CSSI Frameworks: Scalable Modular Software and Methods for High-Accuracy Materials and Condensed Phase Chemistry Simulation

PI: Edgar Solomonik*, co-PIs: Lucas Wagner◇, Timothy Berkelbach†, and Garnet Chan⋆

Contributors: Linjian Ma*, Navjot Singh*, Yang Gao⋆, Phillip Helms⋆

* Department of Computer Science, University of Illinois at Urbana-Champaign

◇ Department of Physics, University of Illinois at Urbana-Champaign

† Department of Chemistry, Columbia University

⋆ Division of Chemistry and Chemical Engineering, California Institute of Technology

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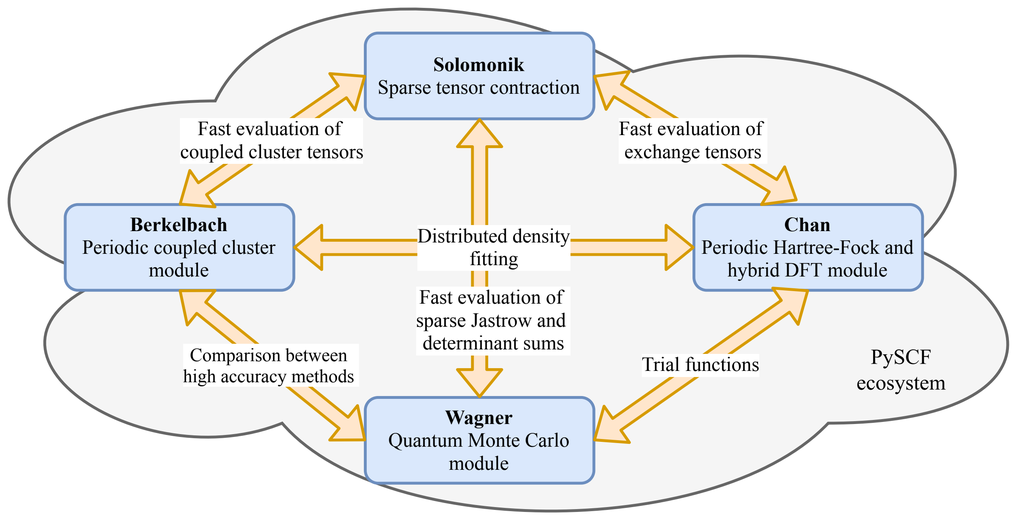
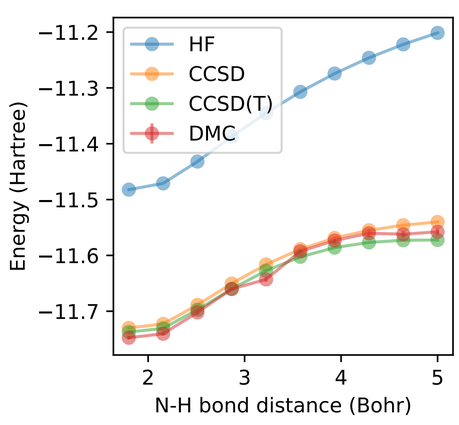
PySCF + QWalk + Cyclops

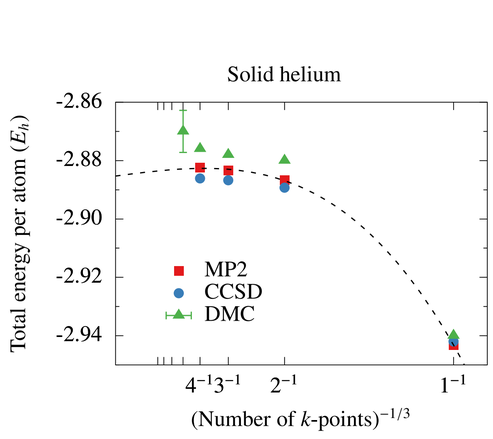


Aim: bring high-accuracy methods to state of practice for materials and condensed phase chemistry by equipping PySCF with robust periodic mean-field and wave-function methods, leveraging reduced-scaling approximations, and innovating in tensor abstractions.

Interoperation of Methods

```
for r in np.linspace(2.0,5.0,10):
    mol = gto.M(atom=f"H 0. 0. 0.; H 0. 0. {r}", basis='cc-pvtz',unit='bohr')
    mf = scf.RHF(mol)
    ehf = mf.kernel()
    edmc, edmc_err = run_qmc(mol,mf)
    mycc = mf.CCSD().run()
    eccsd = mycc.e_corr
    et = mycc.ccsd_t()
```



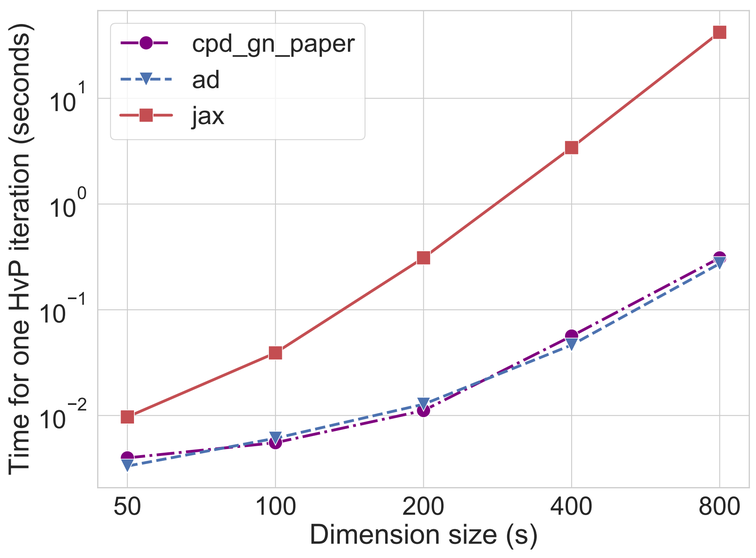


PySCF extended to support QMC methods

Parallel Tensor Abstractions

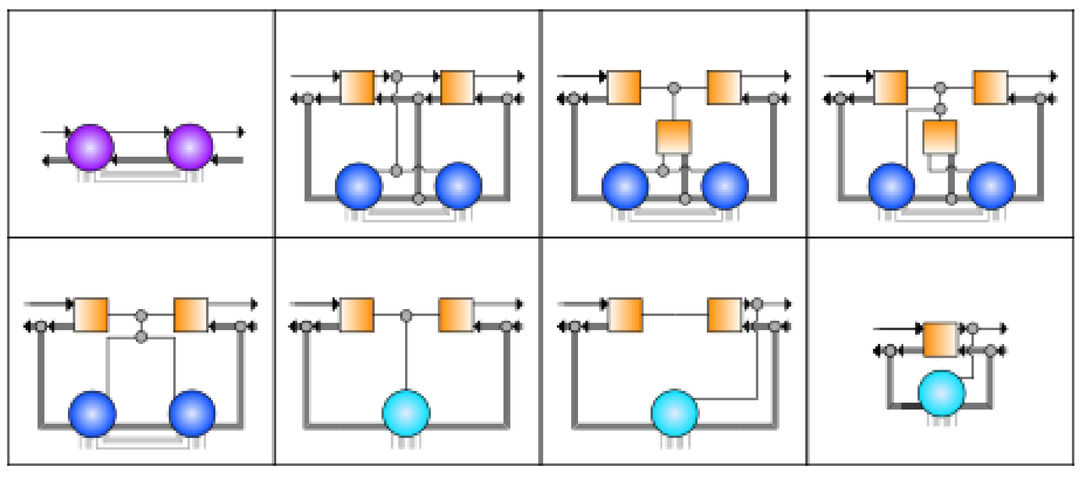
```
import ctf
def Tucker(T,rank):
    [Z,SA,A] = T.i("ijk").svd("ajk","ia",rank)
    [Z,SB,B] = Z.i("ajk").svd("abk","jb",rank)
    [Z,SC,C] = Z.i("abk").svd("abc","kc",rank)
    Z *= ctf.einsum("a,b,c->abc",SA,SB,SC)
    return [A,B,C,Z]
T = ctf.random.random((9,9,9))
[A,B,C,Z] = Tucker(T,3)
r = ctf.norm(T-ctf.einsum("abc,ia,jb,kc->ijk",Z,A,B,C))
print("Residual norm is",r)
```

Automatic Einsum Differentiation

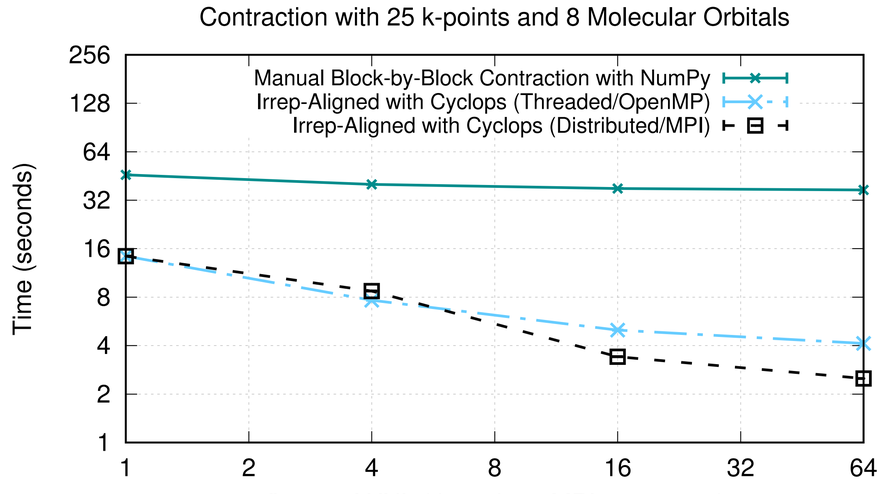


New Python tensor autodifferentiation and optimization library (ad).

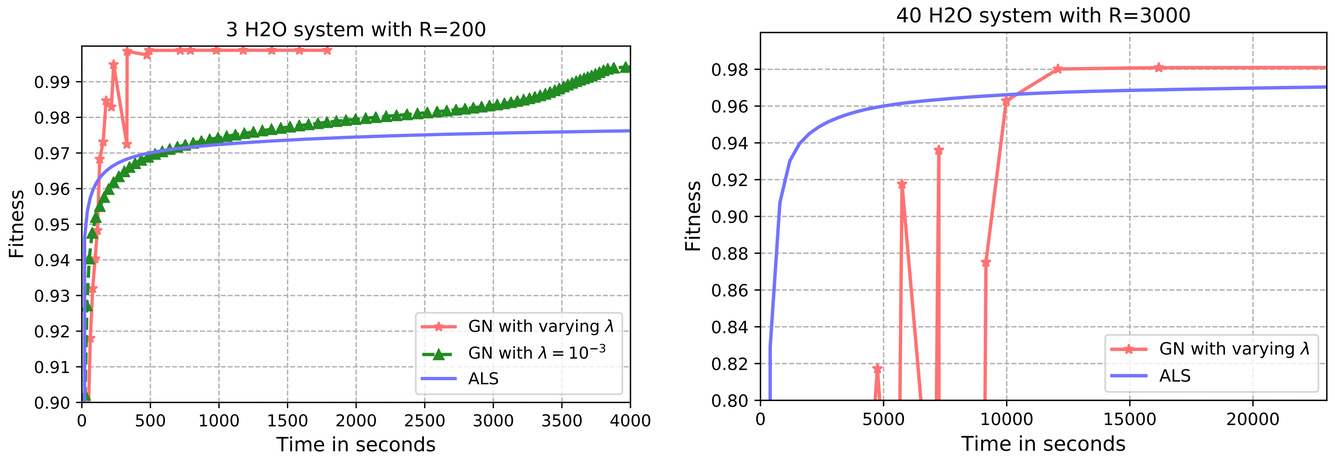
Symmetry by Automatic Irrep Alignment



New cost-efficient algorithm to handle tensor contractions with group symmetry via large dense tensor contractions exposes parallelism to tensor libraries.

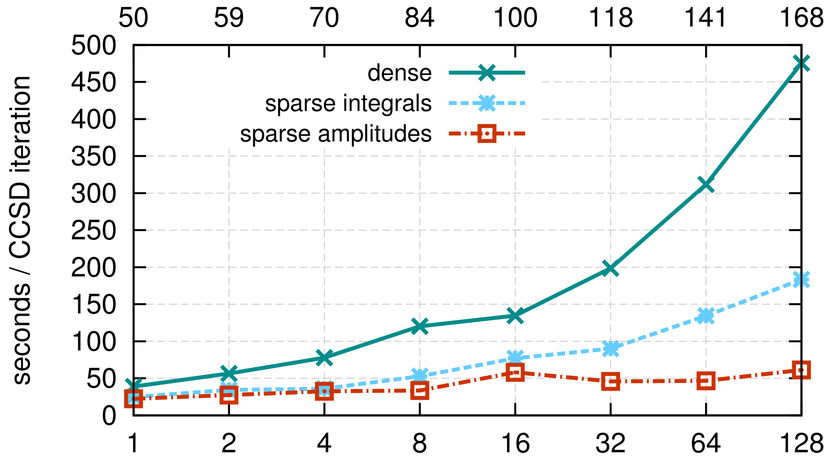


Tensor Decomposition for Post-HF



New parallel Gauss-Newton methods for CP tensor decomposition for tensor hypercontraction factorization to enable reduced-scaling post-Hartree-Fock methods.

Sparse Parallel Local Coupled Cluster



Parallel sparse tensor contractions via Cyclops for localized coupled cluster methods.

References

Parallel Gauss-Newton tensor decomposition (arXiv:1910.12331)

http://github.com/cyclops-community/ctf

http://github.com/pyscf/pyscf