Parallel spin-orbit CI

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Research Effort

- Actinide containing systems. (U, Pu, etc.)
  - Requires high-accuracy
    - c / mass effects
    - spin-orbit (SO) effects
    - structural and dynamic correlation effects.
  - Software must be modified.
    - Calculations require the fastest/biggest machines.
- Chemistry
  - f-f transition energies (+assignments)
  - Large ionization pots. (large formal charges)

Approach.

- Build models using modern formalism.
  - ARECPs-incorporates important c / mass effects in core.
  - SO operator rigorously included. (ARECP-RECP)
  - In a form useable in standard (spin-orbital) CI code
  - Permits valence correlation.
- Build upon available software.
  - F90 and C languages.
  - Global Arrays (GA) for distributed data.
  - Parallel I/O (ChemIO) for distributed out-of-core work.
  - Start with available "legacy" code (CIDBG.X)
    - COLUMBUS system

Conventional SOCI

- Massive, sparse eigenvector problem.
- Symmetric and Real*
- Conventional, i.e., "Direct" approach
  - Construct whole matrix.
  - Store H on disk
- Solve iteratively.
  - (Davidson's method)

- *Can be made real for select point groups

- Construct H in double-group basis.
  - Precompute configuration list.
  - Include all configs satisfying total "J" (neither LS not jj coupling)
  - Store coupling information in memory/disk
    - **fine-grain access.**
- Eigenvectors (~40-50)
  - Blocks of degeneracies
  - all roots under 2-3 eV

Spin-Orbit CI (SOCI)

$$\mathrm{H} = \sum_{\mu} h_{\mu} - \sum_{\mu>\nu} \frac{1}{\mathrm{r}_{u\nu}} + \sum_{l} O_l\, \xi_l(\mathrm{r}) \left(\vec{l} \cdot \vec{s} \right) O_l$$

$$h_{\mu} = \frac{-1}{2} \nabla^{2}_{\mu} + \sum_{\alpha}^{N} \left(\frac{-Z^{eff}{}_{\alpha}}{r_{\alpha\mu}} + U_{\alpha}^{ARECP} \right)$$

H. time-independent hamiltonian operator.

μ,ν index valence electrons. α indexes nuclei.

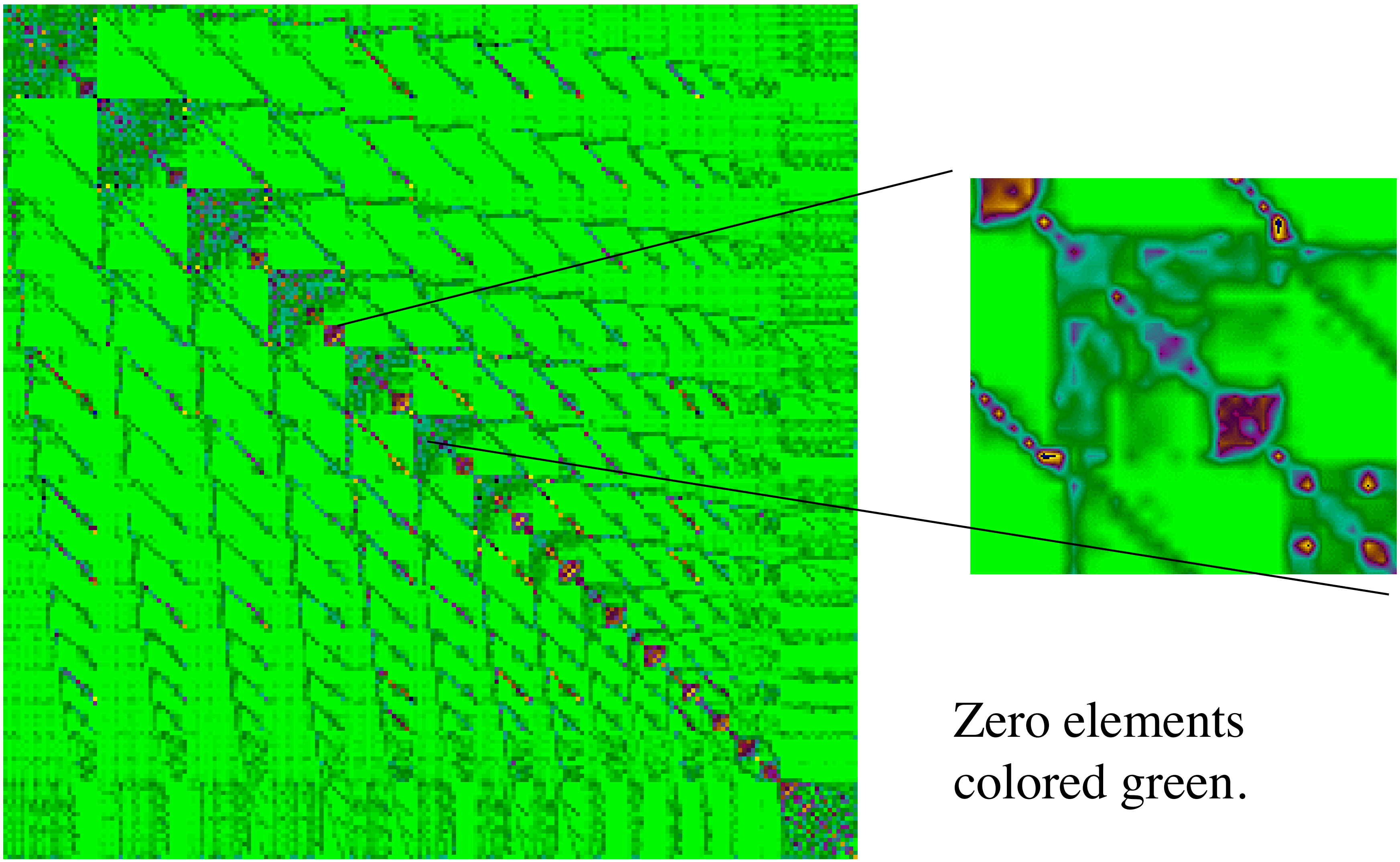
U^{ARECP} is j averaged-RECPs.

$\xi_l\,(\mathrm{r}) = 2\Delta \mathrm{U}_l^{RECP}/(2l+1)$

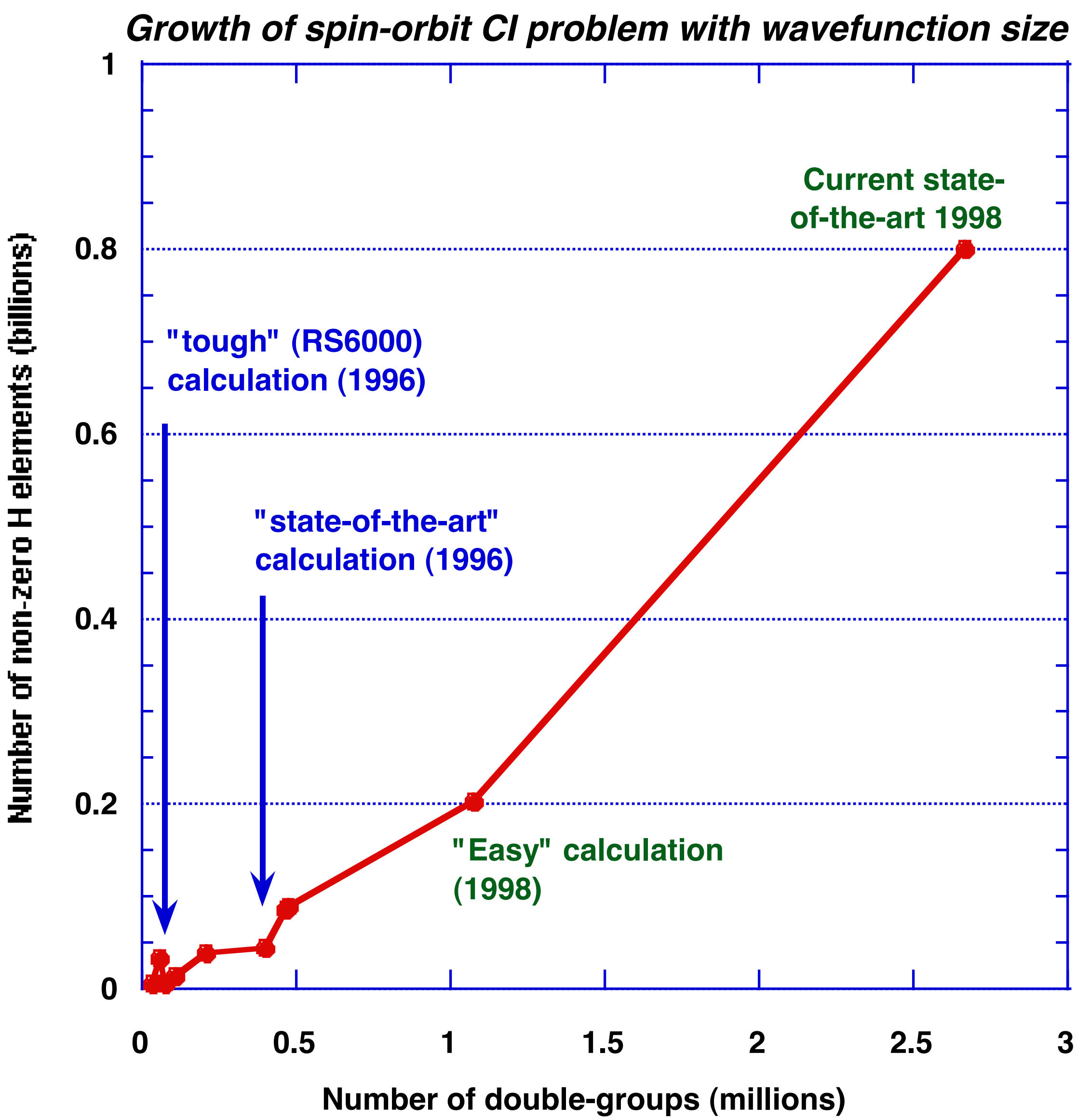
O_l formally projects ξ(r) back into $|lm_l\rangle$.

Rigorous inclusion of spin-orbit terms. AO integrals only in standard basis required.

Sample hamiltonian



Zero elements
colored green.



Growth of spin-orbit CI problem with wavefunction size
Number of non-zero H elements (billions)
Number of double-groups (millions)
0
0.2
0.4
0.6
0.8
1
0
0.5
1
1.5
2
2.5
3
"tough" (RS6000)
calculation (1996)
"state-of-the-art"
calculation (1996)
"Easy" calculation
(1998)
Current state-
of-the-art 1998

Parallel SOCI

- CIDBG.X algorithm changes.
  - Wavefunction description.
    - Precompute couplings in concurrent blocks
    - Store in distributed memory memory*
  - Hamiltonian construction
    - Static load-balancing scheme.
    - Construct in concurrent blocks
    - Store in distributed "storage"
  - Eigenvectors
    - Borrow NWChem parallel Davidson.

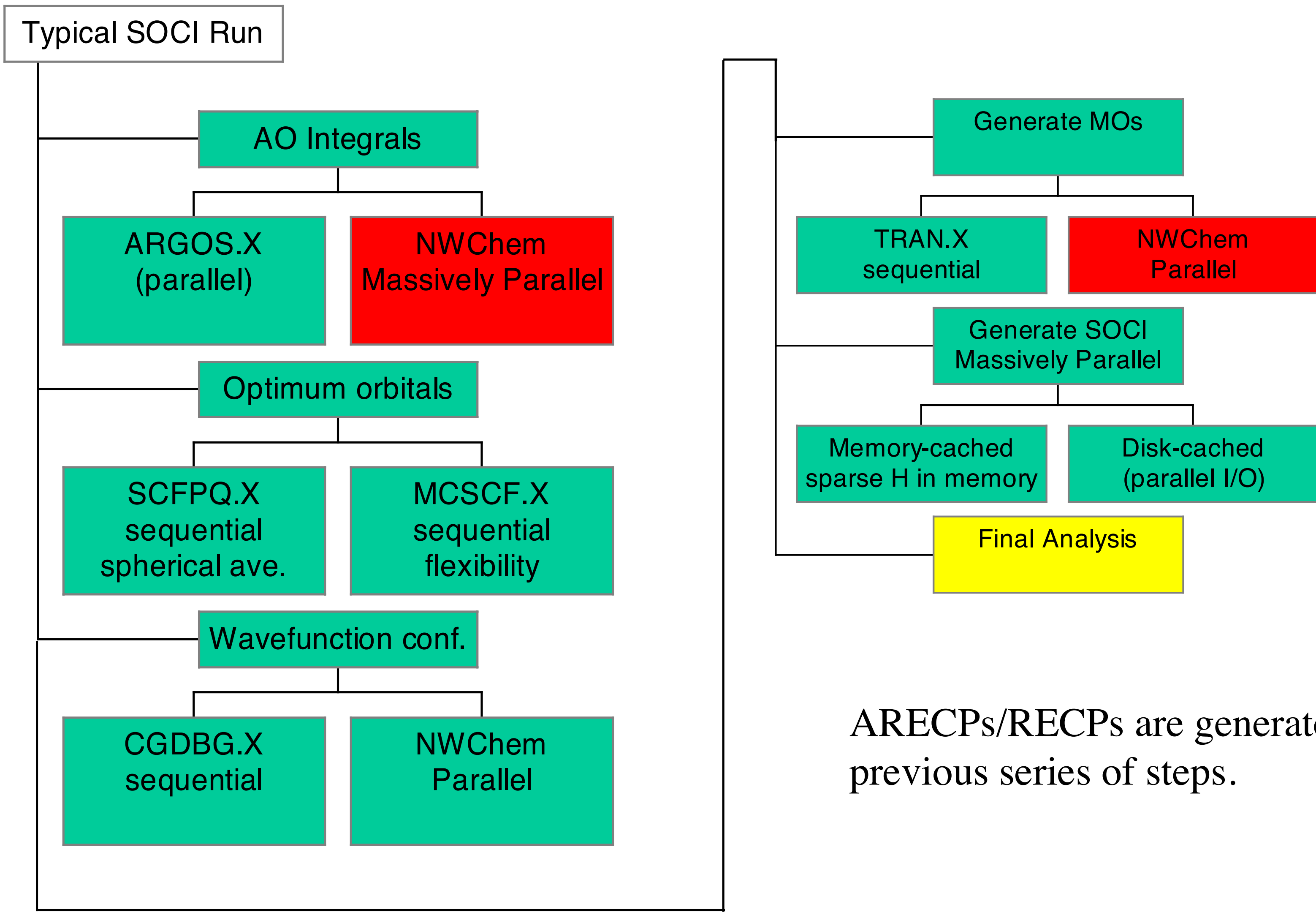
- Global Arrays 2.3 (GA)
  - Constructs and manages distributed-data space.
  - Permits portable imp.
  - Little perceived performance penalty.
  - Simple implementation

*fine grained access. Works very well on the T3E. High latency on the SPs requires the application to chunk data.

Parallel H storage

- Method One - Fastest
  - Store H in aggregate memory using GA
  - Simple distribution changes
- Limited problem sizes.
  - approx. 8 million double-groups. (theoretical)
  - Largest to-date: 3 million
- Method Two - Larger problems.
  - Store H onto disks using ChemIO.
  - Exclusive access model (EAF), no striping.
  - Each node writes "its" part of H to its local-disk.
- I/O times slower than memory access.

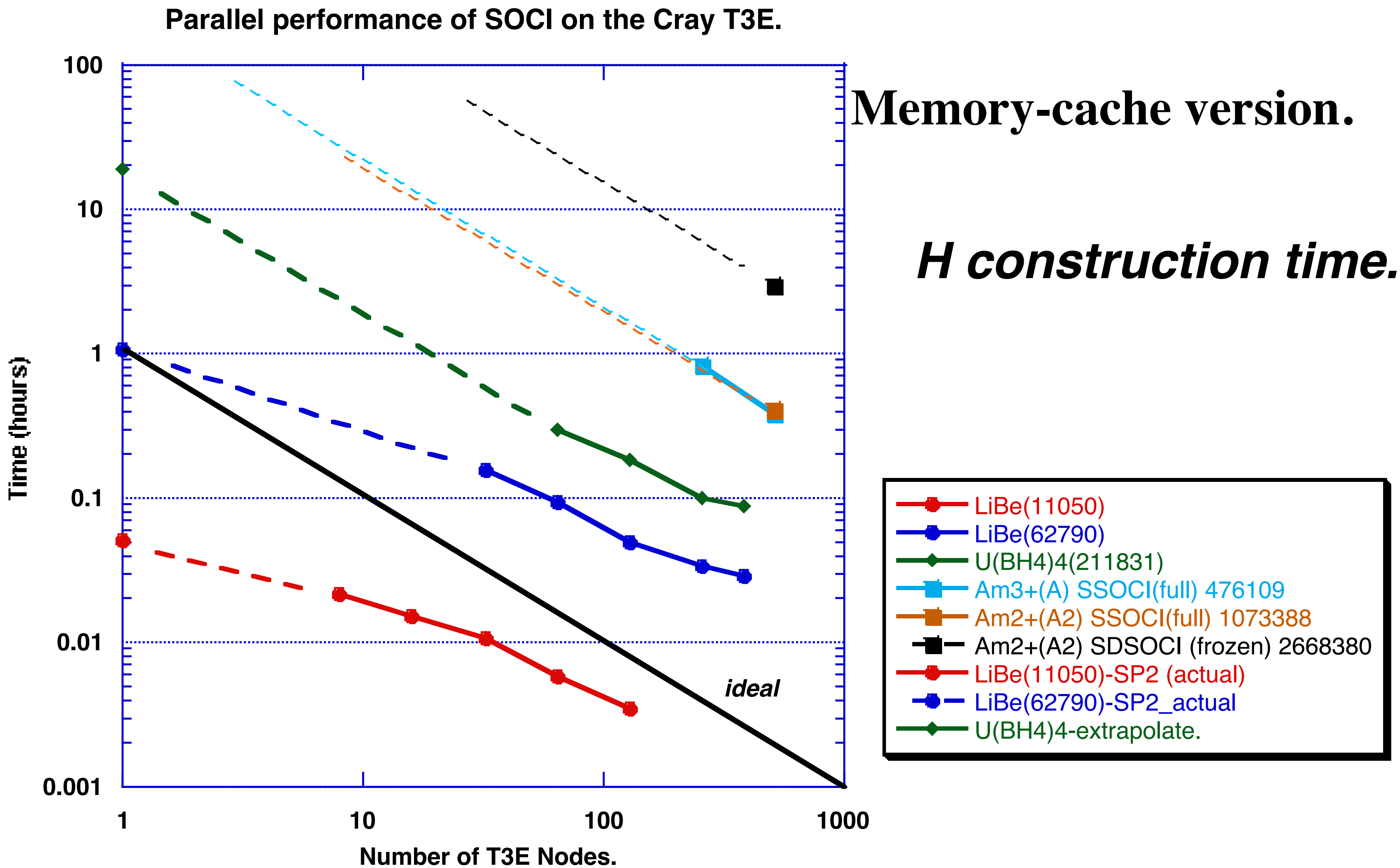
SOCI Procedure. (typical)



ARECPs/RECPs are generated in a previous series of steps.

SOCI Performance

Method 1- Memory cached



Memory-cache version.

H construction time.

Disk I/O SOCI.

- Initial tests
  - Replaced H memory store with H disk store.
  - A simple approach
  - Permits restart
  - BUT ! Subsequent read performance poor.
    - I/O Access too fine-grained
- Prefetching algorithm
  - Increased performance
  - Uses same algorithm.
  - Portable.
- Method.
  - Explicit (application level) prefetching
  - H store still performing single column access.

Application prefetching.

- Attempt to increase *read* performance.
  - by minimizing latency
  - achieving better B.Width utilization.
- Method
  - H columns are contiguous on disk.
  - Hence, Read several H columns at one time.
- Method.
  - Simple additional interface to ChemIO.
  - Specify maximum prefetched rows.
  - Fully in-core if possible.
- Experiments
  - How much should we prefetch ?
  - how good can we get ?

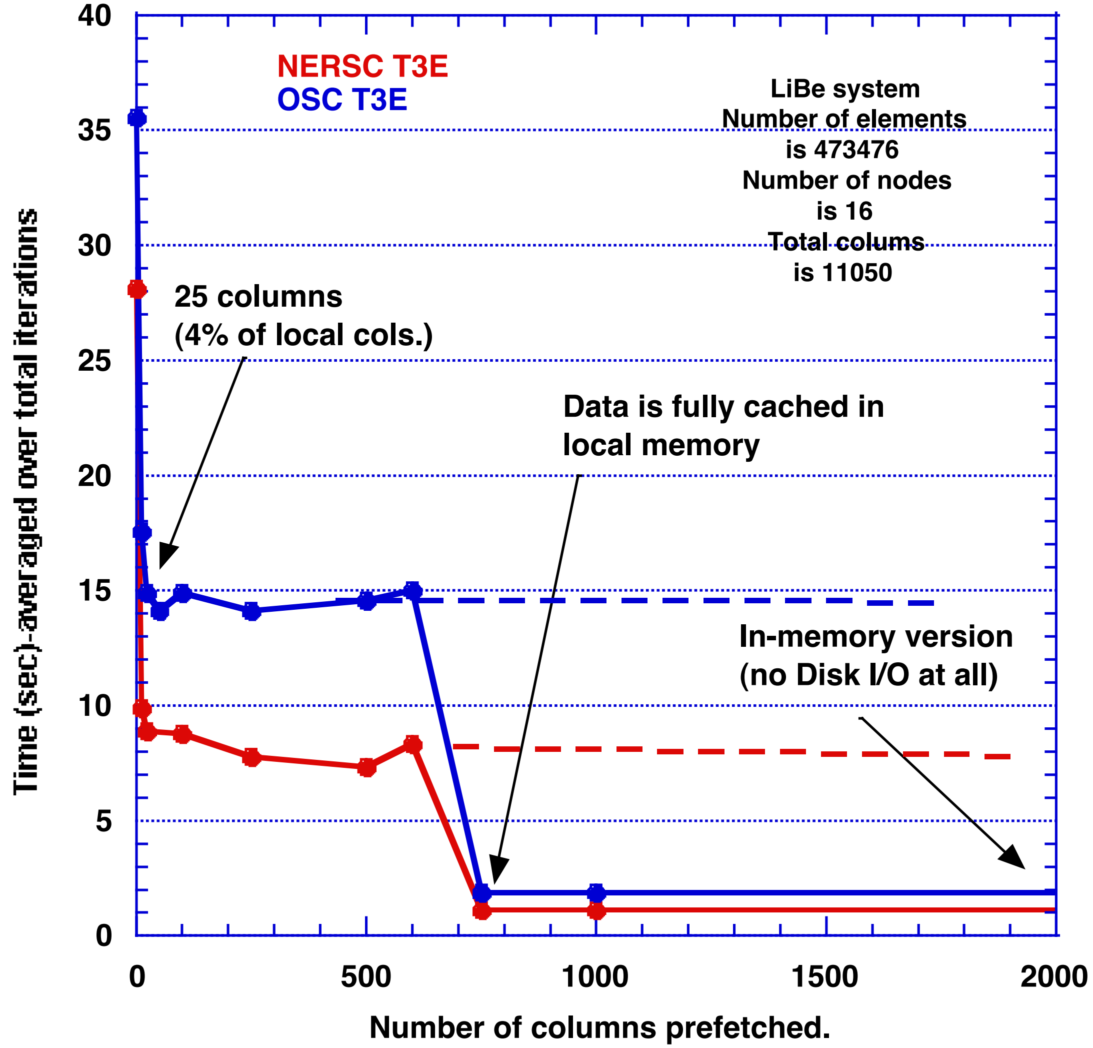
Hamiltonian I/O step

- Performance good.
  - Write 1 column at a time. (non-zeros only)
  - No “chunking” of writes.
  - H sufficiently complicated that 1-column accesses are good.
- No additional modifications (yet) required.

Eigenvector I/O step

- Problem step.
  - Lots of I/O latencies.
  - H columns sparse (10K)
    - Poor utilization of BW
  - Little work per column read.
  - Many vectors/poor guesses/Lots of iterations.
- Requires prefetching or equivalent

Prefetching Tests.
Parallel matrix-vector product.



Prefetching summary.

- Hamiltonian construction.
  - Two times slower than in-core version.
  - Still room for improvement.
  - Good for now.
- Matrix-vector products.
  - 5-8 times slower per product.
    - (nominal prefetching)
  - Still less time than H construction.
  - Lots of new things to try.

Future Plans

- Further optimizations and tuning of SOCI.
- Semi-direct approach.
    - Determine distribution of work w.r.t. stored H blocks.
    - Build this into integrated storage and load description.
- Incorporate dynamic load-balancing.
- Explore MPI-2 implementation.
- Interface/Merge ideas into NWChem.
- SOCI analytic gradients

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Select WWW sites and References

Project: http://www.emsl.pnl.gov:2080/proj/tms/hpcc_actinides/source.html

Global Arrays: http://www.emsl.pnl.gov:2080/docs/global/ga.html
ChemIO: http://www-c.mcs.anl.gov/chemio/

COLUMBUS: http://www.itc.univie.ac.at/~hans/Columbus/columbus_homep.html.
NWChem: http://www.emsl.pnl.gov:2080/docs/nwchem/nwchem.html

RECPs: Ermler, W.C.; Lee, Y.S.; Christiansen, P.A.; Pitzer, K.S. *Chem. Phys. Lett.* **1981**, *81*, 70.

SOCI (sequential): Pitzer, R.M.; Winter, N.W. *J. Phys. Chem.* **1988**, *92*, 3061.

This list is intended to be representative and not complete.