Parallel Software usage on UK National HPC Facilities 2009-2015

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Reusing this material

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Outline

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- Analysis Tool
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- Summary

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  - Particularly Alan Simpson and Stephen Booth
- Thanks also to the Cray Centre of Excellence staff at the University of Edinburgh
  - Particularly Jason Beech-Brandt

Motivation

- Understand the application profile on UK National Supercomputing Services so we can provide a better service
  - Different research areas will have different requirements
- Often stated that applications have trouble scaling to O(10000) cores and beyond
  - Is this true?
  - If so, what are the limiting factors?
- Which areas are growing in usage and which are decreasing?
  - Same question for applications: which new applications have appeared and which old ones have disappeared?

Systems Included

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Systems Included

System (Type)	Processor Arch. (Clock Speed)	Cores per Node (Sockets)	Memory/ Node (Bandwidth/ core)	Nodes (Cores)	R_{peak} (Tflop/s)
HECToR Phase 2a (Cray XT4)	AMD Barcelona (2.3 GHz)	4 (1)	8 GB (3.2 GB/s)	5664 (22656)	63.4
HECToR Phase 2b (Cray XE6)	AMD Magny-Cours (2.1 GHz)	24 (2)	32 GB (3.6 GB/s)	1856 (44544)	372.8
HECToR Phase 3 (Cray XE6)	AMD Interlagos (2.3 GHz)	32 (2)	32 GB (2.7 GB/s)	2816 (90112)	829.0
ARCHER (Cray XC30)	Intel Ivy Bridge (2.6 GHz)	24 (2)	64 GB (4.9 GB/s)	4920 (118080)	2550.5

Analysis Tool

Analysis Tool

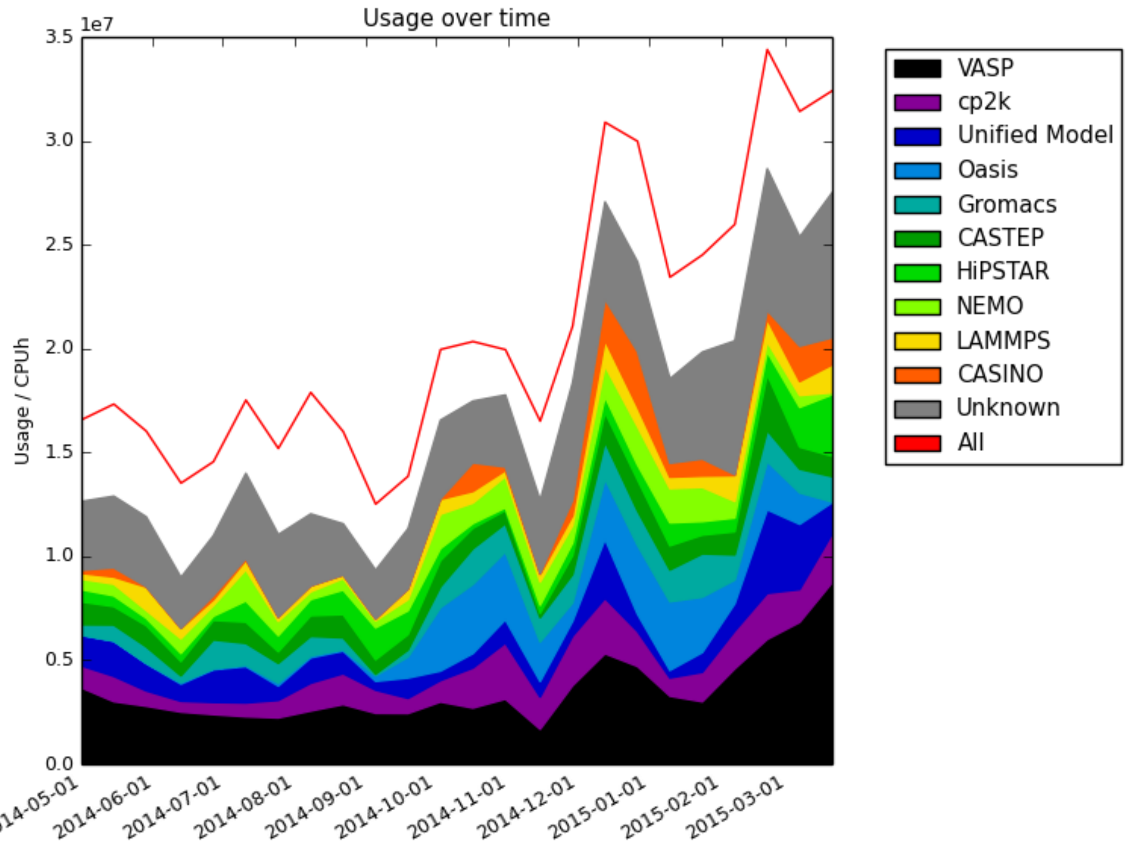
- Poll ALPS on an hourly basis and store:
  - User, size of job, executable name, ALPS ID
- Analyse logs using Python program
  - Extensible descriptions of applications include: programming language, parallel model, code type, research area, license
  - Executable names matched via regex
- Can limit to specific period or project
- Text, graphical and/or CSV output
- Hints to help identify further applications

Analysis Tool: Example Output

Total code usage (ordered by CPUh)

Code	CPUh	% Time	Jobs	% Jobs	Users	Mean	Median
====	==========	======	====	======	=====	====	======
VASP	90128736.0000	17.36	202742	40.78	177	2202.36	240.0000
cp2k	35669040.0000	6.87	21155	4.25	78	3702.55	672.0000
Unified Model	31979904.0000	6.16	18613	3.74	159	2087.09	1392.0000
Oasis	31491624.0000	6.07	2074	0.42	10	6249.98	5232.0000
Gromacs	26942616.0000	5.19	13759	2.77	69	941.73	432.0000
CASTEP	26060376.0000	5.02	74661	15.02	92	2434.20	360.0000
HiPSTAR	24043632.0000	4.63	1146	0.23	11	14439.75	10344.0000
NEMO	21366096.0000	4.12	19498	3.92	21	3589.34	1920.0000
LAMMPS	14493840.0000	2.79	9851	1.98	50	672.84	456.0000
CASINO	13404504.0000	2.58	861	0.17	4	5991.07	5016.0000
ONETEP	12339456.0000	2.38	3190	0.64	23	1079.92	864.0000
Hydra	10611552.0000	2.04	930	0.19	13	2069.26	1248.0000
NAMD	9475416.0000	1.83	8913	1.79	34	613.54	480.0000
CRYSTAL	8659632.0000	1.67	2237	0.45	26	6945.64	2808.0000
PDNS3D	7278528.0000	1.40	755	0.15	9	6721.09	6144.0000
WRF	6611784.0000	1.27	1170	0.24	20	2591.09	2064.0000
OpenFOAM	6474984.0000	1.25	2560	0.51	19	695.84	288.0000
MITgcm	5415576.0000	1.04	8284	1.67	23	571.12	384.0000

Analysis Tool: Example Output



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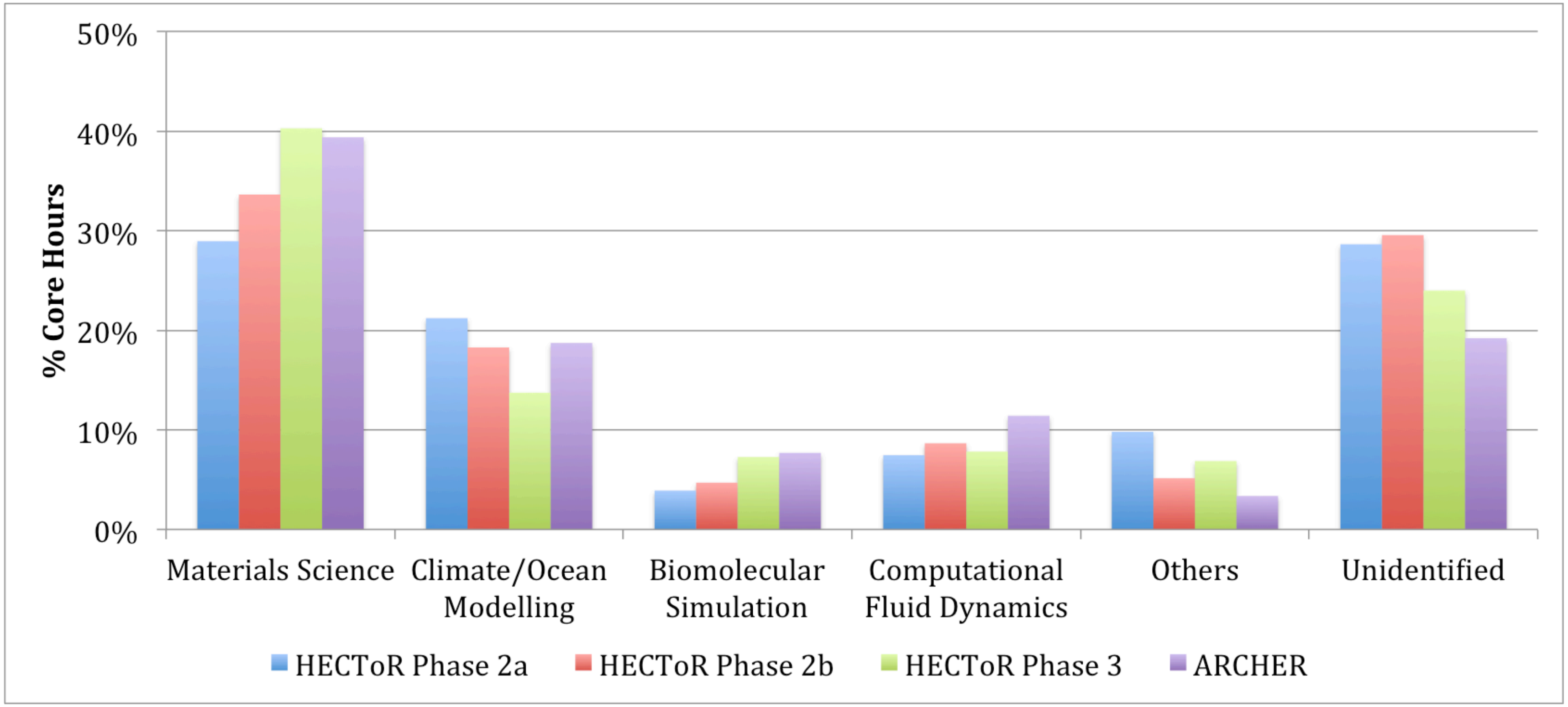
Overall Comparisons

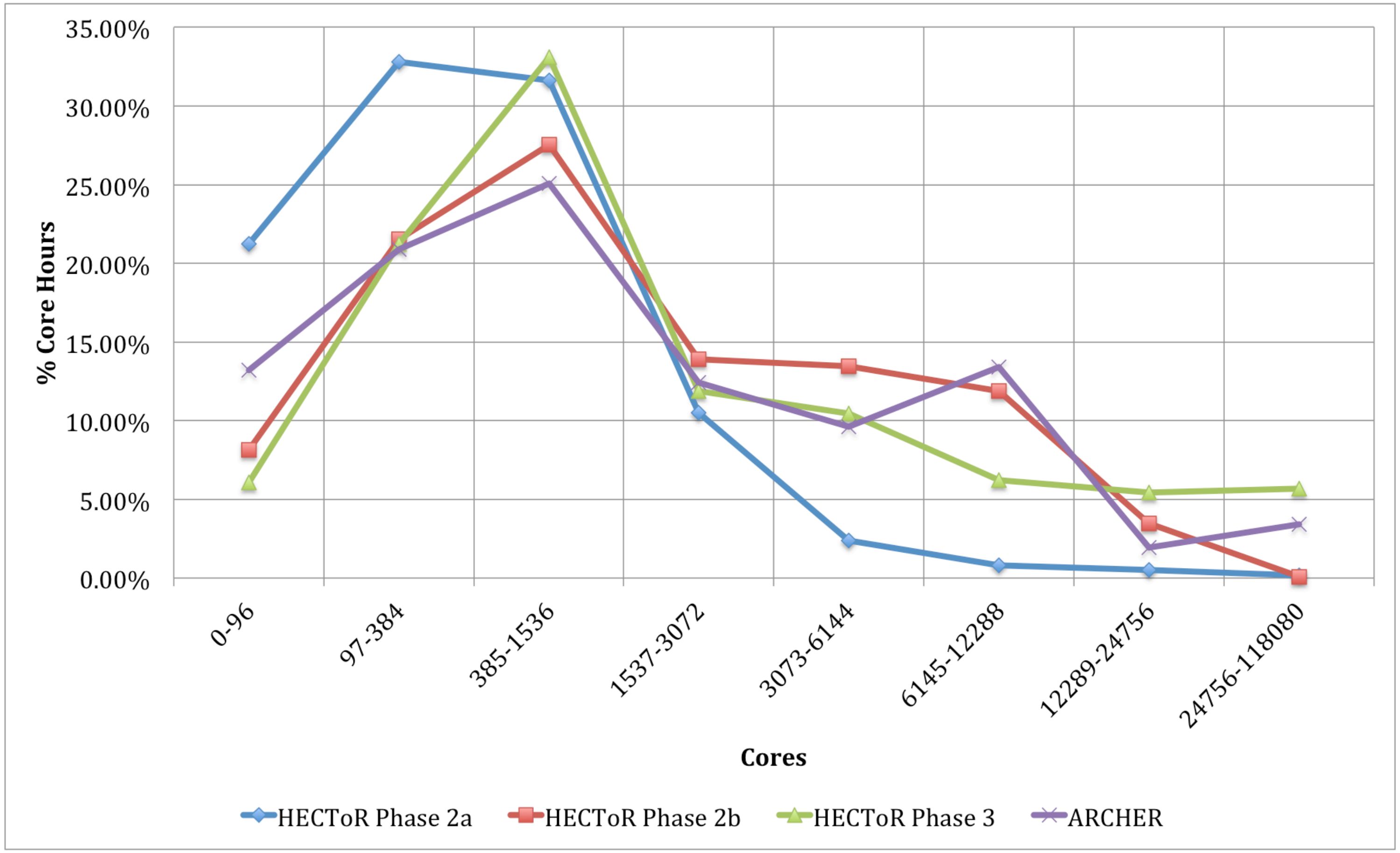
Overall Comparisons: Top Ten Codes

HECToR Phase 2a	HECToR Phase 2b	HECToR Phase 3	ARCHER
UM	VASP	VASP	VASP
VASP	UM	CP2K	CP2K
CASTEP	CASTEP	UM	UM
Hydra	CP2K	CASTEP	Oasis
CP2K	INCOMPACT3D	Gromacs	Gromacs
Chroma	NEMO	DL_POLY	CASTEP
NAMD	Gromacs	PDNS3D	HiPSTAR
ChemShell	MITgcm	MITgcm	NEMO
WRF	ChemShell	NEMO	LAMMPS
DL_POLY	PDNS3D	CRYSTAL	CASINO

Overall Comparisons



Overall Comparisons

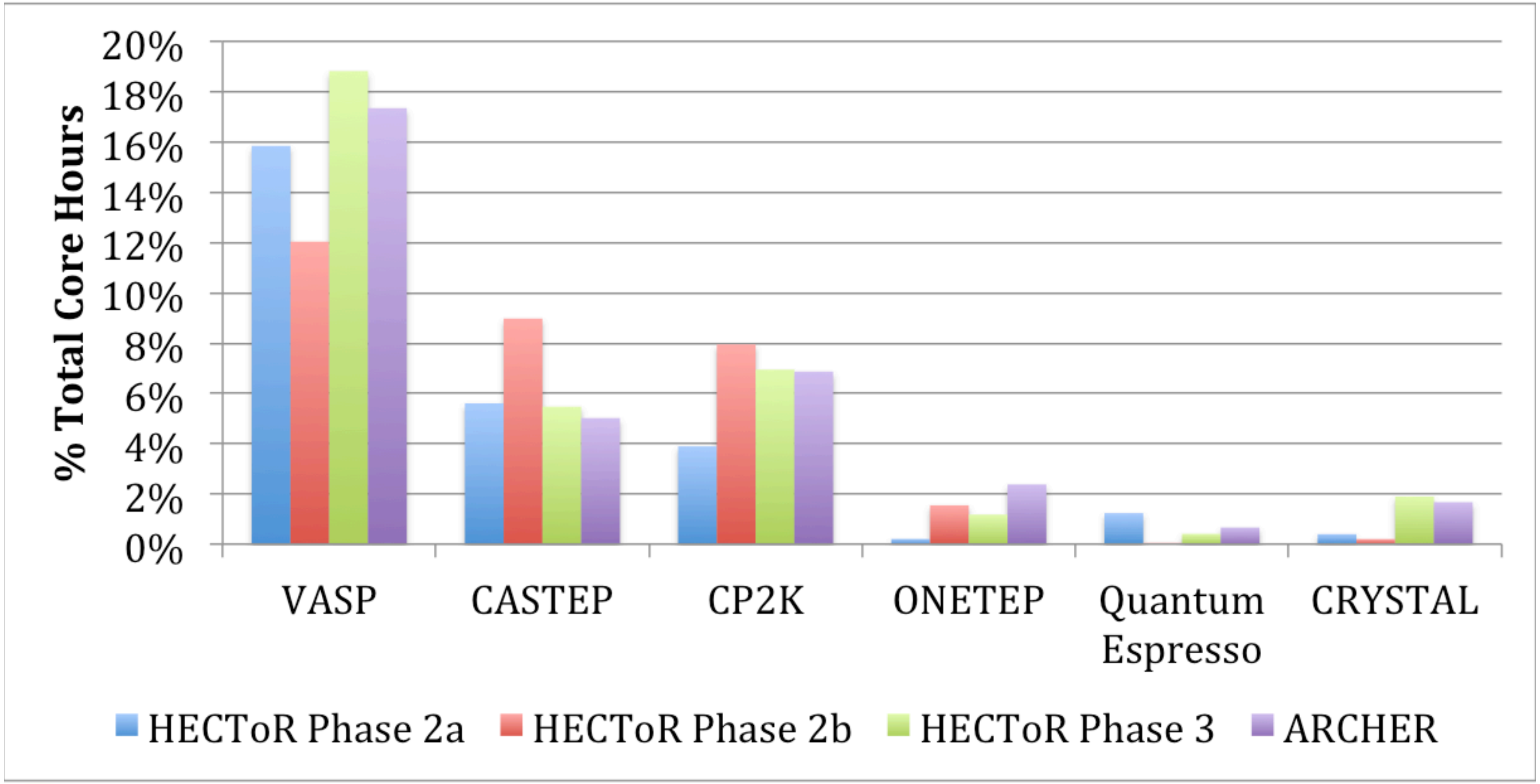


Overall Comparisons: Summary

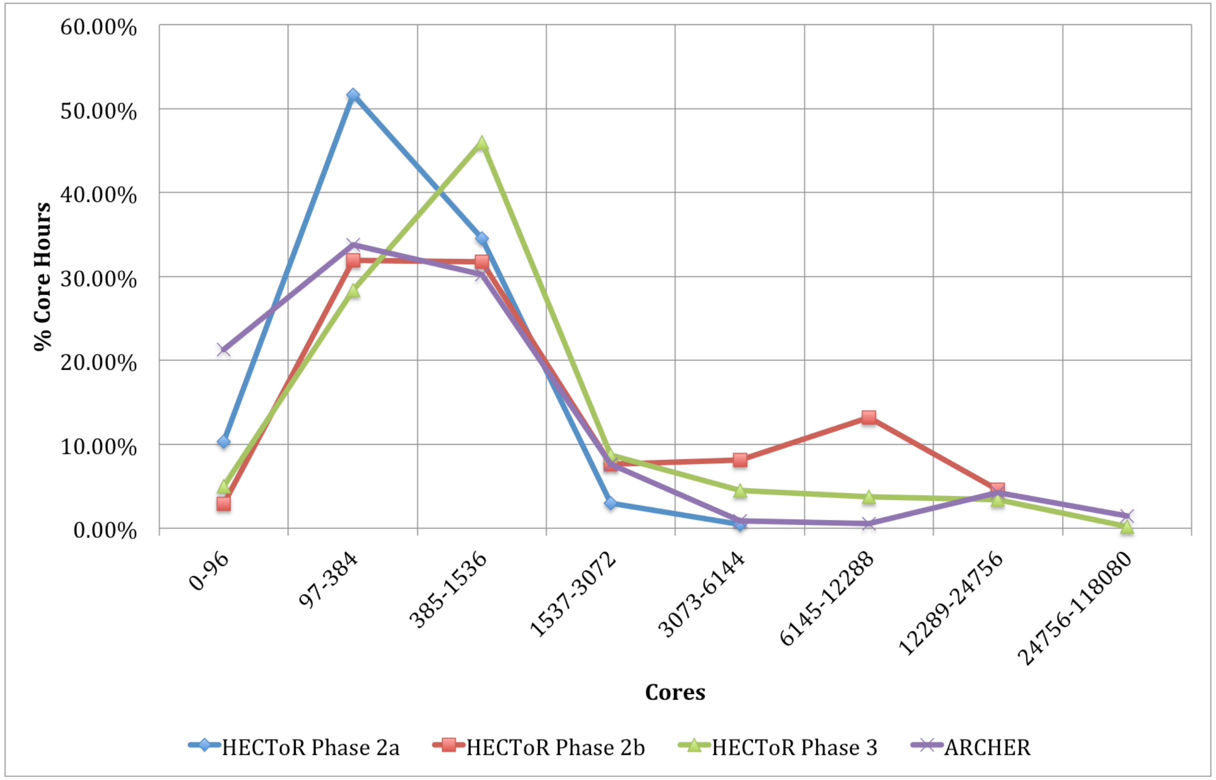
- Biggest growth areas are materials science and biomolecular simulation
  - In “Others” category, Medical Physics has grown from 0.01% to 0.5% and we expect this to carry on growing
- Largest change has been from quad core (phase 2a) to many multicore (phase 2b)
- Modest increase in job size
  - As materials science is majority of usage, it has the largest effect on job size
  - This area has not increased job size as much as others

Application Areas

Periodic Electronic Structure

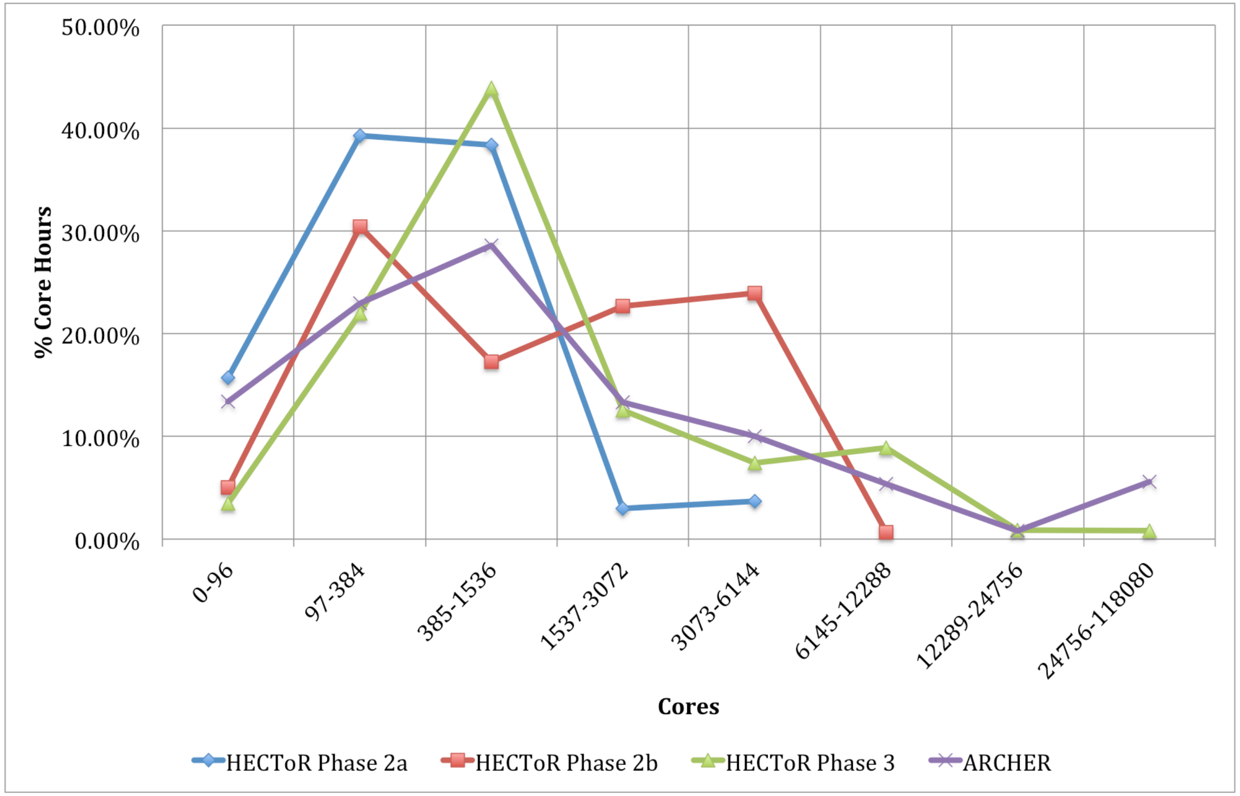


Periodic electronic structure



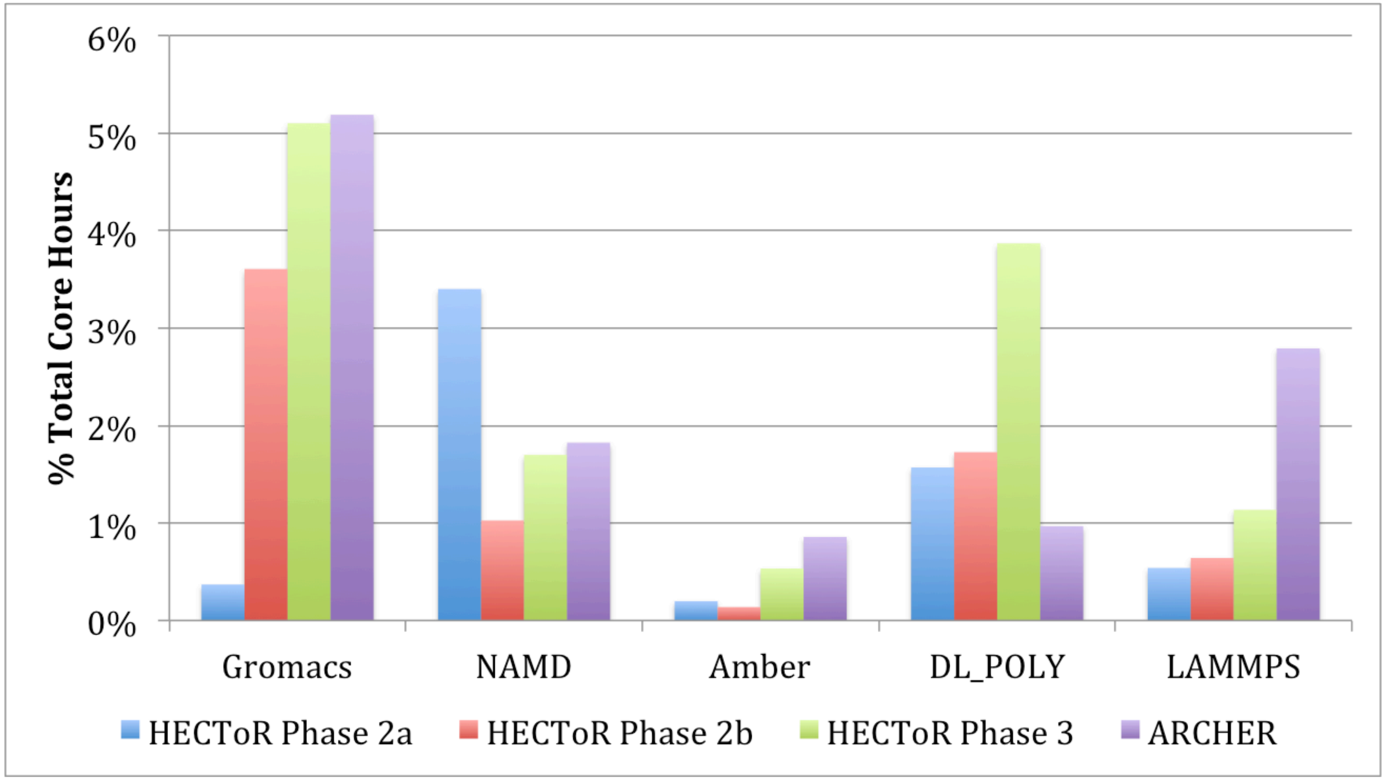
CASTEP job size distribution

Periodic electronic structure



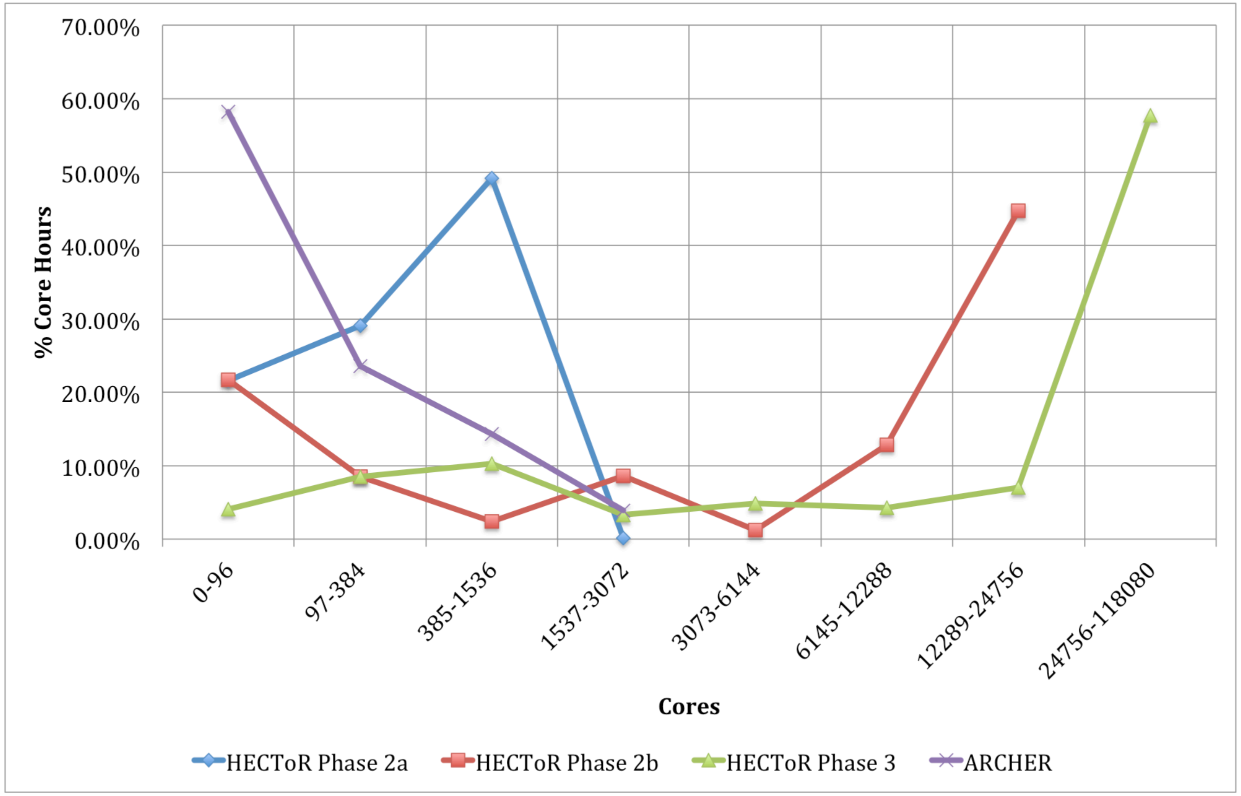
CP2K job size distribution

N-body codes



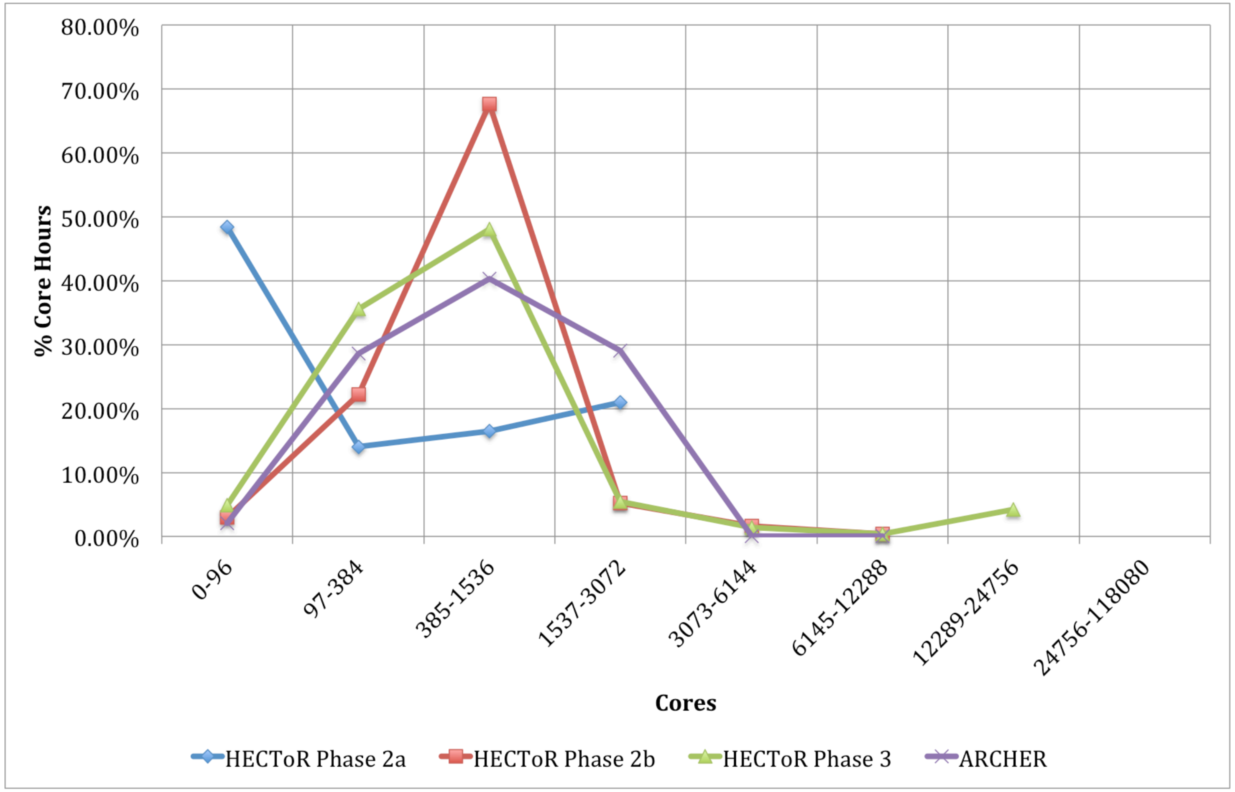
6%
5%
4%
3%
2%
1%
0%
% Total Core Hours
Gromacs
NAMD
Amber
DL_POLY
LAMMPS
HECToR Phase 2a
HECToR Phase 2b
HECToR Phase 3
ARCHER

N-body codes



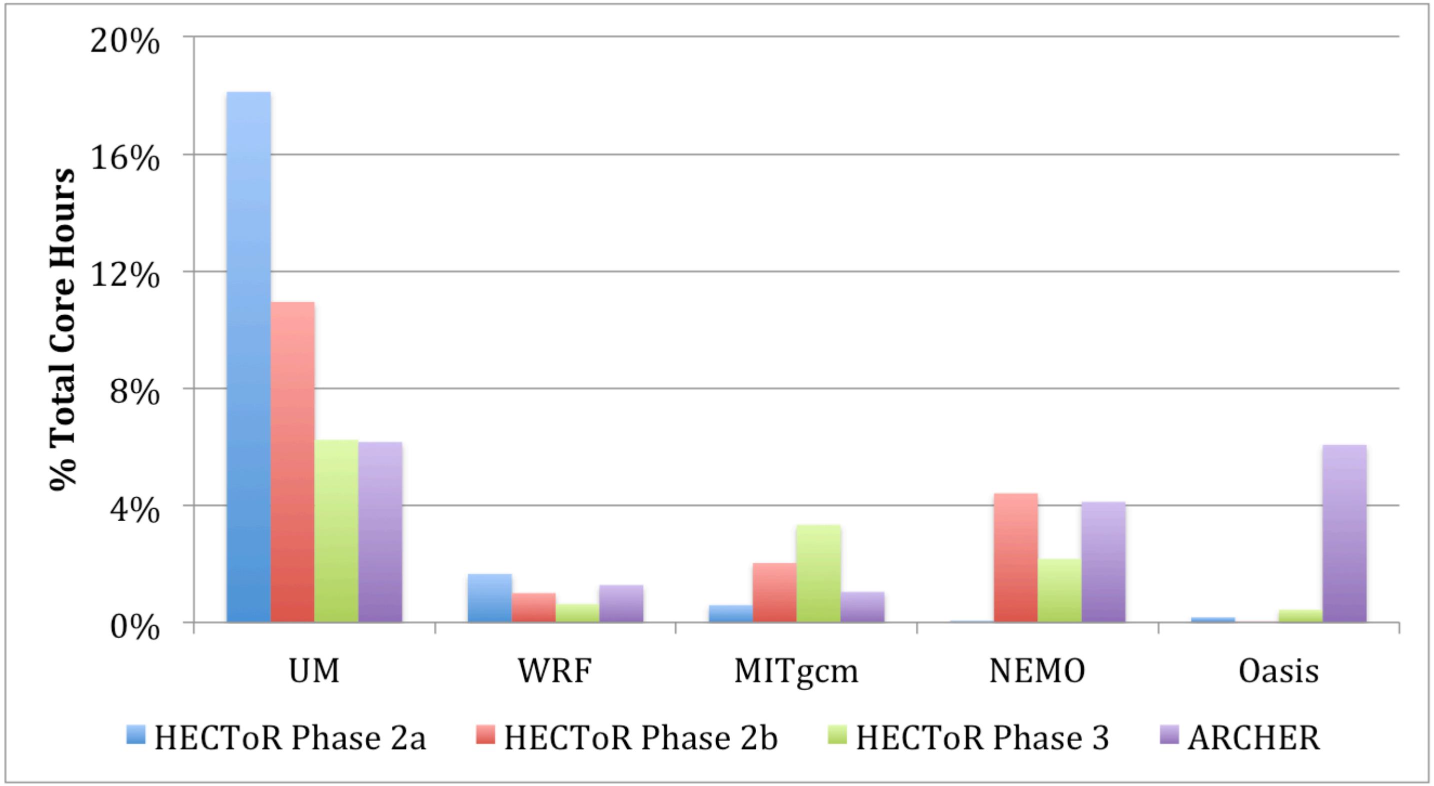
DL_POLY job size distribution

N-body codes

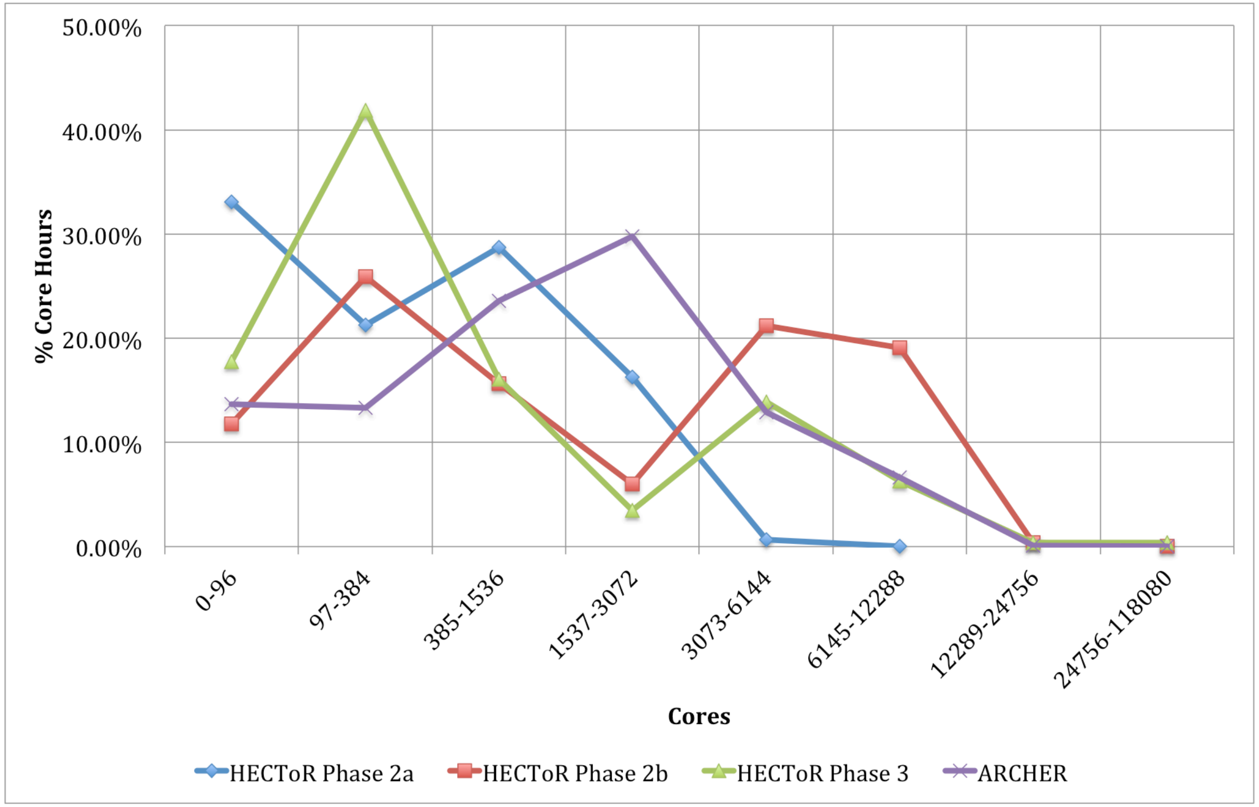


Gromacs job size distribution

Grid-based Codes: Climate

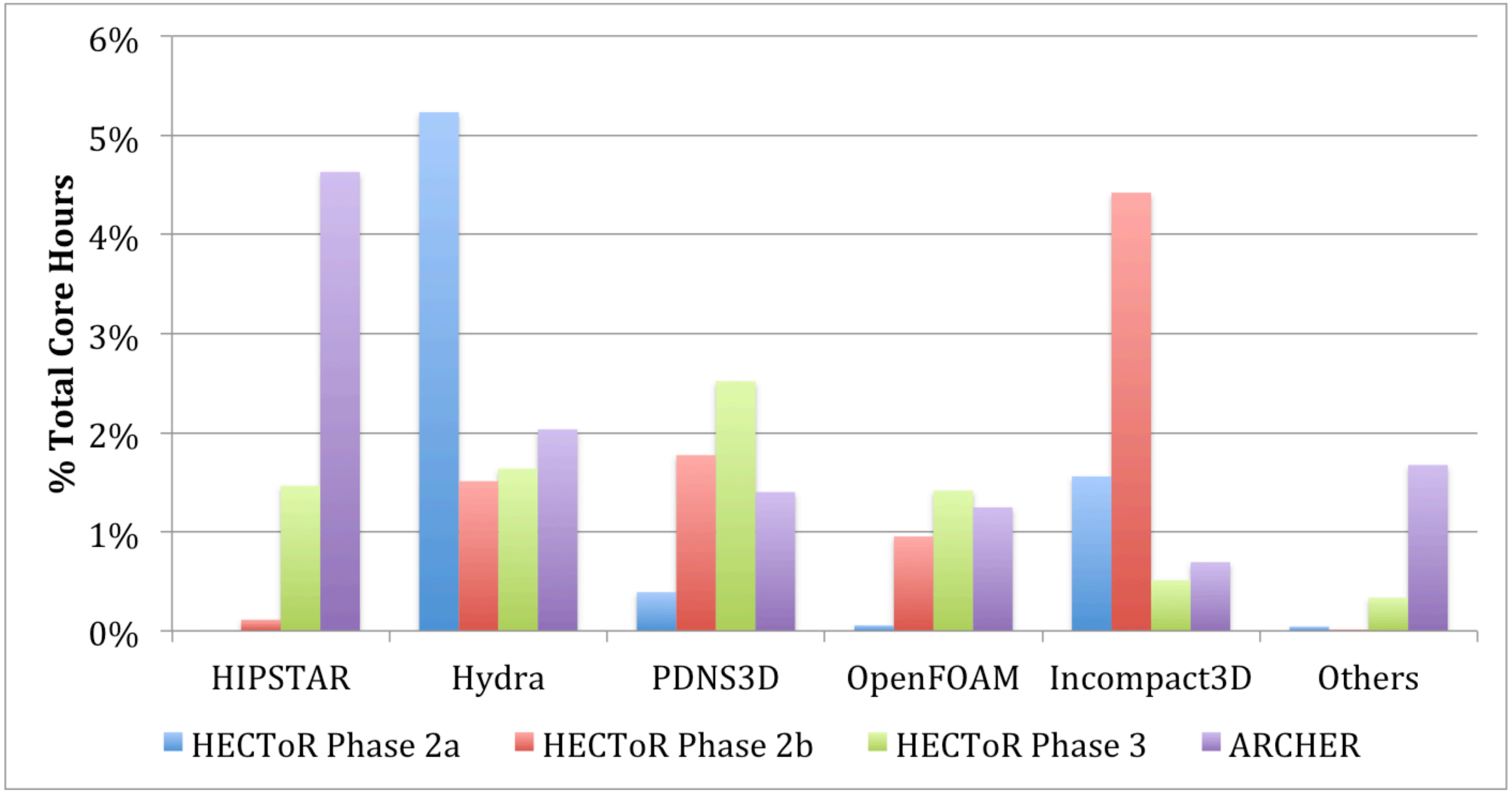


Structured Grid: Climate Simulation



Met Office UM job size distribution

Grid-based Codes: CFD



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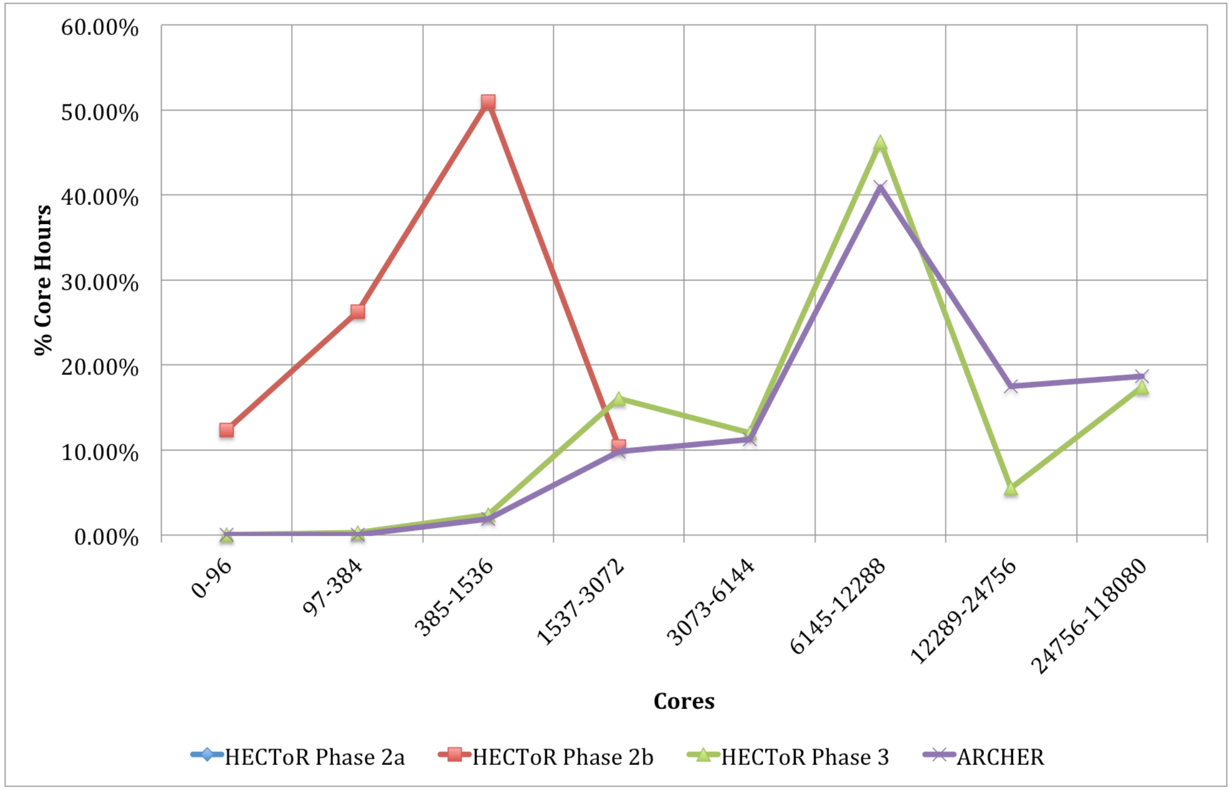
Unstructured Grid: CFD



HiPSTAR job size distribution

Future Look

1. Scaling limited by scientific problem
   - Use additional throughput to access more sophisticated sampling
   - Via application or code agnostic frameworks (e.g. PLUMED)

2. Scaling not limited by scientific problem
   - Opportunity for single calculations to scale to large core counts
   - (As well as exploiting additional throughput)

- In both cases continued software development is obviously key to exploiting future HPC architectures

Summary

- Most applications able to increase scaling with switch from quad core to multicore
  - Generally by 2 times rather than 6 times
- For some areas scaling is generally limited by research problem rather than the application issues
  - Application scaling limits may never be reached for problems that are scientifically relevant
- In other areas application scaling is key to furthering research
- Future HPC systems offer opportunities for applications in both classes
  - In the UK we maybe need to be less focused on single application scaling and look at sampling and coupling frameworks more

Questions?