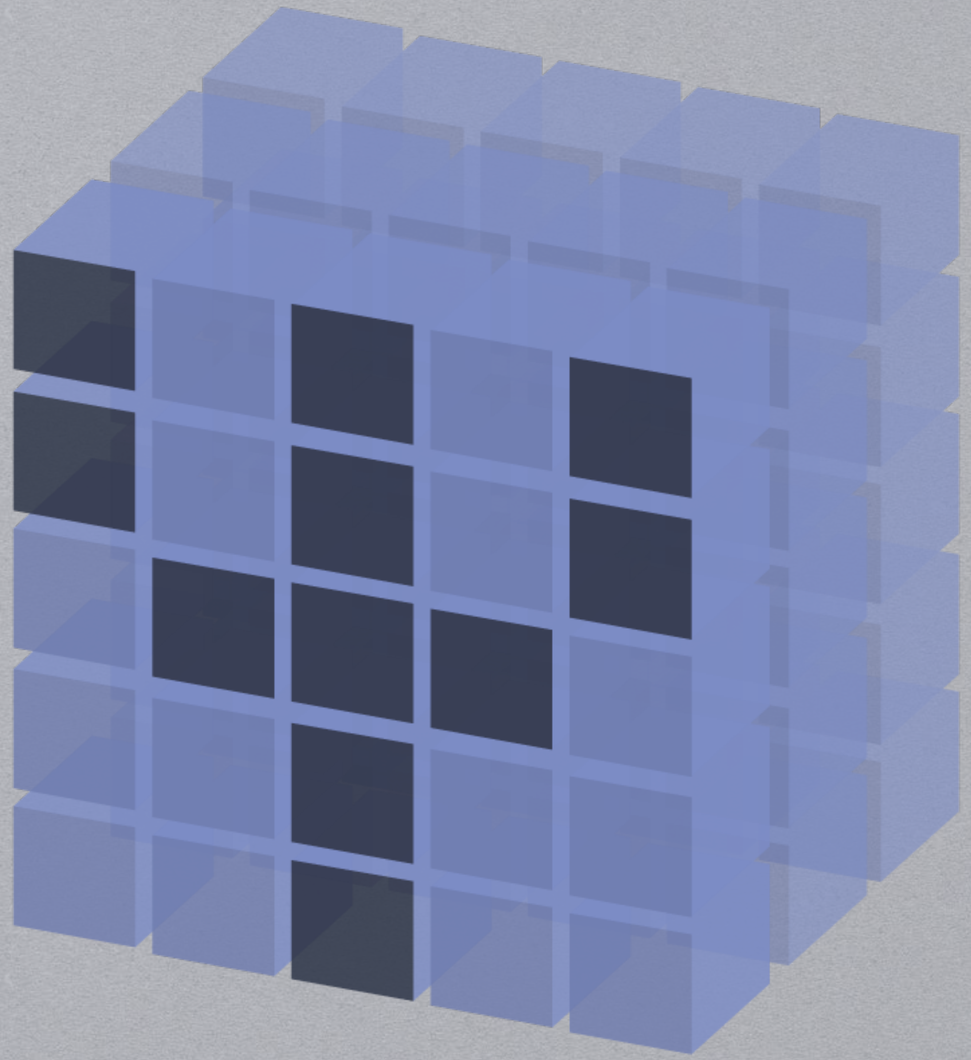
Psi4NumPy:
THE STATE OF THE PROJECT

D. A. SIRIANNI

2017 Psi4
WORLDWIDE DOMINATION CONFERENCE



Psi4NumPy

WHAT IS PSI4NUMPY?

PROJECT OBJECTIVES

REFERENCE IMPLEMENTATION

PROTOTYPING & DEVELOPMENT

EDUCATION

PROJECT OBJECTIVES

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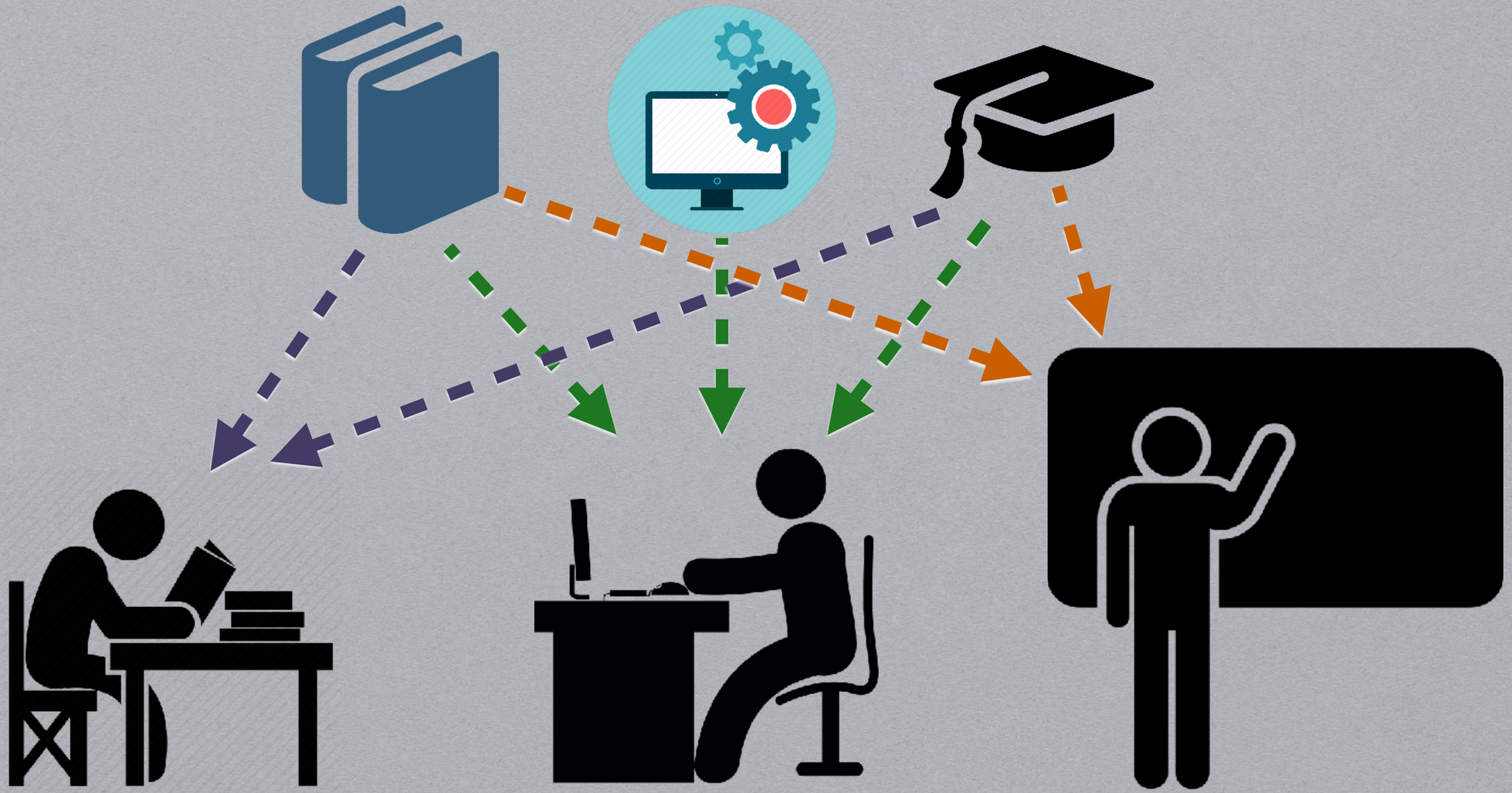
PROJECT OBJECTIVES



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

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

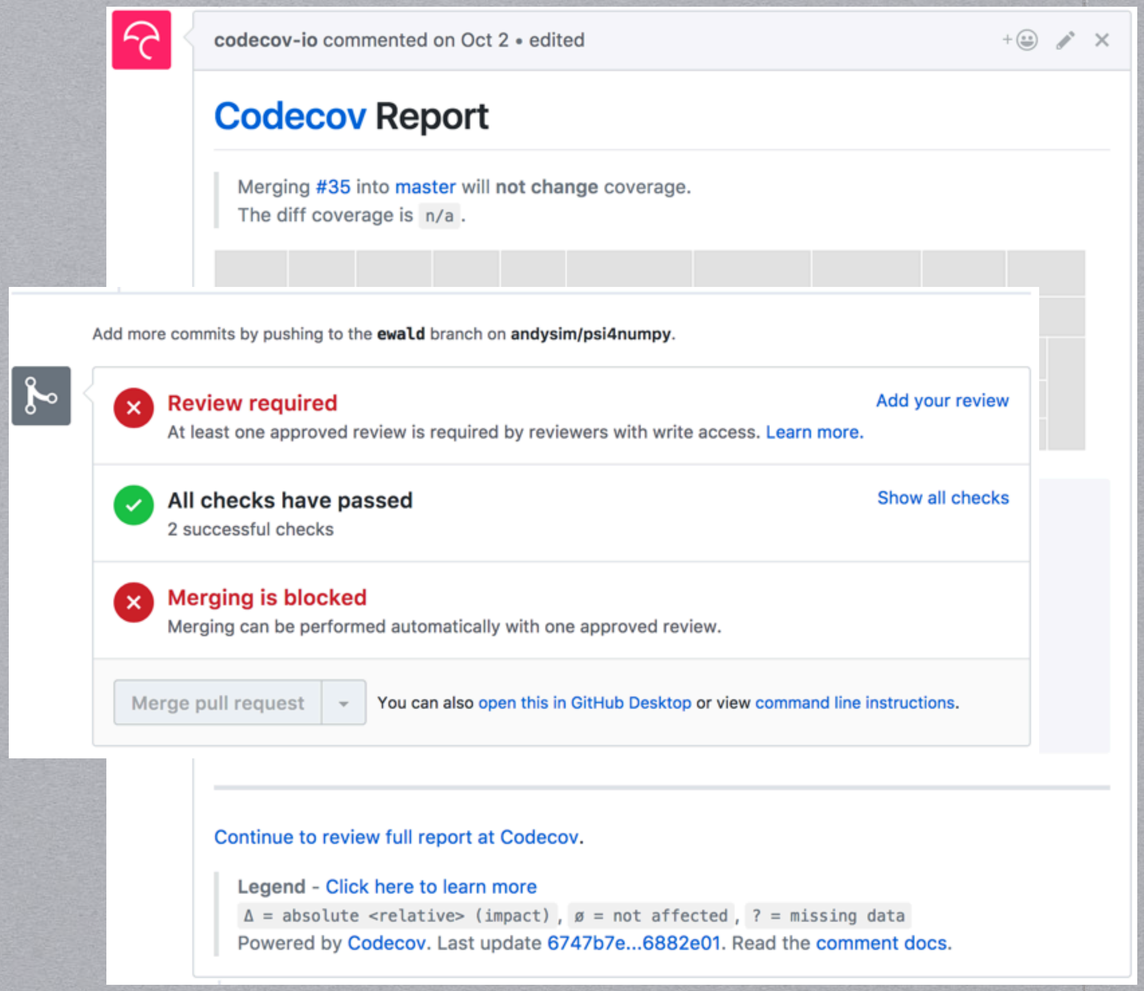
- Hartree–Fock: RHF, ROHF, & UHF w/ DIIS & Second-Order convergence, TDHF
- Moller–Plesset: MP2, DF-MP2, MP3, MP3 w/ Spin Orbitals, MPn
- Coupled Cluster: CCSD, CCSD w/ DIIS, CCSD(T), TD-CCSD, CC Response
- Configuration Interaction: CIS, CISD, CI w/ D-L, FCI
- Electron Propagator: EP2, EP2 w/ Spin Orbitals, 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



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!