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).
2. Return the completed form (as a Word document) to the ARCHER helpdesk (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: Using linear scaling first principles molecular dynamics on 10,000-100,000 atoms: Boron implantation in Si/Ge nanowires

1.2. Application Type: Grant (ARCHER Leadership bid)

1.3. PI Name and Contact Details.

Name:	Dr David R Bowler
Department:	London Centre for Nanotechnology
Institution:	University College London
Position Held:	PI and Reader in Physics
Address:	17-19 Gordon St, London
Postcode:	WC1H 0AH
e-Mail:	david.bowler@ucl.ac.uk
Telephone:	02076797229
Nationality:	United Kingdom

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

Name:	[Please Complete Table]
Department:	
Institution:	
Position Held:	
Address:	
Postcode:	
e-Mail:	
Telephone:	
Nationality:	

1.5. Proposed start date of ARCHER use: 15th October 2015

1.6. Project length (months) of ARCHER use: 12 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?

Cray T3E, CSAR, HPCx

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):

HECToR (using standard VASP) as part of UKCP consortium
Jaguar (Oak Ridge, Conquest code up to 16,384 cores)
Three dCSE projects for CONQUEST on HECToR

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.

CONQUEST (http://en.wikipedia.org/wiki/CONQUEST) and links to papers therein.

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

F90 compilers, ScaLAPACK, MPI, LAPACK, BLAS, BLACS

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)	No

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)	16384	2000	500
Number of tasks used per node	24	24	24
Wallclock time for each job.	48	12	12
Number of jobs of this type	10	50	50
Total memory required.	43712 GB	5376 GB	1344 GB
Amount of data read/written to disk in each job.	10 GB	5 GB	5GB
Amount of data to be transferred to/from ARCHER per job.	10 GB	5 GB	5 GB

Total kAU: 147,702 kAU
Notional Cost: £78,793.00

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)	250 GB
/work (required)	100 GB
RDF (optional)	

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

Period 1 (months 0-6)	47, 702
Period 2 (months 7-12)	100,000
Period 3 (months 13-18)	
Period 4 (months 19-24)	

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)

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

CONQUEST has been shown to scale exceptionally well on HECToR (see for instance J. Phys.:Condens. Matter **22** 074207 (2010)) and the K computer in Japan (reaching almost 200,000 cores – see JASSE **1**, 87 (2014) available at: https://www.jstage.jst.go.jp/article/jasse/1/1/1_87/_article)

CONQUEST has been used previously to perform first principles molecular dynamics previously on K (Japanese supercomputer using 16,384 cores) using similar elements and identical basis set size. During these runs the time per MD time step was 1085 seconds, running for 300fs and time step of 2fs, with a total run time of ~46 hrs and computing 32,768 atoms. Our largest calculations will be of approximately similar size, with smallest job sizes based on smaller test systems and typical job sizes based on investigations of smallest physical system size.

Paper reference; dx.doi.org/10.1021/ct500847y

Typical data files from CONQUEST MD runs are 2-5GB, though this will increase with larger runs and the sizes are reflected in our estimates.

Section 2: Technical Assessment (*To be completed by CSE team).*

Date Received by CSE: 7 September 2015

Is the application, as outlined above, suitable for access to the ARCHER service? **Yes / No**

Comments:

Do the applicants have the technical expertise required for the proposed work?	Yes
The applicants have a large amount of technical expertise with HPC systems and the code described in the application.	

Is the software specified technically suitable for ARCHER?	Yes
The software has been successfully used on large Cray systems before and alos on other MPP architectures.	

Has scaling evidence been provide that shows speedup to required job size for the software specified?	Yes
References provided show good scaling up to the required job sizes for the software on the K supercomputer in Japan.	

Does the project require the technical capabilities of ARCHER?	Yes
The largest parallel jobs cannot be supported on other UK HPC machines.	

Is the compute time requested reasonable and has the job breakdown been technically justified?	Yes
The compute time requested seems reasonable for the project but little detail is provided on the job breakdown.	

Are the storage requests reasonable and has technical justification been provided for the values?	Yes
Storage requests are reasonable however I would recommend adding some RDF space to the project so that the data analysis capability of the UK-RDF DAC can be used to analyse the results.	

Name: Dr Andrew Turner
Position: CSE Team Leader
Date: 9 September 2015