# CDS Group SoC – Day 6 Notes

June 15, 2016

## 1 Discussion of JK build algorithms, black magic, and Psi4 hacks

- GEMM, GEMV routines are both written in Fortran
  - Arguments passed to GEMM & GEMV *must* be in written in Fortran order (opposite of C order)
  - When given a matrix in C order, numpy.dot forces a copy of the matrix into Fortran order, to be compatible with GEMM & GEMV routines
  - This process is **SLOW!!**
- When calling numpy.dot on arrays A and B:
  - Initialize output array C in memory before starting
  - call np.dot(A, B, out=C)
  - This prevents the need to allocate memory & populate the new array (C above) on *each* iteration...much faster this way!
- Instead of doing direct BLAS operations on the entire intermediate tensors (in J and/or K builds in DF-RHF) on each SCF iteration:
  - Can loop over auxiliary basis set index explicitly, and call scipy.linalg.blas.dgemm directly
    - Similar speed as single "all array" dgemm call with np.dot
    - Greatly reduced memory requirement, since the *entire* 3-index intermediate tensor in K build doesn't need to be kept in memory
    - Even with slight loss in speed by employing Python loop, will be exactly same speed when written in C/C++ but drastically reduced memory requirement
- Can also use Psi4 to directly access JK object using numpy syntax
  - Create a numpy view of the Psi4 JK object pointing to the same location in memory

  - Any modification to the numpy view of the JK object *also* modifies the Psi4 JK object itself!

## 2 SOSCF: Second-order Orbital Optimization

- Diagonal elements of the energy gradient are zero.
  - Elements of gradient tensor are the change in energy upon rotating one orbital for another – rotating one orbital to itself (diagonal elemetns) incurs no change in energy
- In constructing Hessian, need to transform inactive Fock matrix, ${}^{I}F_{\mu\nu}$ from AO basis to MO basis
  - To do this, use the C matrix:

$$ {}^{I}F_{pq} = C_{p\mu}^{\mathrm{T}} F_{\mu\nu} C_{\nu q} $$

- Once the whole Hessian is constructed, only actually want the OVOV blocks
  - OO & VV blocks contain orbital rotations that *do not change orbital occupations*, so they have the same energy!
  - OV blocks are identical apart from transpose