Tier-2

Tier-2

- Set of six machines that sit between Archer/Dirac (Tier-1) and University HPC clusters (Tier-3)
- Result of a £20m capital investment from EPSRC, with funding from Universities to provide operational costs
- Cirrus (EPCC), Isambard (GW4), CSD3 (Cambridge), Athena (HPC Midlands+), Jade (Oxford), MMM Hub
- Range of hardware (CPUs, GPUs, storage, networks) and architectures (X86-64, ARM64, Power, DGX-1)
- Free access to EPSRC researchers via regular resource allocation calls – next one in the summer

- Information about Tier-2 is collected together with other UK HPC services at https://www.hpc-uk.ac.uk

UK HPC Facilities

These are HPC facilities in the UK that have defined access processes for external users:

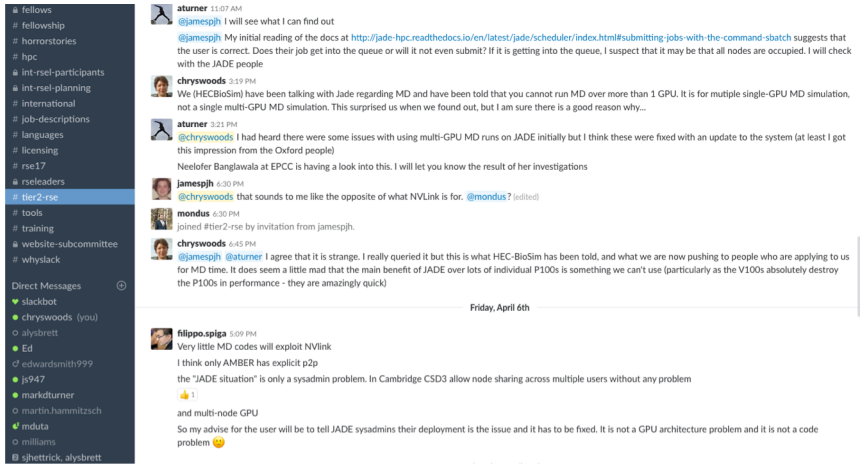
ARCHER, the UK national supercomputing service offers a capability resource for running very large parallel jobs. Based around a 118,080 core Cray XC system, the service includes a helpdesk staffed by HPC experts from EPCC with support from Cray Inc. Access is free at point of use for academic researchers working in the EPSRC and NERC domains. Users can also purchase access at a variety of rates. Industry access is available.

Cirrus at EPCC is one of the EPSRC Tier-2 HPC facilities. The main resource is a 10,080 core SGI/HPE ICE XA system. Free access is available to academic researchers working in the EPSRC domain and from some UK universities; academic users from other domains and institutions can purchase access. Industry access is available.

Isambard at GW4 is one of the EPSRC Tier-2 HPC facilities. Isambard provides multiple advanced architectures within the same system in order to enable evaluation and comparison across a diverse range of hardware platforms. Free access is available to academic researchers working in the EPSRC domain and

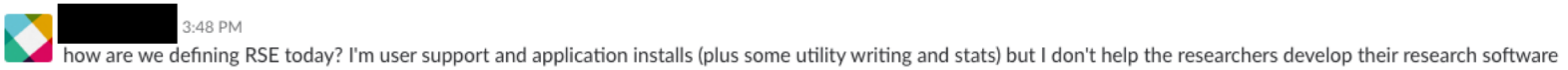
Tier-2 RSEs

- Tier-2 centres were strongly encouraged to fund RSEs to provide support to users
  - They communicate via:
    - #tier2-rse Slack channel on the UKRSE Slack
    - Monthly skype meetings



However, communication is infrequent and a community of RSEs working together to port and develop software across Tier-2 has yet to fully gel…

…still a lot of confusion as to the difference between a sysadmin and an RSE



CIRRUS RSE UPDATE

Andy Turner, EPCC

25 April 2018

a.turner@epcc.ed.ac.uk

EPSRC

Engineering and Physical Sciences Research Council

cirrus

Powered by epcc

CIRRUS RSE UPDATE

- Supporting user requests: software installations, technical help, etc.
- Comparative benchmarking across ARCHER and Tier2 systems
  - Initial focus on CPU-based systems
  - Synthetic benchmarks: HPC Challenge, parallel file system performance (MDS and bandwidth)
  - HPC application benchmarks: CASTEP, GROMACS, OpenSBLI (CFD)
- Installation and configuration of ISV sofware and licences

TIER2 RSE COORDINATION

- EPCC have initiated a regular series of meetings between Tier2 RSE teams and ARCHER CSE
- Initial focus:
  - Sharing experiences and approaches
  - Sharing introductory HPC training material
- Future plans:
  - Group involvement in RSE Leaders workshop submission for RSE2018
  - Sharing best practice and experience with DiRAC RSE group
  - Identifiy opportunities for cross-site collaborations
  - Face-to-face day-long workshop (potentially with DiRAC RSE group) for late 2018

Thomas: MMM Hub

- System updates:
  - Outage for Lustre firmware update (10th-12th April)
  - Rolling kernel updates for Meltdown/Spectre (18th-23rd April)
    - Temporary issue: Gold jobs were higher priority than our reimaging job, so some user jobs tried to run across nodes with a mixture of kernel versions:

      `Trying to connect to a HFI (subnet id – 0)on a different subnet – 1023`

      - There is only one subnet…
      - Increased priority of reimaging jobs
- Software:
  - Users requesting `hrex` supplied by GROMACS+plumed
  - Had to try our existing modules and find it didn't exist
  - Needed the most recent version of GROMACS that had plumed patch available (not so easy to see if `hrex` included)
  - Ended up with GROMACS 2016.4 + plumed 2.4.1
  - Previously encountered Intel compiler bug in plumed 2.4.0 alignment step (RMSD calc), resulted in NaNs in tests. Fixed in 2.4.1

Tier-2 RSE Support on the Cambridge Centre for Data-Driven Discovery

Access to CSD3:

- Quarterly EPSRC calls for science calls details available when the calls are published
- "pump-priming" access available for testing and development: email resources@csd3.cam.ac.uk

Questions or informal advice

- talk to Jeffrey Salmond (head of local RSE team)
- email js947@cam.ac.uk or
- find Jeffrey on the UKRSE slack

RSE Projects on CSD3:

- The RSE team would love to help! RSE support can be requested as part of a science project
- Lots of experience in HPC software projects from both EPSRC and STFC/DiRAC domains
- However we have limited resources. Talk to Jeffrey if you have a project in mind.
- RSE team is also part of the support team and will try to help all users of the system

CSD3 is good for

- Classic MPI-parallelised HPC applications
- Pipelines that can use GPU, CPU and KNL
- Applications that need lots of IO bandwidth
  large flash filesystem will deliver 100s of GB/s

UNIVERSITY OF CAMBRIDGE
Research Computing Services

How do the RSEs work in GW4?

- GW4 runs the Isambard ARM64 cluster
- RSEs at Bath, Bristol, Cardiff and Exeter work closely with engineers at Cray, and help researchers port applications to ARM
- Result is a large and growing ecosystem of HPC software that now runs on Isambard, and demonstration of ability to run a production ARM64 system
- This is one reason why Bristol was one of three universities awarded a free HPE ARM64 supercomputer (Catalyst UK, 4096 cores) – HPE were confident that we had the staff and expertise to immediately run it as a production system

Status of Isambard

Cavium ThunderX2

- **James Price is lead RSE**
- Initial porting using pre-production silicon from Summer 2017
- November 2017 has 8xFoxconn servers containing A0 silicon (2xThunderX2, but with one socket disabled)
- March 2018 replaced with B1 silicon (2 socket) plus pre-release Cray tools and compilers

Full system will depart the factory in the US in early July, and installed in late July. Will comprise >160 nodes based on 2x32cores at >2 GHz per core and >= 2500 MHz memory clock. Will be 10,000+ cores total, with Cray interconnect.

(HPE will arrive at the same time, also be ThunderX2, but will have a Mellanox Infiniband interconnect – will be interesting to compare…)

Hackathons

- Focus of RSE effort has been the Isambard Hackathons
- Three hackathons, with the aim to support researchers as they port and optimize code on Isambard
- James Grant, RSE at Bath, will now provide a summary…

Other RSE work

- In addition to the hackathons, we work continuously to optimize and port key codes
- Also working on porting R and Anaconda Python
- Work closely with Cray engineers, e.g. during porting of R, we discovered that “fortran” is a reserved keywork in the Cray C++ compiler. Notified Cray who are providing a fix…

Discussion Session

- Four questions in Google docs:
  - What do we want to achieve from Tier-2?
  - How do you want to find about about Tier-2?
  - What forums should Tier-2 use to work together?
  - How could Tier-2 RSEs help?
- Please add your answers to the google docs by following this link
  - https://goo.gl/5Kc2EN
- We will capture notes here during live discussion

A Whistle Stop Tour of Isambard Hackathons

Dr James Grant

University of Bath

r.j.grant@bath.ac.uk

Archer Champions
25th April 2018

Overview

Isambard partners

A typical Hackathon

{Is the} Future Hackathon(s)

Partners

UNIVERSITY OF
BATH

CRAY

Met Office

GW4
Isambard

CAVIUM

arm

UNIVERSITY OF
BATH

University of
BRISTOL

EPSRC

CARDIFF
UNIVERSITY
PRIFYSGOL
CAERDYDD

UNIVERSITY OF
EXETER

Developing a Community

- To date 2 Hackathons
- Coincident with delivery (November 2017)
- and upgrade (March 2018)
- Opportunity for meet and greet with other RSEs
- Discussions with suppliers
- and developers

Raising Steam

Raising Steam

UNIVERSITY OF BATH

Stoking the Fire

The plan ...

- Introductions and goals
- The TX2 architecture
- ARM software
- Cray Programming Environment
- Hands on - "Roll up your sleeves"

Objectives

Target "10" highest use codes on ARCHER:

Raising Steam

VASP, GROMACS, CP2K, UM, OpenFOAM

Stoking the Fire

CASTEP, HYDRA, NAMD, Oasis, SBLI, OpenFoam, UM and NEMO

Port, (validate), benchmark, optimise
Find bugs - in libraries; in codes? Profile?

Takehomes

Excellent opportunity to develop the Tier-2 community (RSEs, SysOps, Researchers, Code developers)
Training with/provided by suppliers
Develop collaborations
Share experience
Hackathon teambuilding meal (subject to funding)

Future Hackathon(s)

1. Raising Steam
2. Stoking the Fire
3. Off the rails?

Future Hackathon(s)

1. Raising Steam
2. Stoking the Fire
3. Train wreck?

Future Hackathon(s)

1. Raising Steam
2. Stoking the Fire
3. Tunnel vision?

Plans

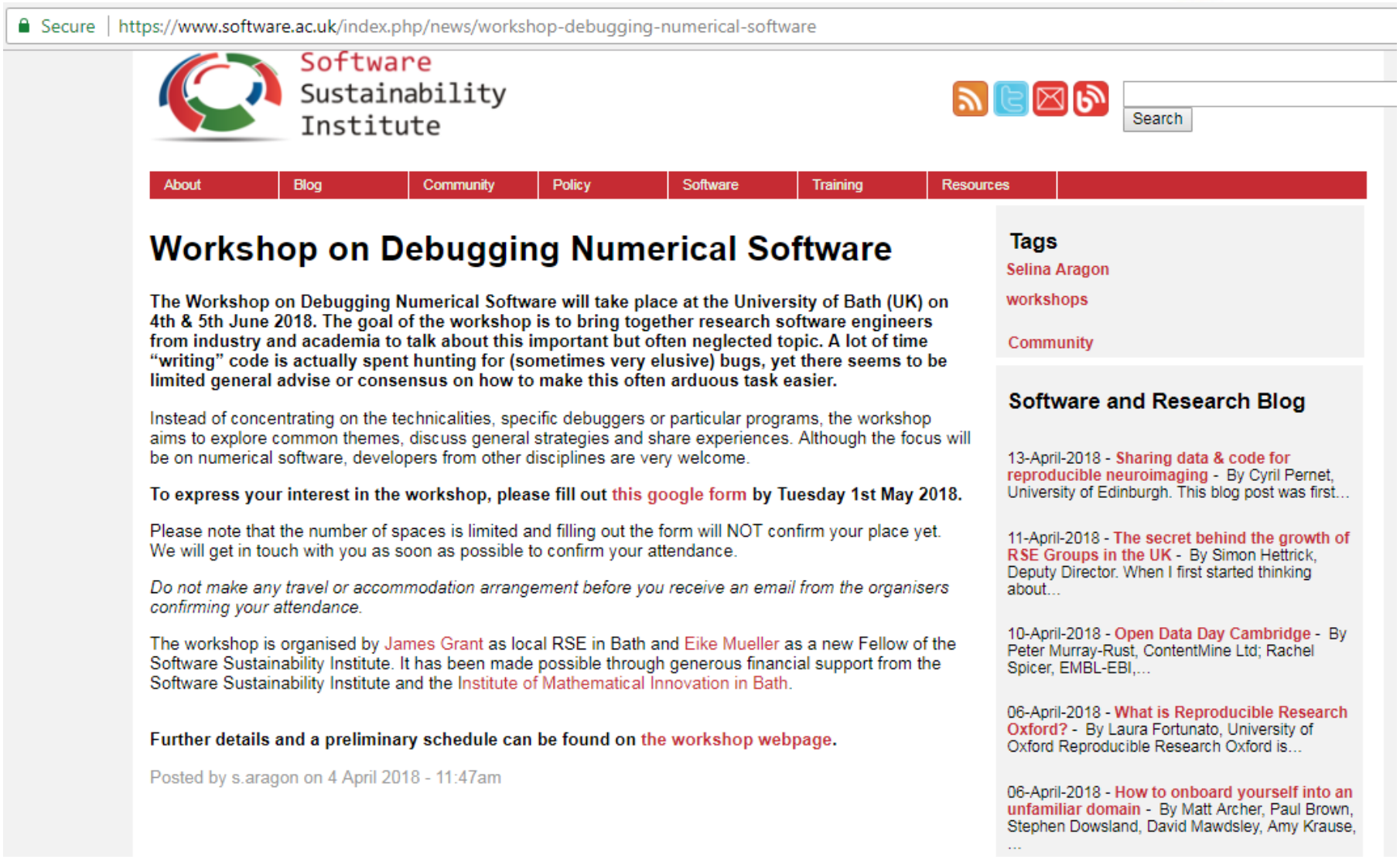
1. Dinner/social event
2. Broader reach: RSE, SysOps, Researchers
3. More on profilers and debuggers (CRAY and ARM)
4. Cheat sheets and other docs
5. Formalising internal and external RAP process
6. Standard software packages, modules, builds, licensing?
7. Future training, hackathon needs

Tier-2 Hackathons

To pre-empt Christopher:

- Is this something that could benefit across Tier-2(s)?
- What would it look like?
- Where will we/you get funding?

Shameless plug



Secure | https://www.software.ac.uk/index.php/news/workshop-debugging-numerical-software

Software Sustainability Institute

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Workshop on Debugging Numerical Software

The Workshop on Debugging Numerical Software will take place at the University of Bath (UK) on 4th & 5th June 2018. The goal of the workshop is to bring together research software engineers from industry and academia to talk about this important but often neglected topic. A lot of time "writing" code is actually spent hunting for (sometimes very elusive) bugs, yet there seems to be limited general advise or consensus on how to make this often arduous task easier.

Instead of concentrating on the technicalities, specific debuggers or particular programs, the workshop aims to explore common themes, discuss general strategies and share experiences. Although the focus will be on numerical software, developers from other disciplines are very welcome.

To express your interest in the workshop, please fill out this google form by Tuesday 1st May 2018.

Please note that the number of spaces is limited and filling out the form will NOT confirm your place yet. We will get in touch with you as soon as possible to confirm your attendance.

Do not make any travel or accommodation arrangement before you receive an email from the organisers confirming your attendance.

The workshop is organised by James Grant as local RSE in Bath and Eike Mueller as a new Fellow of the Software Sustainability Institute. It has been made possible through generous financial support from the Software Sustainability Institute and the Institute of Mathematical Innovation in Bath.

Further details and a preliminary schedule can be found on the workshop webpage.

Posted by s.aragon on 4 April 2018 - 11:47am

Tags

Selina Aragon

workshops

Community

Software and Research Blog

13-April-2018 - Sharing data & code for reproducible neuroimaging - By Cyril Pernet, University of Edinburgh. This blog post was first...

11-April-2018 - The secret behind the growth of RSE Groups in the UK - By Simon Hettrick, Deputy Director. When I first started thinking about...

10-April-2018 - Open Data Day Cambridge - By Peter Murray-Rust, ContentMine Ltd; Rachel Spicer, EMBL-EBI,...

06-April-2018 - What is Reproducible Research Oxford? - By Laura Fortunato, University of Oxford Reproducible Research Oxford is...

06-April-2018 - How to onboard yourself into an unfamiliar domain - By Matt Archer, Paul Brown, Stephen Dowsland, David Mawdsley, Amy Krause, ...

End of the line

Thank you!

Any short questions?