

An Efficient Parallel Implementation of a Hybrid Method for the Advection of High Schmidt Scalars in Flows

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ABSTRACT

We present here a parallel implementation of a hybrid method combining a high order semi-Lagrangian method for the advection-diffusion of scalars and a finite element method for the Navier-Stokes equations. Then, we introduce an overloading strategy to enhance the computational performance of this method. Finally, we present an application test case of a high SCHMIDT scalar in a turbulent jet flow.

1. Introduction

The phenomenon of advection-diffusion equations in turbulent flows manifests in diverse scenarios, including heat transfer [1] or the dispersion of pollutants [2]. Scalars passively advected mainly vary in their diffusivity properties, which are characterized by their SCHMIDT number, defined as the ratio of viscosity to diffusivity. Handling scalars with high SCHMIDT numbers remains a challenge for direct numerical simulation. Specifically, the Kolmogorov scale μ_K , representing the smallest velocity variation scale, is associated with the Batchelor scale μ_B , which denotes the smallest mixing variation scale, through the following relation:

$$\mu_B = \frac{\mu_K}{\sqrt{S_c}} \quad (1)$$

As a consequence, when dealing with SCHMIDT numbers higher than one, scalar dynamics operate at scales smaller than the Kolmogorov scale. Achieving accurate treatment of scalar advection-diffusion at high SCHMIDT numbers requires a finer mesh for the scalar than for the momentum. Consequently, monolithic numerical investigations are limited to moderate SCHMIDT numbers. To address these challenges, we have developed and implemented a method to overcome these limitations.

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2. Equations and numerical method

For incompressible flows, the dynamics of the flow are governed by the Navier-Stokes equations

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p = \mathbf{0} \quad (2)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (3)$$

with $\mathbf{u}$ the velocity field, p the pressure field, and ν and ρ the viscosity and the density, respectively. Those equations are solved on a unstructured grid thanks to a finite-element method with the EMAC formulation [3].

The dynamics of a passive scalar θ advected in the flow are governed by a advection-diffusion equation:

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \kappa \Delta \theta \quad (4)$$

where κ is the diffusion coefficient of θ . The SCHMIDT number is then defined as $S_c = \nu/\kappa$. The scalar advection-diffusion equation is solved on a fine Cartesian mesh. A semi-Lagrangian particle method is used for the scalar transport. It consists in concentrating the transported quantity θ on a set of particles. Particles are then advected thanks to the advection velocity field and remeshed after each time-step on the grid using an interpolation kernel. This methodology has been validated and applied in [4, 5, 6]. In particular, Cottet showed the high order of the method in [7]. Nevertheless, the authors of [6] highlight the presence of load balancing issues when very unstructured velocity mesh are used. The presented parallel implementation aims to solve those problems.

3. Parallel implementation

In the present work, Navier-Stokes and advection-diffusion equations are solved on two different groups of processors. The first group aims to solve Navier-Stokes equations.

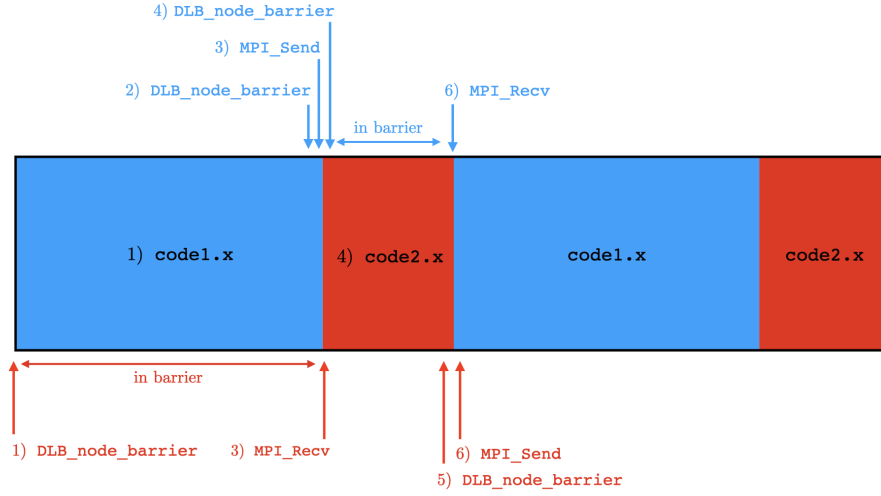


Figure 1: Workflow with or without the use of DLB Barrier.

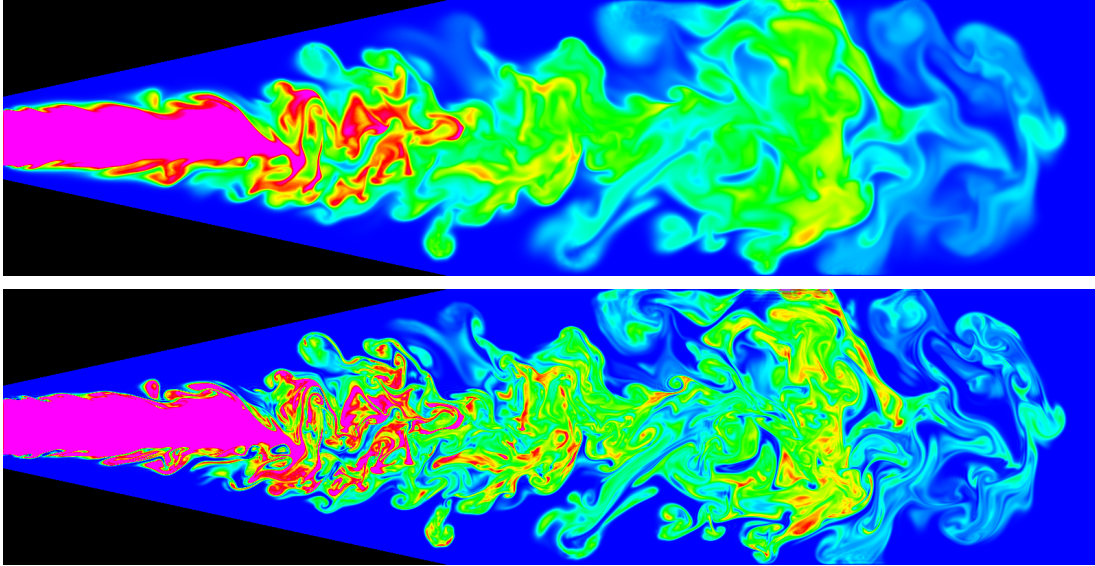


Figure 2: Instantaneous contours of a scalar injected in a turbulent flow. Top picture $Sc = 1$. Bottom picture $Sc = 10$.

The second group deals with the remeshed particles method. At each time step, the velocity field is communicated from the first group to the second group in order to advect the particles with a fourth order Runge-Kutta time scheme. Using this partitioning, we avoid the load balancing issues highlighted in [6] where the partitioning of the particle mesh follows the velocity mesh. However, with this parallel implementation, both groups of processors works in an alternate fashion as the second group needs the velocity field to advect particles. A way to enhance the computational

performance of this implementation is to use an overloading strategy thanks to DLB, a library that improves the performance of hybrid applications by addressing the load imbalance at runtime [8]. With this strategy, all the resources are used for both solvers. Figure 1 shows the workflow when overloading resources. Code1.x represents the tasks for solving Navier-Stokes equations and Code2.x represents the tasks for the remeshed particles method. When Code1.x is running, Code2.x is in a *DLB.node.barrier*, which means that its processes do not do a busy wait and consequently,

do not consume cycles. At the end of Code1.x, the communication of the velocity field is done. Code1.x enters in the *DLB.node.barrier* and Code2.x does its tasks.

4. High Schmidt scalar advection in a turbulent flow

A round jet in transition to turbulence is considered. The flow configuration is defined by its inlet velocity profile. At the inlet, the mean velocity field is non zero only for the streamwise component, which is given by a hyperbolic tangent profile:

$$u_i = \frac{U_1 + U_2}{2} - \frac{U_1 - U_2}{2} \tanh\left(\frac{R}{4\Gamma_0}\left(\frac{r}{R} - \frac{R}{r}\right)\right)$$

where U_1 is the centerline velocity, U_2 is a small co-flow, Γ_0 is the momentum thickness of the initial shear layer, r the radial coordinates, and R the initial jet radius. The REYNOLDS number is fixed at $Re = U_1 \cdot (R/\nu) = 2,000$. A forcing term is added to accelerate the transition. This forcing is first composed by a random part only added in the shear layer of the jet to the three velocity components. It follows a Passot-Pouquet spectrum with an amplitude set to 10% of U_1 . This forcing is then complemented by a deterministic part, which consists in a varicose axisymmetric excitation.

Figure 2 shows instantaneous contours of scalars for values of SCHMIDT number equal to 1 and 10, with 960 CPUs used. The velocity mesh consists of 62M elements and the particles mesh of 115M particles.

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