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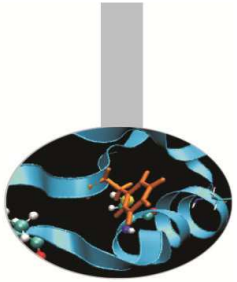
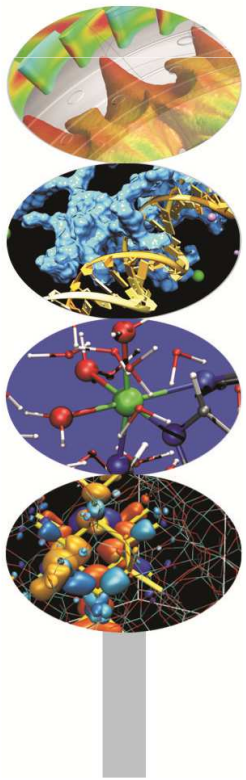
SuperComputing Applications and Innovation



FFT Libraries Hands-on



Massimiliano Guarrasi,
CINECA

Casalecchio di Reno, 17/02/2016

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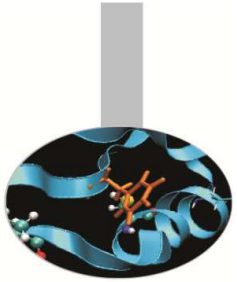
Fast Fourier Transform (FFT)



- FFTPACK
- FFTW
- 2Decomp&FFT
- P3DFFT

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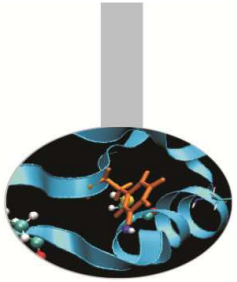
Fast Fourier Transform (FFT)



FFTPACK

FFTPACK is a package of Fortran subroutines for the fast Fourier transform. It includes complex, real, sine, cosine, and quarter-wave transforms. It is included in the general-purpose mathematical library SLATEC.

Language: FORTRAN

Availability: public domain

Developers: Paul N. Swarztrauber, National Center for Atmospheric Research, Boulder, CO

Distributors: NETLIB

Ref.: The University of Tennessee at Knoxville and Bell Laboratories

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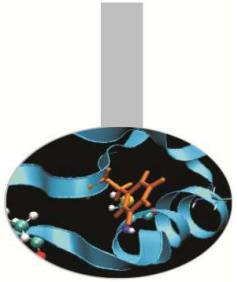
Fast Fourier Transform (FFT)



FFTW

(Fastest Fourier Transform in the West)

FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data (as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST).

The currently most used free library to compute DFTs.

It uses both MPI and OpenMP.

Language: C

Availability: public domain

Developers: Matteo Frigo and Steven G. Johnson.

Distributors: FFTW

Ref.: MIT

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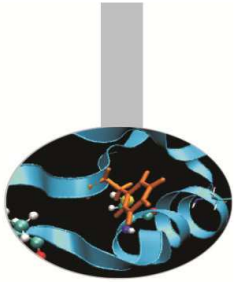
Fast Fourier Transform (FFT)



FFTW

(Fastest Fourier Transform in the West)

- Written in C (FORTRAN 77/90/2003 wrappers are included)
- FFTW adapt itself to your system and your problem: It check both total memory, size of your array, cache size register, CPU type, …
- … and it chose the best algorithm for you!
  - 2 setps is required:
    - Plan creation
    - Execution
- It supports FFTs for any different array size (< total memory)

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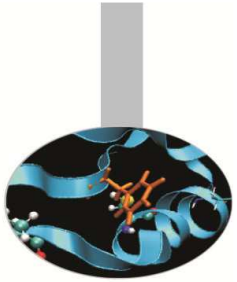
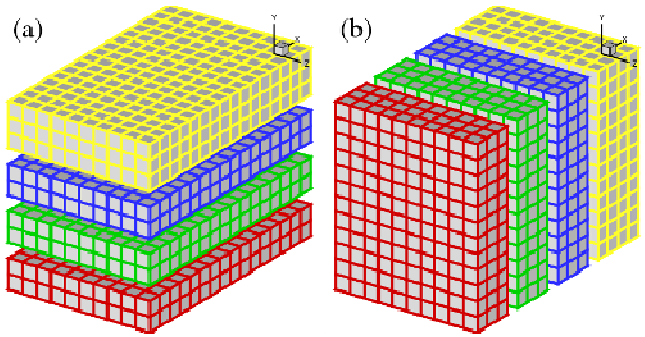
Fast Fourier Transform (FFT)

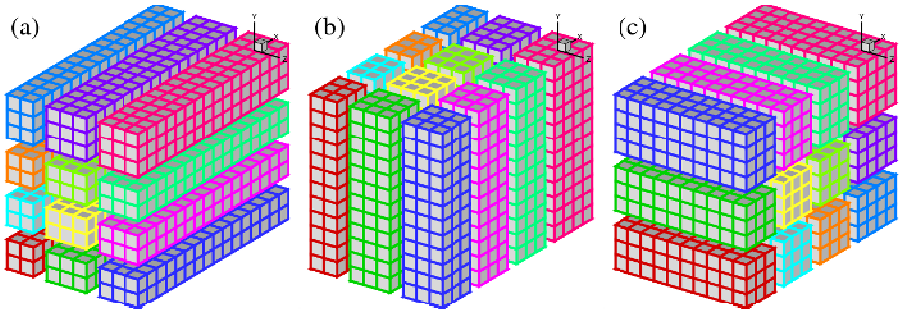


2Decomp&FFT

The 2DECOMP&FFT library is a software framework in Fortran to build large-scale parallel applications. It is designed for applications using three-dimensional structured mesh and spatially implicit numerical algorithms. At the foundation it implements a general-purpose 2D pencil decomposition for data distribution on distributed-memory platforms. On top it provides a highly scalable and efficient interface to perform three-dimensional distributed FFTs. The library is optimised for supercomputers and scales well to hundreds of thousands of cores. It relies on MPI but provides a user-friendly programming interface that hides communication details from application developers.



VS



Language: FORTRAN

Availability: public domain

Developers: Ning LI.

Distributors: 2decomp.org

Ref.: HECToR Distributed Computational Science and Engineering (CSE) Service operated by NAG Ltd.

http://www.2decomp.org/

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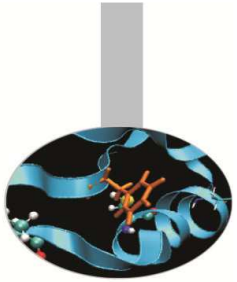
Fast Fourier Transform (FFT)



P3DFFT

3DFFT is a scalable software library implementing three-dimensional spectral transforms. It has been used in a variety of codes from many areas of computational science. It has been tested and used on many high-end computational system. It uses two-dimensional domain decomposition in order to overcome a scaling bottleneck of one-dimensional decomposition. This allows the programs with this library to scale well on a large number of cores, consistent with bisection bandwidth scaling of interconnect of the underlying hardware system.

Language: C

Availability: public domain

Developers: Dimitry Pekurovsky.

Distributors: 2decomp.org

Ref.: San Diego Supercomputer Center (SDSC) at UC San Diego.

https://code.google.com/p/p3dfft/

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