

# HECToR Update

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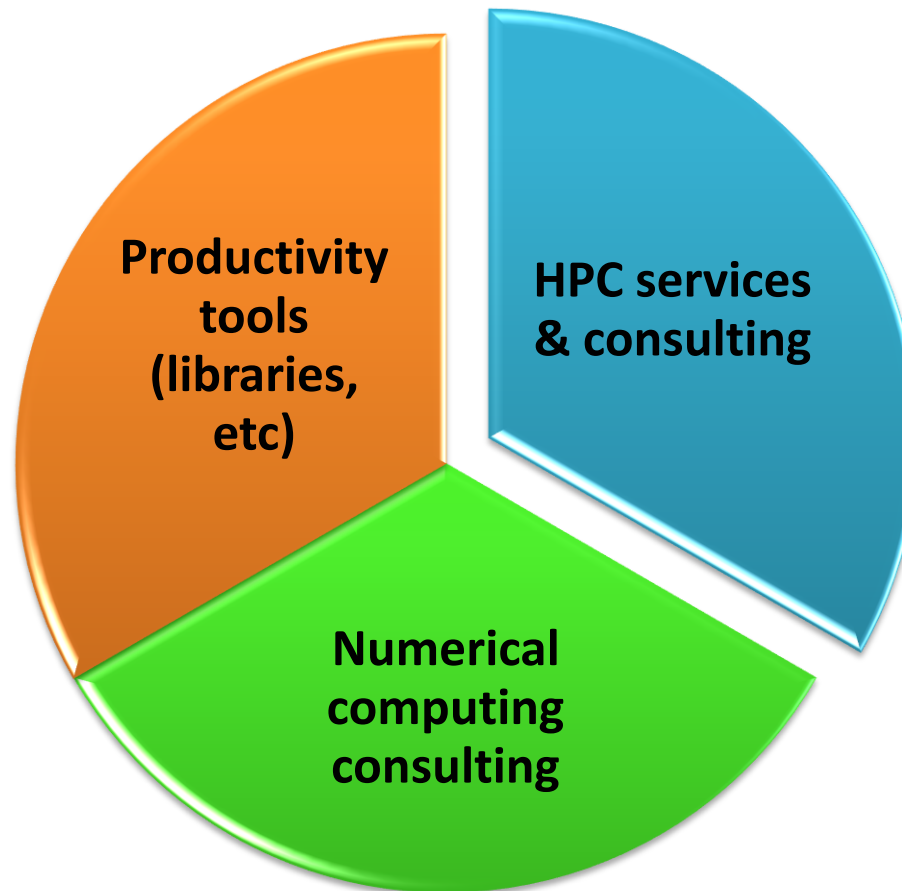
*IDC HPC User Forum  
8-10 September 2009*



Experts in numerical algorithms  
and HPC services

# N A G : what we do

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**HECTOR**

HIGH END COMPUTING TERASCALE RESOURCE

A Research Councils UK High End Computing Service

Capability Science. NAG HPC expertise.

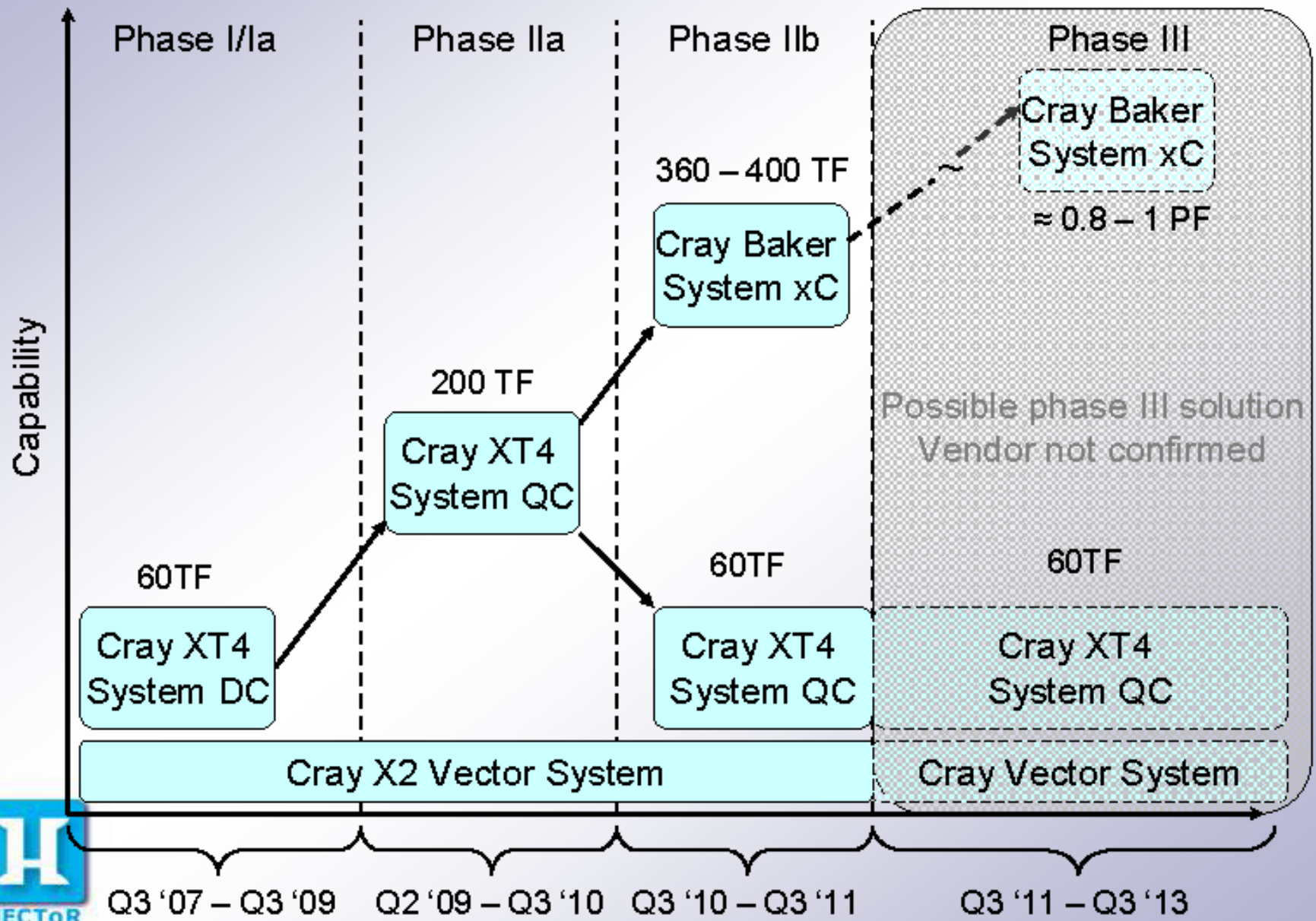
The UK's £113M primary national academic supercomputing service, 2007-2013

“a service to the UK academic community to enable true **capability science**”





# Revised HECToR Upgrade Roadmap



# HECToR: capability CSE support

## Comparable scale investment in expertise

- Computational Science & Engineering
- Capability support model

User requirements capture during HECToR procurement identified the need for strong CSE support



# HECToR service structure

Academic user community

Helpdesk

Training, dCSE

20 FTEs CSE support

( **N A G** )

Cray  
Centre of  
Excellence

System management & hosting (UoE HPCx)

[Phase 2a] 208 TF Cray XT4 plus X2

Phase 3 (Unknown)



# NAG's role in HECToR

## **Independent HPC advisor to procurement project**

Market survey,  
benchmarking, technology  
watch, etc

## **CSE service contract**

120 person-years  
(competitively won)

# NAG HPC Services & Consulting

## **Support the business**

Strategy and procurement  
Technology evaluation &  
benchmarking

## **Support the user/developer**

Software engineering for  
robustness, performance,  
scalability and portability

# Technology driving need for CSE

There used to be 3 main types of HPC

- Vector
- SMP
- MPP

Now we have all these rolled into one

Programming this at scale is hard



# Quiz: A sensible alternative?

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- As an aerodynamics engineer, you decide that the programming skills and effort required to use your CFD code on high end supercomputers are just too much of a diversion from your science
- You decide to only do those simulations that fit on your high end desktop workstation
- Your group hires a pair of good old-fashioned wind-tunnel engineers to test more complex designs

# CSE: Computational Science & Engineering

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The science & engineering of computation ...

- Scaling, optimisation, multi-core enabling, algorithm development & innovation, functional enhancements, re-factoring, software engineering for robustness & performance, ...





# Why CSE investment matters to users

## Faster

Reduce time to solution

Bigger simulation in same time

More simulations in same time

## Better

Larger, more complex models

Better resolutions

Longer model time spans

## Cheaper

More efficient use of hardware

More efficient service costs

More efficient use of people

# Distributed CSE support service

~60% of CSE **embedded in user community**

- secondments to specific research groups
- research group staff funded by HECToR (NAG)

all staff managed by, and part of, NAG team

6-24 months of effort (may be >1 FTE)



# Return on Investment – examples so far

## Materials science code (CASTEP)

- 8 person months
- 4x scalability or 4x faster
- Up to £2.4M savings for remainder of project

## Climate code (NEMO)

- 6 person months
- 25% faster
- Potential £3M savings across all HECToR users



# The future: national services

## Child of HECToR

- Next national service
- On funding roadmap, planning underway

## PRACE: European multi-Petascale service

- UK [EPSRC] is a Principal Partner – likely to host Tier0 system



## Summary



“... **capability science** ...”

capability usage *and* support model



**CSE investment enables better science,  
quicker and at lower cost**

**nag**

NAG's HPC expertise  
underpins HECToR mission



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