ICHEC

ICHEC Consultancy & Services

www.ichec.ie

ICHEC
Irish Centre for High-End Computing

3D Visualisation for Climate Modelling
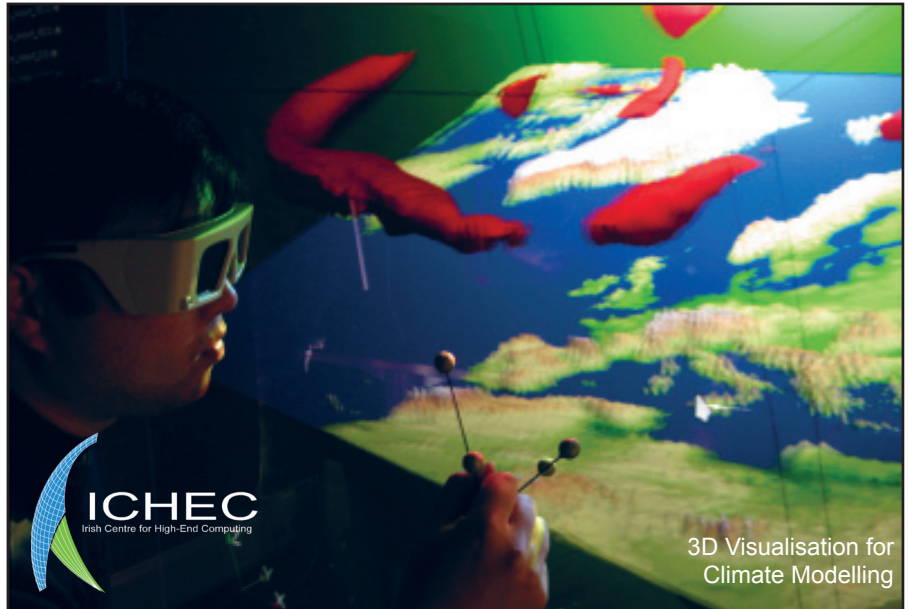
Consultancy & Services For Better Business

ICHEC gives companies efficient and cost-effective access a complete portfolio of consulting services tailored to the needs of industry. ICHEC's extensive facilities are available and support each project. ICHEC's software engineering and problems solving skill sets help solve increasingly more complex and challenging problems. ICHEC's mission is to increase the competitiveness of Irish industry through the innovative use of cutting edge software technologies.

ICHEC offers a wide range of solutions including:

- Mastering business problems through novel applications

- Access to High Performance Computing (HPC) facilities

- Design, development and re-engineering of applications to benefit from HPC

- The management, integration and mining of data

- Optimisation of application performance across a range of computer systems

- Consultancy in numerical modelling, simulation and visualisation

- Training in the use of HPC for industrial applications

- Consultancy and solutions in Grid, distributed and cloud computing

- Bespoke software development

All ICHEC projects are undertaken at a fixed cost with clearly agreed deliverables at the outset ensuring very competitive rates. This enables customers to make a thorough cost-benefit analysis before the work starts. All projects are carefully specified in consultation with the client before any work starts. This approach ensures that client expectations are met both in terms of cost and of business benefits.

ICHEC offers a flexible range of contract options covering the use of computational facilities, consultancy services and application development, porting and optimisation. These options include one-off and periodic use of facilities, fixed-price developments and long-term support. All projects are managed by qualified practitioners using the PRINCE2 framework.

HPC FACILITIES

ICHEC deploys a range of HPC systems including:
a Blue Gene/P (Schrödinger, 1024 nodes x 4 cores - 2GB RAM @ 850Mhz),
a Blue Gene/L (Lanczos, 1024 nodes x 2 cores - 1 GB RAM @ 700 Mhz),
an SGI Altix ICE 8200EX (Stokes, 320 nodes x 2 x 4 cores - 16GB RAM @ 2.8 GHz),
a Bull Novascale R422-E2 (Stoney, 64 nodes x 2 x 4 cores - 48GB RAM @ 2.8
   GHz with 12 Tesla S1070 Nodes for GPGPU-accelerated computing).

ACCESS TO CLOUD AND HPC FACILITIES

- Volume discounts are available.
- Limited use for proof of concept is offered free to new users.
- All systems can be accessed securely over the Internet.

DESIGN, DEVELOPMENT AND RE-ENGINEERING OF APPLICATIONS

Many software applications and codes may not have been implemented using the optimal numerical algorithm, nor designed to use modern multi-core and multi-processor architectures. ICHEC is highly accomplished in moving applications to these new architectures. Furthermore, in many cases, significant improvements can be made by using General Purpose Graphics Processing Units (*GPGPUs*) to accelerate numerically intensive computations.

Recently, ICHEC worked with a major Irish oil exploration company to profile and port a analysis system to run more efficiently and cost-effectively on a modern multiprocessor system.

ICHEC's capabilities include:
- The design and development of numerical applications
- The analysis and redesign of existing applications to improve performance

OPTIMISATION OF APPLICATION PERFORMANCE

Optimisation of the performance of an application to run on a range of computer systems is a key skill of ICHEC. For an application to benefit from a modern multiprocessor system, it needs to be ported to a form suitable for parallel processing. Most applications can be adapted to run on massively parallel multiprocessor systems such as ICHEC's HPC systems. Examples of ICHEC's work in this area include the porting of the protein molecular dynamics in *DL_POLY*, Tyndall Institute's *TIMES* simulator, and custom software for the complex 3D modelling of seismic waves.

ICHEC's services include:
- Application porting and parallelisation
- Application optimisation

CONSULTANCY IN NUMERICAL MODELLING, SIMULATION AND VISUALISATION

The design and development of new products and services increasingly use modelling and simulation. Engineers, in particular, are becoming more familiar with techniques such as *FEA (finite element analysis)* and *CFD (computational fluid dynamics)*. These techniques are used in development processes across a growing number of companies from sectors including aeronautics, automotive, biomedical and wind turbine modelling. ICHEC are experts in optimising and reengineering existing codes to enable faster and larger simulations.

An example of this work is the porting and acceleration of the *DL_Poly* package, allowing it to use *GPGPUs*. *DL_Poly* is a general-purpose molecular -dynamics simulation package used in a range of industries.

Advanced visualisation is an important complement to modelling and simulation. ICHEC has significant expertise in this area, not only for engineering applications, but also for the exploration of complex datasets from diverse businesses.

ICHEC
Irish Centre for High-End Computing

TRAINING IN THE USE OF HPC

ICHEC provides a range of courses in MPI, OpenMP, C/C++, Fortran, and HPC. We offer bespoke training courses upon request.

Advanced courses are available on topics such as:
- **Numerical Libraries**
- **Advanced MPI**
- **Software Engineering for Scientists**
- **HPC in Bioinformatics**

GRID, DISTRIBUTED AND CLOUD COMPUTING CONSULTANCY AND SOLUTIONS

ICHEC provides companies with impartial advice on available commercial and open-source solutions that are available and which best fit their requirements. These could be an in-house option, a cloud-based option, or a hybrid model best suited to the needs of the client.

BESPOKE SOFTWARE DEVELOPMENT

ICHEC offers software development tailored to the scope and needs of its clients. ICHEC's expertise in parallel and distributed computing (using *MPI, Open MP* and *Web services*) is internationally recognised. Its experienced software developers program on Linux, Windows and in various Unix environments using *.NET, Fortran*, *C, C ++, Java, XML, Perl, Pytho*n and other languages.

The most appropriate technologies are deployed on a case-by-case basis. ICHEC staff undertake these developments on a fixed-price basis utilising a comprehensive project-management process based on the PRINCE2® methodology.

ICHEC areas of expertise include:

- *Augmented, immersive & virtual reality*
- *Collaborative reasoning*
- *Science converging technology*
- *Context-oriented information*
- *Data mining in complex sources*
- *Human-technology interfaces*
- *Software engineering & data management*
- *Spatial data collection & management*
- *Visualisation*

DATA-MANAGEMENT, DATA-INTEGRATION, AND DATA-MINING SERVICES

ICHEC is expanding its well established data-management and data-integration services to provide additional data-mining services. The approach focuses on a detailed understanding of the underlying data, utilising standard statistical approaches and decision tree analysis.

"ICHEC has a strong track record in data management. For example, in the field of Numerical Weather Prediction (NWP) it provides an operational capability for Met Éireann, running time-critical NWP models for the national weather service. There is an on going and active research collaboration with Met Éireann in NWP development and climate modelling. Both are partners in the international EC-Earth climate project. ICHEC contributes to the development of model codes related to these activities; it is currently involved in the development of the next generation meso-scale NWP model (HARMONIE) through the HIRLAM international project; it is also involved in the development of the OASIS coupling software for ocean modelling."

Ray McGrath, Head of Research and Applications Division - Met Éireann

Contact Details

If you would like any further information about our consultancy services and what we can do to improve your business, please contact:
Eoin Brazil: eoin.brazil@ichec.ie
Tel: +353-1-5241608 ext 36, Fax: +353-1-7645845
http://www.ichec.ie

GENERAL PURPOSE GRAPHICAL PROCESSING UNITS (GPGPUs)

Programming interfaces such as NVidia's CUDA allow applications to leverage recent advances in graphical processing units. An application can see an order of magnitude speed up in comparison to optimised CPU implementations. GPGPUs can be combined in clusters with this type of processing for large scale-data processing tasks. GPGPU implementations can provide targeted acceleration of specific functions.
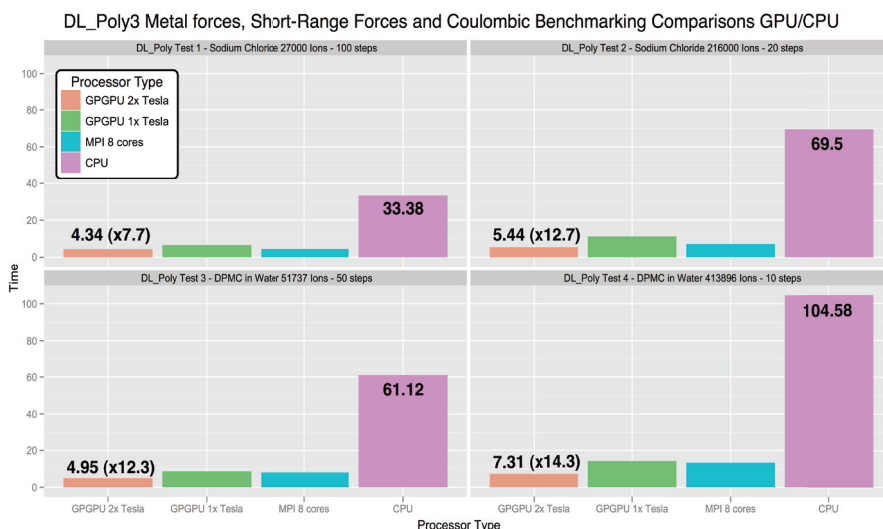
ICHEC's capabilities include:

- Porting and Development of GPGPU applications
- Profiling and Analysis of applications to highlight potential areas where GPGPUs or other techniques may benefit your existing applications
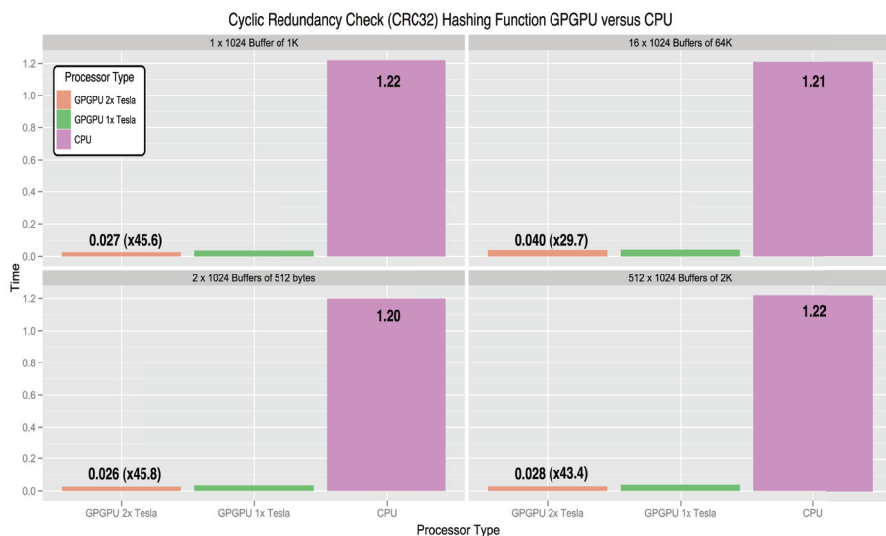
CASE STUDY - GPGPU ACCELERATION OF DL_POLY3

ICHEC software developers are porting the molecular dynamics application, *DL_POLY* to utilise GPGPU hardware.

Early results have shown a five to seven times performance improvement using a single NVidia Tesla card and a seven to fourteen time performance improvement using two NVidia Tesla cards. Further optimisations are ongoing and we expect even higher performance to be realised.

DL_Poly3 Metal forces, Short-Range Forces and Coulombic Benchmarking Comparisons GPU/CPU

DL_Poly Test 1 - Sodium Chloride 27000 Ions - 100 steps

Processor Type
- GPGPU 2x Tesla
- GPGPU 1x Tesla
- MPI 8 cores
- CPU

4.34 (x7.7)   33.38

DL_Poly Test 2 - Sodium Chloride 216000 Ions - 20 steps

5.44 (x12.7)   69.5

DL_Poly Test 3 - DPMC in Water 51737 Ions - 50 steps

4.95 (x12.3)   61.12

DL_Poly Test 4 - DPMC in Water 413896 Ions - 10 steps

7.31 (x14.3)   104.58

Case Study - GPGPU ACCELERATION OF CYCLIC REDUNDANCY CHECK (CRC) HASHING FUNCTION

Cyclic Redundancy Check (CRC32) Hashing Function GPGPU versus CPU

1 x 1024 Buffer of 1K

Processor Type
- GPGPU 2x Tesla
- GPGPU 1x Tesla
- CPU

0.027 (x45.6)   1.22

16 x 1024 Buffers of 64K

0.040 (x29.7)   1.21

2 x 1024 Buffers of 512 bytes

0.026 (x45.8)   1.20

512 x 1024 Buffers of 2K

0.028 (x43.4)   1.22

ICHEC has implemented and benchmarked a standard CRC hashing function. This type of function is typically used within data verification and cryptological algorithms. Early results have shown a 29 to 35 times performance improvement using a single NVidia Tesla card and a 29 to 46 times performance improvement using two NVidia Tesla cards. Similar performance gains are expected for other applications.

ICHEC is hosted by the National University of Ireland, Galway (NUIG) with staff located in Dublin and Galway.

Tower Building,
Trinity Technology & Enterprise Campus,
Grand Canal Quay,
Dublin 2

ICHEC
Irish Centre for High-End Computing

IT 302, IT Building,
NUI Galway, University Road,
Galway City
www.ichec.ie