CCP for NMR Crystallography

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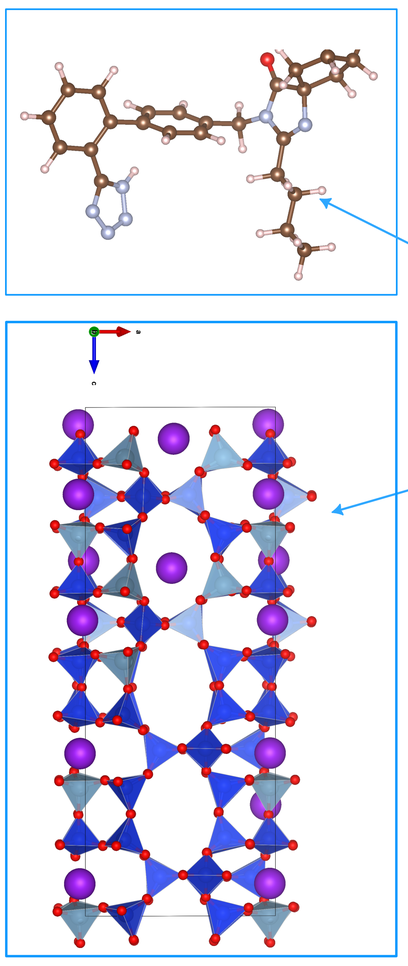
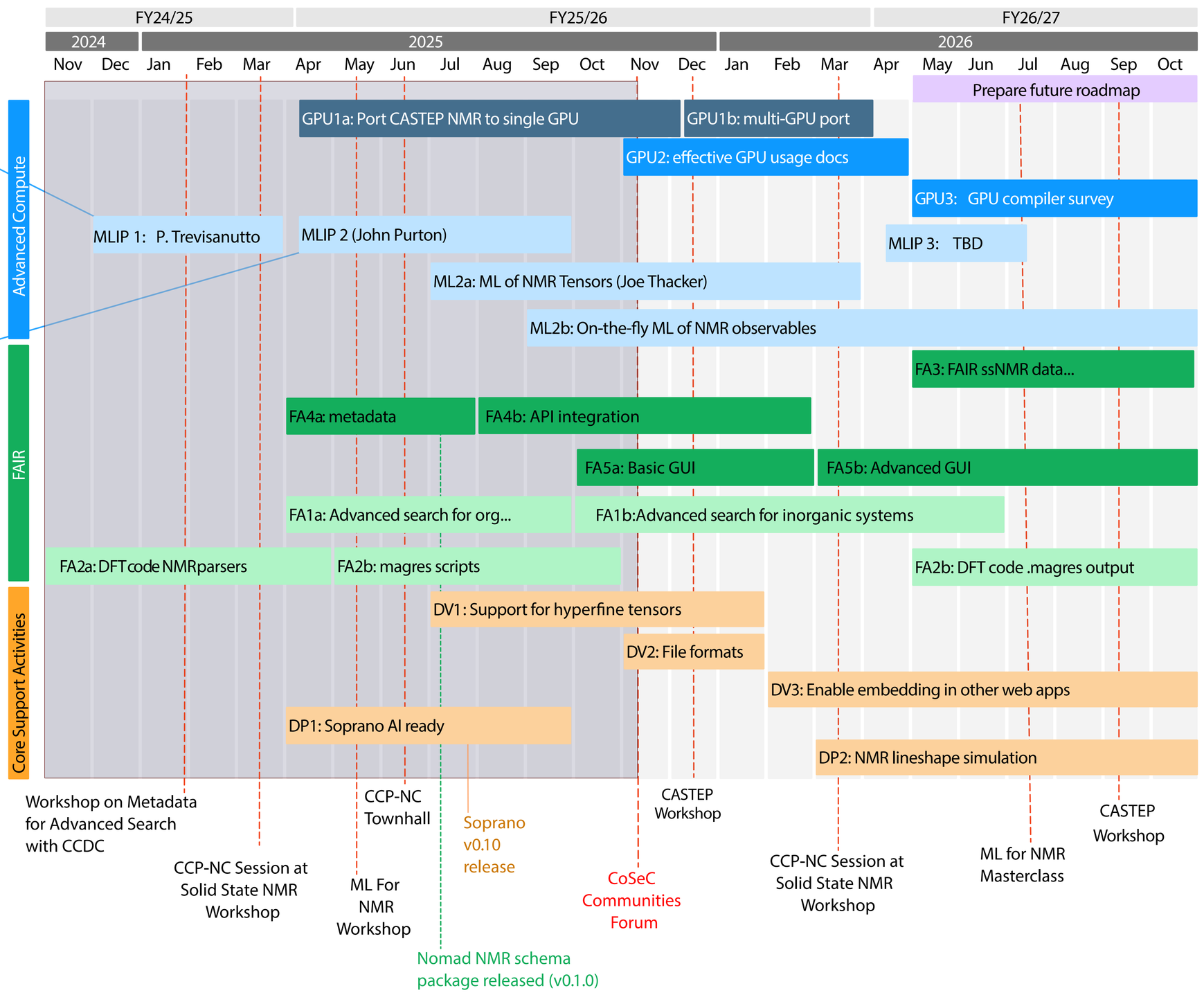
Computational Science Centre for Research Communities



MagresView 2 visualisation of the Euler angle between the backbone amide shielding tensor and the NH bond vector in tripeptide Ala-Ala-Ala.



RSE/Postdoc (1 FTE)

GPU CoSeC staff (0.2 FTE)

ML CoSeC staff (0.4 FTE)

EPSRC-funded CoSeC (0.5 FTE)

FAIR CoSC staff (0.4 FTE)

EPSRC-funded CoSeC (0.8 FTE)

Accelerating CASTEP (NMR) with GPUs

CASTEP

- CASTEP is a widely-used `first-principles' materials modelling software package.
  - Uses Density Functional Theory to predict the properties of solid materials and molecular crystals.
  - Properties include relaxed structures and NMR spectra, with very close match to experiment.
- Widely used in the UK by NMR crystallography community for interpretation of experimental results.

CASTEP with GPUs

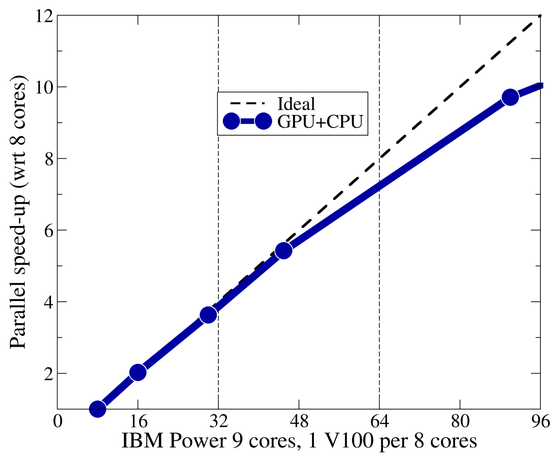
- Initial GPU port of CASTEP successfully released with version 26.
  - Targeted the single point energy calculation.
  - Used OpenACC programming model (NVIDIA only).
  - Used optimised libraries for intensive compute.

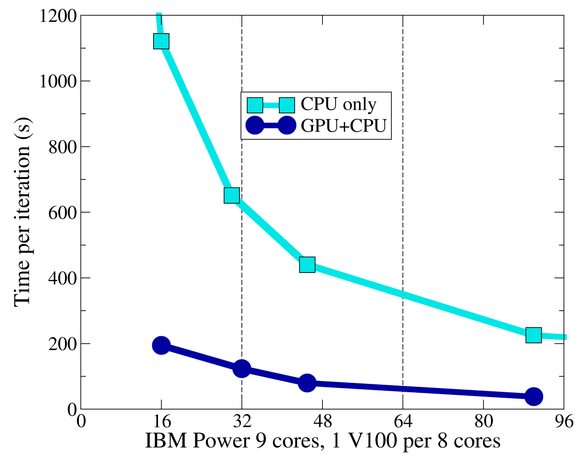
OpenACC

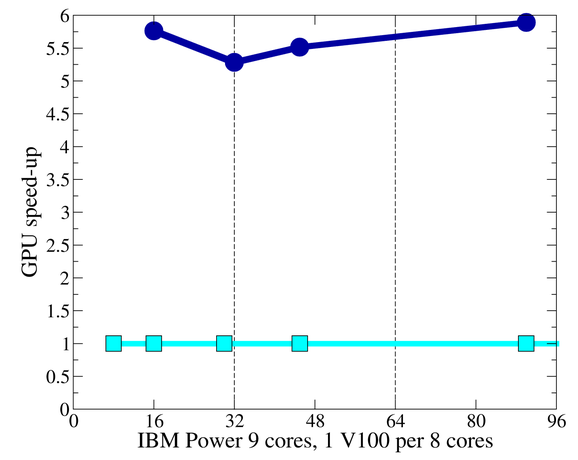
- Progress is being made on rewriting CASTEP GPU to use the OpenMP programming model.
  - Vendor agnostic, i.e. works with AMD GPUs.
  - Will support wider range of calculation types, including NMR.

OpenMP

CASTEP-GPU Performance







- Benchmark computes the ground state DFT energy of the Heusler alloy Fe_2VAl.
  - Uses OpenACC version of CASTEP.
- Run on the UK's Bede Tier-2 HPC facility's IBM Power 9 nodes:
  - 32-core IBM Power 9 CPU + 4 NVIDIA V100 GPUs.

Grace -Hopper Performance:
Bede has recently gained some Grace-Hopper GH200 nodes.
Initial benchmarking shows **10-fold speed up** with GPU.

CCP-NC Collaborative Computational Project for NMR Crystallography

Science and Technology Facilities Council
Scientific Computing