

# ARCHER Technical Assessment Form: Standard Grant and RAP Applications

**Note: this form is for standard grant applications (usually via J-eS) and RAP applications only. Technical Assessment forms for other access routes can be found on the ARCHER website at <http://www.archer.ac.uk/access>**

## Instructions:

1. Complete Section 1 below as fully as possible. If you have any questions or require clarification, please contact the ARCHER helpdesk ([support@archer.ac.uk](mailto:support@archer.ac.uk)).
2. Return the completed form (as a Word document) to the ARCHER helpdesk ([support@archer.ac.uk](mailto:support@archer.ac.uk)) along with a draft of your Case for Support.
3. The ARCHER CSE team will complete Section 2 and will contact you directly for more information if it is required. This may take up to 10 days from receipt of the completed form.
4. The CSE team will return the fully completed form to you so you can include it in your grant/RAP application.

## Notes for Standard Grant Applications:

- You can apply for ARCHER resources for a maximum of 2 years (even if the research grant is longer). Additional resources to support the grant should be applied for through the RAP top-up process at the appropriate time.
- You must supply quantitative evidence that the codes to be used scale to the core counts requested. More details on the evidence required can be found in Section 1, Part 6.

## Notes for RAP Applications:

- You can apply for ARCHER resources for a maximum of 1 year for RAP or 2 years for RAP top up.
- You must request at least 1000 kAU.
- You must supply quantitative evidence that the codes to be used scale to the core counts requested. More details on the evidence required can be found in Section 1, Part 6.
- Further notes can be found at: <http://archer.ac.uk/access/rap/>.

Completion of this form implies permission for user details to be stored in the Service Partners' and Research Councils' databases and to be used for mailing, accounting, reporting and other administrative purposes.

**Section 1: HPC Resources and Case for Support (To be completed by the applicant).**

**1. Project Information.**

**1.1. Project Title:** CP2K-UK

**1.2. Application Type:** RAP Top-up

**1.3. PI Name and Contact Details.**

<b>Name:</b>	<i>Fill in Your details</i>
<b>Department:</b>	
<b>Institution:</b>	
<b>Position Held:</b>	
<b>Address:</b>	
<b>Postcode:</b>	
<b>e-Mail:</b>	
<b>Telephone:</b>	
<b>Nationality:</b>	

**1.4. Contact details for application (if different from PI above)**

<b>Name:</b>	As above
<b>Department:</b>	
<b>Institution:</b>	
<b>Position Held:</b>	
<b>Address:</b>	
<b>Postcode:</b>	
<b>e-Mail:</b>	
<b>Telephone:</b>	
<b>Nationality:</b>	

**1.5. Proposed start date of ARCHER use:** 1-Oct-2015

**1.6. Project length (months) of ARCHER use:** 24 months

## 2. Previous Use of HPC Resources.

**2.1. Are you an existing ARCHER user? Yes**

**2.2. Which other HPC services have you used?**

HECToR, PRACE Tier-0 Services (Jugene, Juqueen, Curie), CSCS Services (Piz Daint, Todi, Monte Rose), Magnus XC40 (UWA), various local HPC clusters

**2.3. If you have used other HPC services please provide a brief summary of the number of core hours used and the types of jobs run (codes, core counts, typical job lengths):**

Wide range of production simulations and benchmarking using CP2K, up to 65536 cores. Typical benchmark jobs are short, lasting between a few hours (on smaller process counts), down to 10 mins or less for large runs. Production runs (e.g. MD) can last for several days in total.

### 3. ARCHER Software and Support Requirements.

#### 3.1. Summary of software requirements.

What are the main codes you will be using? A description of available software on ARCHER is given here <http://www.archer.ac.uk/documentation/software/>. Please provide links to codes/software not presently available on ARCHER.

CP2K

#### Software requirements (e.g. compilers, libraries, tools):

GNU compiler suite, Cray MPT, Libsci, CrayPat

#### 3.2. Support Requirements

How do you plan to port and optimize your code on ARCHER (delete as appropriate)?

Expertise in your group	Yes
ARCHER CSE Support	No
Other (please specify)	We are applying for eCSE support for performance developments identified during the main project (but outside the scope of our workplan)

Please summarise any other support requirements for this project:

None

#### 4. Proposed Use of ARCHER Resources.

##### 4.1. Job size mix for the project

The online kAU calculator (<http://www.archer.ac.uk/access/au-calculator/>) can be used to help complete this table and contains a list of kAU rates.

**Please see notes at beginning of this document regarding the maximum amounts/duration of time that can be applied for and consult any call guidelines.**

	Largest Job	Typical Job	Smallest Job
Number of parallel tasks (e.g. MPI ranks)	12,228	576	96
Number of tasks used per node	24	24	24
Wallclock time for each job.	0.12	10	1
Number of jobs of this type	100	63	100
Total memory required.	32640 GB	1536 GB	256 GB
Amount of data read/written to disk in each job.	< 1 GB	~10 GB	~100 MB
Amount of data to be transferred to/from ARCHER per job.	None	~100 MB	None

**Total kAU: 7,790.4**

**Notional Cost: £4,362.94**

##### 4.2. Disk space requirements.

/home: Small, backed-up. For project critical files (e.g. source code).

/work: Large, high-performance, not backed-up. For input and output from calculations.

RDF: Large, backed-up, long-term. Data analysis and long term data storage.

	Storage
/home (required)	200 GB
/work (required)	500 GB
RDF (optional)	500 GB

## 5. Usage Breakdown by 6-month Periods

**\*This Section does NOT need to be filled in by applicants to the RAP, but is compulsory for grant applicants including top-up applications through the RAP.**

The total number of kAU requested above must be broken down into 6-month *periods* that span the length of access to ARCHER that has been requested (e.g. if you have requested 1 year of access in total then the kAUs must be split into two 6 month periods). The table below has rows for the maximum number of periods for a grant application (4 periods = 2 years), please only complete the number of rows required for your application.

If your application is successful then these period allocations will be enforced on ARCHER in the following way:

- Any unused allocation at the end of a period is lost
- You cannot move kAU between different allocation periods

<b>Period 1 (months 0-6)</b>	2,700 kAU
<b>Period 2 (months 7-12)</b>	2,700 kAU
<b>Period 3 (months 13-18)</b>	1,195.2 kAU
<b>Period 4 (months 19-24)</b>	1,195.2 kAU

## 6. Scaling Evidence to Support Proposed Use of ARCHER

The number of kAUs requested and the job sizes specified in 4.1 above must be backed up by quantitative evidence that the code scales efficiently to the job sizes requested. The evidence must include:

- A graph or table of the *speedup* for a similar problem using the code on ARCHER or another HPC system. The speedup should be provided relative to the smallest number of cores that can be used feasibly (see examples below).

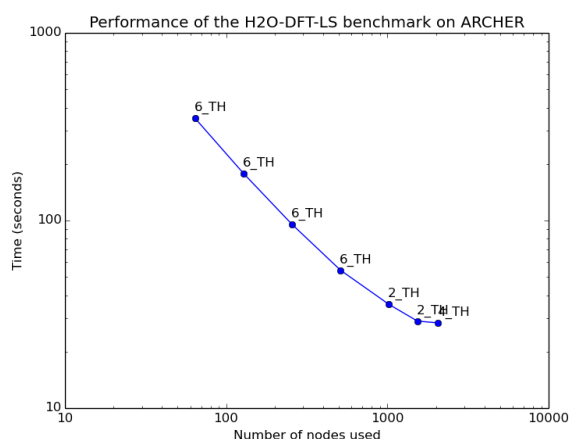
If the application is developing new algorithms for which scaling data is not yet available then the proposed scaling should be justified with appropriate references and descriptions.

If you require help in evaluating the speedup of a code on a particular problem then please contact the ARCHER Helpdesk ([support@archer.ac.uk](mailto:support@archer.ac.uk))

You should also provide brief justification of the storage requirements specified in 4.2 above.

We will run several different types and scales of CP2K calculations during the project. Representative samples of these are as follows:

**Large jobs** – Linear Scaling SCF using DBCSR. For some of the development in WP2 we will run highly expensive and scalable (but short) calculations using the LS-SCF module in CP2K. Scaling for this method is shown below:

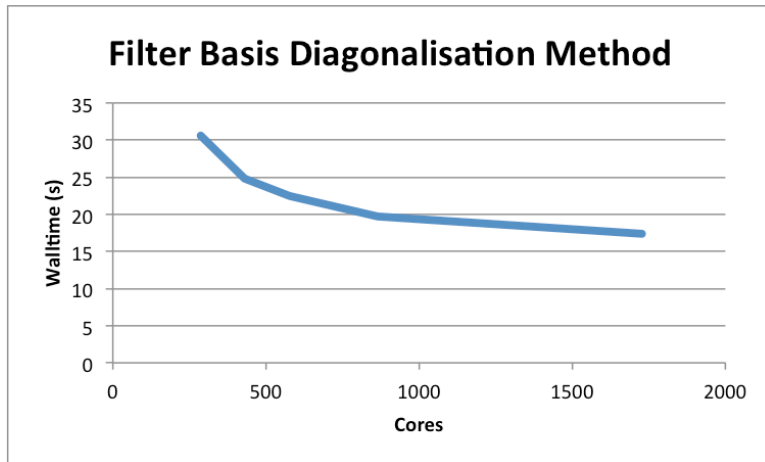


On 512 ARCHER nodes (12,228 cores), 80% parallel efficiency is obtained, and the run takes 415s. As a result, each calculation takes:

$$415 \text{ (s)} * 512 \text{ (nodes)} / 3600 \text{ (s/h)} = 59 \text{ (nh)} * 0.36 = \sim 22 \text{ kAU}$$

We will need to run many of these jobs as we develop the code, as detailed in table 4.1

**Medium jobs** – using the Filtered Basis method developed in WP3. The scaling plot below shows a single SCF cycle of an energy calculation with a system of 5184 atoms (1728 H2O molecules) carried out on ARCHER.



70% parallel efficiency is obtained on 576 cores, and takes 22.5s for this calculation. Based on previous experience that 50 SCF cycles per MD step is typical, and we would run a 1 ps MD using a 0.5fs timestep, a full calculation will require:

$$22.5 \text{ (s)} \times 50 \text{ (SCF)} \times 2,000 \text{ (steps)} \times 24 \text{ (nodes)} / 3,600 \text{ (s/h)} = 6,000 \text{ (nh)} * 0.36 = \sim 5,400 \text{ kAU}$$

We will run these split into 63 10-hour individual batch jobs (see table 4.1).

**Small jobs** – We will run many short jobs on the order of 2-4 nodes for testing and debugging during code development, and these are detailed in table 4.1.

**Storage** – Our current storage needs remain modest, as we are primarily storing code, binaries and a limited amount of scratch space is needed for temporary files generated during execution and debugging. Therefore we request the same amount of storage as in our original 2 year allocation: 200 GB on /home and 500GB on /work and the RDF.