



Award #:
1835885

CSSI Element: Software: Multidimensional Fast Fourier Transforms on the path to Exascale

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Motivation:

- Efficient Fourier Transforms and related algorithms (Spectral Transforms) are in high demand in computational science and key to many simulations at large scale
- Inherent properties of Spectral Transforms limit their adoption at Exascale
- Existing implementations also suffer from limited functionality, such as data structures and usability options

WHAT CAN BE DONE TO RECONCILE SPECTRAL TRANSFORMS AND EXASCALE?

WHAT CAN BE DONE TO INCREASE THE RANGE OF USE BEYOND TRADITIONAL DNS TURBULENCE CODES?

CAN PERFORMANCE AND FLEXIBILITY BE COMBINED?

Goal: create an adaptable software framework for Spectral Transforms, targeting two main criteria:

1. Broader Impact: wide range of options and use cases
2. Performance: minimize the impact of the interconnect and memory bandwidth limitations

Progress:

- P3DFFT++ is an open source package, containing a newly designed library for 3D FFT and generalized spectral transforms at large scale.
- C++/MPI implementation, C and Fortran interface
- Early version available from <http://www.p3dfft.net>

Ongoing and future work:

- GPU-enabled implementation
- Pruned/sparse transforms
- Overlap of communication with computation
- Autotuning etc

