# eCSE Overview

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# Overview

- Programme provides funding to the ARCHER user community to develop software in a sustainable manner for ARCHER
- Objectives
  - To sustain key codes for the UK computational science community
  - To facilitate efficient use of ARCHER resources through enhanced code performance/functionality
  - To offer a not-for-profit service that provides value for money to the HPC user community and beyond
- Also
  - Develop and sustain codes and communities from new areas
  - Support and encourage early career researchers


# Scope - examples

- Addition of new functionality into the code
- Enhanced performance of the code – primarily scalability improvements
- Integration of multiple codes e.g., to provide additional functionality;
- Improved software quality (e.g. reduction in complexity, removal of dependencies)
- Development of support tools / scripts to enhance usability
- Test suite development and/or correctness / accuracy / validation testing
- Code development to take a code from a Tier-2 (Regional) to Tier-1 (National) level bringing new communities onto Archer

- Funding cannot be used for scientific research

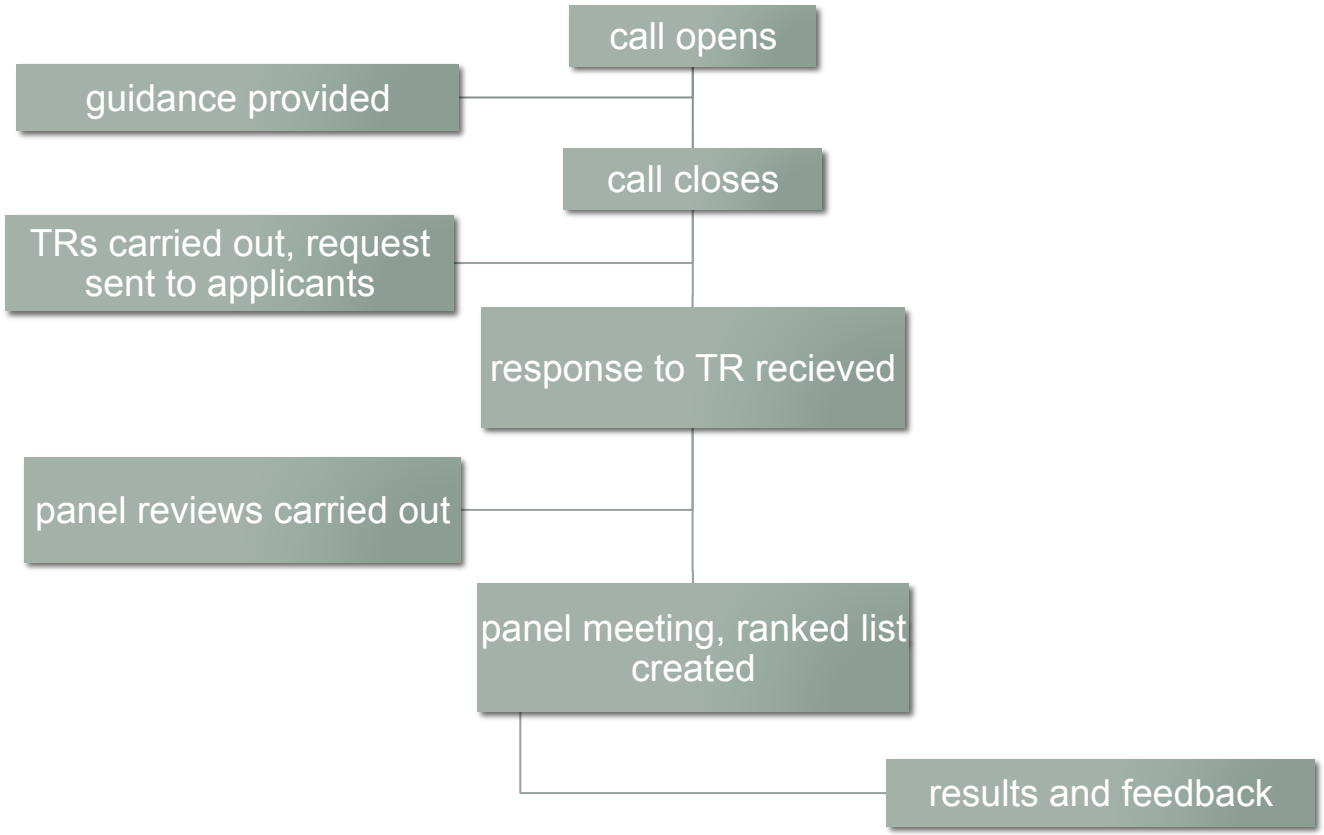

# New communities

- Funding is available for
  - Established ARCHER communities - proposals from these communities are encouraged
  - However, proposals from new scientific communities are also encouraged
- New scientific communities
  - communities from **scientific** areas not currently exploiting the ARCHER system
  - likely to have a scientific need for greater computational power than available at a regional level
- New codes to ARCHER are not necessarily new scientific communities
  - New codes / users from existing communities can apply as an established community
  - Encouraged to contact / join existing appropriate consortia
- Panel will assess whether a project is from a new community
  - If not a new community, this will automatically be considered as an existing community


# Embedded CSE (eCSE)

- 3 regular calls per year
  - Current (6th) call closes 4pm on Tuesday 11th October 2016
  - Most projects between 6 and 12 months
- Can apply to develop on the KNL system
- Funding can be requested for
  - staff located at the institution of the PI, third parties, staff from the centralised CSE support team, or a mixture of the above
- Early career researchers and support staff can be PIs
  - PI institution must be UK based, CO-Is may be elsewhere
- Ability of technical staff to complete the work is assessed
  - Considered together with PI/Co-I expertise and training plan
- Not-for-profit
  - Committed to average of 14 FTE per year. Additional money will be put into further eCSE PMs. Costed at 80% FEC


# eCSE process

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# Reviewing eCSE applications

- Two stage reviews for all eCSE applications
  - Technical Reviews (TRs)
  - Panel Reviews

# Technical review (TR)

- Administrative checks are applied for all submissions before the TRs
- Applications will be reviewed by technical advisors and the ARCHER centralised CSE team
  - Majority carried out by the centralised team
  - If conflicts of interest, proposal reviewed by external advisors
- Looking for missing information or detail

# TR request for further information

- Any requests for further information will be sent to applicants after the admin check and TRs
- Applicants will be given the opportunity to respond
  - Original proposal will not be updated, only additional response can be submitted via SAFE
  - All information supplied to the panel
  - Can also choose to withdraw and submit to a later panel

# Panel reviews & panel meetings

- Each application will be reviewed by two panel members independently prior to the panel meeting
  - Based on the Assessment Criteria
- Panel Meeting will take place within around 8 weeks after the call closed
- For each application, Panel can decide to fund, not fund or if needed fund in part
- Robust conflict of interest and confidentiality process
- A small number of early career researchers may be present as observers
  - Selected from a competitive selection process
  - Will be looking for the next set of observers nearer the end of the year

# Assessment criteria

- Applicants
  - Track record of applicants, including all team members, demonstrate project can be completed
- New Communities Justification
  - Enough detail to justify application is from New Community
- Technical context
  - Sufficient technical information provided
- Benefits
  - Why it is needed, what are the expected benefits
  - Scientific, computational and to ARCHER community
- Pathway to impact
  - Impact activities to ensure potential benefits are achieved
- Work plan
  - Appropriate plan for management, technical work and resources
- Overall
  - Overall quality and objectives


# Points to remember

- Specific Benefit to the ARCHER community
  - Availability of code on ARCHER after the work is complete
  - Who will utilise the improvements and for what activity – be specific
  - License arrangements – shouldn't create a significant barrier for ARCHER users
  - End result must be to use ARCHER
- Objectives are important
  - Where possible should be measurable and quantifiable
- New Communities
  - If a new code but in an existing area, investigate existing consortium
- Technical staffing experience and profile is considered by the panel
  - Experience of PIs/Co-Is relevant as is training plan and/or additional support
- Evidence
  - The panel looks for evidence that the work is achievable e.g. scaling evidence
  - Ask for help from the CSE team if you need – but not 1 day before the deadline
- Existing funding
  - Looking to ensure the work is not already supposed under a different route

# Final decision and feedback

- Final decisions will be sent to applicants together with feedback from the panel
  - Within around 2 weeks after the panel meeting
- Unsuccessful applications
  - Will be provided with constructive feedback
  - If appropriate will be encouraged to contact the CSE team for further advice and support in the preparation for the resubmission to the future call
  - Any resubmission will be treated in the same way as new submissions

# Overview

- What happens if your project is accepted?
  - Contracts set up
  - ARCHER project set up and CPU-hours awarded
  - Contact point established
  - Engagement with ARCHER community expected
  - Reporting
    - Final report
    - https://www.archer.ac.uk/community/eCSE/eCSE-reports.php
  - ARCHER webinar presented
  - All projects are showcased on the ARCHER website
    - Subset of projects chosen for case studies


# Further information

- After calls opens, proposals should be submitted via SAFE using the *eCSE Funding Calls* pages:
  - https://www.archer.ac.uk/safe/
  - Please register first if you are not a registered user in SAFE

- Information and guidelines for applying can be found at:
  - https://www.archer.ac.uk/community/eCSE/
- Applicants can request guidance from the centralised CSE team before submission:
  - Please contact ARCHER helpdesk: support@archer.ac.uk


# Questions?


# Final Reports



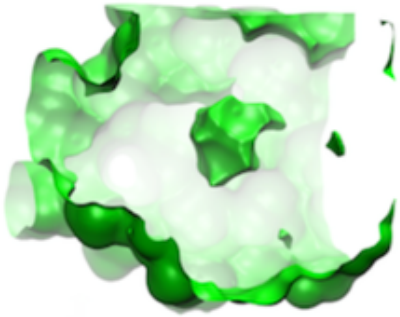



# eCSE programme

- Enhances application codes for the benefit of the ARCHER community
  - Enables new science
- It is important to showcase the work of the eCSE
  - Highlighting the benefits and impact from the work
- However eCSE's are early in the process
  - At the end of an eCSE the code will be improved, but the science is yet to be done
  - Nevertheless it is important to try and demonstrate the benefits and impact of the work – now or in the future

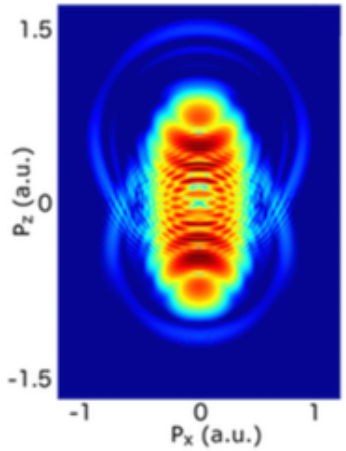

# Final Reports

- Are primarily aimed at showcasing the work of the eCSE
  - Also reviewed by the panel and feedback provided
  - Reports are to be completed within 8 weeks of the end of project
- Contains a technical description of the work carried out
  - Showcases achievements, provides learning opportunity for the community
- Contain a publishable summary
  - Achievement against objectives
  - Project summary
  - Software summary
- Publishable summary is used to provide a summary on the website



## A pinch of salt in ONETEP's solvent model

Chemical reactions, drug-protein interactions, and many chemical and physical processes on surfaces are examples of technologically important processes that happen in the presence of solvents. The inclusion of electrolytes (salt) in solvents such as water is crucial for biomolecular simulations, as most processes (e.g. protein-protein or protein-drug interactions or DNA mutations) take place in saline solutions. This project aimed to develop the capability to model electrolyte-containing solvents in quantum-mechanical simulations of materials from first principles. Using a linear-scaling code such as ONETEP enables simulations to be performed on entire biomolecules or catalysts that typically involve hundreds or thousands of atoms.




## Performance enhancement in RMT codes in preparation for application to circular polarised light fields

One of the grand challenges in physics and chemistry is to understand what actually happens during a chemical reaction. The nuclei in molecules move on the femtosecond ($10^{-15}$ s) timescale, but the electrons in the molecules move on the attosecond ($10^{-18}$ s) timescale. The R-matrix with time dependence (RMT) code is a leading code for the description of ultra-fast processes in general atoms and molecules. Scientists at Queen's University Belfast have been working on the RMT code, increasing its speed by up to a factor of 5 and reducing the amount of memory required by one or more orders of magnitude.

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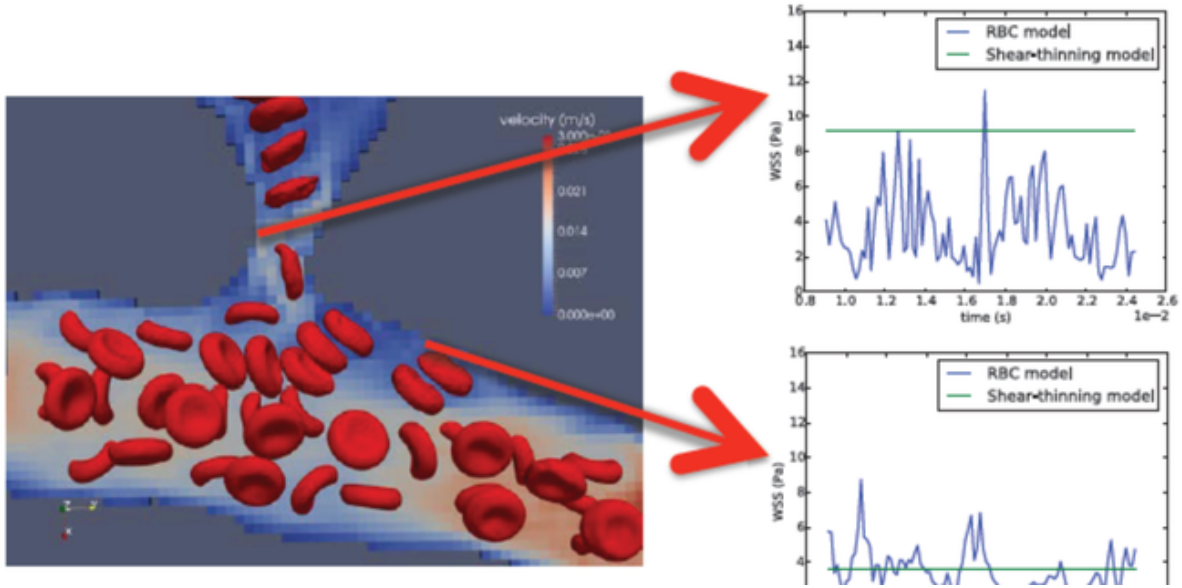
vascular networks.

The main components to be implemented were: a) the immersed boundary method for fluid-structure interaction, b) a finite element model of particle membrane elastic deformation, and c) a procedure for simulation initialisation. An important challenge to be overcome in the project was developing a generic implementation of the previous algorithms that could scale up well in terms of domain complexity and particle volume fraction without undermining the excellent parallel scalability of HemeLB.

Thanks to the work done in this eCSE project, we can now model blood as a suspension of deformable particles. The work represents a substantial leap forward for the simulation of blood flow in microvasculature and enables for the first time the theoretical study of advanced aspects of haemorheology, oxygen transport, and cell trafficking in realistic vascular networks. This has already started to provide a much more accurate picture of the WSS experienced by the microvasculature. Furthermore, this will enable the theoretical study of the collective dynamics of dense RBC suspensions in complex vessel geometries.



# Publishable summary

- Our way of demonstrating the science benefits and impact from the eCSE programme
  - All summaries will go on the web, shows the breadth of science
- Example science benefits
  - Reduced time to solution for simulations carried out on the code
  - Reduction in the cost of a simulation (e.g. in CPU hours and hence monetary terms)
  - Increase in the quantity of science produced for the same cost budget
  - Increase in the novelty and breadth of the science produced (e.g. previously untenable science) on ARCHER


# Case studies

- Small number of reports are converted to full case studies
  - Part of the case study series:
  - http://www.archer.ac.uk/casestudies/
  - We work with you and the designer to produce this
  - Available on the web site and as a flyer. Postcard also produced.
  - Disseminated at conferences and events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# UNDERSTANDING HOW BONES DEVELOP AND RESPOND TO DISEASE AND THE USE OF IMPLANTS

"This new ability

**Scientists at the University of Hull have developed their simulation software to utilise ARCHER to model complete bones or large sections of bones. This**

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