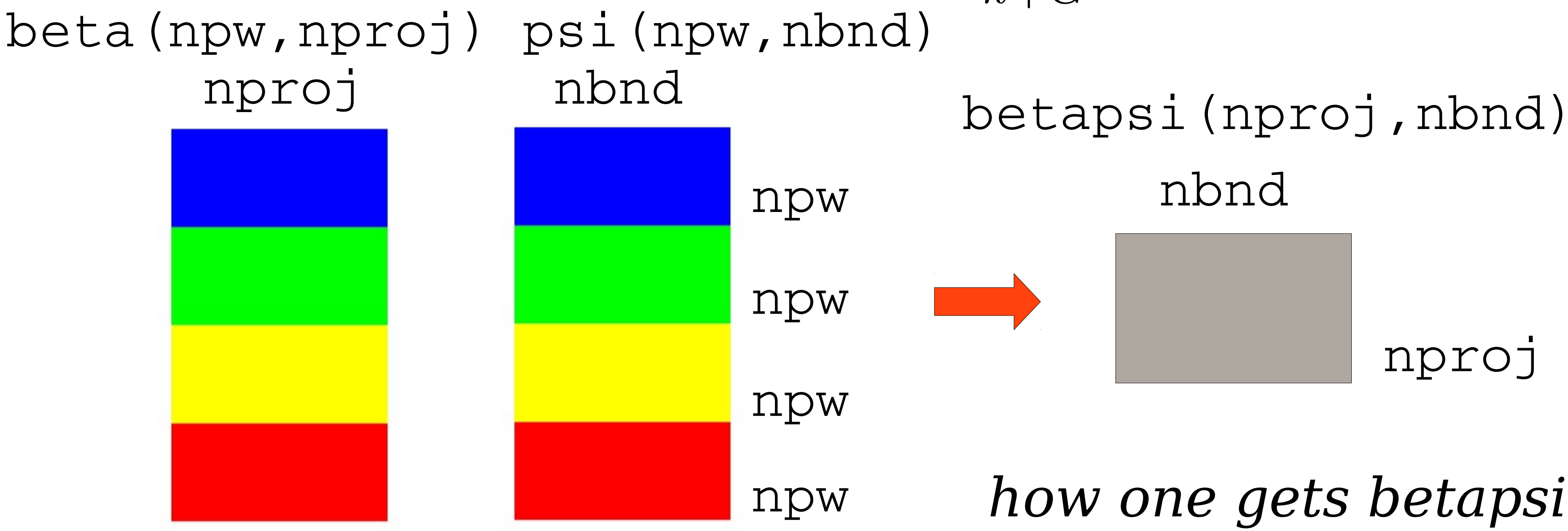
MPI – Message Passing Interface

a simple example

$$\langle \beta_i | \psi_j \rangle = \sum_{k+G} \beta_i^*(k+G)\psi_j(k+G)$$



how one gets betapsi?

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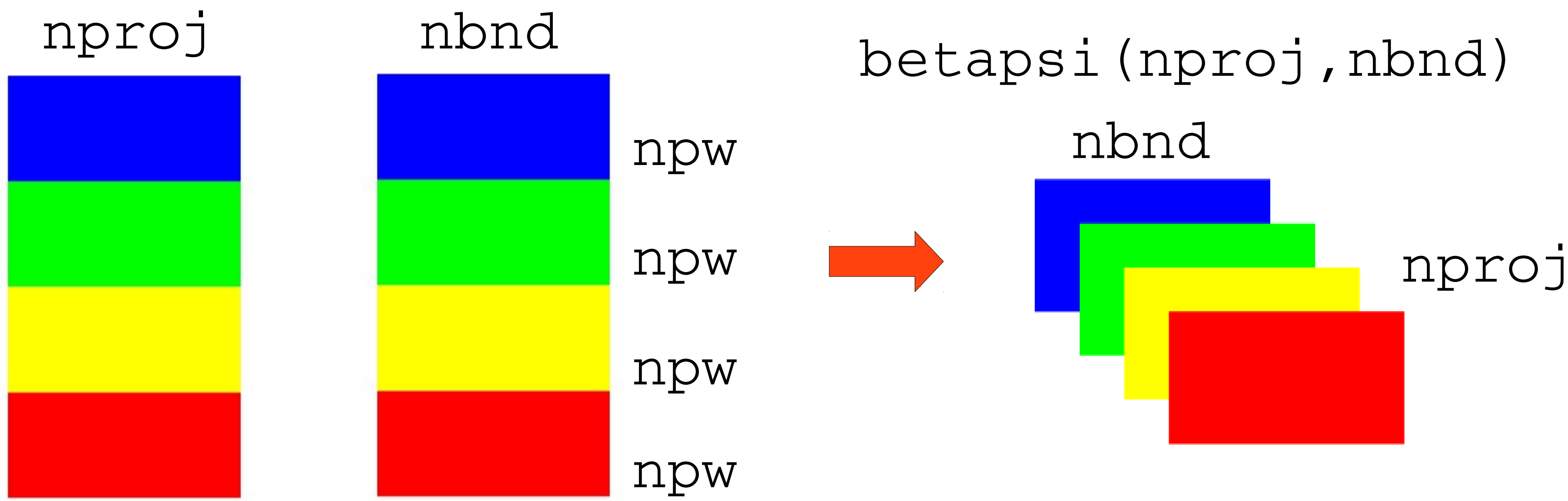
a simple example

$$\langle \beta_i | \psi_j \rangle = \sum_{k+G} \beta_i^*(k+G)\psi_j(k+G)$$

beta(npw,nproj) psi(npw,nbnd)

betapsi(nproj,nbnd)




```
CALL ZGEMM( 'C', 'N', nproj, nbnd, npw, (1.0_DP,0.0_DP), &
                  beta, npwx, psi, npwx, (0.0_DP,0.0_DP), &
                  betapsi, nprojx )
```

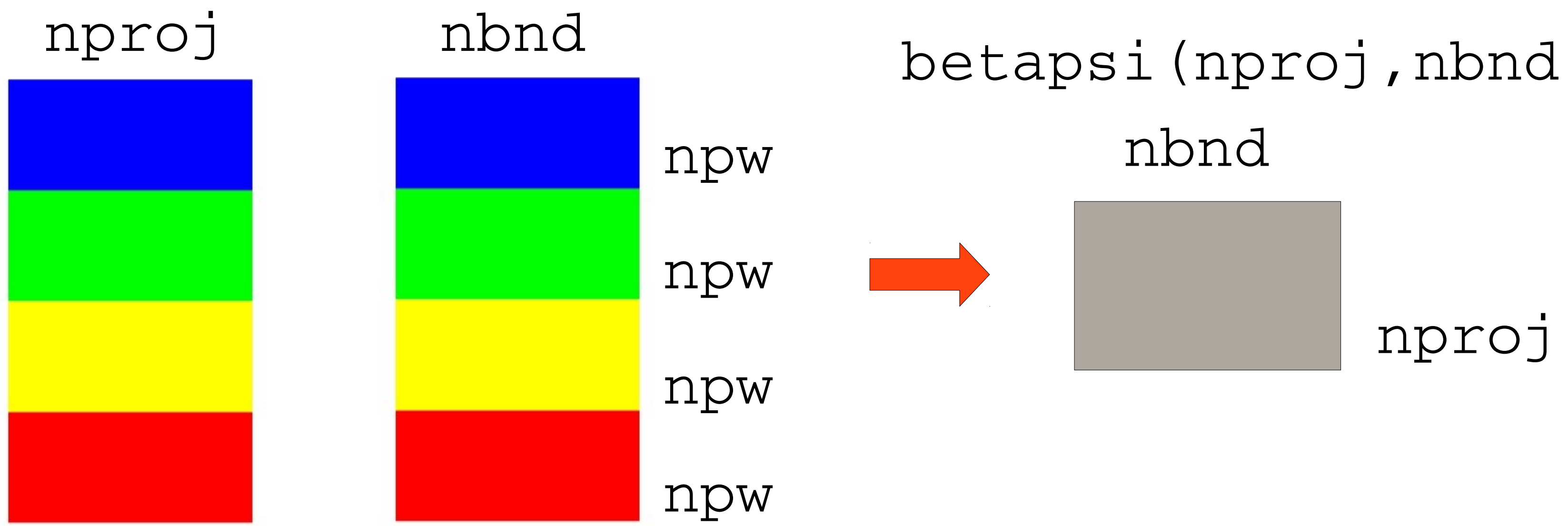
each processor has a partially summed betapsi

MPI – Message Passing Interface

a simple example

$$\langle \beta_i | \psi_j \rangle = \sum_{k+G} \beta_i^*(k+G)\psi_j(k+G)$$

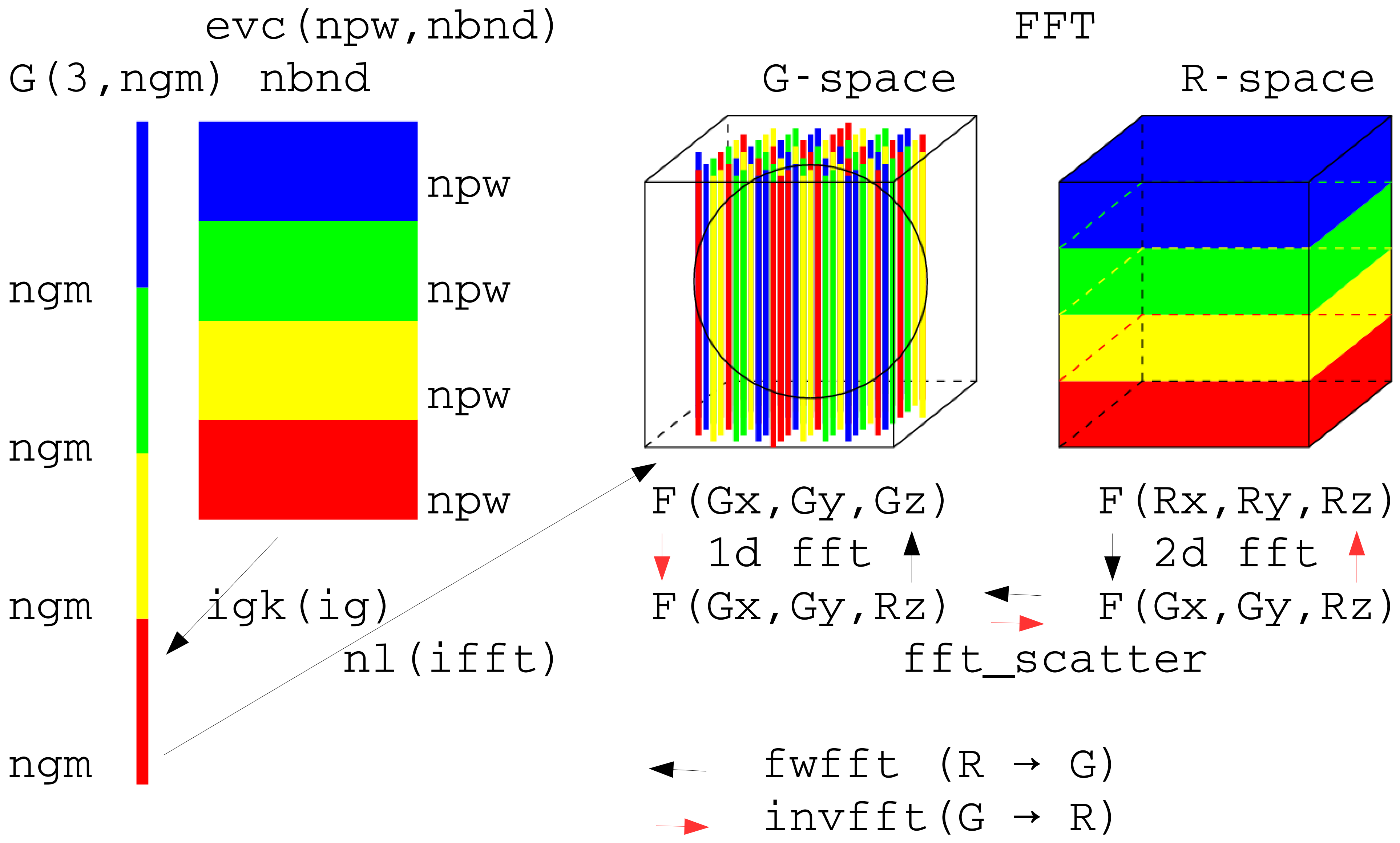
beta(npw,nproj) psi(npw,nbnd)

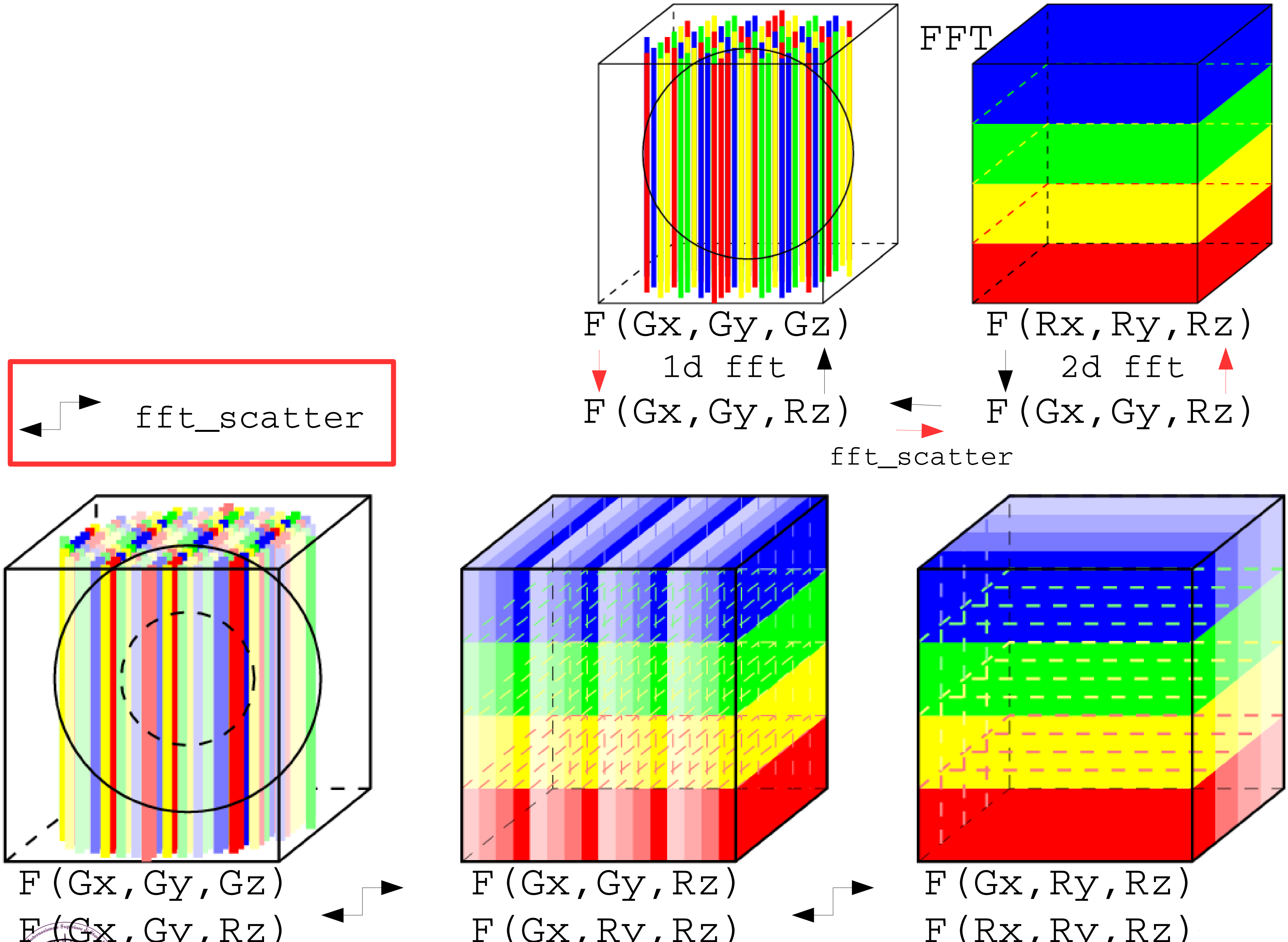



```
CALL ZGEMM( 'C', 'N', nproj, nbnd, npw, (1.0_DP,0.0_DP), &
                 beta, npwx, psi, npwx, (0.0_DP,0.0_DP), &
                 betapsi, nprojx )
CALL mp_sum( betapsi, intra_bgrp_comm )
```

at the end each processor has the complete betapsi !

R & G parallelization




FFT
F(Gx,Gy,Gz)
1d fft
F(Gx,Gy,Rz)
F(Rx,Ry,Rz)
2d fft
F(Gx,Gy,Rz)
fft_scatter
fft_scatter
F(Gx,Gy,Gz)
F(Gx,Gy,Rz)
F(Gx,Gy,Rz)
F(Gx,Ry,Rz)
F(Gx,Ry,Rz)
F(Rx,Ry,Rz)