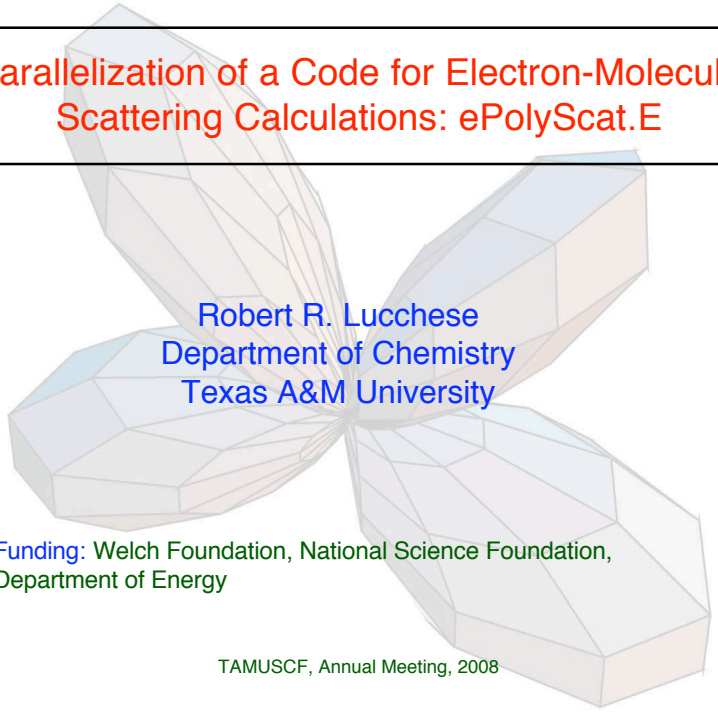
Parallelization of a Code for Electron-Molecule Scattering Calculations: ePolyScat.E



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Design Goals

- ePolyScat.D, a legacy serial code
  - Many separate executables
  - Coarse grained parallelization using shell scripts
  - Low memory usage
    - Heavy use of scratch disk files
    - Communication between executables through disk
  - Static array allocation
- ePolyScat.E, distributed-memory parallel ($N \leq 64$)
  - One executable
  - Limited disk I/O using only the master node
  - Dynamic array allocation
  - All intermediate data held in core
  - Fortran 90, MPI message passing

Basic Equations

The three dimensional Schrodinger equation for an electron interacting with a molecule

$$H\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

Use expansion in the angular coordinates

$$\psi(r,\theta,\phi) = \sum_{l=0}^{l_{\max}} \sum_{m=-l}^{l} \frac{1}{r} f_{lm}(r) X_{lm}(\theta,\phi)$$

Differential equation for radial functions

$$\left\{ -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - E \right\} f_{lm}^{n}(r) + \sum_{l'm'} V_{lm,l'm'}^{\text{static}}(r) f_{l'm'}^{n}(r)$$
$$= \sum_{l'm'} \int_0^{\infty} V_{lm,l'm'}^{\text{exchange}}(r,r') f_{l'm'}^{n-1}(r') dr'$$

Distribute Grid on Processors

The problem is solved on a grid

$$f_{lm}(r) \Rightarrow f_{lmk} = f_{lm}(r_k) \quad k = 1,\text{K}\ ,M$$

Each of the *N* processor then has part of the grid

$$[1,\text{K}\ ,M_1]\ [M_1+1,\text{K}\ M_2]\ \text{L}\ [M_{N-1}+1,\text{K}\ M_N]$$

- The grid has different step sizes in different regions of the molecule
- Different values of $l_{\max}$ are used in different regions
- Different numbers of points are allocated to each processors

Exchange Integrals

The exchange integral contains a term from the Coulomb potential of the form

$$I_l(r) = \frac{1}{r^{l+1}} \int_0^r (r')^l \, g(r') dr' + r^l \int_r^\infty \frac{1}{(r')^{l+1}} g(r') dr'$$

Partial integrations are done independently on each processor and the sums are obtained in VDiff using MPI_SCAN

$$I^k = \sum_{j=1}^{k} P^j$$

Solution of the Inhomogeneous Diff Eq

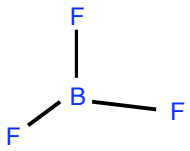
- The solution of the differential equation can also be written as a series of matrix multiplications

$$\mathbf{f}_N = \mathbf{T}_N \mathbf{T}_{N-1} \cdots \mathbf{T}_2 \mathbf{T}_1 \mathbf{f}_0$$

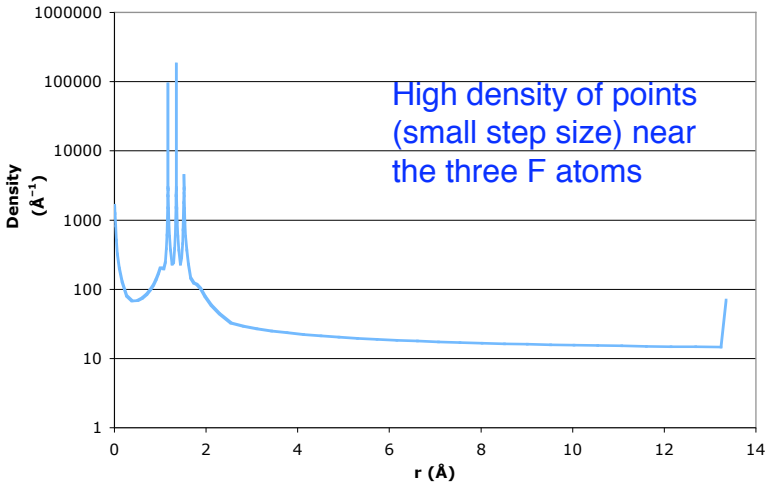
  where each $\mathbf{T}_k$ matrix resides on a different processor.
- Unfortunately, in order to obtain numerical stability, the computation of $\mathbf{T}_k$ depends in part on the value of the vector obtained on the *k*-1 processor.
- Current code in GHomo uses a pipeline for parallelization.

Test Runs on Hydra

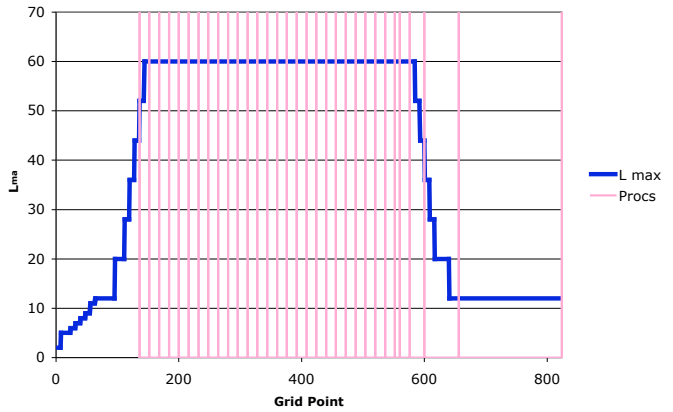
- Tests using 8, 16, 32, and 64 processors with 8 processors per node
- Elapsed time ranged from 3 hours for 8 processors to 1 hour with 64
- Production runs typically use 32 processors
- Test jobs compute the photoionization of BF_3 in an asymmetric planar geometry



Radial Grid Density

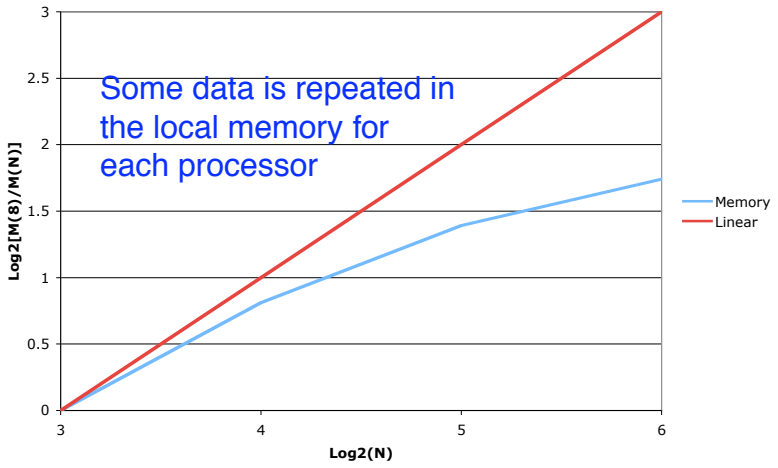


Partial Wave Expansion

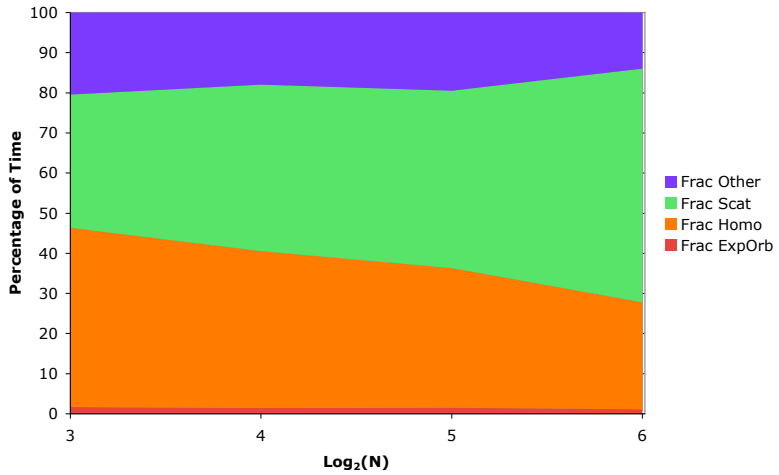


Distribution of grid on 32 processors, work ~ $L^{1.5}$

Memory Usage



Distribution of Time in ePolyScat



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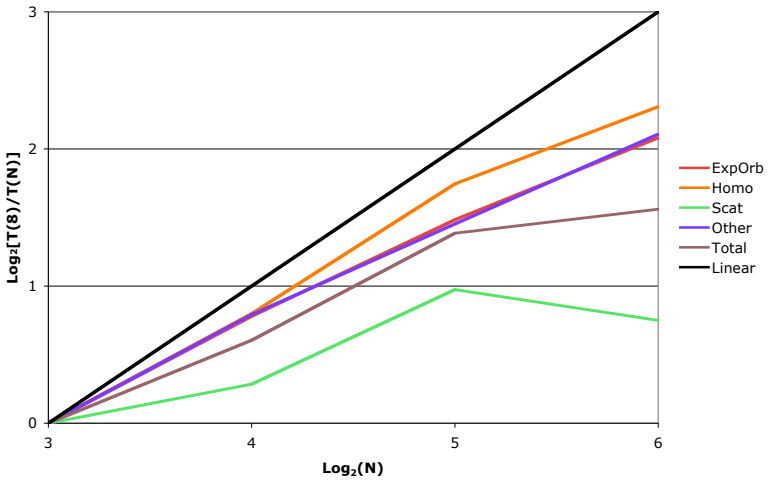
Speedup in ePolyScat



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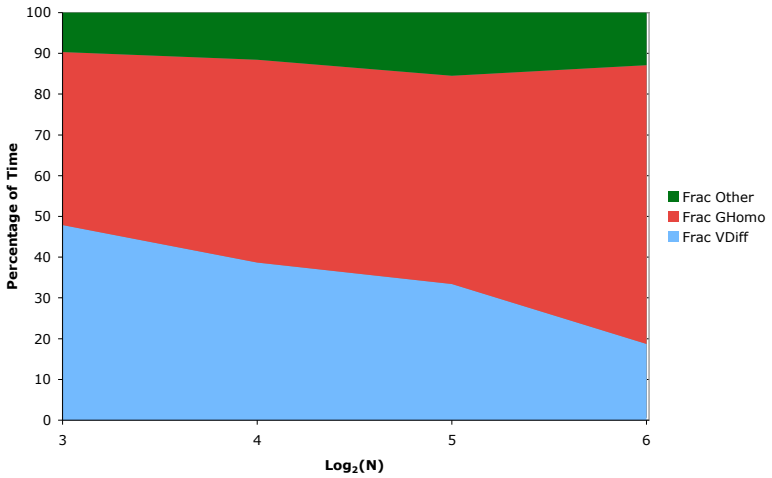
Distribution of Time in Scat



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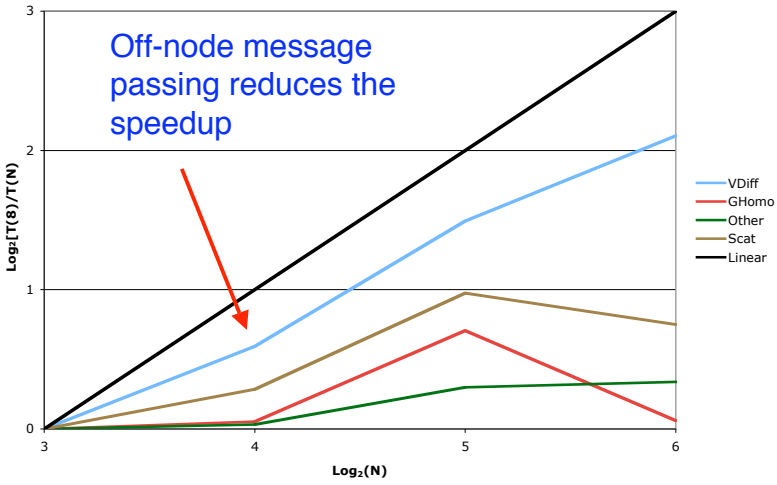
Speedup in Scat



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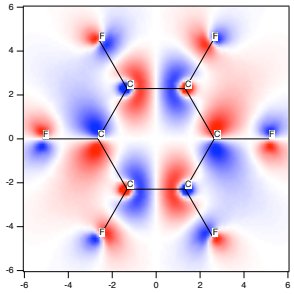
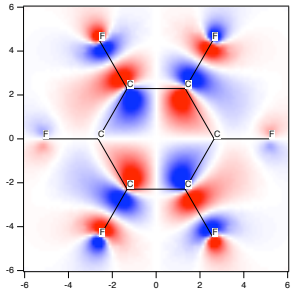
Photoionization of C_6F_6 Leading to the $C\,^2B_{2u}$ State of $C_6F_6^+$

$b_{2u} \rightarrow ke_{2g}$



σ^*(C-F) and σ^*(C-C)
E=18.5 eV, Γ = 0.31 eV



σ^*(C-F) and π^*(C-C)
E=21.0 eV, Γ = 0.49 eV

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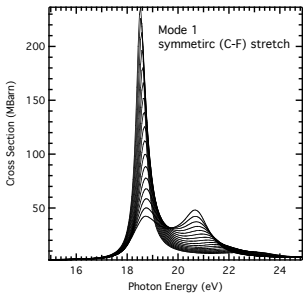
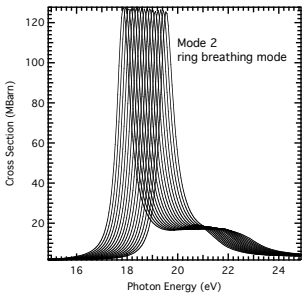
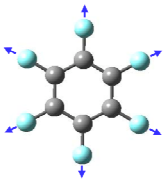
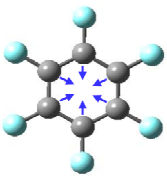
Response to the Two Symmetric Modes









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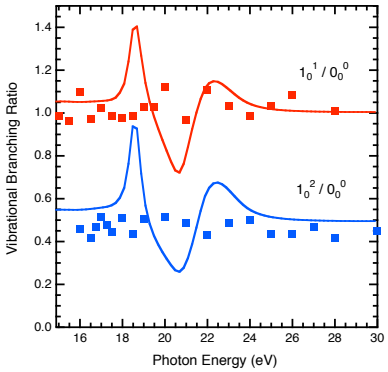
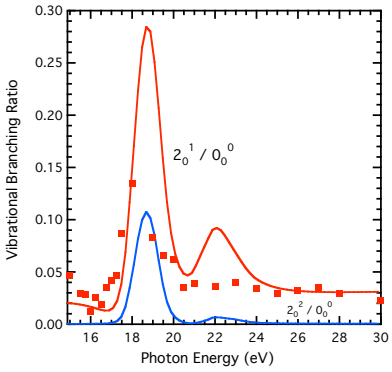
C_6F_6 Vibrational Branching Ratios



Mode 1



Mode 2

Experiments of E. Poliakoff and coworkers, Louisiana State University

Conclusions

- Parallelization has been achieved using up to 32 processors
- The combination of a parallel code and a significant computational resource, i.e. hydra, has allowed us to consider much larger systems
- To go beyond 32 processors
  - Additional work on the bottleneck, GHomo
  - Consider larger systems
    - systems with no symmetry
    - electron correlation, i. e. multichannel
  - Additional coarse grained parallelization, e. g. more that one scattering energy at one time
- http://www.chem.tamu.edu/rgroup/lucchese/ePolyScat.E2.manual/manual.html