HPC on stream

Powering wave energy

Pelamis Wave Power is using EPCC’s INDY cluster to accelerate the designs for the first wave farms

Also in this issue

New MSc in HPC with Data Science
From the Directors

Welcome to the Summer 2014 issue of EPCC News.

The past few months have been a very busy time for EPCC as the ARCHER national computing service has taken over from the HECToR service, which was retired at the end of March 2014. Right until the end, HECToR was full to capacity, delivering results to scientists across the UK and beyond. We’d like to thank our users, Cray and the Research Councils led by EPSRC for making HECToR the success it was.

This has also been a very busy period for many of our projects. As you’ll discover in this issue, CRESTA (p8) is well into its final year while Fortissimo (p9-11) is now at full volume, delivering its first results to the many SMEs engaged in it.

We’re also very proud to have been recently chosen as an Intel Parallel Computing Center.

You can read all about these projects and many others in this issue. We hope you enjoy it!

Alison Kennedy & Mark Parsons
EPCC Executive Directors
a.kennedy@epcc.ed.ac.uk
m.parsons@epcc.ed.ac.uk

Available now: 2014 MSc guest lecture podcasts

The full set of podcasts from this year’s MSc guest lecture series is now available, either from the School’s podcast page or via our iTunesU channel.

Every Friday afternoon throughout March, an invited speaker from industry or academia gave a talk about the use of high-performance computing. Our students got to hear about how Intel is tackling the challenge of Exascale computing, how local company Integrated Environmental Solutions benefitted from using EPCC’s HPC resources and expertise, how big data is revolutionising the field of bioinformatics, and finally details of a newly-standardised extension to C++ for parallel programming of heterogeneous algorithms!

Overall, we had a great series of speakers this year. I certainly found them interesting, and hope you will too.

Iain Bethune
i.bethune@epcc.ed.ac.uk

MSc guest lectures
http://bit.ly/1s2C6V2

Contact us

www.epcc.ed.ac.uk info@epcc.ed.ac.uk +44 (0)131 650 5030

EPCC is a supercomputing centre based at The University of Edinburgh, which is a charitable body registered in Scotland with registration number SC005336.
EPCC at ISC: come and say hello!

EPCC will be exhibiting in Booth 920.

The International Supercomputing Conference (ISC) is one of the main events in the field of high performance computing, networking and storage. It has a diverse programme of keynote talks, research presentations, tutorials, BoFs and satellite events provided by 300 expert speakers along with over 170 exhibitors and 3,000 attendees. As usual, there will be a significant EPCC representation.

EPCC’s exhibition will focus on a few specific projects and areas.

Adept, a 3-year EU-funded project, is addressing energy use in parallel software and hardware. This is a rapidly expanding area, with energy consumption now a key priority for many system operators and users. EPCC is developing measurement and modelling techniques which will allow users to explore the trade-offs between runtime performance and power usage across a range of hardware, from embedded to HPC-class systems. Not only will representatives from Adept be available at the EPCC exhibition booth, we are also hosting a BoF entitled “Measuring Energy Usage in Parallel Software/Hardware” on the Tuesday morning.

Fortissimo (see p9) will also be represented on our booth. This project looks to enable European manufacturing, particularly SMEs, to benefit from simulation services running on cloud infrastructure making use of HPC systems. EPCC’s booth will also hold promotional material from a variety of other projects and partners such as the Software Sustainability Institute, Journal of Open Research Software and Women in HPC network (see pp16-17).

Dr Michele Weiland will give a talk entitled “Is PGAS Ready for Prime Time?”. EPCC is at the forefront of PGAS language research and this talk will start with an introduction to the PGAS programming model and then discuss the different PGAS implementations; programming languages (eg Chapel), language extensions (eg UPC) and libraries (eg OpenSHMEM.) Michele will highlight recent developments and consider whether PGAS languages are becoming a viable alternative to mainstream parallel programming models. Using her own practical experiences of this programming model she will outline where PGAS tends to be a good or poor fit.

EPCC also features in the research paper programme, where I will present my work on programming languages targeted at data-intensive workloads. These have become a popular use of HPC, raising the question of how data scientists, who might not be HPC experts, can effectively program such machines. I will consider encoding all aspects of parallelism via types and the type system, which allows a programmer to write simple PGAS data-intensive HPC codes using the Mesham programming language.

Nick Brown
n.brown@epcc.ed.ac.uk

Team EPCC takes on ISC Student Cluster Competition

Four of our MSc in HPC (see p20) students will compete against 10 other teams in the third ISC Student Cluster Competition (SCC). Teams compete to achieve maximum performance within the power limit of 3kW by running the selected benchmarks and applications on their own self-designed cluster.

Team EPCC’s industrial partner, Boston Ltd, will provide hardware, training and support.

You can find Team EPCC, the only UK team in the SCC this year, at booth 293 of the competition.

Adept project BoF

Measuring Energy Usage in Parallel Software/Hardware

BoF 06, Tuesday, June 24: 9–10am, Hall 5

http://bit.ly/1uKyzso
Next-generation HPC meets big data

EPCC has launched a unique new postgraduate Master’s degree in High Performance Computing with Data Science. Scholarships are available for 2014/15.

EPCC is the major provider of high performance computing (HPC) training in Europe, with an excellent international reputation for education and research.

We are now offering a first-of-its-kind MSc in HPC & Data Science, alongside our well-established MSc in HPC.

Our MSc programmes have a strong practical focus and both are powered by ARCHER, the UK’s primary academic research supercomputer.

Scholarships are available for both MSc programmes.

“EPCC’s MSc in HPC has always been a leader in its field. Coupling it to Data Science responds to the huge increase in demand for graduates with both HPC and data skills from both science and business.”

Professor Mark Parsons, Executive Director, EPCC

MSc in High Performance Computing with Data Science

Data science involves the manipulation, processing and analysis of data to extract knowledge, and HPC provides the power that underpins it.

Students learn the multidisciplinary skills and knowledge in both HPC and data science to unlock the knowledge contained in the increasingly large, complex and challenging data sets that are now generated across many areas of science and business.

MSc in High Performance Computing

HPC is the use of powerful processors, networks and parallel supercomputers to tackle problems that are very computationally or data-intensive.

Students learn leading-edge HPC technologies and skills to exploit the full potential of the world’s largest supercomputers and multicore processors.

Industry-based projects

For more than two decades EPCC has provided consultancy and software development services to industry and commerce. Drawing on our strong links with industry, we offer our students the opportunity to undertake their dissertation project with companies in the local area.

Career benefits

Swapnil Gaikwad graduated in 2013. He is now a software developer at the Irish Centre for High End Computing (ICHEC).

“The MSc in HPC enabled me to get this job and I use knowledge obtained from it in my everyday tasks. I am really glad that I took the course which allowed me to follow my dream career path.

“I highly recommend the MSc to anyone who is passionate about learning parallel computing. It gives excellent knowledge about HPC from the experts. All you need is a basic familiarity with computers and the MSc course will take you from there.”

www.epcc.ed.ac.uk/msc
Future Internet Experimentation: Fed4FIRE

EPCC has been involved in Future Internet Research and Experimentation (FIRE) for a number of years, through its flagship project BonFIRE. For the past 18 months we have been taking this further through the Fed4FIRE project which aims to federate a number of FIRE facilities with different features to provide a rich environment for experimenters.

FIRE facilities exist to satisfy the demand from both academic and industrial communities to bridge the gap between visionary research and large-scale experimentation, through experimentally-driven advanced research. The European Commission has provided support for many FIRE facilities with different characteristics. For example BonFIRE is a multi-cloud experimentation platform that provides control and observability features that are not available on public clouds, but are necessary when testing or benchmarking distributed applications. Other FIRE facilities focus on providing capability to test wireless applications, mobile applications or specialised sensor networks and other distributed computing technologies.

The Fed4FIRE project was conceived to bring these test facilities together in a single federation that will allow experimenters to combine the different features in more challenging experiment scenarios. Bringing these different test facilities together is itself a challenging task, as the underlying technologies and user policies are variable across the facilities. Fed4FIRE is implementing an architecture in stages that is aimed at making it easy for experimenters to access the necessary resources and set up experiments involving multiple test facilities. This covers discovering and provisioning of resources, secure access to resources and user-friendly ways to manage experiments and collect data.

The project is very much aimed at satisfying the needs of real experimenters. To understand these needs better, funding was reserved to support early use of Fed4FIRE by experimenters; a series of ‘open calls’ have been issued, inviting experimenters to submit their proposals. Successful applicants have been able to benefit from early access to the federation, and Fed4FIRE has gained valuable insight into the needs of the experimenter communities. There are currently 8 experiments running from the first open call, with another 10–20 expected from subsequent calls.

The experiments currently underway are wide-ranging, covering areas such as sensor networks in urban areas, processing Earth observation data, dealing with cyber-threats and streaming media in wide area networks. BonFIRE has proved a popular choice among experimenters, with 6 of the 8 experiments wanting to use the facility. Clearly there is a demand to couple BonFIRE with other test facilities – which is good news both for BonFIRE and Fed4FIRE.

Mark Sawyer
m.sawyer@epcc.ed.ac.uk

There is still time for experimenters to submit proposals for experiments: the final call for experiments closes on July 2nd 2014.

Details of how to apply, together with project news and information, can be found on the Fed4FIRE website.

Fed4FIRE is funded by the European Commission’s 7th Framework Programme.

EPCC’s FIRE projects
BonFIRE
www.bonfire-project.eu
CityFlow
www.cityflow.eu
ECO2Clouds
eco2clouds.eu
Fed4FIRE
www.fed4fire.eu
Loosely speaking (and often in IT there isn’t any other way) we can think of research data infrastructure (RDI) as a collection of hardware and software designed to capture, store and manage the enormous volumes of research data gathered by a particular group or community.

And, as research communities struggle with ever-increasing burdens of bits, we increasingly use “an infrastructure” (and therefore some infrastructures, one infrastructure of many) because when we talk about research today, the infrastructure is no longer as common and underpinning as we would all like.

In simple terms, RDIs are about the archiving, sharing, description and discovery of research data for re-use – typically re-use within a discipline as part of the validation and verification of published scientific results.

European infrastructure research

There are 35 RDI projects currently listed on the roadmap of the European Strategy Forum on Research Infrastructures (ESFRI). These infrastructure projects cover a wide range of research disciplines and each focuses on meeting the needs of one particular community.

Each of the ESRFRI RDIs is a “vertical infrastructure”, and in a recent talk at University College London I described these as “RDI Phase I”. In Europe and globally, many efforts are now focusing on what we might term “Phase II”: connecting the vertical RDIs horizontally to create truly common, collaborative data infrastructure that cuts across disciplines. To achieve Phase II we need to harmonise a complex and dynamic set of factors, from how to describe data objects to user identities and legal licences. It is not easy. It’s such a challenge we need to ask if there’s any real value in doing it. Cross-discipline re-use of data? Really?

Research Data Alliance

The Research Data Alliance (RDA) was formed 18 months ago by a group of data-oriented researchers keen to begin the research data harmonisation process. With funding from the European Union, the US National Science Foundation and the Australian National Data Service, the RDA has become the global forum for discussing better cross-disciplinary data sharing.

Collaborative infrastructure

In Europe, the EUDAT project is building the foundations of a truly cross-disciplinary collaborative data infrastructure. It has so far created a resilient network of large-scale high-performance computing and data centres and individual community data repositories to

Cross-disciplinary benefits

A delightful example of the insights possible through the combination of data from different areas is the paper by Ludlow et al from last year: Medieval Irish chronicles reveal persistent volcanic forcing of severe winter cold events, 431–1649 CE. Ludlow’s team successfully cross-correlated volcanic deposit data from Greenland ice cores with monastic chronicles of bad winters and poor harvests. Consider the application of similar approaches to questions about the likely impact on human populations of a large-scale earthquake. Or how to increase wheat yields.

Answers to such big questions transcend any single research discipline.
provide a core set of data replication and management services. It aims to build, step by step, common pieces of infrastructure compatible with the existing investments of its ESFRI partners, weaving existing data repositories together in ways which are as non-disruptive as possible.

Next steps

Phase II of the development of RDIs is thus underway. What’s next?

Arguably Phase III involves the harmonisation not only of data infrastructures but also of computing infrastructure. We want to store and organise these data so other researchers can validate, re-analyse, combine and compute with them.

As the volumes of collected research data increase, moving them around the Internet becomes less feasible, and bringing major RDIs together with significant HPC systems is the next obvious step to take. How best to achieve this strategy is still an open question. We need to balance the risks to data preservation with the need to provide access within a rich analytic environment. Does virtualisation solve every use-case? Are general-purpose computers suitable for data-intensive tasks? Do we need more data-set-specific “Data-Scopes”, built around particular archives?

And what of Phase IV? If the first three phases of RDI development are concerned with better storage of research data, Phase IV may be about not storing it.

Between 1998 and 2008, telescopes participating in the Sloan Digital Sky Survey collected 25 TB of data. This year, the Large Synoptic Survey Telescope (LSST) will produce that in a week, and by 2019 the Square Kilometre Array telescope (SKA) will be producing 10 PB per year of “finished” data from a raw instrument feed of over 6 PB per second. From the current ESFRI roadmap, the EISCAT_3D polar geophysical imaging radar experiment will be generating 100 PB per year by 2020; that same year, the High Luminosity Large Hadron Collider, the upgrade to CERN’s LHC, will come online with estimated data rates of 500 PB annually.

Future directions

Can we store these data? We don’t know. Do we need to invent new ways to filter, process and analyse them as they stream off the detectors? Almost certainly.

The future of research data infrastructures might well lie with neither high-capacity storage nor high-performance computing but with smarter instrument design.

Research Data Alliance
https://rd-alliance.org

EUDAT
www.eudat.eu

European Strategy Forum on Research Infrastructures
http://ec.europa.eu/research/infrastructures
The Collaborative Research into Systemware, Tools and Applications (CRESTA) project is at an exciting time. In this final year, many of the promised software, tools and applications have been produced, at least in prototype form. For the next 6 months we will be finalising these products: ensuring success metrics are met and working on exploiting them beyond the project.

CRESTA has four significant outputs:

- Research portfolio
- Systemware software collection
- Co-design applications
- Co-design methodology

The CRESTA systemware software collection represents a set of software components being developed to utilise future exascale hardware and to exploit current petascale resources effectively. The components are driven by the needs of our co-design applications and many have already been delivered, at least in prototype form. We are thus at an exciting time when components are being enhanced through interaction with the co-design applications and we are seeing early results of their use.

One key focus for the remainder of the year is the exploitation of these components beyond the project and we are looking at a set of pilot studies to test and exploit them.

Considerable effort has gone into preparing the six co-design applications for exascale, with final releases of the codes due near the end of the project. CRESTA has always aimed to demonstrate the social and economic benefit of the work. This is being done through a series of exemplar simulations – each application has prepared a simulation that could not have been achieved without the development work within CRESTA. In turn these simulations represent previously unattainable scientific achievement.

CRESTA also has a research component, which looks at new algorithms and techniques to address the challenges of future exascale technologies. These techniques are driven by the needs of our applications and we are now seeing the results of these efforts in journal and conference publications, white papers and demonstrators.

Finally, CRESTA has always been viewed as a testbed for the co-design methodology. Throughout the project we have developed our management processes to facilitate co-design, developing a series of success metrics to highlight its importance. This final year will see many of these metrics being met and we will disseminate our experiences in co-design to the wider community.

Lorna Smith
l.smith@epcc.ed.ac.uk

CRESTA at ISC
CRESTA is part of the European Exascale Booth at ISC’14. If you are attending do come and visit us in booth 833.

Computing at the exascale
CRESTA is developing techniques and solutions to address the most difficult challenges of computing at the exascale.

The supercomputing community worldwide has set itself the challenge of delivering an exaflop (or a million million million calculations per second) by the end of this decade. CRESTA is committed to ensuring Europe is at the forefront of meeting this challenge.

http://cresta-project.eu
HPC for business: simulation in the cloud

Launched a year ago, the Fortissimo project is helping European businesses, in particular small and medium-sized enterprises, to use HPC in a cost-effective way for modelling and simulation applications.

The benefits of high-performance computing (HPC) in commercial applications have been proven over the years with many companies benefiting. The results are better products brought to market sooner – an obvious competitive advantage.

But for the majority of small and medium-sized enterprises (SMEs), the costs of owning an HPC system will outweigh the benefits of using it. The need for HPC expertise, together with the fact that it may only be utilised at its peak capacity for short periods, make the ownership of HPC too risky for small companies. A much more attractive option would be widely available HPC services where the resources are provided in a pay-per-use, on-demand manner, much in the way that the cloud computing model serves enterprise computing. This is where Fortissimo comes in.

Fortissimo combines the computing muscle of HPC systems with the cloud computing model of access to resources to reduce the cost of entry for companies using HPC. It also adds a further dimension by providing the HPC expertise to help companies in their opening foray into HPC. These things combine to create a marketplace where HPC solutions and users can meet – a one-stop-shop for HPC.

Fortissimo started with 20 experiments to provide requirements for the HPC-cloud infrastructure, and to validate the approach taken. Each experiment deals with a specific business application of HPC, and typically involves an end-user and a technology provider (which includes software vendors). In all, over 30 partners are involved in the experiments (in addition to the ‘core’ partners who provide the HPC resource and know-how). Application areas are diverse, ranging from the redesign of combustion engines to reduce CO₂ emissions to estimating the load on a roof due to snowfall.

The number of experiments has increased following two open calls, and overall there are expected to be around 60 experiments with over 100 partners, making Fortissimo one of EPCC’s most ambitious projects, and giving it potential for major business impact.

The ultimate goal of Fortissimo is to make the marketplace sustainable, with HPC resource providers combining with software companies and domain experts to provide solutions for end users, and all parties sharing the rewards.

Fortissimo is coordinated by EPCC and is funded by the European Commission’s 7th Framework Programme.

Mark Sawyer
m.sawyer@epcc.ed.ac.uk

HPC can speed up processing in modelling and simulation applications, allowing companies to reduce the time taken to design products and to analyse their quality in greater detail.

See overleaf for examples of HPC in action.

Contact
www.fortissimo-project.eu
HPC for business

The Fortissimo project gives companies a low-risk opportunity to try out HPC. By combining it with cloud computing, they can gain the benefits without buying and running their own systems. Here we look at three examples of HPC in action under Fortissimo.

IES: Urban Planning

In EPCC News 74 we reported on EPCC's work with Glasgow-based software and consultancy company Integrated Environmental Systems (IES) to enable its SunCast simulation software (which measures the effect of solar energy on buildings to improve energy efficiency) to run on HPC systems. IES and EPCC are now working together in the Fortissimo project.

IES is developing a planning tool for cities that incorporates dynamic simulation of all aspects of a city including buildings, transport and utility infrastructures. Because of the depth of information associated with multiple buildings, this tool will rely heavily on HPC simulation.

The cloud-based model of HPC is ideal for this application, as end-users typically do not have HPC systems. The pay-per-use service under development in Fortissimo removes the capital costs of an HPC system and the need for the specialist skills to operate it.

For IES, this will open up a whole new market of urban consultants and planners, giving them tools that currently do not exist to support decisions about how to create low carbon cities.

Koenigsegg: Hypercar design

Swedish super-car company Koenigsegg is working with Fortissimo to help it improve the aerodynamics of its performance cars.

Computational Fluid Dynamics is a well-established HPC tool, used by

Mark Sawyer
m.sawyer@epcc.ed.ac.uk

IES
http://www.iesve.com

Koenigsegg
http://www.koenigsegg.com

NUMTECH
http://www.numtech.fr

CERC
http://www.cerc.co.uk
many companies in the aerospace and automotive industries. However because of the high costs of HPC systems, it has been difficult for smaller companies to use CFD to its full potential. As an SME, Koenigsegg can benefit from cloud-based HPC because it can get the massive computational power it needs on demand, and does not need to worry about an expensive computer being idle at other times. The pay-per-user model is highly attractive.

Koenigsegg is using the OpenFOAM CFD application running on systems operated by Italian HPC provider and Fortissimo partner CINECA. Ultimately the aim is to offer this type of simulation service through the Fortissimo marketplace to end-users with similar needs to Koenigsegg.

NUMTECH CERC: Air quality

French environmental consultancy NUMTECH and British software experts CERC (Cambridge Environmental Research Consultants) are taking part in an experiment to use cloud-based HPC services to investigate air quality at city scale. European air quality regulations require many different scenarios to be evaluated. The massive computing capacity required to simulate these scenarios is typically beyond that of the end-users.

NUMTECH and CERC are working with Fortissimo partners Bull and GENCI to use CERC’s air quality modelling software in a cloud-based HPC environment. The result will be cost-effective access to the service, and new business opportunities for the companies.

EPCC is a one-stop-shop for companies looking to understand the potential of HPC to improve their business. We provide the following services to industry:

- On-demand computing
- Software development
- Modelling and simulation
- Big data solutions
- HPC training
- MSc in HPC and an MSc in HPC with Data Science.

We have a wealth of experience in transferring relevant skills quickly to our partners and building competitive advantage for the companies we work with. Our approach is firmly orientated towards collaborative working and agility.
Pelamis Wave Power Ltd, the Edinburgh-based developer of leading wave energy technology, is making use of EPCC’s INDY cluster to accelerate the designs for the first wave farms.

Ross Henderson, Pelamis Wave Power enquiries@pelamiswave.com

EPCC’s INDY cluster

INDY is a dual configuration Linux-Windows HPC cluster aimed at industrial users from the scientific and engineering communities who require on-demand access to mid-range, industry-standard HPC.

To find out more about using INDY, contact George Graham at EPCC: g.graham@epcc.ed.ac.uk

Pelamis and EPCC are working together as part of Supercomputing Scotland, a joint EPCC-Scottish Enterprise initiative. www.supercomputingscotland.org

Pelamis Wave Power generates highly detailed numerical simulations of the hydrodynamics and control of the Pelamis machines to analyse performance and survivability.

A small-scale cluster computing platform has been used by Pelamis for many years to develop designs and control algorithms, and provide engineering load and motion data. These bespoke tools enabled the delivery of two second-generation Pelamis P2 machines, which are currently being demonstrated at the EMEC test centre in Orkney, providing a huge range of data from real sea operations. Research and development of the technology continues, so the next Pelamis design must provide another step up in performance and engineering efficiency.

The power available to a Pelamis machine depends on the incident sea conditions, but the physical design of the machine and the way it is controlled determines how much of that power can be extracted. The movements of the Pelamis machines are monitored in real time, making it possible to maximise their energy yield by controlling the power take off systems within the machine accordingly to tune their dynamic response to the changing wave conditions. Tailoring these control algorithms and settings to perform optimally across the full range of different wave conditions is key to increasing the power absorption, and therefore yield, of the Pelamis machines.

EPCC’s INDY cluster offers a new order of magnitude of computing capacity to Pelamis and is opening up new frontiers of research through numerical optimisation methods that would previously have been too computationally expensive to apply.

Ross Henderson, Technology Director at Pelamis, said: “Our first challenge was adapting our existing core simulation code to compile and run on INDY, which with the help of EPCC was less painful than expected. This allowed us to successfully demonstrate INDY with a real application, conducting batches of hundreds of simultaneously optimising simulation runs. Our next challenge is to fully integrate INDY with our simulation front-end and database tools so such batches can be conducted with auditable inputs, and maximum usability of results. We are also keen to explore the application of specialist skills at EPCC to optimise our code for faster run-times.

“Wave energy is on the cusp of
entering commercial service as part of the wider renewable energy marketplace. We need to impress utility customers with the very first farms and these numerical simulations will play a vital part in delivering machines that can do this. Where we have been running on 40-60 cores on our own in-house cluster, we will soon be able to run on over 1500. This means that numerical optimisation of control systems and geometry of the machines becomes tractable using our ‘virtual machine’ simulations. This is very exciting as it may open up new routes to increasing performance and reducing costs.

“We already know that by increasing the volume of the Pelamis machine we can infinitely increase the power it captures, with no theoretical limits aside from the practical engineering constraints. However, there is an ultimate limit on the amount of power capture we are able to achieve from a Pelamis machine at each set volume and given geometry - a maximum energy output. With the machines which we’re currently demonstrating in Orkney, we’re still quite far from reaching that maximum output. So with the Supercomputing Scotland project with EPCC, we’re looking at both how we can improve the control of existing machines, but also optimising the Pelamis design for future iterations.

“The initial demonstration studies we’ve run on INDY so far have already shed new light on the ultimate limits of wave power absorption for a given geometry of machine - and it is much higher than we’ve achieved to date. While demonstrations of the two machines in Orkney have yielded very positive and valuable test results over the last few years, there is much scope to further enhance our technology before reaching that maximum energy output.

“Wave energy in general, and Pelamis in particular, offers what is perhaps the fastest cost of energy reduction trajectory of any energy technology. This is because in addition to the traditional and accepted route of cost reduction through incremental design improvements and economies of scale, we can deliver major increases in the underlying capture efficiency through control and geometry optimisation. With such a big increase in the parallel computing resources available to us we hope to optimise these aspects of Pelamis technology faster, to get closer to an ultimate absorption limit with the early commercial wave farms.”
Mathematical modelling of complex fluid flows has practical application within many industrial sectors including energy, the environment and health. Flow modelling includes oil and gas flows in long-distance pipelines or refinery distillation columns, liquid cooling of micro-electronic devices, carbon capture and cleaning processes, water treatment plants, or blood flows in arteries. Multi-phase flow modelling models flows consisting of gases, fluids and solids within a single system eg steam and water or oil and gas within a pipe, or coal dust in the air.

Industry, for example, continues to rely on empirical modelling and trial-and-error pilot-scale runs, which incur significant capital cost investments and delays before commissioning.

TPLS

TPLS (Two-Phase Level-Set) is a CFD code developed by Prashant and Lennon. TPLS uses ultra-high 3D Direct Numerical Simulation combined with the Level-Set method for tracking the developing interface between phases. TPLS employs a 2D message passing interface (MPI) process decomposition coupled with a hybrid OpenMP parallelisation scheme to allow scaling to 1000s of CPU cores. TPLS is designed to address the limitations of commercial CFD codes and provide a simulation capability that is unrivalled in computational efficiency and numerical accuracy.

Parallelisation and optimisation

Funded by both HECToR dCSE and EPSRC grants, TPLS was optimised for HECToR in collaboration with EPCC’s Iain Bethune and David Scott. TPLS has now been awarded 8 months funding from the eCSE (Embedded Computational Science and Engineering) scheme of

Authors:

Mike Jackson and Iain Bethune, EPCC, University of Edinburgh m.jackson@epcc.ed.ac.uk i.bethune@epcc.ed.ac.uk

Lennon Ó Náraigh, School of Mathematical Sciences, University College Dublin lennon.onaraigh@ucd.ie

Prashant Valluri, Institute of Materials and Processes, School of Engineering, University of Edinburgh Prashant.Valluri@ed.ac.uk
ARCHER, the new UK national supercomputer. Iain and Toni Collis (also of EPCC) are continuing to improve the robustness, flexibility and performance of TPLS. This includes: implementation of parallel I/O based on NetCDF; addition of a Diffuse Interface Method (DIM) solver; and, updating TPLS to use the PETSc (Portable, Extensible Toolkit for Scientific Computation) solver. The outcomes of this work will be a new release of TPLS and evidence of the scalability, and performance improvements realised. It is predicted that I/O performance will be improved by a factor of 20 and a 15% speedup be delivered for TPLS’s solvers, on 1024 cores.

**Usability, maintainability and sustainability**

The TPLS team applied for free consultancy in software development best practice from The Software Sustainability Institute. It was awarded 2.5 months of effort and Mike is helping to improve the usability, maintainability and sustainability of TPLS. This includes: providing a quick start guide for new users and developers; refactoring TPLS to make it configurable via the command-line or files, so researchers don’t need to hack the source code, or even have to be developers; developing an initial suite of automated tests; and, reviewing a selection of TPLS researcher-specific versions to identify commonality, and so propose how TPLS can be made more modular to support the reuse of its constituent components across different research domains.

**Conclusion**

These parallel collaborations will allow TPLS to continue both to serve Lennon’s and Prashant’s research group, other TPLS users (including Imperial College London, Brunel University London, University of Science and Technology of China, Tata Institute for Fundamental Research, India, and the Université de Lyon) and to provide further incentives for increasing its uptake within both academia and industry. This will be realised by improving both the ease with which users can adopt TPLS and the effectiveness with which TPLS can scale up to exploit powerful HPC resources like ARCHER.

Together, it is hoped these will allow TPLS to provide a simulation capability that is unrivalled in computational efficiency and numerical accuracy. We look forward to reporting on our progress.
The need for action

High-performance computing (HPC) spans multiple traditional science subjects and relies on leading-edge scientific research. It might be expected that gender inequality, which has been identified and quantified in many areas of science, would be overcome by the broad range of disciplines that HPC draws on. However, at two recent UK HPC conferences (EASC 2013 and PGAS 2013), only 8.1% of registered attendees were female.

Many organisations have made great efforts to advance gender equality in science, but so far this appears to have had little impact in HPC. The Women in High Performance Computing (WHPC) network aims to address the gender gap by taking advantage of HPC’s multi-disciplinary roots and encouraging women from diverse backgrounds into the field.

What we do

WHPC supports collaboration and networking, bringing together female HPC scientists, researchers, developers, users and technicians from across the UK. We encourage women in HPC to engage in outreach activities and improve the visibility of inspirational role models. Our activities are complemented by research into the influence of UK equality initiatives on the HPC community.

Launch

The Women in HPC network launched in April with an afternoon of talks from leading women in HPC in the UK. EPCC Director Alison Kennedy kicked off the afternoon by explaining the need to address gender inequality specifically in HPC rather than relying on schemes such as Athena Swann and Project Juno. Other contributors – including Angela Busse (University of Glasgow), Claire Hepwood (AWE), Carole Morrison (University of Edinburgh) and EPCC’s Lorna Smith – provided an insight into their work (including comparing running ARCHER to raising two small boys).

The successful afternoon finished with networking among the participants, giving many of the attendees their first opportunity to meet other women working in HPC.

WHPC at SC14

We will run an international workshop at Supercomputing 2014 on improving the representation of women in the international HPC community.

This half-day event will include invited talks by world-leading women working in the field of HPC, describing the problems facing women in HPC careers and how to improve the representation of women in supercomputing. There will also be peer-reviewed talks and posters to provide early-career women in HPC an opportunity to showcase their work in a prestigious and supportive environment.

Toni Collis
acollis@epcc.ed.ac.uk
Call for Papers

Women in HPC at Supercomputing 2014, Denver, Colorado, Friday 21 November 2014

Closing date: 31/07/2014

WHPC network will run a half-day workshop at Supercomputing 2014 to highlight the work of women in the international HPC community.

We invite submissions from female early career researchers (papers or posters) to present their work in a supportive environment that promotes the engagement of women in HPC research and applications. This will be an opportunity for peer-to-peer networking and to meet female role models. Submissions will be peer reviewed.

Submission categories

- Extended abstract (500 words max) on research in any area that utilises HPC
- Short abstract (250 words max) for a poster in any area that utilises HPC.

Workshop aims

The workshop aims to address gender issues in HPC research and innovation where they impact efficacy of the scientific method and research quality. In addition to talks by early-career researchers, it will bring together HPC scientists and researchers to discuss the challenges facing women in HPC, ways to address the gender imbalance, and strategies to achieve these goals.

The workshop will include invited talks by world-leading women working in the field of HPC, describing the career challenges they have met and how to improve the representation of women in supercomputing.

Registration

Details on how to apply are available from the event website. Applicants must be female and either PhD candidates or early-career researchers who have been awarded their PhD within 5 years of 1st November 2014.

The WHPC network will attempt to identify and address the causes of the gender gap in HPC in the UK.

WHPC website
www.womeninhpc.org.uk

SC14 workshop
www.womeninhpc.org.uk/SC14
Through this new partnership, EPCC will collaborate with Intel to optimise several open source high-performance computing (HPC) applications for Intel’s latest parallel processor architectures.

**Incredible opportunity**

“Designation as an IPCC gives us an incredible opportunity to work on a range of important, and widely used, simulation codes to ensure that they can utilise the latest Intel hardware effectively,” said Professor Mark Parsons, EPCC’s Executive Director (Research & Commercialisation). “ARCHER, the UK’s national HPC service hosted and supported by EPCC is a Cray XC30 system with Intel® Xeon® Processor E5-2697 v2,” continued Mark. “It is therefore essential that mainstream simulation packages, which account for more than half the usage of ARCHER, are properly optimised to get maximum benefit from this technology”.

“The centre will build on a range of world-class projects, collaborations, and initiatives that EPCC is currently involved with, including European HPC projects such as PRACE and CRESTA and global simulation initiatives, such as the G8-funded Nu-FuSE project,” said Adrian Jackson, Research Architect at EPCC and leader for EPCC’s involvement in NU-FuSE.

Dr Michèle Weiland, Project Manager at EPCC, said: “The initial target for optimisation and porting work are codes that EPCC is already very familiar with, have had experience parallelising and optimising for standard distributed memory parallel systems, and are used by a wide community of simulation scientists for world leading science on global challenges such as energy security, climate change, and future manufacturing technologies.”

**Performance tuning**

EPCC’s Application Consultants, who are experts in the performance tuning of HPC modelling and simulation codes, will undertake the code porting and optimisation tasks. A further aim of the IPCC is to leverage the world-leading hardware available at EPCC, and its extensive training programmes, to provide training and expertise to a wider range of academic and industrial participants in the UK and Europe on efficiently using Intel hardware for computational simulation.

“Intel is pleased to expand our Intel® Parallel Computing Center program in collaborating with EPCC.

“This new centre creates an opportunity for Intel and EPCC to innovate and optimize applications which benefit industry and science in Europe and globally.”

Bob Burroughs, Director of Technical Computing Ecosystem Enabling, Intel
ARCHER is go!

The official launch event for the new ARCHER high-performance computing service took place in March at the National Museum of Scotland in Edinburgh.

Over a hundred people attended the event including representatives from the University of Edinburgh, Cray, the National Environmental Research Council and the Engineering and Physical Sciences Research Council. Speakers included David Delpy, Chief Executive of EPSRC; Ian Gillespie, Director of Science, NERC; and Peg Williams, Senior Vice President of HPC at CRAY.

The event also featured bite-sized summary presentations from users and industry showcasing their work on ARCHER and the impacts of HPC.

ARCHER
www.archer.ac.uk

Maureen Simpson
m.simpson@epcc.ed.ac.uk

EPCC at the Museum

The Edinburgh International Science Festival is one of the longest running science festivals in the world and this year EPCC joined the University of Edinburgh Families’ programme at the National Museum of Scotland.

For five days, EPCC staff and students demonstrated a range of hands-on activities for the public to show how supercomputers are used and how high performances are obtained from these systems. The activities used to do this include sorting activities to illustrate how parallelism speeds up calculations, old supercomputing boards to show the physical nature of supercomputers and a dinosaur simulation to show the implementation of an application and because dinosaurs are cool.

For the first time, we had students helping EPCC staff at an event and this proved to work very well, they were approachable and knowledgeable about the subject and to provide them with outreach experience.

Over the five days we were involved, we had three students and four staff members with one member of staff per day to engage with the public that visited our exhibit area. During this period over 3400 individuals from toddlers to pensioners visited the exhibit area at the museum. All these visitors had questions about the concept of supercomputers and were amazed to find out how technology developed for supercomputing has made its way into everyday devices such as tablets and mobile phones.

The event proved to be a success for EPCC with many enquiries over the days about what EPCC does and who we work with. Hopefully we will be back next year with new and improved exhibits.

What our visitors said...
“This is excellent!”
“It makes a difference being able to talk to real scientists.”
“The students are great - so helpful and friendly.”
Postgraduate Master’s Degrees in High Performance Computing

Scholarships available for 2014/15

These MSc programmes are offered by EPCC, an institute at the University of Edinburgh.

EPCC is one of Europe’s leading supercomputing centres and operates ARCHER, a 72,000-processor Cray XC30 system.

ARCHER is the new UK academic High Performance Computer System.

These programmes equip participants with the multidisciplinary skills and knowledge to lead the way in the fields of High Performance Computing and Data Science.

Through our strong links with industry, we also offer our students the opportunity to undertake their Master’s dissertation with one of a wide range of local companies.

The University of Edinburgh is consistently ranked among the top 50 universities in the world*.

*Times Higher World University Ranking

www.epcc.ed.ac.uk/msc