Improving CASINO performance for models with large number of electrons

Dario Alfè, Mike Gillan
UCL, London, UK

Lucian Anton
NAG Ltd, Oxford, UK

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Outline

- Introduction
- Algorithms for distributed data
  - Shared memory
  - MPI two-sided
  - MPI one-sided & SHMEM
- Second Level Parallelism
  - MPI
  - OpenMP
- IO at large scale
- Conclusions

QMC and CASINO

Quantum Monte Carlo techniques are used to compute electronic structure of solids, large molecules, nano-clusters...

- Very precise results
- Good scaling with system size
- Good parallel efficiency

CASINO developed by Theory of Condensed Matter group, Cambridge University.

Fortran 95 +MPI

http://www.tcm.phy.cam.ac.uk/~mdt26/casino2.html

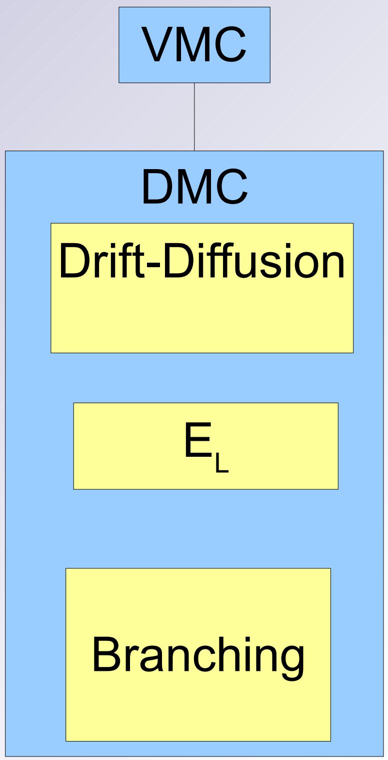
Background

- Quantum many-body systems: N_e electrons, N_I ions.
- Computationally challenging problem and of practical interest.

$$i\hbar \frac{\partial \Psi(R,t)}{\partial t} = -\frac{\hbar^2}{2\mathrm{m}} \sum_{i=1}^{N_e} \nabla_i^2 \Psi(R,t) + V(R, R_I)\Psi(R,t)$$

$$E = \frac{\langle \Psi | H \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

CASINO QMC computational steps



$$\frac{1}{(2\pi\tau)^{3N/2}}\exp\left(-\frac{\left(\boldsymbol{R}-\boldsymbol{R}'-\tau\boldsymbol{v}(\boldsymbol{R}')\right)^2}{2\tau}\right)$$

$$E_L(\boldsymbol{R})=\Psi^{-1}\boldsymbol{H}\Psi$$

$$\exp\left(-\frac{\tau}{2}\left[E_L(\boldsymbol{R})+E_L(\boldsymbol{R}')-2E_T\right]\right)$$

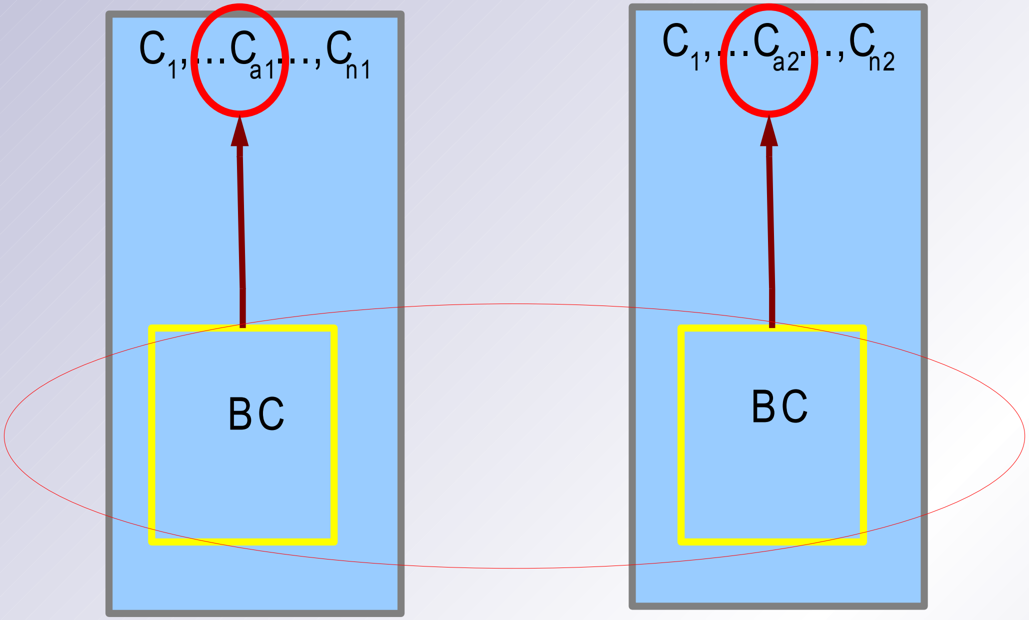
Blip coefficients

$$\Psi = f(t) e^{J} D_{\uparrow} D_{\downarrow}$$

$$D_{\uparrow} = \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \cdots & \phi_1(r_{N_\uparrow}) \\ \vdots & \cdots & \cdots & \vdots \\ \phi_{N_\uparrow}(r_1) & \phi_{N_\uparrow}(r_2) & \ldots & \phi_{N_\uparrow}(r_{N_\uparrow}) \end{vmatrix}$$

$$\mathrm{BC}(N_o, 0:N_{gx}-1, 0:N_{gy}-1, 0:N_{gz}-1, N_s)$$

The origin of the memory problem



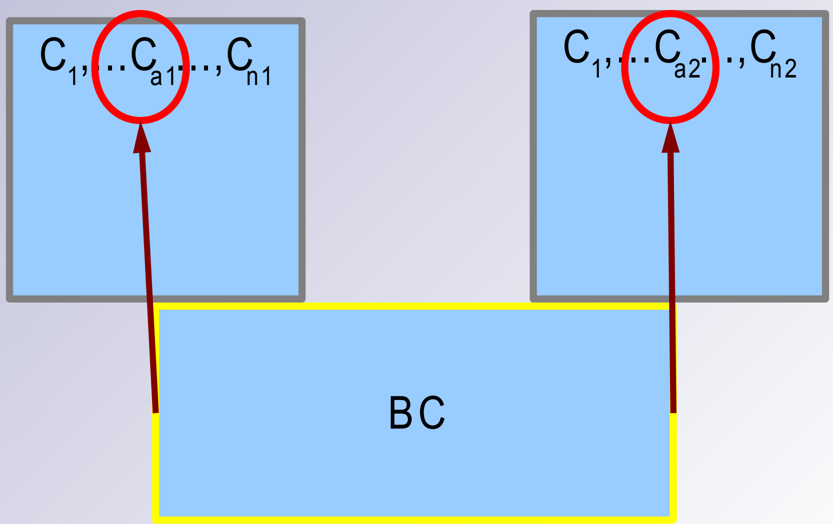
Can BC be shared
on a processor or a node?

1024 electrons need 512 OPO

80 grid points in each direction direction

>2GB in double precision

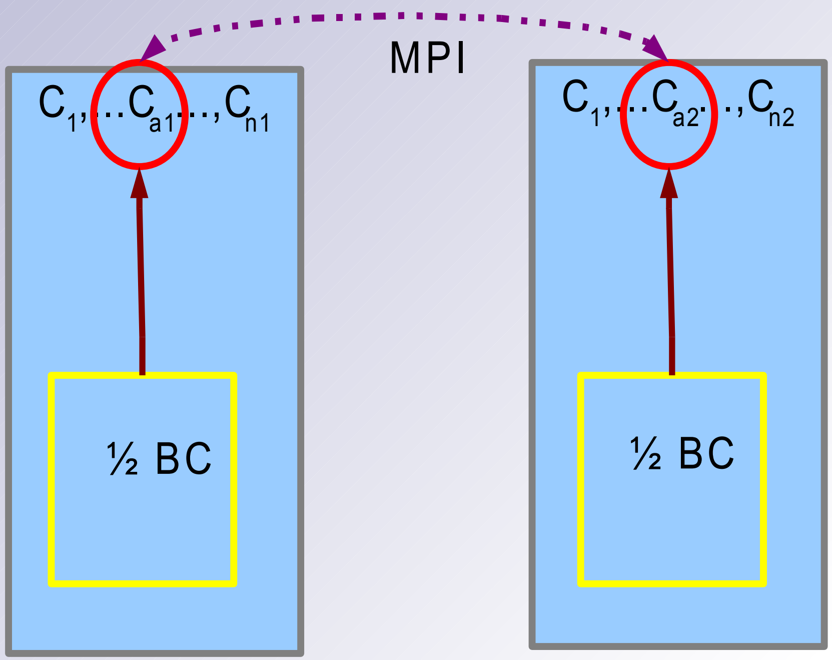
SHM



No MPI solution to share memory on a node, but one can use Unix inter process communication library:

- Easy to implement.
- Needs C functions to allocate the shared memory.
- Cray pointers to pass the reference to the FORTRAN pointers.

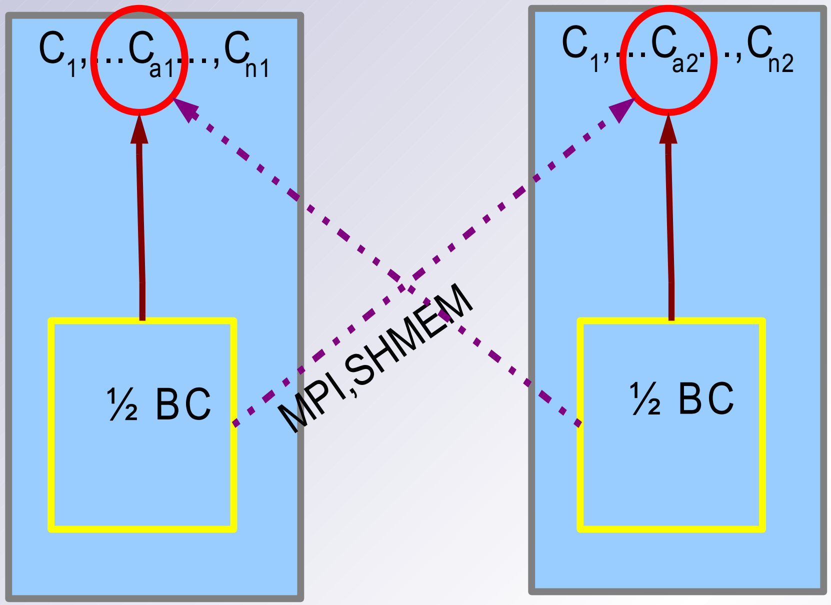
MPI-2Sided



- No need of shared memory
- Fully compliant with CASINO coding standard
- Call for orbital computation must be synchronous

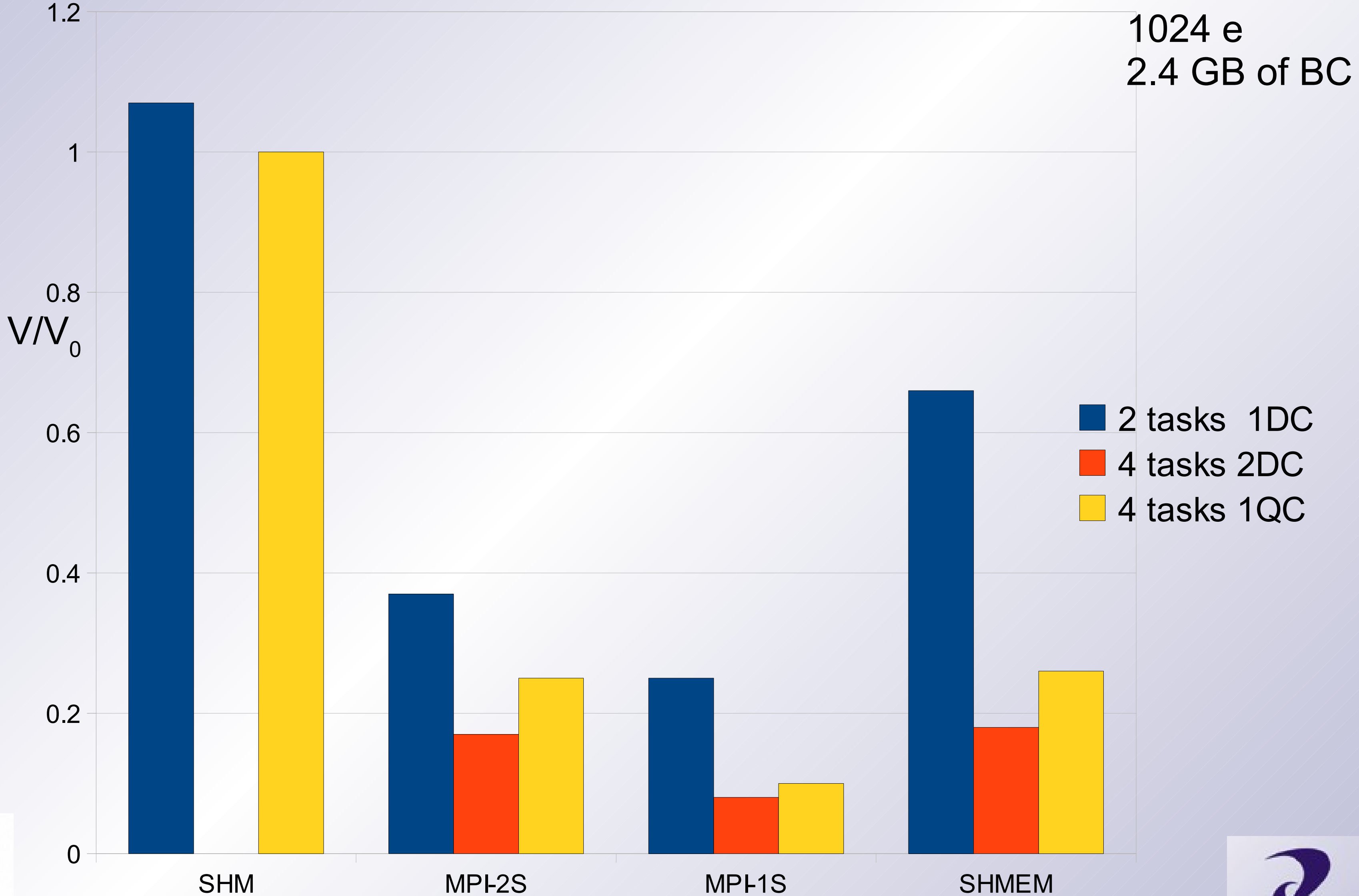
Implemented by Randolph Hood, LLNL, June 2008

MPI-1Sided



Can we avoid the synchronisation of MPI-2S with MPI one-sided or CRAY SHMEM library?

Timing results



Second level parallelism I

Why is needed?

$$t_{\text{total}} \approx N_{\text{step}} \times \frac{N_{\text{pop}}}{P} \times t_{\text{step}}$$

Second level parallelism II

For one configuration step we have to compute:

- The sums involved in computing the energy terms scales as N^2
- Slater matrix elements: N^2
- Slater determinant: N^3 (LU decomposition) or N^2(cofactor matrix)

$$t_{\text{step}}[O(10^4)] \approx 10^{2.x} t_{\text{step}}[O(10^3)]$$

QMC algorithms for electronic structure at the petascale
K P Esler *et al*, J Phys: Conf Series, **125**(2008) 0122057

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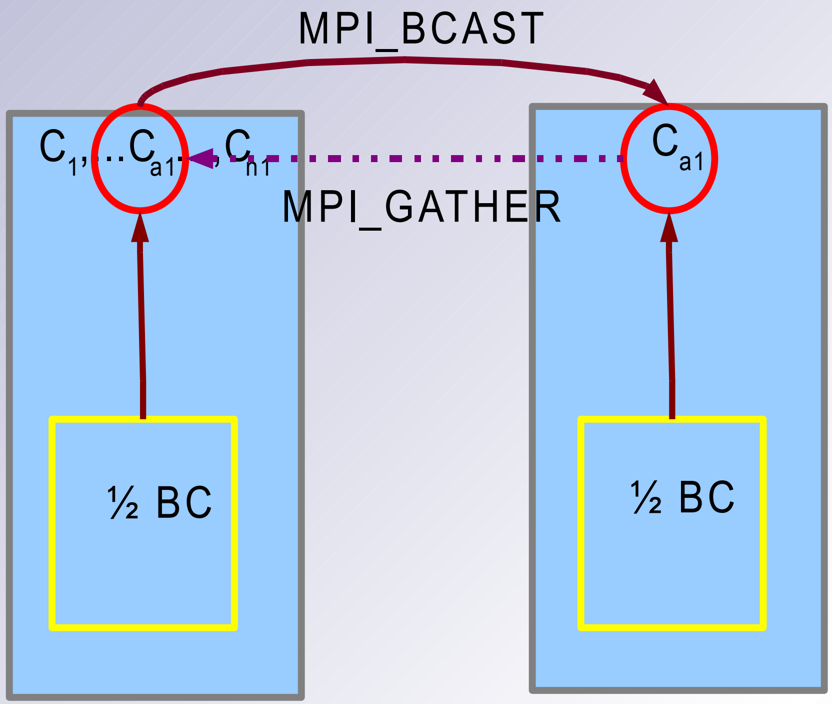
MPI second level parallelism



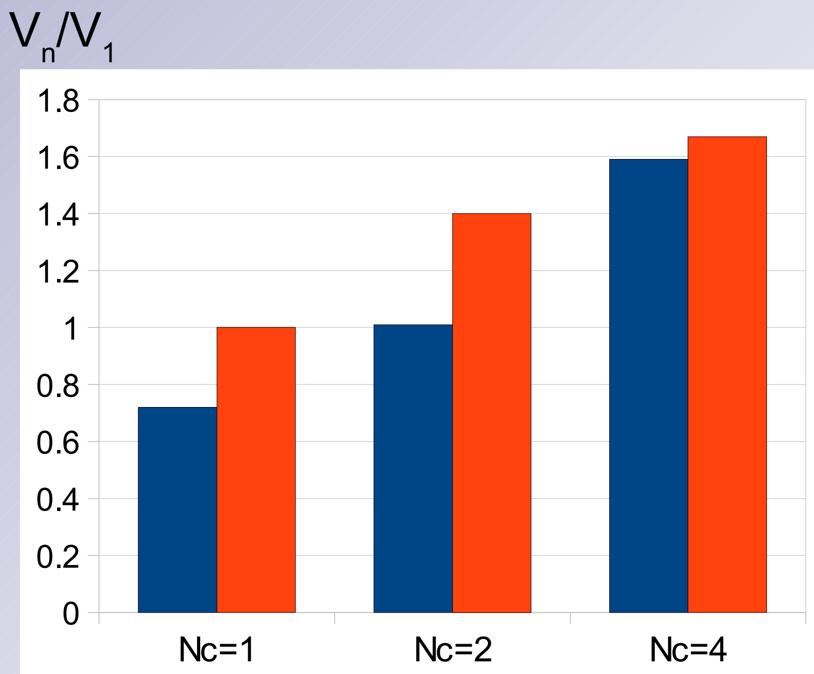
- The pool computes for the same configuration: OPO, Jastrow factor, energy components, Slater determinats.
- The computation is controlled by the pool head.

OpenMP second level parallelism

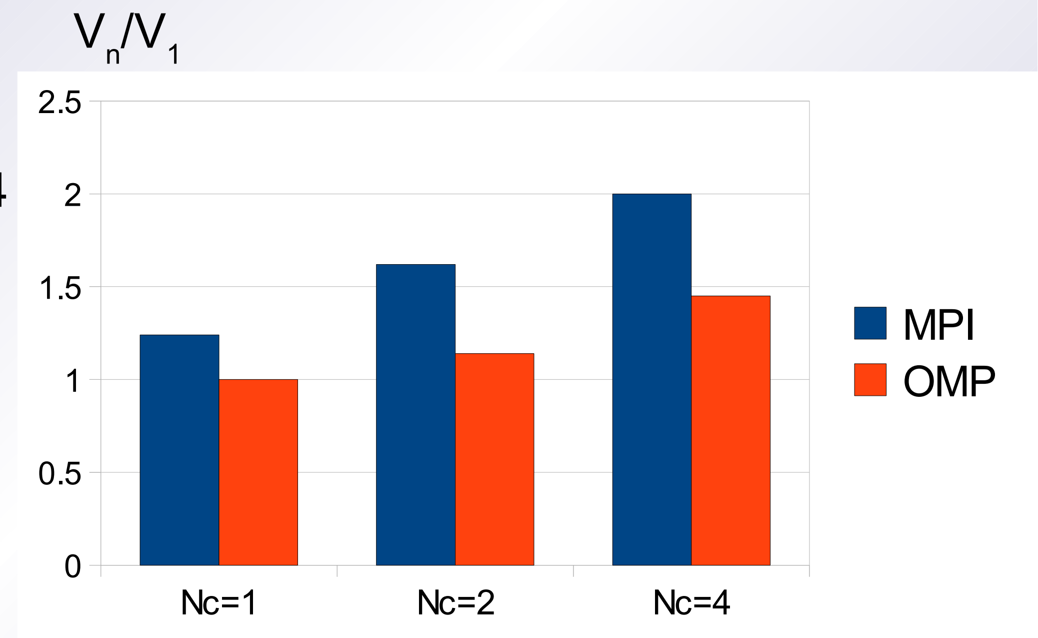
- Loops over the electron index abound in CASINO code and many of them are easy to adapt to parallel computation

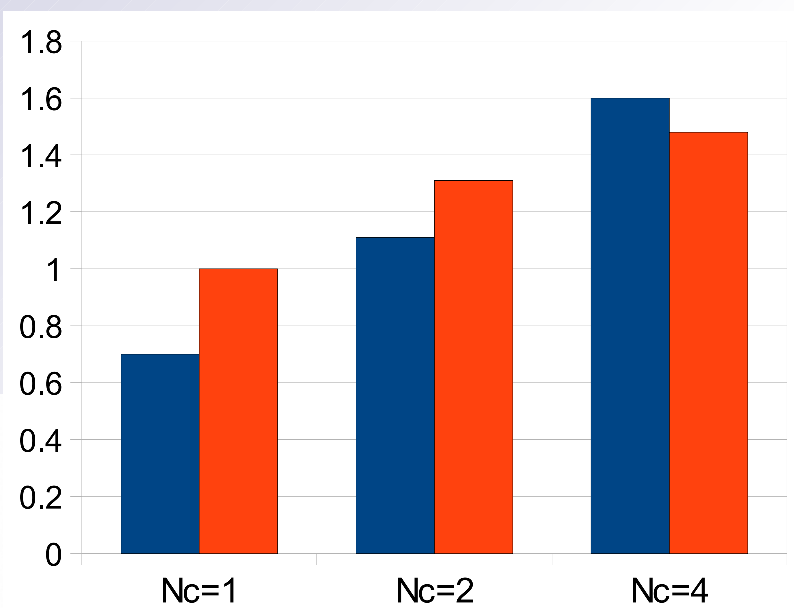
  Higher level OpenMP much harder to implement
- Dependencies in the code (bufferring)
- Compilers cannot handle module subroutines or variables in parallel regions(things are getting better though).

OPO & Jastrow

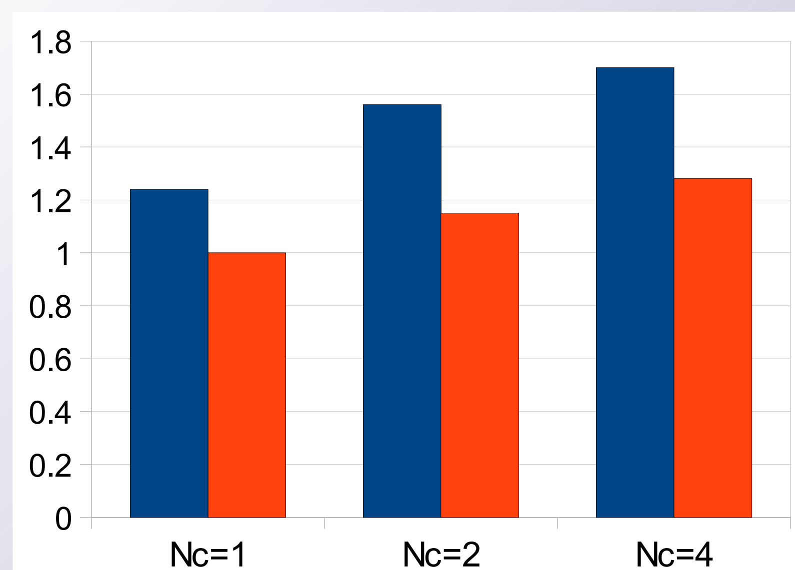


N_e=1024

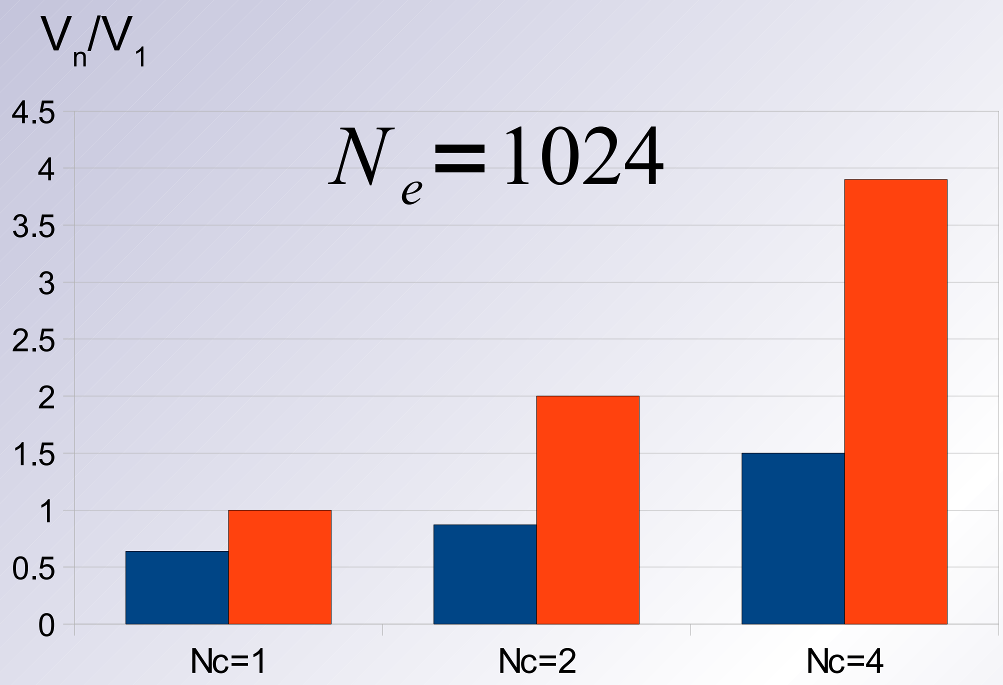




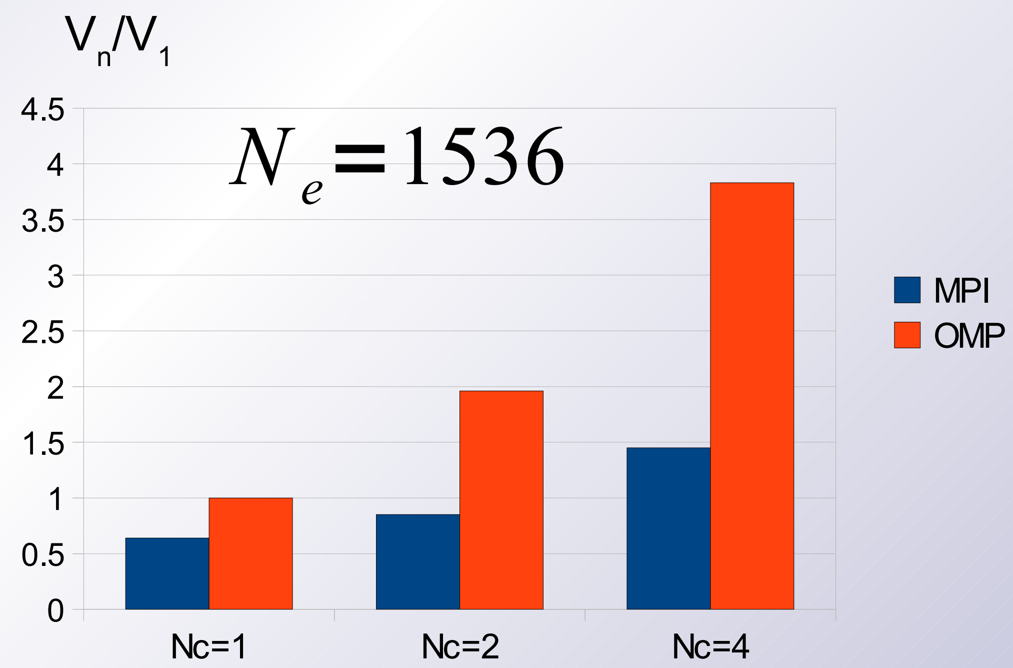
N_e=1536



Ewald sum

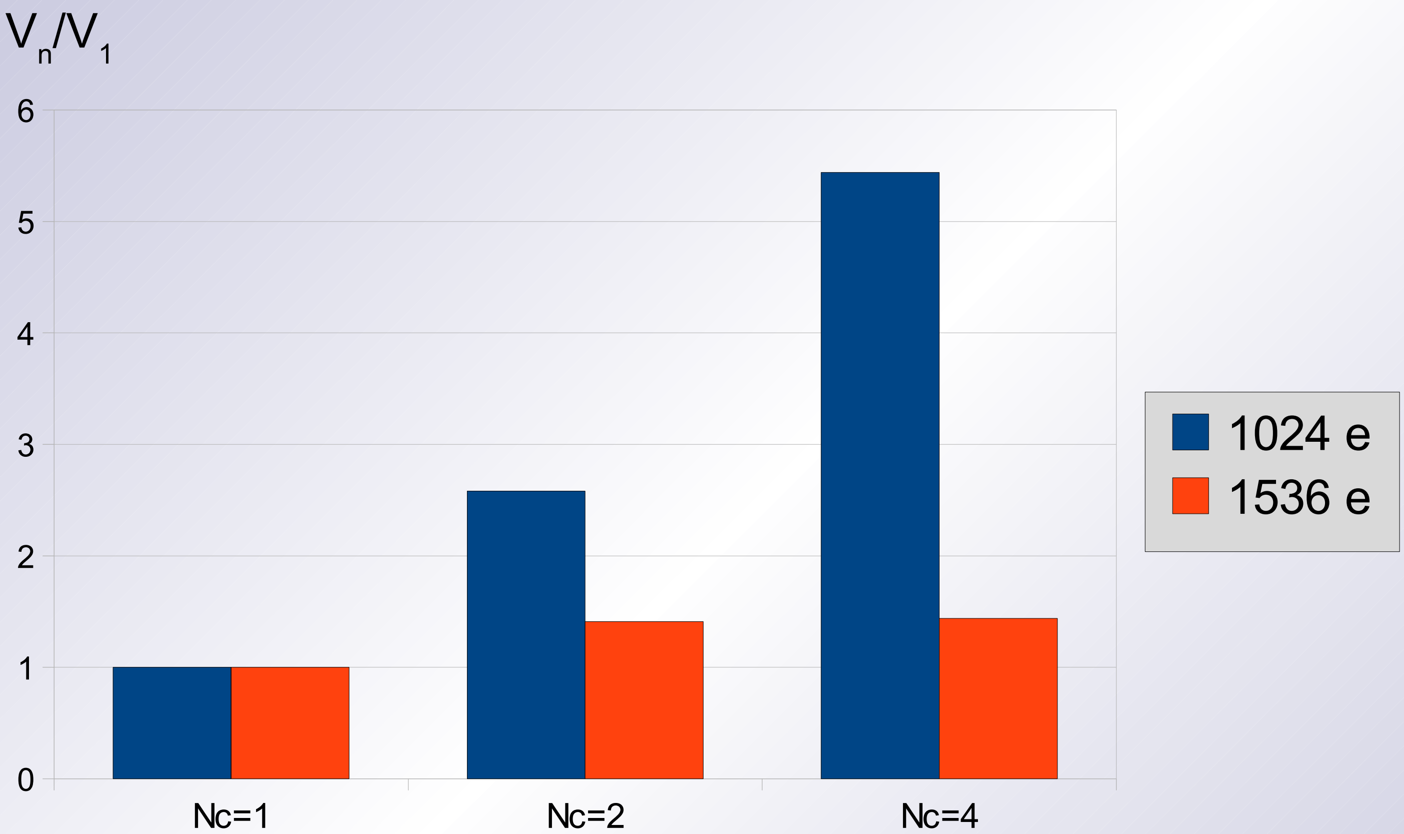


V_n/V_1
$N_e = 1024$
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
Nc=1
Nc=2
Nc=4



V_n/V_1
$N_e = 1536$
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
Nc=1
Nc=2
Nc=4
MPI
OMP

Update $\overline{D}$ & DMC (OpenMP only)



Update $\bar{D}$ for 1024 electrons

Ncores=2

```
USER / slater_update_dbar_.LOOP@li.2770
------------------------------------------------------------------------
  Time%                                   4.5%
  Time                            31.541876 secs
  Imb.Time                          0.415274 secs
  Imb.Time%                               5.2%
  Calls                  0.002M/sec      117869.0 calls
  PAPI_L1_DCM             23.775M/sec    1477514702 misses
  PAPI_TLB_DM              0.441M/sec      27410560 misses
  PAPI_L1_DCA            881.986M/sec   54811035690 refs
  PAPI_FP_OPS            997.309M/sec   61977759711 ops
  User time (approx)      62.145 secs  142933500000 cycles
100.0%Time
  Average Time per Call                     0.000268 sec
  CrayPat Overhead : Time     0.5%
  HW FP Ops / User time   997.309M/sec   61977759711 ops
10.8%peak(DP)
  HW FP Ops / WCT         997.309M/sec
  Computational intensity    0.43 ops/cycle     1.13 ops/ref
  MFLOPS (aggregate)       997.31M/sec
  TLB utilization         1999.63 refs/miss    3.906 avg uses
  D1 cache hit,miss ratios  97.3% hits          2.7% misses
  D1 cache utilization (M)  37.10 refs/miss     4.637 avg uses
```

Ncores=4

```
USER / slater_update_dbar_.LOOP@li.2770
------------------------------------------------------------------------
  Time%                                   2.4%
  Time                            13.466174 secs
  Imb.Time                          0.523796 secs
  Imb.Time%                               6.7%
  Calls                  0.002M/sec      117869.0 calls
  PAPI_L1_DCM             11.380M/sec     611074379 misses
  PAPI_TLB_DM              0.222M/sec      11933068 misses
  PAPI_L1_DCA            510.886M/sec   27431996968 refs
  PAPI_FP_OPS            577.128M/sec   30988879856 ops
  User time (approx)      53.695 secs  123498500000 cycles
100.0%Time
  Average Time per Call                     0.000114 sec
  CrayPat Overhead : Time     1.2%
  HW FP Ops / User time   577.128M/sec   30988879856 ops
6.3%peak(DP)
  HW FP Ops / WCT         577.128M/sec
  Computational intensity    0.25 ops/cycle     1.13 ops/ref
  MFLOPS (aggregate)       577.13M/sec
  TLB utilization         2298.82 refs/miss    4.490 avg uses
  D1 cache hit,miss ratios  97.8% hits          2.2% misses
  D1 cache utilization (M)  44.89 refs/miss     5.611 avg uses
```

Update $\bar{D}$ for 1536 electrons

Ncores=2

USER / slater_update_dbar_.LOOP@li.2770

Time% 12.9%
Time 25.522353 secs
Imb.Time 0.021617 secs
Imb.Time% 0.3%
Calls 464.8 /sec 24017.0 calls
PAPI_L1_DCM 14.540M/sec 751360178 misses
PAPI_TLB_DM 0.267M/sec 13780336 misses
PAPI_L1_DCA 483.841M/sec 25002479245 refs
PAPI_FP_OPS 549.334M/sec 28386821099 ops
User time (approx) 51.675 secs 118852500000 cycles
100.0%Time
Average Time per Call 0.001063 sec
CrayPat Overhead : Time 0.1%
HW FP Ops / User time 549.334M/sec 28386821099 ops
6.0%peak(DP)
HW FP Ops / WCT 549.334M/sec
Computational intensity 0.24 ops/cycle 1.14 ops/ref
MFLOPS (aggregate) 549.33M/sec
TLB utilization 1814.36 refs/miss 3.544 avg uses
D1 cache hit,miss ratios 97.0% hits 3.0% misses
D1 cache utilization (M) 33.28 refs/miss 4.160 avg uses

Ncores=4

USER / slater_update_dbar_.LOOP@li.2770

Time% 12.7%
Time 23.751722 secs
Imb.Time 0.118560 secs
Imb.Time% 0.9%
Calls 253.3 /sec 24017.0 calls
PAPI_L1_DCM 4.040M/sec 383077467 misses
PAPI_TLB_DM 0.075M/sec 7143074 misses
PAPI_L1_DCA 131.908M/sec 12508535695 refs
PAPI_FP_OPS 149.676M/sec 14193410550 ops
User time (approx) 94.828 secs 218103250000 cycles
100.0%Time
Average Time per Call 0.000989 sec
CrayPat Overhead : Time 0.1%
HW FP Ops / User time 149.676M/sec 14193410550 ops
1.6%peak(DP)
HW FP Ops / WCT 149.676M/sec
Computational intensity 0.07 ops/cycle 1.13 ops/ref
MFLOPS (aggregate) 149.68M/sec
TLB utilization 1751.14 refs/miss 3.420 avg uses
D1 cache hit,miss ratios 96.9% hits 3.1% misses
D1 cache utilization (M) 32.65 refs/miss 4.082 avg uses

Update $\bar{D}$ code

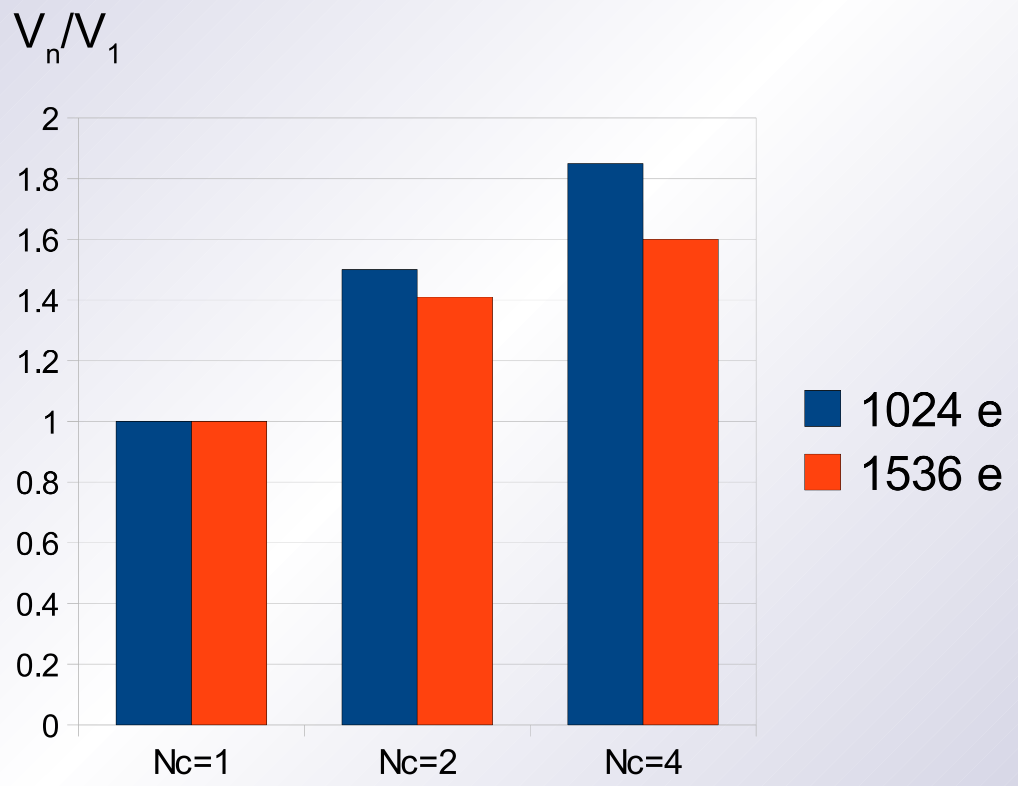
$$\bar{D}_{kj} = \begin{cases} \bar{D}_{kj}/q_i, & \text{if } j=i \\ \bar{D}_{kj} - \dfrac{\bar{D}_{ki}}{q_i}\left[\sum_{l=1}^{N} \bar{D}_{lj}\phi_l(\boldsymbol{r}_i)\right], & \text{if } j \neq i \end{cases}$$

$$q_i = \sum_{j=1}^{N} \bar{D}_{ji}\phi_j(\boldsymbol{r}_i)$$

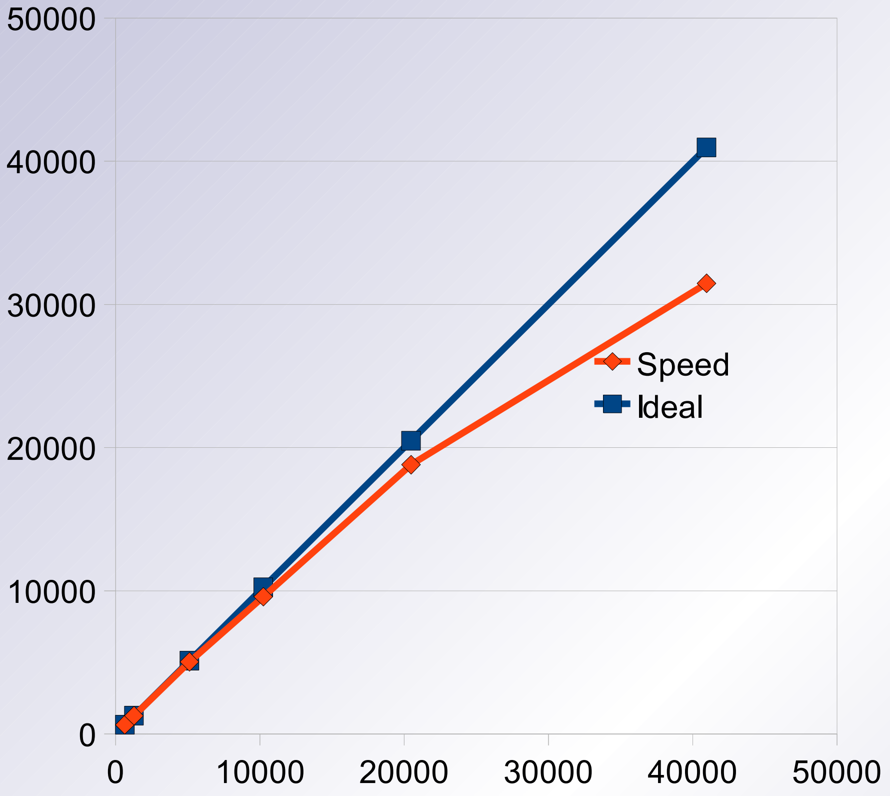
Code:

```
!$OMP PARALLEL DO DEFAULT(none) SHARED(ie,one_over_q_real,nele_uspin,&
!$OMP &dbar,uspin,rpsi) PRIVATE(je,tempr)
    do je=1,nele_uspin
     if(je==ie)cycle
     tempr=-one_over_q_real*ddot(nele_uspin,dbar(1,je,1,uspin),1,rpsi(1,1),1)
     call daxpy(nele_uspin,tempr,dbar(1,ie,1,uspin),1,dbar(1,je,1,uspin),1)
    enddo ! je
!$OMP END PARALLEL DO
```

Aggregated DMC performance



IO at large scale



Improvements:

- OPO data reorder and read/write in binary format (FORTRAN or MPIIO)
- config.in read only by small group of cores

  and data distributed with MPI.

CASINO scaling on Jaguar(ORNL) June 2009.

Conclusions

- The System V shared memory solution allows sharing of the orbitals data and therefore each core of a processor can run a computing task even for very large scale models.
- The input optimisations have eliminated unnecessary waiting time which wasted approximately 200 AU for each 1000 cores in a run.
- The computation using mixed mode second level parallelism reaches speed up factor close to 1.8 on quad core processor for models with a more than 1000 electrons.