**Information**

EPSRC requires an annual report from each of the HEC consortia. The MCC committee needs help to complete this task via:

(i) the completion of annual reports from our members,

(ii) data uploaded to https://www.ucl.ac.uk/klmc/mcc/documents/forms.html for publications, degrees awarded and destinations of staff, and

(iii) the answers to the following four questions for the reporting period:

Q1: If you (or your group) have been involved in software development activities work, please provide brief details on progress of software development and any impact this has had on consortium members and the broader research community, otherwise state “NONE”.

Q2: If your work, as a result of MCC membership (e.g. use of ARCHER2), involved collaboration with industry, then please provide, here I quote directly from EPSRC, “details of the company involved, information on the part ARCHER2 played, a statement on the impact that the work has / is making and, if relevant, details of any in kind or in cash contributions that have been associated with this work”, otherwise state “NONE”.

Q3: Likewise, please provide, again I quote directly from EPSRC, “details of any other activities involving industrial participation e.g. activities involving any Industrial Advisory panels, attendance/participation in workshops and Consortium based activities”, otherwise state “NONE”.

Q4: For strengthening UK’s international position, if your work, because of MCC membership (e.g. use of ARCHER2), involved collaboration with international partners, then please provide, here I quote directly from EPSRC, “a bullet pointed list of projects that have involved international collaboration. For each example, please provide a brief summary of the part that ARCHER and the Consortium have played.” AND “any other international activities ... involved in (workshops, EU projects etc.)”, otherwise state “NONE”.

Note that annual reports from members are required for each budget code, for example, my group has used budget codes e05-nandef-smw and e05-gener-smw on ARCHER2 and MCC\_nandef\_smw on YOUNG, therefore I would need to complete two reports, one for nandef and one for gener as each theme will be collated independently.

In these reports we try to capture: (A) a brief update on statistics and how a project is progressing; (B) information that can be included in our annual report to EPSRC; and (C) information for outreach (webpage).

Part A should be included for all allocations awarded (note that you do not need to copy the description of the project that is already given in your proposals).

Parts B and C should be completed if you can provide useful information that we can include in our annual report to EPSRC.

**Please:**

(a) If you have more than one project within a theme to report on, then create just one document (copy and paste the entire template below to create a series of reports). We rely on the judgment of the group leader to decide on whether it is best or not to combine a number of these. In the case of combining projects, please choose an appropriate title (i.e. it does not need to match that in the original proposal).

(b) Replace all red text without changing the style and re-colour BLACK;

(c) Rename document (all lower case)

report-{year}-{theme code}-{group code}.doc

(d) Delete all blue instructions (entire paragraphs so that extra blank lines do not remain) before sending as a Word document to your group’s coordinator, or group leader.

(e) Once the group leader (full MCC member) is happy with the content, please email all reports for this year as Word documents to [klmc.mcc@ucl.ac.uk](mailto:klmc.mcc@ucl.ac.uk) and include in the email message answers to the four questions listed above under section (iii).

(f) Check that there is no missing data that needs to be captured in our Google forms (use links in address given above in section (ii)).

**Thank you**

**Scott Woodley, on behalf of the MCC committee**

Type the Title of Your Research Here

List investigators in the form: First X. Surname, Second Y. Surname, and Third Z. Surname

**PART A**

**Project start date:** July 2023

**ARCHER2 allocation awarded this year for this project:** 50,000 k AU

**YOUNG allocation awarded this year for this project:** 30,000 k AU

If the project ran over more than one year, then the next lines will report larger numbers than that shown above but can also be smaller if allocation not consumed. Numbers here are not supposed to be precise, just a rough estimate

**Estimate of current total spend on ARCHER2 for this project:** ~100,000 k AU

**Estimate of current total spend on YOUNG for this project:** ~30,000 k AU

To capture current (and future) HEC requirements, please complete the next section.

**Estimate of typical job type for project during this period (size, length, fraction of jobs):**

4 nodes 12hr 60%

8 nodes 12hr 40%

**File space on ARCHER2 (home, work, RDF) in Gb:** 0 1,200 12

**Typical Work Flow:** Software installed by ARCHER (no home space required); over the course of the project I will run ~400 simulations; each simulation requires input file of ~1kB; generates 3 restart files of ~1Gb in size and 1 output file ~1kB in size; all files are stored until project ends (work ~1.2Tb); at end of project restart files deleted, whereas input and output files tarred and transferred to RDF (~12Gb).

If the project used HEC resources obtained elsewhere (not from MCC), then please let us know, for example if 50% MCC-ARCHER2 30% UKCP-YOUNG 20% EUROPA-Barcelona

**Other HEC resources used this year:** 30% UKCP-YOUNG 20% EUROPA-Barcelona

In the next section please give the total number of publications and then list the DOI of papers (one per line) arising from the work of this project. Note that they will still need to be uploaded into our Google form!

**Publications arising from work** 2

10.1021/jp104372j

10.1038/nmat2321

**Brief update** (please include where in the timeline of the project you are)

This project is part of a 3-year EPSRC grant and we are at the half way mark. Tomas has completed 40% of the required simulations and is now preparing the final manuscript. Optimisations were 10M AU cheaper than expected. In the next year we will apply for more time to complete the larger systems. All results will be part of our first paper on this topic.

**PART B**

**Summary or Highlights**

If possible, provide scientific highlights in the form of a sentence or short paragraph that can ideally be used in our report to EPSRC that includes a reference your paper (use 1, 2, ... to reference the first, second, ... DOI listed above), which acknowledges the MCC. The highlight can also be related to software development or porting on HEC systems.

The role of ... has been established, which is important because ... This insight was achieved by ...

**Please indicate whether or not this project is suitable for a 2-page Case Study.**

Although we do not have any industrial partners, we do have international collaborators involved in this project, and the work has a high impact in ....

**Noteworthy Presentations or Announcements arising from work**

Below include details of any other noteworthy outputs that can be included in our report to EPSRC, for example: invited talks, press announcements.

**PART C**

If there is already a publication and/or closure to the particular part of the supported project, then please complete the following table. This table will be used on our webpage for the public (<https://mcc.hec.ac.uk/>)

|  |  |
| --- | --- |
| Add a nice figure here (perhaps a slightly altered graphical TOC from a publication) | Describe in layman terms the project, how HEC resources enabled the successful outcome of the research, and its impact. |