DCAMM High Performance Computing

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Week 3: MPI

Exercise 5

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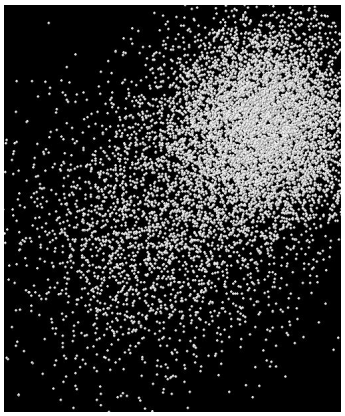
Question 1: Domain Decomposition

Displayed below is a cloud of particles in a 2D-domain. The task is to decompose the



domain into at least *nsub* subdomains such that you could distribute the particles onto different processors using an *adaptive quadtree decomposition*. The algorithm is as follows (starting from the undivided domain) and is sketched in Fig. 1.

{ 1) find the subdomain with the most particles in it, let's call it $D_{\max}$.
2) cut $D_{\max}$ into four equal rectangular subdomains. } repeat until you have $\geq$ *nsub* subdomains.

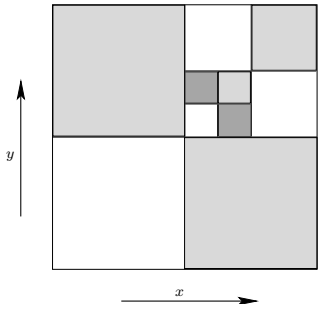


Figure 1: Illustration of adaptive quad tree decomposition

On the course webpage, you can find the binary file `particles.dat` with particle positions and the program skeleton `decompositions.f90` with the input and output sections.

Because we read the particles from a Fortran binary file, your program might throw an error depending on your platform and the compiler. If you are running on the Sun cluster use following command to compile your code:

```
f90 -xfilebyteorder=little4:%all -o d decompositions.f90
```

About the output: There are two output files to choose from: an ASCII file and a PDB file (also ASCII but with extra entries that have nothing to do with our data). The reason we include a PDB output file is that you can use it to nicely visualize the particle cloud, colored according to their subdomains, with the (molecular dynamics) viewer `Jmol` [1]. Please download `Jmol` from `http://jmol.sourceforge.net/` and unpack it in your home folder. To start `Jmol` change into the `Jmol`-directory and type `java -jar Jmol.jar` in your terminal. When you have opened the PDB file in `Jmol`, it will probably look very bad, just go to `Edit` > `Preferences...` and set the default bond radius to zero and then adjust the atom size. Activate the subdomain coloring by going into `File` > `Script...` and type `color property temperature;`.

References

[1] Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/.