

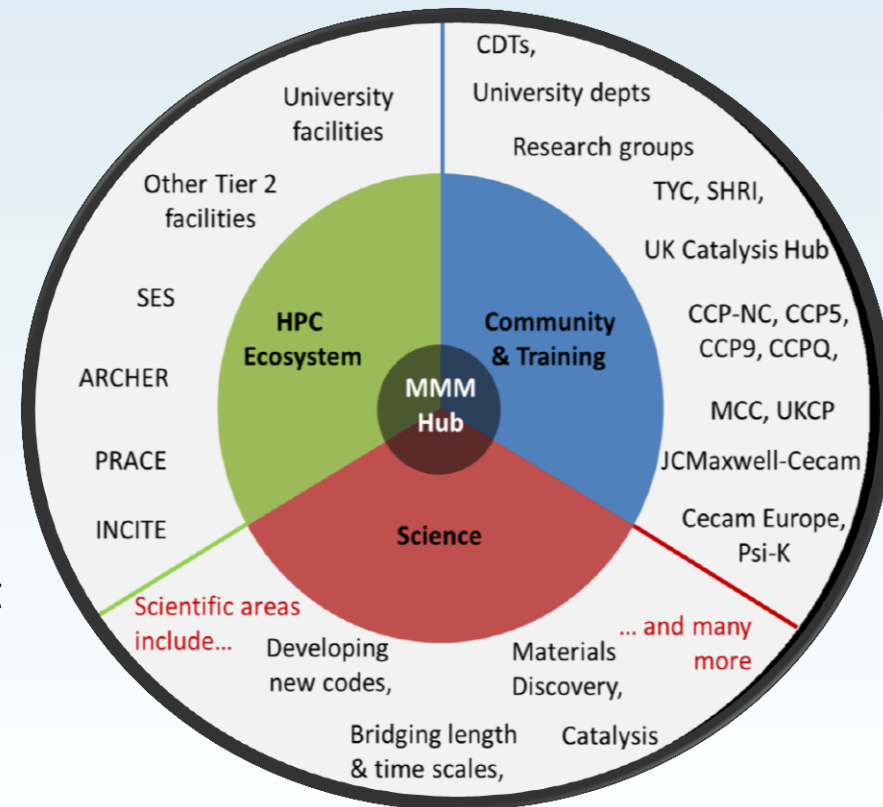
Tier 2 Hub in Materials and Molecular Modelling (MMM)

Service Overview

Dai Jenkins

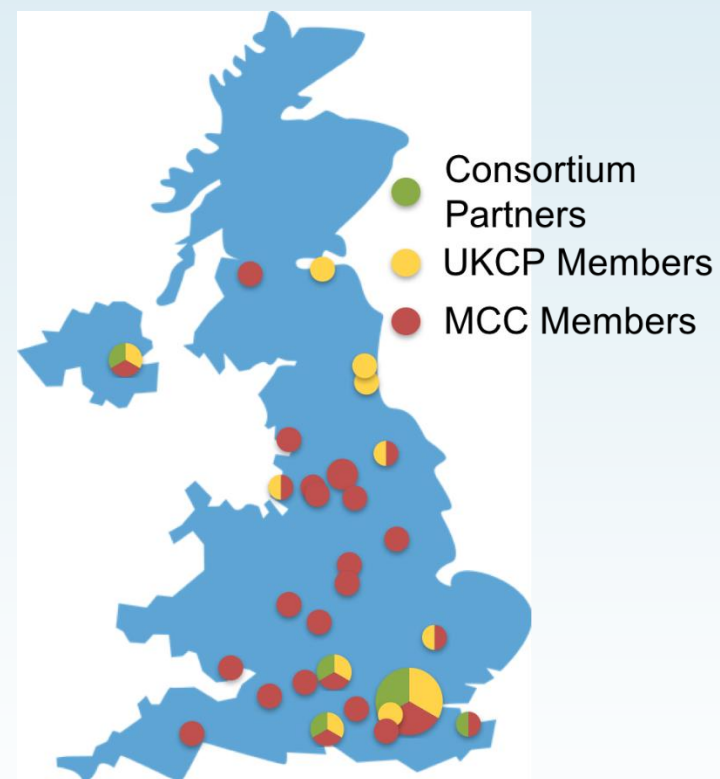
Rationale for a Tier 2 Hub in MMM

- Increasing growth in UK MMM research has created an unprecedented need for HPC, particularly for medium-sized, high-throughput simulations;
- These have been predominantly run on ARCHER (30% VASP), tier 3 sources are too constrained;
- The installation of “Thomas” aims to rebalance the ecosystem for the MMM community;
- It will create a UK-wide Hub for MMM that serves the entire UK MMM community.
- To build a community around the Hub to help foster collaborative research and the cross fertilisation of ideas.
- To provide support and software engineering training

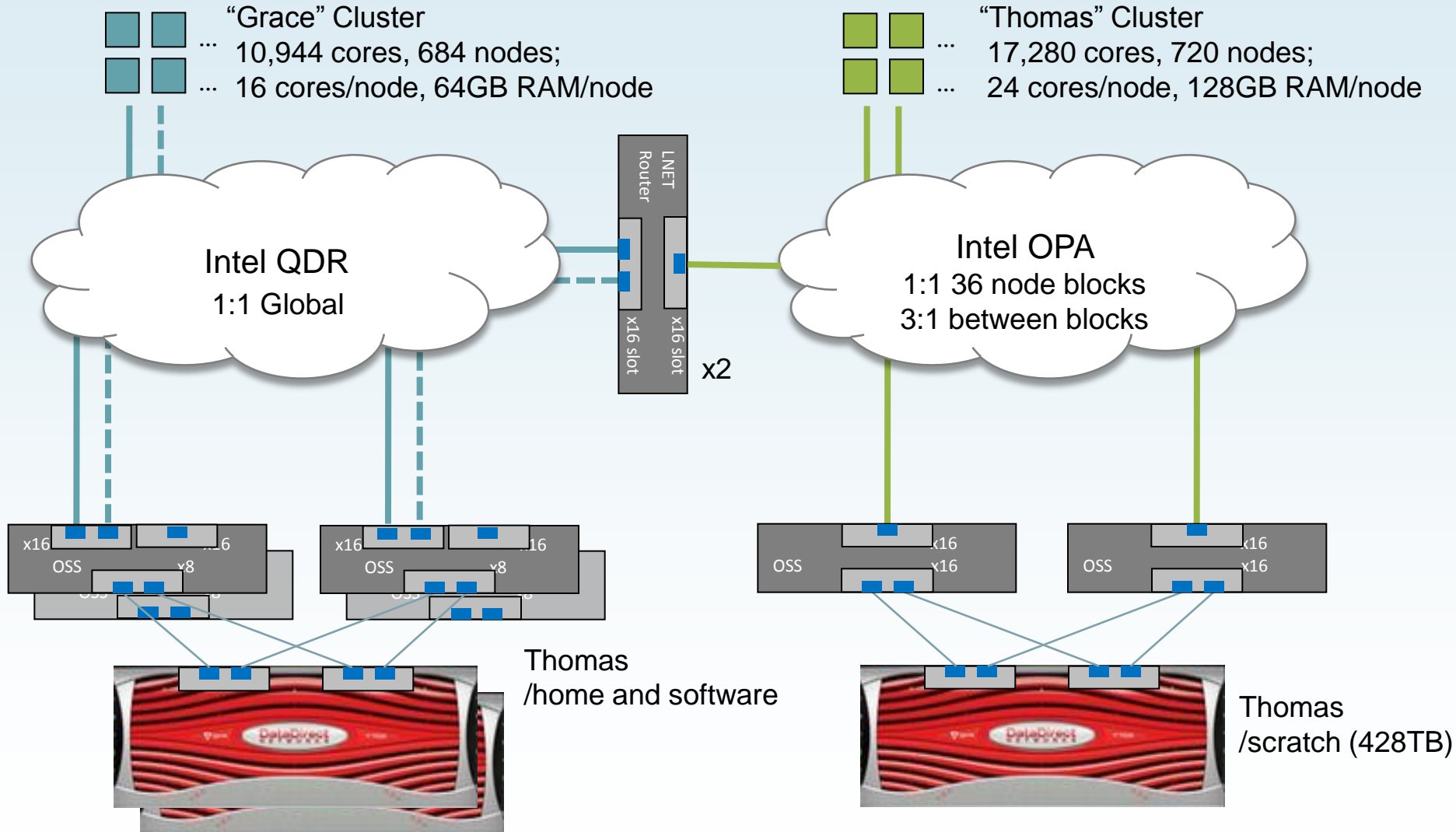


MMM Hub Partner Institutions

- Initial bid development driven by the Thomas Young Centre: *The London Centre for the Theory and Simulation of Materials*: **Imperial, King's, QMUL and UCL**
- During development of the full-bid the team expanded to include: **Belfast, Cambridge, Kent, Oxford, Southampton**
- Funding for operational and hosting costs will be derived from across the partners: **>£2m over initial term**
- **UCL** will provide support and host at the Virtus DC (Slough);
- **OCF-Lenovo** contributing to coordinator post;
- National MMM-HPC Consortia: Materials Chemistry Consortium and UKCP

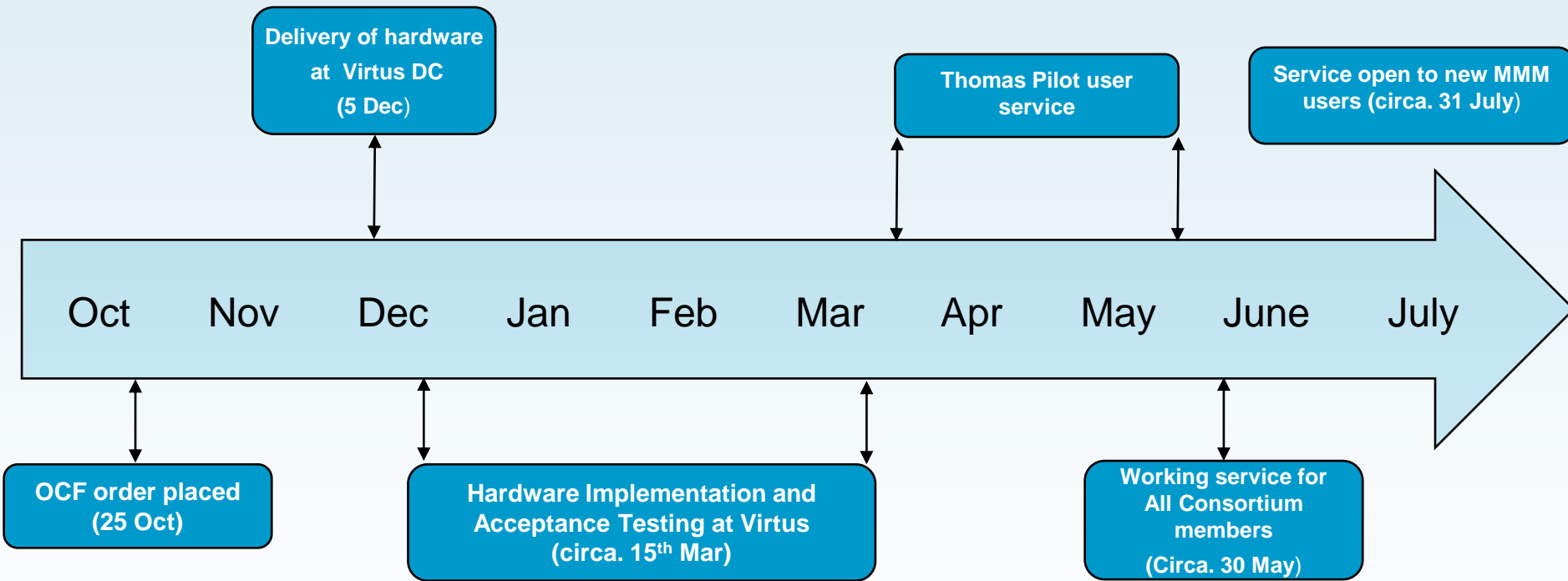


“Thomas” System Overview



External access to Thomas routed via “Bastion” nodes to Login nodes, UCL users route directly to Login nodes via campus network

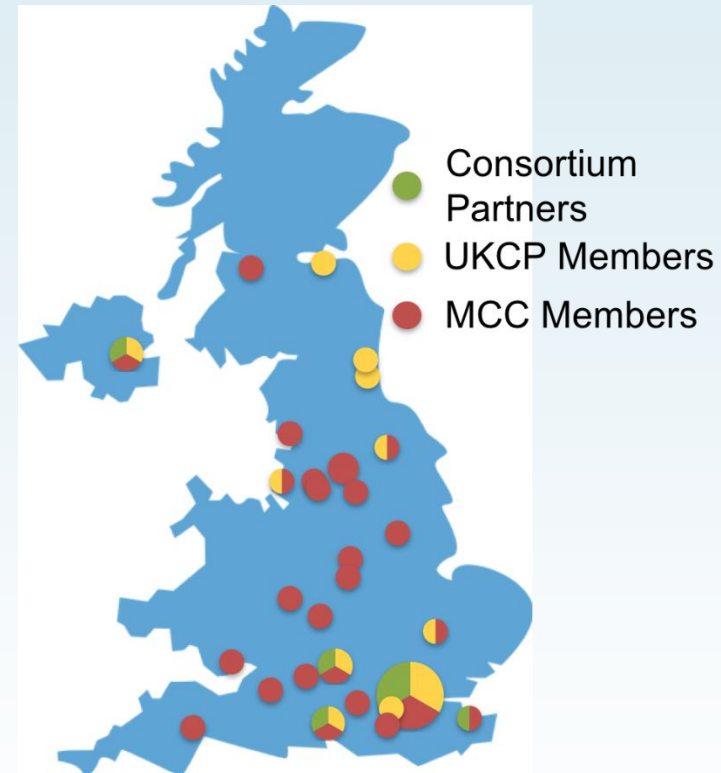
Timeline for delivery of Thomas Service



All hardware has now been delivered, sited, cabled with nodes ready to be discovered and imaged prior to acceptance.

Access and sharing

- Access models/mechanisms being finalised, overall:
 - 75% of machine cycles will be made available to the university partners providing funding for Thomas' hosting and operations costs;
 - 25% of Thomas' cycles will be made available to the wider UK MMM Community;
 - Allocations to non-partner researchers and groups across the UK will be handled via existing consortia (MCC, UKCP...);
 - Tier 2 – 1 integration via SAFE...committed to development, watch this space!



Thank You for listening!
Questions?