Collaborative Research into Exascale Systemware, Tools and Applications

Dr Mark Parsons
EPCC Executive Director
Associate Dean for e-Research
The University of Edinburgh
CRESTA

- **Collaborative Research into Exascale Systemware, Tools and Applications**
- Developing techniques and solutions which address the most difficult challenges that computing at the exascale can provide
- Focus is predominately on software not hardware.
- European Commission funded project
  - FP7 project
  - Projects started 1st October 2011, three year project
  - 13 partners, EPCC project coordinator
  - €12 million costs, €8.57 million funding

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Partnership

- Consortium
  - Leading European HPC centres
    - EPCC – Edinburgh, UK
    - HLRS – Stuttgart, Germany
    - CSC – Espoo, Finland
    - PDC – Stockholm, Sweden
  - A world leading vendor
    - Cray UK – Reading, UK
  - World leading tools providers
    - Technische Universität Dresden (Vampir) – Dresden, Germany
    - Allinea Ltd (DDT) – Warwick, UK
  - Exascale application owners and specialists
    - Abo Akademi University – Abo, Finland
    - Jyvaskyla Yliopisto – Jyvaskyla, Finland
    - University College London – London, UK
    - ECMWF – Reading, UK
    - École Centrale Paris – Paris, France
    - DLR – Cologne, Germany
Key Principles

• Two strand project
  • Building and exploring appropriate systemware for exascale platforms
  • Enabling a set of key co-design applications for exascale

• Co-design is at the heart of the project. Co-design applications:
  • provide guidance and feedback to the systemware development process
  • integrate and benefit from this development in a cyclical process

• Employing both incremental and disruptive solutions
  • Exascale requires both approaches
  • Particularly true for applications at the limit of scaling today
  • Solutions will also help codes scale at the peta- and tera-scales

• World leading hardware vendor as project partner – Cray

• Committed to open source interfaces, standards and new software
Choosing what to study

- As we all know the Exascale research domain is enormous
- A €12 million project can only tackle a small part of the overall problem
- We decided very early not to focus on hardware but on the problems of massive heterogeneous parallelism

Research selection process
- Capture and categorisation of problems
- Each partner asked to indicate their interests
- Topics selected based on
  - Amount of interest
  - Complementary skills
  - Viability within funding constraints

- In supercomputing it is too easy to tie a ribbon around new hardware and much more difficult to tie a ribbon around people
Co-design Applications

- Exceptional group of six applications used by academia and industry to solve critical grand challenge issues
- Applications are either developed in Europe or have a large European user base
- Enabling Europe to be at the forefront of solving world-class science challenges

<table>
<thead>
<tr>
<th>Application</th>
<th>Grand challenge</th>
<th>Partner responsible</th>
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<tbody>
<tr>
<td>GROMACS</td>
<td>Biomolecular systems</td>
<td>KTH (Sweden)</td>
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<tr>
<td>ELMFIRE</td>
<td>Fusion energy</td>
<td>ABO/ JYU (Finland)</td>
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<td>HemeLB</td>
<td>Virtual Physiological Human</td>
<td>UCL (UK)</td>
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<td>IFS</td>
<td>Numerical weather prediction</td>
<td>ECMWF (International)</td>
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<tr>
<td>OpenFOAM</td>
<td>Engineering</td>
<td>EPCC / HLRS / ECP</td>
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<tr>
<td>Nek5000</td>
<td>Engineering</td>
<td>KTH (Sweden)</td>
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Example of incremental and disruptive approaches

• FFTs are a challenge at Exascale because
  • Very large number of HPC applications use them
  • Distributed memory parallel FFT is already a major performance issue today – we accept some FFTs will not scale further

• Two approaches:

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<tr>
<th>Incremental approach</th>
<th>Disruptive approach</th>
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<td>• Through optimisations, performance modelling and co-design application feedback</td>
<td>• Work with co-design applications to consider alternative algorithms</td>
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<td>• Look to achieve maximum performance at Exascale and understand limitations e.g. through sub-domains, overlap of compute and comms</td>
<td>• Crucial we understand maximum performance before very major application redesigns undertaken</td>
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Systemware

- Software components required for grand challenge applications to exploit future exascale platforms
- Underpinning and cross cutting technologies
  - Operating systems, fault tolerance, energy, performance optimisation
- Development environment
  - Runtime systems, compilers, programming models and languages including domain specific
- Algorithms and libraries
  - Key numerical algorithms and libraries for exascale
- Debugging and Application performance tools
  - World leader’s in Allinea’s DDT, TUD’s Vampir and KTH’s perfminer
- Pre- and post- processing of data resulting from simulations
  - Often neglected, hugely important at Exascale
Systemware: integrated set of software components
Conclusion

- CRESTA focuses on software not hardware
- Far too little money is being spent on software worldwide at present
- We need both incremental and disruptive approaches
- Exascale computers challenge our basic understanding of how we model and simulate numerical problems
  - CRESTA can only look at a small number of problems
  - There needs to be much more engagement from the mathematics and computer science communities
- Exascale should enable previously impossible simulations
  - There are a huge number of opportunities - but we need the right tools
- By focussing on co-design of applications and systemware we expect CRESTA to play a key role in the exascale roadmap
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