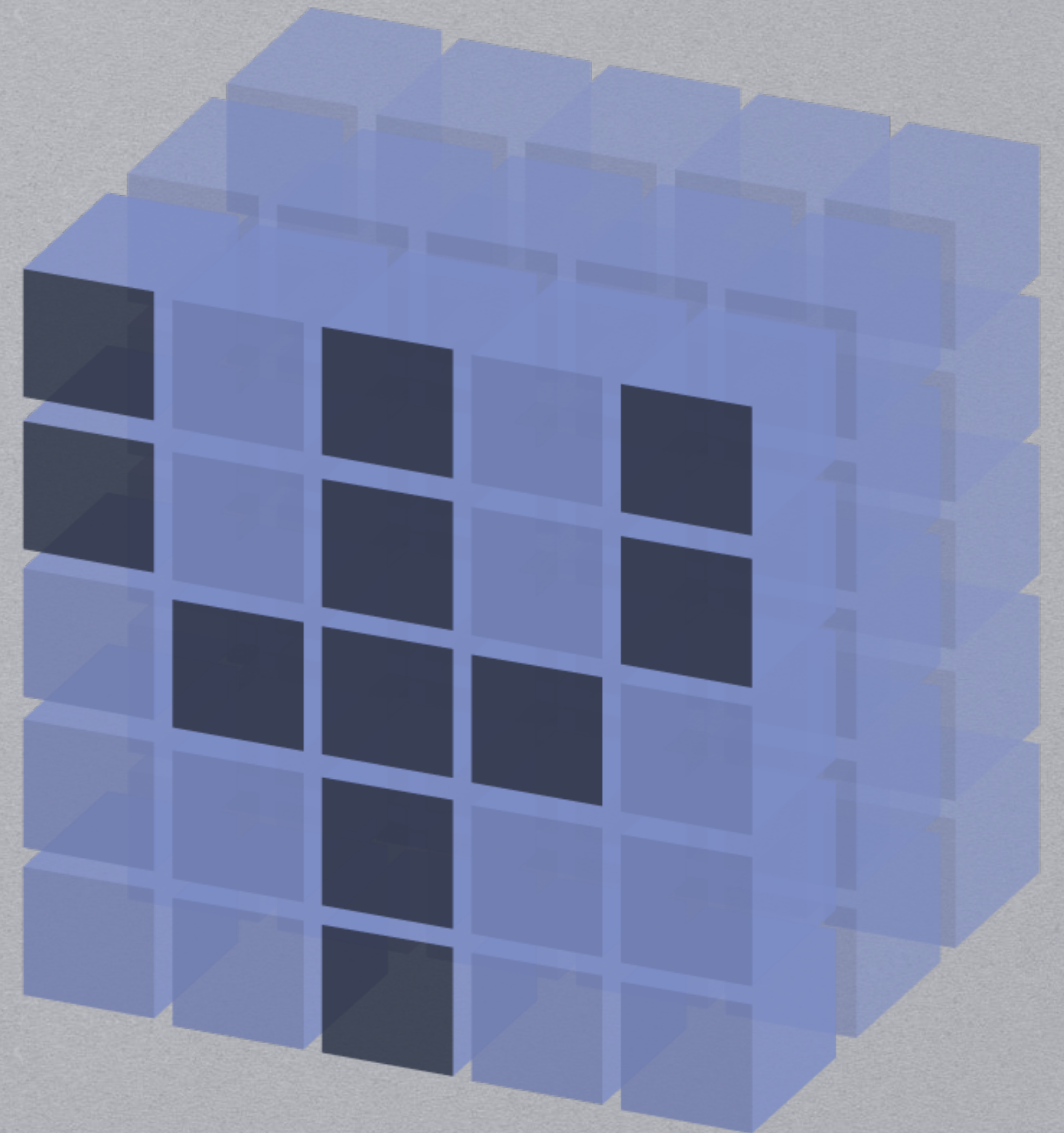


PSI4NUMPY: **THE STATE OF THE PROJECT**

D. A. SIRIANNI

2017 PSI4
WORLDWIDE DOMINATION CONFERENCE



PSI4NUMPY

WHAT IS Psi4NUMPY?



PROJECT OBJECTIVES



**REFERENCE
IMPLEMENTATION**



**PROTOTYPING
& DEVELOPMENT**



EDUCATION

PROJECT OBJECTIVES



**REFERENCE
IMPLEMENTATION**

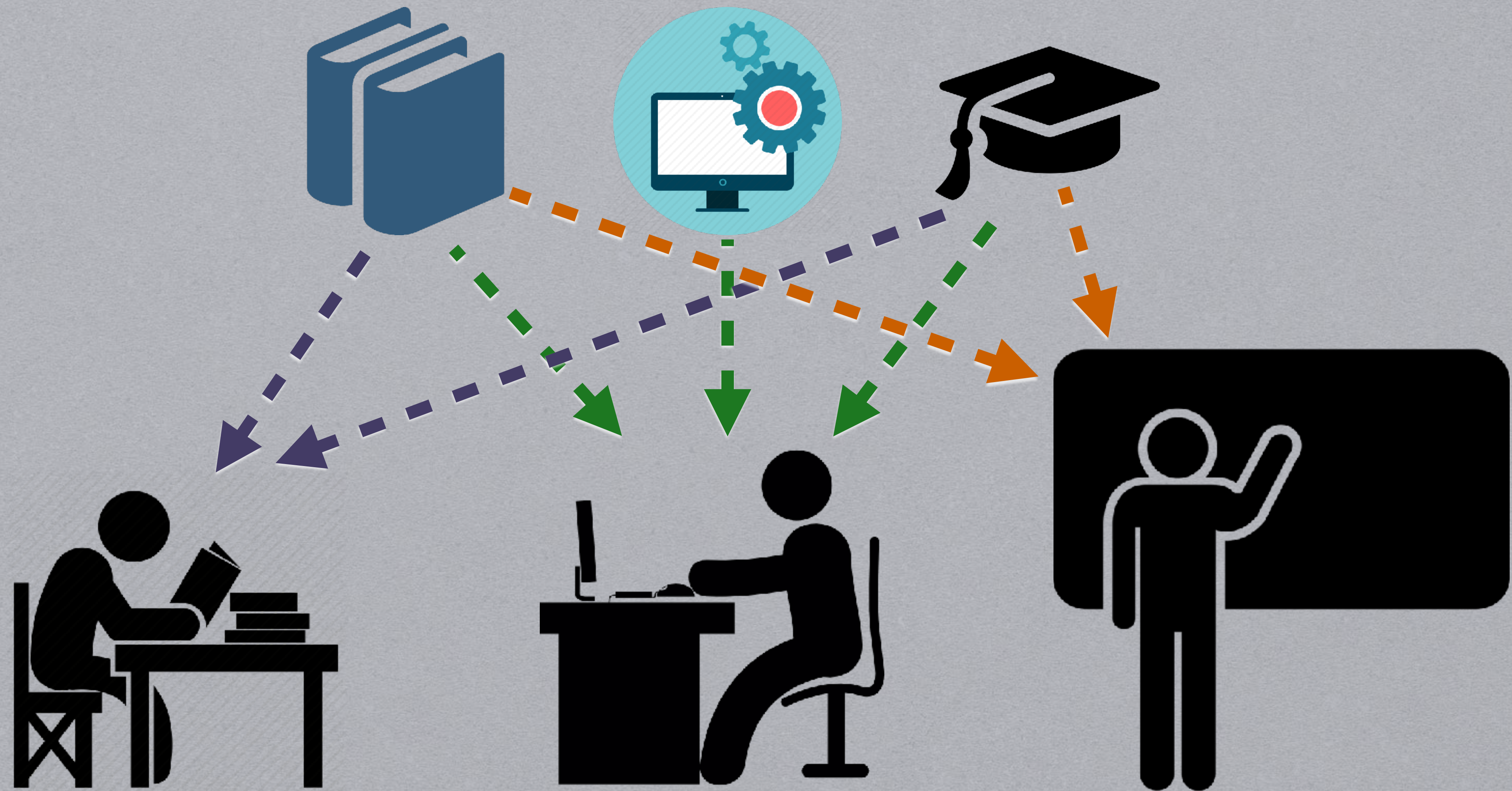


**PROTOTYPING
& DEVELOPMENT**



EDUCATION

PROJECT OBJECTIVES



Students

Researchers

Educators



REFERENCE IMPLEMENTATIONS

Comment on “A new parametrizable model of molecular electronic structure” [J. Chem. Phys. 135, 134120 (2011)]

Ksenia R. Briling^{a)}

[View Affiliations](#)

The Journal of Chemical Physics **147**, 157101 (2017); <https://doi-org.prx.library.gatech.edu/10.1063/1.5000525>



PDF

FIRST PAGE

FULL TEXT

FIGURES

TOOLS

SHARE

METRICS

[Dispersion](#) . [Electrostatics](#) . [Encoding](#) . [Operator theory](#) . [Optical fibers](#)

While implementing the model of Ref. [1](#), we found several inaccuracies in its presentation, which do not allow to reproduce (when using the text directly) the results obtained with the program attached to the original article. Our corrections are proposed below.



REFERENCE IMPLEMENTATIONS

- Hartree–Fock: RHF, ROHF, & UHF w/ DIIS & Second-Order convergence, TDHF
- Moller–Plesset: MP2, DF-MP2, MP3, MP3 w/ Spin Orbitals, MPn
- Coupled Cluster: CCSD, CCSD w/ DIIS, CCSD(T), TD-CCSD, CC Response
- Configuration Interaction: CIS, CISD, CI w/ D-L, FCI
- Electron Propagator: EP2, EP2 w/ Spin Orbitals, EP3 w/ Spin Orbitals
- Symmetry-Adapted Perturbation Theory: SAPT0(RHF), SAPT0(ROHF)
- Molecular Properties: CPHF (1st dipole polarizability & 1st dipole hyperpolarizability)
- *Ab initio* Molecular Dynamics: AIMD w/ Verlet Integrator

INTERACTIVE TUTORIALS

- Hartree–Fock:
 - RHF, RHF w/ DIIS, UHF w/ DIIS, Density Fitting
- Density Functional Theory:
 - DFT grids, LDA kernel, VV10 dispersion, GRAC correction
- Moller–Plesset:
 - Conventional & density-fitted MP2
- Molecular Properties:
 - Coupled-Perturbed Hartree–Fock
- Classical Mechanics:
 - Basics of MD, Particle Mesh Ewald (PME) summation



NEW INFRASTRUCTURE

- Testing – PyTest
- CodeCov
- Continuous Integration
- New tools?
- Binder images of tutorials for online execution

A screenshot of a GitHub pull request interface. At the top, a comment from 'codecov-io' dated 'Oct 2' is shown, containing a 'Codecov Report'. The report states: 'Merging #35 into master will not change coverage. The diff coverage is n/a.' Below this is a progress bar with several grey segments. A secondary overlay box contains three status messages: 'Review required' (with a red 'x' icon), 'All checks have passed' (with a green checkmark icon), and 'Merging is blocked' (with a red 'x' icon). At the bottom of this overlay is a 'Merge pull request' button. Below the overlay, a link says 'Continue to review full report at Codecov.' and a legend explains symbols like Δ for absolute impact and \varnothing for not affected. The footer mentions 'Powered by Codecov' and provides a commit hash and link to comment docs.



PROJECT STATUS

- Paper!
 - New version (last night)
 - Author list? Feedback from the authors?
- Repository
 - Adding equation, papers, etc. references to all scripts & tutorials
 - Reorganization?
 - Always taking contributions, keep them coming!