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Programming with Nonequispaced FFT

Solution 2 **C Library Hands On**

Exercise 1:

The file `pfft_check.x` initialises a plan for a three-dimensional forward FFT with $n_0 \times n_1 \times n_2 = 16 \times 16 \times 16$ Fourier coefficients. The Fourier coefficients $\hat{g}_{k_0 k_1 k_2} \in \mathbb{C}^3$, $k_0 = 0, \ldots, 15$, $k_1 = 0, \ldots, 15$, $k_2 = 0, \ldots, 15$ are generated corresponding to their parallel distribution. Part of the input and output of the FFT and its inverse are displayed. Also, the backward transform is executed, showing that the FFT is a unitary transform.

To allocate 8 processes, we can use the interactive mode:
`msub -I -l nodes=1:ppn=8,walltime=00:30:00`

```
train006@judge048:~> mpiexec -np 8 ~/fourier_lab2/build/pfft_check.x
************************************************************************************************
* Computation of parallel FFT
* for  n[0] x n[1] x n[2] = 16 x 16 x 16 Fourier coefficients
* at   512 equispaced nodes per process
* on   np[0] x np[1] x np[2] = 2 x 2 x 2 processes
************************************************************************************************

Input Fourier coefficients on process 1:
   0. 1.00e+03 + 5.00e+02 I     3.33e+02 + 2.50e+02 I   2.00e+02 + 1.67e+02 I   1.43e+02 + 1.25e+02 I
   4. 1.11e+02 + 1.00e+02 I     9.09e+01 + 8.33e+01 I   7.69e+01 + 7.14e+01 I   6.67e+01 + 6.25e+01 I
PFFT results on process 1:
   0. 5.14e+03 + 4.45e+03 I     3.21e+03 + 1.44e+03 I   2.84e+03 + 1.31e+03 I   2.63e+03 + 1.29e+03 I
   4. 2.48e+03 + 1.30e+03 I     2.37e+03 + 1.33e+03 I   2.28e+03 + 1.37e+03 I   2.20e+03 + 1.41e+03 I
Fourier coefficients after one forward and backward PFFT on process 1:
   0. 1.00e+03 + 5.00e+02 I     3.33e+02 + 2.50e+02 I   2.00e+02 + 1.67e+02 I   1.43e+02 + 1.25e+02 I
   4. 1.11e+02 + 1.00e+02 I     9.09e+01 + 8.33e+01 I   7.69e+01 + 7.14e+01 I   6.67e+01 + 6.25e+01 I

Error after one forward and backward PFFT of size n=(16, 16, 16):
maximum error = 8.04e-14;
```

Exercise 2:

The file `pnfft_test.x` initialises a plan for a three-dimensional parallel NFFT with $N_0 \times N_1 \times N_2 = 16 \times 16 \times 16$ Fourier coefficients and $M = 4096$ nodes. The Fourier coefficients $\hat{f}_{k_0 k_1 k_2} \in \mathbb{C}^3$, $k_0 = 0, \ldots, 15$, $k_1 = 0, \ldots, 15$, $k_2 = 0, \ldots, 15$ and random nodes $\mathbf{x}_j \in [0, 1)^3$, $j = 0, \ldots, 4096$ are generated corresponding to their parallel distribution. Part of the input and output of the NFFT and its adjoint are displayed. Also, the adjoint transform is executed, showing that the NFFT is, in contrast to the FFT, a non-unitary transform.

```
train006@judge048:~> mpiexec -np 8 ~/fourier_lab2/build/pnfft_test.x
************************************************************************************************
* Computation of parallel NFFT
* for  N[0] x N[1] x N[2] = 16 x 16 x 16 Fourier coefficients
* at   local_M = 512 nodes per process
* on   np[0] x np[1] x np[2] = 2 x 2 x 2 processes
************************************************************************************************

Input Fourier coefficients on process 1:
```

```
   0. 1.00e+03 + 5.00e+02 I     3.33e+02 + 2.50e+02 I   2.00e+02 + 1.67e+02 I   1.43e+02 + 1.25e+02 I
   4. 1.11e+02 + 1.00e+02 I     9.09e+01 + 8.33e+01 I   7.69e+01 + 7.14e+01 I   6.67e+01 + 6.25e+01 I
PNFFT Results on process 1:
   0. 2.18e+02 + 1.12e+03 I     -1.17e+02 + -8.73e+02 I -5.86e+02 + -5.89e+02 I 1.19e+02 + -9.76e+02 I
   4. -1.98e+03 + 1.00e+02 I    2.04e+02 + 1.11e+03 I   5.64e+02 + 6.04e+02 I   9.50e+02 + -8.01e+02 I
Fourier coefficients after one forward and backward PNFFT on process 1:
   0. 9.90e+02 + 5.12e+02 I     3.25e+02 + 2.57e+02 I   2.63e+02 + 1.24e+02 I   1.66e+02 + 1.17e+02 I
   4. 1.15e+02 + 1.26e+02 I     9.53e+01 + 9.19e+01 I   7.52e+01 + -1.78e+01 I  7.53e+01 + 3.32e+01 I

Error after one PNFFT and adjoint PNFFT of size N=(16, 16, 16) with nonequispaced nodes:
maximum error = 1.41e+02;
```

Exercise 3:

For example, we can observe the decrease of the error for increasing real space cutoff m.

```
*****************************************************************************************************
* Computation of parallel NFFT
* for  N[0] x N[1] x N[2] = 16 x 16 x 16 Fourier coefficients (change with -pnfft_N * * *)
* at   local_M = 512 nodes per process (change with -pnfft_local_M *)
* with n[0] x n[1] x n[2] = 32 x 32 x 32 FFT grid size (change with -pnfft_n * * *),
*      m = 4 real space cutoff (change with -pnfft_m *),
*      window = 4 window function (PNFFT_WINDOW_KAISER_BESSEL) (change with -pnfft_window *),
* on   np[0] x np[1] x np[2] = 2 x 2 x 2 processes (change with -pnfft_np * * *)
*****************************************************************************************************

pnfft_trafo needs 5.98e-03 s
pnfft_trafo needs 4.50e-03 s
* Results in absolute error = 5.07e-04
* Results in relative error = 6.76e-08


rain006@judge048:~> mpiexec -np 8 ~/fourier_lab2/build/pnfft_check.x -pnfft_m 6
*****************************************************************************************************
* Computation of parallel NFFT
* for  N[0] x N[1] x N[2] = 16 x 16 x 16 Fourier coefficients (change with -pnfft_N * * *)
* at   local_M = 512 nodes per process (change with -pnfft_local_M *)
* with n[0] x n[1] x n[2] = 32 x 32 x 32 FFT grid size (change with -pnfft_n * * *),
*      m = 6 real space cutoff (change with -pnfft_m *),
*      window = 4 window function (PNFFT_WINDOW_KAISER_BESSEL) (change with -pnfft_window *),
* on   np[0] x np[1] x np[2] = 2 x 2 x 2 processes (change with -pnfft_np * * *)
*****************************************************************************************************

pnfft_trafo needs 6.73e-03 s
pnfft_trafo needs 7.82e-03 s
* Results in absolute error = 4.48e-08
* Results in relative error = 5.97e-12


train006@judge048:~> mpiexec -np 8 ~/fourier_lab2/build/pnfft_check.x -pnfft_m 8
*****************************************************************************************************
* Computation of parallel NFFT
* for  N[0] x N[1] x N[2] = 16 x 16 x 16 Fourier coefficients (change with -pnfft_N * * *)
* at   local_M = 512 nodes per process (change with -pnfft_local_M *)
* with n[0] x n[1] x n[2] = 32 x 32 x 32 FFT grid size (change with -pnfft_n * * *),
*      m = 8 real space cutoff (change with -pnfft_m *),
*      window = 4 window function (PNFFT_WINDOW_KAISER_BESSEL) (change with -pnfft_window *),
* on   np[0] x np[1] x np[2] = 2 x 2 x 2 processes (change with -pnfft_np * * *)
*****************************************************************************************************

pnfft_trafo needs 1.08e-02 s
pnfft_trafo needs 1.27e-02 s
* Results in absolute error = 8.50e-11
* Results in relative error = 1.13e-14
```

Exercise 4:

The subroutine `init_equispaced_nodes` can be implemented as follows:

```
static void init_equispaced_nodes(
    const ptrdiff_t *N, const double *lo, const double *up,
    double *x
    )
{
  ptrdiff_t local_N[3], local_N_start[3], m=0;

  for(int t=0; t<3; t++){
    local_N[t] = ((up[t]-lo[t]) * N[t]);
    local_N_start[t] = lo[t] * N[t];
  }

  m=0;
  for(ptrdiff_t k0=local_N_start[0]; k0<local_N_start[0] + local_N[0]; k0++)
    for(ptrdiff_t k1=local_N_start[1]; k1<local_N_start[1] + local_N[1]; k1++)
      for(ptrdiff_t k2=local_N_start[2]; k2<local_N_start[2] + local_N[2]; k2++, m++){
        x[3*m+0] = (double) k0/N[0];
        x[3*m+1] = (double) k1/N[1];
        x[3*m+2] = (double) k2/N[2];
      }
}
```

Then, the check gives the following results

```
train006@judge048:~> mpiexec -np 8 ~/fourier_lab2/build/pnfft_test_adv.x
*****************************************************************************************************
* Computation of parallel NFFT
* for  N[0] x N[1] x N[2] = 16 x 16 x 16 Fourier coefficients
* at   local_M = 512 nodes per process
* on   np[0] x np[1] x np[2] = 2 x 2 x 2 processes
*****************************************************************************************************

Input Fourier coefficients on process 1:
   0. 1.00e+03 + 5.00e+02 I     3.33e+02 + 2.50e+02 I   2.00e+02 + 1.67e+02 I   1.43e+02 + 1.25e+02 I
   4. 1.11e+02 + 1.00e+02 I     9.09e+01 + 8.33e+01 I   7.69e+01 + 7.14e+01 I   6.67e+01 + 6.25e+01 I
PNFFT Results on process 1:
   0. 7.64e+02 + 3.26e+02 I     -7.34e+02 + -3.80e+02 I 7.11e+02 + 4.41e+02 I   -6.96e+02 + -5.10e+02 I
   4. 6.91e+02 + 5.94e+02 I     -7.02e+02 + -7.01e+02 I 7.47e+02 + 8.53e+02 I   -8.93e+02 + -1.11e+03 I
Fourier coefficients after one forward and backward PNFFT on process 1:
   0. 1.00e+03 + 5.00e+02 I     3.33e+02 + 2.50e+02 I   2.00e+02 + 1.67e+02 I   1.43e+02 + 1.25e+02 I
   4. 1.11e+02 + 1.00e+02 I     9.09e+01 + 8.33e+01 I   7.69e+01 + 7.14e+01 I   6.67e+01 + 6.25e+01 I

Error after one PNFFT and adjoint PNFFT of size N=(16, 16, 16) with equispaced nodes:
maximum error = 2.38e-07;
```