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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

\[ \psi(r,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm}(r) \chi_{lm}(\theta,\phi) \]

Differential equation for radial functions

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

**Distribute Grid on Processors**

The problem is solved on a grid

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

Each of the \( N \) processors then has part of the grid

\[
\left[ 1, K, M_1 \right] \left[ M_1 + 1, K, M_2 \right] \ldots \left[ M_{N-1} + 1, K, M_N \right]
\]

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

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Exchange Integrals

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

\[ I_l(r) = \frac{1}{r^{l+1}} \int_0^r (r')^l g(r') dr' + r^l \int_0^\infty \frac{1}{r^{l+1}} g(r') dr' \]

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
  \[ f_N = T_N T_{N-1} L T_2 T_1 f_0 \]
  where each \( T_k \) matrix resides on a different processor.
- Unfortunately, in order to obtain numerical stability, the computation of \( T_k \) 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

High density of points (small step size) near the three F atoms
Partial Wave Expansion

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

Memory Usage

Some data is repeated in the local memory for each processor
**Distribution of Time in ePolyScat**

![Graph showing distribution of time in ePolyScat](image)

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**Speedup in ePolyScat**

![Graph showing speedup in ePolyScat](image)

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Distribution of Time in Scat

Off-node message passing reduces the speedup

Speedup in Scat
Photoionization of C₆F₆ Leading to the C⁺²B₂u State of C₆F₆⁺

\[ b_{2u} \rightarrow \text{k}_{e_{2g}} \]

\( \sigma^*(C-F) \) and \( \sigma^*(C-C) \)
\[ E = 18.5 \text{ eV}, \ \Gamma = 0.31 \text{ eV} \]

\( \sigma^*(C-F) \) and \( \pi^*(C-C) \)
\[ E = 21.0 \text{ eV}, \ \Gamma = 0.49 \text{ eV} \]

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Response to the Two Symmetric Modes

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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 than one scattering energy at one time