2022 Retrospective: Managing Complexity in Psi

Jonathon P. Misiewicz
Emory University

PsiCon
December 9, 2022

Talk Goals

- What in the codebase did I change?

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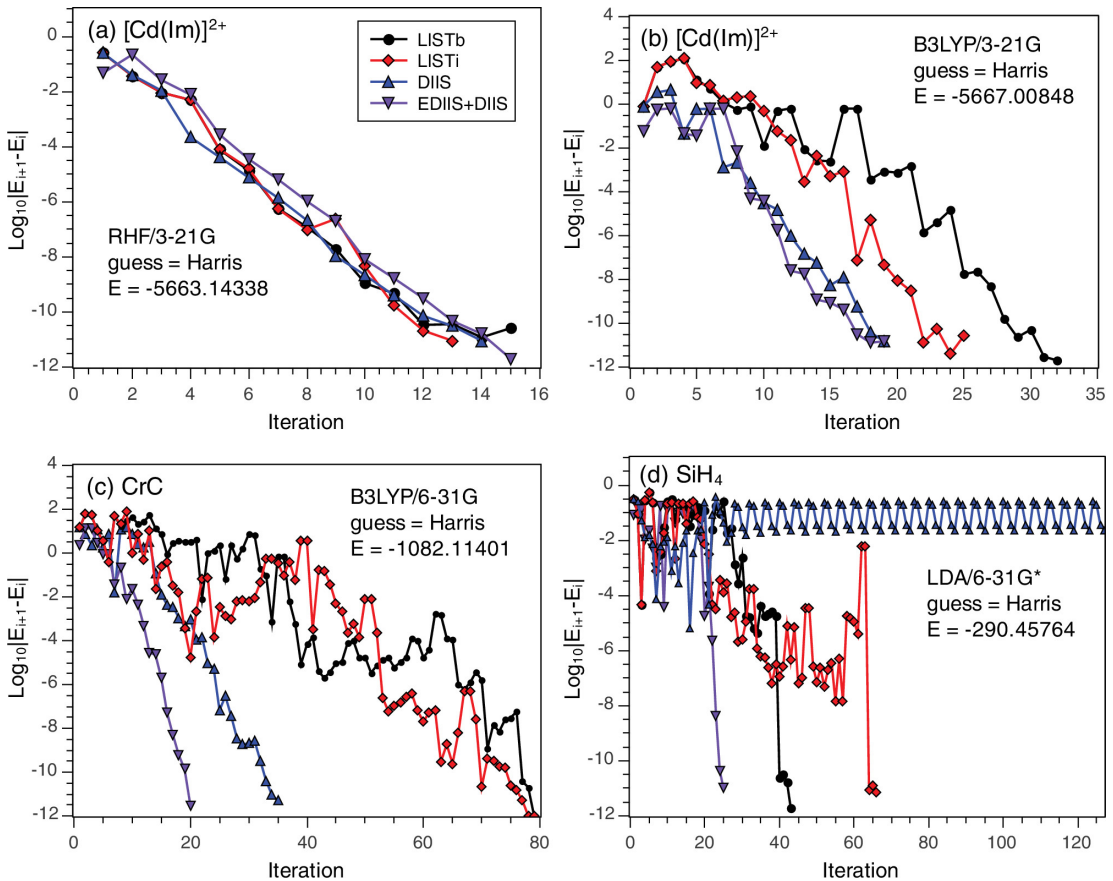
- What in the codebase do I want to change?
- **What in the workflow do I want to change?**

Story 1: ADIIS/EDIIS

ADIIS/EDIIS accelerate SCF convergence when far from converged



DOI: 10.1063/1.4740249; J. Chem. Phys. 137, 054110 (2012); Garza and Scuseria

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- Problem: Users (and test suite) keep reporting the solver fails to work.
- Ver. 2: Use SciPy SLSQP solver on constrained minimization.
- Works for physical geometries!

Everything Else

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- What does Psi need special forces for?
- Dealing with the consequences of our past decisions

Story 2: Pythonizing UHF Instability Following

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- Problem: Code duplication! Both algorithms star the same step.
- By unifying, **we can determine if a KS solution is at a minimum**.
- (UKS-LDA currently supported. RKS and UKS supported for LDA and GGA is planned for 1.8. We can already handle exact exchange and long-range.)

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- Unified them into template classes, so I can change both at once

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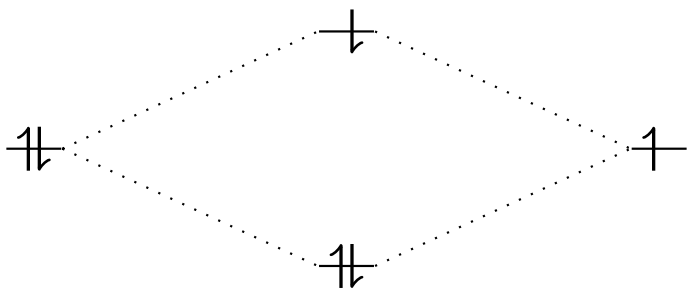

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- Singly occupied beta orbitals **assumed impossible**
- Led to **crashes and tortured MOM-SCF**
- Now we store the alpha and beta occupations and compute the occupations

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- Remaining examples are "big" but highly technical, suggest (to me) Psi workflow should change

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- In 2012, it was proposed that orbitals instead be chosen to minimize the energy

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- γ_{ref} converged when orbitals converged, and we already check that (with lin. dep. accounted for).
- 2006 Orbitals: We already check that the commutator is small
- 2012 Orbitals: It's better to check the orbital gradient

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- **This is not the open-source way.**
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- **How can we reasonably lower the expertise threshhold?**

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- Institutional knowledge failed.

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- Original coder unavailable

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- I reached out to them for the papers...
- Cross-referenced against Psi4Numpy...
- Looked at (sparse) code comments...
- Mostly debugged the function!

Story 8: TD-GGA

```
for (int P = 0; P < npoints; P++) {
    rho_ak[P] = 0.5 * C_DDOT(nlocal, phi[P], 1, Tap[P], 1);
    rho_bk[P] = 0.5 * C_DDOT(nlocal, phi[P], 1, Tbp[P], 1);
}

// Rho^d_k and gamma_k
if (ansatz >= 1) {
    for (int P = 0; P < npoints; P++) {
        // Alpha
        rho_ak_x[P] = C_DDOT(nlocal, phi_x[P], 1, Tap[P], 1);
        rho_ak_y[P] = C_DDOT(nlocal, phi_y[P], 1, Tap[P], 1);
        rho_ak_z[P] = C_DDOT(nlocal, phi_z[P], 1, Tap[P], 1);
        gamma_aak[P] = rho_ak_x[P] * rho_ax[P];
        gamma_aak[P] += rho_ak_y[P] * rho_ay[P];
        gamma_aak[P] += rho_ak_z[P] * rho_az[P];
        gamma_aak[P] *= 2.0;

        // Beta
        rho_bk_x[P] = C_DDOT(nlocal, phi_x[P], 1, Tbp[P], 1);
        rho_bk_y[P] = C_DDOT(nlocal, phi_y[P], 1, Tbp[P], 1);
        rho_bk_z[P] = C_DDOT(nlocal, phi_z[P], 1, Tbp[P], 1);
        gamma_bbk[P] = rho_bk_x[P] * rho_bx[P];
        gamma_bbk[P] += rho_bk_y[P] * rho_by[P];
        gamma_bbk[P] += rho_ak_z[P] * rho_bz[P];
        gamma_bbk[P] *= 2.0;

        // Alpha-Beta
        gamma_abk[P] = rho_ak_x[P] * rho_bx[P] + rho_bk_x[P] * rho_ax[P];
        gamma_abk[P] += rho_ak_y[P] * rho_by[P] + rho_bk_y[P] * rho_ay[P];
        gamma_abk[P] += rho_ak_z[P] * rho_bz[P] + rho_bk_z[P] * rho_az[P];
    }
}
```

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```
// This one is a doozy
for (int P = 0; P < npoints; P++) {
    // V alpha contributions
    if (rho_a[P] > v2_rho_cutoff_) {
        tmp_val = v2_rho_a_gamma_aa[P] * gamma_aak[P];
        tmp_val += v2_rho_a_gamma_ab[P] * gamma_abk[P];
        tmp_val += v2_rho_a_gamma_bb[P] * gamma_bbk[P];
        C_DAXPY(nlocal, (0.5 * w[P] * tmp_val), phi[P], 1, Tap[P], 1);
    }

    // V beta contributions
    if (rho_b[P] > v2_rho_cutoff_) {
        tmp_val = v2_rho_b_gamma_aa[P] * gamma_aak[P];
        tmp_val += v2_rho_b_gamma_ab[P] * gamma_abk[P];
        tmp_val += v2_rho_b_gamma_bb[P] * gamma_bbk[P];
        C_DAXPY(nlocal, (0.5 * w[P] * tmp_val), phi[P], 1, Tbp[P], 1);
    }

    // => Alpha W terms <= //
    if ((rho_a[P] < v2_rho_cutoff_) || (rho_b[P] < v2_rho_cutoff_)) continue;

    // rho_ak
    v2_val_aa = v2_rho_a_gamma_aa[P] * rho_ak[P];
    v2_val_ab = v2_rho_a_gamma_ab[P] * rho_ak[P];

    // rho_bk
    v2_val_aa += v2_rho_b_gamma_aa[P] * rho_bk[P];
    v2_val_ab += v2_rho_b_gamma_ab[P] * rho_bk[P];

    // gamma_aak
    v2_val_aa += v2_gamma_aa_gamma_aa[P] * gamma_aak[P];
    v2_val_ab += v2_gamma_aa_gamma_ab[P] * gamma_aak[P];
```

Moralizing

- Tests work, let's have more of them.
  - Caught numerous issues during my refactoring
  - Would have caught CCSD dipoles, DF-wK

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  - Internal discussion on this point for the best.
  - This is an up-front cost to method addition
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  - This makes debugging so much easier

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  - Comments and Psi4NumPy and paper/equation references
  - Internal discussion on this point for the best.
  - This is an up-front cost to method addition
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  - This makes debugging so much easier
  - Great for new developers

A Word to New Devs

- There's a lot of Psi. Best way to learn is "small projects," e.g., forum topics
- Comments and cleanup welcome as you go

Future Spec. Ops.

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  - Nowadays, difficult to debug and steep learning curve
  - Let's use a standard library!
  - One of our afternoon talks uses `hdf5` I/O

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  - OPDM and Lagrangian down, TPDM to go

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- The answer to "can other people understand this code?" is usually no. This is bad. What are we going to do about that?
- Next targets are refactoring gradients and I/O, and some new DFT tech
- My experience doing so reinforces "can other people understand this code?"

Fin