State of the ~~Union~~ Octopus

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commit 822cf8dccad0d4225bdef51546400ba7c68cc824
Author: Miguel Marques <marques@tddft.org>
Date:   Tue Dec 4 03:51:19 2001 +0000

    Very preliminary version of new tddft code
    now baptized octopus ;))
```

Octopus is 20 years old!

Major milestones since last meeting (June 2019)

- Two major releases (10 and 11) and six bugfix releases
- 822 approved merge requests, more than 5000 commits
- (Numbers from previous meeting: 470 MR and 2700 commits)
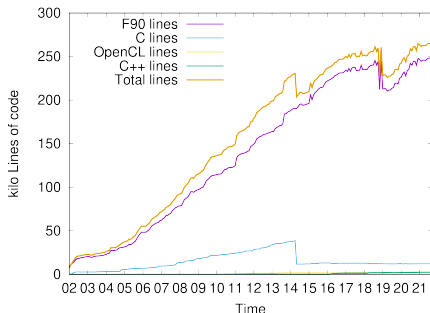
Major milestones since last meeting (June 2019)

- New Octopus paper: N. Tancogne-Dejean *et al*, *"Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems"*, J. Chem. Phys., **152** 124119 (2020)
- Improved GPU support (see talk by Sebastian)
- Improved ground-state calculations
- Many optimizations and bugfixes
- Introduction of OOP features of Fortran 2003/2008
- Major refactoring of core components in progress

Major milestones since last meeting (June 2019)

- New multi-system framework (see talk later today)
- New Maxwell and DFTB+ systems (see talk by Franco)
- Magnons from real-time TDDFT (see talk by Nicolas)
- Hybrid functionals:
    - Support for solids
    - ACE operator and improved parallelization
    - Range-separated functionals
- Several run modes extended to handle photons within QEDFT (see talks by Davis and Johannes)

    Full changelog: https://octopus-code.org/wiki/Changes

Ground-state improvements

Eigensolvers:

- Conjugate gradients
  - Corrected implementation: order of steps
  - Introduce normalizations
  - Adapt convergence criteria of eigensolver loop
- RMMDIIS
  - several corrections and bugfixes
- Improvement in convergence
  - Before, difficulties below 10^{-8} in relative densities
  - Now, convergence to 10^{-15} possible for many systems

Ground-state improvements

Broyden mixing:

- Remove normalization of intermediate quantities
- Enable fast convergence to very high accuracy
- Implement restarting: mixing history is reset after a while, helps finding the right minimum

Preconditioners:

- Filter preconditioner
  - Theoretical understanding in terms of Jacobi iterations
  - Generalization to non-orthogonal cells
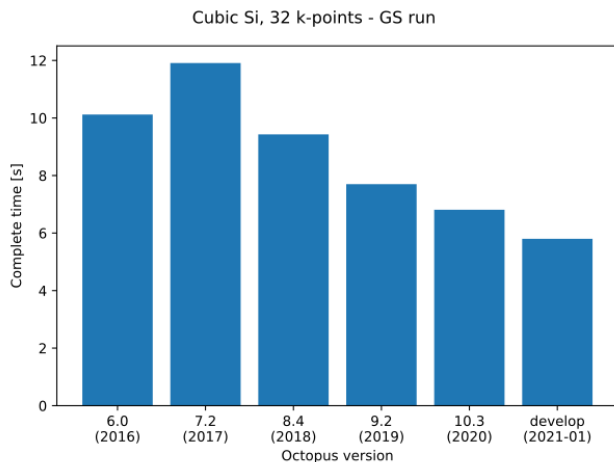- Generalized multigrid preconditioner
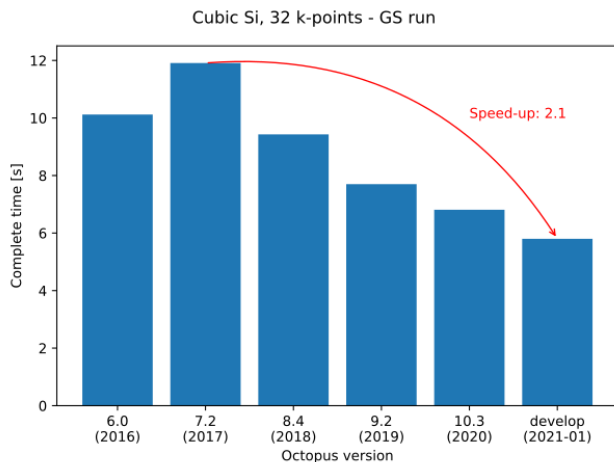
Ground-state improvements
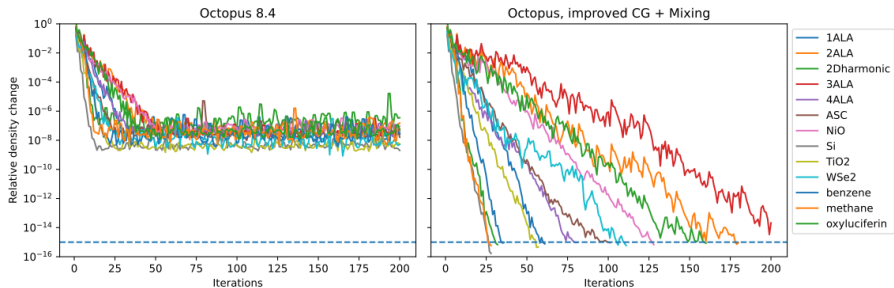
Performance optimizations

- Casida for huge matrices (up to 100k), used for photon coupling
- Improvements of the OpenMP parallelization
  - More pragmas for loops, some are more complicated (e.g. norm)
  - Good scaling up to about 12 threads per rank
  - Only good for large grids, can substitute domain parallelization
- Application of phase for periodic systems
  - Only once at beginning and end of time step
  - Use phase correction for boundary points
  - Can save up to 50-80% of the computing time
- Allocate aligned memory for better vectorization, introduce AVX512 instructions
- Improve finite-difference kernels by using non-temporal store instructions
  - Directly store to memory without cache
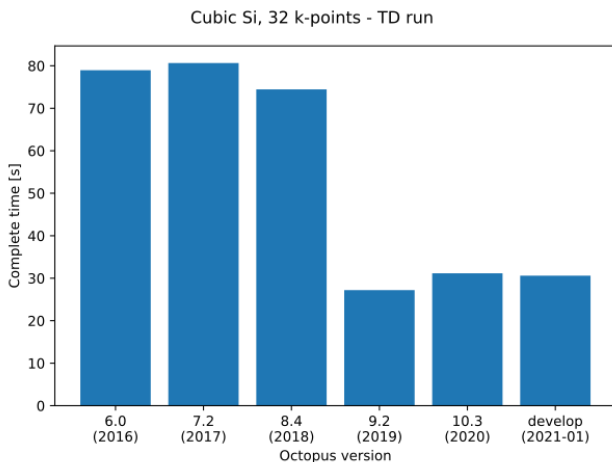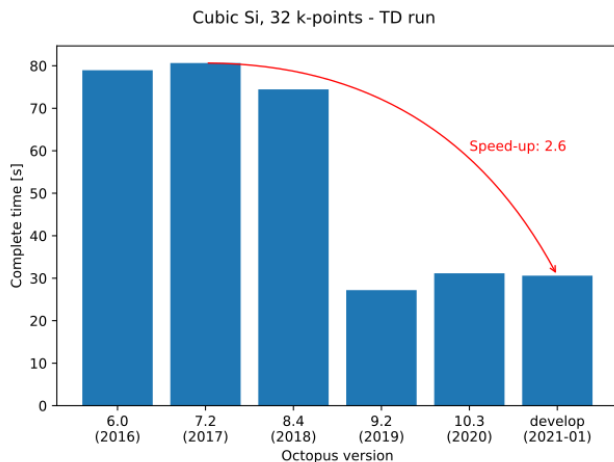 - Improve performance of kernel

Cubic Si, 32 k-points - GS run

Cubic Si, 32 k-points - GS run

Cubic Si, 32 k-points - TD run

Cubic Si, 32 k-points - TD run

Test-suites and test-farm news

Regression test-suite:

- New contidional execution and matches
- Allow for expected execution failures in tests

Performance test-suite:

- Two new Buildbot builders on dedicated hardware
- New web app to visualize results
- Still under development:
  - Only "unit" tests are run, no main run modes (gs, td)
  - Parameter space needs to be reduced (tests take too long)
  - How to determine success/failure?
  - Too large dispersion of timings

Test-suites and test-farm news

Buildbot and test-farm:

- Two new GPU machines with 10 GeForce RTX 2080 Ti cards each
- Next generation of dedicated machines will be available soon
- New builders to check GCC compiler warnings
- New OpenMP+GCC builders

Test-suites and test-farm wishlist

- New compilers?
- Refactorize testsuite to improve coverage and speed
- Meta-tests for regression tests:
    - Detect when tolerances are much too large
    - Detect when test dispersion is too large
- Better integration of EasyBuild with Buildbot
- Builders for all major Linux distributions

Other news

- New website under construction (see talk by Martin)
- MR reviews mandatory since last meeting
- Martin is the new release manager
- Two on-line courses in September:
  - Octopus basics: learn how to use Octopus (39 participants)
  - Octopus advanced: learn how to develop Octopus (25 participants)
- Weekly meetings on Tuesdays at 9:00 am
- Regular hackathons

Other news

Things that did not go so well:

- Still 157 features marked as experimental (159 in Octopus 9.0)
- 211 open issues; 289 closed
- Web server was hacked in July 2019
- Mailing lists are still down