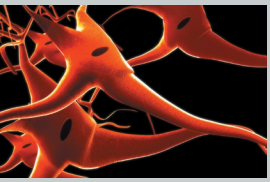
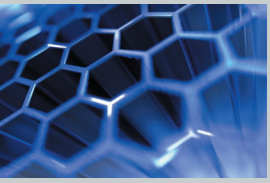
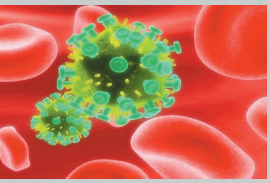
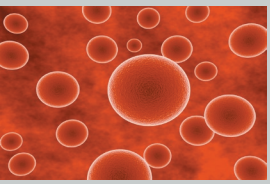
Life Sciences









VPAC is a not for profit registered research agency established in 2000 by a consortium of Victorian Universities and is a leading independent Advanced Computing R&D service provider.

At VPAC, we provide expert services, training and support in High Performance Computing (HPC) as well as professional R&D services in applications of Advanced Computing in the fields of Engineering, Geophysics, Health, Life Sciences, Spatial Information and Grid Computing.

Our aim is to help Australian researchers utilise Advanced Computing to create innovations that will place Australia at the forefront of scientific research and development.

Life Sciences @ VPAC

HPC has revolutionised the Life Sciences by giving researchers the tools necessary for collecting, cross-referencing and visualising huge amounts of biological data. Technological advances in computing have allowed scientist's new insight into fundamental biological processes and the cause of many diseases through visualisation and simulation of these molecular scale phenomena.

Life Science Capabilities

- Biomolecular Simulations
- *in silico* Drug Screening
- Nanotechnology Modelling
- *ab initio* Chemistry

Software

VPAC maintains a wide range of software and hardware for scientific researchers to aid and complement their research efforts. VPAC also offers scientific expertise to help researchers make full use of these resources. * User agreements apply.

- Amber
- DOCK
- Gamess-US
- GROMACS
- NAMD
- NCBI Tookit
- Schrodinger
- MrBayes

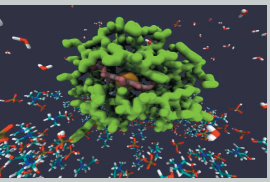
Clients

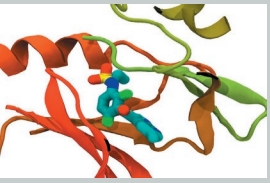
VPAC's clients and collaborative partners in the Life Sciences sector include:

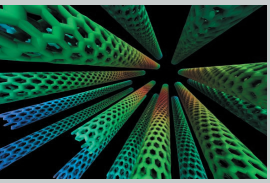
- Burnet Institute
- Department of Primary Industries
- Melbourne Health
- Royal Children's Hospital
- St Vincent's Hospital
- Victorian Infectious Disease Laboratory (VIDRL)

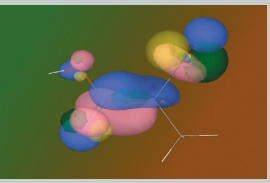
Victorian Partnership for Advanced Computing

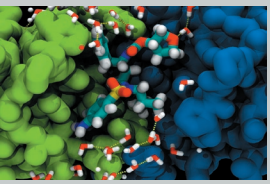
Innovation Powered by Advanced Computing











Life Science Capabilities

VPAC offers a range of academic and commercial software for use in the simulation of life sciences. By offering in-house computation and scientific expertise, VPAC can also assist researchers by utilising the most appropriate software for their needs and provide direct assistance with their modelling.

Biomolecular Simulations

At the core of all biological processes are complex molecules, such as proteins, lipids and nucleic acids, performing a range of essential functions in the living cell. Understanding the multitude of their interactions, especially in diseased states, can be challenging as they are far too small to be observed directly. Building molecular models from supplementary data such as X-ray crystallography, researchers can use HPC to simulate biological phenomena at the molecular level. Visualising these processes can help interpret wet lab experimental results and provide insight for future developments.

In silico Drug Screening

Pharmaceutical activity occurs by a drug molecule interacting with a biomolecule, usually a protein, whereby it either can inhibit or enhance its normal function. In the quest for new pharmaceuticals, HPC has proven useful by rapidly screening millions of drug molecules taken from a database targeted against a known protein to see how well the two “fit” together. High scoring drug models can then be synthesised and screened in wet-lab assays for assessment as lead compound candidates.

Nanotechnology Modelling

Nanotechnology is an exciting multidisciplinary field concerned with materials and devices that are highly ordered at the molecular scale around 1 to 100 nanometres. The physical properties of nanomaterials can be modelled using HPC to gain a better understanding of their molecular interactions as well as to help tailor these materials for specific functions.

ab initio Chemistry Simulations

ab initio chemistry involves calculating molecular properties using quantum chemistry based methods. A variety of *ab initio* methods exist that allow chemists to make predictions of molecular properties of new and existing compounds. The ever increasing level of compute power available to researchers makes the application of *ab initio* methods more practical for larger molecular systems. New hybrid methodologies such as QM/MM (quantum mechanics/molecular mechanics) enable researchers to treat part of a molecular system, such as the active site of an enzyme, with QM for greater detail, while treating the rest of the system with traditional molecular mechanics.

Contact

For further information regarding VPAC’s Advanced Computing solutions for the Life Sciences sector, please email lifesciences@vpac.org or phone +61 3 9925 4645. To view VPAC’s Life Science case studies, visit www.vpac.org.