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Programming with Nonequispaced FFT

Lab 3 **P^{2}NFFT Hands On**

Introduction:
Directory `test/generic/` of the ScaFaCoS source tree includes a program `scafacos_test` that computes the total energy, potentials and fields of a given particle system and compares them with precomputed reference values. Example data for some particle systems are given in directory `test/generic/systems`. In order to save time, we use a precompiled executable of this test program stored in `/homea/hpclab/train006/fourier_lab3`.

The following steps must be done, before you can start with the exercises:

1. Login to Judge via `ssh userid@judge.fz-juelich.de`
2. Copy the tests from `/homea/hpclab/train006/fourier_lab3` to your home directory via `cp -r /homea/hpclab/train006/fourier_lab3 $HOME`
3. Execute `msub -I -l nodes=1:ppn=8,walltime=00:30:00` in order to allocate 8 processes in interactive mode.
4. Go into your copy of the test directory via `cd ~/fourier_lab3/generic`.

Hint: A pdf version of this worksheet and the solutions are available at http://www.tu-chemnitz.de/~mpip/lehre.php.

Exercise 1 (Testing 3dp-P^{2}NFFT):
Compare the direct summation and the P^{2}NFFT method applied to a particle system with three-dimensional periodic boundary conditions. Therefore, run the following commands and compare the run time and accuracy

```
mpiexec -np 1 scafacos_test direct systems/3d-periodic/cloud_wall_8100.xml.gz
mpiexec -np 1 scafacos_test p2nfft systems/3d-periodic/cloud_wall_8100.xml.gz
mpiexec -np 1 scafacos_test p2nfft systems/3d-periodic/cloud_wall_8100.xml.gz \
  -c tolerance_field,1e-5
mpiexec -np 1 scafacos_test p2nfft systems/3d-periodic/cloud_wall_102900.xml.gz
```

Exercise 2 (Testing 2dp-P^{2}NFFT):
Compare the direct summation and the P^{2}NFFT method applied to a particle system with two-dimensional periodic boundary conditions. Therefore, run the following two commands and compare the run time and accuracy

```
mpiexec -np 1 scafacos_test direct systems/2d-periodic/cloud_wall_8100.xml.gz
mpiexec -np 1 scafacos_test p2nfft systems/2d-periodic/cloud_wall_8100.xml.gz
```

Exercise 3 (Testing 0dp-P^{2}NFFT):
Compare the direct summation and the P^{2}NFFT method applied to a particle system with nonperiodic boundary conditions. Therefore, run the following commands and compare

the run time and accuracy

```
mpiexec -np 1 scafacos_test direct systems/nonperiodic/cloud_wall_8100.xml.gz
mpiexec -np 1 scafacos_test p2nfft systems/nonperiodic/cloud_wall_8100.xml.gz \
  -c p2nfft_r_cut,7.4,p2nfft_grid,32,32,32
mpiexec -np 1 scafacos_test direct systems/nonperiodic/cloud_wall_102900.xml.gz
mpiexec -np 8 scafacos_test direct systems/nonperiodic/cloud_wall_102900.xml.gz
mpiexec -np 1 scafacos_test p2nfft systems/nonperiodic/cloud_wall_102900.xml.gz \
  -c p2nfft_r_cut,8,p2nfft_grid,64,64,64
```

Exercise 4 (Testing P^{2}NFFT modules):
Explore the behavior of the 3dp-P^{2}NFFT accuracy for different parameters. Therefore, start the program `scafacos_test` again with the explicitly given default parameters:

```
mpiexec -np 8 scafacos_test p2nfft systems/3d-periodic/cloud_wall_8100.xml.gz \
  -c p2nfft_ignore_tolerance,1,p2nfft_r_cut,4.481387,p2nfft_alpha,0.462344 \
  -c p2nfft_grid,32,32,32,p2nfft_oversampled_grid,32,32,32,p2nfft_cao,4
```

Now, change some of these parameters and observe the differences in accuracy and run time. For example,

- change the size of the near field cutoff radius with the argument `-c p2nfft_r_cut,` followed by one real number,
- change the size of Ewald splitting parameter with the argument `-c p2nfft_alpha,` followed by one real number,
- change the size of the NFFT grid with the argument `-c p2nfft_grid,` followed by three comma separated even integers,
- change the size of the FFT grid with the argument `-c p2nfft_oversampled_grid,` followed by three comma separated even integers,
- change the real space cutoff of the NFFT with the argument `-c p2nfft_cao,` followed by one integer between 1 and 8,
- change the number of processes via `mpiexec -np`,

or add some of the more advanced options, e.g.,

- enable interlaced NFFT with the argument `-c pnfft_interlaced,1` (Note, that the Ewald splitting parameters α must be increased slightly in order to show the improved accuracy in Fourier space),
- enable i**k**-differentiation with the argument `-c pnfft_grad_ik,1` (default is analytic differentiation),
- change the NFFT window function φ with the argument `-c pnfft_window_name,` followed by one of the these strings: `kaiser` (Kaiser-Bessel window), `gaussian` (Gaussian window), `bspline` (B-spline window), `sinc` (Sine Cardinal window - Fourier transform of the B-spline window) and `bessel_i0` (window function based on the modified Bessel function of first kind - Fourier transform of the Kaiser-Bessel window). The default value is `bspline`.

Feel free to play around with different parameter settings and boundary conditions. You can also try to run P^{2}NFFT with some of the noncubic particle systems given in `systems/3d-periodic/noncubic`.

Hint: Find a full list of optional arguments at http://www.scafacos.de/files/pub/libfcs_manual.pdf.