Introduction to QuantumESPRESSO

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QUANTUM ESPRESSO

Quantum ESPRESSO is an open-source suite of computer codes for electronic-structure calculations and materials modeling. It is based on density-functional theory, plane waves, and pseudopotentials.

P. Giannozzi, et al J.Phys.:Condens.Matter, 21, 395502 (2009) http://dx.doi.org/10.1088/0953-8984/21/39/395502 .

`www.quantum-espresso.org`

`www.qe-forge.org`

DEMOCRITOS
DEmocritos MOdeling Center for Research In aTOmistic Simulation INFM

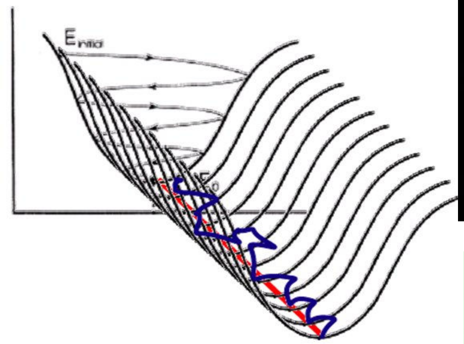
Massachusetts Institute of Technology

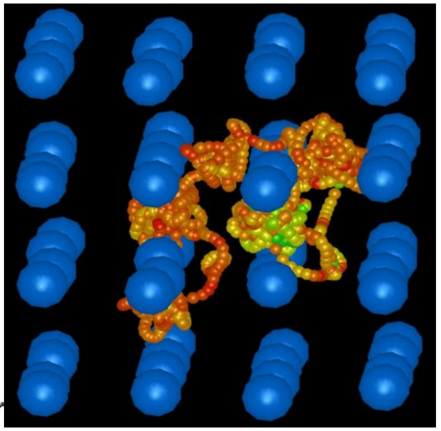
CINECA

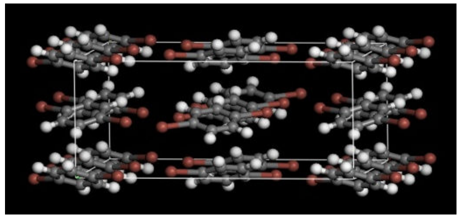
CP (Car-Parrinello)

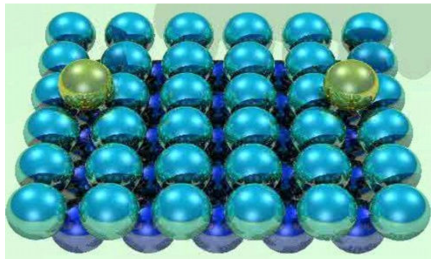
Code for Car-Parrinello MD
Disordered systems
Liquids
Finite temperature

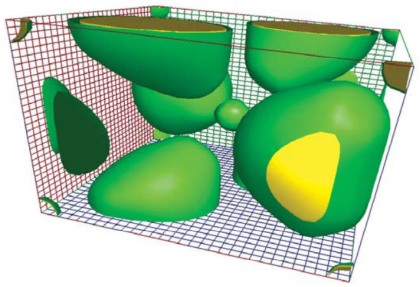
!!! Roberto Car & Michele Parrinello
develop the CP method on a
CRAY machine Installed at CINECA !!!



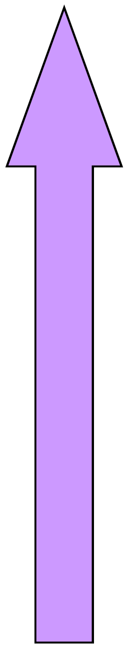








More scalable

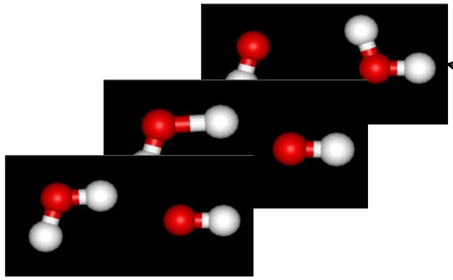


Less scalable

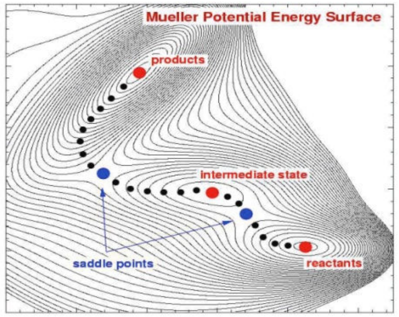
PW (Plane Wave)

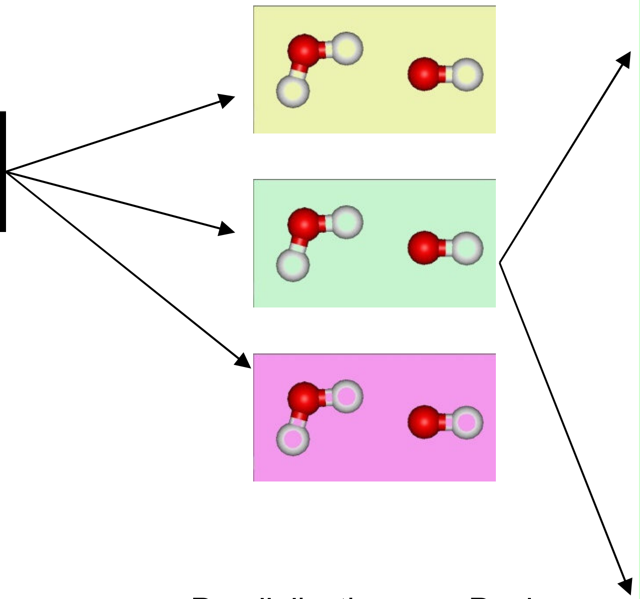
Code for Electronic Structure computation
Structure optimization
Born-Hoppenheimer MD

Parallelization (before OpenMP)



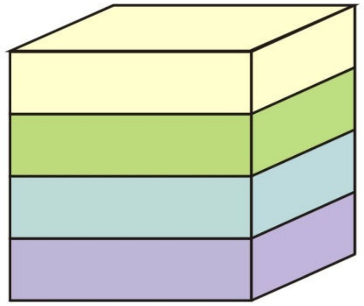
Parallelization over Images
Energy barrier evaluation





Parallelization over Pools:
K-points sempling of
Brillouin Zone.
Electronic band structure

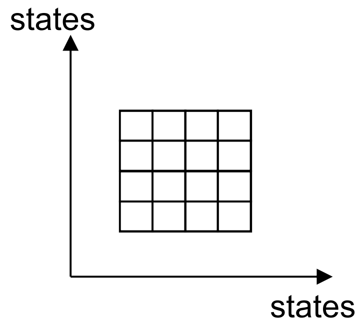
1x1xN proc grid



Charge density

Parallelization of the FFT
Real and Reciprocal Space
Decomposition.
One FFT for each electron

√N x √N proc grid



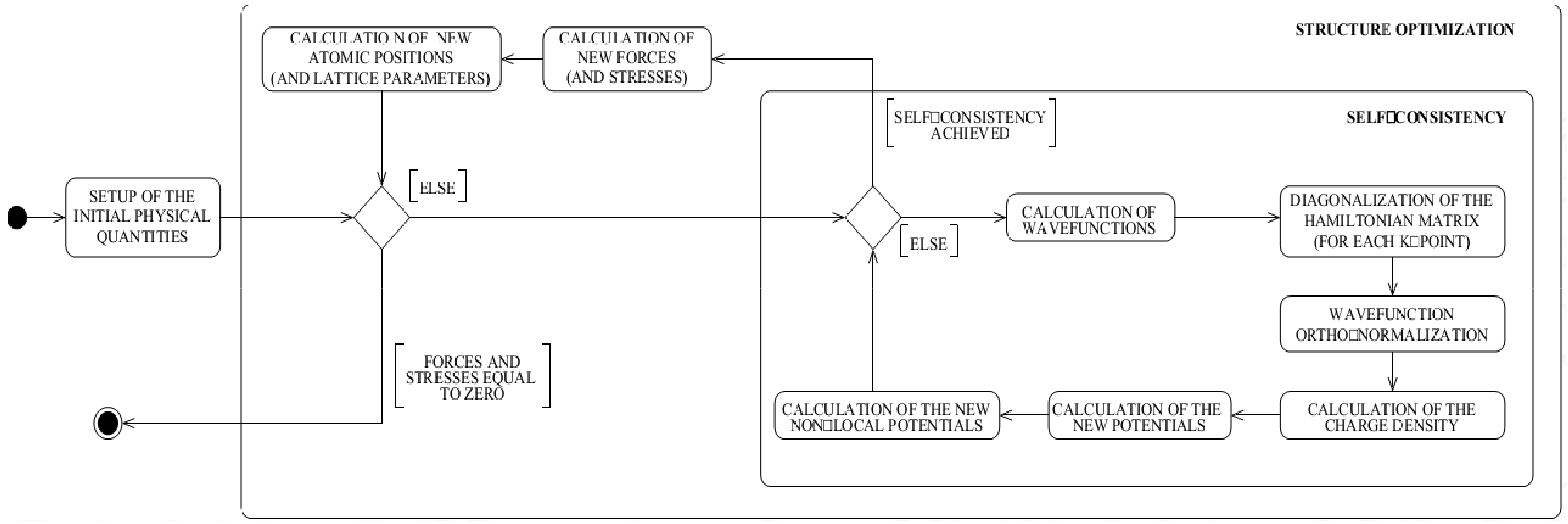
Hamiltonian

Parallelization of
Bands structure.
Matrix Diagonalization
At least one state for
each electron

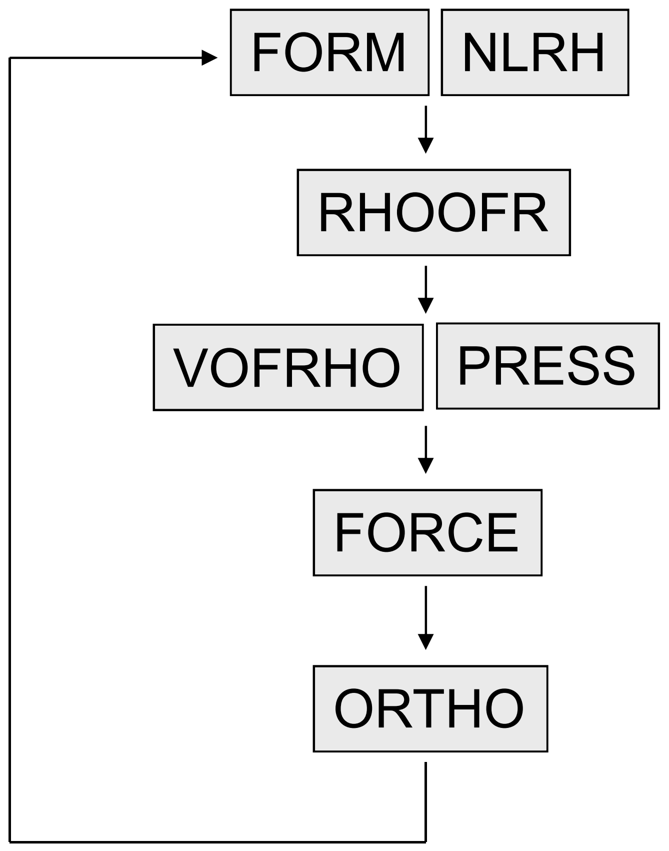
Loosely coupled

Tightly coupled

PW flow chart


STRUCTURE OPTIMIZATION
SELF□CONSISTENCY
SETUP OF THE INITIAL PHYSICAL QUANTITIES
CALCULATIO N OF NEW ATOMIC POSITIONS (AND LATTICE PARAMETERS)
CALCULATION OF NEW FORCES (AND STRESSES)
ELSE
FORCES AND STRESSES EQUAL TO ZERO
SELF□CONSISTENCY ACHIEVED
ELSE
CALCULATION OF WAVEFUNCTIONS
DIAGONALIZATION OF THE HAMILTONIAN MATRIX (FOR EACH K□POINT)
WAVEFUNCTION ORTHO□NORMALIZATION
CALCULATION OF THE CHARGE DENSITY
CALCULATION OF THE NEW POTENTIALS
CALCULATION OF THE NEW NON□LOCAL POTENTIALS

CP Flow chart



Pseudopotential Form factors

$\rho(\mathbf{r}) = \Sigma\, |\psi(\mathbf{r})|^2$

$\mathbf{V}(\mathbf{R}, \psi) = \mathbf{V}^{r}_{DFT}(\mathbf{R}, \rho(\mathbf{r})) + \mathbf{V}^{G}_{DFT}(\mathbf{R}, \rho(\mathbf{G}))$

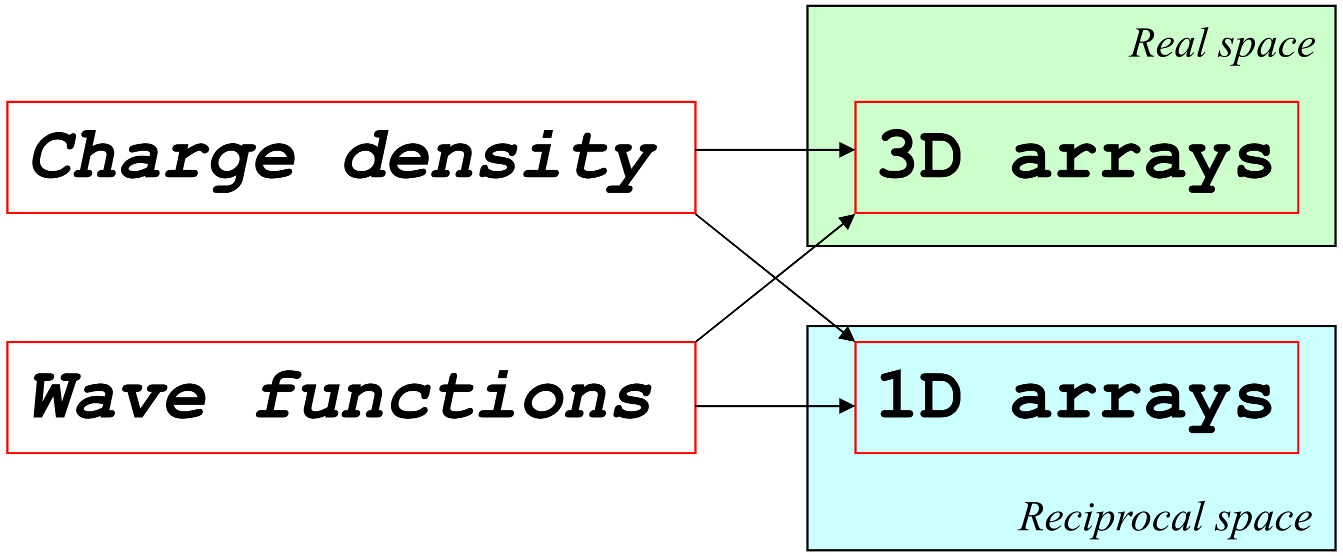
Forces on the electrons: $\mathbf{F}_{\psi}$

Orthogonalize wave functions: ψ

TABLE I: Summary of parallelization levels in QUANTUM ESPRESSO.

group	distributed quantities	communications	performance
image	NEB images	very low	linear CPU scaling, fair to good load balancing; does not distribute RAM
pool	**k**-points	low	almost linear CPU scaling, fair to good load balancing; does not distribute RAM
plane-wave	plane waves, **G**-vector coefficients, **R**-space FFT arrays	high	good CPU scaling, good load balancing, distributes most RAM
task	FFT on electron states	high	improves load balancing
linear algebra	subspace Hamiltonians and constraints matrices	very high	improves scaling, distributes more RAM

Basic Data Type



Reciprocal Space Representation

Wave Functions

$$\psi_i(r) = \frac{1}{\sqrt{\Omega}} \sum_G C_i(G) \exp(iGr)$$

$$|G|^2 / 2 \le E_{cut}$$

To truncate the infinite sum

Charge Density

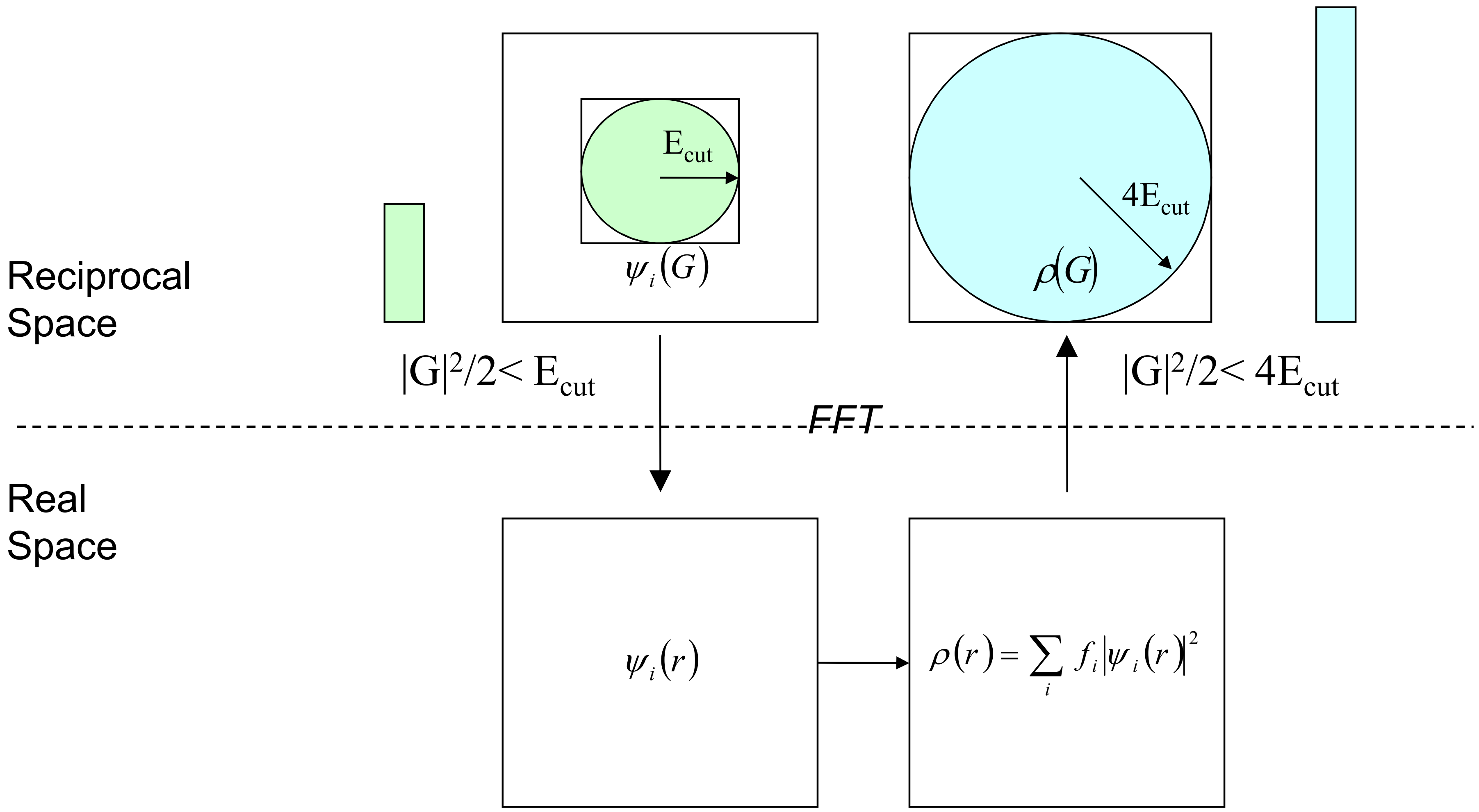
$$\rho(r) = \sum_i f_i |\psi_i(r)|^2$$

$$\rho(G) = \frac{1}{\Omega} \sum_i f_i \sum_{G'} C_i(G') C_i(G - G') \exp(i(G - G')r)$$

$$|G|^2 / 2 \le 4E_{cut}$$

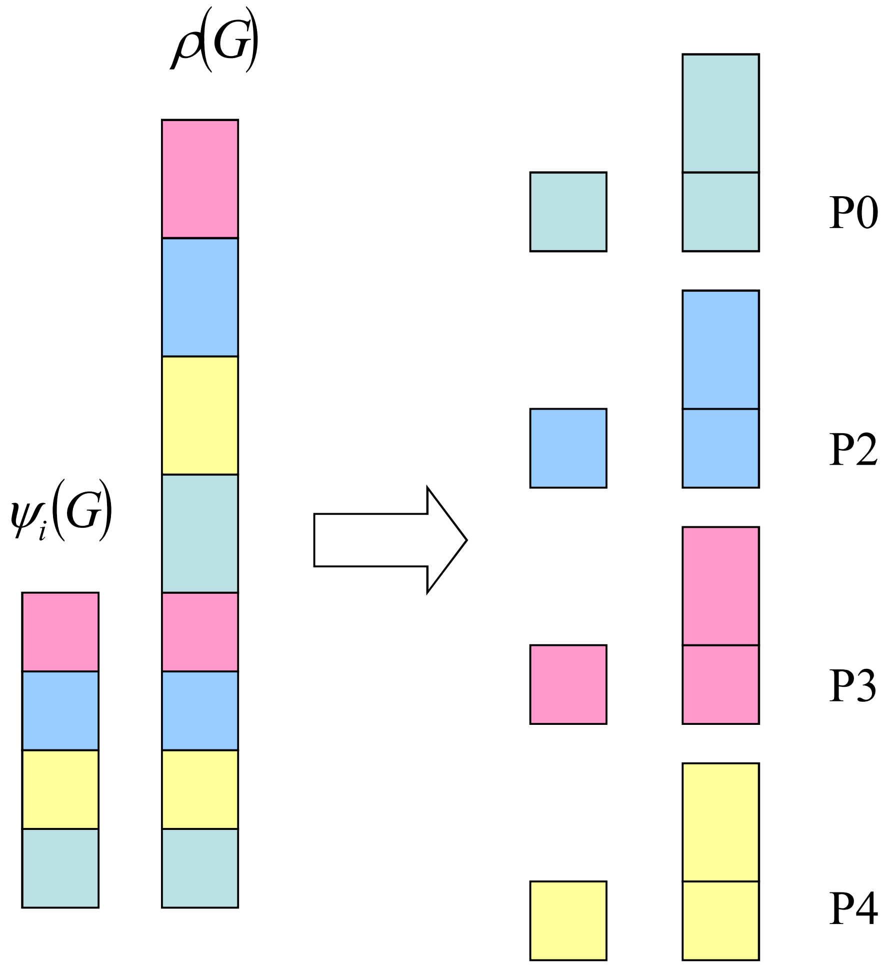
To retain the same accurancy as the wave function

FFTs

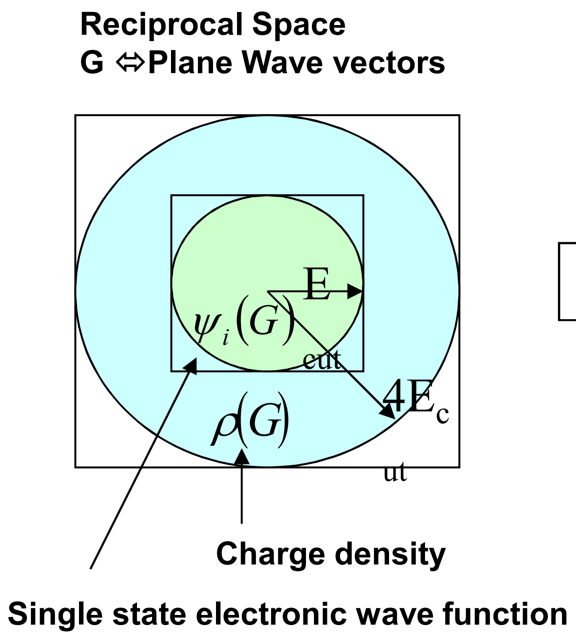


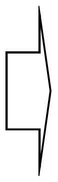
Reciprocal Space
Real Space
E_{cut}
$\psi_i(G)$
$4E_{cut}$
$\rho(G)$
$|G|^2/2 < E_{cut}$
$|G|^2/2 < 4E_{cut}$
FFT
$\psi_i(r)$
$\rho(r) = \sum_i f_i |\psi_i(r)|^2$

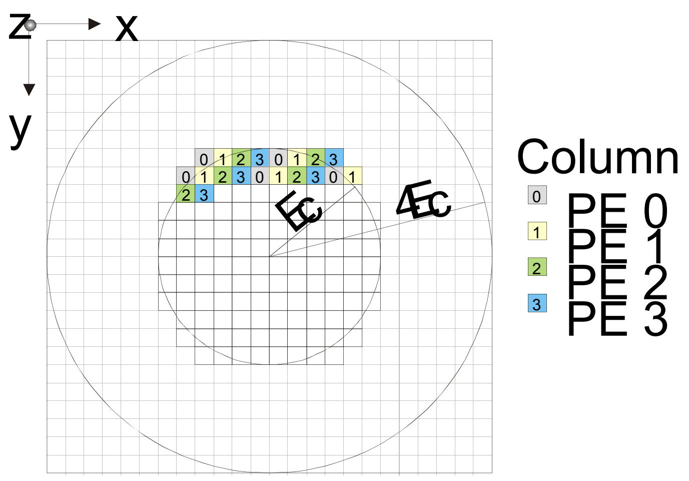
Reciprocal Space distribution



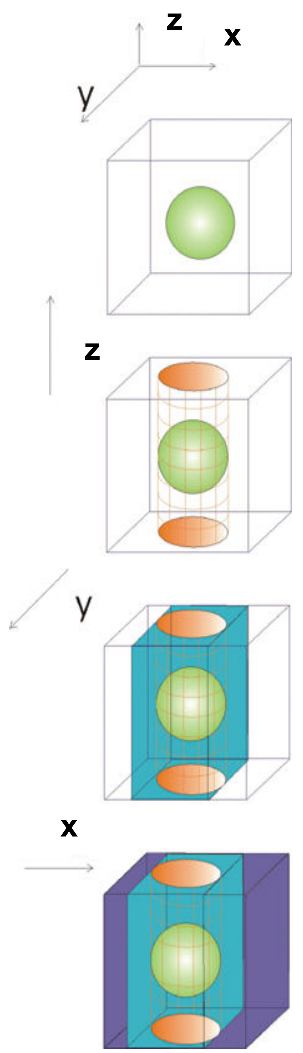
Understanding QE 3DFFT, Parallelization of Plane Wave







~ Nx Ny / 5 FFT along z



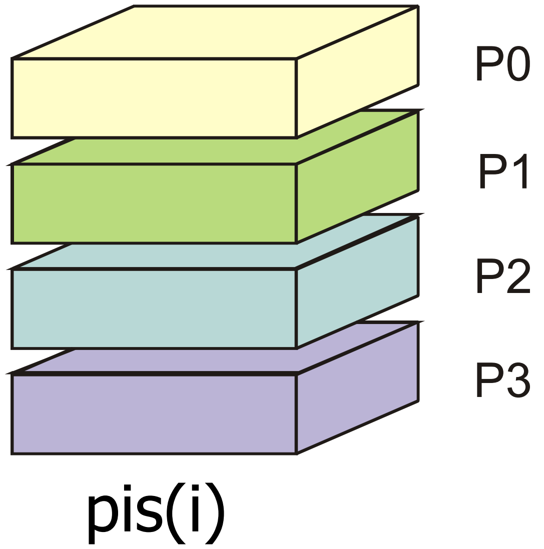
Similar 3DFFT are present in most ab-initio codes like CPMD

Tasks Group technique

This technique is relevant in all applications where you have an external loop over a parallel subroutine that operate on distributed data.

Case Study: parallel 3D FFT

```
do i = 1, n
   compute parallel 3D FFT( psi(i) )
end do
```

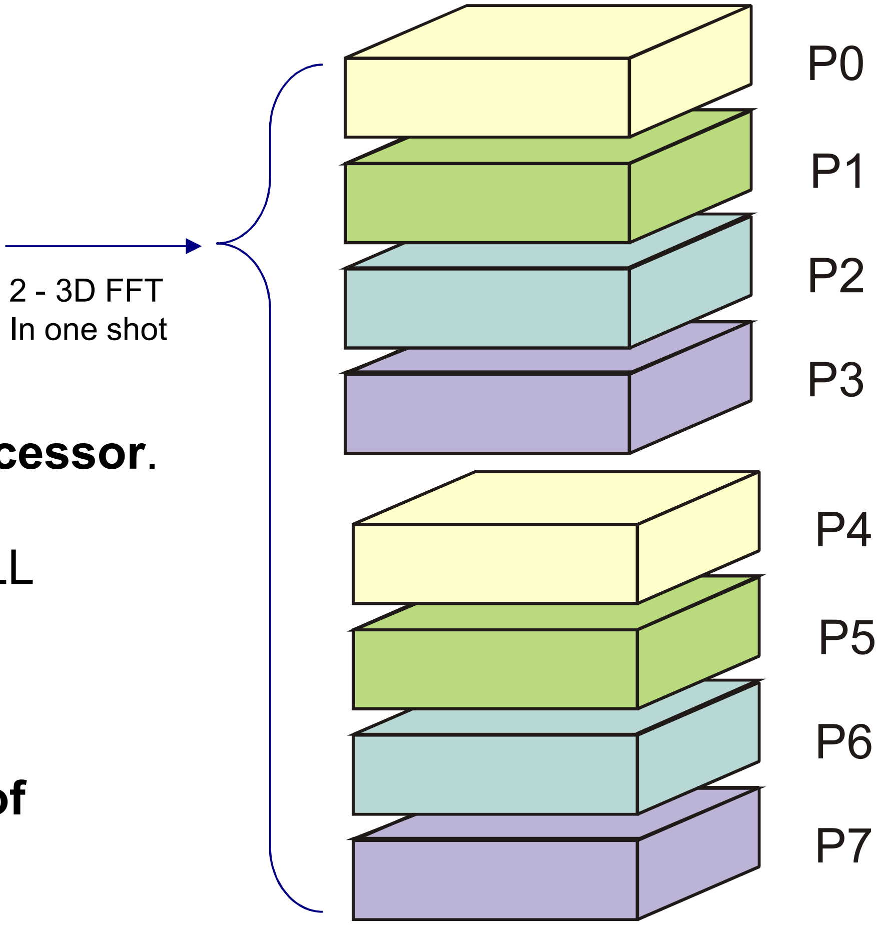


the parallelization is limited to the number of planes in the 3D FFT (NX x NY x NZ) there is little gain to use more than NZ proc

Tasks Group II

The goal is to use more processors than **NZ**.
The solution is to perform FFT not one by one but in group of **NG.**

```
redistribute the n FFT
do i = 1, nb, ng
  compute ng parallel 3D FFT
   (at the same time)
end do
```



we can scaleup to **NZ x NG processor**.

This cost an additional ALLTOALL and memory (NG times the size of the 3D vector).

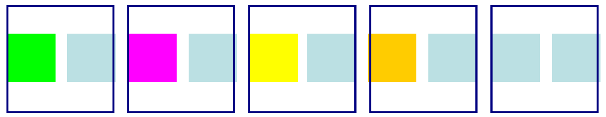
But we have half the number of Loop cycle!

Ortho Group

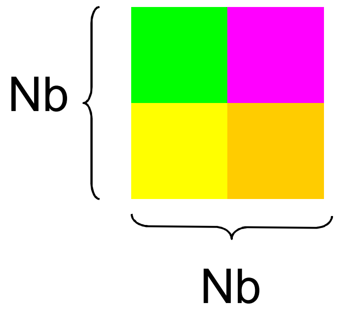
Often, when scaling with the number of nodes, not all part of the code can take advantage of all the processors, or the fastest algorithm may require only a given number of processors.

Case study: iterative diagonalization of hermitian matrixes

Hermitian matrixes are square matrixes, and a square grid of processors can give to optimal performance (communication/computatio)



in a run with 10 processors,
the iter group use 4 procrs (2x2)
one proc every two.



Matrixes are block distributed to the iter group.

In this case is possible to use a mixed parallelization MPI+OpenMP using SMP library

Sample code

```
 ! ... calculates eigenvalues and eigenvectors of the generalized problem
 ! ... Hv=eSv, with H hermitean matrix, S overlap matrix.
CALL pzpotf( S, nx, n, desc ) ! ... Cholesky decomposition of S
CALL pztrtri( S, nx, n, desc ) ! ... S is inverted ( S = S^-1 )
! ... v = S^-1*H
CALL sqr_zmm_cannon( 'N', 'N', n, ONE, S, nx, H, nx, ZERO, v, nx, desc )
! ... H = ( S^-1*H )*(S^-1)^T
CALL sqr_zmm_cannon( 'N', 'C', n, ONE, v, nx, S, nx, ZERO, H, nx, desc )
CALL redistribution
CALL standard_diag ! for Hv=ev problem , Ex: zhpev
CALL back-redistribution
! ... v = (S^T)^-1 v
CALL sqr_zmm_cannon( 'C', 'N', n, ONE, S, nx, H, nx, ZERO, v, nx, desc )
```

The full code can be found in package www.quantum-espresso.org

Main Algorithms in QE

3D FFT

Linear Algebra

- Matrix Matrix Multiplication
- less Matrix-Vector and Vector-Vector
- Eigenvalues and Eigenvectors computation

Space integrals

Point function evaluations

Parallelization Strategy

3D FFT	ad hoc MPI & OpenMP driver
Linear Algebra	ScalaPACK + blas multithread
Space integrals	MPI & OpenMP loops parallelization and reduction
Point function evaluations	MPI & OpenMP loops parallelization

Mixed QE: Implicit *vs* Explicit approach

Implicit

Linking multi-threading libraries

No control of thread creation overhead

Relatively simple

Explicit

OpenMP syntax knowledge

Manage code flow and thread

More efficient

In QE we use both multi-thread parallelization

Multithread libraries (mkl, acml, essl)

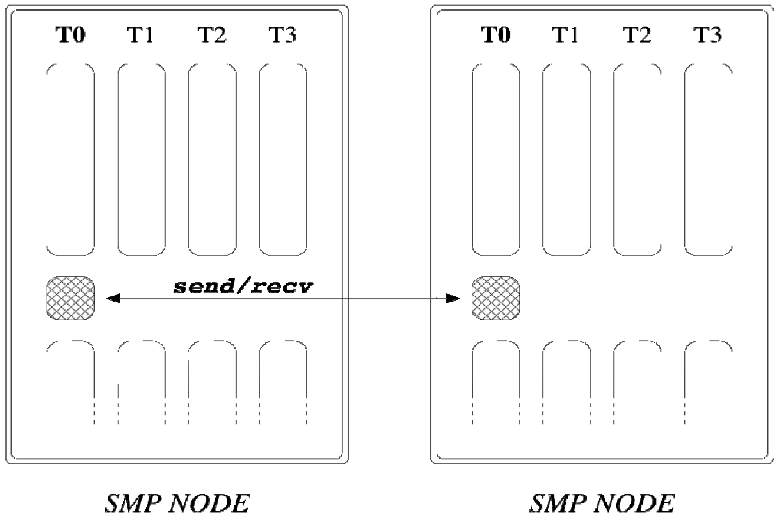
No explicit OpenMP directive

Very efficient (in most cases)

No possibility to mix multithread and non multithread version of the same library (selective call)

Workaround using **omp_set_num_threads() omp_get_max_threads()** not always possible

Understanding QE 3DFFT: *master-only*



```
# begin OpenMP region
   do i = 1, nsl   in parallel
      call 1D-FFT along z ( f[offset] )
   end do
# end OpenMP region

   call fw_scatter( ... )

# begin OpenMP region
   do i = 1, nzl   in parallel
      do j = 1, Nx
            if ( dofft[j] ) then
               call 1D-FFT along y  ( f[offset] )
      end do
      call 1D-FFT along x ( f[offset] )  Ny-times
   end do
# end OpenMP region
```

Local (to each MPI process) number of "z" stick distributed to threads

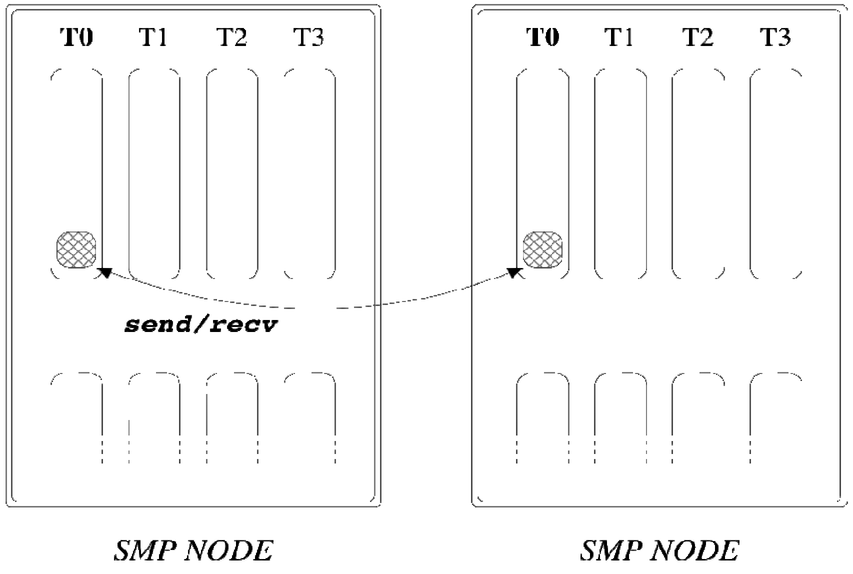
Thread private

Parallel transpose (implemented with isend/irecv)

Local (to each MPI process) number of "xy" plane Distributed to threads

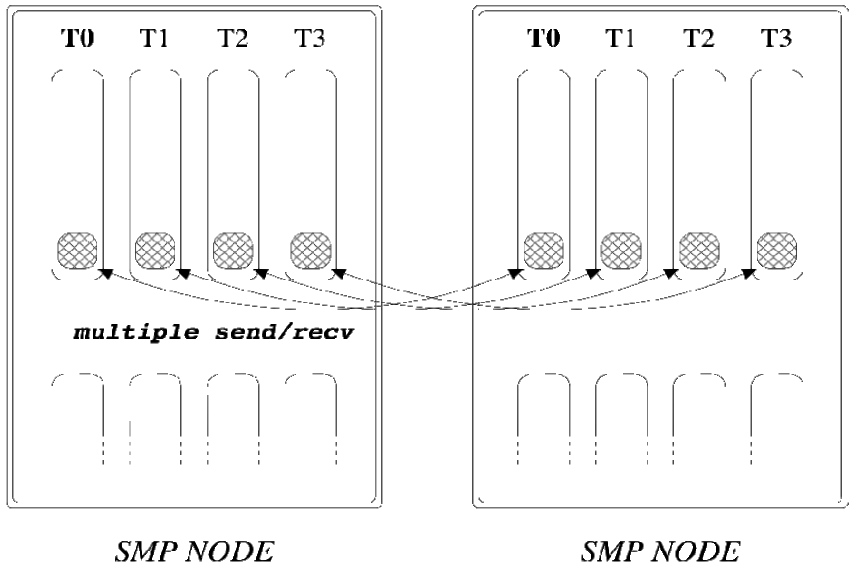
Thread private

QE 3DFFT: *funneled*



```
# begin OpenMP region
   do i = 1, nsl    in parallel
      call 1D-FFT along z ( f[offset] )
   end do

# begin of OpenMP MASTER section
   call fw_scatter( ... )
# end of OpenMP MASTER section
# force synchronization with OpenMP barrier

   do i = 1, nzl    in parallel
      do j = 1, Nx
            if ( dofft[j] ) then
               call 1D-FFT along y ( f[offset] )
      end do
      call 1D-FFT along x ( f[offset] )  Ny-times
   end do
# end OpenMP region
```

QE 3DFFT: *multiple*



Pros:

- Overlap communication and computation
- Less synchronizations between threads and memory flush

- Cons:
  - Do not exploit memory and network hierarchy
  - Stress the network like plain MPI

Not yet completed…

Space Integrals: Electrostatic potential
simple loop parallelization

```
!$omp parallel do default(shared), private(rp,is,rhet,rhog,fpibg), reduction(+:eh,ehte,ehti)
      DO ig = gstart, ngm
        rp   = (0.D0,0.D0)
        DO is = 1, nsp
          rp = rp + sfac( ig, is ) * rhops( ig, is )    Ionic density (reciprocal space)
        END DO
        rhet  = rhoeg( ig )    <----------------------   Electronic density (reciprocal space)
        rhog  = rhet + rp
        IF( tscreen ) THEN
          fpibg     = fpi / ( g(ig) * tpiba2 ) + screen_coul(ig)
        ELSE
          fpibg     = fpi / ( g(ig) * tpiba2 )
        END IF
        vloc(ig) = vloc(ig)  +  fpibg *        rhog                   Hartree potential
        eh       = eh        +  fpibg *        rhog * CONJG(rhog)     Hatree Energy
        ehte     = ehte      +  fpibg *   DBLE(rhet * CONJG(rhet))    Ionic contribution
        ehti     = ehti      +  fpibg *   DBLE(  rp * CONJG(rp))      Electronic contribution
      END DO
```

! IBM xlf compiler does not like name of function used for OpenMP reduction

Space Integral: Non local energy
less simple loop parallelization

Larger parallel region to reduce
The fork/join overhead

```
!$omp parallel default(shared), &
!$omp private(is,iv,ijv,isa,ism,ia,inl,jnl,sums,i,iss,sumt), reduction(+:ennl)
      do is = 1, nsp
         do iv = 1, nh(is)
            do jv = iv, nh(is)
               ijv = (jv-1)*jv/2 + iv
               isa = 0
               do ism = 1, is - 1
                  isa = isa + na(ism)
               end do
!$omp do
               ...
!$omp end do

             end do
          end do
       end do
!$omp end parallel
```

```
!$omp do
               do ia = 1, na(is)
                  inl = ish(is)+(iv-1)*na(is)+ia
                  jnl = ish(is)+(jv-1)*na(is)+ia
                  isa = isa+1
                  sums = 0.d0
                  do i = 1, n
                     iss = ispin(i)
                     sums(iss) = sums(iss) + f(i) * bec(inl,i) * bec(jnl,i)
                  end do
                  sumt = 0.d0
                  do iss = 1, nspin
                     rhovan( ijv, isa, iss ) = sums( iss )
                     sumt = sumt + sums( iss )
                  end do
                  if( iv .ne. jv ) sumt = 2.d0 * sumt
                  ennl = ennl + sumt * dvan( jv, iv, is)
               end do
!$omp end do
```

Point Function evaluation: Exchange and Correlation energy

```
!$omp parallel do private( rhox, arhox, ex, ec, vx, vc ), reduction(+:etxc)
     do ir = 1, nnr
        rhox = rhor (ir, nspin)
        arhox = abs (rhox)
        if (arhox.gt.1.d-30) then
           CALL xc( arhox, ex, ec, vx(1), vc(1) )
           v(ir,nspin) = e2 * (vx(1) + vc(1) )
           etxc = etxc + e2 * (ex + ec) * rhox
        endif
     enddo
!$omp end parallel do
```

Real space electronic charge density

XC functional (external subroutine)

XC Potential

XC Energy

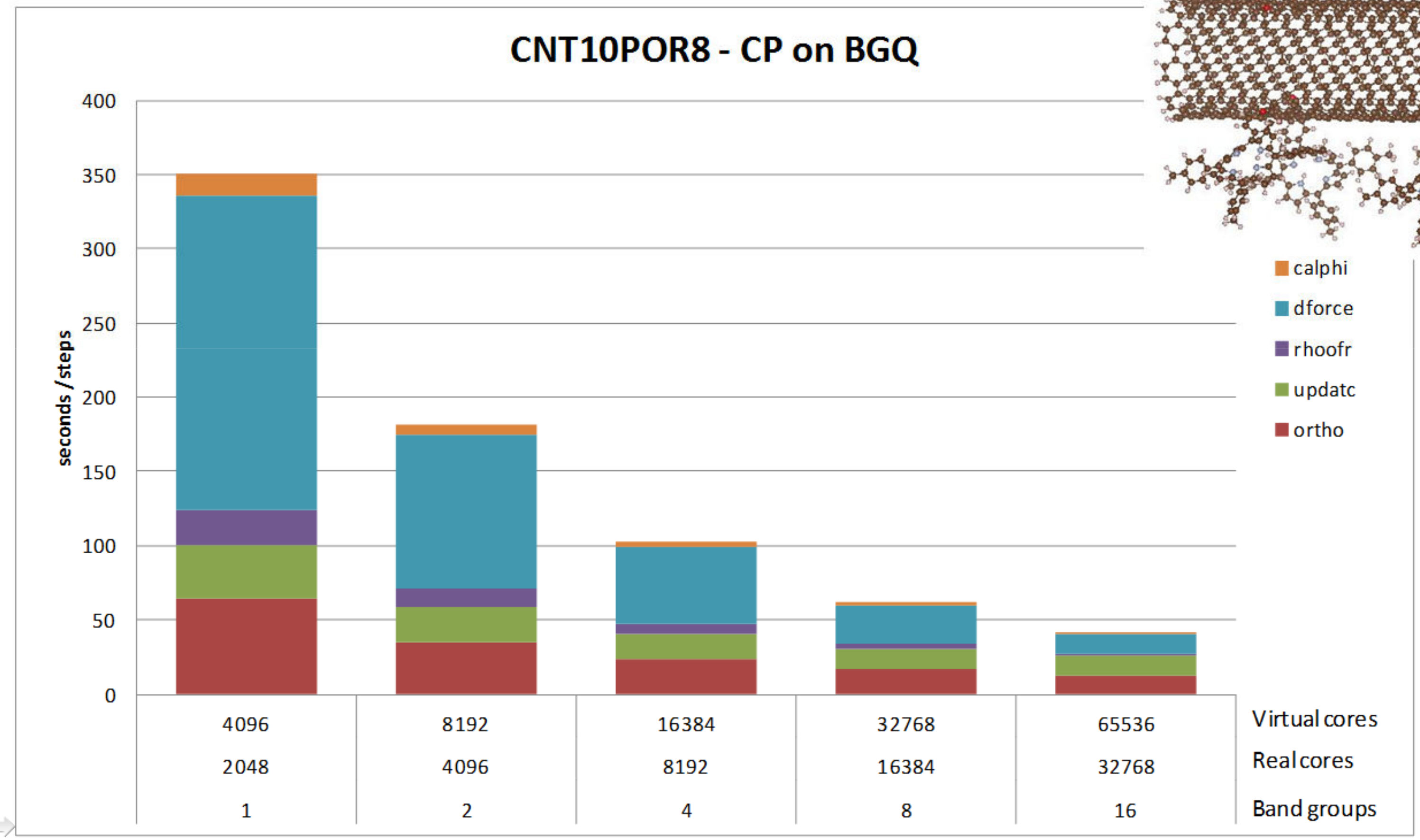
Gram-Schmidt kernel:
dealing with thread private allocatable array

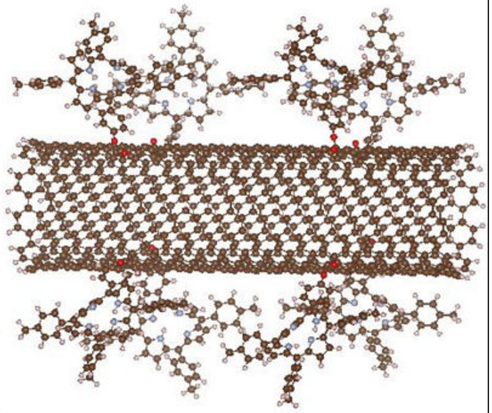
```
!$omp parallel default(shared), private( temp, k, ig )

      ALLOCATE( temp( ngw ) )

!$omp do
      DO k = 1, kmax
         csc(k) = 0.0d0
         IF ( ispin(i) .EQ. ispin(k) ) THEN
            DO ig = 1, ngw
               temp(ig) = cp(1,ig,k) * cp(1,ig,i) + cp(2,ig,k) * cp(2,ig,i)
            END DO
            csc(k) = 2.0d0 * SUM(temp)
            IF (gstart == 2) csc(k) = csc(k) - temp(1)
         ENDIF
      END DO
!$omp end do

      DEALLOCATE( temp )

!$omp end parallel
```

Example of non trivial loop parallelization

```
 DO nt = 1, ntyp
     IF ( upf(nt)%tvanp ) THEN        !
        DO ih = 1, nh(nt)           !
           DO jh = ih, nh(nt)!
              CALL qvan2( ngm, ih, jh, nt, qmod, qgm, ylmk0 )               !
!$omp parallel default(shared), private(na,qgm_na,is,dtmp,ig,mytid,ntids)
#ifdef __OPENMP
              mytid = omp_get_thread_num()          take the thread ID
              ntids = omp_get_num_threads()         take the number of threads
#endif
              ALLOCATE(  qgm_na( ngm ) )             !
              DO na = 1, nat                !
#ifdef __OPENMP
                IF( MOD( na, ntids ) /= mytid ) CYCLE      distribute atoms round-robin to threads
#endif
                IF ( ityp(na) == nt ) THEN
                   qgm_na(1:ngm) = qgm(1:ngm)*eigts1(ig1(1:ngm),na)*eigts2(ig2(1:ngm),na)*eigts3(ig3(1:ngm),na)
                   DO is = 1, nspin_mag
                       dtmp = 0.0d0
                       DO ig = 1, ngm
                          dtmp = dtmp + aux( ig, is ) * CONJG( qgm_na( ig ) )
                       END DO
                       deeq(ih,jh,na,is) = fact * omega * DBLE( dtmp )
                       deeq(jh,ih,na,is) = deeq(ih,jh,na,is)
                    END DO
                 END IF
              END DO
              DEALLOCATE( qgm_na )
!$omp end parallel
           END DO
        END DO
     END IF
  END DO
```

Bands parallelization scaling





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Conclusion

Number of cores double every two years

MPI and OpenMP exploit multi-core nodes

Both implicit and explicit multi-threading

Mixed paradigm: not big effort, good compilers and libraries

Next challenge: beyond Parallel Computing (reliable, hybrid)