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

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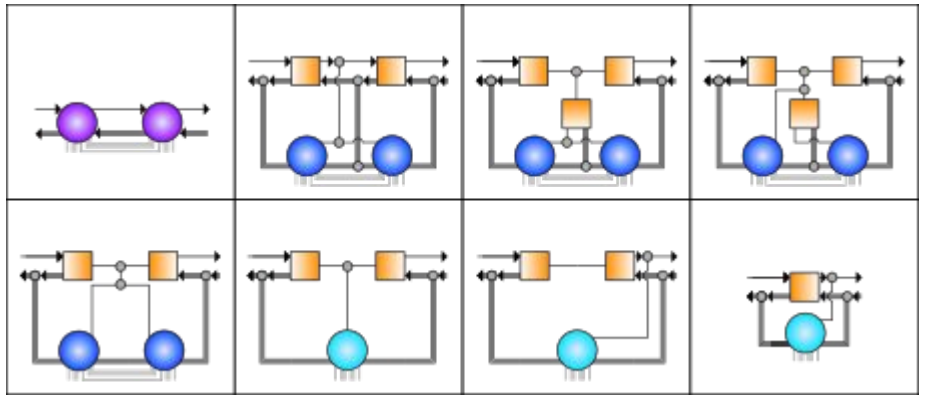
Award #1931258

```python
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()
```



- Productivity via PySCF, parallelism via Cyclops Tensor Framework
- Quantum simulation of materials and condensed phase chemistry
- Hartree Fock (HF) and post-HF methods for periodic systems
- High accuracy: quantum Monte Carlo (QMC), coupled cluster (CCSD)

- New efficient dense representations for group symmetry in tensor contractions

- Low scaling via tensor decomposition and sparse tensors