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### Sharing High Performance Computing, Data Intensive Computing and Novel Computing Resources across Scottish HEIs

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# Sharing High Performance Computing, Data Intensive Computing and Novel Computing Resources across Scottish HEIs

## ERCPool – D-2 Report

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# 1 Document Overview

This document is the D-2 Report deliverable from the ERCPool project. The full title of the ERCPool project is “Pilot Project in Sharing High Performance Computing, Data Intensive Computing and Novel Computing Resources across Scottish HEIs” [1]. For the remainder of this document the project will be referred to as ERCPool.

The two major objectives of the ERCPool project are:

1. To promote and investigate potential opportunities, through equipment pooling initiatives, for the sharing of Edinburgh’s leading-edge high performance and novel computing systems at EPCC with other universities.
2. To deliver a report documenting the strengths, weaknesses, opportunities and threats of a move to a system of resource sharing, as well as looking at the potential benefits to researchers. This report will also look at the practical barriers to resource sharing and undertake a cost/benefit analysis.

This document fulfils this project’s second objective. The content for this document has been derived from the two major activities undertaken in ERCPool.

1. A regional study, based on a pilot programme for resource sharing in novel computing. This has involved opening up two state-of-the-art novel computing resources to researchers from outside Edinburgh. These are the Data Intensive Research (EDIM1) computer and EPCC’s parallel GPGPU resource testbed. This has enabled the identification of some of the operational barriers to the sharing of these novel computing resources with researchers from outside the University of Edinburgh.
2. An investigation into the potential for operating regional or topical HPC resources instead of each University procuring and operating its own machine. Using the researchers from SUPA (which covers all of the Physics departments in Scotland) and other disciplines, ERCPool has investigated and documented the future computing needs of researchers to determine to what extent these could be met by shared resources. It has also looked at the potential tangible benefits for research of sharing research computing resources, such as increased collaboration between institutions, better access to training and consultancy, equality of access to state of the art facilities to researchers from a wide geographical area, integration of university, topical and regional facilities into the UK HPC ecosystem. This has involved contacts with more than 40 staff from HEIs from across Scotland and resulted in three projects running on the state-of-the-art novel computing resources opened up as part of ERCPool’s pilot programme described above.

Section 2 of this document therefore discusses if future computing needs as expressed by contacted IS providers and research groups can be met by resource pooling. Section 3 provides a SWOT analysis, whilst Section 4 discusses the possible cost benefits of resource sharing. Finally, Section 5 discusses the practical barriers to resource sharing and how these could be overcome.

In summary, ERCPool has found that the barriers to sharing of novel and high performance computing resources can be broadly classified into four areas – access, resource management, application-related and costs. Overcoming the access related barriers is primarily about making the resource application process lightweight and timely. Regarding resource management, it must be recognised that traditional techniques such as batch systems and virtualisation are not appropriate for every circumstance. A range of possibilities needs to be provided that includes simple and flexible mechanisms that recognise, for example, that not all applications scale to hundreds or thousands of cores and so may require execution times of longer than 12 hours. Application based training and not just software development training is required since many users do not program but instead run third-party applications, Such users need to know how to use these efficiently and to best effect. Probably the greatest barrier, however, to resource pooling is the lack of clarity around funding models and costs. Once these are better understood

and clear, easy to understand, implement and monitor processes are in place then resource pooling will be far more appealing to researchers. This, however, requires RCUK and HEIs to engage together to resolve this.

## 2 Meeting future computing needs through resource pooling

This section of the report discusses if future computing needs as expressed by contacted IS providers and research groups can be met by resource pooling.

### 2.1 Views of central IS providers

This subsection summarises the views collected from central Information Services (IS) providers at the SUPA Universities other than Edinburgh.

IS providers from all the SUPA partners were contacted and asked if they would meet ERCPool in order to give their views on resource pooling. These providers were also asked to identify research groups at their institution who might be interested in utilising the specialist computing resources and associated staff consultancy available as part of ERCPool.

Responses were only obtained from Aberdeen, Dundee, Glasgow, Heriot-Watt and West of Scotland (UWS). No responses were obtained from St Andrews or Strathclyde despite repeated attempts. Of those that replied only Aberdeen, Glasgow, and Heriot-Watt agreed to a visit by ERCPool. The visits to Aberdeen, Glasgow and Heriot-Watt were minuted and their content agreed with the attendees.

Glasgow has been running a central HPC service but have found that use is falling; a typical usage pattern is for researchers to try out HPC and if this is successful to purchase their own hardware. Glasgow users have also found purchasing their own resources to be easier than accessing national resources such as the National Grid Service (NGS) – even when the NGS resource is located locally in Glasgow!

Aberdeen are looking at providing multi-tiered research computing facilities between IT Services and research groups. At the data centre hosting level, Aberdeen and local HEIs are considering sharing of floor space but this may move into shared compute and storage eventually.

Heriot-Watt provides a central HPC service that is heavily over-subscribed and have issues with providing support for this. Heriot-Watt are open to the idea of sharing an HPC facility but this will obviously depend on the cost models involved.

Dundee and UWS referred ERCPool to staff in academic departments at their institutions.

More details on the interactions with various IS providers are provided in the sub-sections below.

#### 2.1.1 Dr. Brian Robertson, Head of Infrastructure Management, Directorate of Information Technology, University of Aberdeen

Aberdeen DIT has previously not been concerned with the provision of computing for research. Up until recently it had only been concerned with general computing provision with a few research groups having their own clusters. The need for research computing provision by DIT, however, has recently been recognised, with a number of research groups expressing interest in this. Aberdeen DIT are therefore looking at building an infrastructure based on Purdue's example i.e. a scalable infrastructure where Aberdeen DIT provide a basic infrastructure with research groups buying into this and so expanding it. This is seen as being multi-tiered, comprising local level provision, with some middle level provision followed by a high level of supercomputing provision. The existence of these different levels of provision is recognition that one size does not fit all but that collaboration means the whole can be greater than the sum of the parts.

Recently, the University of Aberdeen has been working with other Higher Education institutes in the area on data centre hosting. Robert Gordon's and Aberdeen College are likely to use the University of Aberdeen as their primary data centre. Some other HEIs in the Aberdeen area are looking at using the University of Aberdeen as their secondary data centre. Currently this data centre hosting is only concerned with the sharing of floor space but it may move further and result in shared compute or data storage provision. The belief in Aberdeen is that the higher up

the IT infrastructure stack resource sharing occurs, the more savings there are to be made but this is very much dependent on the amount of trust there is between institutions involved. The University of Aberdeen has been able to build this trust with local HEIs due to its operation over the years of AbMAN - the Aberdeen Metropolitan Area Network. This is why the likes of Robert Gordon's are now willing to use Aberdeen as their data centre.

Brian believes that in all sharing initiatives the key is trust and that is why sharing across sectors is more difficult and less likely to succeed since there has not been the same opportunity for trust to develop.

### **2.1.2 Tom Mortimer, Director of Computing Services, University of Dundee**

Dundee has a strong interest in sharing resources across the sector. Tom referred ERCPool to Jonathan Monk of the College of Life Sciences (see Section 2.3.2).

### **2.1.3 Mark Meenan, Computing Services Grid Manager, University of Glasgow**

A centrally-provided HPC resource has been available in Glasgow since approximately 2008. Use of this resource by research groups is falling. The general pattern has been for research groups to test out their research on the HPC resource and then purchase their own HPC box if the tests have proven successful. Since then:

“researchers have reached a plateau – their existing equipment provides sufficient power for the moment so there is no demand for more.”

“Users who only occasionally want a lot of compute power can get access to such power through easier means than the NGS ie. buy a big desktop.”

This refers to the National Grid Service<sup>1</sup>, which “aims to facilitate UK research by providing access to a broad range of computational and data based resources”.

### **2.1.4 Guilherme De Sousa, Director of Infrastructure Services, Heriot-Watt University**

Infrastructure Services are responsible for hosting many IT services for Heriot-Watt; only part of which is HPC and cluster support. They therefore have many demands on their time. They also provide hosting for many small departmental clusters, this being more time consuming than a single, large, resource due to the inhomogeneous nature of the systems. Specific support for HPC users is sometimes difficult in a general IT department; it's quite a specialised area. Infrastructure Services would be quite open to using some kind of shared facility which could cover general HPC requirements. Their hope is that this would hopefully free up some of their support manpower for other purposes. Before considering this, however, the funding/charging model would have to be carefully worked out and explained.

### **2.1.5 University of Strathclyde**

The Strathclyde IS helpdesk suggested contacting Bruce Rodger, Head of Infrastructure. A number of email attempts were made with no success.

### **2.1.6 University of St Andrews**

The contact email address for St Andrews IT Services was emailed but no reply was received. IT Services were telephoned directly instead and the operator advised contacting Kevin Donnachie, Service Delivery Manager. Email and voicemails were sent to Kevin but received no reply. IT Services were again called but there was no reply. The St Andrews Computer and IT Support helpdesk was therefore contacted. The operator said that Kevin was a busy man and difficult to catch and instead suggested contacting Dean Drew, the new Senior Manager for technical infrastructure. Email and voicemails were sent to Dean but there was no reply. Later an email

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<sup>1</sup> <http://www.ngs.ac.uk/>



was sent to Steve Watt, the Chief Information Officer for St Andrew's IT Services, again no reply was received.

### **2.1.7 Dr Brian Mullins, Director of ICT, University of West of Scotland**

ICT do not provide research computing services such as HPC but referred ERCPool to the School of Computing (see Section 2.3.13).

## **2.2 Views of SUPA partners and SUPA research groups**

This subsection summarises the views from SUPA departments on whether future computing needs can be met by resource pooling.

The members of the SUPA Executive Committee (except Edinburgh) were emailed and asked if they would meet ERCPool in order to give their views on resource pooling and to identify researchers who might be interested in utilising the specialist computing resources and associated staff consultancy available as part of ERCPool.

Responses were only obtained from Aberdeen, Dundee, Glasgow, St Andrews and Strathclyde. No responses were obtained from the Heriot-Watt and UWS's committee members.

Aberdeen emailed a reply stating that they had just purchased a cluster but would forward on the email to the whole department to see if researchers were interested in meeting ERCPool. Unfortunately no Aberdeen SUPA researchers contacted ERCPool. St Andrews emailed a reply stating that they were happy with their existing computing facilities and referred ERCPool instead to the Maths and Chemistry departments.

Dundee, Glasgow and Strathclyde agreed to a visit from an ERCPool project team member. These visits were minuted and their content agreed with attendees.

Dundee would like to have access to shared computing resources but only as a user since they do not have enough of their own resource for others to use. Glasgow run a cluster for the UK-wide GridPP consortium; the utilisation of this is very high and so they are not keen to share with others. Previous attempts at sharing have been problematic but Glasgow see a role for sharing at the infrastructure level ie. machines, rooms, power, cooling, etc. Strathclyde host the newly established West of Scotland Supercomputing Centre also known as ARCHIE-WeSt<sup>2</sup>. The consortium behind this centre is led by the University of Strathclyde and includes the University of Glasgow, Glasgow Caledonian University, University of Stirling and the University of the West of Scotland. Strathclyde believe that shared computing resources offers cost savings for research groups.

More details on the views expressed by the various SUPA departments are provided in the subsections below.

### **2.2.1 Professor Celso Grebogi, Director of Research, Department of Physics, School of Natural and Computing Sciences, University of Aberdeen**

Professor Grebogi replied to the ERCPool email stating that his Institute had just "installed a reasonable size cluster (588 processors and increasing the size)". Professor Grebogi also forwarded on the ERCPool request to everyone in his Institute inviting them to contact ERCPool if they were interested. No replies were received.

### **2.2.2 Professor Mervyn Rose, Head of Division of Electronic Engineering, Physics and Renewable Energy, University of Dundee**

Professor Rose agreed to a meeting with ERCPool. Professor Rose invited interested researchers to the meeting. Two in particular were interested, Dr Trevor Dines and Dr David Goldie, but in the end only Dr Dines accompanied Professor Rose.

Dundee Computing Services do not provide any research computing facilities. Only the Physics and Life Sciences (PaLS) researchers have access to Dundee's Life Sciences computing facilities.

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<sup>2</sup> <http://www.archie-west.ac.uk/>

Other Physics researchers in Dundee do not have access to these facilities. A number of Dundee Physics researchers have simulations that can run for more than a month on a local PC.

Since Dundee currently do not have any computing facilities to share then they could only be a consumer of pooled resources rather than a contributor. Despite this Dundee are keen to participate in any such scheme.

### **2.2.3 Professor David Britton, Professor of Physics, University of Glasgow**

ERCPool were put in contact with Professor David Britton via Professor Andrew Long, Glasgow's SUPA Executive Committee member. Professor Britton is also the Project Leader of the (UK-wide) GridPP project<sup>3</sup>.

Glasgow experimental particle physics have their own cluster which is used specifically for LHC physics as part of the UK GridPP project. In general utilisation of this is very high, over 90% by particle physics, so the opportunities for sharing with others are limited. However they have in the past used spare capacity for other VOs, often making the news with projects such as avian flu studies with the biomedical community, social scientists, archaeology, start-ups, TOTAL etc.

Such shared usage has not been charged, although this means opportunities for sharing are limited. They are happy to take hardware purchased by other people, and integrate into the cluster. The hardware owners get usage of their own resources when required but these can be used by others at other times to get better overall utilisation. Medical projects can only contribute money for independent hardware due to privacy issues. This makes better use of systems support manpower which is expensive compared to hardware.

Speaking as PL of GridPP, Professor Britton has found shared facilities to be much more work. Some GridPP sites have used shared university facilities, some are dedicated to PP. Examples of shared facilities are at Bristol, which failed completely for the project, and Edinburgh where a lot of work was required. The extra work was only economical as PP ends up with more than its share due to utilisation of unused capacity. GridPP, as part of the Worldwide LHC Computing Grid (WLCG)<sup>4</sup>, has stringent requirements on the software stack (from the operating system level upwards) in order to ensure interoperability over the hundreds of sites involved in the project. These requirements make dedicated resources a much more attractive option.

Professor Britton has written a green paper for Glasgow about "condo-computing". He proposes that resource sharing should largely be at the infrastructure level (housing, power, Cooling etc). Individual research groups would "rent rooms" within this to place their own hardware which they still run individually. Rent could be a share of the resource rather than money.

### **2.2.4 Professor Gerald Buller, School of Engineering and Physical Sciences, Heriot-Watt University**

Professor Buller was contacted but no reply was received.

### **2.2.5 Professor Thomas Krauss, School of Physics and Astronomy, University of St Andrews**

Professor Krauss stated that his research group are quite happy with the small-scale computing that they currently do, and are not looking to expand in the near future. There is one other research group that uses more compute but their lead (Prof Ian Bonnell) was on sabbatical. Professor Krauss referred ERCPool instead to the Maths and Chemistry departments at St Andrews.

### **2.2.6 Professor Maxim Fedorov, Professor of Physics and Life Sciences, University of Strathclyde**

ERCPool were put in contact with Professor Fedorov by Professor Robert Martin, Strathclyde's SUPA Executive Committee member. Professor Fedorov is Director of the newly established West of Scotland Supercomputing Centre also known as ARCHIE-WeSt. The centre was

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<sup>3</sup> <http://www.gridpp.ac.uk/>

<sup>4</sup> <http://wlcg.web.cern.ch/>

established in March 2012 by a £1.6M award from the EPSRC e-Infrastructure fund to establish a regional centre of excellence in High Performance Computing. The aim of the centre is to provide High Performance Computing capability for Academia, Industry and Enterprise in the West of Scotland. The Centre is hosted by the University of Strathclyde. The consortium behind the Centre is led by the University of Strathclyde and includes the University of Glasgow, Glasgow Caledonian University, University of Stirling and the University of the West of Scotland.

Dr Fedorov's view is that if a research group runs its own resource then they really need a full-time software support person, in addition to the usual systems support manpower, which they cannot afford. This is required for the installation and configuration of the many different scientific applications, which is a time consuming process, and otherwise replaces valuable research time of scientists. In principle a large shared resource such as ARCHIE-WeSt should be able to provide such support more easily.

### **2.2.7 Professor Frank Placido, School of Engineering, University of the West of Scotland**

Professor Placido was contacted but no reply was received.

## **2.3 Views of non-SUPA Research Groups**

This subsection summarises the views from research groups NOT based in SUPA departments on whether future computing needs can be met by resource pooling. All the research groups are based in Scottish HEIs.

These research groups were identified primarily through the prior contacts with the IS providers and SUPA departments. ERCPool visited the research groups to get their views on resource pooling and to discuss utilising the specialist computing resources and associated staff consultancy available as part of ERCPool.

Visits were made to Aberdeen, Dundee, Glasgow, Heriot-Watt, St Andrews and the University of the West of Scotland. A teleconference was conducted with a researcher the University of the Highlands and Islands.

Aberdeen are actively building an HPC infrastructure to be shared between research groups but note that researchers have concerns over the level of control they have over shared resources as their circle of use expands from departmental through institutional to national. At Dundee, Life Sciences research groups have their own College Computing Service. Similarly School of Engineering researchers at Glasgow have their own HPC service. Despite this, both Dundee and Glasgow noted that researchers will generally share out of necessity and much prefer having their own physical resource due to the level of control. The University of Glasgow HPC group stated the UK's National Grid Service 'was a complete disaster' and that 'No-one likes e-Science certificates'. Researchers in the Schools of Psychology and Chemistry at Glasgow share their resources internally. Petroleum Engineers at Heriot-Watt have their own HPC service and are reluctant to use shared facilities because of data security and software issues. Chemical engineers at Heriot-Watt find the centrally available cluster difficult to use and instead use their own resources or a shared resource at Imperial College. At St Andrews the Schools of Chemistry and Mathematics have a joint HPC service that this is also available generally to researchers at St Andrews though take-up has been limited to physics and computational biology. UHI do not have HPC resource of their own but would like access to some. UWS are part of the ARCHIE-WeSt consortium but need training to use it.

Most researchers spoken to were concerned about the charging model for using external resources. Researchers from Dundee, St Andrews, Glasgow, UHI and Heriot-Watt stated it would be helpful to have access to a zoo of novel machines to experiment. Accompanying staff consultancy to advise on how to work on such machines would also be helpful.

More details on the views expressed by the researchers are provided in the sub-sections below.

### **2.3.1 Naveed Khan, Senior Computer Officer, School of Natural and Computing Sciences, University of Aberdeen**

Mr Khan attended the ERCPool visit to Dr Robertson of Aberdeen DIT (see Section 2.1.1). The School consists of four departments, Chemistry, Computing Science, Mathematics, and Physics. The School and Aberdeen's DIT (see Section 2.1.1) wish to build an infrastructure based on Purdue's; that is, a scalable infrastructure where Aberdeen DIT provides a basic infrastructure with research groups buying into this and so expanding it. To date research groups who wanted HPC facilities have generally relied on external facilities, such as GenePool, however, groups such as the geneticists in particular, have decided they want to have their own resource that they can control. Within Aberdeen, a barrier to sharing and hence resource pooling is that where a research group has a cluster, it does not allow or want others to use it. Such research groups, however, are typically happy to use someone else's cluster in addition to their own.

If there are many hurdles to overcome in order to use a particular resource then this puts researchers off. Whilst there may be an overhead to a researcher managing their own compute facility, they are generally happier to do this compared to using a department level facility where they have less control. Similarly, researchers are happier to use a department level facility compared to a remote, say national, facility where they have even less control and influence. If, however, such remote facilities are the only ones available then researchers recognise they just have to get over any hurdles in order to use it.

### **2.3.2 Jonathan Monk, Head of Life Sciences Computing Services, University of Dundee**

The Life Sciences Computing Services tend not to look at high end computing technology immediately that it becomes available. They prefer to wait until such technology becomes available in commodity platforms since much of the processing on the Services are based on reuse of existing libraries and software.

Outreach visits such as those from the ERCPool project are a valuable way for Life Sciences Computing Services to learn of new developments. Getting access to novel compute services to try out technology before buying it is also very useful. This helps researchers distinguish the wheat from the chaff. For example, earlier access to the GPGPU resources available via ERCPool would have negated the need for the Life Sciences Computing Services to buy a blade to try out GPU-based computing.

Some researchers are better at utilising central resources whilst others prefer to have their own hardware. This is believed to be for operational issues rather than computational reasons; that is, some research leaders prefer to physically have their own resource. A particular example encountered has been where researchers are reluctant to have virtual machine (VM) instances rather than a physical box. Virtualisation has, in effect, aggravated this view point. A further example of this was at the inception of the Scottish Universities Life Science Alliance (SULSA)<sup>5</sup> it had been hoped that a £1million data centre could be set up that would serve all the SULSA partners. This was met with some resistance and the money was instead split across the participating sites. In effect the existence of research groups that have grown up with their own compute provision is a significant hurdle to sharing.

A significant difference between the physical and life sciences is in the source and storage of their data. For physicists, one or two large, expensive research instruments produce data that is processed by many researchers from different HEIs and also shared with the community at large.

In biology, mass spec and next generation sequencing instruments are located in departments at HEIs. These produce masses of data that are stored locally and there is no specific infrastructure in place for sharing this data with the community at large. Whilst the biological and physics communities potentially have similar volumes of data, the difference is in the number of sources, where the data is stored and how it is distributed.

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<sup>5</sup> <http://www.sulsa.ac.uk/>

The number of sources, combined with large data volumes, means data transfer is an issue so the architecture and accessibility of shared resources are important. Despite this, HEIs sharing infrastructure is seen as the future provided such infrastructure is easy for bioscientists to use.

### **2.3.3 Dr Campbell Millar, Device Modelling Group, School of Engineering, University of Glasgow**

Dr Millar manages the HPC service for the School of Engineering assisted by Gordon Stewart. At the time of visit they had about 2000 compute cores in this service. There are some other shared compute resources within the School but the expectation is that the Head of School will not want to share these resources outside of the school, unless there was some sort of quid pro quo in place. The expectation is that this sharing would be for a small amount of cores, maybe 200. Within the College, there has been some talk of resource sharing but nothing definite.

Glasgow do not provide central research computing resources nor do Glasgow researchers like such centralised resources.

Professors might share their kit but they want priority. An important aspect is how academics are assessed by their own institution. This is generally dependant on the amount of income they bring into their own institution. If part of their grant is to another institution to pay for access and running costs of a shared resource then this is detrimental to their career since that portion will not be used in the home institutions assessment of the academic. For example, pay rises for professors at Glasgow are directly related to the amount of money they put into university central resources.

Engineering are looking at shared hosting with other departments i.e. sharing server rooms since it is believed that having a single server room for lots of departments will be cheaper than departments having their own server room. Dr Millar believes that therefore a shared site for universities may be a possibility and would get over professorial issues. This would allow Scotland to have a research computing infrastructure that has flexibility and a service aspect.

Dr Millar lobbied a Glasgow VP about building a shed for compute. This appeared to be getting somewhere but the VP retired and progress stopped. The issue facing this sort of shared space solution is that academics believe that they end up paying twice; firstly, in overheads and, secondly, for actual hosting charges.

### **2.3.4 University of Glasgow HPC Interest Group**

Mark Meenan, Computing Services Grid Manager at Glasgow recommended that ERCPool meet the University of Glasgow's HPC interest group. Members of this group that attended the meeting with ERCPool included:

John McClure – IT Support Manager for the School of Psychology and the CCNi Centre of Neuroimaging.

Peter Bailey – Systems Team Manager, School of Computing Science.

Dr Hans Senn – Lecturer in Theoretical and Computational Chemistry.

The individual views from each of the above on resource pooling are contained in separate subsections below.

The overall views of this group were as follows:

- The development of the charging model for any shared resource needs careful consideration.
- The UK's National Grid Service was a complete disaster - difficult to use, and although Glasgow had resource on this it was never used due to the Globus enforced access mechanism. No one likes e-Science certificates.
- Physics and Astronomy never attend the meetings, although they have large ScotGrid cluster.
- Glasgow researchers will have access to the new ARCHIE-WeSt machine based at Strathclyde - seemingly getting 12 months free access. This, however, is viewed as being very rushed and ad-hoc, and the charging model will need to be developed.

### **2.3.5 John McClure, IT Support Manager, School of Psychology, University of Glasgow**

Psychology department researchers are happy to share their resources internally, maybe due to how their use has developed, and a collegiate atmosphere promoted by the department head. The resources are used for brain imaging analysis (MRI scans), language processing, Matlab, and teaching on their MSc. Researchers previously found it hard to use externally shared resources, hence the purchase of a local resource 7 years ago. There were difficulties using Physics ScotGrid due to privacy issues (NHS data), data disappearing (!) and it being too hard to use in general. Researchers have issues with data due to its sensitivity, eg NHS provided images of brain scans etc.

### **2.3.6 Peter Bailey, Systems Team Manager, School of Computing Science, University of Glasgow**

Research resources generally belong to individuals who need to continually tinker and change things.

### **2.3.7 Dr Hans Senn, Lecturer in Theoretical and Computational Chemistry, School of Chemistry, University of Glasgow**

The School has a cluster for Dr Senn's research group who are the main users. Spare cycles are made available for the rest of the department. Dr Senn would like to try HECToR GPU if particular Molecular Dynamics (MD) codes are already available.

### **2.3.8 Dr Jongrae Kim, Lecturer, Division of Biomedical Engineering and Aerospace Division, University of Glasgow**

Dr Kim was introduced to ERCPool by Dr Millar (see Section 2.3.3) as a candidate for utilising the ERCPool shared computing resources.

Dr Kim's problem is trivially parallel, and he has used Matlab to develop a GPU routine for the analysis which shows a significant speed up. His main issue is that the problem he wishes to run this analysis on would probably take 1-2 days on a single GPU. Dr Kim is therefore keen to use the HECTOR GPU facilities available through ERCPool. This led to a pilot study as described in Appendix A.

### **2.3.9 Dr Ian Chisholm, Director of Computing, Institute of Petroleum Engineering, Heriot-Watt University**

Dr Chisholm attended the ERCPool visit to Guilherme De Sousa, Director of Infrastructure Services (see Section 2.1.4 previously). The data sets for petroleum engineering are usually very large, but often proprietary, so need to be kept very secure. This may preclude usage on a shared facility. A lot of the software used is provided by third parties. This can also make it difficult to use on a shared facility where prolonged negotiations may be required.

### **2.3.10 Dr Robin Westacott, Senior Lecturer, School of Engineering & Physical Sciences, Heriot-Watt University**

Dr Westacott met a member of the ERCPool team at an EPCC roadshow event. Chemical Engineers have access to a local cluster at Heriot-Watt, but this is not optimally supported or administered, therefore is not easy to use. Researchers also have access to machines at the EPSRC UK National Service for Computational Chemistry Software (NSCCS) at Imperial College, where they can use a small cluster which has all the codes they need, including the commercial ones. Typically they use a relatively small number of cores relative to those available on HECToR. Members of Dr Westacott's department were interested in trying out their own scientific code on the EPCC GPU machine. This led to a pilot study as described in Appendix C.

### **2.3.11 Dr Herbert Fruchtl, Scientific Computing Officer, School of Chemistry and the School of Mathematics and Statistics, University of St Andrews**

Dr Fruchtl was recommended to ERCPool by Professor Thomas Krauss (see Section 2.2.5). Dr Fruchtl manages a large computer cluster (~2400 cores) in the School of Mathematics and Statistics. This was bought mainly with an STFC grant to the Solar MHD group (Applied

Mathematics), and with some money from Astronomy (Professor Ian Bonnell, doing Smooth Particle Hydrodynamics, see Section 2.2.5). This cluster replaces the St Andrews half of the EaStCHEM<sup>6</sup> Research Computing Facility, which still exists in a virtual sense, but neither St Andrews nor Edinburgh have their own hardware anymore. In addition there are some sporadic users from Physics (mainly Thomas Krauss' group) and some computational biologists.

At St Andrews there is no central provision of research computing or HPC facilities. The HPC facilities that are available have grown organically within Schools and departments themselves. Researchers, since there is no central provision, have to buy compute resources out of their own grant money. Within St Andrews there is no culture of paying for access to compute resources provided by others.

At present the EASTChem facility only exists on paper since Full Economic Costing (FEC) at Edinburgh means that St Andrews researchers have to pay to use Edinburgh resources and this is too expensive for them. For Edinburgh researchers, the cost of St Andrew resources is the same as it is in Edinburgh under FEC but Edinburgh researchers no longer use the St Andrews cluster. In the past only about 5% of EASTCHEM usage was due to sharing and this was Edinburgh users using St Andrews when Edinburgh was full. The machines were effectively too similar to offer any benefit.

In general, researchers do not know how to apply for funding for compute in any other form. They therefore apply for their own cluster and some percentage of a computing officer to run it.

Chemists often do ad-hoc collaborations which may or may not work so the EPSRC application process is an overly long process that gets in the way of innovation. Moreover chemists are not yet desperate enough for compute power to feel it is their only option. For example, Herbert has HECTOR time available but no-one wants to use it.

A zoo of experimental/novel machines with the necessary consultancy time available to help researchers is good way to allow research groups to more effectively try out new platforms and ideas.

St Andrews has bought an old paper mill at Guardbridge with a view to building a biomass power plant and possibly machine rooms for the University.

### **2.3.12 Dr Edward Graham, Lecturer Sustainable Rural Development Research Theme, University of Highlands and Islands**

Dr Graham wanted access to HPC facilities to investigate using it for his research on the weather and climate change. UHI do not have such facilities. Using the shared computing resources and staff consultancy available through ERCPool, Dr Graham has been able undertake such an investigation, as described in Appendix B.

### **2.3.13 Professor Christos Grecos, Head of School of Computing, University of the West of Scotland**

ERCPool were introduced to Professor Grecos by Dr Brian Mullins, Director of ICT at UWS (see Section 2.1.7. Professor Grecos is also in charge of the Research Computing Strategy for UWS.

Previously at UWS, only the Nuclear Physics group were the only researchers using HPC and facilities at CERN. This group is not as active as it once was.

Whilst UWS are part of ARCHIE-WeSt, researchers at UWS are not interested in sharing since UWS are new to HPC. To date researchers have had sufficient computing resources for their research but it is now recognised that HPC will allow researchers to increase throughput and quality. Even though UWS are part of ARCHIE-WeSt, this does not prohibit them from working with other HPC providers. UWS, in particular, need training in order to use ARCHIE-WeSt.

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<sup>6</sup> <http://www.eastchem.ac.uk/>



### 3 SWOT Analysis of Resource Pooling

This section documents the strengths, weaknesses, opportunities and threats of resource pooling. The content for this section has been gleaned from the visits described in Section 2 and the pilot projects undertaken as part of ERCPool. Whilst the exact categorisation of some of the topics listed is a potential source of debate, the value of the categorisation is in highlighting ways to progress.

#### 3.1 Strengths

- Potential for cost savings in for example, hardware, staff, housing and infrastructure.
- Access to novel platforms that a researcher might not usually have access to eg. I/O intensive vs. CPU intensive applications and architectures.
- The ability to scale up an application without having to buy new hardware and associated costs.
- When there is a community associated with a shared resource there is better support and knowledge transfer.
- Availability of standard software packages without having to provide the personnel to install, maintain and deal with licensing issues.
- Dedicated HPC systems support staff rather than small amounts of effort from staff with a wide range of responsibilities.
- Better overall utilisation of a resource by having many concurrent users.
- Better ancillary services, for instance networking and data backup.
- Possible availability of dedicated application support personnel.

#### 3.2 Weaknesses

- Lack of agreed, well-understood costs/charging models.
- Lack of appropriate licenses from appropriate commercial software vendors.
- Researchers want shared resources that are simple to use.
- Researchers want the application process for shared resources to be simple and quick.
- Researchers want shared resources to be cheap, or even better, free to use.
- Researchers want flexibility in how they use shared resources e.g. extended batch system queue limits.
- Trust between sharing parties is needed and can take a long time to develop, but is easily broken.
- Perceived or real data security and privacy issues, for example for medical or proprietary data.
- Accountability for a remote user.
- Perception that a one-size-fits-all system, centred on a shared, largely homogenous computing centre has been demonstrated to be inadequate for some research projects.
- Administration of local facilities is easier. Using external facilities means a different organisation and operational procedures.
- Lack of debug and development facilities.
- Researchers need training.

#### 3.3 Opportunities

- Researchers are sometimes happy to use someone else's resource if it augments or complements their own.



- Sharing resources provides resilience in the event of failure.
- If remote shared facilities are the only ones available then researchers recognise they just have to get over any hurdles in order to use it.
- Researchers like to try before they buy.
- HPC systems and applications support requires specialist skills whose acquisition impacts on researcher's time or a general IT service.
- HPC applications development requires specialist skills.
- Software as a Service.
- Lots of computing services would like to sell cycles, etc.
- Researchers need training.
- When using any kind of novel technology, a critical part of the support is support for porting and usage. The people providing the hosting are not usually best placed to provide this, and so it often gets overlooked; users initial interest can be lost if they cannot easily make progress.

### 3.4 Threats

- Control and Influence – researchers like to have priority access to their own resource and researchers prefer to take from others rather than give away their own. Researchers like to have control of their own resource and are happier to use a department level facility compared to a remote, say national, facility, where they have even less control and influence.
- Existing career development is based on researchers bringing funds into their own institution rather than in going elsewhere on a shared resource. If part of their grant is to another institution to pay for access and running costs of shared resource then this could be detrimental to their career since that portion will not be used in their home institution's assessment of the academic. For example, pay rises for professors at Glasgow are directly related to the amount of money they put into university central resources.
- Some researchers believe they have reached a plateau where their existing equipment provides sufficient power for the moment and so there is no demand for more.
- Data transfer costs. For huge data flows you need to have access to a higher level in the JANET hierarchy than your local institution.
- Tracking Impact – with an experimental machine, this can be difficult since the machine owners are unlikely to get co-authorship or cited in papers. If they are lucky they might get an acknowledgement. A citation therefore depends on an existing paper about the machine already being out there. Moreover, with an experimental machine there is a very good chance of there being a lot of null results, or simply "it didn't work results" thus further reducing the possibility of tracking impact since such results are unlikely to get published even if they provide valuable information for future hardware/software decisions for research groups. This difficulty in tracking impact is that it will in all likelihood affect sustainability.
- When you buy local resource you can use it for more than just the single project that bought it. If you spend money on shared resource at another HEI then the computing time cannot be used on other projects once it has run out.
- There is a perception that Edinburgh gets a larger share of the supercomputing hosting and support and that this is not fair.
- Geographical remoteness can be perceived to be a barrier to sharing.

## 4 Cost-Benefit Analysis

A true cost benefit analysis is beyond both the scope and resources of the project. In particular, a quantitative analysis of the benefits of sharing novel compute resources is particularly hard; most of the evidence gathered for this report is somewhat anecdotal in nature, particular with respect to the benefits of resource sharing. In addition, due to the novel computing aspect, there is no real prospect of performing any direct comparisons of the costs of a shared resource against a dedicated one – for instance the researchers involved in some of the case studies did not have access to a suitable dedicated resource at all, so no comparison could be made. Likewise, obtaining a measure of the true costs of a compute time is difficult to do, although is clearly important in a world where shared resources are becoming more common. Instead this section will concentrate on some of the comments received during the visits with regard to costs and charging. The benefits of resource sharing are already largely covered in Section 3 in the SWOT analysis.

### 4.1 Cost Models

Any discussion of charging for usage of compute resources clearly needs to take into account cost models – it is impossible to charge for usage until a well formed cost model of a resource has been developed. However, a review of the relevant literature shows this to be a non-trivial exercise. The EU funded e-FISCAL project [6] is studying such problems, and have gathered a useful collection of references [7]. Most of these studies look at the cost of local cluster resources against commercial cloud-computing providers, so are less relevant when considering novel compute resources, which usually have no commercial alternative anyway. The e-FISCAL deliverable D2.2 [8] sums up this literature review nicely, as well as giving a review of some of the costs that need to be taken into account when calculating a resource cost model. These include the obvious capital cost of the resource itself, but then there are several ongoing costs to consider; additional data storage, power, networking, cooling, rental of hosting space, software licences, and most importantly personnel. In addition the depreciation of the resource has to be taken into account if it is to become sustainable – novel resources can quickly become out of date.

The cost of personnel is very important when thinking about costs. All too often these are underestimated, leading to a situation where a resource is less than optimally maintained due to lack of systems-support effort, and therefore the initial capital outlay may be to a large extent wasted. Discussions have also shown that application support effort is critical in enabling efficient usage of novel resources – too often this is completely overlooked, with the assumption that the scientists will just be able to make use of a system themselves. This is a rather naïve view, and easily leads to frustration and a waste of valuable research time.

### 4.2 Benefits

To develop a cost-benefit analysis requires a full understanding of the benefits of using a shared resource in such a way as to allow a direct comparison with a dedicated resource. As already stated this is rather a complex task, and is not attempted here. The benefits of using a shared resource are already covered in Section 3.1. Quantitative studies are rather difficult – how is a benefit measured? A simple method might consider some measure of compute time delivered, however even this is non-trivial, requiring the adoption of an agreed benchmark, which may not be suitable for a novel system. Is this the whole story though, or should the impact be measured in some way? For instance, through the number of scientific publications resulting from the research carried out on a system? These are some of the questions which should be addressed during any follow-up study.

### 4.3 Comments on Costs and Charging

Clearly both the adoption and sustainability of a shared resource depends heavily on the charging model applied to its usage. The visits discussed in Section 2 highlight some opposing views which are not easy to reconcile. On the one hand infrastructure providers are aware of the cost benefits of moving towards larger, shared resources. On the other, many researchers are still reluctant to spend valuable grant money on something that is not owned by them. To change this attitude likely requires a carrot and stick approach – highlighting the benefits of larger, dedicated resources, whilst at the same time funding agencies being less willing to fund personal compute resources as part of grant applications.

As cloud computing gains traction, then the idea of paying for compute time by the CPU hour will become more familiar. It is therefore important that the charging model for shared resources is at least as easy to understand as for commercial cloud providers. This will require those hosting shared resources to have a well developed understanding of their costs in order to develop such a model. Providers have to understand the implications of VAT exemption, both within and outside their institution, as raised by some interviewees. Professor Britton (Section 2.2.3) raised the complication of Full Economic Costing (FEC), and the impact this can have on both resource providers and consumers.

Professor Fedorov (Section 2.2.6) raised the point that he was not so interested in the cost of using a shared resource, more that this cost was easy to find and understand, in order to help the proposal preparation process. He also raised the prospect of different charging models appropriate for different levels of access – although again these should not be complicated nor should there be too many. There could be developer access, where access is provided on an “in-kind” basis to software developers, in return for documentation and usage examples for the scientific application being developed. For users there should be two levels of access, a pump-priming level whereby the feasibility of research may be examined, with a simple application mechanism, before standard charges apply for the main body of the research, which would be granted after a more formal application process.

The funding by EPSRC of several regional HPC centres will lead to a growing expertise in the development of costing and charging models. It is important that this knowledge is gathered and made available to the community in order to facilitate the provision of shared resources by others in the future.

## 5 Overcoming the Practical and Operational Barriers to Resource Sharing

This final section looks at the practical and operational barriers to resource sharing and how they might be overcome, as gleaned from the ERCpool visits and pilot projects. Section 5.1 describes the barriers that have been identified whilst Section 5.2 describes the possible solutions that have been identified.

### 5.1 Barriers to Resource Sharing

The specific barriers gleaned from the visits described in Section 2 and the pilot projects undertaken as part of ERCpool are described briefly below. These are classified into four areas – access, resource management, application-related and costs.

#### Access barriers

- If there are too many hurdles for a researcher to overcome to get access to a shared resource then this puts them off. For example, researchers at Glasgow hate e-science certificates and have therefore been reluctant to use resources such as the National Grid Service that use these, even when such resources are local to them.
- Some researchers much prefer an informal approach to obtaining access to machine rather than the formal RCUK HECToR style process. For example, chemists at St Andrews view the HECToR application process as too cumbersome since they often do ad-hoc collaborations which may or may not work. They therefore view the EPSRC application process as an overly long process that gets in the way of innovation.
- Formal mechanisms for access to EPSRC supplied computing resources are seen to be both advantageous and a hindrance.

#### Resource Management barriers

- Batch processing software can be a barrier to use since researchers often have only used Macs or Windows and never written scripts
- Centralised and bureaucratic resources are not popular with researchers. For example, chemists, generally, hate the 12 hour job length limit on HECTOR since their codes do not scale in a manner that can work within this limit.
- Some academics don't care about SLAs, power outages, etc. and believe that these aspects of a service are not critical.
- EPSRC mechanisms for certifying that a shared resource is suitable for usage on an award are a hindrance. For example, it is not possible to charge ARCHIE-WeSt usage on grant applications until it is certified by EPSRC as a shared resource! This needs a full year's running to determine costs.
- Windows VMs on a shared resource are popular with users but harder to manage since they are not under batch system control.
- Some researchers are reluctant to have VM instances rather than a physical box.
- For some researchers virtualisation is not currently a viable route since it affects I/O and adds an extra layer that affects performance.

#### Application-related barriers

- Shared facilities have been found to be much more work to use.
- The provision of debug/development facility is often forgotten about in national service provision and so the lack of such a facility is real barrier to software engineers using such services.

- Training in HPC is crucial, and needs to be more widely available to potential users.
- More training on the usage of scientific applications should be provided, rather than concentrating mainly on scientific application development.

### Cost barriers

- Users who only occasionally want a lot of compute power can get access to such power through easier means than for example the National Grid Service i.e. buy a big desktop.
- In some HEIs there is no culture of paying for access to compute resources provided by others.
- Researchers do not want to pay for access to other's shared resources.
- For some researchers it is cheaper to buy hardware suited to a code than to re-develop code to fit a particular architecture.
- Billing of debug/develop time vs. productions runs.
- VAT from buying hardware can be claimed back provided the hardware is for internal use. If you sell on services on this hardware to another institution, even a VAT-exempt one, then you are no longer VAT exempt for that hardware.

## 5.2 Overcoming the barriers

Overcoming the access related barriers is primarily about making the resource application process much more lightweight and timely. Regarding resource management, the way to overcome these barriers is to recognise that traditional techniques such as batch management and virtualisation are not appropriate for every circumstance. A range of possibilities needs to be provided that includes simple mechanisms such as email agreements that a research group has exclusive access for a limited period. Pump-priming time is also appreciated by users, so that they can evaluate the feasibility of research before putting a bid for large amounts of compute time. This can include evaluating their own software's suitability to a particular machine's architecture, or testing a range of third-party applications for suitability.

Whilst education and training can overcome these resource management issues, it must be recognised that the undertaking of such adds a further hurdle and potentially time-consuming activity that impacts on research. However, researchers did say that more courses for scientific applications should be provided. Many users don't program but just run third-party applications, and need to know how to use these efficiently, along with help on task farms, data processing etc. This also requires flexibility in the types of jobs that can be run e.g. there needs to be machines where different types of jobs can be run that do not fit the usual 12 hour rule or scale to thousands or even hundreds of cores.

This will therefore help overcome application-related barriers however it must still be recognised that a significant user base will want debug/development facilities and any resource management system needs to be in place that makes this easy to do.

Probably the greatest barrier to resource pooling is the lack of clarity around funding models and costs. Once these are better understood and clear, easy to understand, implement and monitor processes are in place then resource pooling will be far more appealing to researchers. This, however, requires RCUK and HEIs to engage together to resolve this.

This is where a solution based on a shared hosting site for universities may be a possibility and might get over professorial issues. This would allow Scotland to have a research computing infrastructure that has flexibility and a service aspect.

Such a site could host a variety of clusters with differing architectures and formality of service thus matching the range of researcher needs.

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## Appendix A Pilot Study with Jongrae Kim of The University of Glasgow

Our collaborator for this pilot study was Jongrae Kim of the University of Glasgow. His research in Systems Biology concentrates on "stochastic effects and Monte-Carlo simulation using parallel computing algorithms"<sup>7</sup>.

### A.1 Organisation and Non-Technical Considerations

#### A.1.1 Machine access

Access to the HECToR GPGPU machine is administered via the SAFE administration interface<sup>8</sup>. It was very straightforward to give access to our collaborator, with the following steps:

- Request a new group for the ERCPool project.
- Send the prospective user an email with instructions on how to sign up to the SAFE interface. The sign up page is a simple web form taking less than five minutes to complete.
- Approve the user's membership of the ERCPool group.

This led to the relevant machine account on HECToR GPGPU being created.

#### A.1.2 Software Selection and Licensing

The software code used in Dr. Kim's work is a combination of MathWorks MATLAB and nVidia's Compute Unified Device Architecture (CUDA)<sup>9</sup>. It was therefore necessary to license a copy of MATLAB for HECToR GPGPU.

The most appropriate product for this purpose was MathWorks MATLAB Distributed Computing Server (MDCS)<sup>10</sup>. MDCS is a simple batch system which accepts one MATLAB job at a time. Using MATLAB's built in parallelisation capabilities it divides up the work of the task and hands it out to a number of worker processes.

Once installed and configured, MDCS makes it easy for a user to submit compute jobs using MATLAB on their local computer. Results are returned to the user's local MATLAB environment. This allows for a degree of interactivity, though submission of MDCS tasks can also be automated.

MDCS is licensed per number of worker processes available to work on the current task. The cheapest license for MDCS is for eight workers. For an academic license, this costs £1500 for the first year, plus a license maintenance fee of 20% (i.e. £300/year) for subsequent years. However, it was a condition of this license that all users be within a single institution. For the license to cover users outside the institution, the maintenance fee increased to 100% (i.e. £1500/year).

The process of purchasing this license took some time as MathWorks had to draft a legal rider to attach to the software license. The terms of the license restrict use of the software to UK based users only.

### A.2 Technical Work

#### A.2.1 Software Configuration

The first task was to install MDCS on HECToR GPGPU. The installation itself was straightforward, though some work was required to get the license manager to run correctly.

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<sup>7</sup> <http://www.robustlab.org/>

<sup>8</sup> <https://www.hector.ac.uk/safe/>

<sup>9</sup> [http://www.nvidia.com/object/cuda\\_home\\_new.html](http://www.nvidia.com/object/cuda_home_new.html)

<sup>10</sup> <http://www.mathworks.co.uk/products/distriben/>

It was necessary to integrate MDCS with the existing batch system on HECToR GPGPU, Sun Grid Engine (SGE)<sup>11</sup> so that MATLAB jobs did not conflict with other non-MATLAB jobs run on the machine. While SGE is not a fully supported batch system for MDCS, there is example integration code on the MathWorks website.

The other obstacle was the SGE batch system itself which does not allocate GPUs as a resource. This led to a failure mode where a slot was free for the job to run, but when it ran it would find that all of the GPUs were occupied. A workaround was used, telling SGE to allocate an entire node to the job, thus guaranteeing use of all the GPUs. In order to do this a specific node had to be requested, which was not ideal as it did not allow the batch system to allocate nodes optimally.

### A.2.2 Adapting User Software

Dr. Kim provided a small, simple example of the kind of program which he runs on GPGPUs. This was adapted by dividing the code into a server portion which generated data for plots, and a client portion which took these data and generated the data.

It was also intended that the software be adapted to use multiple GPGPUs, but this was not completed due to lack of time.

## A.3 Conclusions

Software licensing can be a problem for equipment sharing. In this example, MathWorks' licensing policy could be an impediment to inter-institution collaboration and resource sharing, by charging vastly more for a license which is open to users outside a single institution. Whilst it is outside the scope of this study, as the license is restricted to the UK, it could also be a problem for international resource sharing.

From this experience, it would appear that MATLAB is currently in transition. Having a strong history of being used interactively on workstations, there is now demand for it to be used in a manner more typical in HPC – that is, on a larger machine, in batch. While MDCS is a big step toward this, the process is by no means complete. For example, lack of officially supported integration with SGE/OGE is surprising given Grid Engine's widespread use in the HPC community.

As well as MATLAB, other "high level" languages such as R and Python are gaining traction in computational science. Some of these languages implement parallelism with minimal changes to the code. For example, MATLAB supports parallel execution of iterations of a loop. In R, it is possible to use SPRINT<sup>12</sup> (5) to easily parallelise some common tasks. Those supporting a shared resource should be prepared to support these technologies in order to attract a diverse user base.

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<sup>11</sup> Since the acquisition of Sun by Oracle, the latest versions of this software are known as Oracle Grid Engine.

<sup>12</sup> <http://www.biomedcentral.com/1471-2105/9/558>



## Appendix B Pilot Study with Eddie Graham of UHI

Our collaborator for this pilot study was at Edward Graham of the University of the Highlands and Islands (UHI). He wished to use the Weather Research and Forecasting Model (WRF)<sup>13</sup> to study rainfall in the west of Scotland, particularly around the Isle of Skye. WRF is a weather research and prediction framework developed by the USA National Center for Atmospheric Research (NCAR)<sup>14</sup> along with a large number of other USA government agencies, and research institutions. It is in widespread use around the world.

### B.1 Organisation

Access to EDIM1 is arranged on an informal basis, as there is no funded support at present. It was easy for our external collaborator to obtain an account on the machine via an email request.

### B.2 Technical Work

#### B.2.1 Software Build

EDIM1 is set up such that nodes are installed with "software appliances". Each software appliance is essentially a variation on the base Linux distribution, ROCKS 5.4<sup>15</sup>. Once such an appliance is created, it can then be copied to all of the nodes which have been allocated to the relevant project.

The cleanest way to do this in terms of compatibility with the base operating system is to use RPM<sup>16</sup> packages. Unfortunately the underlying operating system is relatively old. This meant that a lot of software packages had to be built from source code, in order to use more recent versions. This included the Fortran compiler, gfortran. This is not intended as a criticism of ROCKS or the decision to install ROCKS 5.4 on EDIM1, but more a reflection on the fact that the underlying Linux distribution, Red Hat Enterprise Linux, chooses stability over frequent software updates.

The package building software, rpmbuild, was relatively easy to use for an experienced software developer. It takes a source package and a package description file. Debugging package description files was relatively time-consuming, as testing each change to the description file involves rebuilding the package from the start. Users without experience of building software from source code might find this process challenging.

It is also possible to build node configurations without using the package management system. This possibility was not explored; given the large number of software dependencies involved, it was thought better to use the package management system, which manages such dependencies automatically.

#### B.2.2 Weather Research and Forecasting Model

WRF relies on the WRF Preprocessing System (WPS)<sup>17</sup>. WPS is a set of software applications which help to get the input data for the model into the correct format for a WRF model run.

As supplied, WRF and WPS do not fit well into a packaging system. Throughout, the software applications assume that they are being run in the location where they were built. For the purposes of this project, this was worked around by creating an RPM package which simply unpacks the whole build directory to a single location. This solution is adequate, though not ideal, as it leaves libraries and binaries in a custom directory rather than system default locations.

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<sup>13</sup> <http://www.wrf-model.org/index.php>

<sup>14</sup> <http://ncar.ucar.edu/>

<sup>15</sup> ROCKS is based on CentOS, which in turn is based on Red Hat Enterprise Linux.

<sup>16</sup> Red Hat Package Manager

<sup>17</sup> <http://www.mmm.ucar.edu/wrf/users/wpsv3/wps.html>

The data to be used for the model were from the European Centre for Medium-range Weather Forecasting (ECMWF)<sup>18</sup>. There are groups known to use data from ECMWF with WRF, but support for this seems to still be in its early stages. Some custom software development effort was required to convert the data into the format expected by the WPS tools.

In general the WRF documentation is written for meteorologists rather than software developers. It also assumes knowledge of modelling in general, and the impression was gained that the vast majority of its user base has been trained academically in weather modelling. While this is perfectly sensible given its audience, it sometimes impeded progress where extra research was required to understand a particular concept in the model.

The configuration of WPS/WRF (in particular the custom software development required) took much longer than expected, and so it was not possible to get WRF running on EDIM1 before the end of the project.

### **B.3 Conclusions**

WPS and WRF both proved difficult to build and configure. A scientist without modelling experience would have found this more so, and therefore taken more time, losing valuable research opportunities. This illustrates the importance of having dedicated application support for shared resources.

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<sup>18</sup> <http://www.ecmwf.int/>

## Appendix C Pilot Study with Dirk Mütter

Our collaborator for this study was Dirk Mütter of Heriot-Watt University. Dirk is modifying his simulation code to use GPGPU acceleration, programmed using CUDA, and required access to a more modern generation of GPGPU cards.

Dirk was provided with access to the HECToR GPGPU machine in the same way as Jongrae Kim. He was able to run his application with no further assistance. This produced a 2-3 times speedup over the earlier generation GPGPU card he had access to in his home institution. This was also a significant speedup (7-10 times) over a serial version running on a general purpose cluster node.

A small barrier encountered was the maximum runtime for jobs of twelve hours. This required the workflow to be slightly modified to allow job restarts. A longer queue length would be preferred if possible.