Proposal for a Workshop at 2024 CHPC National Meeting.

- This year the workshops run on **Sunday** 1 December only.

Please provide the following information for the proposed short course or tutorial workshop. It is not necessary to fill in everything, complete as much as you can to help us evaluate the proposal.

Title of Workshop: Exploiting exascale HPC for materials modelling; UK's Excalibur Project

Lecturer(s): Name, Affiliation, Email Address

1. GULP and KLMC: Scott Woodley (and Alexey Sokol), University College London (UCL), Scott.Woodley@ucl.ac.uk
2. CP2K: Marcello Puligheddu, Harwell (SFTC), Marcello.Puligheddu@stfc.ac.uk
3. CASTEP: Matthew Smith, University of York, Matthew.J.Smith@york.ac.uk
4. CHEMSHELL: Thomas Keal (and Rajany KV), Daresbury Laboratory (STFC), Thomas.Keal@stfc.ac.uk

Description: *As will appear on the conference web site and programme.*

Come and learn state-of-the-art materials modelling techniques implemented in internationally leading software suitable for running on local and high-performance platforms. The software introduced will include GULP, CASTEP, CP2K, KLMC and CHEMSHELL. The morning session will be devoted to covering both classical atomic and electronic structure, how to automate such calculations using KLMC and APIs. The afternoon session will cover how to combine these techniques in multiscale approaches. Both morning and afternoon sessions will be composed of lectures followed by hands-on exercises led by developers of the software. The team, funded under the PAX-HPC Excalibur project, are all part of the active efforts in the UK to ensure our community and software are exascale ready, i.e. can exploit exascale HPC platforms as and when they become available. Recent developments for materials modelling carried out under the PAX-HPC project will also be highlighted and, time allowing, explored.

Duration:

- ~~□ ¼ day (90 min)~~
- ~~□ ½ day (3h)~~
- □ full day (6h)

Size: *(max number of delegates)* limited to size of room for lectures and CHPC accounts/resources

Target Audience: *(who should attend this tutorial)*

Postgraduate students, scientists new to the field and other interested scientists with knowledge of solid-state physics/chemistry, quantum mechanics, some experience of running materials software

[If available, include or attach a list of names and email addresses of anyone who has already expressed interest in attending this tutorial or that the CHPC should specifically invite.]

Prerequisites: *(what previous knowledge or skills should the attendees have)*

Knowledge of solid-state physics/chemistry or materials modelling, use of HPC, have an account on CHPC

Type of workshop:	~~Lectures only / Hands-on~~ / Mix of lectures and Hands-on sessions
Special requirements: *(will the attendees need to bring a laptop; have access to the cluster, or specific software; etc.)*	If you want to run any of the exercises, then you will need to bring a laptop and have access to/an account on the CHPC platform. We are also happy for users without a laptop to attend the lectures and ask questions.

Timetable: Please provide an outline of full syllabus

Sunday (1 Dec 2024)

08:00	Registration
	Lectures on Modelling Materials
09:00	GULP: Introduction to modelling materials using IPs
09:30 10:00	CASTEP: Introduction to modelling materials using a planewave basis sets to describe the electronic structure. CP2K: Introduction to modelling materials using atomic centred Gaussian basis sets to describe the electronic structure, complemented by plane waves.
10:30	Morning Refreshment Break
11:00	Hands on session Exercises and assistance will be available so delegates can choose to either learn how to (a) use KLMC to automate GULP calculations for predicting atomic structures or (b) run electronic structure calculations using CP2K or CASTEP.
12:30	Lunch
	Lectures on Modelling Materials
13:30	Introduction to ChemShell ChemShell for materials modelling, including how to employ CP2K or CASTEP within the central region describing the active site or region of interest
15:00	Afternoon Refreshment Break
15:30	Hands on session Exercises and assistance will be available so delegates can choose to either learn how to (a) use ChemShell or they can continue earlier exercises, i.e. (b) use KLMC to automate GULP calculations for predicting atomic structures or (c) run electronic structure calculations using CP2K or CASTEP.
17:00	End of Day

For 90 minute workshop, only complete <u>one</u> session black; for a half-day workshop only fill in <u>two</u> session blocks. We cannot guarantee that your preferred session choice (morning or afternoon) will be available as we have to schedule the timetable according to available venues.

Additional Comments: