MHPC
Master in High Performance Computing

FFT IN PRACTICE

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Fields of Application

- The FFT is used in physics, astronomy, engineering, applied mathematics, cryptography, and comp. finance
- Method to solve differential equations
- Digital Signal Processing & Image Processing
  - Receive signal in the time domain, but want the frequency spectrum
- Convolutions/Filters
  - Filter can be efficiently represented mathematically by a convolution
- Benchmarking

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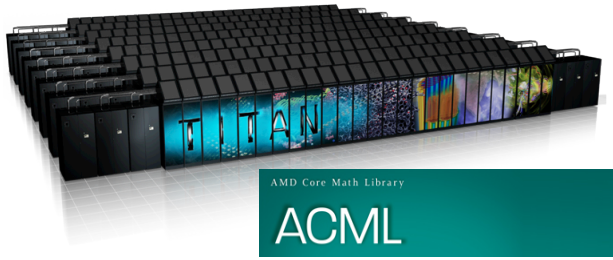
Existing Libraries for Scientific High Performance Applications

MathKeisan

ESSL and Parallel ESSL



AMD Core Math Library
ACML
AMD
The future is fusion

cuFFT

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SDSC
P3DFFT

FFTE

FFTW

2DECOMP & FFT

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FFTW, WHY?

- Freely available open-source package. Most used on Linux environment for High Performance Computing
- FFTW is written in portable C and runs well on many architectures and O.S.
- FFTW computes DFTs in O (*n logn*) time for any length *n* and supports arbitrary multi-dimensional data
- Includes parallel (multi-threaded) transforms for shared-memory systems and distributed-memory parallel transforms using MPI libraries
- FFTW supports multiple and/or strided DFTs; for example, to transform a 3-component vector field or a portion of a multi-dimensional array.
- FFTW supports DFTs of real data, as well as of real symmetric/anti-symmetric data (also called discrete cosine/sine transforms).

FFTW basic usage

```
[...]
use, intrinsic :: iso_c_binding
!
implicit none
include 'fftw3.f03'
!
integer, intent( in ) :: n1,n2,n3
!
type(C_PTR) :: plan
complex(C_DOUBLE_COMPLEX), dimension(:,:,:), pointer :: in, out
type(C_PTR) :: p_in, p_out
!
! Aligned memory allocation
p_in = fftw_alloc_complex( int( n1 * n2 * n3, C_SIZE_T ) )
p_out = fftw_alloc_complex( int( n1 * n2 * n3, C_SIZE_T ) )
!
call c_f_pointer( p_in, in, [ n1, n2, n3 ] )
call c_f_pointer( p_out, out, [ n1, n2, n3 ] )
!
! Definition of a FFTW plan
!
plan = fftw_plan_dft_3d( n3, n2, n1, in, out, FFTW_FORWARD,FFTW_ESTIMATE )
!
call fftw_execute_dft( plan, in, out )
!
call fftw_destroy_plan( plan )
call fftw_free( p_in )
call fftw_free( p_out )
```

FFTW from FORTRAN (remarks)

- Function in C became function in FORTRAN if they have a return value, and subroutines otherwise. All C types are mapped via the iso_c_binning standard.
- FFTW plans are type(C_PTR) in FORTRAN.
- The ordering of FORTRAN array dimensions must be reversed when they are passed to the FFTW plan creation
- For example, consider the three-dimensional (L M N) arrays:

```
complex(C_DOUBLE_COMPLEX), dimension(L,M,N) :: in, out
```

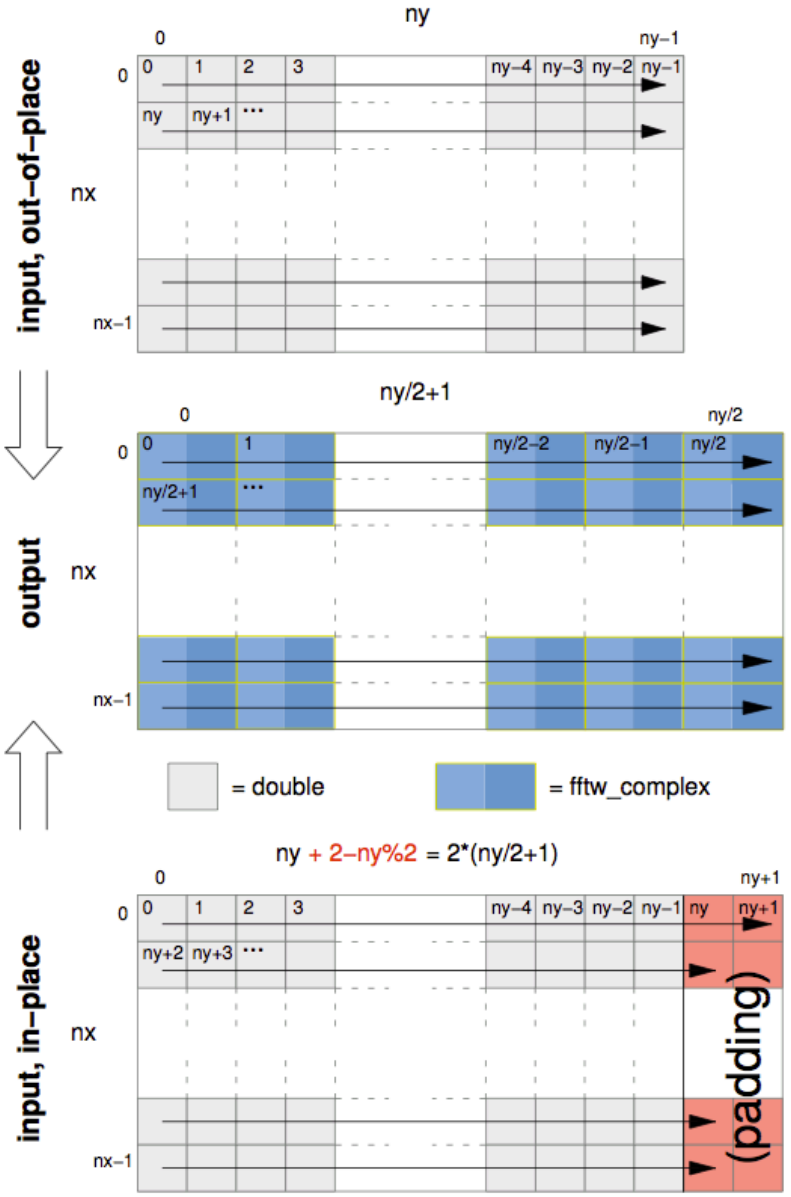
- To plan a DFT for these arrays using fftw_plan_dft_3d, you could do:

```
plan = fftw_plan_dft_3d(N,M,L, in,out, FFTW_FORWARD,FFTW_ESTIMATE)
```

- That is, from FFTW's perspective this is a N M L array. No data transposition need occur, as this is only notation.

Transform Real Data

- The DFT output satisfies the “Hermitian” redundancy: out[i] is the conjugate of out[n - i]
- Substantial optimization
- From r2c, the input is in real numbers, while the output is composed by n/2+1 complex numbers (developers must handle the different data types)



Multithread

- Works on shared-memory multi-cores system that supports POSIX threads and/or OpenMP
- Quick access to scalable FFT (How many threads?)
- Uses the same execution schema as for sequential but the following

```
[...]
/* Initialize FFTW multithreaded environment (to be called before call any FFTW routines) */
int fftw_init_threads(void);

[...]
/* Set the MAX number of threads the for creations of next plans */
void fftw_plan_with_nthreads(int nthreads);

[...]
/* Clean FFTW multithreaded environment */
void fftw_cleanup_threads(void);
```

- Calling FFTW from a thread region, developers must consider *fftw_execute(...)* is the only thread-safe subroutine

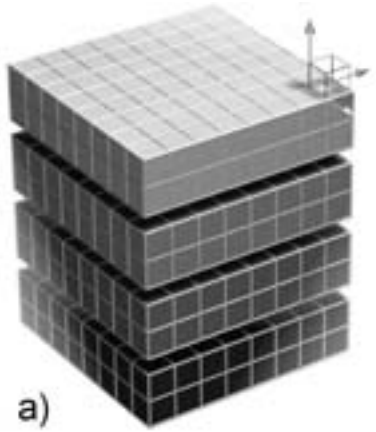
FFTW (MPI)

- each process only stores a portion of the data to be transformed => data structures and programming-interface are quite different from the serial or threads versions

```
#include <fftw3-mpi.h>

[...]
MPI_Init(&argc, &argv);
/* Initalizes FFTW_MPI environment. Must be included between MPI_Init & MPI_Finalize
fftw_mpi_init();

[...]
/* get local data size and allocate */
alloc_local = fftw_mpi_local_size_2d(N0, N1, MPI_COMM_WORLD, &local_n0, &local_0_start);
data = fftw_alloc_complex(alloc_local);

[...]
/* create plan for in-place forward DFT */
plan = fftw_mpi_plan_dft_2d(N0, N1, data, data, MPI_COMM_WORLD, FFTW_FORWARD, FFTW_ESTIMATE);
/* compute transforms, in-place */
fftw_execute(plan);

fftw_destroy_plan(plan);
MPI_Finalize();
```

FFTW (MPI)

- With a distributed-memory FFT, the inputs and outputs are broken into disjoint blocks, one per process
- In particular, FFTW uses a *1d block distribution* of the data, distributed along the *first dimension*



Installation and linking

- Download the package from www.fftw.org
- By default only double precision sequential FFT are compiled and included into the -lfftw3
- Other possible version must be enabled at ./configure time:
  - --enable-float, --enable-long-double for single/long-double precision
  - --enable-threads, --enable-openmp for multithread versions
  - --enable-mpi for MPI version (-lfftw3_mpi)
  - --enable-avx for SIMD extensions (many others available)

References

- FFTW3 manual @ www.fftw.org
- Matteo Frigo and Steven G. Johnson, *The design and implementation of fftw3*, Proc. IEEE, 93(2):2168211;231, 2005
- Matteo Frigo and Steven G. Johnson, Implementing FFTs in practice, http://cnx.org/content/m16336/latest/