Journal of Computational Physics 260 (2014) 127–142

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

# Hybrid spectral-particle method for the turbulent transport of a passive scalar

J.-B. Lagaert [a], G. Balarac [a], G.-H. Cottet [b,*]

[a] Grenoble-INP/CNRS/UJF-Grenoble 1, LEGI UMR 5519, Grenoble, F-38041, France
[b] Grenoble-INP/CNRS/UJF-Grenoble 1, LJK UMR 5224, Grenoble, F-38041, France

ARTICLE INFO

*Article history:*
Received 29 April 2013
Received in revised form 28 November 2013
Accepted 8 December 2013
Available online 18 December 2013

*Keywords:*
Direct numerical simulation
Hybrid method
Particle method
Turbulent mixing
Passive scalar
Universal scaling

ABSTRACT

This paper describes a novel hybrid method, combining a spectral and a particle method, to simulate the turbulent transport of a passive scalar. The method is studied from the point of view of accuracy and numerical cost. It leads to a significative speed up over more conventional grid-based methods and allows to address challenging Schmidt numbers. In particular, theoretical predictions of universal scaling in forced homogeneous turbulence are recovered for a wide range of Schmidt numbers for large, intermediate and small scales of the scalar.



## 1. Introduction

The prediction of the dynamics of a scalar advected by a turbulent flow is an important challenge in many applications. The scalar field can be used to represent various quantities transported by the flow. In combustion, the mixture fraction is a conserved scalar used to describe mixing between fuel and oxidizer [1]. The prediction of scalar in environmental flows is also of great importance [2]. The temperature field is another type of advected scalar which is critical in many applications, e.g. to simulate the cooling systems used for nuclear reactors [3]. Passive scalars can finally be used to capture interfaces in multiphase flows [4] or determine the dynamical properties of turbulent flows [5].

A passive scalar, $\theta$, is governed by an advection–diffusion equation,

$$\frac{\partial \theta}{\partial t} + \vec{u} \cdot \vec{\nabla}\theta = \vec{\nabla} \cdot (\kappa \vec{\nabla}\theta) \tag{1}$$

where $\kappa$ is the molecular scalar diffusivity and $\vec{u}$ the flow velocity field. The phenomenology of passive scalar convection–diffusion depends on the molecular Schmidt number, the viscosity-to-diffusivity ratio, $Sc = \nu/\kappa$. For turbulent flows, the Kolmogorov scale, $\eta_K$, is defined as the smallest length scale of the turbulent motion. Similarly, for Schmidt numbers higher than one, the Batchelor scale, $\eta_B$, is defined as the smallest length scale of the scalar fluctuations. The Batchelor and Kolmogorov scales are related by $\eta_B = \eta_K/\sqrt{Sc}$.

The Batchelor scale is thus smaller than the Kolmogorov scale. This means that, for Schmidt number larger than one, scalar dynamics can occur at scales smaller than the smallest velocity eddy, and therefore requires important computational resources. Donzis et al. [6] performed DNS of turbulent transport by means of pseudo-spectral methods using up to 4096 modes in each direction to study universal scaling laws of a passive scalar.

* Corresponding author.

0021-9991/$ – see front matter 
http://dx.doi.org/10.1016/j.jcp.2013.12.026

In the above reference the same grid resolution and numerical method are used for the momentum and the scalar equations. The two-scale nature of turbulent scalar transport, however, makes it natural to use different grids and different numerical methods for the scalar and the momentum. In a recent work, Gotoh et al. [7] describe a hybrid method combining a spectral method for the Navier–Stokes equation and compact finite-difference schemes for the scalar advection. This hybrid method is validated and applied for simulations of decaying turbulence at Schmidt numbers of 1 and 50. Significant gains were obtained in comparison with methods using spectral discretizations for both the momentum and the scalar.

For large Schmidt numbers, the scalar dynamics is essentially governed by advection, a regime for which Lagrangian or semi-Lagrangian methods are ideally suited. An important feature of these methods, which makes them particularly appealing in the case of high Schmidt numbers, is that they are stable under conditions that are related to the flow strain and not to the grid-size. In practice this means that the time-step used for the scalar equation will depend on the grid resolution used for the momentum equation even if a much finer grid is used for the scalar. Inspired by this observation, we proposed in [8] to couple semi-Lagrangian particle methods at different grid-resolutions for both the scalar transport and the Navier–Stokes equations. This reference provides a proof of concept that scalar spectra and structures are resolved with the same accuracy and much less computational effort in a hybrid method using a coarse resolution for the momentum than in a fully resolved high resolution method. This work was pursued in [9], to investigate the universal laws for large, intermediate and small scales of the scalar for Reynolds numbers (based on the Taylor micro-scale) between 80 and 160 and Schmidt numbers between 0.7 and 16. In this reference, a particle method for the scalar equation was coupled with a pseudo-spectral method for the Navier–Stokes equations.

The purpose of the present paper is to describe and validate the hybrid spectral-particle numerical approach used in [9], and to discuss its efficiency, in particular in comparison with fully resolved methods using spectral discretizations for both the scalar and momentum equations, and with the hybrid method proposed in [7].

An outline of this paper is as follows. In Section 2, we describe the semi-Lagrangian particle method used for the scalar equation, the pseudo-spectral method used for the momentum equation and the coupling strategy. We also indicate the approach to run the hybrid method on massively parallel machines. In Section 3, we test our method in decaying turbulence experiments similar to those in [7] and discuss its accuracy, cost and overall efficiency. In Section 4, we apply our method to investigate the physics of turbulent transport in forced homogeneous turbulence over a wide range of Schmidt numbers. Section 5 is devoted to concluding remarks and future directions that we are currently exploring.

## 2. Hybrid spectral-particle method

In this section we first describe the particle method used to solve the scalar equation, then the pseudo-spectral method used for the Navier–Stokes equation and the coupling strategy. We also explain our strategy to optimize the parallel performance of the hybrid method.

### 2.1. Semi-Lagrangian particle methods

The principle of particle methods for the advection of a given quantity is to concentrate this quantity on a set of particles and to follow these particles with the advection field. These methods are conservative by nature and free of CFL stability conditions. Continuous fields or grid values are recovered from the particles by mollification or interpolation [10]. The numerical analysis of these methods shows that a strong strain in the advection field can create distortions in the particle distribution and deteriorate the accuracy of the method. To overcome this difficulty, it is common practice to remesh particles on a regular grid through interpolation [11,10]. In the context of the advection of a vorticity field to solve the incompressible Navier–Stokes equation in vorticity form, these methods have been validated against spectral or finite-difference methods and applied in bluff body flows [11–14], in homogeneous decaying turbulence [15] and in vortex dynamics [16,17]. In the context of scalar advection they have been used for Lagrangian discretizations of level set methods [18–20] and for the determination of Lyapounov exponents of flow maps [5].

When particles are remeshed at every time-step, which is often the case in practice, one obtains a class of conservative semi-Lagrangian methods that can be analyzed as CFL-free finite-difference methods [20]. Remeshing is performed through interpolation. In one dimension it can be expressed by the following formula:

$$\theta_i = \sum_p \theta_p \Lambda\left(\frac{x_i - x_p}{\Delta x^\theta}\right),$$

where $\Lambda$ is the interpolation kernel, $x_i$ denote the grid points and $x_p$ the particle locations after advection. The summation concerns particles which belong to the support of the kernel around a given grid point. In the present paper, particles are advected by a second order Runge–Kutta scheme and we use the following kernel, derived in [19],

$$\Lambda(x) = \begin{cases} \frac{1}{12}(1-|x|)(25|x|^4 - 38|x|^3 - 3|x|^2 + 12|x| + 12) & \text{if } 0 \leqslant |x| < 1 \\ \frac{1}{24}(|x|-1)(|x|-2)(25|x|^3 - 114|x|^2 + 153|x| - 48) & \text{if } 1 \leqslant |x| < 2 \\ \frac{1}{24}(3-|x|)^3(5|x|-8)(|x|-2) & \text{if } 2 \leqslant |x| < 3 \\ 0 & \text{if } 3 \leqslant |x|. \end{cases} \tag{2}$$