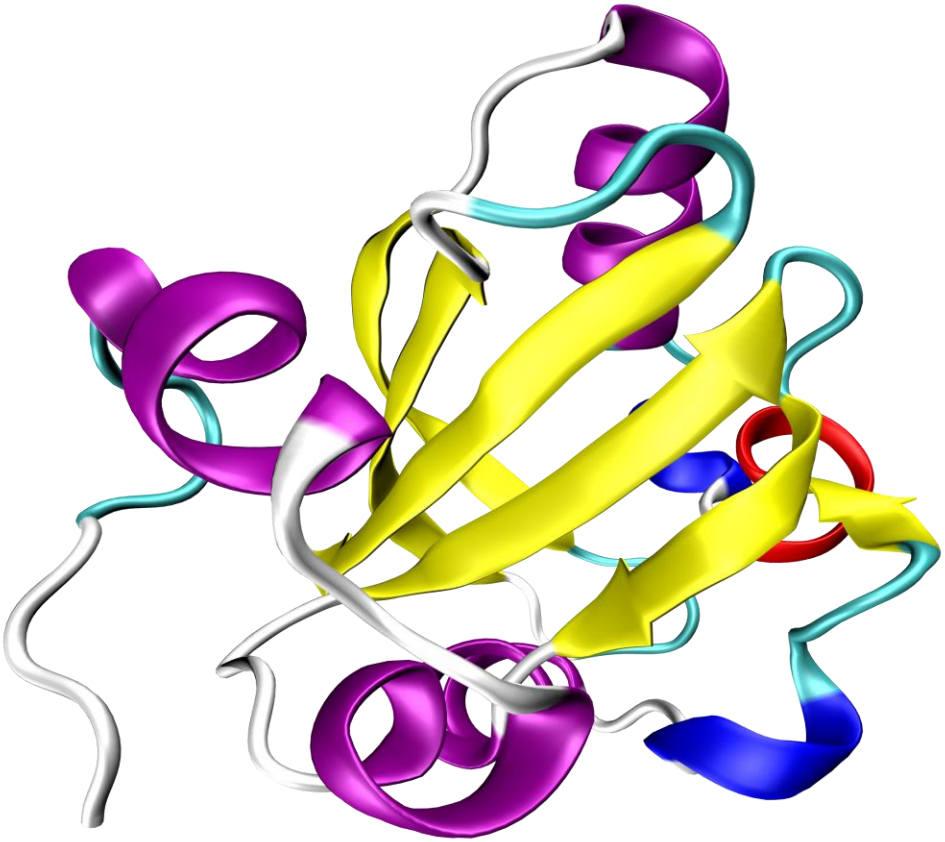
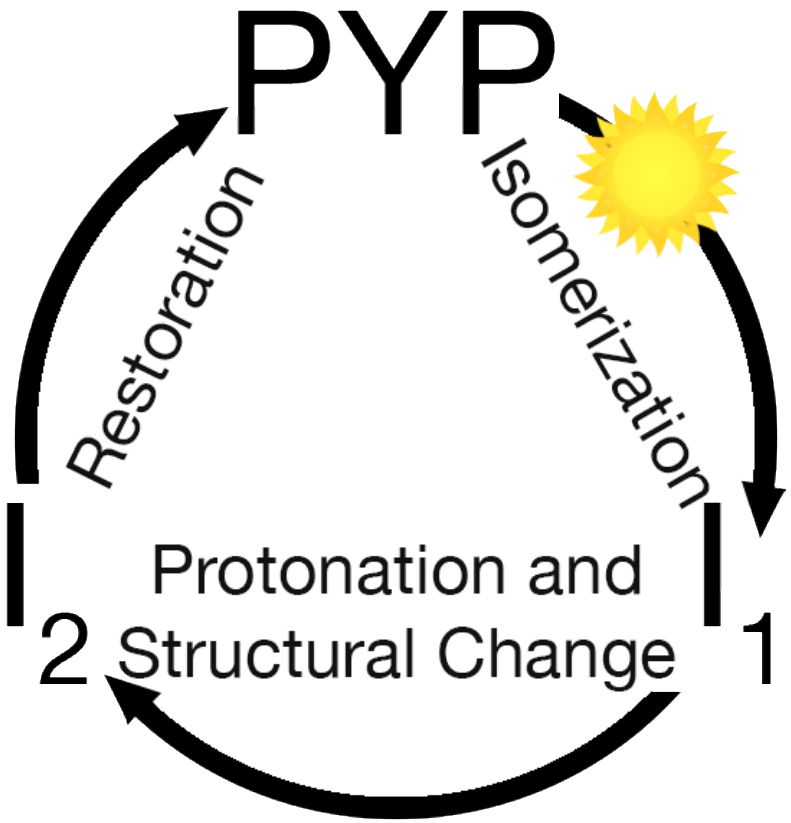
GPU Accelerated Quantum Chemistry: A New Method to Determine Absorption Spectra

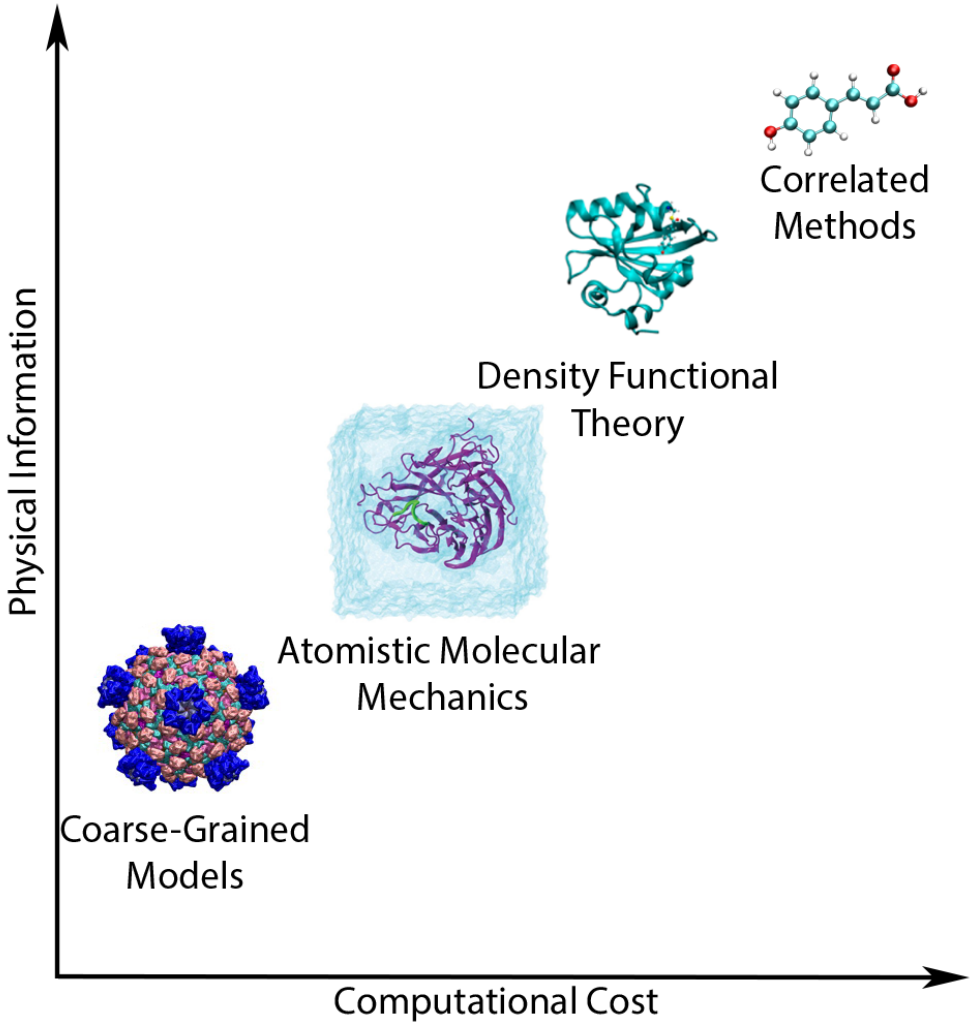
Sara Kokkila Schumacher

Photoactive Yellow Protein (PYP)



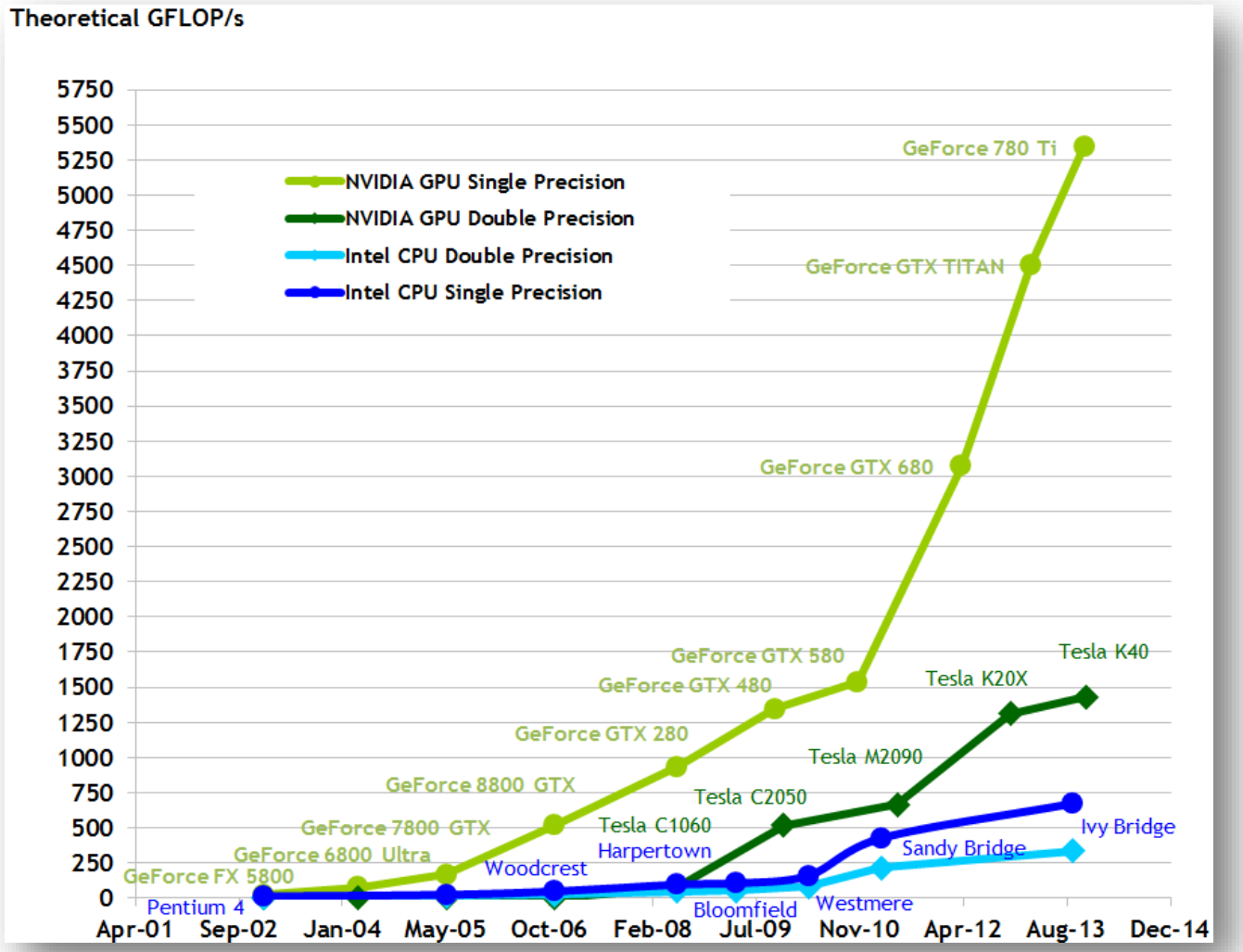


Accuracy vs. Cost



Arkhipov, P. L. Freddolino, and K. Schulten, *Structure*, **14**, 1767 (2006).
C. M. Isborn, et al., *JCTC*, **7**, 1814 (2011).

GPU Acceleration

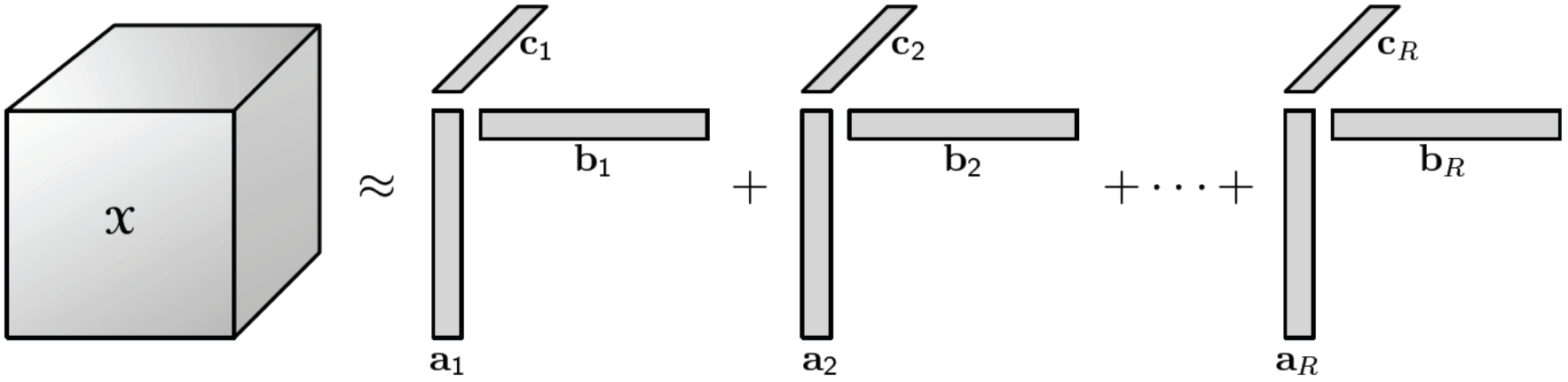


CUDA C Programming Guide [Online], version 6.5, www.nvidia.com, 2014.

Tensor Hypercontraction (THC)

Electron Repulsion Integral (ERI):

$$(mn|ls) = \int\int dr_1\, dr_2 f_m(r_1) f_n(r_1) \frac{1}{r_{12}} f_l(r_2) f_s(r_2) \approx \sum_{PQ} X_m^P X_n^P Z^{PQ} X_l^Q X_s^Q$$



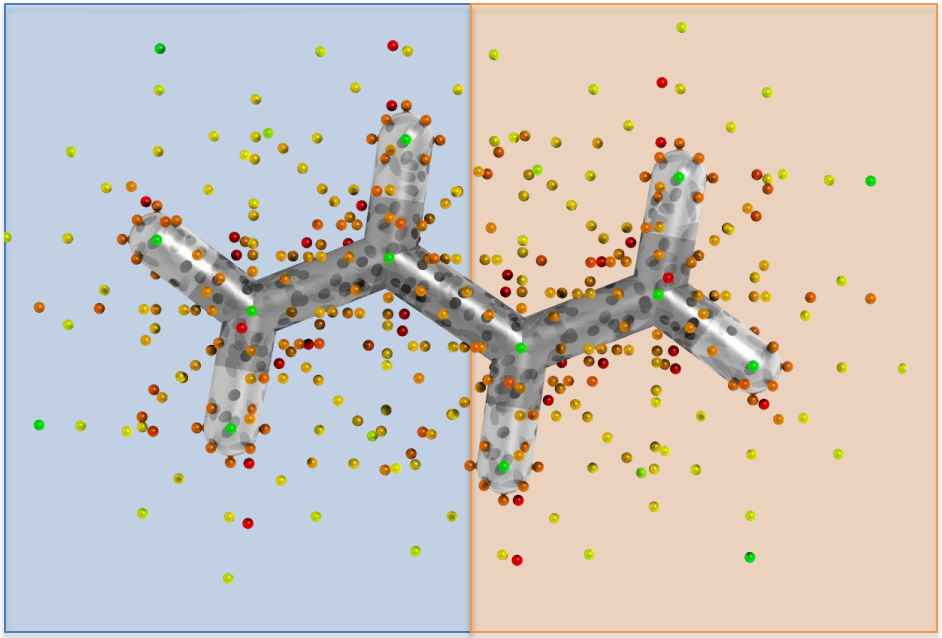
T.G. Kolda and B.W. Bader, *SIAM Rev.*, **51,** 455 (2009)

E.G. Hohenstein, R.M. Parrish, T.J. Martínez, *J. Chem. Phys.*, **137**, 044103 (2012)

E. G. Hohenstein, R. M. Parrish, T.J. Martínez, and C. D. Sherrill, *J. Chem. Phys.*, **137**, 224106 (2012)

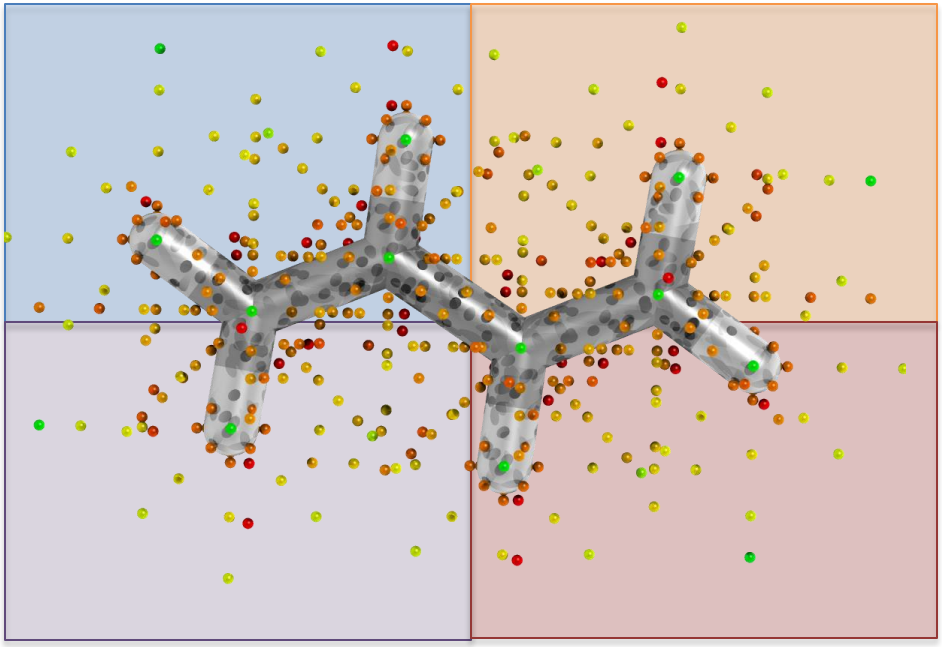
GPU Accelerated THC-CC2

$$(mn|ls) \approx \sum_{PQ} X_m^P X_n^P Z^{PQ} X_l^Q X_s^Q$$

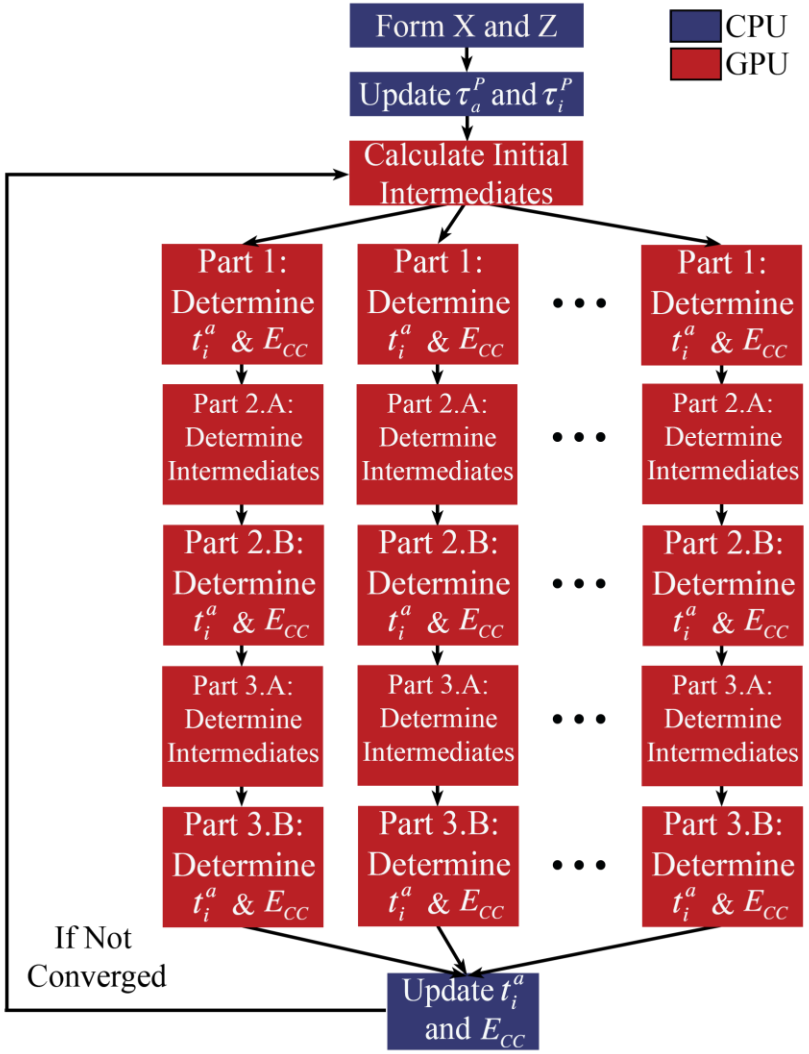


GPU Accelerated THC-CC2

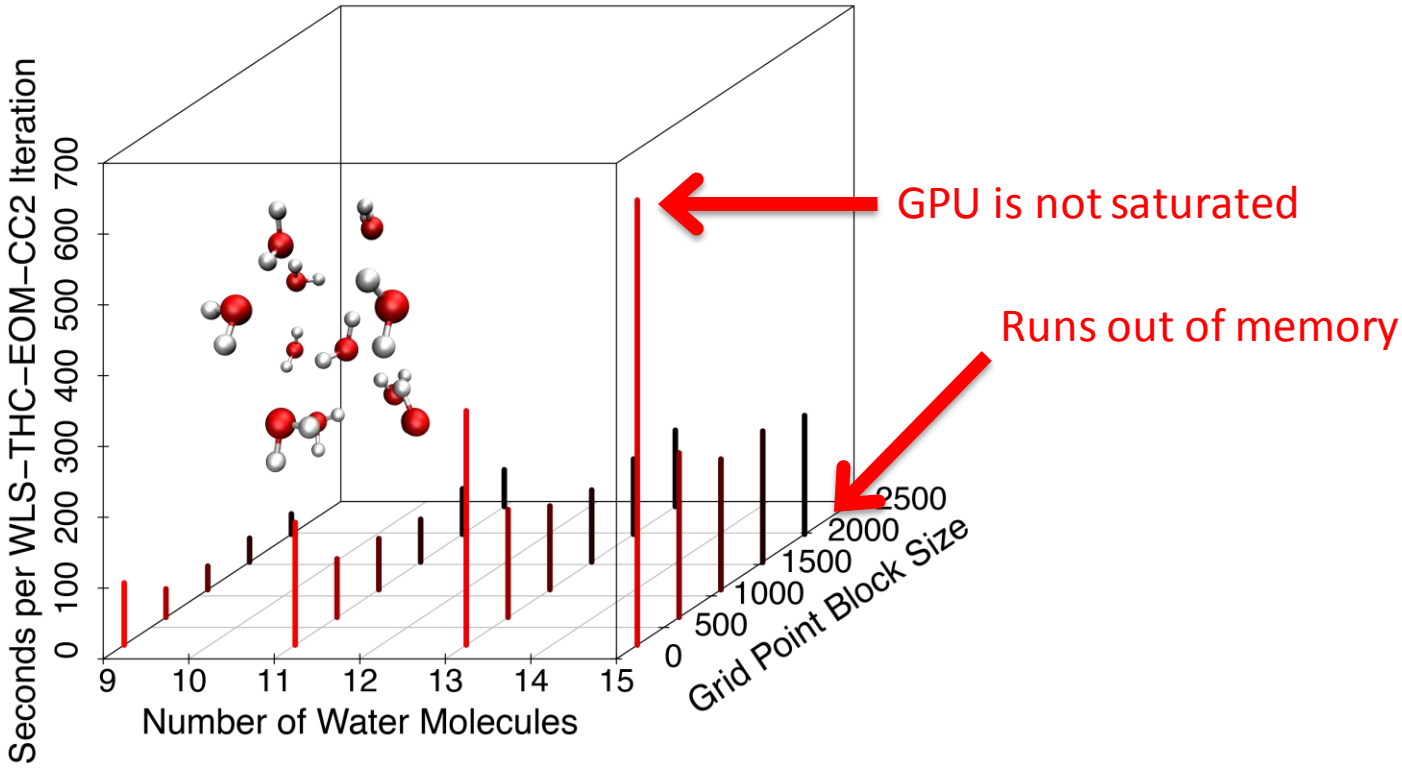
$$(mn|ls) \approx \sum_{PQ} X_m^P X_n^P Z^{PQ} X_l^Q X_s^Q$$



GPU Accelerated THC-CC2



GPU Accelerated THC-EOM-CC2 Timings



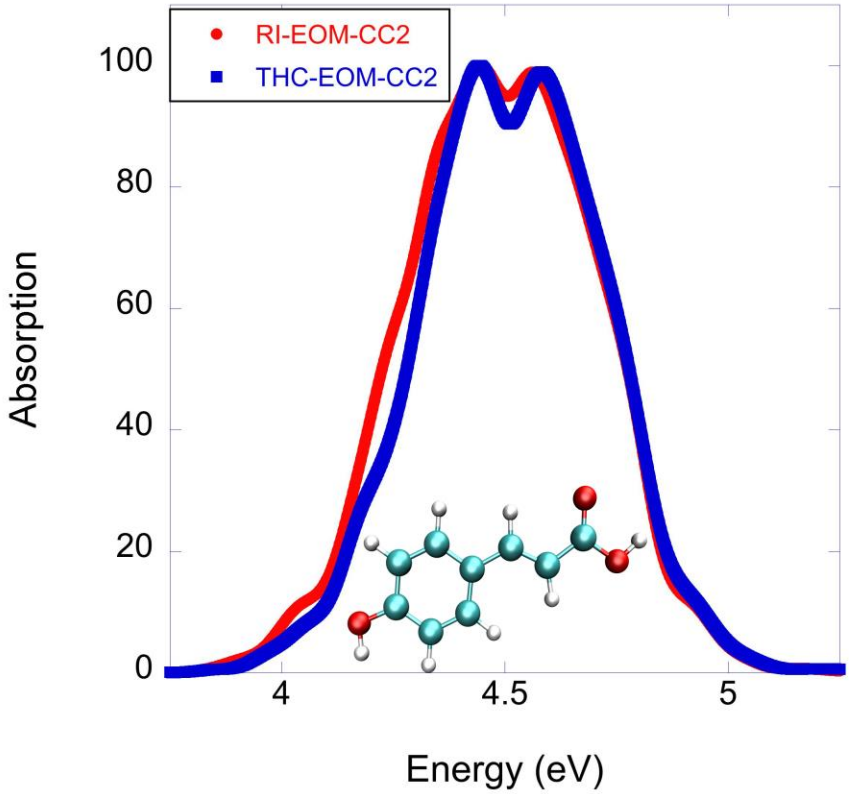
Basis Set: cc-pVDZ

Number of Grid Points per H_2O Molecule: 220

GPU: NVIDIA S2050s

Absorption Spectra Benchmark

Photoactive Yellow Protein(PYP) Chromophore

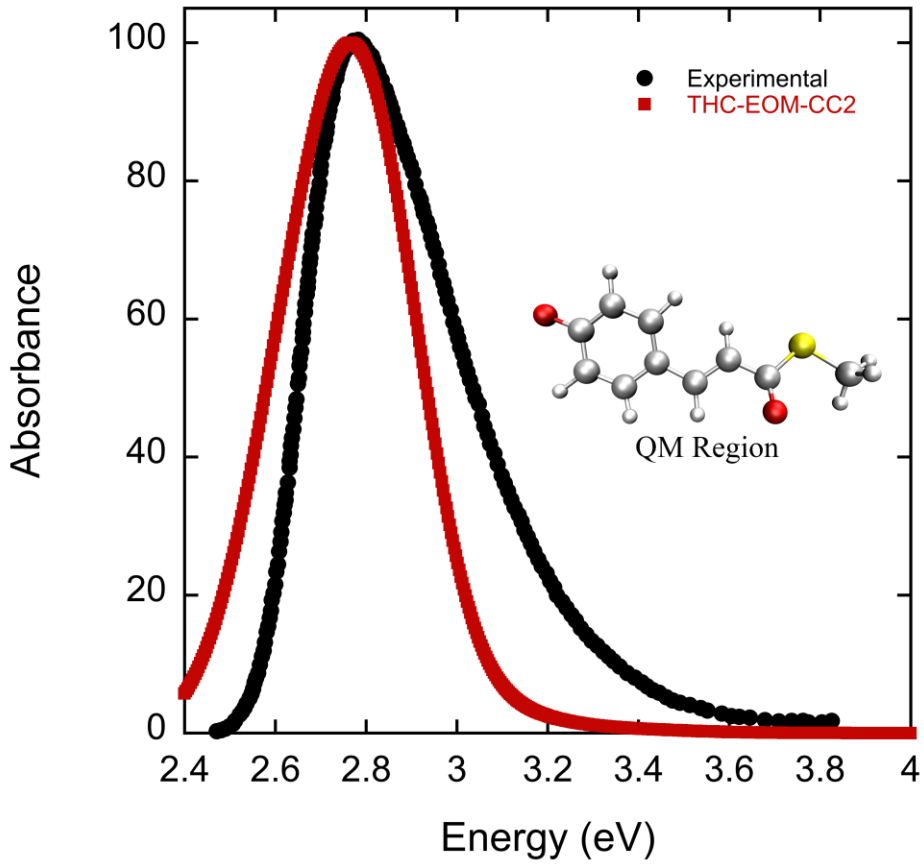


- Geometries : Wigner Distribution, 500 per spectra
- Single point energy calculations convoluted with Gaussians
- 5 Excited states per geometry
- THC-EOM-CC2 Dipole Moment ≈

$$< F_0 | \hat{R}^{(0)} \hat{m} \hat{R}^{(n)} | F_0 >^2$$

QM/MM PYP Absorption Spectra

- Experimental: wild-type PYP
- 100 geometries sampled from 100 ns of a DFT trajectory
  - 2 excited states per geometry
  - protein environment
- TDDFT
  - 6-31G*, wPBE
  - $\lambda_{max} = 3.51\,eV \pm 0.04$
- THC-EOM-CC2
  - cc-pVDZ
  - 0.04 eV shift



C. M. Isborn, et al., *JCTC*, **7**, 1814 (2011).
B. Borucki, et al., *J. Phys. Chem B*, **109**, 629 (2004).

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- Martínez Group

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