Building ONETEP

Software design, development practices and capabilities

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University of Warwick

Preamble

Slides will soon be available online at
http://www.onetep.org/Main/Workshops

See slides online for bibliography

Outline for this talk

How we build ONETEP and how you can use it

1. Thoughts on scientific software development
   - What defines scientific software?
   - What is “good” scientific software?
2. ONETEP as a research tool
   - The motivating problem
   - Linear-scaling density functional theory
   - A tour of capabilities
3. ONETEP as a software package
   - Distribution, usage and governance
   - Design and supporting infrastructure
   - Software development practices

Scientific software

What defines scientific software?

Some common attributes of scientific software packages:

1. Motivated by needs of developers
   - Developers and users often overlap
2. Not developers' main "product"
   - A means to perform research
3. Continually developed, extended
   - Always a prototype, never finished
   - Nature of problem changes

These are some general characteristics I have observed: they are not unique to scientific software (e.g. Linux kernel), nor are they universal to all scientific software.

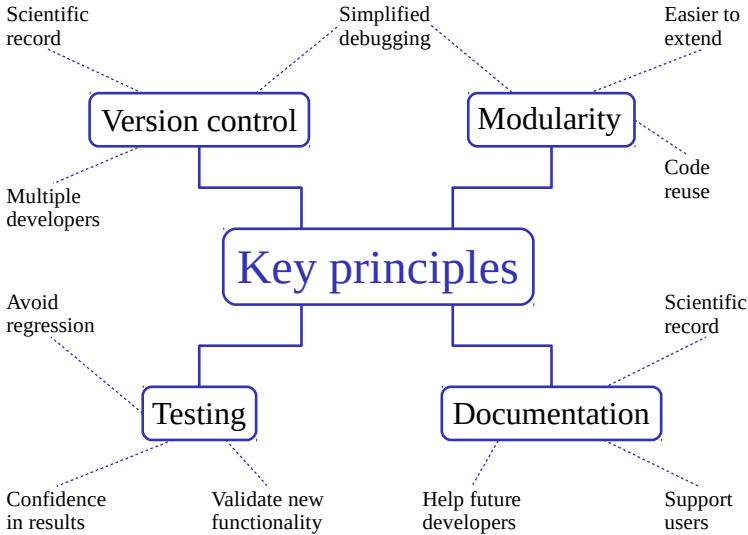
What defines scientific software?

Contrast this with software to control an ATM. . .

1. Designed for users, not developers
2. Software is developers' product
3. Clear, fixed specification

Image: "Nice ATM" by Flickr user Jason Cupp, used under CC BY 2.0

Scientific software: some key principles



Scientific software is scientific infrastructure

A scientific software package is similar to a large shared scientific facility:

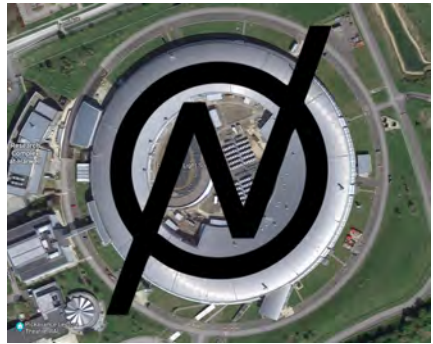
1. Designers (of experiments) are users
2. The product is research, not the instrument itself
3. New experiments add new capabilities

Image: Google Maps, Imagery (c)2018 Google, Map data (c)2018 Google

Scientific software is scientific infrastructure

Not just a metaphor. . .

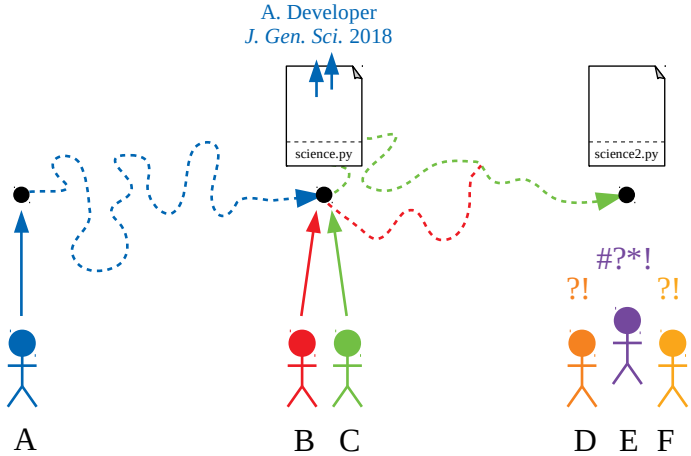
- Research tools for scientific communities
- Significant investment of human-time
- Requires maintenance and long-term planning
- Enables applications beyond those possible for any individual researcher or group



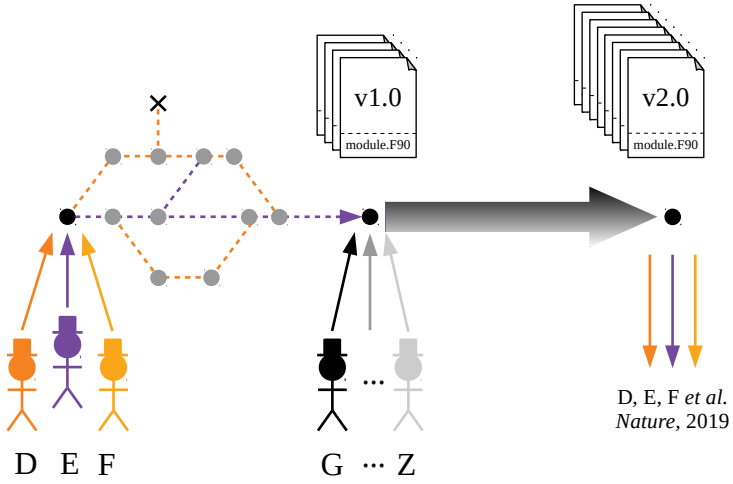
e.g. EPSRC's "Software as Infrastructure" strategy

Image: Google Maps [with logo overlaid], Imagery (c)2018 Google, Map data (c)2018 Google

Scientific software: the good, the bad and the ugly



Scientific software: the good, the bad and the ugly



Scientific software: the good, the bad and the ugly

- Be experimental, but then refine and clean up
- Plan development to avoid unmaintainable messes
- Well-written code is easier to extend and maintain

ONETEP as a research tool

Quantum chemistry

Time-independent electronic Schrödinger equation

$$\hat{H}\Psi = E\Psi$$

- Solutions provide information about properties of materials and molecules
- Intractable many-body problem for all but the smallest atomic system

Self-consistent field approach (SCF)

$$\hat{H}\psi_i = \varepsilon_i\psi_i$$

- Convert N-body problem into N more-tractable 1-body problems
- Electrons interact through a mean field which is self-consistently solved for

Density functional theory (DFT)

$$E[n] = T_s[n] + E_{es}[n] + E_{xc}[n]$$

- A popular and widely adopted SCF method
- Balances accuracy and computational expense
- Conventional DFT: $O(N^3)$ scaling

The $O(N^3)$ scaling of conventional DFT rapidly becomes problematic for > 1000 atoms. . .

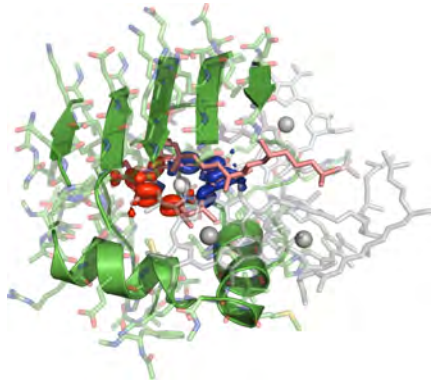


Image: Fig. 1 from D.J. Cole *et al.*, J. Phys. Chem. Lett. 4, 4206 (2013) [CC-BY-4.0 license] [1]

Linear-scaling DFT in ONETEP

Motivation: Practical quantum chemical methods for modelling large systems

Premise: Reformulate DFT to achieve $O(N)$ scaling

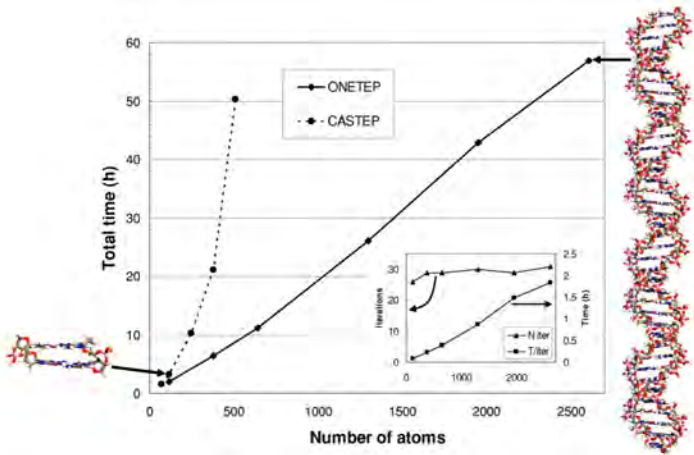
- Possible due to "nearsightedness" [2] of electronic interactions
- Locality of interactions manifested in the density matrix, $\rho(\mathbf{r}, \mathbf{r}')$
- ONETEP expresses DFT as a direct energy minimization wrt $\rho(\mathbf{r}, \mathbf{r}')$

$$E = \min_{\rho} E\left[\rho(\mathbf{r}, \mathbf{r}')\right]$$

Many interesting theoretical and computational techniques are used to implement this in practice [3, 4].

We will focus on the result...

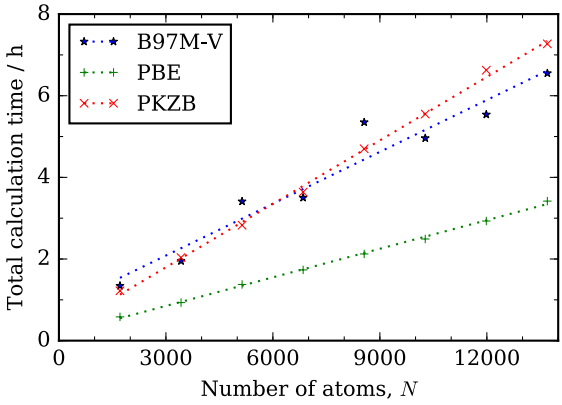
Linear-scaling DFT in action (2005)

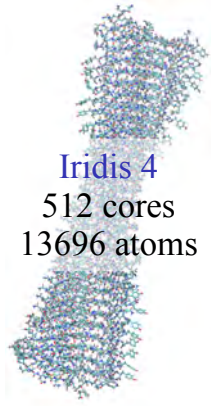


64 processors

2606 atoms

Linear-scaling DFT in action (2016)





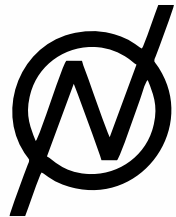
Iridis 4
512 cores
13696 atoms

A tool for researchers

ONETEP computes and analyses quantities relevant to physical scientists

- Many distinct capabilities
- All built upon LS-DFT framework
- See website for documentation

And now, a brief tour. . .



www.onetep.org

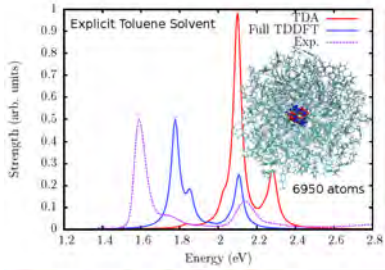
Linear-Response TDDFT

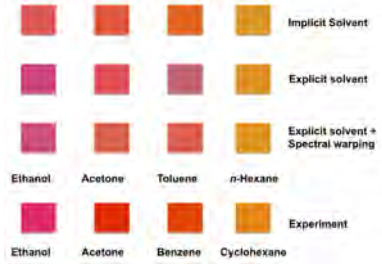
Capabilities:

- Calculate localised excitations and optical spectra
- Analysis of excitations via Quantified Natural Transition Orbitals
- Absorption spectra used to predict colours and exciton dynamics

People: Tim Zuehlsdorff, Jian-Hao Li, David Turban, Matt Turner, Peter Haynes, Nicholas Hine

References: 5, 6 (LR-TDDFT); 7 (QNTO); 8, 9 (colour prediction); 1, 10 (exciton dynamics)





Electron Energy Loss Spectroscopy

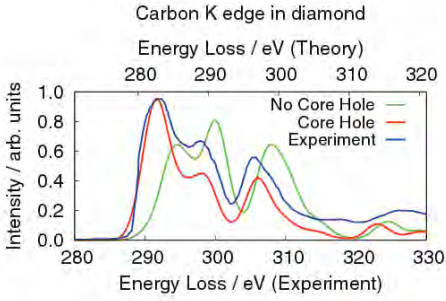
Capability: Predict spectra from EELS measurements

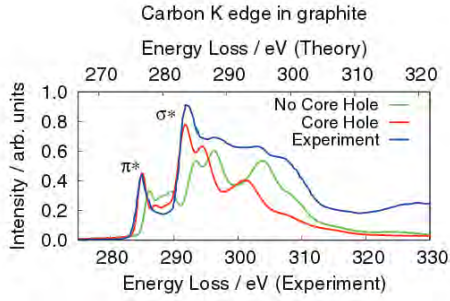
People: Edward Tait, Laura Ratcliff, Nicholas Hine

References: 11

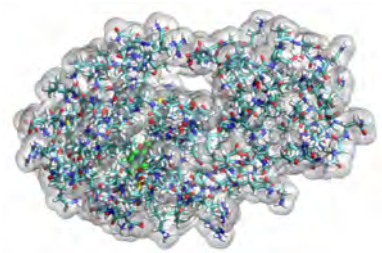
$$\epsilon_2(\omega) = \frac{1}{\Omega}\sum_c \sum_i |\mathbf{q}\cdot\langle\psi_i|\mathbf{r}|\psi_c\rangle|^2 \delta(E_i - E_c - \omega)$$

$$\langle\psi_i|\mathbf{r}|\psi_c\rangle = \langle\widetilde{\psi}_i|\mathbf{r}|\psi_c\rangle + \sum_{\nu} \langle\widetilde{\psi}_i|\widetilde{p}_\nu\rangle(\langle\varphi_\nu|\mathbf{r}|\psi_c\rangle - \langle\widetilde{\varphi}_\nu|\mathbf{r}|\psi_c\rangle)$$





Implicit solvent



Capability: Simulate molecules, nanostructures etc in a polarizable dielectric medium, calculate ΔG_{solv}

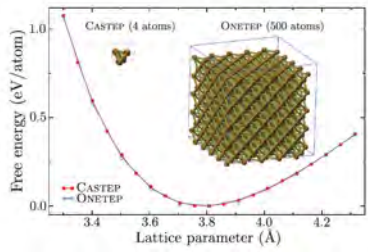
People: Jacek Dziedzic, James Womack, Arash Mostofi, Chris Skylaris

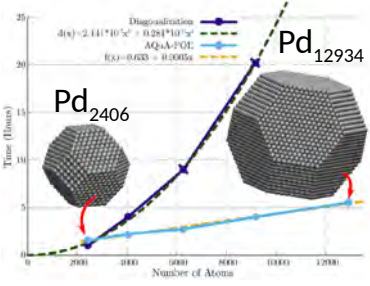
References: 12, 13, 14, 15

Coming soon: Solvation in solvent + ions (Poisson-Boltzmann model)

Metallic Systems

Capability: Treatment of large metallic systems, e.g. metallic nanoparticles, using ensemble DFT (EDFT)





People: Jolyon Aarons, Alvaro Ruiz-Serrano, Chris Skylaris

References: 16, 17, 18; 19 (AQuA-FOE)

New linear-scaling method:
"Annealing and QUenching Algorithm FOE"

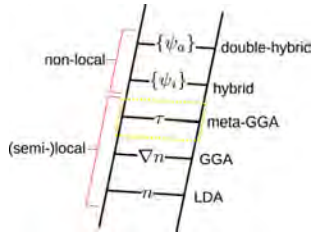
Advanced exchange-correlation models

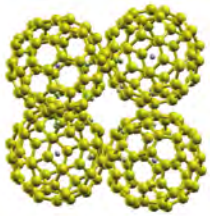
Capability: Functionals with orbital dependence via exact exchange (e.g. B3LYP) or τ (e.g. B97M-rV)

People: Jacek Dziedzic, James Womack, Chris Skylaris

References: 25 (hybrids) 26 (meta-GGAs)

Coming soon: Greatly reduced computational cost!





Capability: Fully non-local van der Waals density functionals, e.g. VDW-DF1/-DF2, VV10

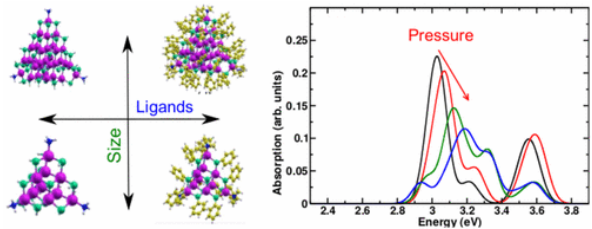
People: Lampros Andrinopoulos, Gabriel Constantinescu, Fabiano Corsetti, Nicholas Hine, Arash Mostofi

References: 20; used in 21

$$E_c^{\mathrm{nl}} = \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\rho(\mathbf{r})\phi(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}') \Rightarrow E_c^{\mathrm{nl}} = \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\rho(\mathbf{r})\phi(q,q',r)\rho(\mathbf{r}')$$

External Pressure

Capability: Simulated systems under external pressure, via enthalpy method



People: Niccolo Corsini, Nicholas Hine, Peter Haynes

References: 22, 23, 23

Projector Augmented Wave

Capability: Use PAW treatment of core electrons rather than norm-conserving pseudos

People: Nicholas Hine

References: 24; used in 21

Effectively an all-electron treatment.
Enables accurate calculations on high-Z elements & transition metals.

Molecular Dynamics

Capability: Perform dynamics on large systems, with density matrix extrapolation

People: Valerio Vitale, Simon Dubois, Chris Skylaris

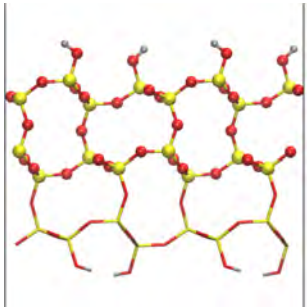
References: 27, 28

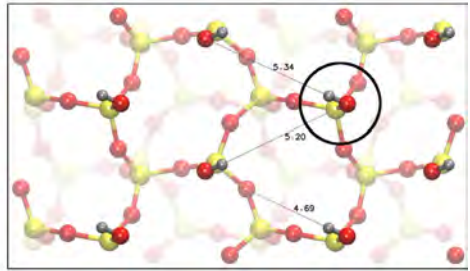
$$1: \quad \mathbf{v}' = \mathbf{v}_n + \frac{\Delta t}{2m} * \mathbf{F}_n \tag{2}$$

$$2: \quad \mathbf{r}_{n+1} = \mathbf{r}_n + \Delta t * \mathbf{v}' \tag{3}$$

$$3: \quad \text{Compute ionic forces } \mathbf{F}_{n+1} \tag{4}$$

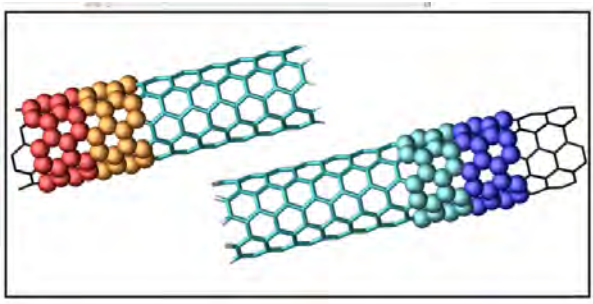
$$4: \quad \mathbf{v}_{n+1} = \mathbf{v}' + \frac{\Delta t}{2m} * \mathbf{F}_{n+1} \tag{5}$$

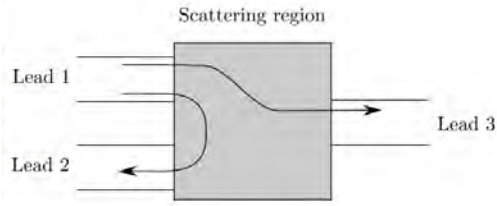




Transport

Capability: Compute electronic transport for multi-lead devices on a large scale



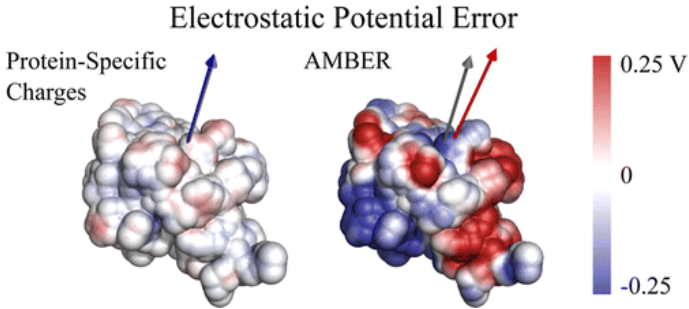


People: Simon Dubois, Rob Bell, Arash Mostofi

References: 29

Population Analysis & Energy Decomposition

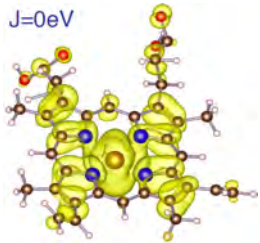
Capability: Natural Population Analysis, Hirschfeld, DDEC, etc, for forcefield fitting and electrostatics



People: Louis Lee, Danny Cole, Max Phipps, Chris Skylaris

References: 30, 31, 32, 33, 34

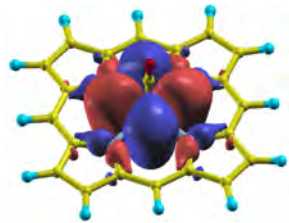
Strong Correlations



Capability:
DFT+U (penalise non-integer occupations); Dynamical Mean Field Theory

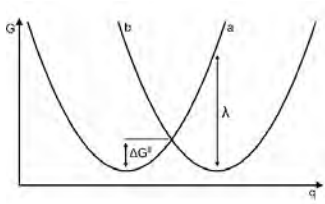
People:
David O'Regan, Cedric Weber, Nicholas Hine, Arash Mostofi

References:
35, 36, 37, 38, 39, 40



Constrained DFT

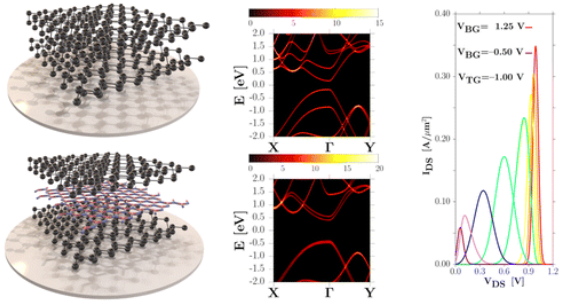
Capability: Constrain populations & spins of certain regions of a system (e.g. for studying charge transfer reactions)



People: Gilberto Teobaldi, David O'Regan, David Turban, Nicholas Hine

References: 41, 42

Spectral Function Projection



Capability: Perform supercell calculation, project result onto primitive bandstructure

People: Gabriel Constantinescu, Nicholas Hine

References: 21, 43, 44

Phonons

Capability: Calculate vibrational frequencies, free energies, phonon modes etc, via a) finite-difference approach, b) linear-response methods

People:
Fabiano Corsetti, Gabriel Constantinescu

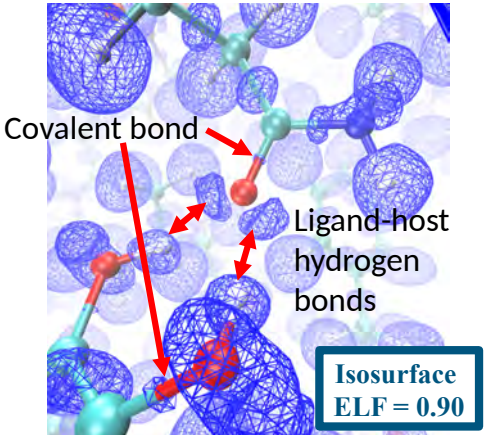
References: 45

$$E^{\mathrm{tot}} = E^{\mathrm{eq}} + \frac{1}{2} \sum_{a,\alpha,\kappa,a',\alpha',\kappa'} u_{a,\alpha,\kappa} \phi^{\alpha,\alpha'}_{\kappa,\kappa'}(a,a')\, u_{a',\alpha',\kappa'},$$

$$\phi^{\alpha,\alpha'}_{\kappa,\kappa'}(a,a') = \frac{\partial^2 E}{\partial u_{a,\alpha,\kappa} \partial u_{a',\alpha',\kappa'}}.$$

$$D^{\alpha,\alpha'}_{\kappa,\kappa'}(\mathbf{q}) = \frac{1}{\sqrt{M_\alpha M_{\alpha'}}} \sum_a \phi^{\alpha,\alpha'}_{\kappa,\kappa'}(a,0)\, \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R}_a},$$

New in v5.2: Electron localisation descriptors



Capability:
Visualisation of electron pair localisation, providing a quantum VSEPR-like representation for prediction of interactions

People:
Rebecca Clements, James Womack, Chris Skylaris

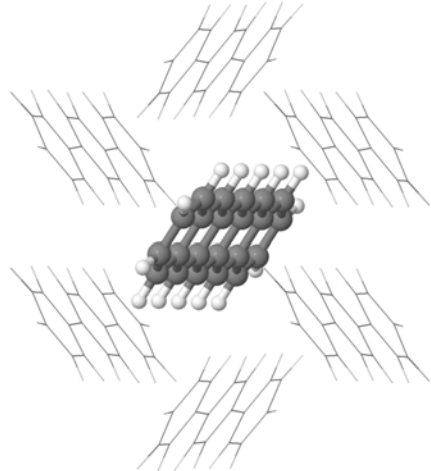
References:
Article in preparation

New in v5.2: Quantum embedding

Capability:
Embedded mean-field theory (EMFT) treats parts of a system with different levels of theory (e.g. hybrid + GGA), reducing cost whilst maintaining accuracy

People:
Joe Prentice, Rob Charlton, Peter Haynes, Arash Mostofi

References:
Article in preparation



ONETEP as a software package

Distribution and licensing

License	Cost	Usage
Collaborator	-	Individual, specific project Includes source
Academic	£500	Entire research group Includes source
Commercial	Purchase of Materials Studio	Non-academic users GUI interface

- All members of the CCP9 community are entitled to collaborator agreements.
- Daussault Systèmes BIOVIA Materials Studio packages ONETEP into a suite of materials science tools with a single GUI.

Usage

150
academic licenses
(individuals and groups)

20-30
academic collaborations
(PIs and groups)

Daussault Systèmes BIOVIA's products have
high market penetration
in top chemical companies
(pharma, oil, automotive, materials, etc.)

Data from ~2016–17

Developers

ONETEP Developer's Group (ODG)

Group of core developers who manage licensing, releases, relationship with BIOVIA:

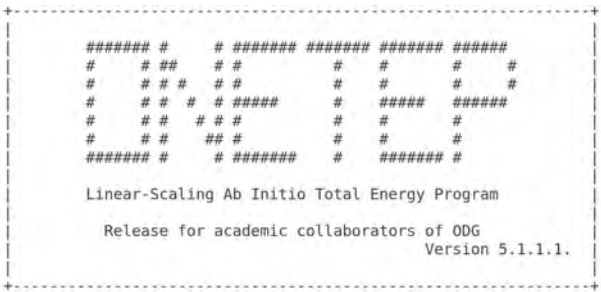
Jacek Dziedzic,[1,2] Peter D. Haynes,[3] Nicholas D. M. Hine,[4]
Arash A. Mostofi,[3] Mike C. Payne[5] and Chris-Kriton Skylaris[1]

1 University of Southampton, **2** Gdańsk University of Technology,
3 Imperial College London, **4** University of Warwick, **5** University of Cambridge

41
code contributors
(past and present)

37
active users of repository
(developers and expert users)

Source code



154
source files

450 000
lines of code

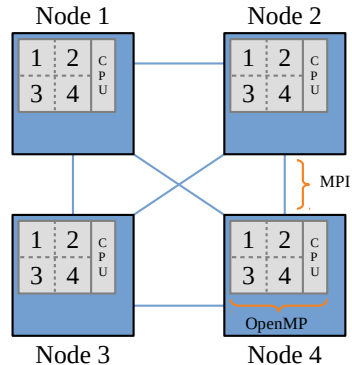
- Written in Fortran (2003 standard), built using GNU Make
- Bundled support utilities written in other languages (e.g. Bash scripts)
- Fortran modules used to encapsulate related procedures and data types

Parallelism

- Designed to run on parallel (super)computers
- Necessary for large-scale calculations
- Combined MPI [46] and OpenMP [47] parallelism.

MPI Work divided between processes which communicate by *message passing*

OpenMP Processes subdivided into threads, with *shared memory* access



Interaction with other software

Designed for Unix-like systems: Linux, Mac OS X (Windows via WSL)

Supporting software is required to build and run ONETEP:

Software/library	**Examples**
Fortran compiler (F2003, OpenMP)	Intel Fortran, GNU Fortran
MPI library	Intel MPI, OpenMPI
Linear algebra libraries	BLAS, LAPACK ScaLAPACK, Intel MKL
Fast Fourier transform (FFT) library	FFTW, FFTW3 Vendor-specific FFT libraries
Multigrid solver library	DL_MG

DL_MG

DL_MG [15] is an open-source Poisson solver library distributed with ONETEP

- Solves several variants of the Poisson equation in real-space:

$$\nabla \cdot (\varepsilon(\mathbf{r})\nabla\phi(\mathbf{r})) = -4\pi\,(n(\mathbf{r})+n_{\text{ions}}[\phi](\mathbf{r}))$$

- Designed for use in large scale electronic structure calculations
- Multigrid approach [48] scales well with problem size and converges rapidly
- Iterative high-order defect-correction reduces discretization error

Enables **open BC electrostatics** and **implicit solvent** functionality in ONETEP

Source code available at
www.dlmg.org

Hardware

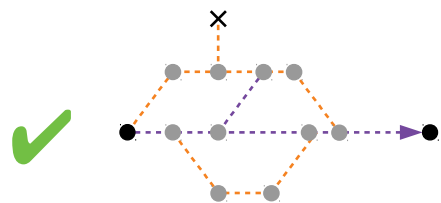
- ONETEP runs well on conventional CPU-based machines
- Scales to 1000s of cores [47]
- More cores and more memory per core are generally advantageous
- GPU-port is a work-in-progress [49]
- Can also run on desktops/laptops

Software development practices

How do we manage day-to-day development?

Follow the key principles:

1. Version control
2. Testing
3. Documentation
4. Modularity

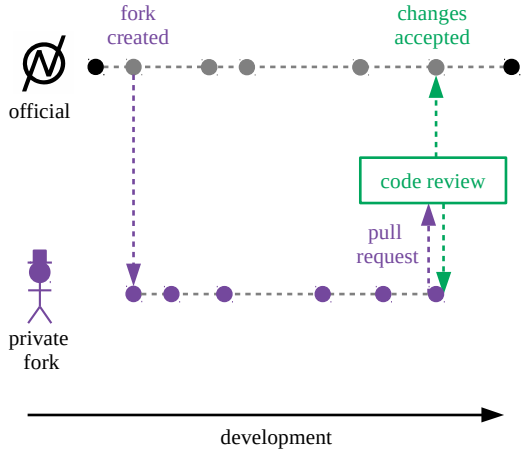


Version control

We have a Git repository hosted on Bitbucket and use a forking workflow:

- Single “official” server-side repository
- Private fork for each contributor
- Changes contributed via pull request
- Pull requests undergo review

New developers don’t need to worry about breaking the official repository!



Testing

We have a growing suite of regression tests:

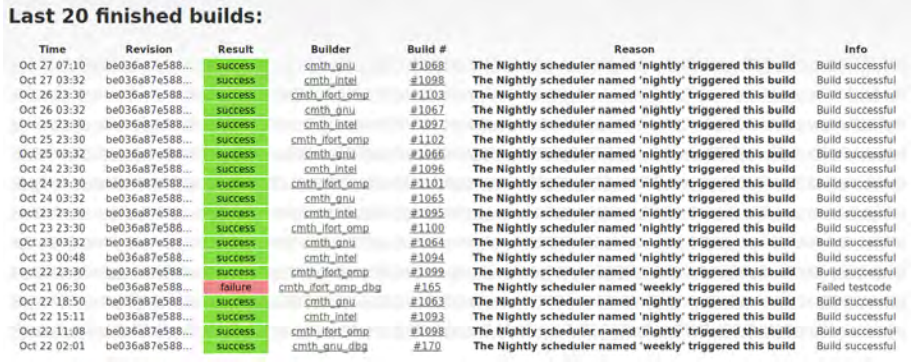
- When new functionality is added, require a new regression test (“QC” test)
- Each test runs a calculation to produce known results (benchmarks)
- QC test suite is run by a Python program called testcode
- A test fails if outputs are outside of allowed tolerance (wrt benchmarks)

The test suite allows new builds of ONETEP to be validated.

Testing

We use the Buildbot package to automate testing of the software:

- A Buildbot instance regularly pulls the official master branch and starts a build
- Each build includes compilation, code quality checks and QC test suite
- If any step fails, core developers are notified by e-mail



Last 20 finished builds:

Time	Revision	Result	Builder	Build #	Reason	Info
Oct 27 07:10	be036a87e588...	success	cmth_gnu	#1068	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 27 03:32	be036a87e588...	success	cmth_intel	#1098	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 26 23:30	be036a87e588...	success	cmth_ifort_omp	#1103	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 26 03:32	be036a87e588...	success	cmth_gnu	#1067	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 25 23:30	be036a87e588...	success	cmth_intel	#1097	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 25 23:30	be036a87e588...	success	cmth_ifort_omp	#1102	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 25 03:32	be036a87e588...	success	cmth_gnu	#1066	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 24 23:30	be036a87e588...	success	cmth_intel	#1096	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 24 23:30	be036a87e588...	success	cmth_ifort_omp	#1101	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 24 03:32	be036a87e588...	success	cmth_gnu	#1065	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 23 23:30	be036a87e588...	success	cmth_intel	#1095	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 23 23:30	be036a87e588...	success	cmth_ifort_omp	#1100	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 23 03:32	be036a87e588...	success	cmth_gnu	#1064	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 23 00:48	be036a87e588...	success	cmth_intel	#1094	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 22 23:30	be036a87e588...	success	cmth_ifort_omp	#1099	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 21 06:30	be036a87e588...	failure	cmth_ifort_omp_dbg	#165	The Nightly scheduler named 'weekly' triggered this build	Failed testcode
Oct 22 18:50	be036a87e588...	success	cmth_gnu	#1063	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 22 15:11	be036a87e588...	success	cmth_intel	#1093	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 22 11:08	be036a87e588...	success	cmth_ifort_omp	#1098	The Nightly scheduler named 'nightly' triggered this build	Build successful
Oct 22 02:01	be036a87e588...	success	cmth_gnu_dbg	#170	The Nightly scheduler named 'weekly' triggered this build	Build successful

Documentation

Developer documentation:

- Template module file to encourage consistent documentation
- Each new module/procedure should be documented
- Encourage developers to comment their code as they write it

```
subroutine example_priv_proc(example_arg1,example_arg2,example_arg3)
 !=========================================================================!
 ! # DESCRIPTION                                                           !
 ! Write a description of the purpose and functionality of this procedure  !
 ! here.                                                                   !
 !-------------------------------------------------------------------------!
 ! # ARGUMENTS                                                            !
 ! <name> <in/out/inout> <arg descrption>                                  !
 ! example_arg1   out    An example argument with intent out.              !
 ! example_arg1   inout  An example argument with intent in.               !
 ! example_arg2   in     An example argument with intent in (optional)     !
 !-------------------------------------------------------------------------!
 ! # AUTHORS & CHANGELOG                                                  !
 ! Author(s):         <Author name(s)>                                     !
 ! Date of creation: <Date of creation>                                    !
 ! List of major changes:                                                  !
 ! <date> <change description> <author>                                    !
 !=========================================================================!
```

User documentation:

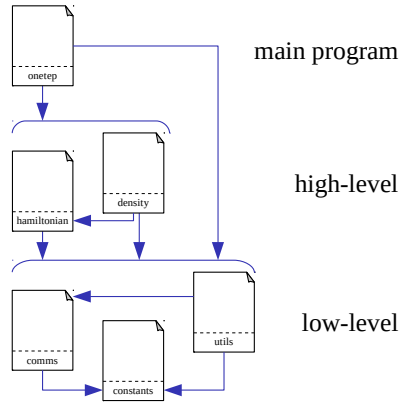
- User documentation is required for substantial new functionality
- Distributed with the code and at www.onetep.org
- Daussault Systèmes BIOVIA provide documentation for Materials Studio

Modularity

ONETEP's source code is organized as a loose hierarchy of modules:

- Modules encapsulate related functionality
- High-level modules depend on low-level modules
- Low-level modules provide basic functionality
- High-level modules perform sophisticated tasks

A module can often be developed without needing to consider the behaviour of the entire program.



Closing remarks

Summary

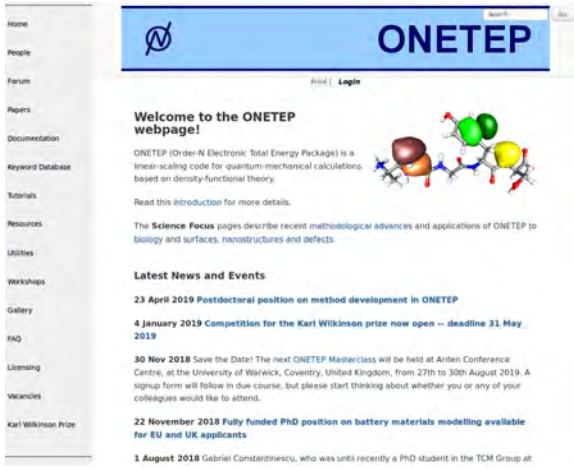
Building ONETEP

1. ONETEP is a tool for large-scale quantum simulation of matter
2. An extensive and expanding list of capabilities
3. Development of ONETEP follows a few key principles
4. These principles keep ONETEP usable and maintainable

Further details

ONETEP

www.onetep.org →



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EPSRC
Engineering and Physical Sciences Research Council

UNIVERSITY OF Southampton

MATERIALS AND MOLECULAR MODELLING HUB

archer

Thank you for your attention!

. . . any questions?

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