Shenfun: High performance spectral Galerkin computing platform

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Summary

`Shenfun` is an open-source computing platform for solving partial differential equations (PDEs) by the spectral Galerkin method. The user interface to `shenfun` is very similar to FEniCS (https://fenicsproject.org), but applications are limited to simple, yet multidimensional, tensor product grids.

With `shenfun` one can solve a wide range of PDEs, with the limitation that one dimension can be inhomogeneous (with Dirichlet/Neumann type of boundaries), whereas the remaining dimensions are required to be periodic. The periodic dimensions are discretized using Fourier exponentials as basis functions. For the inhomogeneous direction, we use combinations of Chebyshev or Legendre polynomials, as described by J. Shen (Shen, 1994, 1995).

The code is parallelized with MPI through the mpi4py-fft (https://bitbucket.org/mpi4py/mpi4py-fft) package, and has been run for thousands of processors on various supercomputers. The parallelization is automated and highly configurable (slab, pencil), using a new algorithm (Dalcín, Mortensen, & Keyes, 2018) for global redistribution of multidimensional arrays.

`Shenfun` is documented, with installation instructions and demo programs, on readthedocs (http://shenfun.readthedocs.org). Extended demonstration programs are included for, e.g., the Poisson, Klein-Gordon and Kuramato-Sivashinsky equations.

`Shenfun` has been designed as a low entry-level research tool for physicists (Mortensen, 2017a) in need of highly accurate numerical methods for high performance computing. The primary focus for the development has been for turbulence and transition to turbulence, where simulations are extremely sensitive to disturbances, and numerical diffusion or dispersion are unacceptable. Spectral methods are well known for their accuracy and efficiency, taking advantage of fast transform methods, like the Fast Fourier Transforms (FFTs). Combined with the Galerkin method and Shen's robust composite bases, this leads to well conditioned linear algebra systems and numerical schemes that are truly exceptional. Highly efficient direct solvers (Mortensen, 2017a) are provided for Poisson, Helmholtz and Biharmonic systems of equations, arising naturally with the current bases for a wide range of problems.

In the spectralDNS repository (https://github.com/spectralDNS/spectralDNS) there are applications utilizing `shenfun` for forced isotropic turbulence (Navier-Stokes equations), turbulent channel flows (Mortensen, 2017b), Magnetohydrodynamics (MHD) and Rayleigh-Bénard flow. However, `shenfun` is by no means limited to the equations for fluid and plasma flows and it should be equally efficient for other scientific applications.

Acknowledgements

References

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