Computer Aided Implementation of Many-Body Methods: The Tensor Contraction Engine

Oak Ridge National Laboratory

David E. Bernholdt,
Venkatesh Choppella,
Robert Harrison

Pacific Northwest National Laborator

So Hirata

Ohio State University

Gerald Baumgartner, Daniel Cociorva,
Russ Pitzer, P Sadayappan,
a small army of graduate students

Louisiana State University

J Ramanujam

University of Waterloo

Marcel Nooijen, Alexander Auer

ab initio Quantum Chemistry

Array of new methodological developments:

Excited States
Explicitly correlated methods
Local correlation methods
Multireference methods
Relativistic effects
Combining low- and high-accuracy regimes

Computed quantities:

Energies
Energy gradients
Properties, ...

Variety of computer architectures:

PC’s and workstations
Small clusters
Massively Parallel machines

The (re-)Coding Bottleneck of Quantum Chemistry

New ideas are emerging continuously.
Developing and testing new ideas is time consuming.

Good ideas should be incorporated (all the way) in efficient production-level codes.

Much of actual coding is fairly routine.

Can we teach the computer to do the job?

Can we train the computer to do the job
better than we could ever do it ourselves?

Automation will support ***evolving*** technology.

Advantages of computer aided implementations

A) Developing new methodologies:

- Codes expected to be robust and free of errors.
- Develop and test new ideas quickly.
- Generation of *many* similar pieces of code.

B) Develop High Performance implementations:

- Explore variety of algorithms in convenient way.
- Computer codes can evolve and improve over time.
- Parallelization is important but “technical” issue

Compare TCE to “compiler - *BLAS* - *EIGPACK*”

A) Operator Contraction Engine (*OCE*): Generating Many-Body equations

- General set of tools to derive many-body equations, based on second quantization and Wick's theorem.

- Additional manipulations of equations, e.g.
  - Derive energy gradients, second derivatives.
  - Obtain AO-based expressions for local methods.
  - … active orbitals … Choleski factorization of integrals … MRCC … Spin-adaptation …

Input from users

B) Tensor Contraction Engine (*TCE*):
Generate efficient computer codes

Methods in *ab initio* quantum chemistry: sums of tensor contractions $\longrightarrow$ Uniform automated implementation.

- Factorization of tensor expressions.
- Prepare precise list of intermediates and tensor contractions (operation tree).
- Synthesize Fortran code to evaluate sequence of tensor contractions.
- Various strategies to develop parallel codes.

Task for TCE team

PNNL prototype version of OCE/TCE (So Hirata)

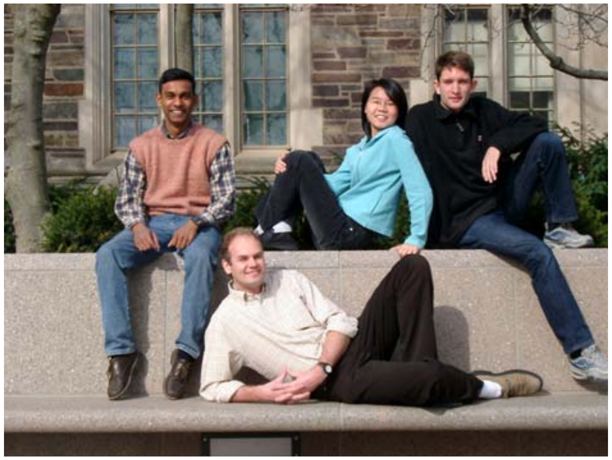
Programming language ***Python***
Interfaced to NWChem (PNNL) and UTChem (University of Tokyo)

Spin-orbital based, Abelian spatial symmetry
Full treatment of permutational symmetry and antisymmetry.
Parallellization using Global Arrays *or* Replicated Data Structures *or* Global File System.

High-order canonical MO-based CC / CI / MBPT
Production level codes up to quadruple excitations (CCSDTQ) in NWchem
Equation-of-Motion CC and excited state properties.

Relativistic Douglas-Kroll and 4-component Fock-Dirac in UTchem

Waterloo directions for OCE / TCE (Alexander Auer)



Local correlation approaches:

Enveloping (atomic-like) non-orthogonal occupied orbitals.
Pure AO’s for the virtual space.

Hierarchy of methods:
Local PT
Local Coupled Cluster

Use PT results to select amplitudes to be treated at CC level.

Dynamical construction of intermediates & screening

Parallel CCSD(T) code

“Loop fusion,
reduced communication,
evolving code,
partially hand-coded”

Ohio State / ORNL version of TCE

Computer Science approach:

Algorithms for
- Operation minimization (factorization)
- Memory Minimization (loop fusion)
- Space-Time trade-off (recomputation)
- Data locality
- Effective parallellization

TCE analogous to compiler

Contents of the TCE work shop

- Introduction (Marcel Nooijen)
- Overview of the prototype TCE (So Hirata)
- A practical example: CCSD (Alex Auer)
- Optimizations in the second generation TCE (Sadayappan)

- Discussion