Element Project Workshop
Welcome and Introduction
Professor Mark Parsons, EPCC Director
ExCALIBUR and ELEMENT

- Exascale Computing: Algorithms & Infrastructures Benefitting UK Research
- Funded by UK Government Strategic Priorities Fund
- £50m over 4 years
- One of a small number of Exascale Projects funded to date
- ExCALIBUR is focussed on Exascale software challenges faced by
  - UK Met Office
  - UK Atomic Energy Authority (represented by Culham Centre for Fusion Energy)
- Project led jointly by the UK Met Office and EPSRC
- ELEMENT is one of 10 High Priority Use Case projects funded in early 2020
ExCALIBUR High Priority Use Cases

1. ELEMENT: Exascale Mesh Network
2. Materials And Molecular Modelling Exascale Design And Development Working Group
3. Gen X: ExCALIBUR working group on Exascale continuum mechanics through code generation
5. Massively Parallel Particle Hydrodynamics for Engineering and Astrophysics
6. BASE: Benchmarking for AI for Science at Exascale
7. EXA-LAT: Lattice Field Theory at the Exascale Frontier
8. ExaClaw: Clawpack-enabled ExaHyPE for heterogeneous hardware
10. Turbulent Flow Simulations at the Exascale: Application to Wind Energy and Green Aviation

20/10/2020 Welcome and introduction
Led by EPCC, The University of Edinburgh in partnership with University of Cambridge, Imperial College London, University of Exeter and Swansea University.

Focusses on the high priority use case of meshing for the Exascale.

- Developing highly scalable solutions to create meshes on Exascale systems.
- Partitioning efficiently to minimise load imbalance.
- Ensuring meshes are of sufficient quality to represent Exascale problems.

Objectives

- To build a community around meshing practice by establishing a collaborative network.
- Undertake a small number of proof of concept studies.
- Publish a Vision Paper which will inform a Strategic Research Agenda.

Strategic Research Agenda will cover the full meshing workflow at the Exascale including mesh generation, adaptation, partitioning, and visualisation.
# Workshop Day 1

## Morning Session: Introduction to ELEMENT & Exascale System Technologies

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker and Affiliation</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:30-11:00</td>
<td>Mark Parsons, EPCC</td>
<td>Introduction to ELEMENT &amp; The UK Exascale Project</td>
</tr>
<tr>
<td>11:00-11:20</td>
<td>Simon McIntosh-Smith, University of Bristol</td>
<td>The evolution of computer architecture and its implications for meshing</td>
</tr>
<tr>
<td>11:20-11:40</td>
<td>Bernhard Homoelle, SVA</td>
<td>Memory technologies, what comes next?</td>
</tr>
<tr>
<td>11:40-12:00</td>
<td>Nic Dube, HPE</td>
<td>Exascale and Beyond: Supercomputing Heterogeneity</td>
</tr>
<tr>
<td>12:00-12:50</td>
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<td>Breakout groups &amp; discussion</td>
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<tr>
<td>12:50-13:00</td>
<td></td>
<td>Summary of breakout groups</td>
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## Workshop Day 1

### Afternoon Session: Parallel mesh generation

<table>
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<tr>
<th>Time</th>
<th>Speaker(s)</th>
<th>Title</th>
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<tbody>
<tr>
<td>14:00-14:20</td>
<td>Trevor Robinson, Queen's University Belfast</td>
<td>Applying Simulation Intent to Parallel Mesh Generation</td>
</tr>
<tr>
<td>14:20-14:40</td>
<td>Christos Tsolakis, Polykarpos Thomadakis and Nikos Chisochoides, Old Dominion University</td>
<td>Exascale-Era Parallel Adaptive Mesh Generation and Runtime Software System Activities at the Center for Real-Time Computing</td>
</tr>
<tr>
<td>14:40-15:00</td>
<td>Christophe Geuzaine, University of Liege</td>
<td>Towards (very) large scale finite element mesh generation with Gmsh</td>
</tr>
<tr>
<td>15:00-15:20</td>
<td>Tzanio Kolev, Lawrence Livermore National Laboratory</td>
<td>Large-scale Finite Element Applications on High-Order Meshes</td>
</tr>
<tr>
<td>15:20-15:40</td>
<td>ELEMENT project talk</td>
<td>Meshing towards the Exascale</td>
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<tr>
<td>15:40-16:30</td>
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<td>Breakout groups &amp; discussion</td>
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<tr>
<td>16:30-16:45</td>
<td></td>
<td>Summary of breakout groups</td>
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# Workshop Day 2

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Description</th>
<th>Presenter</th>
<th>Company</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:30-10:50</td>
<td>Morning Session: End user stories</td>
<td>Paul Cusdin</td>
<td>Renault F1</td>
</tr>
<tr>
<td>10:50-11:10</td>
<td>Practical CFD and Meshing. An Inconvenient Truth</td>
<td>Paolo Adami</td>
<td>Rolls-Royce</td>
</tr>
<tr>
<td>11:10-11:30</td>
<td>A view from Rolls Royce</td>
<td>Carolyn Woeber</td>
<td>Pointwise</td>
</tr>
<tr>
<td>11:30-11:50</td>
<td>A Mesh Generation Perspective on Exascale CFD</td>
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<tr>
<td>11:50-12:45</td>
<td>ELEMENT project talk</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12:45-13:00</td>
<td>Translating high order spectral/hp element methods from academia to industry</td>
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</tbody>
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# Workshop Day 2

## Afternoon Session: Geometry definition, CAD interaction and mesh adaptivity

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<tr>
<td>14:00-14:20</td>
<td>Henry Bucklow, ITI</td>
<td>Geometry for mesh generation</td>
</tr>
<tr>
<td>14:20-14:40</td>
<td>Xevi Roca, Barcelona Supercomputing Centre</td>
<td>Meshing from CAD vision: curved adaption to geometry and solution</td>
</tr>
<tr>
<td>14:40-15:00</td>
<td>Adrien Loseille, INRIA</td>
<td>Parallel anisotropic mesh adaptation in complex geometries and extreme anisotropy</td>
</tr>
<tr>
<td>15:00-15:20</td>
<td>Bob Haimes, MIT</td>
<td>A lightweight geometry kernel for distributed mesh generation and adaptation</td>
</tr>
<tr>
<td>15:20-15:40</td>
<td>ELEMENT project talk</td>
<td>Mesh Adaptation towards the Exascale</td>
</tr>
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<td></td>
<td>Summary of breakout groups</td>
</tr>
<tr>
<td>16:45-17:00</td>
<td></td>
<td>Conclusion - Summary of Workshop</td>
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THE UK EXASCALE PROJECT

ELEMENT Workshop – October 2020

Professor Mark Parsons
EPCC Director
EPSRC Director of Research Computing
### The Exascale era – international context

<table>
<thead>
<tr>
<th>Country or Region</th>
<th>Timescale</th>
<th>Detail</th>
</tr>
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<tbody>
<tr>
<td>China</td>
<td>2020 / 2021</td>
<td>Little known at present – updated CPU plus accelerator as per Sunway</td>
</tr>
<tr>
<td>Japan</td>
<td>2020</td>
<td>Fugaku: based on A64FX Arm processor</td>
</tr>
</tbody>
</table>
| USA               | 2021/2    | Frontier: based on AMD EPYC CPU + AMD GPU  
Aurora: based on Intel A21 CPU + Intel GPU |
| Europe            | 2020  
2023/4 | Pre-Exascale hosting sites chosen (Finland / Spain / Italy)  
Future Exascale systems will use Europe’s own CPU |
Building the case for Exascale computing in the UK

- Europe Union is investing heavily in Exascale through EuroHPC
- UK scientists mustn’t be left behind
- In mid-2018 UK Government decided it needed a strategy
- Established Exascale Project Working Group to develop Business Case for investment
- Parallel review of e-Infrastructures by UKRI led by EPSRC
- Supercomputing Science Case developed to understand scientific needs
Supercomputing Science Case themes

Computational biology
Expanding the frontiers of fundamental sciences
Climate, weather and earth sciences
Mathematics and science of computation
Computational biomedicine
Engineering and materials
Digital humanities and social sciences
Exascale Project Specific Requirements from Government

• System should support both traditional Modelling & Simulation and Artificial Intelligence / Deep Learning applications
  • Technology choices may be impacted by this
  • But future technologies blur the distinction

• System should support both scientific user communities and industry users
  • A greater focus is proposed with regard to industry use for research
  • Pay-per-use production access will be supported
  • Specific support for SMEs

• System should be operational by 2023
Infrastructure takes time and money

£20m – New computer room
£8m – 30MW additional power

Opening Dec 2020
Aiming for Net Zero

Bilston Glen Colliery, 670m, 15.0C, Minewater
Monktonhall, 866m, 25.5C, Rock
Lady Victoria, 768m, 18C, Minewater

All National HPC services are already 100% Green Electricity
On the road to Exascale …

- USA’s SUMMIT system was the world’s fastest supercomputer from June 2018 – June 2020 according to Top500 HPL benchmark
- 2,414,592 CPU cores and 27,000 GPUs
- $R_{\text{peak}} = 201$ Petaflop/s
- Power consumption of 13 Megawatts
- To reach the Exascale with this technology
  - 12 million CPU cores + 68,000 GPUs
  - 65 Megawatts
- … very high levels of parallelism

… but at ISC in June 2020 Japan’s Fugaku system took the crown
… Fugaku takes the crown

- Fugaku became the world’s fastest supercomputer in June 2020 with a cores-only approach based on the Fujitsu A64FX Arm CPU
- Processor developed in long-term co-design (10 years) with Japanese computational science community led by Riken CCS
- 7,299,072 Arm CPU cores
- 4.866 Petabytes of RAM
- $R_{\text{peak}} = 513.9$ Petaflop/s
- Power = 28.3 Megawatts
- Single precision > 1 Exaflop
Why GPUs are good at AI – and how CPUs are catching up

• Keys operation in computer graphics are matrix multiplications
• All GPUs support General Matrix Multiplication (GEMM) operations of the form \( D = (A \times B) + C \)
• For computer graphics these are generally low precision FP16 calculations
• It turns out that for many AI Deep Learning algorithms – which use GEMM operations – low precision is good enough
• It’s the ability to do lots of calculations in parallel that is key
• CPUs focus on excellent FP64 arithmetic – although many designs have now added 16-bit (often the BFloat16 format) and GEMM operations (often called MMA)
Technology – two routes to the Exascale

• Cores-only route
  • Favoured by Japan
  • Evidence this approach leads to longer lifetimes of systems
  • Hardware support for AI increasing – main focus traditional simulation
  • Larger power requirements and physical dimensions

• Cores plus accelerator route
  • Favoured by the USA
  • Traditional multi-core processors coupled to accelerator
  • Sweet spot seems to 10 cores per GPU – pushes towards 1 socket + 4 GPU blades at the Exascale
  • Strong AI performance – traditional simulation more challenging
## Technology – Japanese versus American model

- Japanese model has attractions but difficult to sell to Government
- Lower peak performance but much longer science lifetime

HPCG Results (June 2019 and June 2020)

<table>
<thead>
<tr>
<th>Rank</th>
<th>Site</th>
<th>Computer</th>
<th>Cores</th>
<th>HPL Rpeak</th>
<th>HPL Rmax (Pflop/s)</th>
<th>Top500 Rank</th>
<th>HPCG (Pflop/s)</th>
<th>Rmax to Rpeak</th>
<th>Fraction of Rmax</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Riken CCS JAPAN</td>
<td>Fugaku</td>
<td>7,299,072</td>
<td>513.9</td>
<td>415.5</td>
<td>1</td>
<td>133.7</td>
<td>80.9%</td>
<td>32.17%</td>
</tr>
<tr>
<td>2</td>
<td>DOE/SC/ORNL USA</td>
<td>Summit</td>
<td>2,414,592</td>
<td>200.8</td>
<td>148.6</td>
<td>2</td>
<td>2.9</td>
<td>74.0%</td>
<td>5.73%</td>
</tr>
<tr>
<td>5</td>
<td>Riken CCS JAPAN</td>
<td>K-Computer</td>
<td>705,024</td>
<td>11.3</td>
<td>10.5</td>
<td>22</td>
<td>0.6</td>
<td>93.2%</td>
<td>5.73%</td>
</tr>
</tbody>
</table>
Technology – key insights from recent Exascale vendor briefings

- **High Bandwidth Memory is coming**
  - Many Exascale blades include HBM
  - Some designs have no DRAM at all

- **Four-way competition for CPUs and/or GPUs**
  - Intel versus AMD versus Arm versus NVIDIA

- **GPUs are getting ever more powerful**
  - We’re already seeing the market broaden

- **Cabinet energy densities are rocketing**
  - Today’s 80-100KW cabinets will be eclipsed by cabinets at 300KW+
  - Density of blades is a key battleground

- **Multicore CPUs are also getting AI Deep Learning features**
Exascale systems – How parallel? How large?

- For a cores only approach it should be possible to get to 1 Exaflop theoretical peak with 4-5 million cores.
- A cores plus GPU approach will reduce the number of cores but overall parallelism will increase as GPUs have much higher parallelism – better for AI less so for simulation.
- 1 Exaflop power requirements range from 20MW to 160MW.
- Size of systems is highly dependent on density of blades and cabinet design.
  - Number of cabinets ranges from circa. 60 to over 800!
- Key metric is always usefulness for both science and industry.
Conclusions

- The next generation of blade designs focus on moving data to and from the processor faster than ever before.
- This is just as relevant for modelling and simulation applications as it is for AI deep learning applications.
- Supercomputing and data science computing are converging.
- Need to focus on data processing performance not flops in future.
- Exascale is driving much of this convergence but so are AI applications that use large amounts of data.
- For the most demanding problems the Cloud Hyperscaler world and Supercomputing are converging.