N8 HPC

Annual Report 2013

Executive Summary

A survey of all Principal Investigators who have a project registered on N8 HPC was carried out over July – August 2013. The findings demonstrated that N8 HPC is providing a good reliable appreciated service although there is concern over the length of time taken to run jobs and the capacity of the machine.

Impact of the use of N8 HPC was demonstrated through:

- The average usage since October 2012 was 88.4% of machine uptime. This time period includes the pilot phase during which users were invited onto the machine in a controlled manner. The machine was not opened to all until March 2013.
- These are early days in terms of research paper production however so far 3 research papers have been published, 2 are in press, 5 have been submitted and 17 are in preparation.
- We have also been notified of 7 conference papers, 1 book and 1 commissioned review produced acknowledging N8 HPC
- Even though the machine has only been open to all for 7 months, 17 grants have been submitted which specifically mention the use of N8 HPC.
- The largest grant to mention the use of N8 HPC is a joint EPSRC / BBSRC grant involving the University of Liverpool entitled "*Biological and bio-inspired systems with applications in energy and sustainable chemistry*" with a value of £12.9M which is currently "under review".
- In addition grants totalling over £5M mentioning the use of N8 HPC have been awarded with grants totalling over £14M currently submitted.
- So far there are 7 existing industry-related PhD studentships utilising N8 HPC resources with another 7 studentships due to start in 2013/4 involving multi-national companies.
- Currently 60% of research performed on N8 HPC has industrial involvement with 37 individual companies, over 50% of who know of the usage of N8 HPC.

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

- 60% of projects on the N8 HPC facility involve industrial collaboration with 37 individual companies named. Over 50% of industrial collaborators were aware of their usage of N8 HPC.
- 7 existing industry-related PhD studentships making use of N8 HPC resources with another 7 due to start very soon
- Use of N8 HPC resources has been directly responsible for 6 instances of collaboration with UK industry and one overseas industry including companies such as EDF and the La Farge Group.
- Currently two joint industry / academia papers have been published / accepted with a further 4 in preparation.
- There have been 6 knowledge transfer projects which have made use of N8 HPC:

Developing skills in the use of e-infrastructure across N8

- The use of N8 HPS has enabled 10 PI's to gain access to Tier 1 resources such as Hector and Hartree.
- A further 2 PI's have applied for access to Hector and are currently awaiting confirmation.

Sharing skills across N8

- Use of N8 HPC has enabled 8 instances of collaboration between N8 universities and 9 collaborations with non-N8 UK institutions including Imperial College London, University of Cambridge and STFC.

N8 HPC Annual Survey 2013

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 begin 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 is now fully utilised.

In order to assess the impact the usage of N8 HPC has had on research at the N8 Institutions during the first year, a survey was devised with input from all 8 institutions and sent to the PI's of all registered projects on N8 HPC. The survey had an 88.5% response rate with only 7 non-respondents.

The survey was split into two parts as it not only investigated the impact N8 HPC has had on research but also looked at how the facility was performing in terms of service.

Part 1: Impact

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. Given the early stage of usage by many of the respondents, there were a number of papers in a state of preparation or in submission. A full list of papers is given in Appendix 1.

In summary 27 papers, 7 conference papers, 1 book and 1 commissioned review have been produced acknowledging N8 HPC.

In the future further investigation can be undertaken regarding the impact of published papers e.g. impact rating of the journals. A 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.

Again due to the early stage of usage by many PI's, a large number of grants mentioning N8 HPC are in varying stages of completion. 17 grants have been submitted which specifically mention the use of N8 HPC and they range in value up to £12.9M.

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. Some of these studentships may have already been in place before N8 HPC was available. In total there are 7 existing industry-related PhD studentships with another 7 due to start soon.

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.

Use of N8 HPC has enabled 8 instances of collaboration between N8 universities and 9 collaborations with non-N8 UK institutions including Imperial College London, University of Cambridge and STFC. Overseas collaborations have been enhanced with 10 instances of collaboration due to N8 usage.

Industrial collaboration has also occurred with 6 instances of collaboration with UK industry and one with overseas industry. Companies include EDF and the La Farge Group.

Industrial Collaboration

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

Q6 Is your industrial partner aware of your usage of N8 HPC?

60% of projects on the N8 HPC facility involve industrial collaboration with 37 individual companies named. PI's were asked if their industrial collaborators were aware of their usage of N8 HPC. The results are shown in the chart below which indicates that most industrial collaborators know of N8 HPC usage.

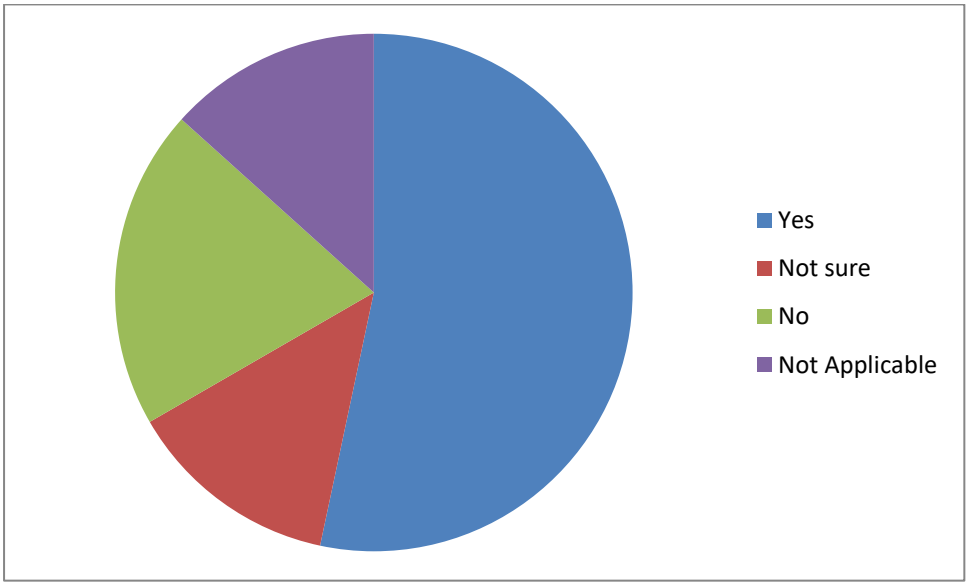


Fig. 1. Industrial collaborators awareness of N8 HPC use by their academic partner.

Industrial Collaborative Papers

Q7 Have you produced any joint academic-industry publications? If so please provide details.

Currently two joint industry / academia papers have been published / accepted with a further 4 in preparation.

Published

- With DLR, German Aerospace Centre:

Da Ronch A, McCraken A, Badcock KJ, Widhalm M, Campobasso MS. Linear Frequency Domain and Harmonic Balance Predictions of Dynamic Derivatives, AIAA Journal of Aircraft, Vol. 50, no. 3, 2013, pp. 694-707. DOI: 10.2514/1.C031674.

- With EDF:

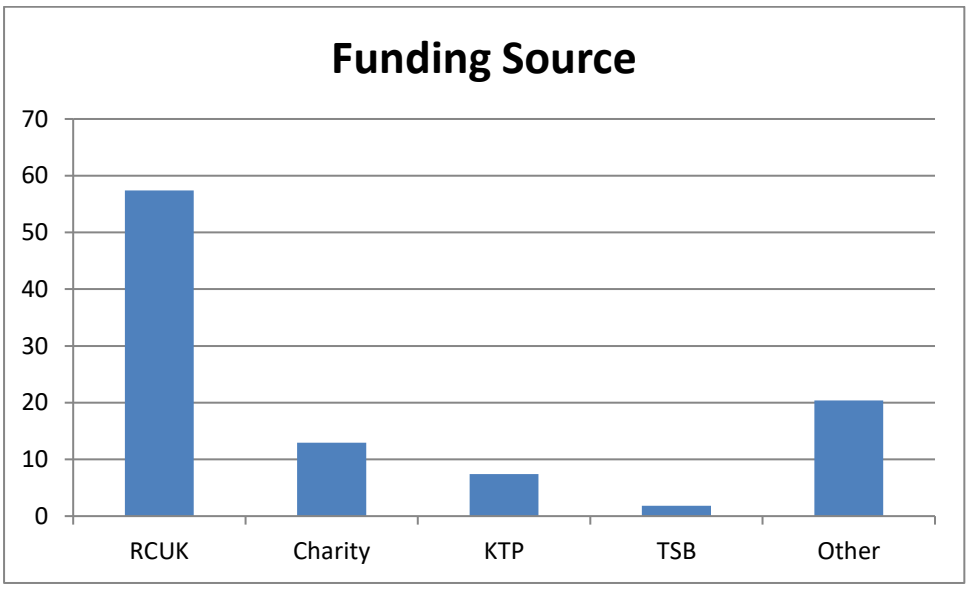
Mayrhofer A, Rogers BD, Violeau D, Ferrand M. Investigation of wall bounded flows using SPH and the unified semi-analytical wall boundary conditions, Computer Physics Communications. DOI: 10.1016/j.cpc.2013.07.004 In Press.

Funding Sources

Q8 Does your research involve any of the following? Please tick the appropriate box.

- RCUK
- Charity grants
- TSB grants
- Knowledge Transfer Partnerships

Almost 13% of funding was obtained from charities whilst the "other" category included funding sources such as European funding and the Food Standards Agency.



Knowledge Partnership Grants

Q9 Have you had any knowledge transfer projects? If so please provide details.

There have been 6 knowledge transfer projects which have made use of N8 HPC:

- Richard Bryce, Manchester, BBSRC Industry Interchange grant with AstraZeneca examining protein plasticity using MD simulations. (Finished Feb 2013)
- Peter Buxton, York, KTP between Tokamak Solutions, the University of York and Peter Buxton (post-doc).

Chris Greenwell from Durham University has had several grants -

- Joint industry grants
    - Royal Society Industry Fellowship (£130K) 'Mineral Interface Determination during Shale Hydration' with M-I SWACO (Schlumberger). Approved and start date of May (2013-2017).

    - EPSRC Knowledge Transfer Account funding was received (£36K) for an outgoing Industrial Fellowship for Dr Dawn Geatches to the Lafarge Group to study molecular modelling methods for understanding hydration in clays (2011).
- Specific KT grants:
    - EPSRC Pathways to Impact funding (£14K) 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);
    - EPSRC Knowledge Transfer Account funding was received (Â£19K) for an incoming Industrial Fellowship for Dr Alain Jacquet from Lafarge Group to study molecular modelling methods for understanding hydration in clays (2010).

Contact with university Business Engagement Managers

Q10 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?

All Business Engagement Managers have received a list of researchers who are utilising N8 HPC resources at their institution. They have been encouraged to open dialogue with these researchers. Only two researchers have noted contact from their BEM.

Access to Tier 1 Resources

Q11 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.

Ten PI's had gained access to Tier 1 resources such as Hector and Hartree resources through their use of N8 HPC with another 2 PI's having applied for access and currently awaiting confirmation. This demonstrates that there is a progression from local to national through regional resources.

Part 2: Service Satisfaction

Project Applications

Q11 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 involves the PI completing an online project application form (http://n8hpc.org.uk/research/gettingstarted) containing information on the project, funding and the resources required. The average score was 4.37 showing a high level of satisfaction with the procedure.

Comments were also solicited with 11 praising the straight forward application procedure and quick confirmation time. Two comments mentioned the length of the form and the inability to save the form during completion. Four comments, of which 3 were from Newcastle, raised issues regarding knowing the amount of resource usage for the form and communication gaps regarding the status of the application.

User Applications

Q12 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 4.48 showing a 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.

Technical Documentation

Q13 Does the technical documentation on the website meet your needs?

Q14 Is there anything missing from the technical documentation or further explanation required?

The website is under review and we were keen to solicit feedback from PI's as to the type and quality of information provided on the website. The majority of users (80.39%) were happy with the technical documentation provided on the website. The remainder of the users were somewhat happy with the documentation with only one respondent being unhappy.

Feedback for improving the technical documentation included making it more obvious on the website, providing more detail on the queuing system, an FAQ for less experienced users and more examples of running jobs.

Running Jobs

Q15 Have you or your researchers run a job on the N8 HPC?

92% of the respondents or their researchers had run a job on the system. Due to projects being able to apply for access to the machine at any point in the year, some of the respondents had only just had their applications approved.

Support and Helpdesks

Q16 Did you require support at any point?

62% of respondents have required help to use N8 HPC. The information received in the survey from these respondents will be cross checked with previous responses to identify why they required help and what with.

Of the people that required assistance 90% received the help they required.

Q17 Did you know how to contact the correct 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 N8 HPC website under "Research" and also the "Contacts" section. 89% of respondents knew how to contact the correct helpdesk.

Q18 Was your helpdesk query handled in a satisfactory and timely manner?

Of the people that contacted their local helpdesk query for assistance, 92% reported that their query was handled in a satisfactory manner. Only 3 people had problems with their local helpdesk – two from Durham and one from Newcastle. Both of these sites currently have issues due to lack of sufficient support staff.

Training

Q 19 Do you or your research team require any training that could be provided locally or within N8? If so please give details.

A list of training recommendations from the PI's is listed below. Only 8 PI's suggested topics –

- Standard methodology for the installation of new codes on the system.
- MPI related programming training
- A short course for non-experienced users on the hardware possibilities offered by N8 HPC.
- Maximizing use of Lustre fs
- Unix/bash course
- Aspects of parallel programming, optimisation of codes for the N8 machine, OpenMP as well as parallel code debugging.
- Any HPC tutorials such as coding sessions especially CUDA programming.

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 suggestions from researchers that use the machine on a regular basis.

Personal Recommendations

Q20 Would you recommend the use of N8 HPC to colleagues?

94% of respondents would recommend the use of N8 HPC to their colleagues. Only 3 people said that they would be unable to recommend using the resource. This was mainly due to dissatisfaction with the length of time it takes to run a job.

Looking to the Future

Q21 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?

33 feedback comments were received. Two main issues were raised - the length of time it now takes to run jobs (12 comments) and a requirement or desire for a larger machine (10).

Seven comments praised the machine and the level of support received with 3 comments highlighting small issues. These issues were –

- 48 hour time limit being too short although we also received feedback that this time limit was very much appreciated
- Clarity in how the job priority is assigned
- The requirement to have a N8 institutional IP address

Several comments provided suggested improvements to the service relating to –

- Having nodes which could be reserved for code development and testing

- Narrowing down the purpose of the machine given the high usage and difficulty running large jobs due to demand e.g. offering short periods of access to limited numbers of groups to enable leading research to be done and to allow benchmarking and testing of codes prior to accessing national facilities.
- Very early access to emerging technologies
- remote visualization capability
- Email alert when users are reaching a certain percentage of disk usage
- A more comprehensive output file e.g. details of job start and completion time.

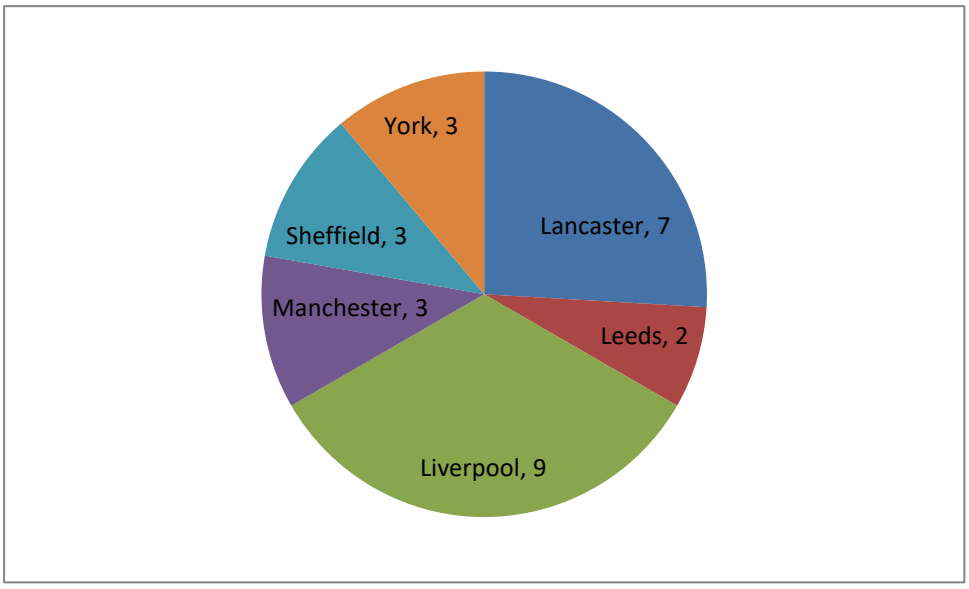
Conclusion

Overall researchers were happy with both the machine and the level of service provided. Several areas will be investigated such as the lack of support at some institutions – some of which has been addressed during the survey period.

The future usage of the machine has to be addressed given the limited resources available. Access criteria may be required to ensure that the research performed on the machine is of sufficient impact in order to demonstrate value for money to N8 and the enhancement of industrial collaboration.

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

Academic Papers



Number of Papers produced by each N8 Institution acknowledging N8 HPC.

Lancaster

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

M. S. Campobassoa, A. Piskopakisb, J Drofelnikb, A Jacksonc Turbulent navier-stokes analysis of an oscillating wing in a power-extraction regime using the shear stress transport turbulence model Computers & Fluids (2013)

H. Sadeghi, S. Bailey, D. Visontai, D Manrique, J. Ferrer and Colin J Lambert Graphene Sculpturenes Nanopores for Nucleotide Sensing, ACS Nano Letters. Submitted.

N.D. Drummond, V. Zolyomi and V.I. Falko, Electronic properties of monolayer hexagonal boron nitride , in preparation (2013).

N.D. Drummond, V. Zolyomi and V.I. Falko, Vibrational behaviour of monolayer gallium chalcogenides , in preparation (2013).

E. Mostaani, N.D. Drummond and V.I. Falko, Quantum Monte Carlo calculation of the binding energy of bilayer graphene , in preparation (2013).

N.D. Drummond and R.J. Needs, Energy of the homogeneous relativistic electron gas , in preparation (2013).

Liverpool

M. Carrion, M. Woodgate, R. Steijl and G. Barakos, Implementation of All-Mach Roe-type Schemes in Fully Implicit CFD Solvers - Demonstration for Wind Turbine Flows. Int. J. Num. Meth. Fluids, May 2013. Accepted for publication.

A. Tagliabue, L. Bopp and O. Aumont, The impact of different external sources of iron on the global carbon cycle, Geophys. Res. Lett., Submitted., 2013.

J. Elliott and G. Teobaldi, Structural and electronic characterisation of imogolite nanotubes with inner organic functionalization: a linear scaling DFT study, in preparation.

J. Elliott and G. Teobaldi, Structural and electronic characterisation of Fe-doped imogolite nanotubes: a linear scaling DFT study, in preparation.

E. Poli and G. Teobaldi, Geometry and electronic properties of cation-vacancy induced defects in imogolite nanotubes: a linear scaling DFT study, in preparation.

S. Devoy and G. Teobaldi, Local polarisability of imogolite nanotubes: a linear scaling DFT study, in preparation.

E. Poli, V. C. Nguyen and G. Teobaldi, High Energy-density self-healing ferroelectric polymers: a linear scaling DFT study, in preparation.

A. Tagliabue and Y. Balkanksi, How does dust mineralogy impact the ocean's iron cycle? Glob. Biogeochem. Cyc., In preparation. 2013

I. Scivetti and M. Persson . A new density functional approach for atoms and molecules on insulating films supported by metal substrates: NaCl bilayer on Cu(100). J. Phys. Cond. Matt. In preparation.

Leeds

D. Toroz, R. Hammond, K. Roberts, S. Harris and T. Ridley. Molecular dynamics simulations of organic crystal dissolution: The lifetime and stability of Para-amino benzoic acid polymorphs in aqueous environment. *Journal of Crystal Growth*. Submitted.

D. Toroz, I. Rosbottom, R. Hammond and K. Roberts. Conformational analysis of Para Aminobenzoic-Acid using Gas-Phase and Solvent Continuum Calculations of single molecules and Clusters, Journal of Physical Chemistry B. In preparation.

Manchester

A. Mayrhofer, B.D. Rogers, D. Violeau, M. Ferrand. Investigation of wall bounded flows using SPH and the unified semi-analytical wall boundary conditions, Computer Physics Communications. DOI: 10.1016/j.cpc.2013.07.004 In Press.

Ll.M. Evans, L. Margetts, V. Caselagno, M. Ferraris, L. Lever, J. Bushell, T. Lowe, A. Wallwork, P. Young, A. Lindemann, M. Schmidt, P.M. Mummery. Transient Thermal Finite Element Analysis of CFC-Cu ITER Monoblock from X-ray Tomorgraphy Data. J. Nuc. Mat. In prep.

Ll.M. Evans, L. Margetts, J. Bushell, T. Lowe, A. Wallwork, W.E. Windes, P. Young, P.M. Mummery Thermal finite element analysis on massively parallel computing platforms. Finite Elem. Anal. Des. In prep.

Sheffield

Z.J. Chen, N. Qin, Planform Effects for Low-Reynolds-Number Thin Wings with Positive and Reflex Cambers, Journal of Aircraft: 1-13, 10.2514/1.C032102W.

Wang, S. Siouris, N. Qin, Hybrid RANS/LES for active flow control, Aircraft Engineering and Aerospace Technology, submitted.

J.H. Harding, C.L. Freeman and D.M. Duffy. Commissioned review - Oriented crystal growth on organic monolayers. CrystEngComm. Submitted.

York

R. Chantrell. Temperature dependent properties of NdFeB permanent magnets (In preparation)

R. Chantrell. Atomistic simulation of Heat Assisted Magnetic Recording with ECC media (In preparation)

R. Chantrell. On-site magnetic moments enhancement of FePt-L10:MgO(001) interfaces: a first principles study (In preparation)

Books

Manchester

I.M. Smith, D.V. Griffiths and L.Margetts. Programming that Finite Element Method 5th Ed (2013);

Conference Papers

Lancaster

M.S. Campobasso, A. Piskopakis, M. Yan, Analysis of an Oscillating Wing in a Power-Extraction Regime Based on the Compressible Reynolds-Averaged Navier-Stokes Equations and the K â^' ! SST Turbulence Model, ASME paper GT2013-94531, presented at the ASME/IGTI Turbo Expo 2013 Technical Conference, 3rd-7th June 2013, San Antonio, Texas, USA.

Manchester

A Skillen, A Revell, J Favier, A Pinelli, U Piomelli. LES Study into the Flow Physics of an Undulating Leading-Edged Wing. In Proceedings of the ERCOFTAC international symposium - Unsteady separation in fluid-structure interaction, Mykonos, Greece, June 17-21, 2013;

A Skillen, A Revell, J Favier, A Pinelli, U Piomelli. Investigation of Wing Stall Delay Effect Due to an Undulating Leading Edge: an LES Study. In Proceedings of the 8th international symposium on turbulence and where flow phenomena. Poitiers, France. August 28 - 30, 2013

Ll.M. Evans, L. Margetts, L. Lever, W.E. Windes, P.M. Mummery. NAFEMS NWC13 - Parallel Processing for Time-dependent Heat Flow Problems (June 2013)

Sheffield

S. He and M. Seddighi, A DNS Study of Effects of Reynolds Number on Unsteady Channel Flow, 8th International Symposium on Turbulent Shear Flow Phenomena, 28-31 August 2013, Poitiers, France

M. Seddighi, S. He, A. E. Vardy, T. O'Donoghue, D. Pokrajac, DNS of a Transitionally Rough Channel Flow with a 3D Roughness, 8th International Symposium on Turbulent Shear Flow Phenomena, 28-31 August 2013, Poitiers, France

S. He and M Seddighi, Energy Growth in Transient Channel Flow, 14th European Turbulence Conference, 1-4 September 2013, Lyon, France.

Commissioned Reviews

J. Harding Commissioned review - Controlling crystal growth using arrays of organic molecules. Submitted August 2013.