Computers & Fluids 82 (2013) 122–131

Contents lists available at SciVerse ScienceDirect

Computers & Fluids

journal homepage: www.elsevier.com/locate/compfluid

Analysis of interpolation schemes for the accurate estimation of energy spectrum in Lagrangian methods

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ARTICLE INFO

Article history:
Received 22 November 2012
Received in revised form 29 April 2013
Accepted 1 May 2013
Available online 14 May 2013

Keywords:
Lagrangian methods
Energy spectrum
Turbulence modelling

ABSTRACT

Direct evaluation of energy spectra in purely Lagrangian meshless methods is a challenging task. On the other hand, improvement of turbulence modeling in a Lagrangian framework relies strongly on our ability to estimate energy spectra up to the maximally resolved wavenumber. In this paper we compare different strategies to extract energy spectra from a velocity field defined on a scattered set of points. Spectra can be directly evaluated from irregularly distributed sample by using Discrete Fourier Transform (DFT) and their regularized versions. Alternative procedures require a preliminary interpolation into a grid where, on a second stage, a Fourier analysis can be performed. As a last approach a Moving Least Squares (MLSs) technique for preliminary interpolation is investigated and the results are discussed. Although exhibiting good accuracy in the low-moderate wavenumber window, the first two strategies introduce unacceptable large errors in the near-maximal-resolved wavenumber, where the highest accuracy is often required. Here we propose a second-order Moving Least Squares (MLSs) scheme as an optimal tool that allows us to reproduce precisely the energy spectrum over the entire wavenumber window. We discuss the importance of this result with respect to the development of accurate turbulence models for purely Lagrangian meshless methods.

1. Introduction

Turbulence modeling is the key issue for most computational fluid dynamics simulations. Several turbulence models were developed in the past for grid-based Eulerian methods, but little progress has been made in the context of a Lagrangian framework. Although meshless Lagrangian methods have been developed since more than 30 years, turbulence modeling in a purely Lagrangian framework has been studied only recently. Wagner and Liu have derived multiple scale sub-grid models for Reproducing Kernel Particle Method (RKPM) [1]. In 2004, Shao and Gotoh applied a turbulence model [2] to Moving Particle Semi-implicit method (MPS), a scheme proposed originally by Koshizuka and Oka in [3]. A Lagrangian meshless method for hydrodynamic flow problems which is receiving increasing attention is Smoothed Particle Hydrodynamics (SPH) [4]. Although the early development of SPH is dated back to the 1970s, its first application to the study of compressible turbulent flows has been presented by Welton and Pope [5] who in 1997 coupled the scheme with a Monte Carlo/PDF (probability density function) method. In 2002, Monaghan proposed an SPH version of the α-model [6] devised initially by Foias et al. to describe compressible turbulent flow [7]. In 2003, a very interesting LES approach for SPH turbulence modeling has been presented by Pumir and Shraiman [8]. Recently, Violeau and Issa solved a set of SPH–RANS equations based on an eddy viscosity model (EVM) commonly used in classical CFD [9].

Although much effort have been devoted in the past to test the effect of Lagrangian turbulent models in complex free-surface flows situations, few systematic studies have been conducted under isotropic turbulence. A simple but strong benchmark case that allows us to test the accuracy of different turbulent models is provided by the energy spectrum analysis under homogeneous isotropic turbulent flow conditions [10]. Unfortunately, until now accurate results can be obtained only in the low-to-moderate wavenumber range (large scale motion). The drawback lies in the post-processing analysis and it is mainly due to the fact that velocity field defined on a scattered set of data (particle positions) must be interpolated first on a grid, introducing uncontrollable errors specially near the maximal resolved wavenumber.

In [11], an SPH interpolation was employed to map the velocity field from scattered positions onto a grid and then FFT routine was applied to extract the energy spectrum. An alternative idea is to avoid interpolation and use DFT to direct calculate the energy spectrum from the scattered data [12]. Both methods introduce large

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http://dx.doi.org/10.1016/j.compfluid.2013.05.003

errors in high wavenumber range, masking out therefore all the effects caused by the adopted turbulent model. It should be remarked that the correct description of the sub-grid energy transfer in the near maximal-resolved regime is critical in large eddy simulations to discriminate among turbulence models [13]. As a consequence, an advanced data analysis, i.e. a stage of reconstruction of the whole flow field which does not introduce spurious effects, plays a crucial role in determining the accuracy of turbulent models developed for Lagrangian meshless methods. The presented work aims at establishing a most accurate and reliable method for reconstructing the spectra from scattered data. As a result of the analysis performed here, we propose a second-order moving-least-squares (MLSs) interpolation scheme as an optimal tool that allows to reproduce *exactly* the energy spectrum (up to the maximal resolved wavenumber) of a predefined velocity field on a scattered set of data. The presented tool can be directly applied to analyze the performance (and the accuracy) of the existing turbulence model for Lagrangian methods.

The paper is organized as follows. In Section 2, the Kolmogorov theory and the formulations of spectra are introduced. In Section 3, five methods, namely DFT, regularized DFT, SPH interpolation, Remeshed interpolation and MLS, which are used to calculate the energy spectrum in this work, are discussed. The performance of the five methods are compared in Section 4. Finally, conclusions are given in Section 5.

2. Formulation of energy spectrum

A stringent benchmark for turbulence models is represented by their ability to reproduce the correct energy spectrum under homogeneous isotropic turbulent conditions up to the maximally resolved wavenumber. A turbulent flow is characterized by a hierarchy of scales through which the energy cascade takes place. The dissipation of kinetic energy takes place finally at scales of the order of Kolmogorov length where the flow becomes laminar, while the injection of energy in turbulent flow occur generally at much larger scales. The range between these two scales is the so called inertial range, where the kinetic energy is essentially not dissipated by the viscosity, but it is merely transferred to smaller scales via a non-linear mechanism presented in the Navier–Stokes equation, until viscous effects become important. Within this range, inertial effects are much larger than viscous effects, and it is reasonable to assume that viscosity does not play a role. Through dimensional analysis, Kolmogorov derived the so-called 5/3 law, namely the energy spectrum $E(k)$ must fall off as $k^{-5/3}$ for 3D isotropic turbulence. His findings have been supported by considerable experimental evidence.

The standard way to evaluate $E(k)$ in grid-based methods is through application of FFT to the velocity field. Let $\mathbf{v}(\mathbf{r})$ be the velocity field defined in the whole physical space L^3. The integral Fourier transform of $\mathbf{v}(\mathbf{r})$ is defined as

$$\mathbf{V}(\mathbf{k}) = \left(\frac{1}{L}\right)^3 \int e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}(\mathbf{r})d\mathbf{r} \tag{1}$$

with $d\mathbf{r} = dxdydz$ in 3D and $d\mathbf{r} = dxdy$ in 2D. Using these definitions the velocity spectrum is defined as

$$E(\mathbf{k}) = \frac{1}{2}|\mathbf{V}(\mathbf{k})\cdot\mathbf{V}^*(\mathbf{k})| \tag{2}$$

where $\mathbf{V}^*$ is the complex conjugate of the transformed velocity. $\mathbf{k} = (k_x, k_y, k_z)$ is the wavenumber vector. The energy spectrum $E(k)$ in isotropic situations can be defined as

$$E(k) = 4\pi k^2\langle E(\mathbf{k})\rangle, 3D \tag{3}$$

$$E(k) = 2\pi k\langle E(\mathbf{k})\rangle, 2D \tag{4}$$

where <. . .> denotes averaging over a thin spherical shell of radius $k = |\mathbf{k}|$. Although this strategy presents no problem for grid-data, problems arise while dealing with scattered set of points.

3. Methods

In this section we discuss five different numerical approaches to calculate the energy spectrum from irregularly distributed samples. These methods can be divided in two general classes, adopting, respectively, the following strategies: (1) the energy spectrum is directly calculated from the scattered samples; (2) the velocity field is first estimated on the grid and then Fast Fourier Transformation (FFT) applied.

3.1. Discrete Fourier Transform methods

In order to obtain the full information over the entire wavenumber range without preliminary interpolation, Discrete Fourier Transform (DFT) of velocity field can be employed. In the following we review two popular approaches highlighting advantages and drawbacks.

3.1.1. Standard Discrete Fourier Transform

In a standard Discrete Fourier Transform (DFT) method, the DFT of a the velocity field $\mathbf{v}(\mathbf{r})$ defined on a scattered set of points $\mathbf{r}_j$, $(j = 1, \ldots, N)$ is defined as

$$\begin{bmatrix} \mathbf{V}(\mathbf{k}_1) \\ \mathbf{V}(\mathbf{k}_2) \\ \vdots \\ \mathbf{V}(\mathbf{k}_N) \end{bmatrix} = \begin{bmatrix} e^{-i\mathbf{r}_1\cdot\mathbf{k}_1} & e^{-i\mathbf{r}_2\cdot\mathbf{k}_1} & \cdots & e^{-i\mathbf{r}_N\cdot\mathbf{k}_1} \\ e^{-i\mathbf{r}_1\cdot\mathbf{k}_2} & e^{-i\mathbf{r}_2\cdot\mathbf{k}_2} & \cdots & e^{-i\mathbf{r}_N\cdot\mathbf{k}_2} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-i\mathbf{r}_1\cdot\mathbf{k}_N} & e^{-i\mathbf{r}_2\cdot\mathbf{k}_N} & \cdots & e^{-i\mathbf{r}_N\cdot\mathbf{k}_N} \end{bmatrix} \begin{bmatrix} \mathbf{v}(\mathbf{r}_1) \\ \mathbf{v}(\mathbf{r}_2) \\ \vdots \\ \mathbf{v}(\mathbf{r}_N) \end{bmatrix} \tag{5}$$

which, in a simplified form reads

$$\mathbf{V} = B\cdot\mathbf{v} \tag{6}$$

where B is the matrix of $e^{-i\mathbf{r}\cdot\mathbf{k}}$. The inverse Fourier Transform is written as

$$\mathbf{v} = \frac{1}{N}\cdot B^H\cdot\mathbf{V} \tag{7}$$

If we insert Eq. (7) into Eq. (6), we obtain $\mathbf{V} = \frac{1}{N}\cdot(B\cdot B^H)\cdot\mathbf{V}$ which holds, only when

$$\frac{1}{N}\cdot(B\cdot B^H) = I \tag{8}$$

in other words, B must be orthogonal and $B^H = N\cdot B^{-1}$. When the points are on the grid, Eq. (8) holds exactly, however if they are disordered, $\frac{1}{N}\cdot(B\cdot B^H) \neq I$ generally, and DFT suffers from an ill-posed problem for a scattered set of data.

3.1.2. Regularized discrete fourier transform

Tikhonov regularization [14,15] is the most commonly used regularization method to solve the ill-posed problems mentioned above. For the DFT, we have $\frac{1}{N}\cdot B^H\cdot\mathbf{V} = \mathbf{v}$ and a linear least squares is proposed in the attempt to minimize the residual

$$\|\frac{1}{N}\cdot B^H\cdot\mathbf{V} - \mathbf{v}\|^2 \tag{9}$$

when B^H is ill-conditioned or singular. In this latter case this strategy does not produce any improvement with respect to the original DFT problem. Therefore the regularization term is included in the minimization and a Tikhonov regularization is performed to find the solution that minimizes the following objective function:

$$\Psi(\mathbf{V}) = \|\frac{1}{N}\cdot B^H\cdot\mathbf{V} - \mathbf{v}\|^2 + \|\Gamma\mathbf{V}\|^2 \tag{10}$$