Introduction to CP2K:

a first principles electronic structure simulation package

L. Tong[1], M. Watkins[2], I. Bethune[3] and L. Kantorovich[1]

[1] Department of Physics, Kiing's College London, United Kingdom
[2] Department of Physics and Astronomy, University College London, United Kingdom
[3] EPCC, University of Edinburgh, United Kingdom

www.cp2k.org

A first principles simulation package for atomic structures

A wide variety of models Hamiltonians

- DFT (GGA, PBE, vdW, Hybrid)
- MP2, RPA
- Semi-Empirical (DFTB)
- Classical Force Fields (FIST)
- Combinations (QM/MM)

Swiss Army Knife of molecular simulation

- Geometry and cell optimisation
- Molecular Dynamics (NVE, NVT, NPT, Langevin)
- Simulating STM image
- Sampling energy surface (Metadynamics)
- Finding transition state (Nudged Elastic Band)
- Path Integral Molecular Dynamics
- Kinetic Monte Carlo

Fast and accurate DFT solver

- Gaussian basis functions
  - Small and sparse matrices
  - Multi-grids for Gaussians of different width
- Plane waves for electron densities
  - FFT for electrostatics
- Orbital Transform method for direct energy minimisation
  - Avoids expensive diagonalisation
  - Guaranteed to find the minimum
- Standard Diagonalisation
  - Needed for solving metallic systems
  - Significant speed up for large systems using **Filter Matrix Algorithm** [2]

Figure 3: Periodic electronic structure code usage across systems as a function of % core hours used.

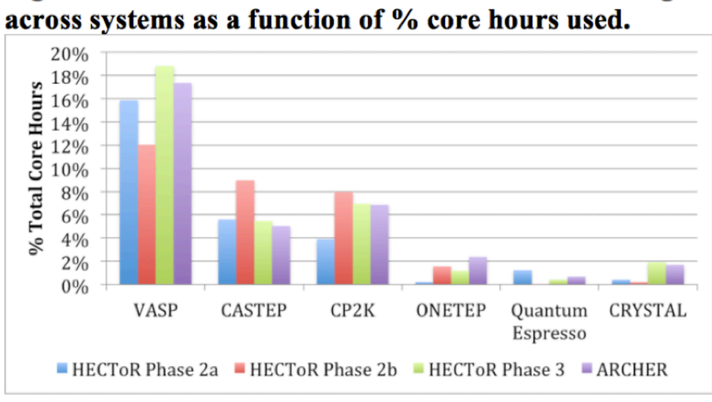


Table 5: Median job sizes (in cores) for periodic electronic structure codes on each of the systems.

	HECToR Phase 2a	HECToR Phase 2b	HECToR Phase 3	ARCHER
VASP	240	456	480	240
CASTEP	252	720	512	360
CP2K	224	1320	608	672
ONETEP	104	504	416	864
Quantum Espresso	60	72	448	192
CRYSTAL	144	4032	3648	2808

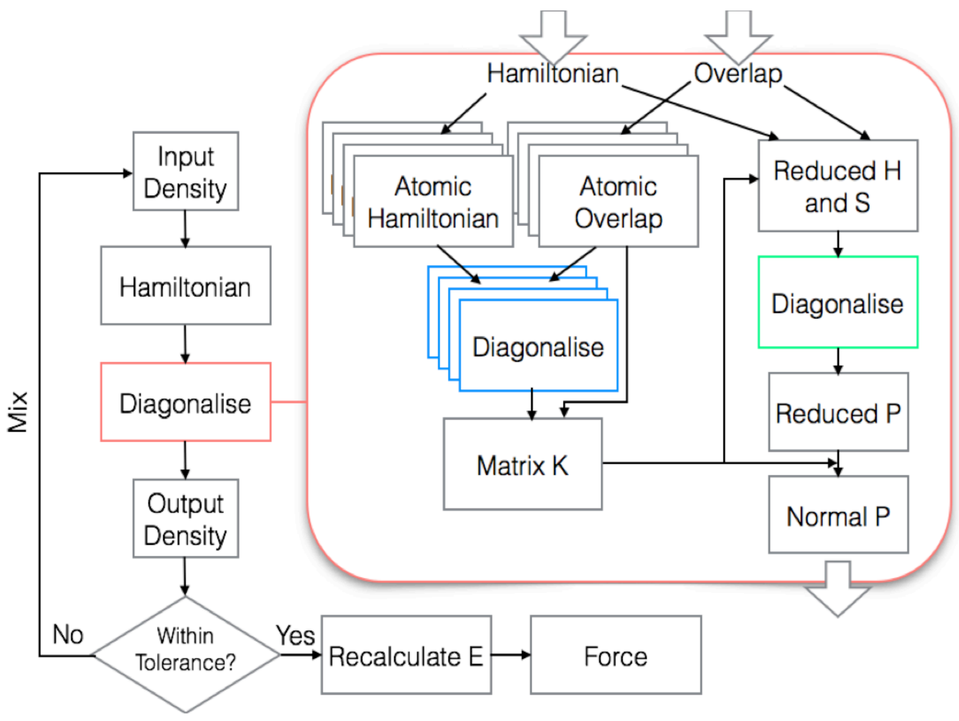
Large user base and active development

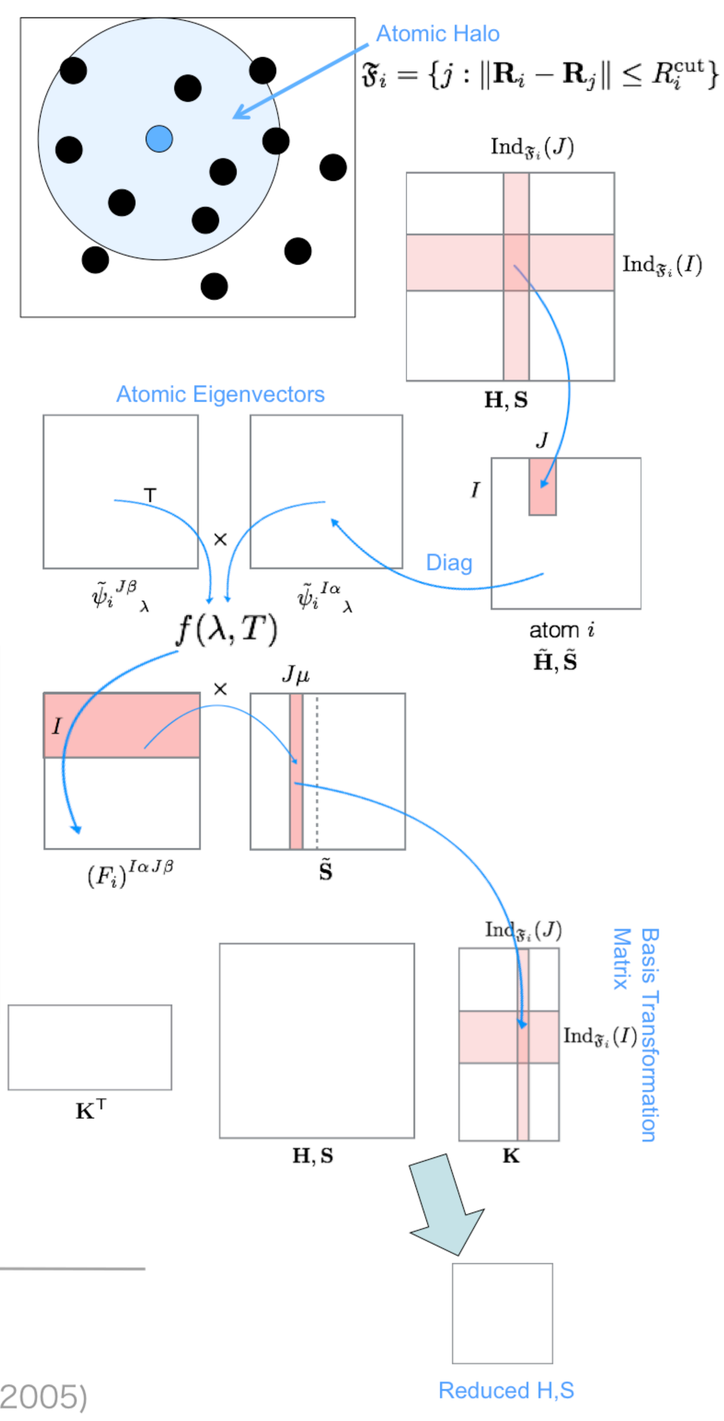
- Second most used electronic structure code on UK's national HPC service HECToR (phase 3), as well as the new ARCHER [3]
- Usage has continued to increase as ARCHER replaced HECToR [3]
- Median job size used CP2K on ARCHER is almost double that of the major planewave codes. [3]
- Over 1 million lines of code, daily commits

Filter Matrix Algorithm: General Idea

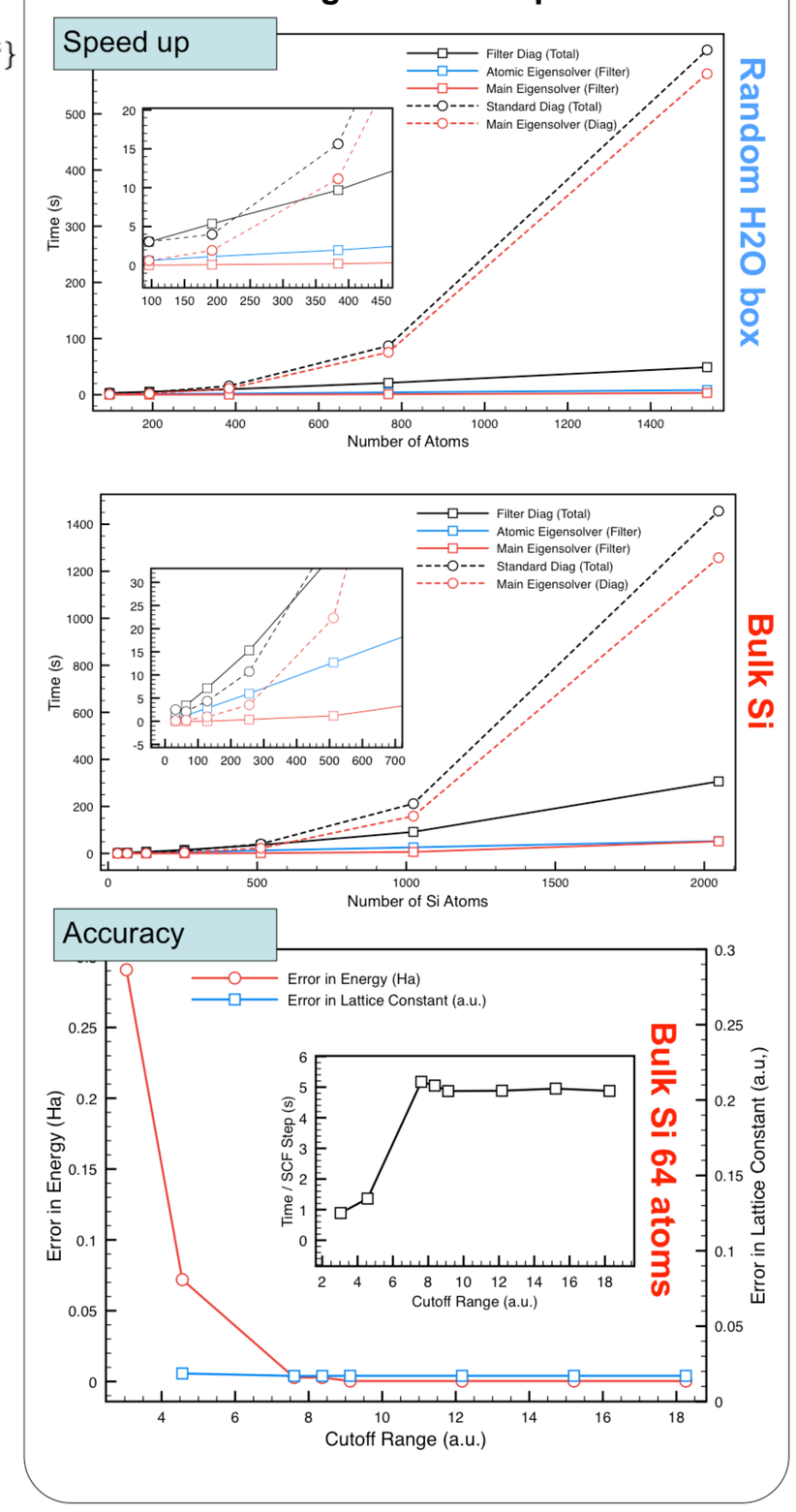
- Dynamically reduce the basis set for each atom, size matters!
  - Optimised minimal basis for each atom
  - Takes into account the electronic structure and interaction with neighbouring atoms
- Consider sub-problems involving an atom and its neighbours in the system
  - Use sub matrices of the density matrix corresponding to each atom and its interacting neighbours as a projector to map a normal basis function into the space spanned by the eigenvectors of the sub problem thus obtaining a new basis for each atom
- Because the new basis is in the eigenspace, we can take much fewer number of them to accurately describe ground state

Overall Scheme of Implementation





Filter matrix diagonalisation performance



References

[1] J. VandeVondele, et al., Comput. Phys. Commun. 167, 103 (2005)

[2] Rayson and Briddon, Phys. Rev. B 80, 205104 (2009)

[3] A, Turner, https://www.archer.ac.uk/documentation/white-papers/app-usage/UKParallelApplications.pdf (2015)

This project is funded by EPSRC grant EP/K038222/1