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A Memory-Saving Algorithm for Spectral Method of Three-Dimensional Homogeneous Isotropic Turbulence

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Abstract. Homogeneous isotropic turbulence has been playing a key role in the research of turbulence theory. And the pseudo-spectral method is the most popular numerical method to simulate this type of flow fields in a periodic box, where fast Fourier transform (FFT) is mostly effective. However, the bottle-neck in this method is the memory of computer, which motivates us to construct a memory-saving algorithm for spectral method in present paper. Inevitably, more times of FFT are needed as compensation. In the most memory-saving situation, only 6 three-dimension arrays are employed in the code. The cost of computation is increased by a factor of 4, and that 38 FFTs are needed per time step instead of the previous 9 FFTs. A simulation of isotropic turbulence on 2048^3 grid can be implemented on a 256G distributed memory clusters through this method.

AMS subject classifications: 80M22, 76F05, 76F65, 65T50

Key words: Spectral method, homogeneous isotropic turbulence, DNS, FFT.

1 Introduction

Homogeneous and isotropic (HI) turbulence has been a paradigm theoretically since it was introduced by G. I. Taylor [1] and it assumed even greater importance after the fundamental work of Kolmogorov [2–4]. Due to predicted "universality" at small-scales, turbulent motions smaller than those at lengths where production occurs are expected to be approximately HI in many applications. Nevertheless, even this simplest state of turbulence has resisted intensive efforts at complete understanding. Large scale direct

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numerical simulations (DNS) of HI turbulence are urgently needed for the understanding of the small scale behaviors in turbulence. It is well know that the most popular numerical method for the simulation of HI turbulence is pseudo-spectral method [5, 6]. The simulation scales from 64^3 [7], 128^3 [8–10] to 512^3 [11–15]. NEC's Earth Simulator at 36 teraflops led the TOP500 super computing list for two and a half years, from June 2002 until September 2004, when it was overtaken by IBM's Blue Gene. The landmark 4096^3 simulation performed on the Earth Simulator [16–20] remains the highest-resolution computation of three-dimensional (3D) homogeneous isotropic turbulence conducted to date.

The rapid progress of super computers has made the simulation of turbulence more and more powerful although it is still far from the resolution of Kolomogorov scale. With spectral method, the major problem is the large demand of memory instead of CPU time. For example, in order to simulate a three dimensional incompressible turbulence on a N^3 mesh, now the best code needs 12.5 real arrays of size N^3, which may still need another one in 3D fast Fourier transform (FFT) as a work array [11]. After that, the total memory in bytes will be $4\times 12.5N^3 = 50N^3$ (assuming only single precision real number is used). If $N=1024$, the total amount will be about 54G, if $N=2048$, this amount will be up to about 429G. This makes it impossible to simulate a 2048^3 size flow on a 256G memory machine (the clusters we used have 256G memory, which is a popular configuration for university machines). In order to do this, we must reduce the number of arrays from 12.5 to at least to 7, then $4\times 7N^3 = 28N^3$, which will be about 241G when $N = 2048$. If additional array is needed in FFT program, this amount will be 275G, which is a little large. This means we must design a method with only use at most 7 arrays of size N^3 in order to finish this task. From the published papers, such as [15] and others, the number of arrays is more than ten. Through precise design, a memory-saving algorithm for spectral method of three-dimensional homogeneous isotropic turbulence is present, and the coding details are listed in Appendix.

The outline of the paper is as follows: in the next part, the standard algorithm of pseudo-spectral method will be introduced briefly, and the idea of our new algorithm will also be presented as well. Subsequently in the third part, we show the numerical results and performance. Finally, the summary and discussions are given in the forth part.

2 Numerical method

Almost all DNS of fluid turbulence are implemented based on the pseudo-spectral method, which solves the Navier-Stokes equation directly in the Fourier space. We review briefly the standard algorithm [5, 6], and then point out the basic idea of our new algorithm. The incompressible Navier-Stokes equation can be written as

$$\begin{cases} \nabla\cdot\mathbf{v}=0, \\ \dfrac{\partial \mathbf{v}}{\partial t}-\mathbf{v}\times\boldsymbol{\omega}=-\nabla P+\nu\Delta\mathbf{v}+\mathbf{f}, \end{cases} \tag{2.1}$$