Accelrys Materials Studio and Discovery Studio
- Schrödinger Software
- IBM Discovery Link Solutions
- Bio -Mirror - APAC

VPAC are proud to announce that in collaboration with BioMelbourne Network and IBM we will be officially launching the BioPlatform in the format of an early evening cocktails event. The event will host a variety of keynote speakers who are experts in the field of advanced life science research and will also pose as an excellent networking event. Keep an eye out on the VPAC website at [www.vpac.org](http://www.vpac.org) and the BioMelbourne Network website at [www.biomelbourne.org](http://www.biomelbourne.org) for more information on the official launch. To subscribe to our launch mailing list, please email [maria@vpac.org](mailto:maria@vpac.org) and type *BioPlatform Launch Mailing List* in the subject title box.

Access to the BioPlatform is easy and cost effective and is based on an initial proof of concept scheme. For further information regarding accessing this powerful research tool, please contact Bill Yeadon on 03 9925 4719 or email at [b.yeadon@vpac.org](mailto:b.yeadon@vpac.org), or visit the VPAC website at [www.vpac.org](http://www.vpac.org).

Over the past few months the Life Science (LS) Team has been involved with projects in Large Scale Bioinformatics, Medical Informatics and Molecular Modelling solutions. VPAC is currently working with the Victorian Infectious Diseases Reference Laboratory (VIDRL) developing computational models of evolving drug resistance to Human Immunodeficiency Virus (HIV) protease inhibitors. Current anti-HIV drugs are becoming less effective with the rise of resistant HIV strains, leaving less treatment options available. It is hoped that greater understanding of HIV resistance mechanisms can lead to optimized patient treatment regimes.

The VPAC LS team is also working with the Department of Primary Industries (DPI) on an Advanced Computing Project that will support large-scale genomic data analysis and pipelining of this analysis with in-house and public genomic data.

VPAC is also involved in implementing a state of the art clinical informatics project, bringing together the major hospital groups in Melbourne. VPAC has identified a gap in the industry in terms of skilled expertise in the area of Medical Informatics and plans to get more involved in this area with a focus on integrating clinical data.

In July, Dr Mike Kuipers, Molecular Modeller, represented VPAC at the ninth Molecular Modelling 2004 conference in Sydney, a combined meeting of the biomolecular Chemistry division of the RACI, (Royal Australian Chemical Institute) and MGMS (Molecular Graphics Modelling Society).

Australian and International speakers presented a variety of current molecular modelling topics, including advances in protein modelling, quantum mechanics/molecular mechanic (QM/MM) methods, and large scale molecular dynamics simulations. The breadth of work presented highlighted the impact of high performance computing in chemical simulations with ever larger and more complicated systems being modeled to higher levels of accuracy. Of particular interest was the implementation of QM/MM methods, whereby large protein systems with catalytic active sites or photosynthetic centers are modeled with high levels of quantum theory, while outlying regions of the protein complex are modeled with computationally cheaper molecular mechanics. These methods provide additional insight into protein mechanisms than previously possible with molecular mechanical methods alone. Some of these simulations required tens of thousands of CPU hours to complete and future work will undoubtedly use order of magnitudes more, again highlighting the ever-increasing need for high performance computing centers in Australia, such as APAC, VPAC and AP3.

In September, the VPAC Life Science team will, in association with the VBC, officially launch its advanced computational BioPlatform incorporating a supercomputing infrastructure and a growing range of advanced computational life science hardware and software products, support services and expertise in scientific programming. This will increase the international competitiveness of Victorian companies and research organisations involved in molecular biology and drug development research (see feature article).

For more information on VPAC Life Science projects please contact Bill Yeadon on 03 9925 4719 or email [b.yeadon@vpac.org](mailto:b.yeadon@vpac.org).

# Molecular Modelling Studies of HIV Protease Drug Resistance

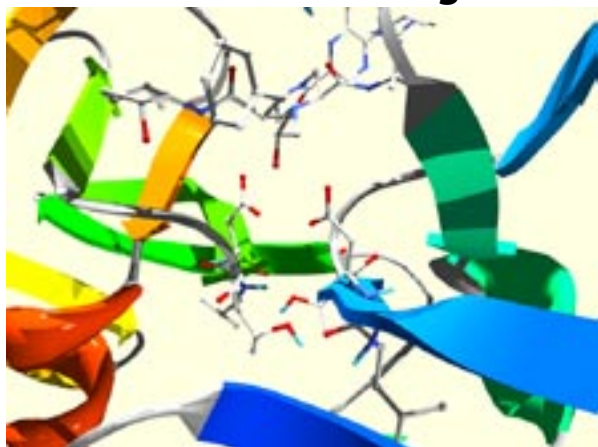


Figure 1 HIV protease with inhibitor

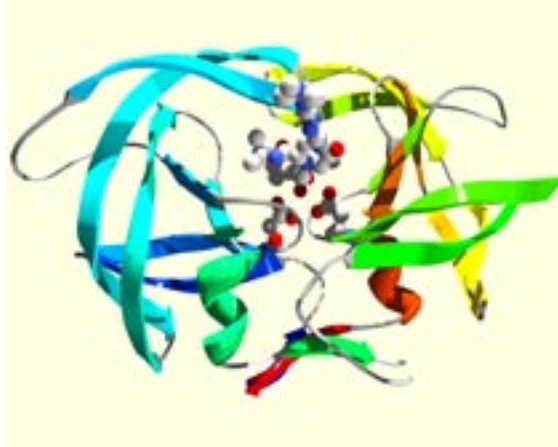


Figure 2 Active site of HIV protease

**Collaborators:** Dr Chris Birch, Victorian Infectious Diseases Reference Laboratory, (VIDRL)  
Dr. David Chalmers, Victorian College of Pharmacy (VCP).

## Objective:

To understand the effects of resistance mutations on the human immunodeficiency virus (HIV) protease specific drugs on the structure of this enzyme, and use this information to aid in drug choices for patients currently undergoing HIV therapy.

## Background:

More than 40 million people were infected with HIV at the end of 2003, according to data supplied by the World Health Organization, and many of these individuals had already progressed to full-blown AIDS. Antiviral drugs are available to only a small proportion of those infected, in most cases people living in developed countries. These drugs have, to some extent, changed HIV infection from a uniformly fatal disease to a chronic infection. The requirement for their lifelong use, however, results in adverse side effects and the emergence of drug resistance virus in many patients. Once resistance develops, a change in drug therapy is required to maintain an appropriate virological and immunological response. This may be problematic because the generation of cross-resistance within the drug classes used to treat HIV infection is common. HIV protease, an essential enzyme required for the replication of HIV in host cells, is one of the key targets of current drug therapies. Depending on the type of drug used in treatment, one or more amino acid mutations can occur in the protein structure of the HIV protease, conferring resistance to that drug and cross-resistance to other protease-directed drugs. By modelling these mutations and understanding their mechanisms it is hoped that drug therapies can be better tailored to patients with drug resistant HIV strains.

## Method:

The solved crystal structure of HIV protease was used as a starting model for molecular minimization and dynamics simulations (PDB code 2BPY). After adding approximately 7,000 water molecules and minimizing the system, multi-nanosecond simulations of the wild type and mutant HIV protease were run using NAMD\* 2.5 at VPAC. Each simulation typically used 8 processors and ran for about 7 days or about 1400 CPU hours.

Analysis of the dynamics simulations using VMD\*\* revealed certain mutations increased instability at the active site, possibly contributing to weakening the affinity for the protease drugs. Other modelled mutations sites presented clear steric hindrance for certain protease inhibitors such as glycine 48 to valine giving resistance to Saquinavir.

## Outcomes:

Our dynamics simulations have identified mutations responsible for HIV protease dimer stability, which along with active site mutations, are implicated in reduced drug affinity. Verification is hoped to be gained with experimental work, providing more insight into resistance mechanisms and eventual implementation into the design of more effective drug regimes for the treatment of HIV.

\* NAMD Laxmikant Kalé, Robert Skeel, Milind Bhandarkar, Robert Brunner, Attila Gursoy, Neal Krawetz, James Phillips, Aritomo Shinozaki, Krishnan Varadarajan, and Klaus Schulten. NAMD2: Greater scalability for parallel molecular dynamics. *Journal of Computational Physics*, 151:283-312, 1999.

\*\* VMD Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", *J. Molec. Graphics*, 1996, vol. 14, pp. 33-38.



# Environmental Science and Geographic Information Systems News



The Environmental Science and Geographic Information Systems (EGIS) team at VPAC has grown significantly during the past year due to the growing demand for advanced computing services for the analysis and visualisation of large volumes of Spatial Information.

Marcus Reston heads this team with support from Shoaib Burq, Roger Ting and more recently Carly Lambert. This team has a wide range of experience and expertise in Remote Sensing, Geographic Information Systems, Geomatics and Earth Sciences. The supercomputing and extensive software platform maintained by VPAC offers a significant resource for organisations wishing to analyse and visualise large data sets for a wide range of Geospatial applications.

The team's primary focus has been working with the Departments of Primary Industries & Sustainability & Environment in the migration of a variety of resource intensive software applications from desktop workstations to the newly commissioned DPI/DSE supercomputing installation located at the DPI regional centre at Bendigo.

Additionally, VPAC is developing a spatial information mapping project in partnership with the Land Information Group and the CRC for Spatial Information to monitor and model Victoria's public and private water resources using temporally refreshed high resolution satellite imagery.

Base data generated by this project may also be repurposed to extract information regarding other topical environmental issues such as crop health & vigour, soil salinity, and soil erosion for both government and rural communities.

More recently VPAC has commenced working with the Bureau of Emergency Services Telecommunications group in collaboration with RMIT's Interactive Information Institute (I-Cubed) in developing new capabilities to use Real-Time positional information for search and rescue planning, monitoring and debriefing. This technology is also under investigation in association with the Country Fire Authority using Global Positioning Technology (GPS) linked with GIS databases to improve positional accuracy of moving fire fronts and proximity to available water resources under emergency situations.

This collaborative work with RMIT's I-Cubed is now extending into the use of GIS and GPS technologies to develop more effective tools for the Victoria Police for criminal investigations, coronial inquiries and crime prevention. (*HyMap imagery courtesy of HyVista Corporation*). For more information on EGIS projects please contact Marcus Reston on 03 9925 4905 or email at [marcus@vpac.org](mailto:marcus@vpac.org).

# Computational Software Development News

Earlier this year, VPAC's software development research team was renamed the Computational Software Development (CSD) group. Over the past year, the CSD Group has continued to work on a variety of Australia-based and international projects. The group has also been strengthening its collaborations with international research groups, including the PETSc Group at Argonne National Labs in the United States, visited by CSD computational scientist Luke Hodgkinson as part of a three-month intern program.

In Australia, *St Germain* is a VPAC developed open-source framework for developing computational codes and provides an environment that supports extensibility, a feature that is somewhat absent in scientific codes. The framework is proving extremely fruitful, forming the basis of both Snark and Snac (see below), and being science neutral, is under consideration for other projects.

*Snark*, VPAC'S collaborative project with Monash Cluster Computing, is another of CSD's Australia-based projects. Snark is a software framework for 3D Particle-In-Cell geodynamic modelling, but the larger context of the project is a continual process of developing and deploying the numerical and computational techniques to allow researchers to explore new ideas in their research.

The focus of the team for the next few months will be on producing a fully documented release of Snark to allow new user groups to make use of our technology, and implementing a Multigrid solver to allow tackling of much higher resolution problems.

The CSD team has also been working closely with ACcess, the Australian Computational Earth Systems Simulator, on the Australia-based SPMoel project. SPMoel is an extensible framework for building fluvial erosion applications, customisations and extensions. The SPMoel has many important applications, from modelling large-scale interactions with tectonic processes to modelling why particular catchment basins evolved in a particular manner and how they might change in the future.

## International (GeoFramework) projects

GeoFramework is an NSF ITR-funded effort to develop a suit of tools to model multi-scale, multi-physics deformation for Earth science problems. It is a collaborative project between Caltech's Centre For Advanced Computational Research (CACR), Geology and Planetary Sciences (GPS) and VPAC.

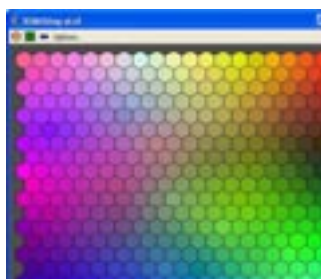
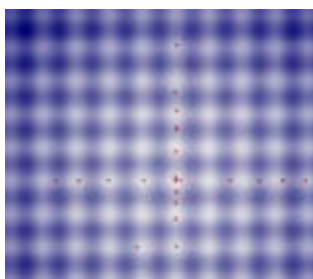
*Snac*, a key CSD project, is a completely new code based off Poliakov's FLAC algorithm in 3D. Being lagrangian and explicit (amongst other things), Snac is suited to region- scale crustal deformation modelling, that is, it models mountain building, plate subduction, plumes, rifts and so on. Snac is currently parallel, 3D Cartesian and spherical, with elastic, plastic, viscoelastic and temperature plug-ins. The remesher is near complete.

## Generic Mapping Tools status

A new collaboration with the GeoFramework team began in March this year, when Patrick Sunter, CSD's project leader, spent three months at California Institute of Technology working on adding an interface between GeoFramework and Genetic Mapping Tools (GMT). GMT is a very widely used toolkit for plotting and data projections, particularly in the Geosciences. With this new project, GMT should become much more accessible to new users through a Python scripting interface and more readily available to visualise other GeoFramework software. Patrick has completed a first-cut version with interfaces to the core GMT functionality, and will be continuing to work with the GeoFramework team to improve it.

To learn more about the above projects and all our other news, head to the CSD homepage at <http://csd.vpac.org>.

## Interactive Inversion Software for Geoscience



**Student:** Tim Robinson **Discipline:** Geoscience

**Supervisor(s):** Patrick Sunter, VPAC, Steve Quenette, VPAC

### Research Objective

The aim of this project was to work with the Nimrod/O development team to develop a prototype interactive inversion front end to the Snark/Underworld (VPAC/Monash Cluster Computing) Geoscience finite element/particle-in-cell software package. This was achieved by implementing an evolutionary algorithm that works within the Nimrod/O framework and the creation of a self-organising maps generator/viewer to aid in visual analysis of the results.

### Motivation / Significance

With the advent of the modern supercomputer, it has become possible to perform quite sophisticated geological forward modelling experiments. Frequently there is a need to work in the other direction, however. The sort of problems a geoscientist commonly deals with is to seek the set of material properties and initial conditions that lead to a modern day geological formation. This is a more complicated problem requiring successive trial and error methods. Since the forward modelling processes are quite computationally expensive, an efficient way of searching through the parameter space is required. This process of optimising the search for an answer is called inversion. One approach to inversion that has been used extensively in many fields is to employ an evolutionary algorithm. Evolutionary algorithms mimic the natural process of evolution by combining properties of good 'parent' solutions to produce 'child' solutions with more refined properties. In this way, an initially random population of potential solutions evolves toward an optimal solution. The use of genetic algorithms requires an evaluation of 'fitness' of a particular solution, which in the case of geological modelling is often very difficult to quantify. For this reason, it has become necessary to develop methods of interactive inversion. Rather than trying to get a computer to rank a population of solutions, which may be difficult or infeasible, the expertise of a geoscientist is introduced into the loop by allowing them to visualise the potential solutions and rank them. This leads to far more efficient searches for an optimal solution.

### Results

The main results of this project are an extension to the Nimrod/O code in the form of a genetic algorithm and a stand-alone self-organising maps generator/viewer both of which are to be integrated into the Nimrod/OI web portal for use in interactive inversion.

The self-organising maps package allows for generation and viewing of hexagonal and square SOMs with the option of including distance nodes.

### Discussion

With the use of the genetic algorithm and the SOM package, the existing Snark software can now be used within the Nimrod/OI framework to perform inversion experiments. This should allow a geoscientist with minimal computing skill to use this software to search large parameter spaces for initial conditions and material properties that have led to existing geological formations. This is a natural step forward in geological modelling and will hopefully lead to many new and exciting discoveries.

### Conclusion

The initial testing, done locally, has been very positive. The software is now at the stage where it can be fully integrated into the Nimrod/OI environment and further testing can be conducted. If the software performs well with these tests then it will be trialled on a 'real-world' problem. This promises to be an exciting new development in both geological modelling and optimisation in general.

# CENTRE FOR COMPUTATIONAL PROTOTYPING NEWS UPDATE

## **The Centre for Computational Prototyping (CfCP) Turns 1 Year Old.**

The CfCP has just had its first birthday and what a year it has been. The CfCP was developed as part of VPAC's charter to provide Engineering, IT, academic and R&D services to the automotive industry. Currently, the CfCP has formed close collaborative relationships with many Automotive partners and the team has been successful in evaluating and designing new computational engineering processes through proof of concept projects. Automotive OEM's and suppliers, as well as Higher Education Institutions (through the Summer and Winter Internship programs) and technology vendors, have benefited from the work completed by the CfCP. Aerospace organisations have also begun to show strong interest in the work of the CfCP with several projects underway and some completed.

The CfCP continues to encourage cross industry collaboration by inviting key industry partners to join in collaborative environments such as the Cooperative Research Centre for Advanced Automotive Technologies (Auto-CRC) and the Virtual Engineering Forum. The CfCP has made significant contributions to the Auto-CRC, encouraging Aerospace and technology partners to participate. The CRC has now completed stage two of the CRC Selection process with CfCP and VPAC represented on the executive committee and chairing the sub-committee for Virtual Engineering and Design.

## **Virtual Engineering Forum**

The Virtual Engineering (V.E.) Forum is a joint initiative between VPAC and Holden Innovation and was inaugurated via a breakfast meeting in March 2004 in Port Melbourne. The goal of the V.E. Forum is to advance the international competitiveness of the Manufacturing and Engineering sector in Australia through innovation and collaboration. Members of the forum range from across a number of key manufacturing companies, universities, government and research organisations. The forum has met on two occasions since March 2004. The forum aims to foster collaborative R&D projects as well as exchange experience through means such as case studies, pilot projects and presentations on VE and Virtual Manufacturing.

In the past two forums both Holden and VPAC (CfCP) have presented on the future of Virtual Engineering and what place it has in design and manufacturing. It was during CfCP's keynote speech that the vision of Virtual Integrated Design Environments (VIDE) was launched.

The third meeting is scheduled for 3rd of August with guest speaker Dr Nemes from CSIRO (CMIT) who will be presenting on "Manufacturing Sector Outlook for Australia".

Should you wish to find out more information about the forum please visit the website [www.vpac.org/veforum](http://www.vpac.org/veforum) or contact Dr Thomas Ting, the VE Forum Web Site Moderator on 96475431 or [thomas@vpac.org](mailto:thomas@vpac.org).

# CENTRE FOR COMPUTATIONAL PROTOTYPING NEWS UPDATE continued

## Virtual Integrated Design Environments

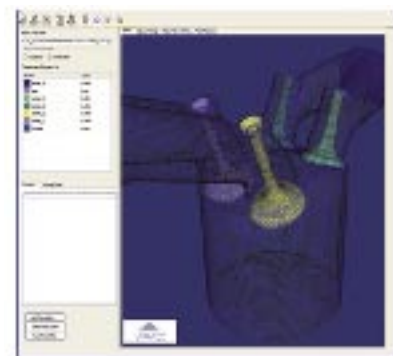
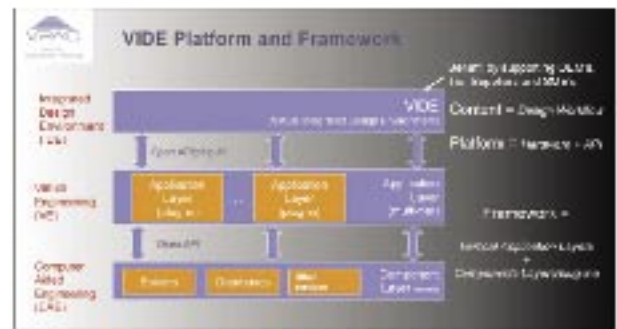
The rationale of VIDE is to use advanced computational and visualization tools to implement rapid lean design and simulation for new product development and processes linked with advanced technology validation and testing tools.

The design environments of today are highly heterogeneous, and these environments lack integration of the different functions and data streams that need to be applied in order to drive product development efforts from market need - to concept - to manufacture, and even to after market service. Indeed the organization and implementation of today's design environments are subverted by such tool chains due to lack of resource and simulation sharing mechanisms. This leads to loss of competitiveness from the resulting blow out in development time, rework and other manufacturability-related areas.

VIDE is a new paradigm that not only seeks to address these barriers but also points to a path of development and adoption. Such a path is important since Australian OEM's and large tier suppliers are crying out for a new solution. The CfCP believes that VIDE can deliver on this need.

Early demonstrators of VIDE technology have reduced development times by up to 80% to 90%.

The diagram below shows the framework for VIDE. VIDE development proceeds in a top-down manner by focusing on the design process rather than the functionality of individual tools (e.g. CAE).



An early VIDE Demonstrator

For more information regarding the VIDE concept please contact:

-For technical enquiries Chris Seeling at [chs@vpac.org](mailto:chs@vpac.org)

-For business enquiries Jon Carroll at [jon@vpac.org](mailto:jon@vpac.org).

# Conceptual design tool chain for branched network turbulent flow



**Student:** Stephen Dibb **Discipline:** Engineering  
**Supervisors:** Chris Seeling, VPAC, Jarrod Sinclair, VPAC

## Research Objective

The project aims to research the development of a tool chain for the conceptual design of branched networks containing turbulent flow conditions. The tool chain will streamline prototyping of possible network configurations by linking CAD (Unigraphics), meshing (Gambit) and CFD (Fluent) elements. This project was conducted solely as a VPAC CfCP project, however, on completion the tool chain would have potential application to several contracted industry projects.

## Motivation / Significance

The tool chain was originally conceived as a packaging together of software elements, such as CAD and CFD, commonly used in the conceptual design phase of turbulent flow branched networks (such as pneumatic pipe systems). By forming these elements into a single package operated through a single GUI, the design process can be accelerated through automation of normally repetitive tasks such as the forming of volumetric geometry from altered centreline paths.

Further, by embedding engineering knowledge into the tool chain the need for the operator of the tool chain to possess specialist knowledge in fluid flows, CAD and CFD operation knowledge can – to some degree, and with appropriate caution – reduced or eliminated. These two results of reduced time and user knowledge required would, in an industrial context, allow resources to be more efficiently employed on other more complex tasks, thus saving money and improving product performance.

Further significance is added to the development of such a tool chain as currently the only similar packages readily available operate much less sophisticated elements. As well as providing the full range of functionality, the use of sophisticated elements will also allow the conceptual tool chain files to be enhanced and updated, rather than entirely new models created as with a less sophisticated conceptual design package.

## Conclusion

The investigations completed in this project have found that all the elements are in place for production of an efficient and accurate tool chain for pipe network flow simulation. By using the geometric construction abilities of Unigraphics, an unstructured mesh tailored to optimise the Fluent wall functions and the k- $\epsilon$  viscosity model turbulent pipe flow can be simulated to a level of accuracy more than sufficient for the conceptual design phase. Further, it was found that by simplifying the mesh and solver settings (using the Spalart-Allmaras viscosity model) a rapid simulation could be run that, whilst lacking absolute accuracy, was capable of accurately ranking (in terms of pressure loss) various different pipe configurations. Thus, the final tool chain can be constructed from elements now well understood from the investigations of this project.

# FACILITIES UPGRADE *goodbye* Grendel

One could be forgiven for thinking the team at VPAC would be sad to see the shutdown of one of our oldest, most loyal members, our 3 ½ year old Alpha Server, Grendel. On the contrary! We at VPAC are buzzing with excitement with the knowledge that within the next 3-6 months we will be saying Goodbye Grendel. You may think us insensitive but the truth is our sadness to see Grendel go has been overtaken by feelings of anticipation and excitement over the up and coming adoption of a brand new, state of the art HPC machine.

Although it is too early to specify with any certainty the exact machine model VPAC will be purchasing, it is safe to say that the machine will certainly be running on a 64-bit platform, allowing for faster processing time for some applications and a larger memory store. The machine will also most likely run Linux, due to consumer demand and, of course, be cluster-based. The machine is also likely to feature a fast central switch and may contain Itanium, Opteron or Power chips.

The upgrade is aimed at improving the performance of VPAC's HPC infrastructure for all our Members, Partners and Users and will allow for the improved running of the advanced software packages available through VPAC, including VPAC's BioPlatform.

At present, Grendel contributes only 20% of VPAC's total CPU hours. VPAC, however, is aware that Grendel does cater to a number of users with specific needs and for this reason is working diligently with those users to move their application to Brecca or, if their need is 64-bit, to our 32CPU Opteron cluster.

## **What's next for Grendel?**

VPAC is interested in hearing proposals from our members on how to use the existing Grendel components in alternative value added schemes. Alternatively, our hardware vendors may offer to buy back certain components of Grendel.

VPAC always welcome user input into matters concerning our facility upgrades. Please feel free to phone David Bannon, the Systems Manager on 03 9925 4733 or email on [D.Bannon@vpac.org](mailto:D.Bannon@vpac.org) with any enquiries regarding the up and coming systems upgrade or other HPC machines available through VPAC's HPC infrastructure.

# The VPAC Access Grid

## A *Virtual* World Supporting Human *Interaction* & Collaboration

VPAC houses an Access Grid node that provides a state of the art videoconferencing facility aimed at fostering distance-immune, immersive training and collaboration among research groups and industry experts. The Access Grid aims to improve current video conferencing experiences by providing a sense of presence and supporting human interaction.

VPAC Partners, Members and Users are able to use this exciting, advanced video conferencing facility free of charge. To learn more about the global Access Grid Project or to view a listing of all participating institutions housing an Access Grid node visit <http://www.accessgrid.org>.

Initially developed by the Futures Laboratory at Argonne National Laboratory, the Access Grid is a system designed to support group-to-group interactivity across a distributed grid. The system was developed to broaden the capabilities of traditional online collaboration systems. This is achieved by providing access to resources through other distributed computing grids currently in use.



The VPAC Access Grid room is equipped with high end audio and visual technology and is complimented by the GrangeNet effort for high speed data transmission and seamless communication.

Virtual meetings using the Access Grid can be conducted with as few as one participant, who could be located on the other side of the world or in the next building. Each meeting is easy to set-up, comfortable and is as interactive as a conventional face-to-face meeting. This is enabled by a user interface that is intuitive, easy to use and navigate.

For more information on the VPAC Access Grid Node, or to make a booking, please contact the VPAC Access Grid Network Engineer, Nelsie Fernandes, by phone on 03 9925 4947 or by email on [nelsie@vpac.org](mailto:nelsie@vpac.org) or visit that VPAC website at [www.vpac.org](http://www.vpac.org).

# VPAC Training Courses

VPAC is committed to ensuring our Partners and Members get the most out of our HPC facility. As part of this commitment, VPAC holds a number of free of charge training courses throughout the year aimed at providing users with the necessary skill sets to maximize the utility of the VPAC facility.

Some of the training courses offered include:

- Introduction to VPAC
- Parallel Programming Workshop
- Message Passing Interface Course

The Program for the next three months is:

- Introduction to VPAC:
  - Tuesday 7th September 2004 at 10:00 am at the VPAC Offices
  - Thursday 30th September 2004 at 1.30pm at the VPAC Offices
- Parallel Programming Workshop:
  - Tuesday 17th August 2004 at 10:00am at the VPAC Offices.
- MPI Course:
  - Wednesday 18th August 2004 at 2:00pm at the VPAC Offices.

VPAC is interested in developing training courses that meet the needs of our users and invites you to email any suggestions to [david@vpac.org](mailto:david@vpac.org).

VPAC also has a number of conference and training facilities available to industry and academia. Choose from any of our fully equipped meeting rooms, all with comfortable seating and ample lighting and some with in-built data projectors for presentations and seminars.

For further details on each of the training courses and facilities, please visit the Service & Support section of the VPAC website at [www.vpac.org](http://www.vpac.org). All Training Courses are free of charge to VPAC Members. Interested parties will need to register online at: [www.vpac.org/content/services\\_and\\_support/training/courses.php](http://www.vpac.org/content/services_and_support/training/courses.php).

# Upcoming Events

## AUGUST 2004

### **VPAC Access Grid Official Launch**

Details To Be Announced. Keep an eye out on the VPAC website at [www.vpac.org](http://www.vpac.org) for further details regarding the official date of this event.

## **SAGE AU 2004**

**When:** 16th to 20th August 2004

**Where:** Brisbane, QLD

**Website:** <http://www.sage-au.org.au>

## **2004 Western Pacific Geophysics Meeting**

**When:** 16th to 20th August 2004

**Where:** Honolulu, Hawaii, USA

**Website:** <http://www.agu.org/meetings/wp04/>

## SEPTEMBER 2004

### **4th International Conference on Engineering Computational Technology**

**When:** 7th to 9th September 2004

**Where:** Lisbon, Portugal

**Website:** <http://www.civil-comp.com/conf/ect2004.htm>

### **7th International Conference on Computational Structures Technology**

**When:** 7th to 9th September 2004

**Where:** Lisbon, Portugal

**Website:** <http://www.civil-comp.com/conf/ect2004/htm>

### **Pacific Rim Conference in Nano-Sciences**

**When:** 7-12 September 2004

**Where:** Broome, Western Australia

**Website:** <http://physchem.ch.ic.ac.uk/broome/>

### **30th Design Automation Conference**

**When:** 28th September to 2nd October 2004

**Where:** Salt Lake City, Utah, USA

**Website:** <http://www.detc2004.me.byu.edu/index.htm>

**For more** event listings visit [www.vpac.org](http://www.vpac.org).

# comic relief *Quotes of the Quarter*



The world is full of willing people, some willing to work, the rest willing to let them.

Robert Frost (1874 - 1963)

Computers can figure out all kinds of problems, except the things in the world that just don't add up.

James Magary

If computers get too powerful, we can organize them into a committee -- that will do them in.

Bradley's Bromide

Home computers are being called upon to perform many new functions, including the consumption of homework formerly eaten by the dog.

Doug Larson

Computers are magnificent tools for the realization of our dreams, but no machine can replace the human spark of spirit, compassion, love, and understanding.

Louis Gerstner

*And just for fun...*

I've wrestled with reality for 35 years, Doctor, and I'm happy to state I finally won out over it.

Jimmy Stewart (1908 - 1997), in "Harvey", 1950

Quotes taken from <http://www.brainyquote.com>.

## Want to Hear More?

The Victorian Partnership for Advanced Computing (VPAC) was established by a consortium of six leading Victorian Universities to provide High Performance Computing (HPC) facilities to support its academic shareholders, industry and other organisations involved in research and development that required HPC capabilities.

If you would like to be updated with regular newsletters and workshops on various tools and technology register your details with the Victorian Advanced Computing Association (VACA), an incorporated association sponsored by VPAC whose objectives are to lift the awareness of High Performance Computing within Victoria by providing regular lecturers 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 Expertise and Education 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 03 9925 4645 or by email at [cammie@vpac.org](mailto:cammie@vpac.org). VPAC News is distributed quarterly.

For article submissions please contact Maria Kambourakis on 03 9925 4630 or email [maria@vpac.org](mailto:maria@vpac.org).

