



Update on Bede / NICE

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EPSRC Tier-2 response



- Call that ran over summer 2019
- Secured £3.2M to establish Tier-2 HPC facility: NICE19
- Key Objective
 - **Enable data from observation and models to inform each other, more effectively, in support of scientific discovery.**
 - Deploy hardware architecture that extends capabilities of accelerated computing.
 - Community of expertise to enable best use
- N8 contribution
 - Electricity and system administration costs
 - 1FTE RSE effort per site
 - Coordination from N8-CIR
- IBM (training / software) and OCF support
- Collaboration & co-location with DiRAC
- 62% N8 allocation, 38% National access



DiRAC



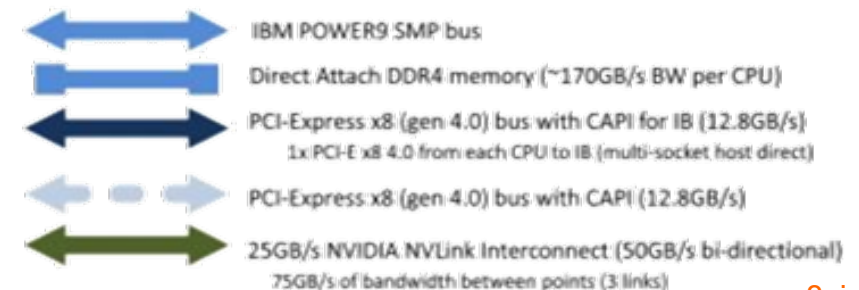
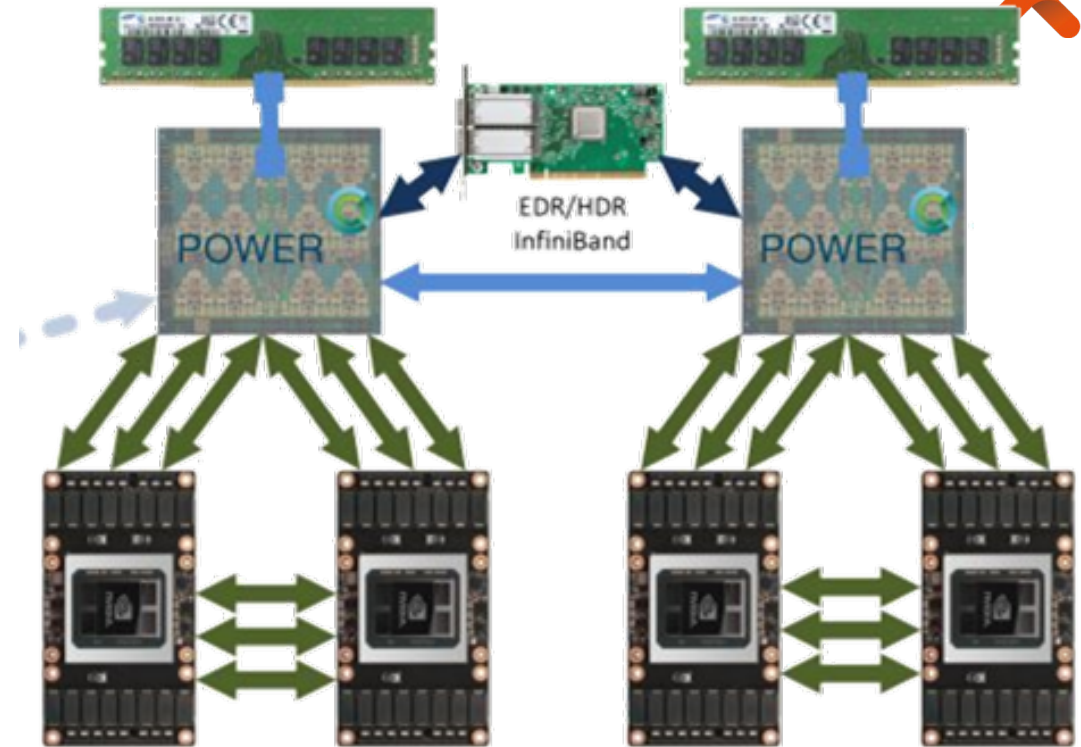
Bede

- Scholar and Historian 673 – 735 AD
- Most widely known for work focusing on role and increasing influence of the church in what was contemporary society.
- Also produced scientific writing
 - Not afraid of challenging wisdom of the time.
 - Wrote a text for teaching students on what was known of the physical sciences at the time.
 - Wrote clear explanation of the evidence that the Earth was a globe (well understood at the time)
 - Established the connection between the tides and the moon.
 - Performed calculations to calculate the age of the world and the dates of the Easter festival
- Currently buried in the Galilee Chapel, Durham Cathedral
- His main problem, apparently, was his students had a tendency to skip lessons to go fox-hunting



System architecture

- IBM AC922 main building block – 32 compute Nodes & 2 login nodes.
- 2x Power9 CPUs per node (18-core 3.15Ghz)
- 0.5TB Memory/node
- 4x NVidia V100 per node
- CAPI – memory coherence between accelerator and CPU.
- Also 4 nodes of IC922
 - 20core 2.9GHz Power9
 - 4 with 4 x Nvidia T4, PCIe Gen 4 Mellanox EDR connected nodes
- 2Pb/ 10GB/s Lustre parallel filesystem



Access mechanisms



- EPSRC Consortia:
 - HECBioSim award 190kGPU hours/year through calls every 6 months.
 - UKCP and MCC pump-priming access.
 - Being requested/formalised as part of current HEC Consortia call
- EPSRC Resource Allocation Panel
 - Through Access to HPC call every ~6 months, alongside other Tier 2 and ARCHER2
- N8 partner access (<https://n8cir.org.uk/supporting-research/facilities/bede/bede-application/>)
 - Application via N8 website, facilitated by local institution.
 - 1 FTE RSE support available locally.
- Director's share
 - Cross institutional/pump-priming/strategic access.
- Bede Driving test (to come).

Training & support



- N8 CIR training specifically for Bede
 - Bede introductory event
 - IBM training for Bede – AI
 - Fundamentals of Accelerated Computing with CUDA + C/C++
 - IBM training for Bede – HPC
 - Cryo-EM, Genomics & other Life science workload on Bede
- Online at: <https://www.youtube.com/c/N8CIR> Other training at: <https://n8cir.org.uk/events/past-events/>
 - Includes carpentry-style train the trainer for Bede RSEs
- Documentation at: <https://bede-documentation.readthedocs.io/en/latest/>
- Early user survey undertaken 24th March – 14th May 2021
- User groups held quarterly

Update on service



- Support via:
 - Distributed helpdesk
 - Slack work space
 - Email lists
- Collaborative task-forces
 - AMBER / GROMACS - closing
 - Documentation - ongoing
 - Driving test – will release 1st test over summer
 - Possible benchmarking/performance TF
- User survey:
 - <https://forms.office.com/r/kjiibq7fra>
- PI survey:
 - Maintain correct project information
 - Update grant support & outputs information



Next 6 months



- Coordinate 3 task forces arising from feedback from user group and survey
 - Improving and extending documentation
 - Setup of Bede driving test
 - Improving access to GROMACS and AMBER
- OS from RHEL 7.6 upgrade to RHEL 8
 - Latest ML tools require later version of CUDA only on RHEL 8 on Power.
 - Watson Machine Learning Community Edition tied to RHEL 7.6
 - Extended memory & DDL support for ML becomes equivalent to on x86
 - May still be able to use Large memory support in Pytorch and Tensorflow, but not maintained by IBM
- IBM facilitated CryoEM/life sciences workshop
- Actions arising from WHPC chapter application

Keep In Touch



- Website – n8cir.org.uk
- Case studies - <https://n8cir.org.uk/supporting-research/rse/case-studies/>
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