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Programming with Nonequispaced FFT

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

Exercise 1:

```
Initializing FCS, method direct...
    Average time: 4.075688e+01
    Total time:   4.075688e+01
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
         abs_rms_field_error =    1.576721e-02
         abs_max_field_error =    4.332013e-02
     abs_rms_potential_error =    2.790704e+00
     abs_max_potential_error =    6.098140e+00
            abs_energy_error =    3.553589e+02

  RELATIVE ERRORS (from 8100 of 8100 particles)
         rel_rms_field_error =    3.672597e-03
         rel_max_field_error =    1.009040e-02
     rel_rms_potential_error =    7.539153e-01
     rel_max_potential_error =    1.647427e+00
            rel_energy_error =    8.836555e-02

            total_energy_ref =    4.021464e+03
                total_energy =    4.376823e+03
```

```
Initializing FCS, method p2nfft...
    Average time: 1.021841e-01
    Total time:   1.021841e-01
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
         abs_rms_field_error =    9.830651e-03
         abs_max_field_error =    3.829890e-02
     abs_rms_potential_error =    3.982203e-03
     abs_max_potential_error =    1.061833e-02
            abs_energy_error =    1.038400e+01

  RELATIVE ERRORS (from 8100 of 8100 particles)
         rel_rms_field_error =    2.290622e-03
         rel_max_field_error =    8.923956e-03
     rel_rms_potential_error =    1.846829e-03
     rel_max_potential_error =    4.924468e-03
            rel_energy_error =    2.582144e-03

            total_energy_ref =    4.021464e+03
                total_energy =    4.031848e+03
```

```
Initializing FCS, method p2nfft...
    Average time: 2.024260e-01
    Total time:   2.024260e-01
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
         abs_rms_field_error =    1.269773e-05
         abs_max_field_error =    2.571326e-05
     abs_rms_potential_error =    2.617172e-06
     abs_max_potential_error =    6.746318e-06
            abs_energy_error =    6.039146e-03

  RELATIVE ERRORS (from 8100 of 8100 particles)
         rel_rms_field_error =    2.956367e-06
         rel_max_field_error =    5.986727e-06
     rel_rms_potential_error =    1.214787e-06
     rel_max_potential_error =    3.131372e-06
            rel_energy_error =    1.501728e-06

            total_energy_ref =    4.021464e+03
                total_energy =    4.021470e+03
```

```
Initializing FCS, method p2nfft...
    Average time: 1.380877e+00
    Total time:   1.380877e+00
  ABSOLUTE ERRORS (from 102900 of 102900 particles)
         abs_rms_field_error =    8.707156e-03
         abs_max_field_error =    3.679576e-02
     abs_rms_potential_error =    3.841221e-03
     abs_max_potential_error =    9.852075e-03
            abs_energy_error =    1.328007e+02

  RELATIVE ERRORS (from 102900 of 102900 particles)
         rel_rms_field_error =    2.028866e-03
         rel_max_field_error =    8.573828e-03
     rel_rms_potential_error =    1.781436e-03
     rel_max_potential_error =    4.569078e-03
            rel_energy_error =    2.599475e-03

            total_energy_ref =    5.108749e+04
                total_energy =    5.122029e+04
```

The direct summation takes longer than all the P^{2}NFFT runs. Even for the higher accuracy and for the larger system size P^{2}NFFT is a lot faster.

Exercise 2:

```
Initializing FCS, method direct...
    Average time: 1.287987e+01
    Total time:   1.287987e+01
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
          abs_rms_field_error =    2.056811e-01
          abs_max_field_error =    2.293834e-01
       abs_rms_potential_error =    1.205946e+00
       abs_max_potential_error =    2.802046e+00
              abs_energy_error =    1.442260e+02

  RELATIVE ERRORS (from 8100 of 8100 particles)
          rel_rms_field_error =    5.100132e-02
          rel_max_field_error =    5.687862e-02
       rel_rms_potential_error =    4.564652e-01
       rel_max_potential_error =    1.060608e+00
              rel_energy_error =    3.896687e-02

              total_energy_ref =    3.701246e+03
                  total_energy =    3.845472e+03
```

```
Initializing FCS, method p2nfft...
    Average time: 9.597588e-02
    Total time:   9.597588e-02
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
          abs_rms_field_error =    2.057253e-02
          abs_max_field_error =    8.388797e-02
       abs_rms_potential_error =    1.348259e-02
       abs_max_potential_error =    8.236404e-02
              abs_energy_error =    1.007187e+01

  RELATIVE ERRORS (from 8100 of 8100 particles)
          rel_rms_field_error =    4.952019e-03
          rel_max_field_error =    2.019270e-02
       rel_rms_potential_error =    5.557085e-03
       rel_max_potential_error =    3.394778e-02
              rel_energy_error =    2.721210e-03

              total_energy_ref =    3.701246e+03
                  total_energy =    3.711318e+03
```

Again, the P^{2}NFFT is faster and reaches higher accuracy.

Exercise 3:

```
Initializing FCS, method direct...
    Average time: 1.044040e+00
    Total time:   1.044040e+00
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
          abs_rms_field_error =    2.144149e-14
          abs_max_field_error =    1.263026e-13
       abs_rms_potential_error =    1.614742e-14
       abs_max_potential_error =    9.059420e-14
              abs_energy_error =    6.821210e-12

  RELATIVE ERRORS (from 8100 of 8100 particles)
          rel_rms_field_error =    5.041171e-15
          rel_max_field_error =    2.969537e-14
       rel_rms_potential_error =    4.901409e-15
       rel_max_potential_error =    2.749909e-14
              rel_energy_error =    1.821154e-15

              total_energy_ref =    3.745543e+03
                  total_energy =    3.745543e+03

Initializing FCS, method direct...
    Average time: 1.706608e+02
    Total time:   1.706608e+02
  ABSOLUTE ERRORS (from 102900 of 102900 particles)
          abs_rms_field_error =    9.289615e-14
          abs_max_field_error =    7.808651e-13
       abs_rms_potential_error =    2.130021e-13
       abs_max_potential_error =    1.412204e-12
              abs_energy_error =    1.840817e-09

  RELATIVE ERRORS (from 102900 of 102900 particles)
          rel_rms_field_error =    2.105974e-14
          rel_max_field_error =    1.770237e-13
       rel_rms_potential_error =    3.276131e-14
       rel_max_potential_error =    2.172074e-13
              rel_energy_error =    3.523983e-14

              total_energy_ref =    5.223683e+04
                  total_energy =    5.223683e+04
```

```
Initializing FCS, method p2nfft...
    Average time: 2.325690e-01
    Total time:   2.325690e-01
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
          abs_rms_field_error =    4.909207e-03
          abs_max_field_error =    1.460276e-02
       abs_rms_potential_error =    3.331898e-03
       abs_max_potential_error =    1.202156e-02
              abs_energy_error =    3.551864e+00

  RELATIVE ERRORS (from 8100 of 8100 particles)
          rel_rms_field_error =    1.154816e-03
          rel_max_field_error =    3.435075e-03
       rel_rms_potential_error =    1.011858e-03
       rel_max_potential_error =    3.650804e-03
              rel_energy_error =    9.482908e-04

              total_energy_ref =    3.745543e+03
                  total_energy =    3.741991e+03

Initializing FCS, method direct...
    #0 time: 3.252705e+01
    Average time: 3.252705e+01
    Total time:   3.252705e+01
  ABSOLUTE ERRORS (from 102900 of 102900 particles)
          abs_rms_field_error =    6.638876e-14
          abs_max_field_error =    9.176450e-13
       abs_rms_potential_error =    9.182183e-14
       abs_max_potential_error =    8.126833e-13
              abs_energy_error =    5.093170e-11

  RELATIVE ERRORS (from 102900 of 102900 particles)
          rel_rms_field_error =    1.505047e-14
          rel_max_field_error =    2.080320e-13
       rel_rms_potential_error =    1.412288e-14
       rel_max_potential_error =    1.249967e-13
              rel_energy_error =    9.750151e-16

              total_energy_ref =    5.223683e+04
                  total_energy =    5.223683e+04
```

```
Initializing FCS, method p2nfft...
    Average time: 4.204461e+00
    Total time:   4.204461e+00
  ABSOLUTE ERRORS (from 102900 of 102900 particles)
         abs_rms_field_error =    7.908770e-03
         abs_max_field_error =    1.944398e-02
     abs_rms_potential_error =    5.279158e-03
     abs_max_potential_error =    1.872120e-02
            abs_energy_error =    8.347581e+01

  RELATIVE ERRORS (from 102900 of 102900 particles)
         rel_rms_field_error =    1.795161e-03
         rel_max_field_error =    4.413463e-03
     rel_rms_potential_error =    8.119951e-04
     rel_max_potential_error =    2.879536e-03
            rel_energy_error =    1.598026e-03

            total_energy_ref =    5.223683e+04
                total_energy =    5.215336e+04
```

For the 8100 particle system, both methods are comparable with respect to run time, but the direct method is much more accurate. However, we can see already at the 102900 particle test case, that the N^2 scaling of the direct methods permits the application to larger systems. Even if we use 8 processes, the direct method is still much slower than the P^{2}NFFT.

Exercise 4:

We present some selected examples here.

With interlacing and increased α we gain an order of accuracy at the same run time.

```
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,0.57 \
  -c p2nfft_grid,32,32,32,p2nfft_oversampled_grid,32,32,32,p2nfft_cao,4 \
  -c pnfft_interlaced,1

    Average time: 1.115122e-01
    Total time:   1.115122e-01
  ABSOLUTE ERRORS (from 8100 of 8100 particles)
         abs_rms_field_error =    1.580598e-03
         abs_max_field_error =    3.765933e-03
     abs_rms_potential_error =    5.248671e-04
     abs_max_potential_error =    1.140644e-03
            abs_energy_error =    1.587127e+00

  RELATIVE ERRORS (from 8100 of 8100 particles)
         rel_rms_field_error =    3.680610e-04
         rel_max_field_error =    8.769421e-04
     rel_rms_potential_error =    2.435946e-04
     rel_max_potential_error =    5.293812e-04
            rel_energy_error =    3.946639e-04

            total_energy_ref =    4.021464e+03
                total_energy =    4.023051e+03
```