

N8 HPC Annual Report 2014



Executive Summary

A survey of all Principal Investigators who have a project registered on N8 HPC was carried out over July – August 2014. 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 130 research papers produced acknowledging the use of N8 HPC resources.
- We have also been notified of 29 conference paper produced acknowledging N8 HPC
- After 18 months of full open service, 36 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 "Application to the Individualised Multi-Scale Simulation of the Musculoskeletal System".
- In addition grants totalling over £16M mentioning the use of N8 HPC have been awarded or are active with grants totalling over £3.2M under review and a further £1.2M worth of grants in preparation.
- There are 13 industry-related PhD studentships utilising N8 HPC resources double that of 2013.



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

- 35% of projects on the N8 HPC facility involve industrial collaboration with 36 individual companies named. Over 50% of industrial collaborators were aware of their usage of N8 HPC.
- 13 industry-related PhD studentships making use of N8 HPC resources
- Use of N8 HPC resources has been directly responsible for 7 instances of collaboration with UK industry and 3 overseas industry including companies such as the La Farge Group.
- There have been 3 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 9 PI's to gain access to Tier 1 resources such as ARCHER and Hartree.
- A further 4 PI's have applied for access to Tier 1 resources and are currently awaiting confirmation with another 4 expecting to apply in the future.

Sharing skills across N8

• Use of N8 HPC has enabled 12 instances of collaboration between N8 universities and 10 collaborations with non-N8 UK institutions including University of St Andrews, Imperial College London and the University of Bristol.



N8 HPC Annual Survey 2014

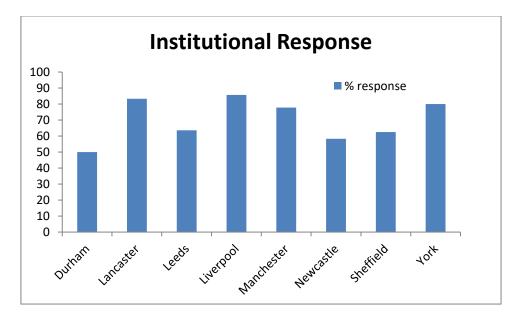
Introduction

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 2014 survey was based on the 2013 survey with only minor modifications and it 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 68.4% response rate compared to last year's 88.5% which may be due to some projects no longer being active on N8 HPC. 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 papers that are associated with the use of N8 HPC.

PI's were asked for details of research papers that were associated with and / or acknowledged the use of N8 HPC. In comparison to last year when many of the papers were "in preparation", many have now been published or are in press. A full list of papers is given in Appendix 1.

In summary 130 papers and 29 conference papers have been produced acknowledging N8 HPC. This is in contrast to 27 papers and 7 conference papers as reported in the 2013 survey – an increase of more than 480%. The substantial increase is to be expected as the number of projects has increased by approximately one third and many projects have been using the resource for over a year.

Further investigation will be undertaken regarding the impact of the published papers e.g. impact rating of the journals. The full list of all published papers and links will be published on the N8 HPC website in the future.

Research Grants

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

After 18 months of full service there are now 21 active grants which stated the use of N8 HPC facilities with 9 more submitted and 5 in the preparation stage. This leads on from last year's annual survey which stated that 17 grants had been submitted specifically mentioning the use of N8 HPC. The value of the grants varies from £10,000 to £4 million with the majority being funded by EPSRC. The full list of grants which state the use of N8 HPC resources can be found in Appendix 2.

Industrial Studentships

Q3 Do you have any industry-related PhD studentships who use N8 HPC resources? If so please give details of the PhD including start and finish dates, title, industry collaborator, funding body and title of PhD.

PI's were asked for the details of any industry related PhD studentships which made use of N8 HPC resources. This area has shown substantial growth compared to 2013 figures. Last year there were 7 existing industry-related PhD studentships with another 7 due to start. In 2014 there are 13 industry-related PhD studentships, almost double the figure recorded last year. A full list together with the industry partners is available in Appendix 3.

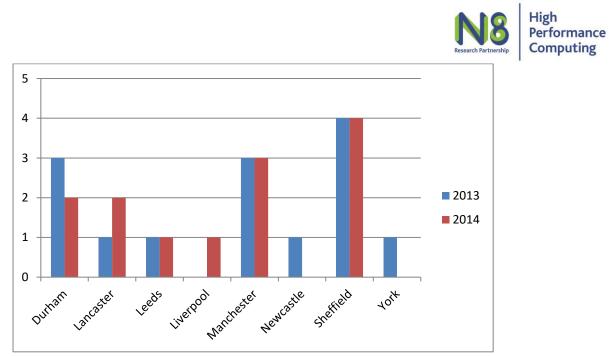


Fig. 1 Number of existing and forthcoming industry studentships at N8 institutions.

Enabling Collaboration

Q4 Have you collaborated with another researcher, institution or industrial partner due to your use of N8 HPC? If so please give details.

Compared to 2013 there has been an increase in the amount of industrial collaboration through the use of N8 HPC facilities as well as academic collaborations. It has been interesting to note that collaboration between (and also within) N8 institutions continues to grow. Some examples of overseas collaborators include San Paulo University; University of Florence; Lamont-Doherty Earth Observatory, USA; Pacific Northwest National Laboratory, USA. The UK industrial collaborators include Sun Chemical, Lafarge, Schlumberger, BP and Jaguar LandRover.

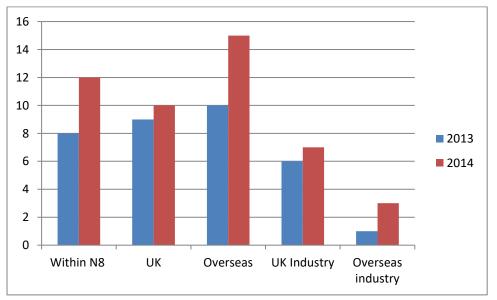


Fig. 2 Collaboration as a result of N8 HPC usage



Industrial Collaboration

Q5 Does your research involve any industry collaborations (funding etc)?

Q7 Is your industrial partner aware of your usage of N8 HPC?

In 2014 only 35% of projects confirmed some sort of industry involvement compared to 60% in 2013 demonstrating a substantial decrease. However there was only a decrease of 1 individual company – 36 in 2014 compared to 37 in 2013. Industrial collaborators awareness of N8 HPC usage has remained constant at around 52%.

Industrial Collaborative Papers

Q8 Have you produced any joint academic-industry publications? If so please provide details.

In 2013 2 joint industry / academia papers had been published with another 4 in preparation by the time of the annual survey. In 2014 details of 1 published and 3 submitted joint industry / academia papers were received. The slight decrease in the number of joint industry / academia papers may be due the decrease in industry collaborative projects.

Funding Sources

Q9 Does your research involve any of the following? Research Councils; Charity grants; TSB grants; KTPs; Other

The majority of projects utilising N8 HPC are funded by EPSRC with the next largest group being unfunded research. The "other" category included funding from industry, EU, NSF, The Royal Society and researchers own universities.

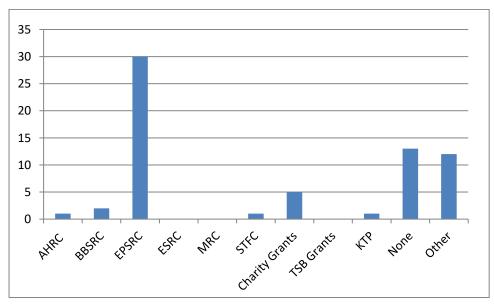


Fig. 3 Funding sources for N8 HPC projects



Knowledge Partnership Grants

Q10 Have you had any knowledge transfer projects (KTPs, KTNs etc) that involve N8 HPC? If so please provide details.

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

- Chris Greenwell, Durham University
 - EPSRC Knowledge Transfer Account Industrial Fellowship, Dr Dawn Geatches to the Lafarge Group to study molecular modelling methods for understanding hydration in clays (2011).
 - EPSRC Pathways to Impact funding was received for Dawn Geatches to develop computational methods to study reactivity between clays and inorganic swelling inhibitors in partnership with Dr Stewart Clark (PI, Physics) and M-I SWACO (2010).
- Alistair Revell, University of Manchester
 - Impact Acceleration Account Transfer of turbulence modelling developments to Industrial commercial code with CD adapco.

Contact with university Business Engagement Managers

Q11 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?

94% of project PIs have had no contact from their Business Engagement Manager. One researcher had had a useful discussion but concerns were raised from PIs regarding the understanding and applications of HPC amongst Business Engagement Managers.

Interaction with CDTs

Q12 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 a new question introduced to the survey this year. Eleven project PIs identified themselves as having involvement with CDTs. The involvement included being a co-Investigator and an Associate Director of a CDT. Possible usage by PhD students was suggested by several PIs through this question. Further work will be undertaken to make the most of our links with CDTs at N8 institutions.

Access to Tier 1 Resources

Q13 Has your use of N8 HPC allowed you to move upwards and gain access to any Tier 1 (HECTOR, ARCHER, Hartree) and Tier 0 (PRACE/Tianhe/Xsede) resources? If so please give details of the resource used.

In 2013 10 Pl's had gained access to Tier 1 resources such as Hector and Hartree through their use of N8 HPC with another 2 Pl's having applied for access and currently awaiting confirmation. In 2014,



use of N8 HPC has allowed 9 PI's to move onto Tier 1 resources including ARCHER, PRACE, Hartree resources (BlueGene), IFERC-CSC machine HELIOS (Japan) and RES (Spain). In addition 4 PI's are in the process of applying for access, 6 PIs already have access and a further 4 are expecting to apply in the future to use Tier 1 resources.

Many PI's explicitly commented that the use of N8 HPC resources had helped them gain access to Tier 1 resources.



Part 2: Service Satisfaction with N8 HPC

Project Applications

Q14 How easy did you find the 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 current procedure requires the PI to complete an online project application form (<u>http://n8hpc.org.uk/getting-started/</u>) containing information on the project, funding and the resources required. The average satisfaction score was 4.32 which is comparable to last year's score of 4.37 showing that there is still a high level of satisfaction with the procedure.

Comments such as "efficient", "good and straightforward" and "like it - light touch" were received. Where there were issues (3 cases), all PIs commented on how good the support was and how quickly the issues were resolved.

User Applications

Q16 How easy did you find the 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 4.38 compared to the 2013 score of 4.48 showing a continuing high level of satisfaction with the procedure. However not all PI's have applied for a user account with many of them leaving the machine usage to their researchers. Again comments received remarked on how smooth and easy the procedure was.

Technical Documentation

Q18 Does the technical documentation on the website meet your needs?

Q19 Is there anything missing from the technical documentation or further explanation required?

The website has recently been revamped and feedback was sought on the type and quality of information provided on the website. The majority of users (81.8% compared to 80.4% in 2013) were happy with the technical documentation provided on the website. The remainder of the users were somewhat happy with the documentation with no unhappy respondents.

Feedback for improving the technical documentation included the provision of a short 2-3 page guide for new users with basic information on compilation, job handling and data/disk limits; more clarification on the compiling of code; instructions on how to set up a job to write the output to /nobackup; information on task jobs and more details on the installation of codes.



Running Jobs

Q20 Have you or your researchers run a job on the N8 HPC?

95% of the respondents or their researchers had run a job on the system compared to 92% in 2013. The small increase may have been due to the more established nature of the projects compared to the same time last year. The high usage figures suggest that those researchers who register a project on the machine are actively using N8 HPC resources.

Support and Helpdesks

Q21 Have you or your researchers required support at any point to run a job on N8 HPC?

63% of respondents have required help to use N8 HPC which is up slightly from 62% in 2013 possibly due to the much larger number of projects using the service. The information received in the survey from these respondents will be cross checked to identify why they required help and what with. Of the people that required assistance 95% received the help they required which is an increase from 90% in 2013.

Q23 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". All respondents knew how to contact the correct helpdesk compared to only 89% of respondents last year.

Q24 Was your helpdesk query handled in a satisfactory and timely manner?

Only one person who contacted their local helpdesk for assistance felt that their query was not handled in a satisfactory and timely manner. This compared to 92% last year who felt that their query was handled appropriately.

Training

Q25 Do you or your research team require any training that could be provided locally or within N8? If so please give details.

Nine PIs (an increase of 1 compared to 2013) said that their research team would benefit from training. A list of training recommendations from the PI's is listed below. Only 7 PI's suggested topics –

- Porting FORTRAN CPU codes to GPUs.
- Parallel programming in Fortran using MPI and/or openMP
- Introduction to HPC (requested twice)
- MPI



- Periodic training on N8 HPC resources and programming languages (Fortran, C++, MPI OPenMP) and scripting (python, perl scripting)
- Using N8 as a private cloud (if this feature is possible) would be helpful to prepare for use of Virtual Machines
- Specific training on submitting jobs to N8 HPC
- Courses on advanced parallel programming, visualization of data would be helpful for the students and RAs.

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

Q26 Would you recommend the use of N8 HPC to colleagues?

95% of respondents would recommend the use of N8 HPC to their colleagues (up from 94% in 2013). Only 3 people said that they would be unable to recommend using the resource. The main reason for not recommending the use of N8 HPC was due to the length of the queues.

Looking to the Future

Q27 Do you have any further feedback you would like to provide? Are there any improvements you would like to see? Would a larger machine benefit your research and if so in what way?

31 feedback comments were received with two main issues raised – queues and the requirement or desire for a larger machine. There were also several comments praising N8 HPC and the support provided. Full details of the comments received are in Appendix 4.

Success Stories

Q28 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 the TSB. If you have a story then please leave brief details below and we will get in touch.

This is a new question added into the survey at the request of EPSRC. We received 9 replies, several of which were PIs confirming that they had already provided information on their research which had been made into case studies. However there are 5 possible new case study leads which will be followed up.

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. Concerns have been raised again regarding the length of queues and the capacity of the machine. Plans are well advanced regarding an equipment refresh for N8 HPC.



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

Durham, 5 York, 9 Lancaster , 15 Sheffield, 28 Leeds, 25 Newcastle, 20 Liverpool, 17 Manchester, 11

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

Durham

J. McElwaine, Rotational bulldozing of granular material doi:10.1017/jfm.2014.181J. Fluid Mech. (748) 143--174 2014

J. McElwaine, From episodic avalanching to continuous flow in a granular drum. Submitted to J. Fluid Mech. (2014)

J. Funke. Noncongruence subgroups and Maass waveforms In preparation (2014)

B. Gregoire, V. Erastova, D.L. Geatches, H.C. Greenwell, S.J. Clark, D. Fraser 'The adsorption of aspartate on layered hydroxide minerals: insight into early Earth chemical evolution', Geochim. Cosmo. Acta, submitted (2014)

X. Mao, Effects of base flow modifications on receptivity and nonnormality: flow past a backward-facing step, Journal of Fluid Mechanics. Submitted (2014)

Lancaster

V. Zolyomi, N. D. Drummond and V. I. Falko, Electrons and phonons in single layers of hexagonal indium chalcogenides from ab initio calculations, Phys. Rev. B 89, 205416 (2014).

A. Kormanyos, V. Zolyomi, N. D. Drummond and G. Burkard, Spin-orbit coupling, quantum dots and qubits in transition metal dichalcogenides , Phys. Rev. X 4, 011034 (2014).

F. Liu, H. Shimotani, H. Shang, T. Kanagasekaran, V. Zolyomi, N. D. Drummond, V. I. Falko and K. Tanigaki, High-sensitivity photodetectors based on multilayer GaTe flakes , ACS Nano 8, 752 (2014).

A. Kormanyos, V. Zolyomi, N. D. Drummond, P. Rakyta, G. Burkard and V. I. Falko, Monolayer MoS2: trigonal warping, Gamma-valley and spin-orbit coupling effects, Phys. Rev. B 88, 045416 (2013).

Academic Papers



V. Zolyomi, N. D. Drummond and V. I. Falko, Band structure and optical transitions in atomic layers of hexagonal gallium chalcogenides , Phys. Rev. B 87, 195403 (2013).

N. D. Drummond, V. Zolyomi and V. I. Falko, Quantum Monte Carlo study of the electronic properties of single layers of hexagonal boron nitride , to be submitted to Phys. Rev. B. In preparation (2014)

E. Mostaani, N. D. Drummond and V. I. Falko, Quantum Monte Carlo Calculation of the Binding Energy of Bilayer Graphene, to be submitted to Phys. Rev. Lett. In preparation (2014)

N. D. Drummond, V. Zolyomi and V. I. Falko, Vibrational Behavior of Monolayer Gallium Chalcogenides, to be submitted to Phys. Rev. B. In preparation (2014)

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S. Bailey, GOLLUM: a next generation simulation tool for electron, thermal and spin transport, New Journal of Physics In press (2014)

Leeds

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

PI Institution		Grant Title	Funding Body	Grant Status	
Chris	Durham	Mineral interfaces in Shale	Royal Society	Active	
Greenwell		hydration	50		
Steven Bailey	Lancaster	FP7 ITN MOLESCO	EC	Active	
Ruza Ivanovic	Leeds	Forward modelling of past abrupt climate transitions (IRF)	NERC	Awarded	
Ruza Ivanoivc,	Leeds	From pre-bomb to post-bomb:	NERC	Under	
Lauren		using radiocarbon to examine the		review	
Gregoire		ocean carbon cycle			
Peter Leeds		SEAMSEW	Axa Research	Ended May	
Knippertz			Fund	2014	
Martyn Chipperfield	Leeds	NCEO	NERC	Awarded	
Dmitry Leeds		Quantum mechanical effects in	EPSRC	Under	
Shalashilin		excited state dynamics of biological		review	
		building blocks. Reaching			
		agreement between first principle			
		theory and experiment			
Gilberto	Liverpool	Advanced new linear-scaling	Royal Society	Active	
Teobaldi		constrained density-functional	-,,		
		theory approaches			
Gilberto Liverpool		INSPIRE Physical Sciences: A	EPSRC	Active	
Teobaldi		synergy for next generation			
		materials science			
Gilberto Liverpool		Impact Acceleration Account	EPSRC	Active	
Teobaldi		(Liverpool)		, lotive	
Ming Li	Liverpool	Morphological modelling of mix	NERC	In	
	Liverpoor	sediment transport	NEINE	preparation	
Peter Lee	Manchester	Structural evolution across multiple	EPSRC	Awarded	
reter Lee	Wanchester	time and length scales	LI SILC	Awarueu	
Peter Lee	Manchester	EXOMET: Physical Processing of	EU	Awarded	
	Wallenester	Molten Light Metals Nano-	10	Awarueu	
		Particulate Reinforced Alloys under			
		the influence of External Fields			
Paul Bushby	Newcastle	Cosmic rays in the multi-phase	STFC	Awarded	
Paul Bushby	Newcastle	interstellar medium with dynamo-	SIFC	Awarueu	
Jacek Cala	Newcastle	generated magnetic fields	EC	In	
Jacek Cala	Newcastie	EU / Brazil Cloud infrastructure -	EC		
		Connecting Federated Resources		preparation	
N111		for Scientific Advancement	50000		
Nilanjan	Newcastle	Fundamental understanding and	EPSRC	In	
Chakraborty		modelling of differential diffusion		preparation	
		effects in turbulent premixed			
		combustion: A Direct Numerical			
		Simulation (DNS) based analysis			
Nilanjan	Newcastle	Fundamental understanding and	EPSRC	In	

resources



Chakraborty		modelling of natural convection of		preparation
		visco-plastic fluids: A combined		
		experimental and numerical		
		approach		
Nilanjan Newcastle		Fundamentals and modelling of	EPSRC	Under
Chakraborty		turbulent spherical flames: A		review
		combined experimental, numerical		
		and theoretical approach		
Jaume	Newcastle	Model-driven Software Engineering	EPSRC	Under
Bacardit		for GPU Data Mining (MAGENTA);		review
Marcus Kaiser	Newcastle	Modelling Human Brain	EPSRC	Awarded
		Development		
Mehmet Atlar	Newcastle	SONIC	EU-FP7	Awarded
Mehmet Atlar	Newcastle	SEAFRONT	EU-FP7	Awarded
Mehmet Atlar	Newcastle	Foil Cat	M-Technic	In
			(Local industry)	preparation
Mehmet Atlar	Newcastle	Propeller Shear Stress	International	Awarded
			Paints (Local	
			industry)	
Mehmet Atlar	Newcastle	Multi-Purpose Flume design	International	Awarded
			Paints (Local	
			industry)	
Ning Qin	Sheffield	Mesh Adjoint	Rolls Royce	Awarded
Ning Qin	Sheffield	MARS EC		Awarded
Ning Qin	Sheffield	Rooftop Wind Turbine	Solar Europa	Under
				review
Ning Qin	Sheffield	Wind Turbine Noise	EPSRC	Submitted
Ning Qin	Sheffield	Unstructured adjoint DSTL		Under
				review
John Harding	Sheffield	Mineral-Microbe interaction role	NERC	Ended
		on concentration and fractionation		
		of Rare Earth Elements		
Labor Harriber	Choffiold	(MM_FREE);		Culture it to al
		SoS RARE	NERC	Submitted
John Harding	Sheffield		FRERC	A
Damien	Sheffield	Modelling Complex and Partially	EPSRC	Active
		Identified Engineering Problems -	EPSRC	Active
Damien		Identified Engineering Problems - Application to the Individualised	EPSRC	Active
Damien		Identified Engineering Problems - Application to the Individualised Multi-Scale Simulation of the	EPSRC	Active
Damien Lacroix	Sheffield	Identified Engineering Problems - Application to the Individualised Multi-Scale Simulation of the Musculoskeletal System		
Damien		Identified Engineering Problems - Application to the Individualised Multi-Scale Simulation of the Musculoskeletal System Technology Options for Closed Th-	EPSRC EPSRC	Active Submitted
Damien Lacroix Shuisheng He	Sheffield Sheffield	Identified Engineering Problems - Application to the Individualised Multi-Scale Simulation of the Musculoskeletal System Technology Options for Closed Th- U233 Fuel Cycles	EPSRC	Submitted
Damien Lacroix Shuisheng He Roy Chantrell	Sheffield Sheffield York	Identified Engineering Problems - Application to the Individualised Multi-Scale Simulation of the Musculoskeletal System Technology Options for Closed Th- U233 Fuel Cycles Atomistic modelling of MRAM	EPSRC Samsung	Submitted
Damien Lacroix Shuisheng He	Sheffield Sheffield	Identified Engineering Problems - Application to the Individualised Multi-Scale Simulation of the Musculoskeletal System Technology Options for Closed Th- U233 Fuel Cycles	EPSRC	Submitted

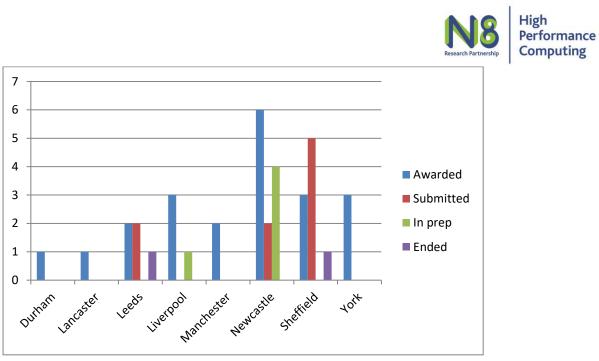


Fig. 5 Number of research grants and their state at the time of the survey per institution.



Appendix 3 – list of industrial studentships involving N8 HPC

PI	Institution	Funders	Industrial Involvement	Title	Dates
Chris	Durham	Durham Uni	BP	Nanogeochemistry of low	2013 -
Greenwell		Scholarship		salinity EOR	2017
Chris Greenwell	Durham	NERC-CASE	M-I SWACO	Understanding shale swelling	2011 - 2015
Steven Bailey	Lancaster	BP	BP	Pushing Reservoir Limits: The Simonstone Project'	2010 - 2013
Jamshed Anwar	Lancaster	EPSRC CASE	Astra Zeneca	Molecular simulation of crystal growth	2014 - 2018
Sarah Harris	Leeds	EPSRC	Astra Zeneca	Importance of Entropy in Drug Design	2013 - 2017
Ming Li	Liverpool	EPSRC	EDF-RD	3D modelling morphological impact of Offshore wind farm	2013 - 2017
Benedict Rogers	Manchester	EDF	EDF	An Investigation into Wall boundary Conditions and Three-dimensional Turbulent Flows using Smoothed Particle Hydrodynamics	2010 - 2013
Richard Bryce	Manchester	BBSRC	Janssen	Unravelling the molecular mechanisms that underpin regulatory kinase function using new computational tools	2010 - 2014
Alistair Revell	Manchester	iCASE	National Grid	Application of recently developed Embedded Large Eddy Simulation for detailed investigation of flow physics	2014 - 2018
Ning Qin	Sheffield	EPSRC	Airbus	Robust Optimisation of Shock Control Bumps	2013 - 2016
Ning Qin	Sheffield	EPSRC	Airbus	Parameterisation and optimisation of aircraft winglet	2013 - 2016
Ning Qin	Sheffield	EPSRC	Airbus	Adjoint mesh sensitivities and optimisation	2014 - 2017
Ning Qin	Sheffield	Rolls Royce	Rolls Royce	Adaptive mesh using adjoint	2014 - 2018



Appendix 4 – feedback comments received

Expansion of resources

- More nodes.
- We need more resources! Expand the N8
- Expansion of the system, if possible
- The system should now be substantially upgraded to be real use for the community.
- A bigger machine would be nice
- More cores please :-)
- Need a larger machine for true capability calculations
- More cores.
- We have found the performance of the system varies a great deal, to the point that at some times it is almost unusable. I put this down to simply too many users on the system.
- During the first year we had good turn-around times of jobs. No the machine is practically useless to us since the time it takes for a job to start running is weeks! The machine is also flooded by 1-core jobs. Such jobs should be banned on a parallel computer.
- The system is already too busy and my jobs get killed after being in a queue for 2 days. Some reserved access quotas could be established in order to be sure that I can run my jobs. Else, I will not rely purely on the N8 to run the jobs of my funded projects if I am not guaranteed that I will have enough time to run them.

Queues

- A short test queue
- Test queue?
- Better queuing system can take a long to run jobs due to queue
- It would be useful to publish an explanation of the scheduling policies used in N8 HPC. Of lately the waiting time before an experiment starts to run has been quite variable, so it would be useful to know why.
- I would like to see differing queue structures on the N8 places where jobs and new compilations can be tested on small amounts of cores with minimal waits. Currently, there can be a variable amount of waiting time and it can be very frustrating to have a job finish in 5 minutes due to a misplaced decimal point after 48 hours in a queue.
- Just some time the queue time was more than 1 weeks and if we could know why this situation happened in advanced. That will be brilliant.
- I would like to see a node or two dedicated to a test-queue. I always struggle at the start of projects, when i need to test model developments or new experimental set-ups. Simulations can queue for hours to days. This considerably slows down my work. I have met many other researchers throughout the university who come across the exact same problem. We would all benefit from having a test queue on which we can run very short (i.e. 1h) tests.

Technical Requests

- GPUs
- High memory machine for visualisation



- It would probably be good to have the same OS on both login and computing nodes. This would make compilation of own code much easier.
- Only that the automatic deletion on /nobackup could perhaps occur on a slightly longer time period or using different criteria. I have forcing fields for my model that are essential, but not accessed; their deletion would be very annoying and means i have to constantly 'touch' them to avoid this.
- Our current research is slightly limited with the N8 cluster. The quantum mechanical calculations can take significant computational time i.e. over a week. However jobs are not allowed to run for more than 2 days and get killed if they have not finished. It is not really possible to know how long the job will run for either. Unfortunately, the quantum mechanical software does not scale with the number of processors and so 16 is about the most that can be used to try and complete the calculation within the 2 day time frame. I appreciate that this is a fairly unique problem and that changes could cause issues with the advanced reservation system.

Miscellaneous

- How about light-weight access for short placement students/final year/masters students?
 E.g. access to a separate with a low core limit and hd space? I could provide ~10 students / year in this
- A clearer framework of time budget or use would be handy.
- As stressed in point 4, we had severe problems with the queueing time and was hard to use a large number of cores so at the time we used HECTOR instead. However, we recently learnt that these problems have been solved now. In the future, we would like to come back and use Polaris resources
- Better communication with business engagement team is required.
- I and many users at my institution have been very frustrated by the excessively long queuing times on Polaris. This was finally traced to a bug in the scheduling software back in April, which meant that the way certain users were using array jobs was being mis-calculated and drastically reducing the priority for all users at my institution. This took a very long time (and a lot of prodding from me) for this to be made clear to the users involved, and has resulted in many potential users leaving the service & as far as I know, no attempt has been made to woo them back. The lack of communication from the service administration to the users on this has been a major missed opportunity to build bridges and reassure users that the N8 HPC is a useful service.
- It would be useful if a log was kept containing the run time and memory usage of each job, that way the job run times and memory usage passed in to qsub could be more accurate. Likewise if a job was prematurely finished for over usage of memory or run time a log could be kept (or even an automated email although this could possibly lead to spam) to explain why.

Thank you!

- Excellent tech support, short queue times.
- I am very pleased with the N8 service.



- The N8 is a very useful tool which allows us to access computing resources otherwise not available.
- The support has been excellent.
- We feel N8 provides a very valuable platform that allows us to perform many HPC tests and model applications. Without such resources, many of our research work will not be possible. The services provided are also very satisfactory to us. The system is very reliable and fairly straightforward to use, unlike many other similar systems. The help we received are also very helpful to resolve the problems we had. So overall we are very impressed with the system and hope it can continue to support our research in the future.
- Excellent service.