1. Executive Summary

This report covers the period: 1 July 2014 to 30 September 2014 inclusive.

- Centralised CSE Team:
  - The CSE team resolved 413 queries during this reporting period.
  - The number of In-Depth queries resolved fell from 80 in Q2 to 46 in Q3 (97 were resolved in Q1 2014). The lower number of queries indicates that users are more familiar with the system and that there are fewer requests to install new software.
  - The median resolution time for In-Depth queries is 4 weeks.
  - The median completion time for Technical Assessments is 4 days.

- Summary of feedback:
  - Feedback on query handling uniformly rated the service as "Excellent".

- Training:
  - Provided 22 days (631 student-days) of face-to-face training in the quarter, at 7 different locations.
  - Provided 1.5 days of virtual tutorials as interactive webinars with more than 80 attendees in total, an increase over the previous quarter’s attendance of 60.
  - GPU course in Sheffield used as “train the trainers” event: ARCHER material was delivered by local staff but additional tutorial support was provided by EPCC.
  - Joint ARCHER/DiRAC training course on manycore / Xeon Phi programming agreed in principle, and will form part of proposed 2015 training plan.
  - Survey for measuring longer-term impact of training approved by ARCHER Training Panel. This will be circulated to course attendees on a regular basis; first set of attendees have been contacted. See [http://archer.ac.uk/training/feedback/follow-up-survey.php](http://archer.ac.uk/training/feedback/follow-up-survey.php)
  - Meeting of ARCHER Training Panel arranged for 15 October to discuss proposed training plan for 2015.

- eCSE:
  - Of 14 projects accepted for the first call, 13 have started with all associated contracts signed and costs agreed. The one remaining project is undergoing a change of staffing.
  - Of 9 projects accepted for the second call, 8 have started with all associated costs agreed. Contracts are in the process of being agreed and signed. The one remaining project is undergoing a change of staffing.
  - The third eCSE call opened on 5 August 2014 and closed on 16 September, receiving 16 proposals.
  - Templates for interim eCSE reports have been agreed.
  - Outline of final eCSE reports has been agreed along with outline of reviewing process for completed projects.
2. Impact Summary

- Outreach Activities:
  - 26 September 2014: Meet the Experts, Our Dynamic Earth, Edinburgh (http://www.explorathon.co.uk/edinburgh/meet-the-experts)
  - 14 September 2014: Bang Goes the Borders, Melrose (http://www.bgtb.org/)
  - 6-11 September 2014: British Science Festival, Birmingham (https://www.epcc.ed.ac.uk/blog/2014/09/10/epcc-british-science-festival-2014)
  - 10 July 2014: Sutton Trust, Medical School, University of Edinburgh (http://www.ph.ed.ac.uk/news/sutton-trust-04-08-14)

- Papers from Centralised CSE Team:
  - Linear instability, nonlinear instability and ligament dynamics in three-dimensional laminar two-layer liquid-liquid flows, L. Ó Náraigh (Dublin), P. Valluri (Engineering Edinburgh), D. Scott (EPCC Edinburgh), I. Bethune (EPCC Edinburgh) and P. D. M. Spelt (Lyon), Journal of Fluid Mechanics, 750, p464-506

- Conference Presentations from Centralised CSE Team:
  - Ultra-high resolution direct numerical simulations of stratified flows: From waves to droplet pinch-off, First Thermapower Workshop, Shanghai (Aug 2014)

- Meetings Attended by Centralised CSE Team:
  - UK Turbulence Consortium Annual Review (22-23 September 2014). Consortium Contact met users and discussed how CSE service can help them and opportunities for code improvement.
  - HPC-SIG (30 September 2014, Imperial College, London). Discussed links between regional/institutional HPC and national HPC. Continue to build links with UK HPC community.

- Presentations by Centralised CSE team:
  - Lecture on "HPC Architectures" at the EPSRC-funded "HPC Autumn Academy" (15-26 September 2014, Cambridge). This school is aimed at EPSRC-funded PhD students and early-stage researchers in computational science.
3. Continual Service Improvement

- Centralised team:
  - Reduction in volume of In-Depth technical queries has allowed us to put more effort into proactive technical activities. For example, producing documentation on best practice in parallel IO, on monitoring power consumption by user jobs, and on using Python in HPC.
  - Plans to produce short online "how to" screencast videos on using particular tools: debuggers, profilers, etc. to complement the online written documentation.

- Consortium Contacts:
  - Start developing links with major users from Consortia as well as with PI’s.
  - Monitor and report on Consortium usage profiles to PIs.

- Performance monitoring:
  - Analysis of time to completion of Technical Assessments now included in this report. Should help inform metric development in future.

- Website development:
  - Knowledgebase of compilation instructions for scientific software packages now available on website. Will continue to expand and improve this information. This aids ARCHER users, staff and the worldwide HPC community.
  - CSE staff profiles now available on the website. Plan to add photographs and publicise to users. Aim to give “faces” to the ARCHER service.

- Technical Forum:
  - Presentations in TechForum Webinar series from first batch of eCSE projects. Showcase the advances made possible through eCSE funding.
  - Initial set of webinar recordings now available on website. Remainder are being processed.
  - Mailing list renamed to “hpc-techforum” to encourage sharing of expertise from all HPC users, ARCHER and otherwise.

- New Scientific Python training developed due to increased demand
  - Extra day on Python programming added to July's Software Carpentry course.
  - August virtual tutorial on Python attracted in excess of 45 attendees.

- Online material
  - Material from all ARCHER courses now available online after each course run.
  - Recordings of virtual tutorials are now being posted on youtube channel “ARCHER High Performance Computing Service.”
  - Designed a feedback form tailored for online courses which we will use after all virtual tutorials. It will also be available for people to fill in after they have watched any of the online videos.

- eCSE:
  - Based on feedback from the previous eCSE panel meeting, review functionality being improved in the SAFE for reading the associated proposal and review documents.

- Raising profile of science enabled by ARCHER
  - ARCHER Image Competition opened; closing at end of October. Images will be used to promote the scientific impact of ARCHER.
4. Contractual Performance Report

This is the contractual performance report for the ARCHER CSE Service for the Reporting Periods: July 2014, August 2014 and September 2014.

The metrics were specified by EPSRC in Schedule 2.2 of the CSE Service Contract.

CSE Query Metrics

- **QE1**: The percentage of all queries notified to the Contractor by the Help Desk in a Quarter that the Contractor responds to, and agrees a work plan with, the relevant End User within 3 working hours of receiving the notification from the Help Desk. *Service Threshold: 97%; Operating Service Level: 98%.

- **QE2**: The percentage of all queries notified by the Help Desk to the Contractor that have been satisfactorily resolved or otherwise completed by the Contractor within a 4-month period from the date it was first notified to the Contractor. *Service Threshold: 80%; Operating Service Level: 90%.

- **TA1**: The percentage of all technical assessments of software proposals provided to the Contractor by the Help Desk in any Service Period that are successfully completed by the Contractor within 10 days of the technical assessment being provided to the Contractor by the Help Desk. *Service Threshold: 85%; Operating Service Level: 90%.

- **FB1**: The percentage of End User satisfaction surveys for CSE queries carried out in accordance with the Performance Monitoring System by the Contractor showing the level of End User satisfaction to be “satisfactory”, “good” or “excellent”. *Service Threshold: 30%; Operating Service Level: 50%.

<table>
<thead>
<tr>
<th>Period</th>
<th>Metric</th>
<th>Jul-14</th>
<th>Aug-14</th>
<th>Sep-14</th>
<th>Q3 2014</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Perf.</td>
<td>Perf.</td>
<td>Perf.</td>
<td>Perf.</td>
<td>Total</td>
</tr>
<tr>
<td>QE1</td>
<td>100%</td>
<td>-2</td>
<td>100%</td>
<td>-2</td>
<td>100%</td>
</tr>
<tr>
<td>QE2</td>
<td>100%</td>
<td>-2</td>
<td>100%</td>
<td>-2</td>
<td>100%</td>
</tr>
<tr>
<td>TA1</td>
<td>100%</td>
<td>-1</td>
<td>92%</td>
<td>0</td>
<td>100%</td>
</tr>
<tr>
<td>FB1</td>
<td>100%</td>
<td>-2</td>
<td>100%</td>
<td>-2</td>
<td>100%</td>
</tr>
<tr>
<td>Total</td>
<td>-7</td>
<td>-6</td>
<td>-7</td>
<td>-20</td>
<td></td>
</tr>
</tbody>
</table>

*Pink – Below Service Threshold
Yellow – Below Operating Service Level
Green – At or above Operating Service Level*
**Training Metrics**

- **FB2**: The percentage of all training satisfaction carried out in accordance with the Performance Monitoring System by the Contractor in each Quarter that are rated “good”, “very good” or “excellent”. *Service Threshold: 70%; Operating Service Level: 80%.*

<table>
<thead>
<tr>
<th>Metric</th>
<th>Jul-14</th>
<th>Aug-14</th>
<th>Sep-14</th>
<th>Q3 2014</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perf.</td>
<td>SP</td>
<td>Perf.</td>
<td>SP</td>
<td>Perf.</td>
</tr>
<tr>
<td>FB2</td>
<td>100%</td>
<td>-1</td>
<td>100%</td>
<td>-1</td>
</tr>
<tr>
<td>Total</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
</tbody>
</table>

*Pink – Below Service Threshold
Yellow – Below Operating Service Level
Green – At or above Operating Service Level*
5. CSE Queries

Queries Resolved in Reporting Period

Metric Descriptions

<table>
<thead>
<tr>
<th>Metric</th>
<th>Jul-14</th>
<th>Aug-14</th>
<th>Sep-14</th>
<th>Total</th>
<th>% Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>In-Depth</td>
<td>20</td>
<td>12</td>
<td>14</td>
<td>46</td>
<td>11.1%</td>
</tr>
<tr>
<td>Course Registration</td>
<td>223</td>
<td>26</td>
<td>38</td>
<td>287</td>
<td>69.5%</td>
</tr>
<tr>
<td>Technical Assessment: &lt;Category&gt;</td>
<td>10</td>
<td>4</td>
<td>9</td>
<td>23</td>
<td>5.6%</td>
</tr>
<tr>
<td>Technical Assessment: RAP</td>
<td>0</td>
<td>6</td>
<td>14</td>
<td>20</td>
<td>4.8%</td>
</tr>
<tr>
<td>Technical Assessment: Instant</td>
<td>5</td>
<td>2</td>
<td>3</td>
<td>10</td>
<td>2.4%</td>
</tr>
<tr>
<td>Technical Assessment: HEC</td>
<td>1</td>
<td>0</td>
<td>7</td>
<td>8</td>
<td>1.9%</td>
</tr>
<tr>
<td>eCSE Application</td>
<td>6</td>
<td>3</td>
<td>10</td>
<td>19</td>
<td>4.6%</td>
</tr>
</tbody>
</table>

A total of 413 queries were resolved by the CSE service in the reporting period.

All of the feedback left by users on queries was rated “Excellent”. 9 query feedback responses were received on In-depth queries in the reporting period. This represents a 20% return rate for feedback forms.

Resolved In-Depth queries fell into the following categories:

<table>
<thead>
<tr>
<th>Category</th>
<th>Number of Queries</th>
<th>% Queries</th>
</tr>
</thead>
<tbody>
<tr>
<td>3rd Party Software</td>
<td>31</td>
<td>67.4%</td>
</tr>
<tr>
<td>Compilers and system software</td>
<td>4</td>
<td>8.7%</td>
</tr>
<tr>
<td>User Programs</td>
<td>3</td>
<td>6.5%</td>
</tr>
<tr>
<td>Performance and scaling</td>
<td>2</td>
<td>4.3%</td>
</tr>
<tr>
<td>Batch system and queues</td>
<td>2</td>
<td>2.5%</td>
</tr>
<tr>
<td>Other</td>
<td>2</td>
<td>4.3%</td>
</tr>
<tr>
<td>User behaviour</td>
<td>1</td>
<td>2.2%</td>
</tr>
<tr>
<td>Porting</td>
<td>1</td>
<td>2.2%</td>
</tr>
</tbody>
</table>

A histogram of the time to resolution for In Depth queries (see below) reveals that the median resolution time is 4 weeks.
A histogram of the time to completion for Technical Assessments (see below) reveals that the median completion time is 4 days.
6. Training

The CSE Service has provided a total of 22 days (631 student-days) of face-to-face training across seven different locations in the reporting period, plus 1.5 days of interactive web-based training. The table below summarises the training delivered in Q3 2014.

<table>
<thead>
<tr>
<th>Month</th>
<th>Dates</th>
<th>Course</th>
<th>Location</th>
<th>Days</th>
<th>Attendees</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jul 2014</td>
<td>30 Jun - 4 Jul</td>
<td>ARCHER Summer School</td>
<td>EPCC</td>
<td>5</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>GPU Programming with CUDA</td>
<td>Sheffield</td>
<td>1</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>Virtual Tutorial: Make and Compilation issues</td>
<td>Online</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-23</td>
<td>Software Carpentry and Scientific Python</td>
<td>Cranfield</td>
<td>3</td>
<td>37</td>
</tr>
<tr>
<td>Aug 2014</td>
<td>13</td>
<td>Virtual Tutorial: Python for High Performance Computing</td>
<td>Online</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>18-19</td>
<td>Introduction to F95</td>
<td>Culham</td>
<td>2</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>20-21</td>
<td>Introduction to OpenMP and MPI</td>
<td>Culham</td>
<td>2</td>
<td>13</td>
</tr>
<tr>
<td></td>
<td>27-28</td>
<td>NSCCS/ARCHER CP2K Workshop 2014</td>
<td>London</td>
<td>2</td>
<td>41</td>
</tr>
<tr>
<td>Sep 2014</td>
<td>1-2</td>
<td>GPU Programming</td>
<td>Edinburgh</td>
<td>2</td>
<td>45</td>
</tr>
<tr>
<td></td>
<td>2-3</td>
<td>Efficient Parallel IO on ARCHER</td>
<td>Daresbury</td>
<td>2</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Introduction to ARCHER</td>
<td>Edinburgh</td>
<td>1</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Virtual Tutorial: Tools for Building and Submitting an eCSE Proposal</td>
<td>Online</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>16-17</td>
<td>Software Carpentry</td>
<td>London</td>
<td>2</td>
<td>34</td>
</tr>
</tbody>
</table>

On the feedback forms, attendees rated the course on a scale of 1-5 (“Very bad”, “Bad”, “Good”, “Very good” and “Excellent”. The average feedback using this metric was 4.3, i.e. better than “Very Good”. Users provided 192 feedback forms on the CSE courses.

Figure 1: Breakdown of feedback responses from training course surveys for Q3 2014.
13.5 days of training are currently planned for the following quarter. Details are provided in the table below. All face-to-face courses have been opened for registration except for “Shared-Memory Programming with OpenMP” in Durham where we are in the process of finalising local arrangements.

<table>
<thead>
<tr>
<th>Month</th>
<th>Dates</th>
<th>Course</th>
<th>Location</th>
<th>Days</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oct 2014</td>
<td>8</td>
<td>Virtual Tutorial: Parallel I/O and the ARCHER Filesystem</td>
<td>Online</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>21-22</td>
<td>Hands-on Introduction to HPC</td>
<td>London</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>23-24</td>
<td>Message-Passing Programming with MPI</td>
<td>London</td>
<td>2</td>
</tr>
<tr>
<td>Nov 2014</td>
<td>12</td>
<td>Virtual Tutorial: Software Revision Control</td>
<td>Online</td>
<td>0.5</td>
</tr>
<tr>
<td>Dec 2014</td>
<td>3-4</td>
<td>Shared-Memory Programming with OpenMP</td>
<td>Durham</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>Software Carpentry Workshop</td>
<td>Edinburgh</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>Virtual Tutorial: Intro to GPU Programming</td>
<td>Online</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>16-17</td>
<td>Hands-on Introduction to HPC</td>
<td>Southampton</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>16-17</td>
<td>Single Node Performance Optimisation</td>
<td>Cambridge</td>
<td>2</td>
</tr>
</tbody>
</table>
7. Embedded CSE (eCSE)

eCSE Call 1

- 13 out of 14 projects agreed/contract signed and started.
- Costs agreed for 13 out of 14 projects
- For the one exception, Panel agreed that PI and eCSE team were to identify alternative staffing.

<table>
<thead>
<tr>
<th>eCSE ID</th>
<th>PI</th>
<th>Title</th>
<th>PMs</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>eCSE01-001</td>
<td>Michail Stamatakis</td>
<td>Zacro Software Package Development: Pushing the Frontiers of Kinetic Monte Carlo Simulation in Catalysis</td>
<td>12</td>
<td>Started 01/09/14</td>
</tr>
<tr>
<td>eCSE01-002</td>
<td>Dr Alan Gray</td>
<td>Introducing Thread and Instruction Level Parallelism into Ludwig</td>
<td>12</td>
<td>Started 01/09/14</td>
</tr>
<tr>
<td>eCSE01-003</td>
<td>Dr Benedict Rogers</td>
<td>Developing highly scalable 3-D incompressible SPH</td>
<td>12</td>
<td>Started 01/09/14</td>
</tr>
<tr>
<td>eCSE01-004</td>
<td>Chris-Kriton Skylaris</td>
<td>A pinch of salt in ONETEP's solvent model</td>
<td>3</td>
<td>Started 01/06/14</td>
</tr>
<tr>
<td>eCSE01-005</td>
<td>Mark van Schilfgaarde</td>
<td>QuasiParticle Self-Consistent GW calculations of many-atom systems</td>
<td>6</td>
<td>Started 01/08/14</td>
</tr>
<tr>
<td>eCSE01-008</td>
<td>Dr. Prashant Valluri</td>
<td>TPLS: Optimised Parallel I/O and Visualisation</td>
<td>8</td>
<td>Started 01/04/14</td>
</tr>
<tr>
<td>eCSE01-009</td>
<td>Dr Gerard Gorman</td>
<td>Scalable and interoperable I/O for Fluidity</td>
<td>6</td>
<td>Started 01/07/14</td>
</tr>
<tr>
<td>eCSE01-010</td>
<td>Dr Miguel O. Bernabeu</td>
<td>Adding a resolved deformable particle model to a highly-parallel blood flow solver for sparse vascular networks</td>
<td>12</td>
<td>Started 01/09/14</td>
</tr>
<tr>
<td>eCSE01-013</td>
<td>Jimena Gorfinkel</td>
<td>Efficient computation of two-electron integrals in a mixed Gaussian/B-spline basis.</td>
<td>12</td>
<td>Started 16/06/14</td>
</tr>
<tr>
<td>eCSE01-015</td>
<td>Professor Michael J Fagan</td>
<td>Large scale voxel based modelling</td>
<td>15</td>
<td>Started 01/04/14</td>
</tr>
<tr>
<td>eCSE01-016</td>
<td>Dr Massimo Bollasina</td>
<td>Porting and enabling use of the Community Earth System Model on ARCHER</td>
<td>4</td>
<td>Started 01/04/14</td>
</tr>
<tr>
<td>eCSE01-017</td>
<td>Dr Matt Probert</td>
<td>Hybrid OpenMP and MPI within the CASTEP code</td>
<td>12</td>
<td>Started 01/07/14</td>
</tr>
<tr>
<td>eCSE01-018</td>
<td>Scott M. Woodley</td>
<td>Tuning FHI-Aims for complex simulations on CRAY HPC platforms</td>
<td>12</td>
<td>Started 01/06/14</td>
</tr>
<tr>
<td>eCSE01-019</td>
<td>Ilian Todorov</td>
<td>DL_POLY_4: Multiple Time Stepping Development Support</td>
<td>6</td>
<td>Waiting staffing change</td>
</tr>
</tbody>
</table>
eCSE Call 2

- 17 Proposals received through SAFE (1 subsequently withdrawn due to staffing issues in the project)
  - Withdrawn proposal planned for resubmission once appropriate local staff can be identified by PI.
- 9 proposals were successful
- 8 out of 9 projects agreed/contract signed and started
- One exception due to member of proposed staff taking up new post; PI in process of recruiting new employee

<table>
<thead>
<tr>
<th>eCSE ID</th>
<th>PI</th>
<th>Title</th>
<th>PMs</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>eCSE02-2</td>
<td>Prof Jason M Reese, Edinburgh</td>
<td>Multi-Scale Engineering Flow Simulation: Hybrid MPI/OpenMP Optimization on ARCHER</td>
<td>12</td>
<td>Started 20/09/14</td>
</tr>
<tr>
<td>eCSE02-3</td>
<td>Dr. Patrick E. Farrell, Oxford</td>
<td>Scalable automated parallel PDE-constrained optimisation for dolfin-adjoint</td>
<td>8</td>
<td>Started 01/09/14</td>
</tr>
<tr>
<td>eCSE02-6</td>
<td>Prof Hugo van der Hart, QUB</td>
<td>Performance enhancement of RMT codes in preparation for the treatment of circular polarization</td>
<td>9</td>
<td>Started 01/10/14</td>
</tr>
<tr>
<td>eCSE02-8</td>
<td>Dr David Dickinson, York</td>
<td>Optimising Field Solves in GS2: Improved load balancing and non-blocking communications for maximal efficiency at high #core</td>
<td>7</td>
<td>Started 01/09/14</td>
</tr>
<tr>
<td>eCSE02-9</td>
<td>Dr Matt Probert, York</td>
<td>Optimising van der Waals simulations with the CASTEP code</td>
<td>7</td>
<td>Started 01/08/14</td>
</tr>
<tr>
<td>eCSE02-11</td>
<td>Dr Nicolae Panoiu, UCL</td>
<td>Fast and Massively Distributed Electromagnetic Solver for Advanced HPC Studies of 3D Photonic Nanostructures</td>
<td>12</td>
<td>Awaiting recruitment</td>
</tr>
<tr>
<td>eCSE02-13</td>
<td>Prof Spencer Sherwin, Imperial College</td>
<td>Communication and I/O masking for increasing the performance of Nektar++</td>
<td>12</td>
<td>Started 01/10/14</td>
</tr>
<tr>
<td>eCSE02-15</td>
<td>Dr Nicholas Hine, Cambridge</td>
<td>Calculating Excited States of Extended Systems in LR-TDDFT</td>
<td>6</td>
<td>Started 01/10/14</td>
</tr>
<tr>
<td>eCSE02-17</td>
<td>Dr James Harle, Proudman Oceanographic Laboratory</td>
<td>NEMO Regional Configuration Toolbox</td>
<td>9</td>
<td>Started 01/10/14</td>
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eCSE Call 3

- 16 proposals received
- 162 person months requested in total

<table>
<thead>
<tr>
<th>eCSE ID</th>
<th>PI</th>
<th>Title</th>
<th>PMs</th>
<th>Status</th>
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<tr>
<td>eCSE03-1</td>
<td>Prof. Tony Arber</td>
<td>Optimisation of the EPOCH laser-plasma simulation code</td>
<td>12</td>
<td>Submitted</td>
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<tr>
<td>eCSE03-2</td>
<td>Dr. Michele Sergio Campobasso</td>
<td>Reducing the run-time and improving the ease-of-use and portability of the COSA 3D harmonic balance Navier-Stokes solver for open rotor unsteady aerodynamics</td>
<td>7</td>
<td>Submitted</td>
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<td>eCSE03-3</td>
<td>Dr David J Huggins</td>
<td>Algorithmic Enhancements to the Solvaware Package for the Analysis of Hydration</td>
<td>6</td>
<td>Submitted</td>
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<td>eCSE03-4</td>
<td>Prof George Barakos</td>
<td>Discrete velocity methods for the Helicopter Multi-Block CFD solver</td>
<td>12</td>
<td>Submitted</td>
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<tr>
<td>eCSE03-5</td>
<td>David R Bowler</td>
<td>The first general release of the linear-scaling DFT code Conquest with focus on the emerging field of biological simulations</td>
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<td>Submitted</td>
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<tr>
<td>eCSE03-6</td>
<td>Dr Ozgur Yazaydin</td>
<td>QM/MM Interfacing and Parallelisation of RASPA Molecular Simulation Package</td>
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<td>eCSE03-7</td>
<td>Dr Matthew Piggott</td>
<td>Delivering a step-change in performance and functionality to the Fluidity shallow water solver through code generation</td>
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<td>eCSE03-8</td>
<td>James R. Maddison</td>
<td>Parallel supermeshing for multimesh modelling</td>
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<td>eCSE03-9</td>
<td>Dr Dan Jones</td>
<td>Providing the ARCHER community with adjoint modelling tools for high-performance oceanographic and cryospheric computation</td>
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<td>eCSE03-10</td>
<td>Dr Garth Wells</td>
<td>High performance multi-physics simulations with FEniCS/DOLFIN</td>
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<td>eCSE03-11</td>
<td>Dr Matthew B Watkins</td>
<td>Local excitement in CP2K</td>
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<td>eCSE03-12</td>
<td>Xuerui Mao</td>
<td>Full parallelism of calculations of optimal flow control</td>
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<td>eCSE03-13</td>
<td>Dr Rupert Nash</td>
<td>Grids in grids: hierarchical grid</td>
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<td>13</td>
<td><a href="mailto:rupert.nash@ed.ac.uk">rupert.nash@ed.ac.uk</a> (EPCC)</td>
<td>generation and decomposition for a massively parallel blood flow simulator</td>
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<td>eCSE03-14</td>
<td>Dr Irene Moulitsas <a href="mailto:i.moulitsas@cranfield.ac.uk">i.moulitsas@cranfield.ac.uk</a> (Cranfield University)</td>
<td>PGAS Fortran Coarray parallelisation strategies for CFD applications</td>
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<td>eCSE03-15</td>
<td>Dr Justin R Finn <a href="mailto:J.Finn@liverpool.ac.uk">J.Finn@liverpool.ac.uk</a> (University of Liverpool)</td>
<td>CFD2LCS: A general purpose library for integrated computation of Lagrangian coherent structures during massively parallel hydrodynamic simulations.</td>
<td>12</td>
<td>Submitted</td>
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<td>eCSE03-16</td>
<td>Prof Jonathan W Essex <a href="mailto:j.w.essex@soton.ac.uk">j.w.essex@soton.ac.uk</a> (University of Southampton)</td>
<td>Implementation of Dual Resolution Simulation Methodology in LAMMPS</td>
<td>6</td>
<td>Submitted</td>
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**Future eCSE Calls**

eCSE calls are run to a regular schedule. The upcoming calls are:

- eCSE Call 4: Opens 25 Nov 2014, Closes 13 Jan 2015