



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

Track B: Particle Methods – Part 4

PRACE Spring School 2012

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PART 4: Hybrid parallelization and scalability testing

- Hybrid parallelization and execution on the Blue Gene/P architecture ~ 30 min
- Scalability testing ~ 30 min

Hybrid parallelization

- Our particle code is using only MPI for parallelization so far
- We will prepare MPI+OpenMP implementation and execute it on Notos system

In which part of the code should we insert the OpenMP pragmas?

Force computations loops

Local interactions

```
int compute_forces(){  
  
    int i,j,k;  
    float dist;  
    struct vector3d min,max;  
    int numprocs;  
    int procs[size];  
    struct export_list_data export_list[4*lnp];  
    int nexp=0;  
  
    /* Compute local interaction */  
    for(i=0;i<lnp;i++) {  
        for(j=0;j<lnp;j++) {  
            if(i==j) continue;  
            force(&particles[i],&particles[j]);  
        }  
    }  
}
```

Remote interactions

```
int compute_remote_forces(int nexp,struct  
    export_list_data *export_list) {  
...  
    /* Compute remote interaction */  
    for(i=0;i<size;i++) {  
        for(j=0;j<nimport[i];j++) {  
            for(k=0;k<lnp;k++) {  
                force(&import[i][j],&particles[k]);  
            }  
        }  
    }  
}
```

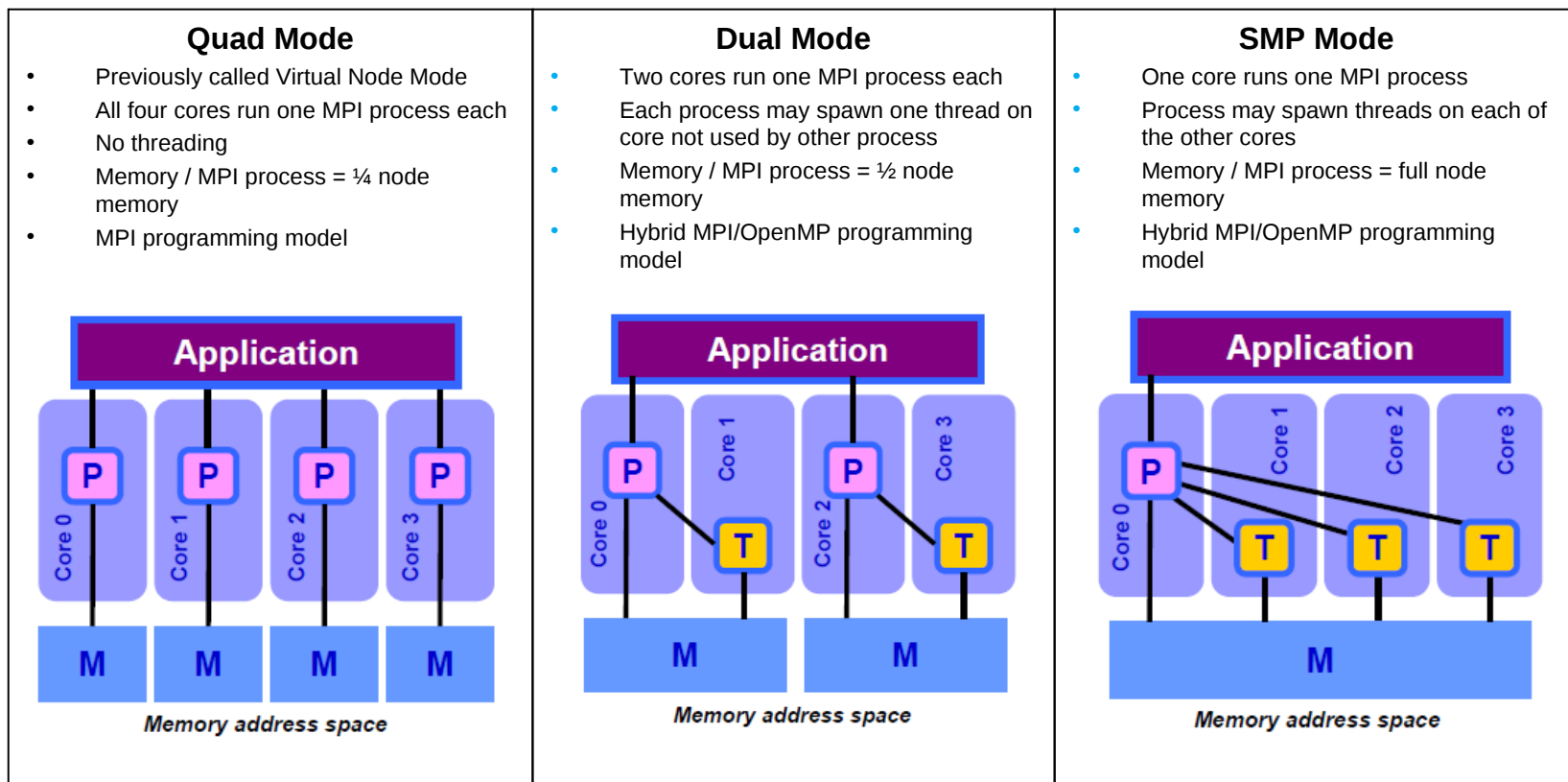


OpenMP parallel loops

```
#pragma omp parallel for <clauses>  
<for loop>
```

- for loop iterations distributed over available OpenMP threads
- Very common way of shared memory parallelization
- Popular clauses:
 - private, shared
 - reduction
 - schedule

Blue Gene/P execution modes



Basic mpirun options (*mpirun -h*)

Option	Description
-np ranks	Number of MPI ranks.
-exe <executable>	Executable file name.
-args „program args”	Program arguments.
-cwd <path>	Work directory.
-mode <SMP,DUAL,VN>	Blue Gene/P execution mode. <ul style="list-style-type: none"> • SMP – 1 rank, 4 threads • DUAL – 2 ranks, 2 threads each • VN – 4 ranks, 1 thread each

Relationship between execution mode, partition size and number of MPI ranks:

- VN mode: number of MPI ranks = 4 x partition size
- DUAL mode: number of MPI ranks = 2 x partition size
- SMP mode: number of MPI ranks = partition size

Hands-on hybrid – Exercise 5

1. Insert two **OpenMP pragmas** and parallelize force computations loops
2. Edit **Makefile** and add **-qsmp=omp** compiler option
3. Change the execution mode and adjust the number of processes in the **Makefile (use SMP mode)**
4. Execute the code and measure the execution time (3 cases: VN, DUAL, SMP)

Hands-on scalability – Exercise 6

- We will try to prepare scalability charts
- Please check the scalability of our code on following partitions:
 - 4 nodes
 - 16 nodes
 - 32 nodes
 - 64 nodes