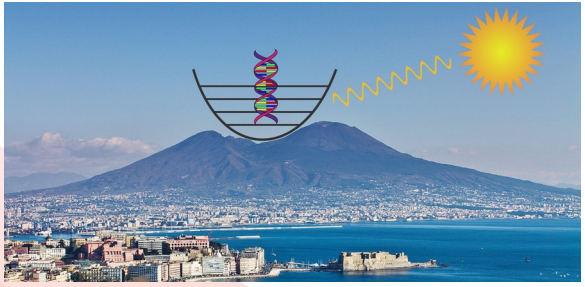
Reports from the UK on the status of FHI-aims

NOMAD Coffee Talk, 27 May 2024

James Green, MS1P e.V.

About Me

- Born in Manchester, UK
- 2010-2014 MChem at Durham University - method development in DFT
- 2014-2018 PhD University of Leeds. Method development in trajectory guided quantum dynamics.
- 2019-2022 Postdoc CNR-IBB Napoli. Method development in diabatisation. Excitonic and quantum dynamical modelling of DNA.
- 2022-2024 AvH postdoc Goethe University, Frankfurt. Quantum chemical & dynamical modelling of organic semiconductors, photovoltaics and photoswitches



About Manchester

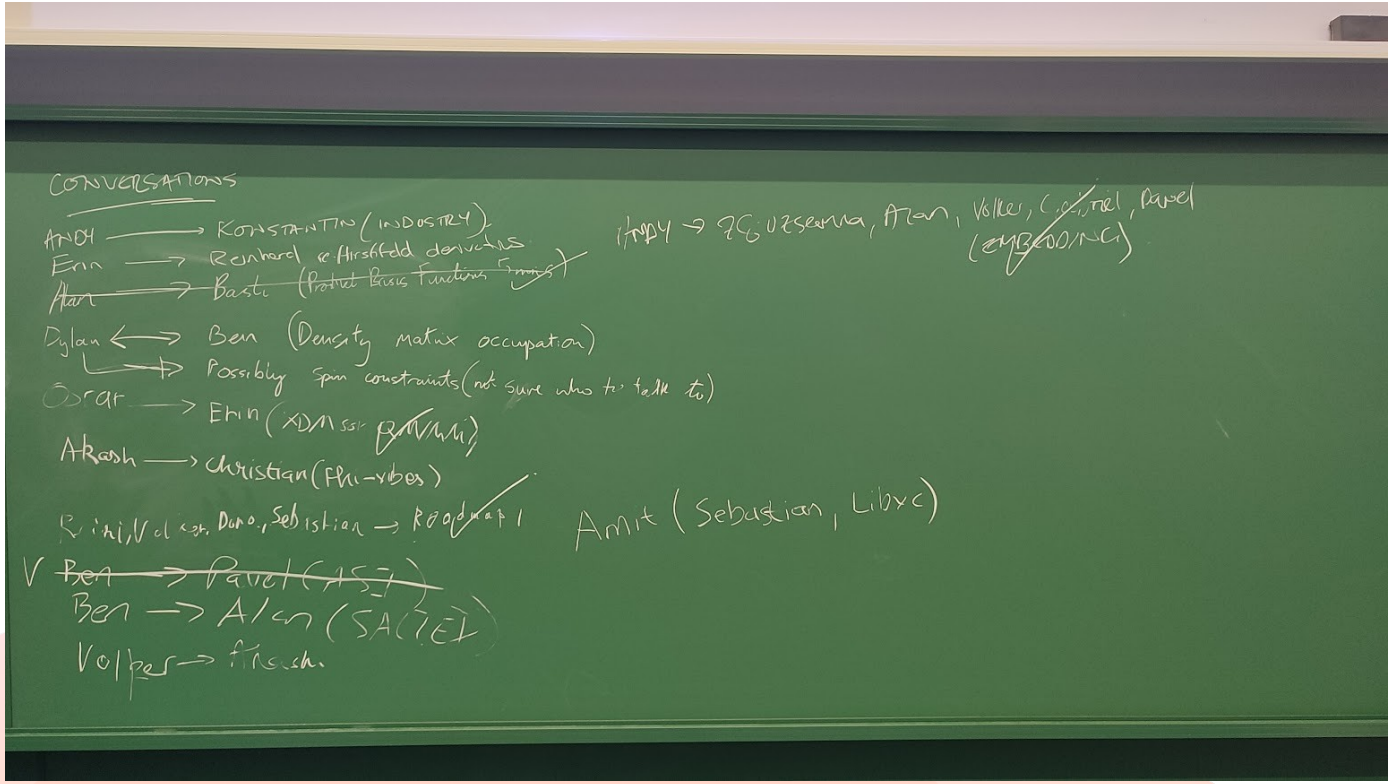
About MS1P

- Platform for the FHI-aims community:
  - Infrastructure – Gitlab, slack, website, tutorials
  - Maintaining social media - publication of new developments/papers
  - Organisation of workshops, conferences, seminars etc
  - Responsible for licensing
  - Support of scholarships
  - Aiding development and maintenance of code

If there is something not working in the code, or you want to implement something – speak to us!

Overview of UK Meeting

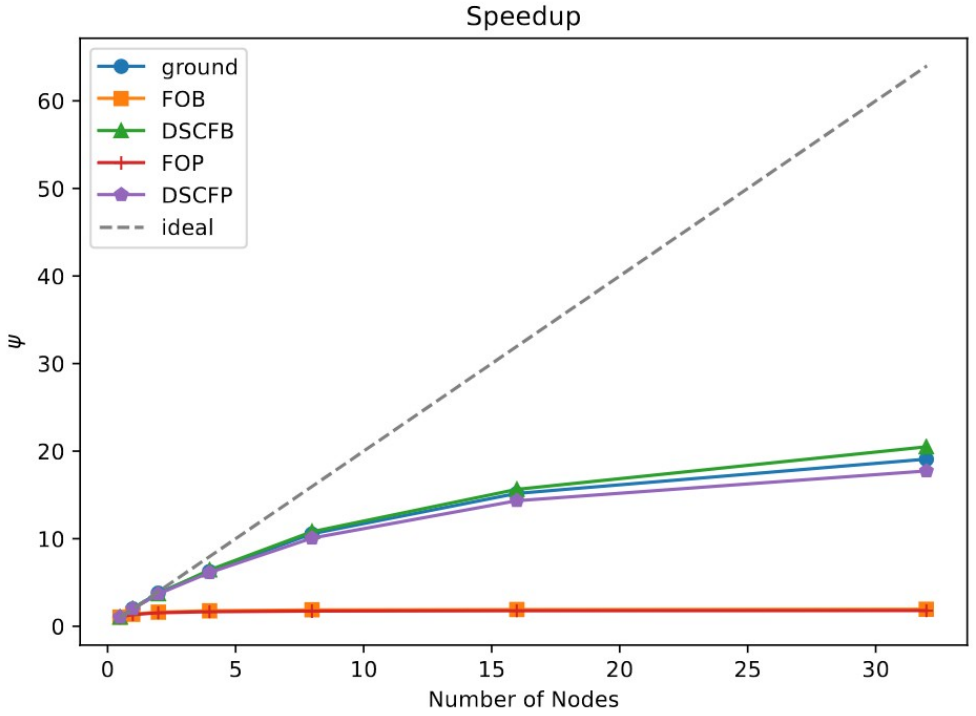
- Start: tutorials on hybrids + GW
- Talks and poster session
- “Hack” at the end – presentation of how to develop the FHI-aims code, discussion groups for specific implementation intentions
- UK community uses FHI-aims a lot for catalysis. Two main groups – Andrew Logsdail and Reinhard Maurer



ΔSCF speedup – Dylan Morgan University of Warwick

- Code refactored and 3000+ lines removed
- New keywords introduced `deltascf_projector` and `deltascf_basis` to be used instead of the old `force_occupation_basis` and `force_occupation_projector`
- Much better scaling and availability now (FOB+FOP old, vs DS(CF)B and DS(CF)P new)
- Tutorial on core-hole spectroscopy

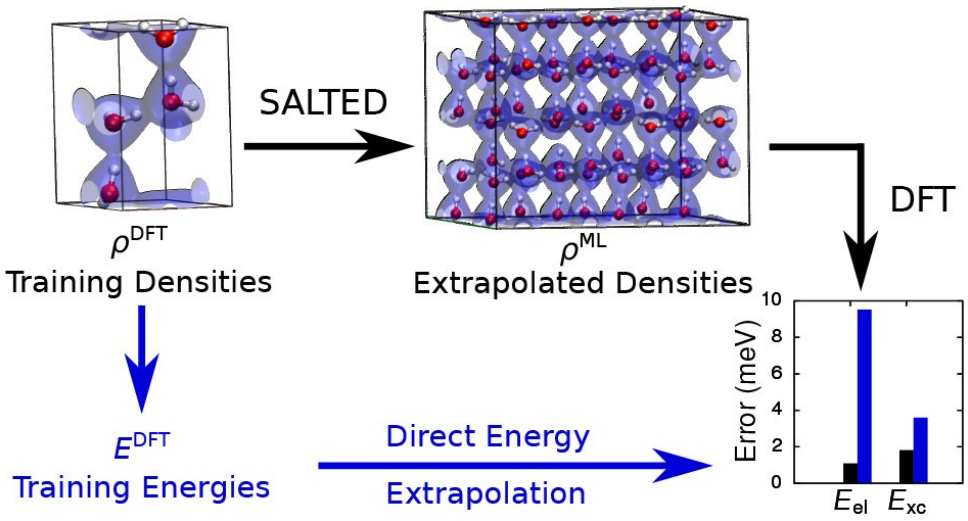
Structure	KS Method	FOP	FOB	DSP	DSB
Aperiodic	serial	✓	✓	✓	✓
	parallel	✗	✗	✓	✓
Periodic	serial	✓	✗	✓	✗
	parallel	✗	✗	✗	✗



ARCHER2-eCSE04-3, elativistic all-electron orbital-constrained Density Functional Theory to simulate x-ray photoemission and absorption spectroscopy, S. J. Hall, D. B. Morgan, and R. J. Maurer, 2023, https://doi.org/10.5281/zenodo.8247288

Symmetry-Adapted Learning of Three-Dimensional Electron Densities (SALTED) – Alan Lewis University of York

- Learning of electron densities in periodic systems with symmetry adapted Gaussian process regression
- Updated tutorial shows how to use SALTED:
  - How to use FHI-aims to generate data
  - How to generate descriptors and do regression
  - Use SALTED to make predictions



A. M. Lewis, et. al., J. Chem. Theory Comput. 2021, 17, 11, 7203–7214

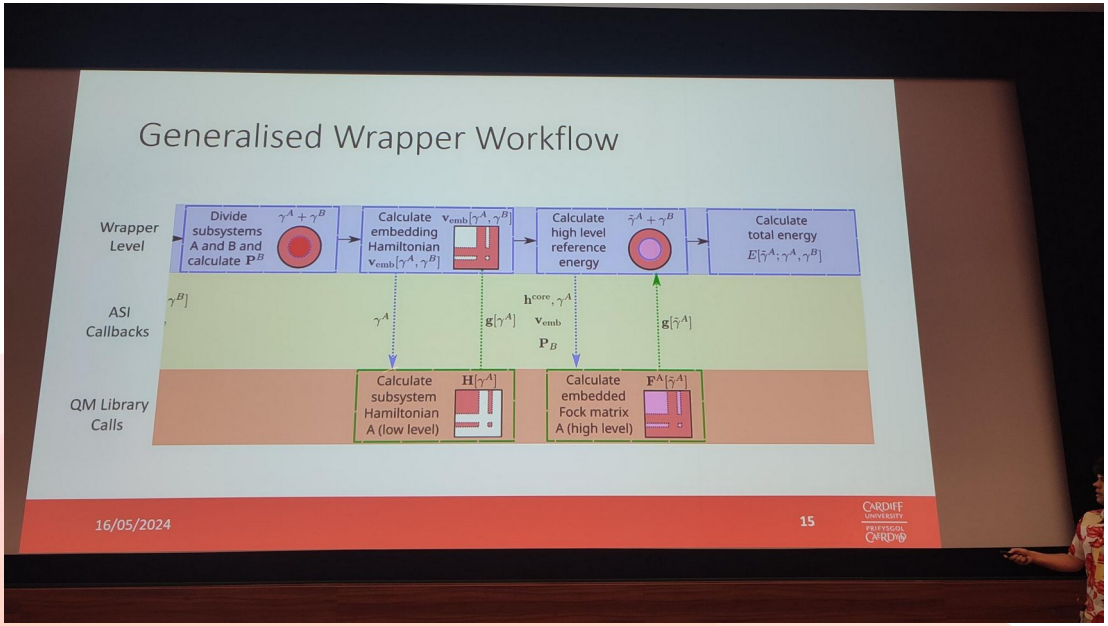
- **Electronic Structure Machine Learning with SALTED**

Symmetry-Adapted Learning of Three-Dimensional Electron Densities (SALTED) method 10.1021/acs.jctc.1c00576 is designed to predict electron densities in periodic systems using a locally and symmetry-adapted representation of the density field.

QM/QM Embedding – Gabriel Bramley
Cardiff University

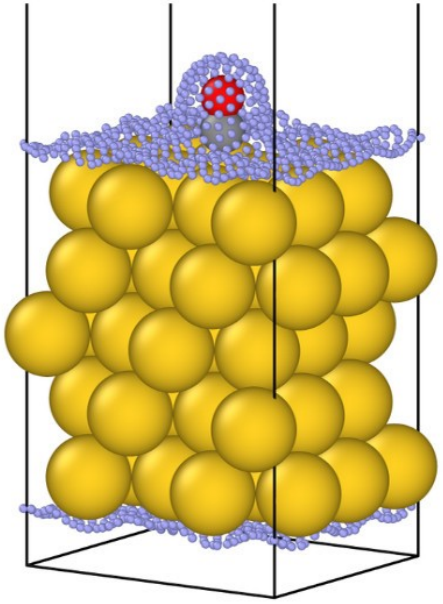
- Compute some important part with a more expensive scheme (e.g. hybrid, GW), and the rest with lower cost scheme (e.g. GGA)

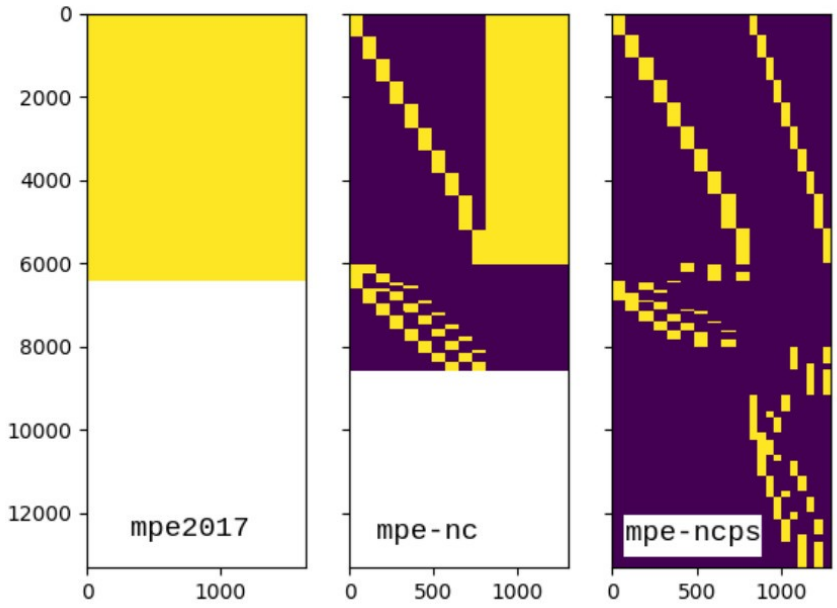
- Use a wrapper, with atomic simulation interface calls
- Currently work in progress, QM/MM has already been implemented with ChemShell



Multipolar expansion model of implicit solvent for periodic systems and clusters – Pavel Stishenko Cardiff University

- New MPE implementation with solute subcavities and piecewise solvent to increase sparsity of matrix and make solution more numerically efficient





ARCHER2-eCSE08-3, Improvements in periodic representation of solvated systems with FHI-aims, P. V. Stishekno, J. Filser, G. Bramley, R. Maurer, V. Blum, H. Oberhofer, A. Logsdail 2024, https://doi.org/10.5281/zenodo.10589628

- Periodic boundary conditions now supported for MPE model

Implementation, benchmarking, and applications of the XDM dispersion model in FHI-aims – Erin Johnson Dalhousie University

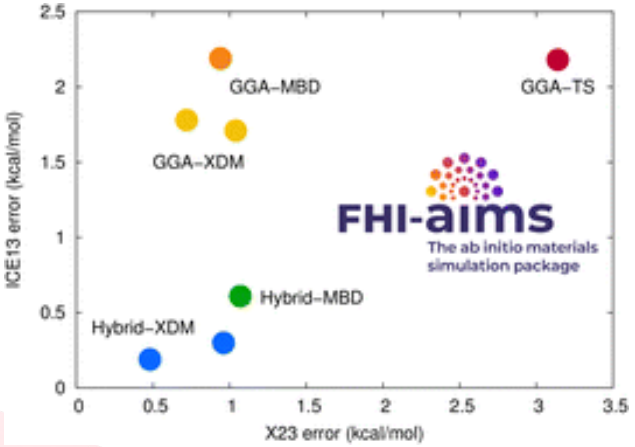
- Developments of XDM in the last months have lead to increased efficiency

- Highly accurate benchmarks e.g. the X23 set of molecular crystal energies and ICE13 set of ice phases

- Some wishlist items for future development:

  - Hirshfeld weight derivatives for improved XDM forces and stresses
  - Exact exchange-energy density at all grid points for local hybrid functionals and B05-type real-space correlation functionals

$$\varepsilon_{X\sigma}^{\text{exact}}(\mathbf{r}_1) = -\frac{1}{2}\phi_{i\sigma}(\mathbf{r}_1)\phi_{j\sigma}(\mathbf{r}_1)\int \frac{1}{r_{12}}\phi_{j\sigma}(\mathbf{r}_2)\phi_{i\sigma}(\mathbf{r}_2)\,d\mathbf{r}_2$$



A. J. A. Price, A. Otero-de-la-Roza and E. R. Johnson, Chem. Sci., 2023, 14, 1252-1262

Things that would be good to implement

- Issue item with requests opened: https://aims-git.rz-berlin.mpg.de/aims/FHIaims/-/issues/549
- Create estimations for hybrid calculations and the needed resources (During runtime or prior?)
- Integrate more generalized k-grid generation
- Allow for spin constraints on atoms (important for difficult to converge systems)
- Functionality of constraining magnetism within SCF – VASP has this https://www.vasp.at/wiki/index.php/I_CONSTRAINED_M
- Density extrapolation for geometry optimisations
- Implementation of correct Ewald summation for MPE solvent

Future meetings in the UK?

- Try to involve more people in FHI-aims beyond the groups of A. Logsdail and R. Maurer
- What format should future meetings have? Best way to organise in future?
- Hack was successful, combine with tutorial in future meeting? Have longer introduction to gitlab to support new developers?

Thank you for listening!