N8 HPC

Annual Report 2015

Executive Summary

A survey of all Principal Investigators who have a project registered on N8 HPC was carried out over August – September 2015. The findings demonstrated that N8 HPC is providing a good reliable service with good support which is very much appreciated. There are some concerns over the length of time taken to run jobs and demand for the expansion of resources.

Impact of the use of N8 HPC was demonstrated through:

- Research outputs are increasing rapidly with 182 research papers acknowledging the use of N8 HPC resources.

- 31 grants have been submitted, prepared or awarded which specifically mention the use of N8 HPC.

- The largest grant to mention the use of N8 HPC is an EPSRC funded project from the University of Sheffield called which has a value of £5.3M.

- The total value of all grants is £22.4M

- There are 12 industry-related PhD studentships utilising N8 HPC resources.

Aims of N8 HPC

N8 HPC was funded in 2012 with 3 main aims –

- seed engagement between industry and academia around research using e-infrastructure
- develop skills in the use of e-Infrastructure across the N8 partnership
- share the asset of skills and equipment across the N8 partnership via the facilitation of networks of people

This survey has demonstrated that we are meeting these aims.

Seeding Engagement between Industry and Academia

- 24% of respondents stated that their projects on N8 HPC facility involve industrial collaboration with 17 individual companies named. 76% of industrial collaborators were aware of their usage of N8 HPC.
- 12 industry-related PhD studentships making use of N8 HPC resources
- Use of N8 HPC resources has been directly responsible for 2 instances of collaboration with UK industry and 3 overseas industry collaborations
- There have been 2 knowledge partnership grants which have made use of N8 HPC.

Developing skills in the use of e-infrastructure across N8

- The use of N8 HPC has enabled 19 PI's to gain access to Tier 1 resources such as ARCHER and Hartree compared to 9 in 2014.
- A further 2 PI's have applied for access to Tier 1 resources and are currently awaiting confirmation

Sharing skills across N8

- Use of N8 HPC has enabled 7 instances of collaboration between N8 universities and 13 collaborations with non-N8 UK institutions as well as 30 overseas academic collaborations.

N8 HPC Annual Survey 2015

Introduction

N8 HPC began in October 2012 with a pilot phase which lasted approximately 5 months. During this phase each institution invited selected researchers to start using the facilities with the aim of trouble shooting any initial problems and ensuring that the machine was running properly.

After the initial pilot phase, the facilities were opened up further to key researchers from all N8 institutions. The machine usage has increased to the point where the machine has been fully utilised over the last year.

In order to assess the impact the usage of N8 HPC has had on research at the N8 Institutions during the last 2 years, a survey was sent to the PI's of all registered projects on N8 HPC. The 2015 survey was again based on the 2013 and 2014 surveys with only minor modifications. The survey was again split into two parts – part one to investigate the impact N8 HPC has had on research; part two to examine how the facility was performing in terms of service.

The survey had a 56% response rate compared to last year's 68.4%. This may have been partly due to the implementation of a new system which sent a personalised link to each PI. This reduced the amount of admin work required to keep track of who had still to respond. However it did mean that group reminder emails could not contain a link to the survey and if the PI had deleted or misplaced the email a generic survey link could not be sent. Many reminders were sent out to all PIs containing their individual survey links. The response rates from the individual institutions are shown below in Fig.1.
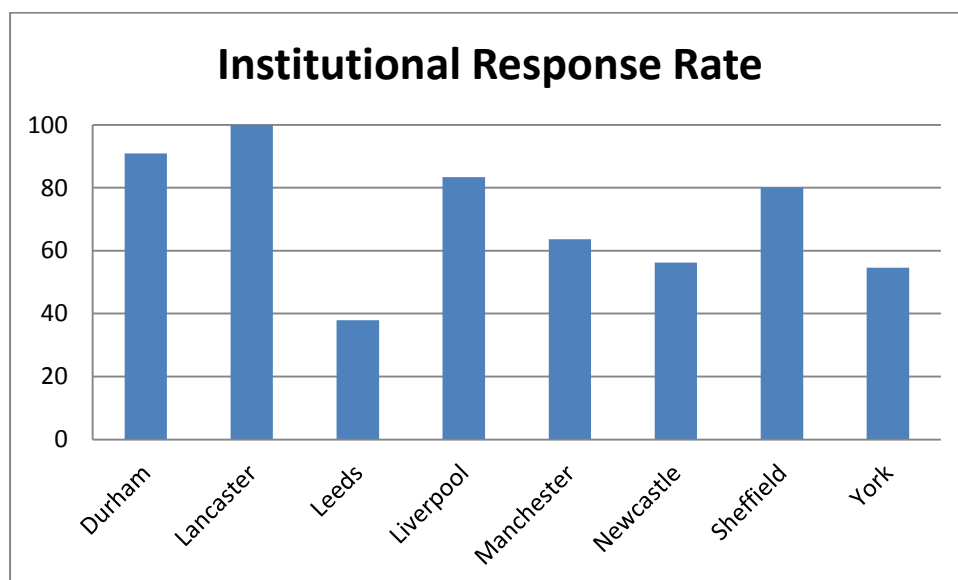
Part 1: Impact of N8 HPC on Research Outputs

Research Papers

> *Q1. Please list the details of any publications (including those in in preparation, submitted or in press) that are associated with the use of N8 HPC.*

PI's were asked for details of any papers that were associated with and / or acknowledged the use of N8 HPC.

In summary 182 papers have been produced in the last 12 months and comparisons against previous year's numbers can be seen in Fig. 1.
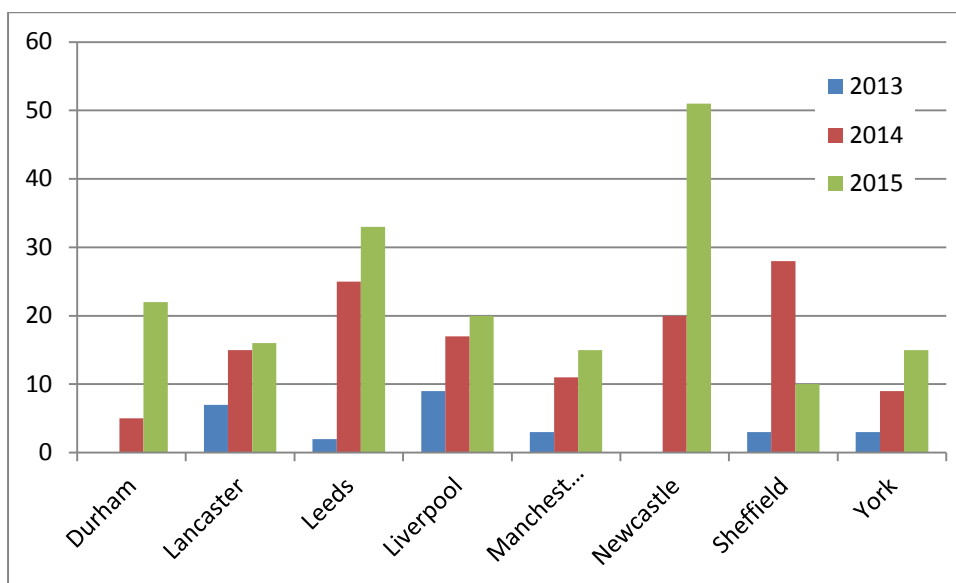

Fig. 1. Number of papers acknowledging use of N8 HPC over the last 3 years.

Research Grants

> *Q2. Please list the details (including funding body) of any grant applications which state the use of N8 HPC and indicate the status and monetary value of these grants.*

There are currently 16 active grants that state the use of N8 HPC facilities with 9 more submitted and 6 in the preparation stage. There were also another 3 grants that stated the use of N8 HPC that have come to an end in the last 12 months. The value of the grants ranges from £7,000 to £5.3M with the total value of grants in all stages being £22.4M. The full list of grants which state the use of N8 HPC resources can be found in Appendix 2.

Industrial Studentships

PI's were asked for the details of any industry related PhD studentships which made use of N8 HPC resources. 12 industry related PhD studentships were reported compared to 13 in 2014 and 7 in 2013. A full list together with the industry partners is available in Appendix 3.
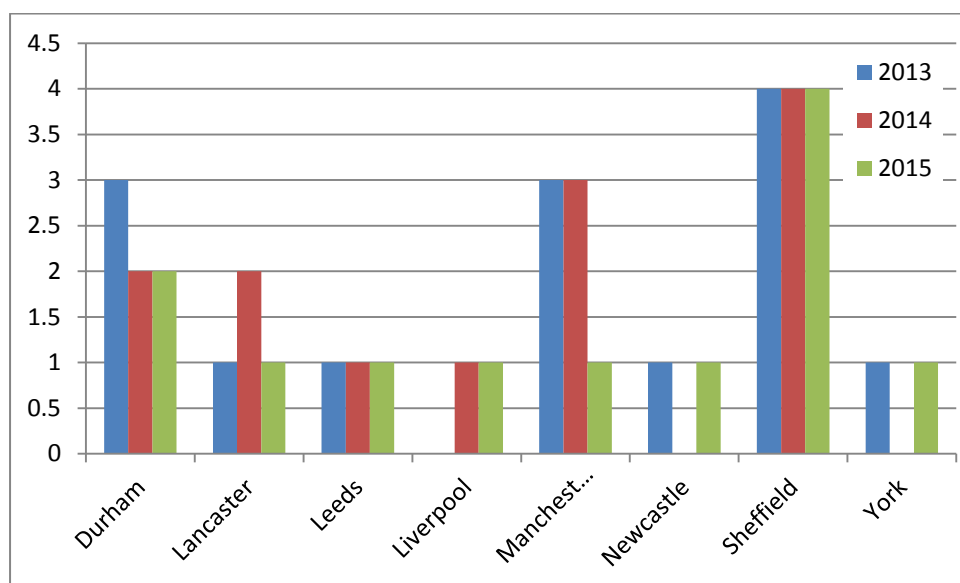

Fig. 2 Number of existing and forthcoming industry studentships at N8 institutions.

Enabling Collaboration

The first three categories in the graph below refer to academic collaboration enabled by the use of N8 HPC services. There has been a slight decrease from previous years regarding collaboration within N8 universities but collaboration between academics from UK non-N8 universities and overseas especially continues to grow. Industry collaboration has remained static or decreased since last year.
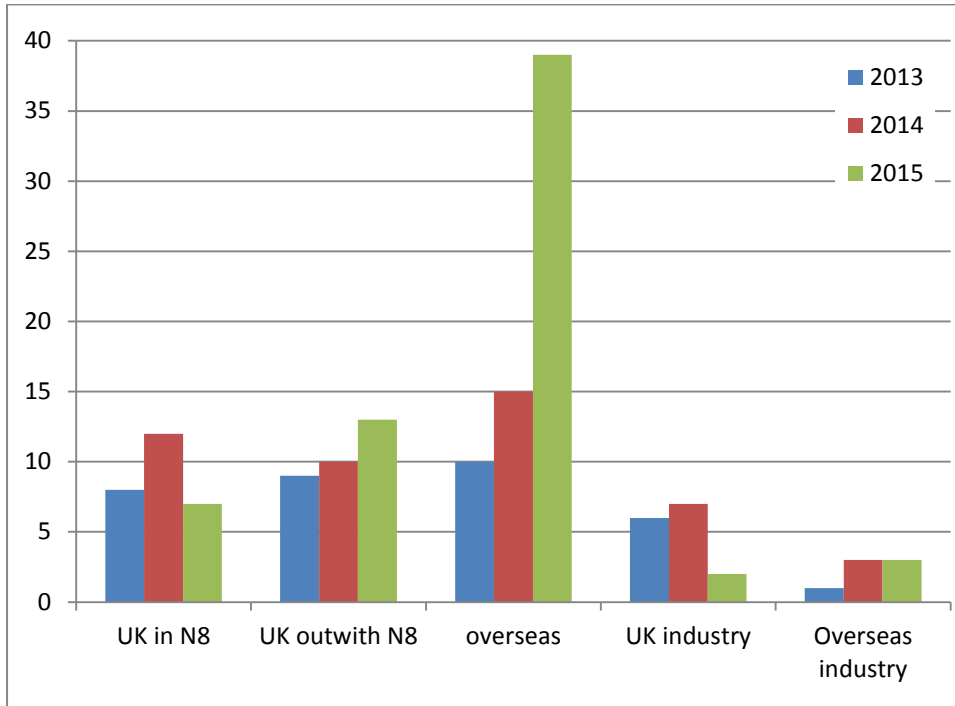
Fig. 3 Collaboration as a result of N8 HPC usage

Industrial Collaboration

> *Q5. Does your research using N8 HPC involve any industry collaborations (funding, joint research projects etc)?*

> *Q6. Do any of your N8 HPC projects involve the NHS? If so please give details.*

> *Q7. Do any of your N8 HPC projects involve the Met Office? If so please give details.*

> *Q8. If applicable, is your industrial partner aware of your usage of N8 HPC?*

In 2015 only 24.3% of projects confirmed some sort of industry involvement compared to 35% in 2014 and 60% in 2013 demonstrating a substantial decrease. 17 companies were named with Samsung and EDF mentioned twice. This is a substantial decrease in the 36 companies named in last year's survey.

Only two projects have any NHS involvement with the same number having Met Office involvement. Industrial collaborators awareness of N8 HPC usage has increased with 76% of PIs stating that their industry collaborators were aware of their use of N8 HPC compared to 52% last year.

Industrial Collaborative Papers

> *Q9. Have you produced any joint academic-industry publications involving the use of N8 HPC? If so please provide details.*

This year there are 6 published joint academic-industry publications with another 2 in preparation. This compares with 1 published and 3 submitted in 2014 and 2 published and 4 in preparation in 2013.

Funding Sources

> *Q10. Does your N8 HPC associated research involve funding from any of the following channels? AHRC, BBSRC, EPSRC, ESRC, MRC, NERC, STFC, Charity grants, TSB grants, Knowledge Transfer Partnerships, Other, please specify*

For the first time the majority of projects utilising N8 HPC are funded by "other" which includes The next largest funding group is EPSRC and then NERC.

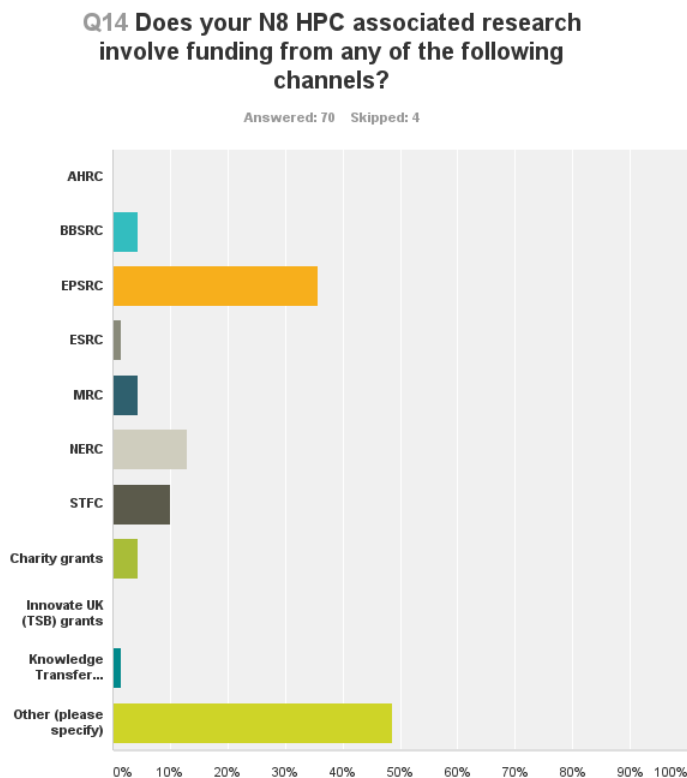In the "other" category the biggest source of funding was the EU followed by "none".

Fig. 4 Funding sources for N8 HPC projects

Knowledge Partnership Grants

> *Q11. Have you had any knowledge transfer projects (KTP, KTNs etc) that involve N8 HPC?*

In 2015 there were 2 projects that came under this category:

- Jaume Bacardit, Newcastle University
  - KTP - Applying Data Mining to create intelligent CAD tools. Start date: June 2013, End date, June 2015

In 2014 the following Knowledge Partnership Grants made use of N8 HPC.

- Alistair Revell, University of Manchester
  - Impact Acceleration Account - Transfer of turbulence modelling developments to Industrial commercial code.

Contact with university Business Engagement Managers

> *Q12. Have you had any contact from your institution's Business Engagement team regarding N8 HPC? If so please provide details. Have these discussions proved fruitful?*

97% of project PIs have had no contact from their Business Engagement Manager up from 94% in 2014.

Interaction with CDTs

> *Q13. Are you involved in a Centre for Doctoral Training (CDT) at your institution? If so please give details of the CDT, your role and if N8 HPC is used or could be used within the CDT.*

This was only the second year that this question has been asked. In 2014 11 project PIs identified themselves as having involvement with CDTs. This year the number was reduced to 8 with involvements including Deputy Director and teaching staff.

Access to Tier 1 Resources

> *Q14. Has your use of N8 HPC allowed you to move upwards and gain access to any Tier 1 (ARCHER, Hartree) and Tier 0 (PRACE/Tianhe/Xsede) resources? If so please give details of the resource used.*

This year 19 PIs and researchers have gained access to Tier 1 resources such as ARCHER and Hartree through their use of N8 HPC with another 2 PIs having applied for access and currently awaiting confirmation. This is in contrast to 10 PIs gaining access in 2013 and 9 in 2014.

Part 2: Service Satisfaction with N8 HPC

Project Applications

> *Q15. How easy did you find the N8 HPC project application procedure? (1- difficult; 5 – easy)*

Respondents were asked to rate the N8 HPC project application procedure on a scale of 1- difficult; 5 easy. The project application form was replaced in October 2015 but the responses to this survey relate to the retired application form.

The average satisfaction score was 4.31 which is comparable to the previous year's results of 4.32 in 2014 and 4.37 in 2013 showing that there is still a high level of satisfaction with the procedure. The majority of comments were positive with 1 user experiencing difficulties in obtaining a project code. This matter was dealt with by the relevant institution and procedural reviews put in place.

User Applications

> *Q16. If you have applied for a user account, how easy did you find the N8 HPC user application procedure? (1- difficult; 5 – easy)*

Once a project has been approved it is issued with a code by the local institution N8 HPC helpdesk. This code must be entered into the user application form by researchers associated to that project who wish to apply for an account.

Respondents were asked to rate the user application procedure on a scale of 1- difficult; 5 easy. The average score was 4.42 up slightly on 4.38 from last year. A couple of issues on problems with the application procedure working smoothly once the form had been submitted were raised. These will be passed onto the relevant institutions.

Both the project and the user application pages will be revised in December 2015 to make them easier to navigate.

Technical Documentation

> *Q17. Does the technical documentation on the N8 HPC website meet your needs?*

> *Q18. Is there anything missing from the technical documentation or is further explanation required in any area?*

The website has been present in its new form for about a year and feedback was sought on the type and quality of information provided on the website. 83% of respondents felt that the technical documentation met their needs, an increase from 81.8% last year and 80.4% in 2013. Two users were unhappy with the technical documentation on the website – one stated that they hadn't used the documentation and the other gave no reason. This will be followed up.

Running Jobs

> ### Q19. Have you or your researchers run a job on the N8 HPC?

86% of the respondents or their researchers had run a job on the system compared to 95% in 2014 and 92% in 2013. 8 PIs replied to say that their researchers had not run a job on N8 HPC and 2 more were unsure. It is unclear why there has been a drop in researchers running jobs on N8 HPC. The respondents were spread across several sites – Durham (2), Lancaster (2), Manchester, Sheffield and York (2).

Support and Helpdesks

> ### Q20. Have you or your researchers required support at any point to run a job on N8 HPC?

46% of respondents have required help to use N8 HPC which is down from 63% in 2014 and 62% in 2013. This may reflect the maturity of the projects and users on the machine.

Of the people that required assistance 92% received the help they required. The remaining 8% (3 respondents) will be contacted to find out more information.

> ### Q21. If you required support did you know how to contact the correct helpdesk (i.e. your local helpdesk)?*

The helpdesk provision at N8 HPC is devolved to the local institution with researchers asked to contact their local N8 HPC helpdesks in the first instance. The email addresses for the helpdesks are listed on the new N8 HPC website under "Help" and then under "Helpdesk". This year 95.5% of respondents knew how to contact the correct helpdesk compared 100% last year. The help pages on the website are earmarked for revision which will hopefully make it easier for users to know who to contact.

> ### Q22. Was your helpdesk query handled in a satisfactory and timely manner?

86.7% of respondents who contacted their local helpdesk for assistance felt that their query was handled in a satisfactory and timely manner. Four respondents felt that their query had not been handled satisfactorily and follow up will take place with these PIs.

Training

> ### Q23. Do you or your research team require any training that could be provided locally or within N8? If so please give details.

Eight PIs (a decrease of 1 compared to 2014) said that their research team would benefit from training. A list of training recommendations from the PI's is listed below –

- GPU and MPI training
- Parallel programming in FORTRAN
- Training on GPU programming, possibly starting from OpenACC.
- Python course

- Courses on HPC and serial/parallel programming (e.g. fortran, MPI, OpenMP)
- Code profiling training
- Abaqus
- Training is always useful, especially for new PhD students.

We will be carrying out a user survey in the near future in which we will ask the users if there is any additional training they require. We may receive further answers from the researchers that use the machine on a regular basis.

Personal Recommendations

> *Q24. Would you recommend the use of N8 HPC to colleagues?*

98.6% of respondents would recommend the use of N8 HPC to their colleagues (up from 95% in 2014 and 94% in 2013). Only 1 PI said that they would be unable to recommend using the resource but no reason was given.

Looking to the Future

> *Q25. Do you have any further feedback you would like to provide? Are there any improvements you would like to see?*

22 feedback comments were received with most comments being categorised under "praise and thank you". Queuing issues and various technical requests were the next two most popular categories. Full details of the comments received are in Appendix 4.

Success Stories

> *Q26. We are always looking for success stories and case studies to publicise on the N8 HPC website and further afield to organisations such as the Department of Business, Industry and Skills (BIS) and Innovate UK. If you have a story then please leave brief details and we will get in touch.*

Several PIs volunteered to help with case studies of which there are 5 good leads that will be followed up soon.

Conclusion

Overall researchers were happy with both the machine and the level of service provided. Particular praise was given to the quality of local helpdesk support and the ease of application. There were decreases in some aspects of industry collaboration and this may need to be addressed by the institutions. Examples of researchers transitioning between HPC Tiers continues to rise demonstrating that regional centres can play an important role in aiding researchers access to larger resources.

Appendix 1 – list of academic output acknowledging the use of N8 HPC
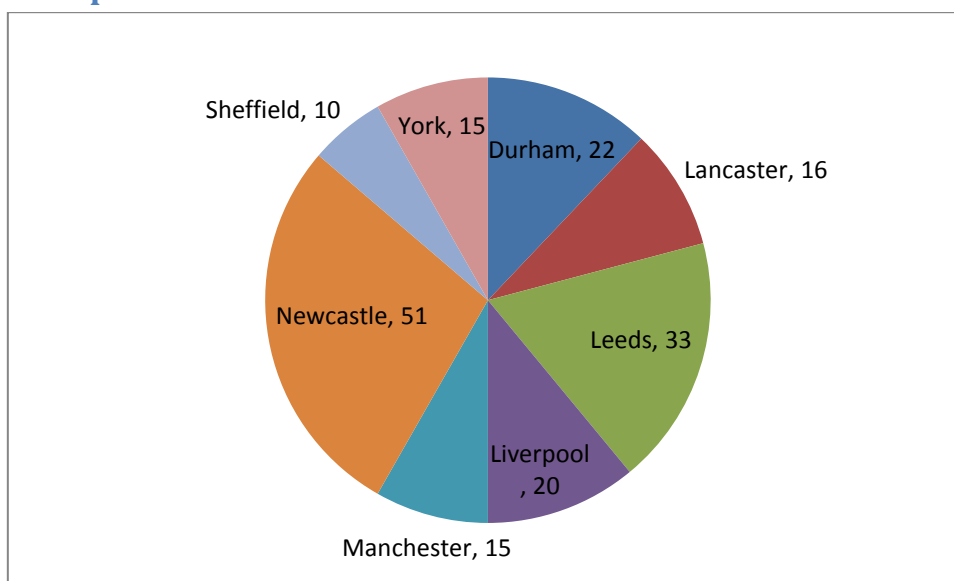
Academic Papers

Fig. 4 Number of papers produced by each N8 institution acknowledging N8 HPC.

Appendix 2 – List of research grants mentioning the use of N8 HPC resources

PI	Institution	Grant Title	Funding Body	Grant Status
Anthony Yeates	Durham	Dynamics of Complex Magnetic Fields: From the Corona to the Solar Wind	STFC	Active
Stewart Clarke	Durham	EP/I029907/1 Castep: Advanced spectroscopies using high-performance computing	EPSRC	Ended
Stewart Clarke	Durham	EP/J011533/1 New transition metal oxychalcogenides	EPSRC	Ended
Stewart Clarke	Durham	EP/K013718/1 Support for the UKCP consortium	EPSRC	Active
Stewart Clarke	Durham	EP/M010953/1 Strong correlation meets materials modelling:DMFT and GW in Castep	EPSRC	Active
Mark Booth	Durham	Health, environmental change and adaptive capacity: mapping, examining and anticipating future risks of water-related vector-borne diseases in eastern Africa (Healthy Futures)	EU FP7	Ended

Halim Kusumaatmaja	Durham	Modelling Liquid Infused Surfaces	EPSRC	In prep
Halim Kusumaatmaja	Durham	Wetting on Structured Surfaces	Industry	Active
Jamshed Anwar	Lancaster	EPSRC CASE studentship with AZ	EPSRC	Active
Chris Lingwood	Lancaster	Microwave filters with improved power handling capabilities for satellite applications	STFC	Active
Ruza Ivanovic	Leeds	Forward modelling of past abrupt climate transitions	NERC	Active
Andy Nowacki	Leeds	The Secret History of the Earth's Mantle	Leverhulme Trust	Active
Zlatko Papic	Leeds	ERC Starting Grant 2015	ERC	Submitted
Prof C A Jones	Leeds	Rapid Dynamics in the Earth's core	NERC	Ended
Lauren Gregoire	Leeds	Constraining ice sheet evolution during the last deglaciation	NERC - NSF	In prep
Gilberto Teobaldi	Liverpool	Advanced new linear-scaling constrained density-functional theory approaches	Royal Society	Active
David Schultz	Manchester	Palaegeography and Palaeoclimate Through The Ages	NERC	Submitted
William Sellers	Manchester	The Mechanics of Hand Use and the Evolution of Modern Humans	Leverhulme Trust	Submitted
William Sellers	Manchester	Marie Skłodowska Curie 2015 fellowship: RPG-2015-323 "IMPACT" Inside out: unravelling the Miocene PrimAte loComoTion through their internal skeletal design	EU	In prep
Paul Bushby	Newcastle	Solar and planetary physics at Newcastle University	STFC	Submitted
Carlo Barenghi	Newcastle	Superfluid Dynamics of Quantum Ferrofluids	EPSRC	Active
David Swailes	Newcastle	'Multiphase flows in boundary layers: The development fundamental models based on advanced numerical and experimental studies'	EPSRC	In prep
Jacek Cala	Newcastle	EU-Brazil Cloud infrastructure Connecting federated resources for Scientific Advancement	EU	Active

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Nilanjan Chakraborty	Newcastle	Fundamental understanding and modelling of differential diffusion effects in turbulent premixed combustion: A DNS based analysis	EPSRC	Submitted
Nilanjan Chakraborty	Newcastle	Numerical and experimental investigation of oxy-fuel coal combustion simulation	EU H2020	In prep
Graeme Sarson	Newcastle	Magnetic fields and cosmic rays in high-redshift and nearby spiral galaxies	STFC	Submitted
Prof Ning Qin	Sheffield	DRAGY: Turbulent Boundary Layer Drag Reduction	EC H2020	Active
Prof Ning Qin	Sheffield	IDREA: Adjoint optimisation		In prep
John Harding	Sheffield	Hard-soft matter interfaces; from understanding to engineering	EPSRC	Active
John Harding	Sheffield	In-Situ Formation of Advanced Nanoparticulate Materials	EPSRC	Submitted
John Harding	Sheffield	SoS RARE: Multidisciplinary research towards a secure and environmentally sustainable supply of critical rare earth elements (Nd and HREE)	NERC	Active
Shuisheng He	Sheffield	On the theory of transition of transient channel flow	EPSRC	Submitted
Robert von Fay-Siebenburgen	Sheffield	Consolidated Grant Support for the Solar Physics and Space Plasma Research Centre (SP2RC)	STFC	Active
Vlado Lazarov	York	EP/K03278X Half-metallic ferromagnets: materials fundamentals for next-generation spintronics	EPSRC	Active
Vlado Lazarov	York	EP/K013114/1 Half metal oxides: In search for 100% spin polarised materials	EPSRC	Ended
Jon Hill	York	Feeling under the weather: what are the health and wellbeing effects of extreme weather events?	NERC	Submitted
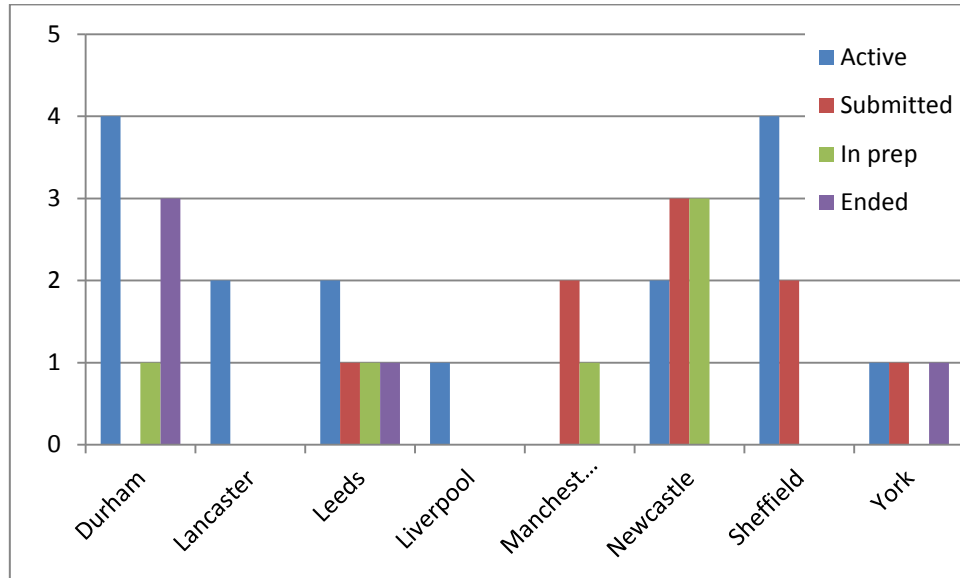
Fig. 5 Number of research grants and their state at the time of the survey per institution.

Appendix 3 – list of industrial studentships involving N8 HPC

PI	Institution	Funders	Title	Dates
Chris Greenwell	Durham	Durham Uni Scholarship	Nanogeochemistry of low salinity EOR	2013 - 2017
Halim Kusumaatmaja	Durham		Lattice Boltzmann simulations of liquid infused surfaces	2015 - 2019
Jamshed Anwar	Lancaster	EPSRC CASE	Molecular simulation of crystal growth	2014 - 2018
Sarah Harris	Leeds	EPSRC	Importance of Entropy in Drug Design	2013 - 2017
Ming Li	Liverpool	EPSRC	3D modelling morphological impact of Offshore wind farm	2013 - 2017
Alistair Revell	Manchester	iCASE	Application of recently developed Embedded Large Eddy Simulation for detailed investigation of flow physics	2014 - 2018
Patrick Briddon	Newcastle	EPSRC	Modelling Diamond CASE project	2013 - 2017
Ning Qin	Sheffield	EPSRC	Robust Optimisation of Shock Control Bumps	2013 - 2016
Ning Qin	Sheffield	EPSRC	Parameterisation and optimisation of aircraft winglet	2013 - 2016
Ning Qin	Sheffield	EPSRC	Adjoint mesh sensitivities and optimisation	2014 – 2017
Ning Qin	Sheffield		Adaptive mesh using adjoint	2014 - 2018
Roy Chantrell	York		Advanced materials for Magnetic Random Access Memory	2013 - 2017

Appendix 4 – feedback comments received

Expansion of resources

More cores please.

Queues

The queue times for York users seem to be getting worse again …

Queue time too long. Sometimes the queue time exceeded the run time and so it was more effective to run the code on a desktop. If the code crashes you have to queue again. Once the resource is given it should be kept to allow quick bug fixes.

It is a concern that the turn-around time of jobs is getting longer and longer. This is perhaps the result of having more users on the system.

Technical Requests

48 hours for the maximum time of a job seems to be quite a short job. My PIC simulations can take over 10 days so I keep having to log back in and restarting it every two days. The code only dumps data at regular intervals, so if its half way between that interval when it gets to 48 hours the job will just cut out and that data is thrown away. So longer job submissions would be really useful.

Allow (short) jobs with massive core counts to pass easier/faster

Integrate our local HPC directly to the N8 so that it just requires a specific queue to send the job directly to N8 supercomputer

Latency should be improved between nodes to allow latency sensitive applications to scale. Also larger groups of topologically close nodes (>256 CPUs) should be requestable from the queuing system.

More standard modules, e.g. Python, Scipy, PETSc, Zoltan, VTK, SCOTCH, Parmetis, for CFD

Much of our work has been undertaken using GPUs hosted at The University of Sheffield. A limitation with the N8 facility is the availability of sufficient storage for ensembles of long time period MHD models. (i.e. some analysis is undertaken using IDL before moving data back to local institutional storage.

Support

The quality of support received by my group was varied, ranging from excellent to less so.

Since applying in June, and after numerous follow up emails, we still haven't been given the access we need to run a job.

Miscellaneous

The N8 meetings are very useful.

Thank you!

Please do not shut the service. It has been useful in our research for publications, and we are using this to pump prime potential grant applications (the first one we submitted happened to be rejected). However, since we have used this service only recently, we do not have much to show, and yet there are several manuscripts and research grant applications that are in the pipeline at the moment. We are optimistic that they will be fruitful in the near future.

Very happy with service

This continues to be a very useful service which fills a void in the capabilities, particularly with the industrial spin.

We have always received a good level of support when using the N8, queries are answered promptly and helpfully. Support staff have given us advice as to how to check our model performance etc. This is very important for our group as we are continually developing new code and running the model in different ways.

The system works excellently for me. It has facilitated a number of high profile publications in the last year or so and it integral to my research activities.

For my purposes, working with N8 has been very efficient.

Great resource!

Great service. I'm really pleased my Leeds collaborator told me about it & having used it over the past couple of months for a small masters project I can now imagine using it in the future for new projects. One of the best aspects is that it is shared between Universities facilitating collaborations.

N8 HPC has provided an excellent and reliable service.

It has been an easy to use and very useful resource.