



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
- Fields impacted: CFD, astrophysics, oceanography, MD/biochemistry/material science, X-ray crystallography, medical imaging
- Inherent properties of Spectral Transforms makes is a challenging algorithm for **Exascale**

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?

Leverage existing open-source package P3DFFT(supported by SI2 in the past), in use by 100's of groups.

Goal 1: increase use to 1000's groups through wider range of options and use cases

Goal 2: push for performance at Exascale

Progress:

- P3DFFT++ is an **open source package** (<http://www.p3dfft.net>) , newly designed library for spectral transforms at large scale.
- C++/MPI implementation, C and Fortran interface

Opportunities for training and outreach

- Undergraduate students involvement

Ongoing and future work:

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

