New trends in Multi-Scale Simulation using Hybrid Grid-Particle Vortex Methods

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New trends in Multi-Scale Simulation using Hybrid Grid-Particle Vortex Methods

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Abstract. *The purpose of this talk is to present a multi-scale Vortex-in-Cell method, for direct numerical simulation of three dimensional fluid flows. Vortex methods are Lagrangian. They are among the most challenging particle method, and have been dramatically improved during the last decade. This talk will present the main ideas of these methods, implemented in the open source package* COMMA, *funded by ANR and based on high performance packages* FISHPACK *and* AGRIF.

Among numerical methods aiming at solving the equations of fluid dynamics, the particle methods are renowned for their ability to compute accurately transport and convective effects. Most of the current challenges focus on the Navier-Stokes equations and their generalizations : multi-fluids, reactive flows, combustion, complex boundary conditions. In this short communication, one focuses on the basic three-dimensional Navier-Stokes equations, for an incompressible fluid, given by

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} = \frac{\mathbf{f}}{\rho} - \frac{\nabla p}{\rho} \tag{1}$$

where $\mathbf{u}$ is the divergence-free velocity field satisfying the no-slip condition $\mathbf{u} = 0$ on Γ, p the pressure, ρ the density, ν the kinematic viscosity, and $\mathbf{f}$ the external force.

For an incompressible fluid of constant density and viscosity, taking the curl of equation (1) and introducing the vorticity as $\boldsymbol{\omega} = \mathrm{curl}\mathbf{u}$, leads to

$$\frac{\partial \boldsymbol{\omega}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\omega} - \boldsymbol{\omega} \cdot \nabla \mathbf{u} - \nu \Delta \boldsymbol{\omega} = 0 \tag{2}$$

with kinematic no-slip boundary conditions $\mathbf{u} = 0$, for external forces deriving from a potential (*ie* is the gradient of a scalar function).

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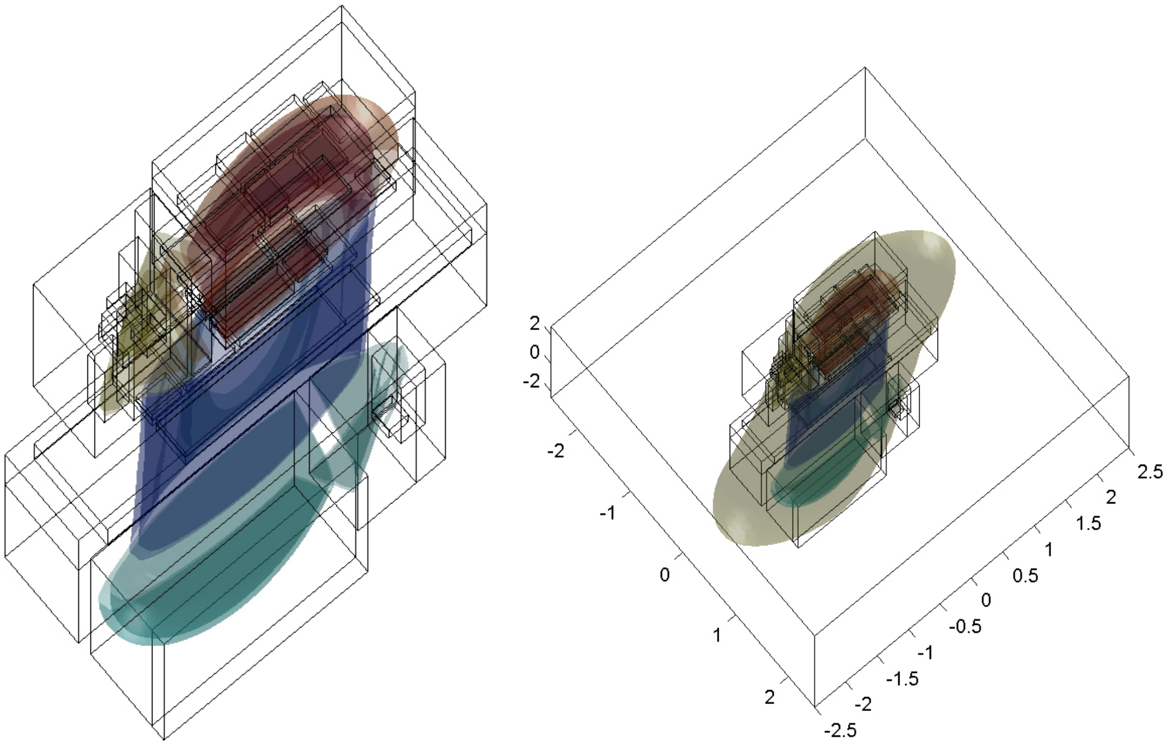

Figure 1: Three level multi-scale computing of a 3D column vortex.

The particle discretization consists in the approximation of vorticity by a set of Dirac functions :

$$\boldsymbol{\omega}^h(t) = \sum_p \boldsymbol{\omega}_p(t) v_p(t) \delta_{\mathbf{x}_p(t)} \tag{3}$$

The set $(\boldsymbol{\omega}_p, \mathbf{x}_p, v_p)$, called particle, denotes local vorticity, location and volume. Moreover, such a particle description of vorticity is called Vortex-in-Cell method.

In practice, modern Vortex-in-Cell methods use time-splitting algorithm of the Navier-Stokes equations : On the one hand, a linear diffusion equation with full no-slip boundary condition (described and analysed in [3]). On the other hand, one considers the convective part of equation (2), whose particle discretization leads to the following ODE system:

$$\frac{\mathrm{d}\boldsymbol{\omega}_p}{\mathrm{d}t} = [\boldsymbol{\omega} \cdot \nabla \mathbf{u}]_{\mathbf{x}_p(t)}, \qquad \frac{\mathrm{d}\mathbf{x}_p}{\mathrm{d}t} = [\mathbf{u}]_{\mathbf{x}_p(t)} \tag{4}$$

where $\boldsymbol{\omega}_p$ must satisfy $\boldsymbol{\omega}_p = \mathrm{curl}\mathbf{u}(\mathbf{x}_p)$. The velocity field $\mathbf{u}$ has been historically performed by means of integral methods using multipole expansion, but it has been shown in the last decade that hybrid grid-particle techniques are more efficient.

Among the main interests of the method, one can notice that transport $\mathbf{u} \cdot \nabla \boldsymbol{\omega}$ vanished in the Lagrangian formulation, thus making the associated CFL vanish as well, leading to robust schemes, that is to say stable for large time step, especially interesting for slightly viscous flows. This has been successfully used for large time scale simulation and flow control [5, 2].

Furthermore, accuracy is strongly dependent of a particle lattice homogeneity and accurate computation of wall effects. It follows that if particles are remeshed frequently, all Lagrangian

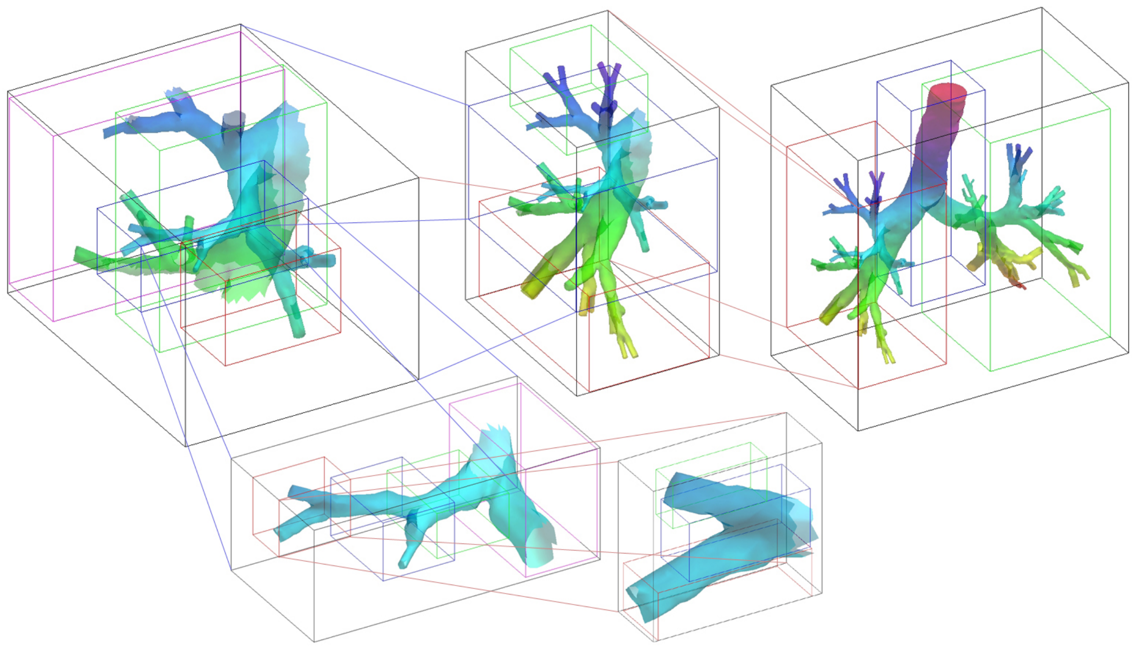

Figure 2: Challenge on multi-scale simulation: real three-dimensional lung geometry.

methods, such as Particle-in-Cell (PIC) or Smoothed-Particle-Hydrodynamics (SPH) give accurate results [4].

In order to have the set of ODEs (4) well defined, one has to be able to compute a velocity field $\mathbf{u}$ from a vorticity field $\boldsymbol{\omega}$. The particles of vorticity are interpolated to a grid $\tilde{\boldsymbol{\omega}}$, and one considers the vorticity-to-velocity operator $\mathcal{A}$ defined on a grid (that is to say $\mathbf{u} = \mathcal{A}\tilde{\boldsymbol{\omega}}$).

$$\frac{\mathrm{d}\boldsymbol{\omega}_p}{\mathrm{d}t} = [\tilde{\boldsymbol{\omega}} \cdot \mathcal{A}\tilde{\boldsymbol{\omega}}]_{\mathbf{x}_p(t)}, \quad \frac{\mathrm{d}\mathbf{x}_p}{\mathrm{d}t} = [\mathcal{A}\tilde{\boldsymbol{\omega}}]_{\mathbf{x}_p(t)} \tag{5}$$

where the brackets means an interpolation back to particles, by means of a sufficiently high order kernel [6].

The vorticity-to-velocity operator $\mathcal{A}$ is defined on a grid by means of the stream function $-\Delta\boldsymbol{\psi} = \boldsymbol{\omega}$ and $\mathbf{u} = \mathrm{curl}\boldsymbol{\psi}$. Operator $\mathcal{A}$ is asked to satisfy the no-flow-through condition $\mathbf{u} \cdot \mathbf{n} = 0$, and boundary conditions compatible with divergence free hypothesis.

The multi-scale computation is natural since it has to be introduced only in the Poisson equation $-\Delta\boldsymbol{\psi} = \boldsymbol{\omega}$. The adaptivity is based on $\nabla\boldsymbol{\omega}$ and implemented using the AGRIF package. Each level of the grid tree is a Poisson equation in a cube, using the efficient FISHPACK package, whose boundary condition is a non-homogeneous Dirichlet condition inherited from the coarse grid containing it. The ANR project COMMA has been aiming at providing an open source software implementing this multi-scale method.

The overall algorithm computational cost scales linearly with the number of particles [1]. This has been put in practice for moderate Reynolds numbers (fig. 1), and a special challenge for computation of air circulation in lungs (fig. 2), in collaboration with INRIA-REO team.

In order to be able to consider complex geometries, it is helpful to write the velocity as $\mathbf{u} = \mathcal{A}\boldsymbol{\omega} = \mathrm{curl}\boldsymbol{\psi} - \nabla\phi$ where the potential velocity ϕ is solution $-\Delta\phi = T$, and where T is

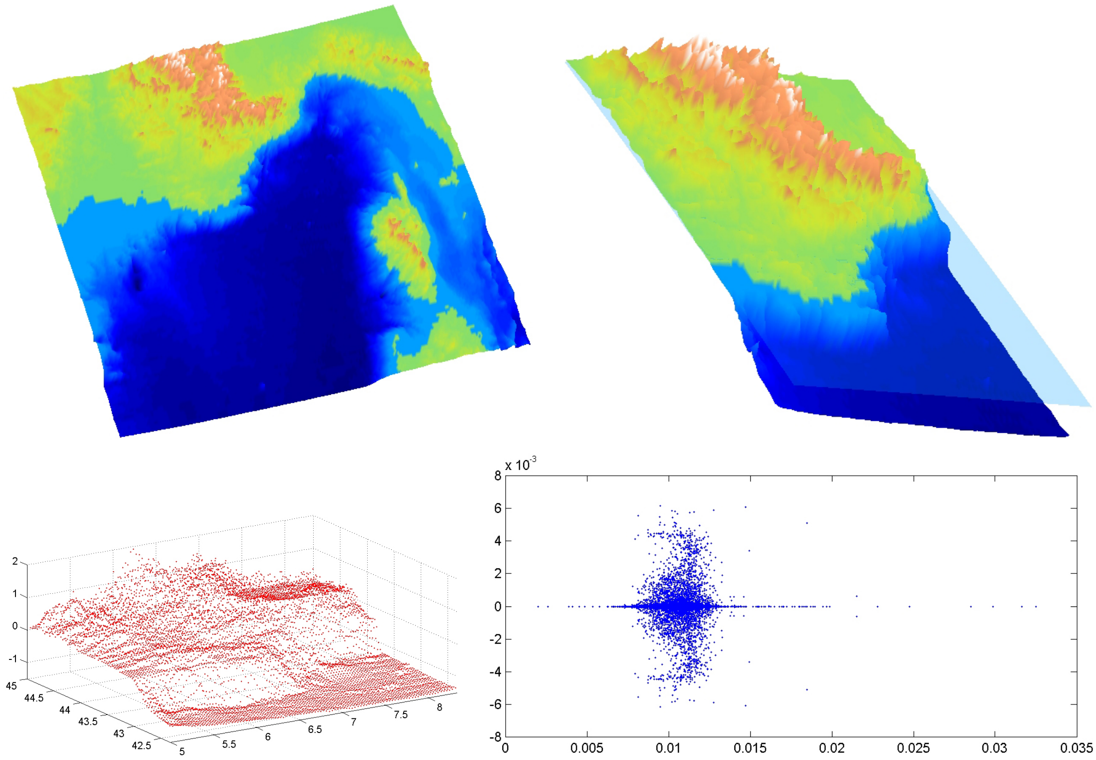

Figure 3: Immersed boundary and immersion spectrum (bottom right) : there is no discrepency in conditioning, even for complex geometries, such as geophysical context.

a generalized function hold by a surface (the domain boundary) : this is an immersed boundary method. The application taking the distribution of the singular source T and giving the flow-through $\mathbf{n} \cdot \nabla\phi$ on the fluid side is well conditioned and leads to very efficient algorithms, even for geometries as complex as geophysical context (fig. 3).

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