HPC Update from the UK:
News, Success Stories and Lessons

IDC HPC User Forum, Dearborn

17-19 Sep 2012

Andrew Jones
VP, HPC Services & Consulting, NAG

nag®

Experts in numerical algorithms and High Performance Computing services

HECToR

HPC Update from the UK

- News
- Success Stories
- Lessons

HPC as a strategic national asset

- Led by the Government Department for Business, Innovation and Skills (BIS)
- [new] E-Infrastructure Leadership Council (ELC)
  - Co-chaired by Minister of State for Universities & Science
  - Industry, Academia, Government, HPC & Non-HPC
  - “Advice to the minister”
  - Minister (and co-chair) “own” national HPC strategy
  - Strategy executed by appropriate agencies (e.g. RCUK)
  - 10 year plan for e-Infrastructure (HPC)

New £158m capital investment in 2011/12

- ARCHER (next National Supercomputing Service)
- Hartree Centre at STFC Daresbury
- Themed (DiRAC, Climate, …)
- Data
- Networking
- …

Also from the £158m …

EPSRC

- West of Scotland Supercomputing Centre for Academia and Industry (**ARCHIE**)
- **N8** e-Infrastructure Interconnectivity
- **Midlands** Centre of Excellence for **HPC**
- **MidPlus** Centre of Excellence for Computational Science, Engineering & Mathematics
- **e-Infrastructure South** Centre for Innovation
- **CORE** (Imperial & Cambridge)

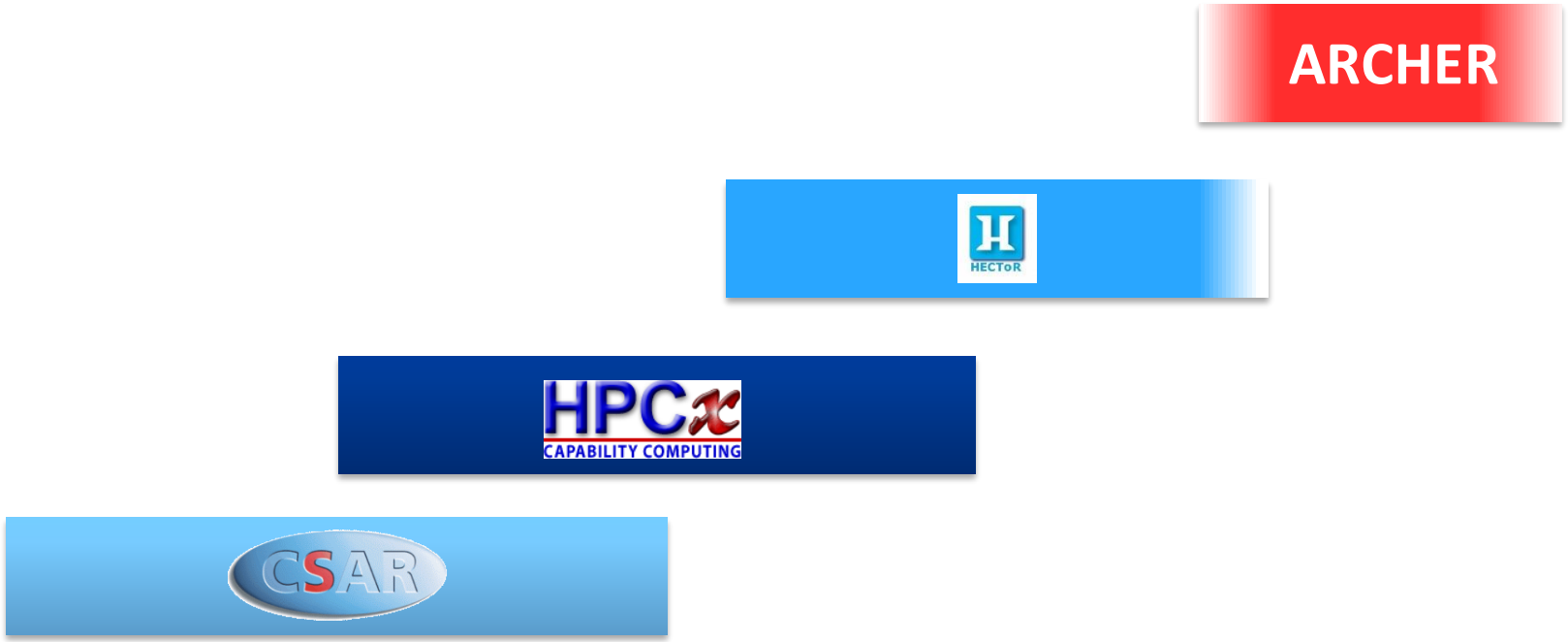
Some other UK HPC …

HPC Wales	UK Met Office	AWE	Industry
			

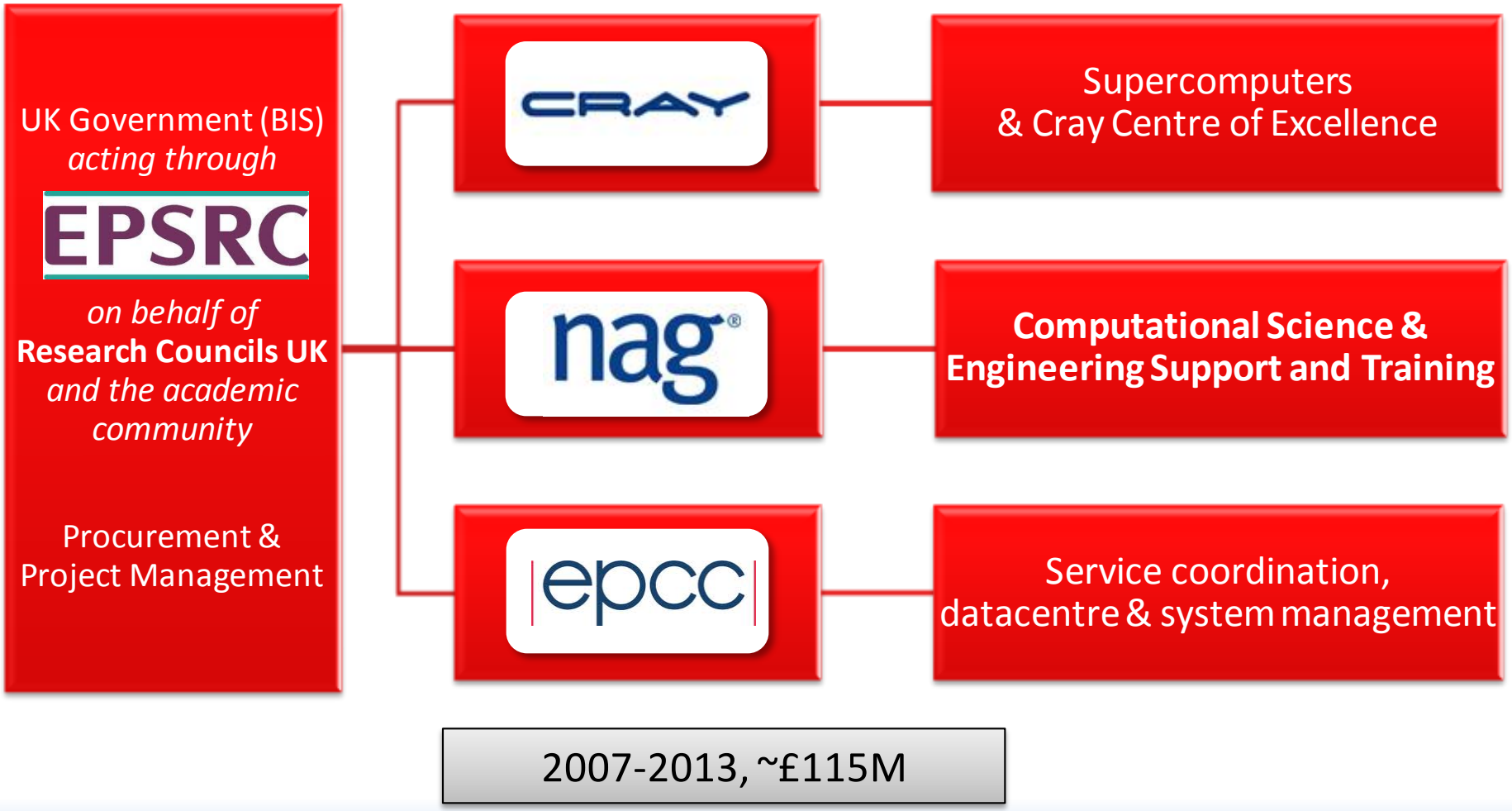
HECToR:
The UK National Supercomputing Service

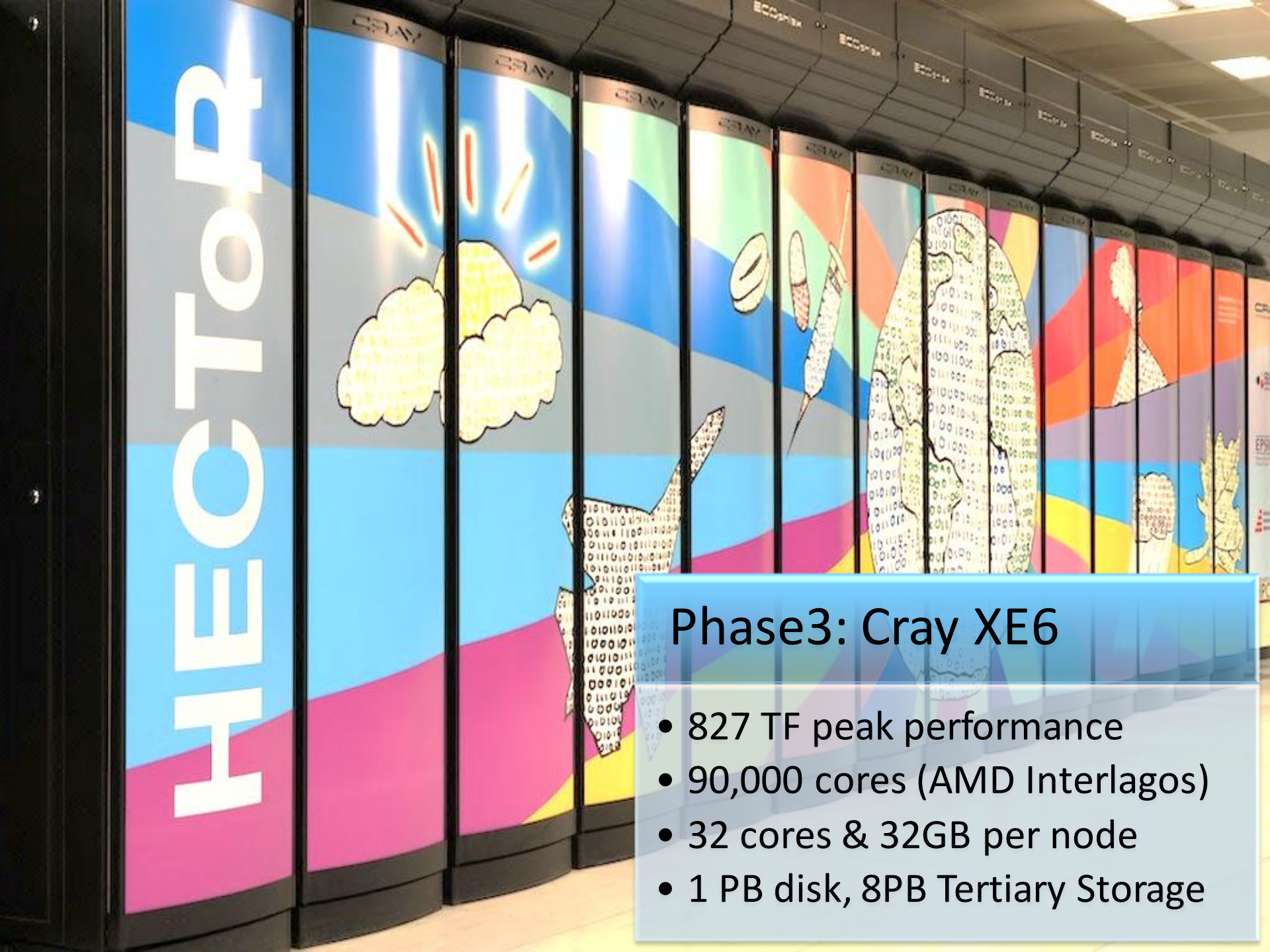
Proving the benefits of investment in application software performance and capabilities

UK national supercomputing services



The UK national supercomputing service





Phase3: Cray XE6

- 827 TF peak performance
- 90,000 cores (AMD Interlagos)
- 32 cores & 32GB per node
- 1 PB disk, 8PB Tertiary Storage

NAG CSE Support Service for HECToR

- ~20 FTE
- In-depth support queries
- Short projects
  - Porting, tuning, benchmarking, profiling, testing
- dCSE projects
  - 6-48 months
  - Performance, scalability, algorithms, …
  - Embedded -> sustainability and dissemination of skills, codes, …
- Training courses
  - Delivered by experienced practitioners
  - So far >1100 attendees, >50 institutions
  - Mainly delivered at user sites (over 20 so far)

Driving science with HPC

Enhanced scientific capabilities -> new science & discoveries

Better models of real world phenomena	Explore new regions of parameter space	Discover new relationships and behaviour

Improved computational modeling capability

Larger & more complex models	Finer resolutions and fidelity	More complex physics	Uncertainty quantification

Improved application software performance

Code optimization	Enhanced scalability	Algorithm development

Just a few of the >50 successes so far …

HECToR

- ✓ **Speed and Scalability** of Key Materials Science Code (CASTEP) Quadrupled
- ✓ Speed and **I/O Performance** of Oceanography Code (NEMO) Enhanced
- ✓ Performance of Quantum Monte-Carlo Application (CASINO) **Quadrupled**
- ✓ **Speed and Scalability** of Materials Science Simulations (CP2K) Enhanced
- ✓ **Performance** of Atmospheric Chemistry Simulations (GLOMAP/TOMCAT) Enhanced
- ✓ **Performance** of Geodynamic Thermal Convection Simulations (CITCOM) Enhanced
- ✓ Scalability of Fluid Turbulence Simulations (EBL) **Enhanced up to 40x**
- ✓ Simulations of Catalytic Chemistry with ChemShell **8x Faster**
- ✓ Scalability of Ocean Modelling Application (Fluidity-ICOM) **Dramatically Improved**
- ✓ Performance of Molecular Dynamics Application (DL_POLY_3) **20x Faster**
- ✓ **Capabilities** of Key Materials Science Application (CASTEP) Significantly Enhanced
- ✓ Performance of Heart Modelling Application (CARP) **20x Faster**
- ✓ Performance of Turbulent Fluid Flow Simulations (Incompact3D) **Improved by factor of 6x**
- ✓ **Performance and Capabilities** of Materials Science Code (Conquest) Enhanced
- ✓ Aircraft Noise Simulations (CABARET) **Get Faster and Reach Bigger Models**

http://www.hector.ac.uk/cse/reports/

SUMMARY

Why HPC?

HPC is used to do a job, not [just] interesting in itself

Getting more **performance** from current process is immediately valuable

hardware *or* software

Enabling a **new capability** (step change) might be *enormously* valuable

hardware ***and*** software

people, training, education, …

Key messages

HECToR & NAG proving the **science and cost benefit** of investing in hardware *plus* software development

$80m supercomputer + $20m CSE investment delivers more science than $100m supercomputer alone

NAG now also delivering this HPC expertise to **other national HPC centres** & **industry internationally**

Follow me: @hpcnotes

END

www.nag.com | blog.nag.com | @NAGtalk