EMSL

Parallelization and benchmarks

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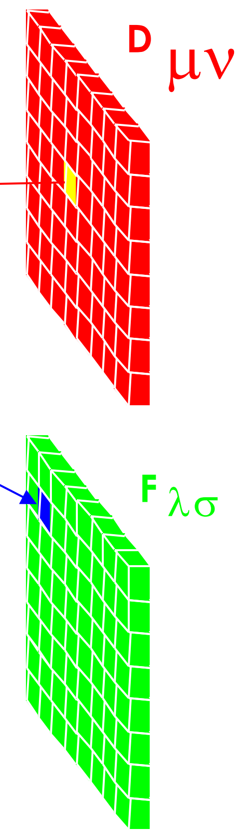
Gaussian DFT computational kernel Evaluation of XC potential matrix element

$$\rho(\mathbf{x}_Q) = \sum_{\mu\nu} D_{\mu\nu}\, \chi_\kappa(\mathbf{x}_Q)\, \chi_\nu(\mathbf{x}_Q)$$

$$F_{\lambda\sigma} += \sum_Q w_Q\, \chi_\lambda(\mathbf{x}_Q)\, V^{XC}[\rho(\mathbf{x}_Q)]\, \chi_\sigma(\mathbf{x}_Q)$$

```
my_next_task = SharedCounter()
   do i=1,max_i
      if(i.eq.my_next_task) then
         call ga_get()
            (do work)
         call ga_acc()
         my_next_task =
SharedCounter()
      endif
   enddo
barrier()
```



Both **GA operations** are greatly dependent on the communication **latency**

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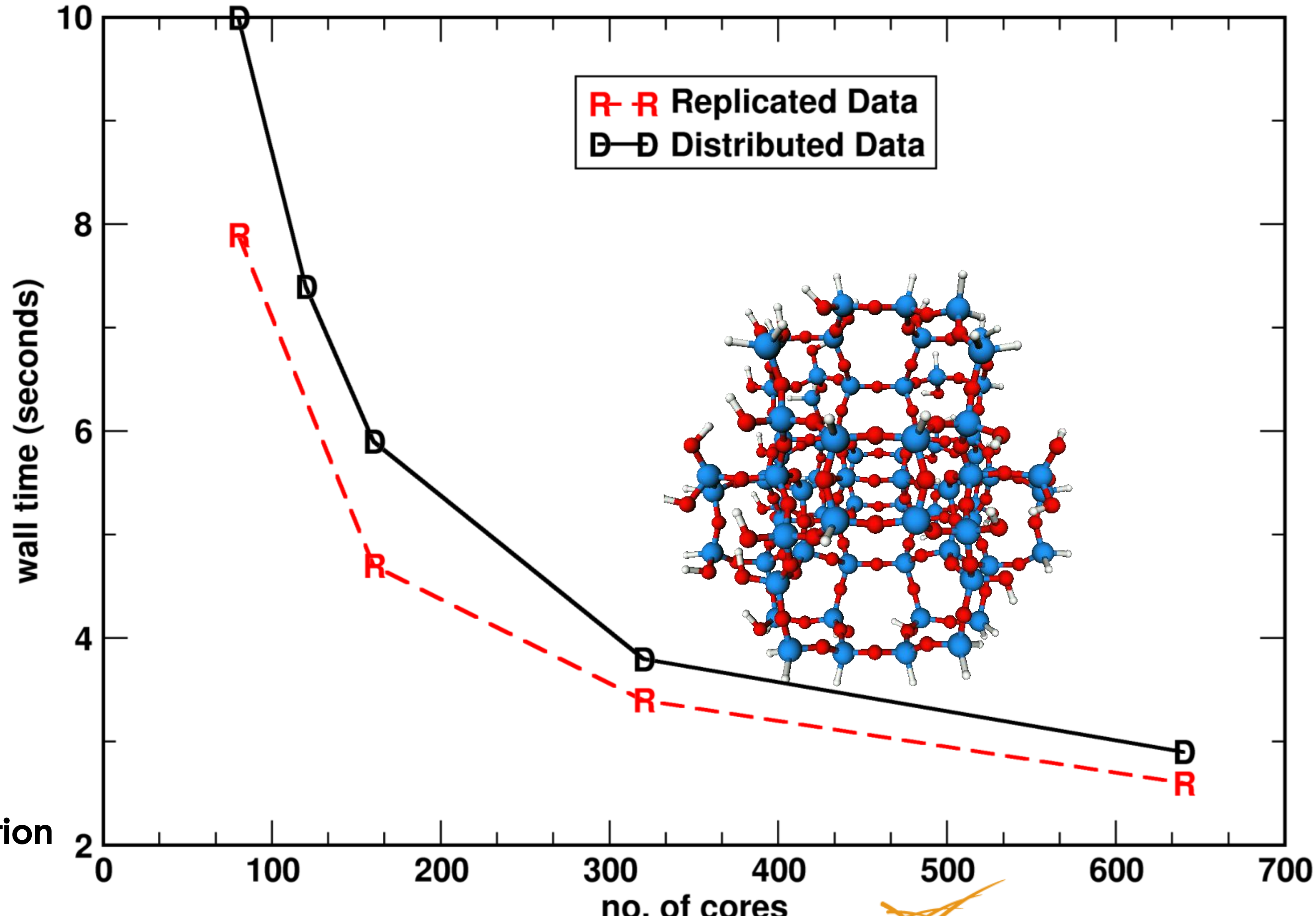
Parallel scaling of the DFT code



$Si_{28}O_{148}H_{66}$

3554 Basis functions

LDA wavefunction

XC build

Benchmark run on

Cray XK6

Parallel scaling of the DFT code

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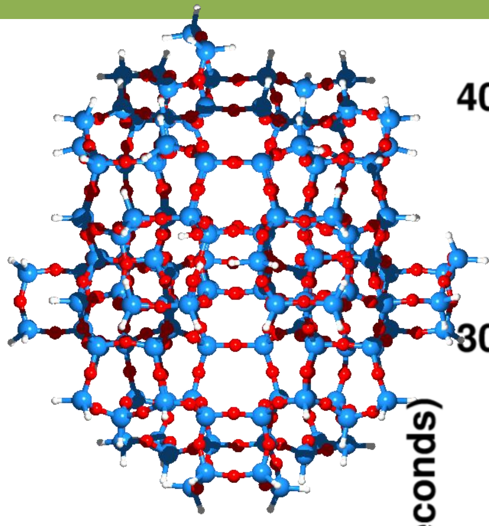

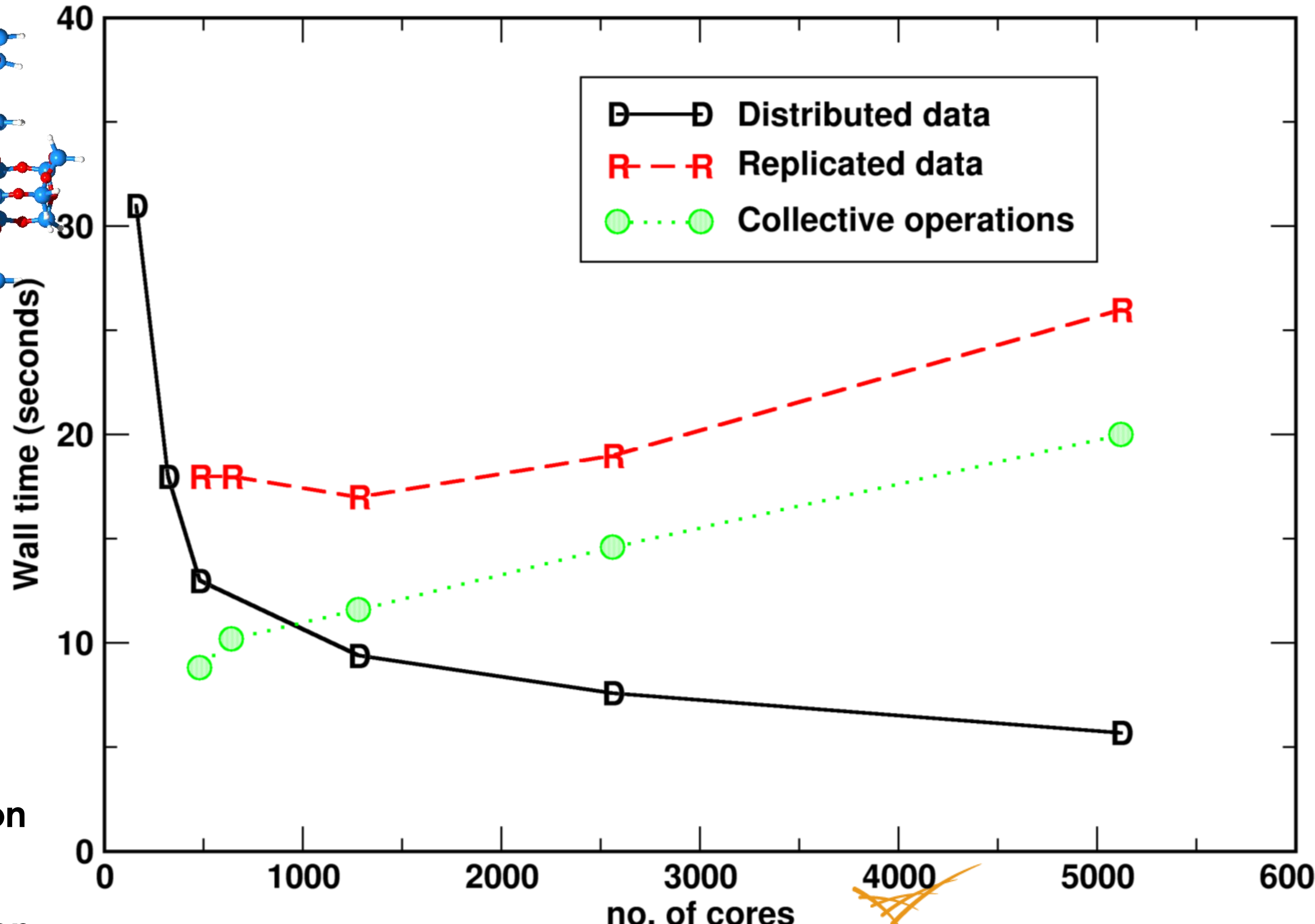

$Si_{159}O_{264}H_{110}$

7108 Basis functions

LDA wavefunction

XC build

Benchmark run on

Cray XK6

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CCSD(T) run on Cray XT5 : 24 water

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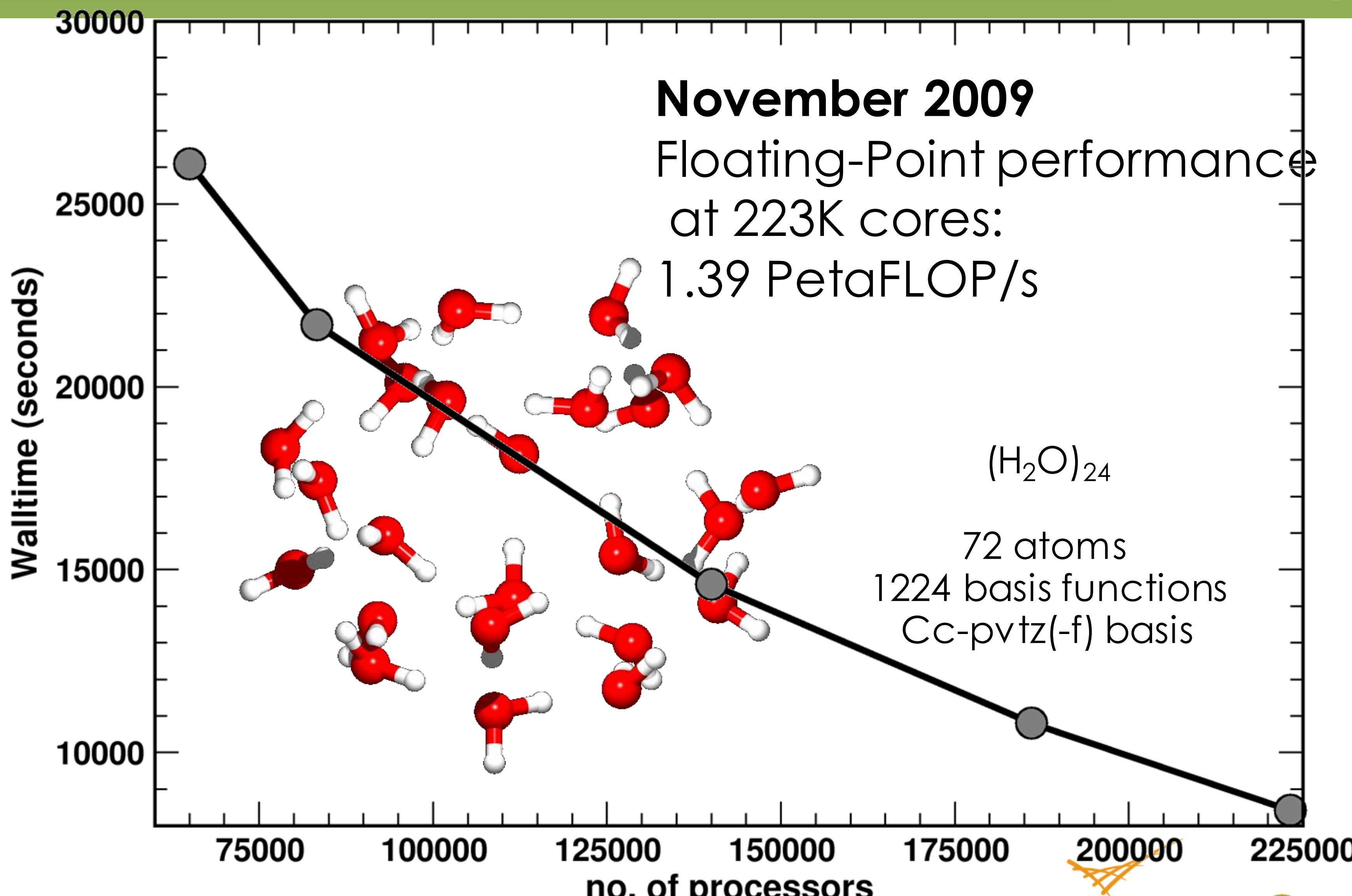

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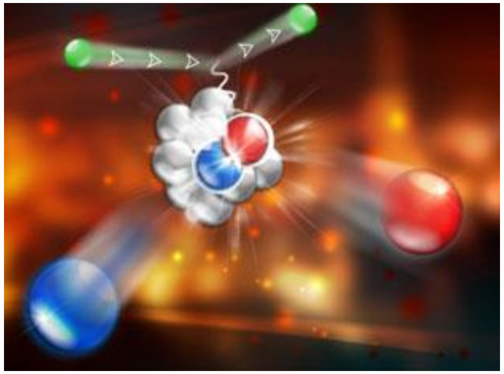
What we want to solve

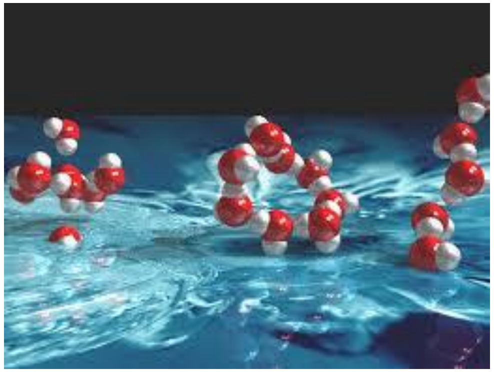
$$\hat{H}\left|\Psi(1,\ldots,N)\right\rangle = E\left|\Psi(1,\ldots,N)\right\rangle$$

Many Particle Systems

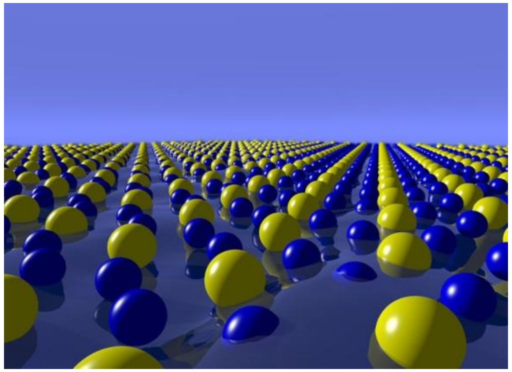
Nuclear Physics



Quantum Chemistry

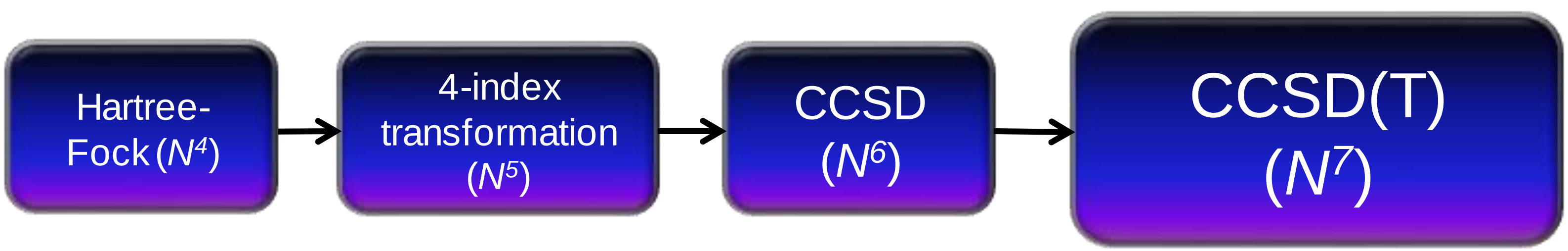


Solid State Physics



Coupled Cluster method

Method	Numerical complexity
CCSD (singles & doubles)	N^6
CCSD(T) (perturbative triples)	N^7
CCSDT (singles & doubles & triples)	N^8
CCSDTQ (singles & doubles &triples & quadruples)	N^{10}



What is Tensor Contraction Engine (TCE)

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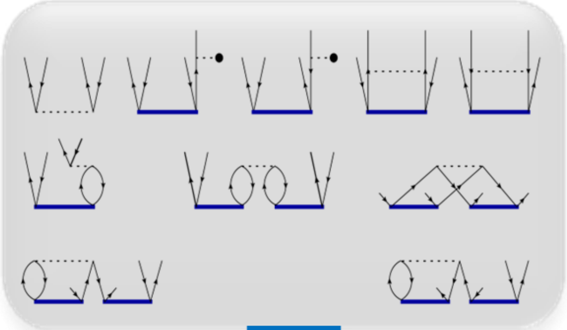
- Symbolic manipulation & program generator
  - Automates the derivation of complex working equations based on a well-defined second quantized many-electron theories
  - Synthesizing efficient parallel computer programs on the basis of these equations.

- Granularity of the parallel CC TCE codes is provided by the so-called tiles, which define the partitioning of the whole spinorbital domain.



OCE

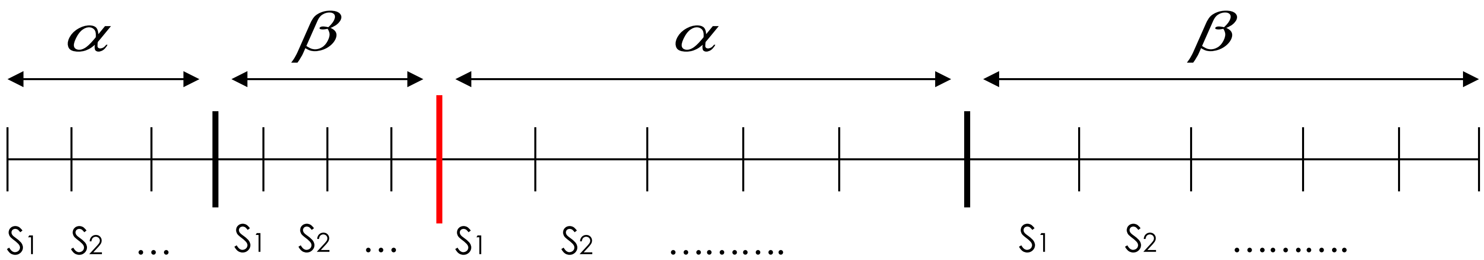
$$+\frac{1}{4}v^{mn}_{ef}t^{ef}_{ij}t^{ab}_{mn}-\frac{1}{2}v^{mn}_{ef}t^{ef}_{mi}t^{ab}_{nj}+$$

TCE

```
next = NXTASK(nprocs, 1)
DO p3b = noab+1,noab+nvab
DO p4b = p3b,noab+nvab
DO h1b = 1,noab
DO h2b = h1b,noab
IF (next.eq.count) THEN
CALL GET_HASH_BLOCK(d_a,dbl_mb(k_a),dim
- 1 + (noab+nvab) * (h1b_1 - 1 + (noab+
+nvab) * (p3b_1 - 1)))))
CALL GET_HASH_BLOCK_I(d_a,dbl_mb(k_a),d
```

What is Tensor Contraction Engine (TCE)

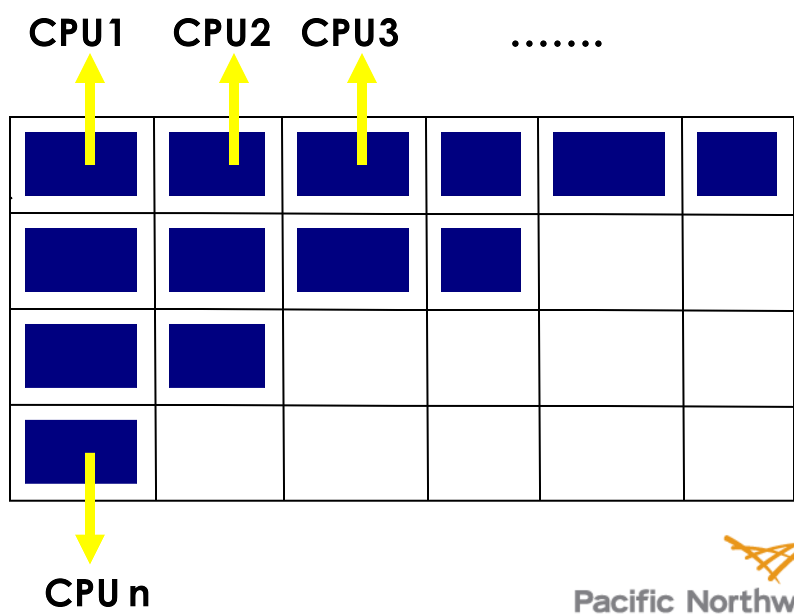
Tile structure:



Occupied spinorbitals **unoccupied spinorbitals**

Tile-induced block structure of the CC tensors:

$$T_a^i \Rightarrow T_{[p_n]}^{[h_m]}$$



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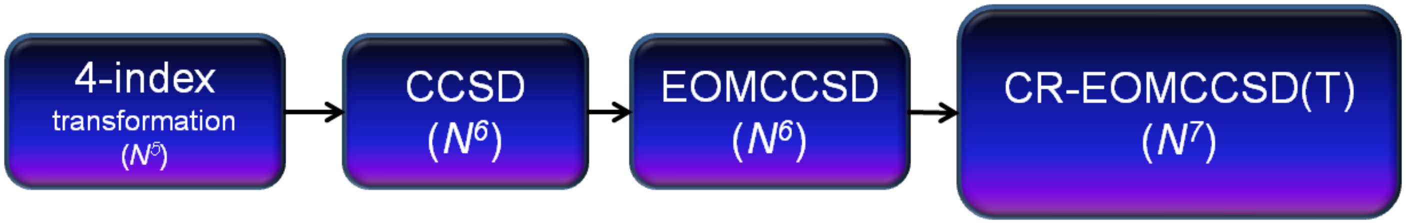
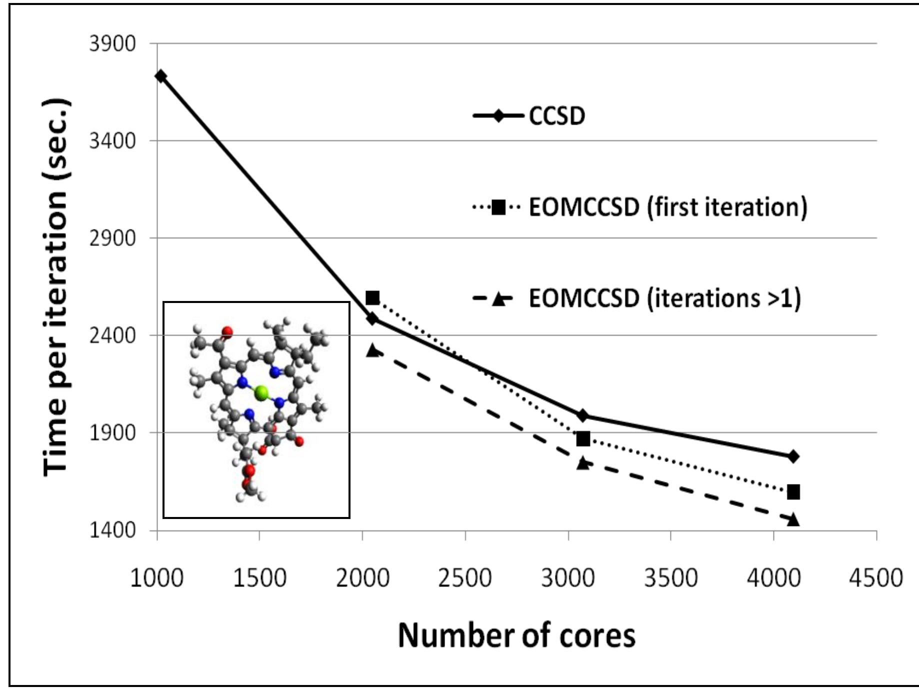
New elements of parallel design for the iterative CCSD/EOMCCSD method

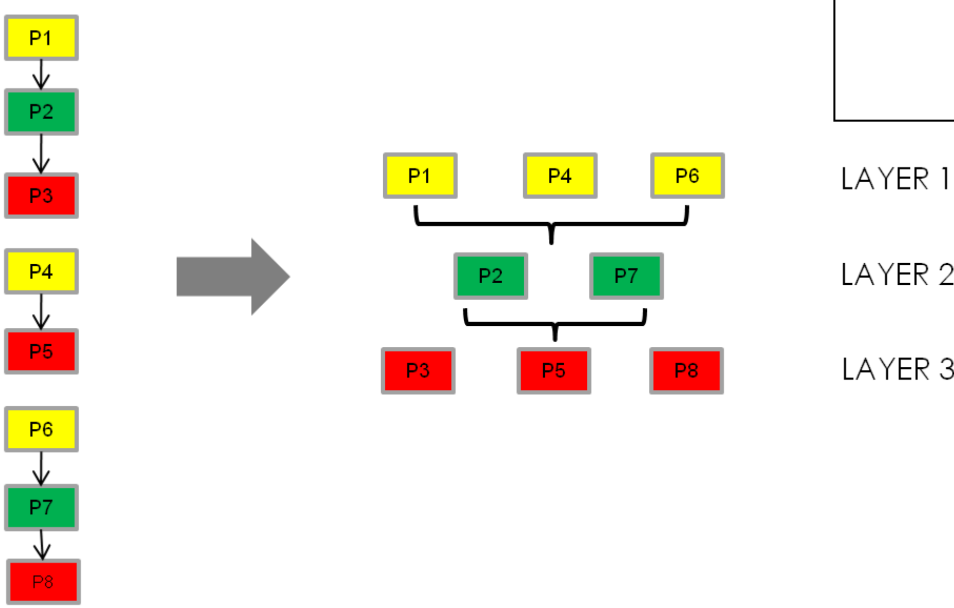


- Use of Global Arrays (GA) to implement a distributed memory model
- Iterative CCSD/EOMCCSD methods (basic challenges)
  - Global memory requirements
  - Complex load balancing
  - Complicated communication pattern: use of one-sided `ga_get,ga_put,ga_acc`
- Implementation improvements
  - New way of representing antysymmetric 2-electron integrals for the restricted (RHF) and restricted open-shell (ROHF) references
  - Replication of low-rank tensors
  - New task scheduling for the CCSD/EOMCCSD methods

Scalability of the iterative EOMCC methods

- Alternative task schedulers
  - use "global task pool"
  - improve load balancing
  - reduce the number of synchronization steps to absolute minimum
  - larger tiles can be effectively used





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New elements of parallel design for the non-iterative CR-EOMCCSD(T) method

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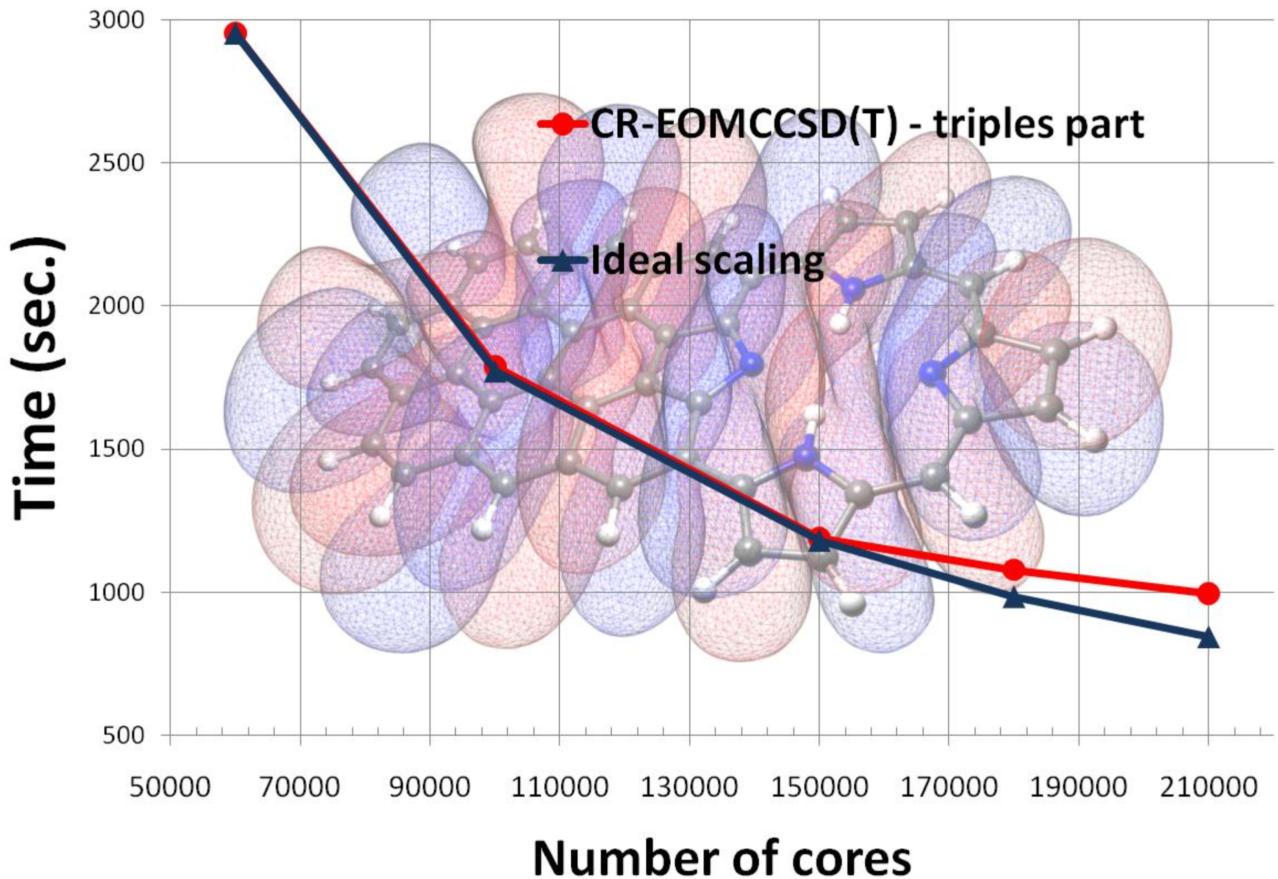
- Use of Global Arrays (GA) to implement a distributed memory model
- Basic challenges for Non-Iterative CR-EOMCCSD(T) method
  - Local memory requirements: $(\text{tilesize})^4$ (EOMCCSD) vs. $M^*(\text{tilesize})^6$ (CR-EOMCCSD(T))
- Implementation improvements
  - Two-fold reduction of local memory use : $2^*(\text{tilesize})^6$
  - New algorithms which enable the decomposition of six-dimensional tensors

Scalability of the non-iterative EOMCC code

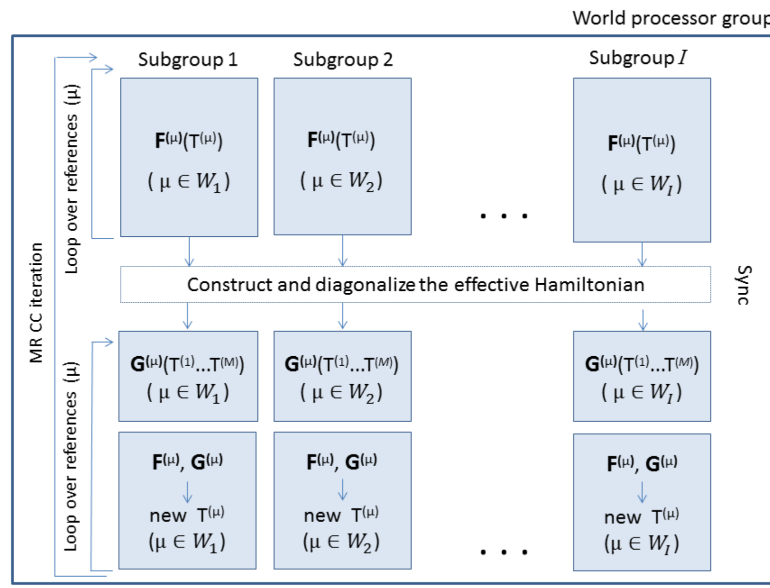
94 %parallel efficiency using 210,000 cores

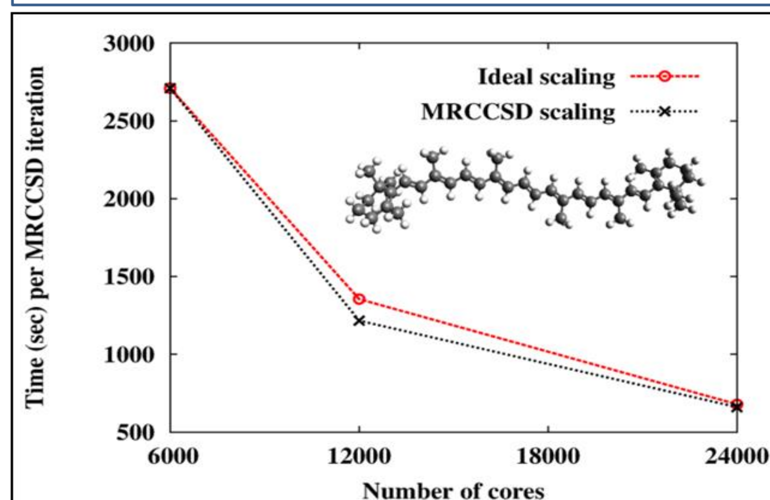


- Scalability of the triples part of the CR- EOMCCSD(T) approach for the FBP-f-coronene system in the AVTZ basis set. Timings were determined from calculations on the Jaguar Cray XT5 computer system at NCCS.

Multireference CC methods

- Multireference CC methods in NWChem (next release)
  - Strongly correlated excited states
  - Implemented MRCC approaches
    - Brillouin-Wigner MRCCSD
    - Mukherjee Mk-MRCCSD approach
    - State-Universal MRCCSD (under testing)
    - Perturbative triples corrections MRCCSD(T)
  - Novel paralellization strategies based on the processor groups
  - Demonstrated scalability of MRCCSD across 24,000 cores





Multireference CC methods

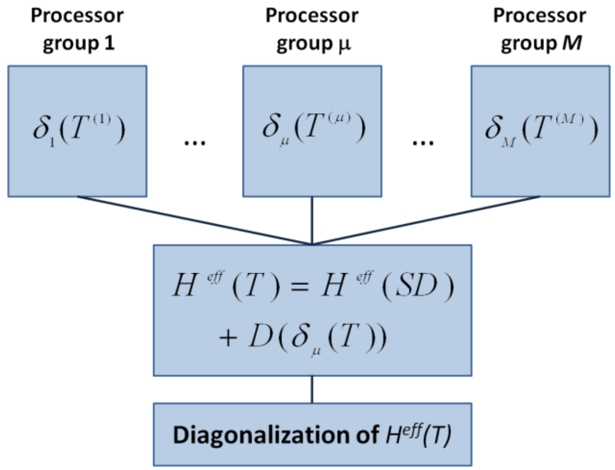
- Improve the quality of the MRCCSD approaches
- Counteract the intruder-state problem

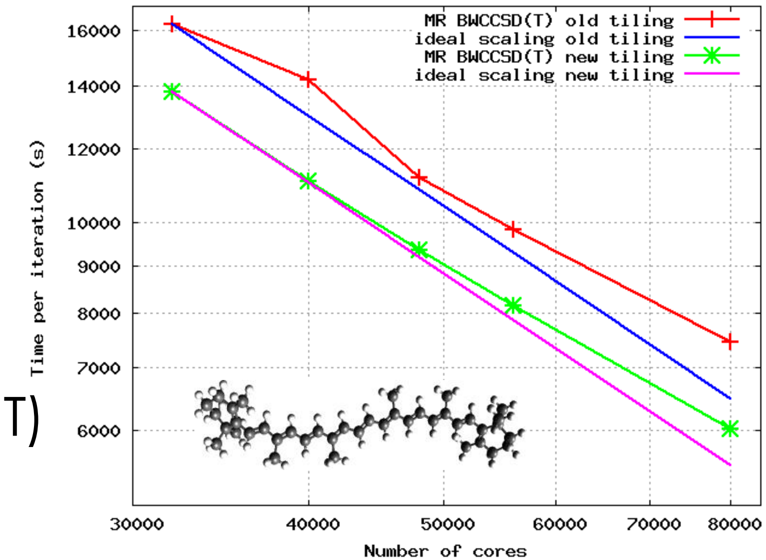
$$H^{eff}_{\mu\mu}(T) = H^{eff}_{\mu\mu}(SD) + \delta_{\mu}(T^{(\mu)})$$

Numerical complexity $\sim M \times N^7$

Scalability $\sim M \times$ *(scalability of the CCSD(T) approach)*

GPU implementations of the MRCCSD(T) approaches are currently tested





K. Bhaskaran-Nair, J. Brabec, J. Pittner, H.J.J. van Dam, E. Apra, K. Kowalski, JCP (accepted).

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Questions?