CATALYST UK AT EPCC

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THE UNIVERSITY of EDINBURGH

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The CATALYST UK programme

- Collaboration between
  - Hewlett Packard Enterprise, Arm & SUSE
  - EPCC, The University of **Edinburgh**
  - University of **Bristol**
  - University of **Leicester**
- Deploy Arm-based HPC systems across the 3 academic sites in the UK
- Programme running for 3 years from December 2018

The aim of the programme

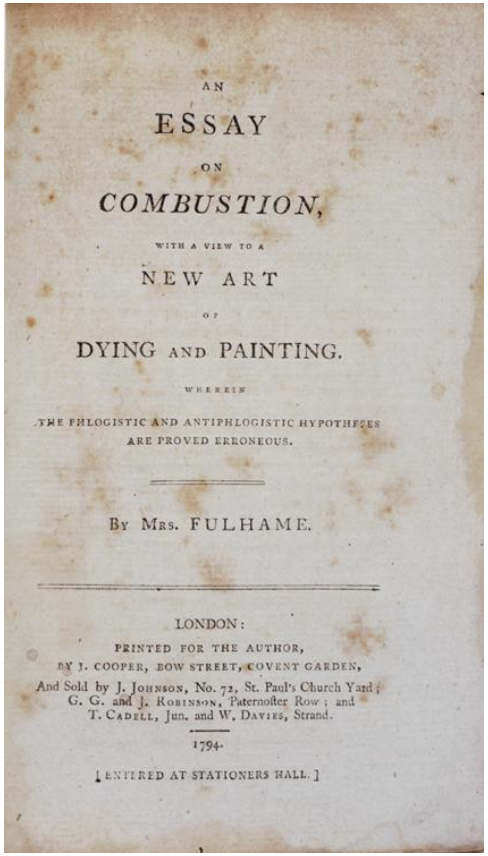
- To investigate and showcase the potential of Arm-based HPC systems
- To further drive supercomputer adoption in the UK in general, and in the commercial sector in particular
- To cooperate with the UK industry to jointly develop critical applications and workflows to best exploit the Arm system capabilities
- To provide training for researchers to successfully and productively work with Arm-based systems in the future

The systems

- HPE Apollo 70
- The clusters at each university are largely identical
  - Designed, built and supported by HPE
- 64 nodes (i.e. 4096 cores) per cluster
  - 2 racks
  - Dual-socket nodes with Cavium ThunderX2 CPUs (32 cores per CPU)
  - 128GB (16 x 8GB) DDR4 per node
  - Mellanox EDR InfiniBand

EPCC's system

- Fulhame was delivered and installed at the end of Nov'18
  - Named after Elizabeth Fulhame - 18th century Scottish chemist, first to describe the process of catalysis
- It was used for a PRACE Advanced Training Centre course on the 3rd & 4th December
  - **Less than 1 week after delivery!**
- Since then, work has focused on code porting & benchmarking


AN
ESSAY
ON
COMBUSTION,
WITH A VIEW TO A
NEW ART
OF
DYING AND PAINTING.
WHEREIN
THE PHLOGISTIC AND ANTIPHLOGISTIC HYPOTHESES
ARE PROVED ERRONEOUS.
By Mrs. FULHAME.
LONDON:
PRINTED FOR THE AUTHOR,
BY J. COOPER, BOW STREET, COVENT GARDEN,
And Sold by J. Johnson, No. 72, St. Paul's Church Yard;
G. G. and J. Robinson, Paternoster Row; and
T. Cadell, Jun. and W. Davies, Strand.
1794.
[ENTERED AT STATIONERS HALL.]

Porting & benchmarking

- Port most heavily used ARCHER and Cirrus packages
  - Make them available as modules
  - Built with different compilers, libraries, etc
- No specific performance optimisation in the first instance
  - Focus on making as many applications available as possible

Rank	Code Name	Usage / Nh	% Usage	Jobs	% Jobs	Users	Mean Job Size / nodes	Median Job Size / nodes
1	VASP	451961	16.73	9055	20.58	87	43.27	17
2	Gromacs	188732	6.99	1976	4.49	31	20.93	21
3	cp2k	155805	5.77	3762	8.55	39	38.64	22
4	CASTEP	139383	5.16	6177	14.04	31	168.06	16
5	Quantum Espresso	116045	4.30	614	1.40	10	95.66	68
6	NEMO	107968	4.00	1256	2.86	12	63.95	25
7	iIMB	102601	3.80	350	0.80	3	41.50	27
8	LAMMPS	79910	2.96	2857	6.49	26	9.31	5
9	ONETEP	65543	2.43	68	0.15	5	52.04	60
10	MITgcm	44673	1.65	761	1.73	7	15.03	12
11	WRF	44028	1.63	99	0.23	7	42.14	4
12	EPOCH	40176	1.49	85	0.19	4	181.53	80
13	Oasis	38625	1.43	231	0.53	6	19.21	17
14	NAMD	37336	1.38	178	0.40	6	18.17	21
15	Met Office UM	36773	1.36	354	0.80	9	11.37	6
16	SBLI	36258	1.34	74	0.17	3	130.63	32
17	OpenFOAM	31593	1.17	231	0.53	19	29.62	20
18	Code_Saturne	23527	0.87	201	0.46	5	16.51	11
19	SENGA	22347	0.83	54	0.12	4	53.85	9
20	CASINO	18572	0.69	80	0.18	1	13.67	8
21	CRYSTAL	17013	0.63	386	0.88	8	11.98	9
22	Nektar++	15614	0.58	19	0.04	3	98.15	50
23	FHI aims	14238	0.53	157	0.36	1	40.97	20
24	ChemShell	9855	0.36	170	0.39	6	11.45	8
25	JOREK	8946	0.33	11	0.03	1	249.04	210
26	CESM	6636	0.25	92	0.21	4	5.70	3
27	OSIRIS	5357	0.20	16	0.04	5	413.89	324
28	HYDRA	4713	0.17	61	0.14	2	12.13	2
29	Nek5000	3520	0.13	6	0.01	1	80.00	80
30	GS2	3042	0.11	18	0.04	2	35.03	22

```
mwngio@eslogin005:~> module avail gromacs

---------------------- /opt/modules/packages-archer -----------------------
gromacs/4.6.5                   gromacs/5.1.2-plumed2.3b
gromacs/4.6.5-plumed            gromacs/5.1.4
gromacs/4.6.7-plumed            gromacs/5.1.4-plumed2.3.3
gromacs/5.0.2                   gromacs/5.1.4-plumed2.4.1-adjmat
gromacs/5.1                     gromacs/2016.3(default)
gromacs/5.1-plumed              gromacs/2016.4
gromacs/5.1.1-plumed            gromacs/2018.2
gromacs/5.1.2                   gromacs/2018.2-plumed2.4.2
mwngio@eslogin005:~>
```

```
[mweiland@cirrus-login0 ~]$ module avail netcdf

--------------------------- /lustre/sw/modulefiles ---------------------------
netcdf/4.4.1                        netcdf-parallel/4.5.0-intel17
netcdf-parallel/4.5.0               netcdf-parallel/4.5.0-intel17-mpt214
netcdf-parallel/4.5.0-gcc6-mpt214
[mweiland@cirrus-login0 ~]$
```

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HPCG - High Performance Conjugate Gradient

- Kernel benchmark aiming to exercise
  - Floating point performance
  - Memory bandwidth
  - Network bandwidth and latency
  - Implemented with C++, MPI & OpenMP
  - Performance measured in Gflop/s

Single node

System	Performance
HPE Apollo 70	30.529
SGI ICE XA	21.115
Cray XC30	15.650
Dell EMC (AVX512)	34.581
Dell EMC (AVX2)	28.120

Multi-node

Nodes	HPE Apollo 70	SGI ICE XA	Cray XC30	Dell EMC (AVX2)
2	61.185	40.491	32.048	56.505
4	120.972	80.317	61.617	111.598
8	241.363	158.774	120.749	214.358
16	482.202	305.534	245.870	400.320
32	939.109	602.092	491.101	747.066

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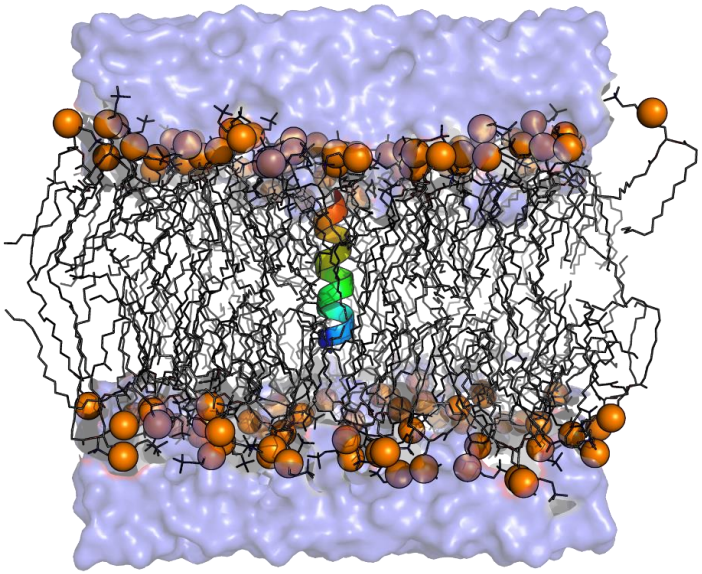
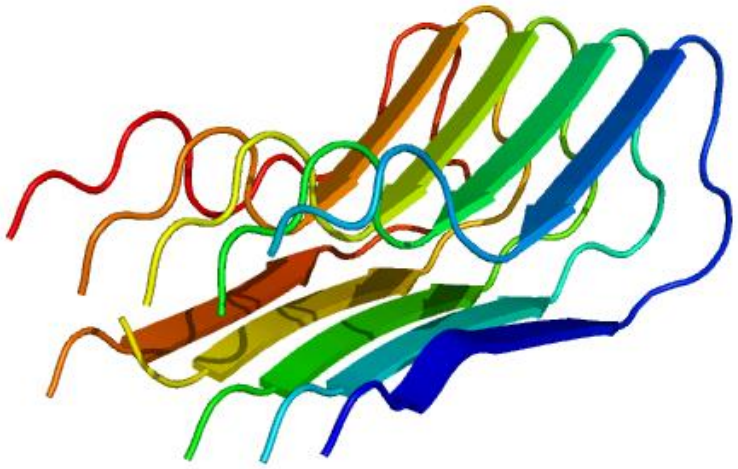
GROMACS

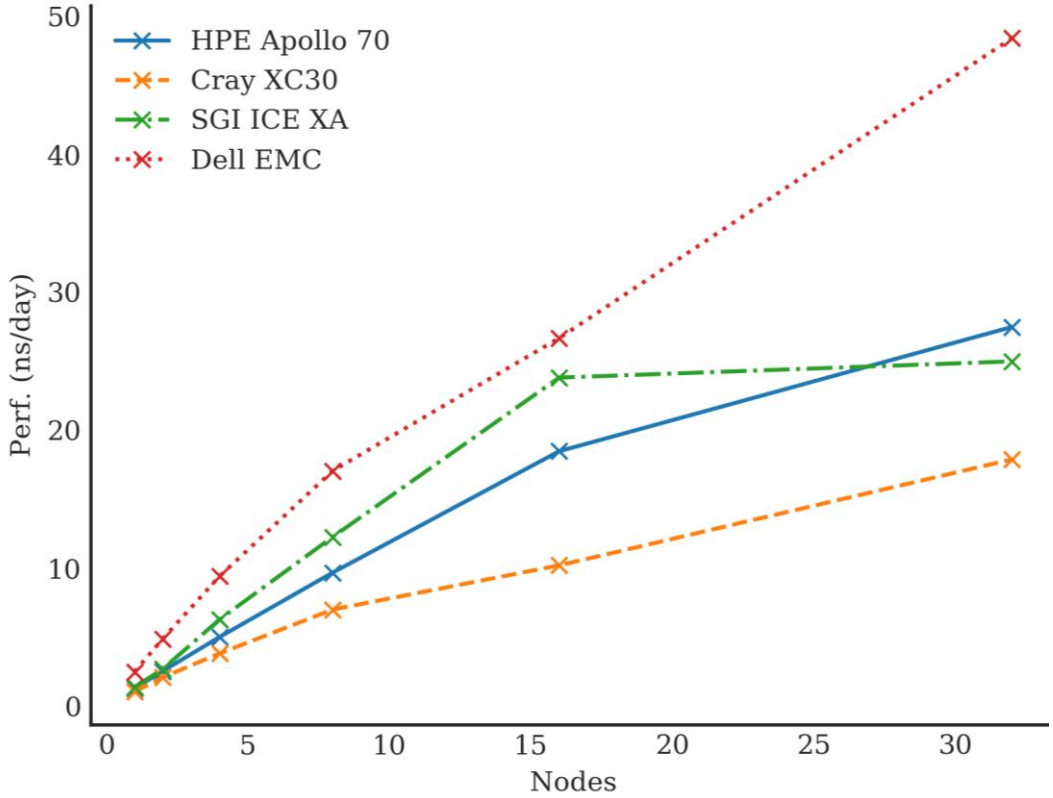
- Molecular dynamics simulations
- Primarily designed for biochemical molecules but also used on systems like polymers
- Implemented in C with MPI & OpenMP





GROMACS 1400k atom benchmark

GROMACS			
HPE Apollo 70	Arm Clang 19.0.0	-std=c++11 -mcpu=native -O3 -DNDEBUG -funroll-all-loops -fexcess-precision=fast -fPIC -O3	OpenMPI 4.0.0 FFTW 3.3.8
SGI ICE XA	GCC 6.2.0	-march=core-avx2 -std=c++0x -O3 -funroll-all-loops -fexcess-precision=fast	SGI MPT 2.16 FFTW 3.3.5
Cray XC30	GCC 6.3.0	-mavx -static -O3 -ftree-vectorize -funroll-loops -std=c++11 -O3 -funroll-all-loops -fexcess-precision=fast	Cray MPICH2 7.5.5 FFTW 3.3.6
Dell EMC	Intel 17.4	-xCORE-AVX512 -mkl=sequential -std=gnu99 -std=c++11 -O3 -ip -funroll-all-loops -alias-const -ansi-alias -no-prec-div -fimf-domain-exclusion=14 -qoverride-limits	Intel MPI library 17.4 Intel MKL 17.4



Detailed results

ACM DL DIGITAL LIBRARY

Evaluating the Arm Ecosystem for High Performance Computing

Full Text: PDF

2019 Article
Research
Refereed limited

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Summary

- In general porting was very straightforward
  - GNU compilers and Arm performance library help significantly
  - Arm compilers can bring performance benefits
- Performance is generally good
  - Not necessarily better than top end Intel
  - But reasonably comparable and potentially much cheaper
- Memory bandwidth dominated codes benefit significantly
- The Catalyst UK programme will give the Arm HPC-ecosystem a significant boost by creating a mature and stable environment for high-performance scientific and industry applications