

UNIVERSITE CATHOLIQUE DE LOUVAIN
Faculté des Sciences Appliquées
Département de Mécanique
Unité de Thermodynamique et Turbomachines (TERM)



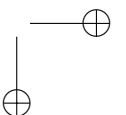
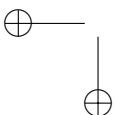
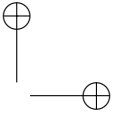
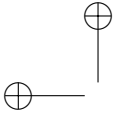
**Combining the vortex-in-cell and parallel fast multipole
methods for efficient domain decomposition simulations:
DNS and LES approaches.**

Roger Cocle

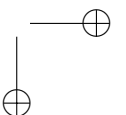
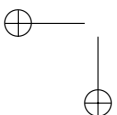
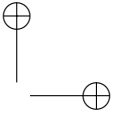
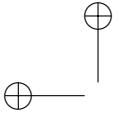
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Thèse présentée en vue
de l'obtention du grade de
Docteur en Sciences Appliquées

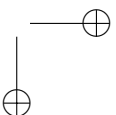
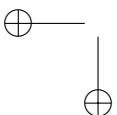
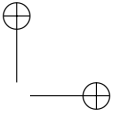
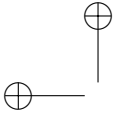


To my parents,
Christiane Goblet and Raymond Cogle



"Life grants nothing to us mortals without hard work."

Horace (65 BC - 8 BC), Satires

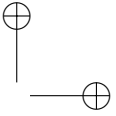
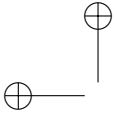


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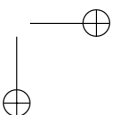
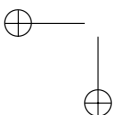
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Introduction

This thesis is concerned with the numerical simulation of high Reynolds number, three-dimensional, incompressible flows in open domains. Many problems treated in Computational Fluid Dynamics (CFD) occur in free space: e.g., external aerodynamics around vehicles, bluff bodies or aircraft; shear flows such as shear layers or jets. In observing all these flows, we can remark that they are often unsteady, appear chaotic with the presence of a large range of eddies, and are mainly dominated by convection.

Objectives

For years, it was shown that Lagrangian vortex element methods are particularly well appropriate for simulating such flows. First, as they are based on the vorticity-velocity formulation of the Navier-Stokes equations, computational vortex elements are required only in regions where the vorticity field is non zero. Vortex methods thus require much less computational elements than grid-based methods (that usually solve the velocity-pressure formulation). Second, as they solve the equations in the Lagrangian framework, the computational elements are convected with the local velocity field, and, so, the flow structures are convected without dispersion errors and with very low numerical diffusion (in opposition to grid-based methods that cannot entirely avoid the dispersion errors, even with high-order methods). Finally, as they make use of the Biot-Savart law to evaluate the velocity field from the vorticity field, vortex methods have the ability to correctly satisfy the open domain condition.

Unfortunately, vortex methods do not only have advantages. First, the use of the Biot-Savart law leads to a high computational cost. To compensate for this drawback, much achievements were done since the middle of the eighties, leading to the implementation of "fast codes". The computational cost was thus reduced

by the use of multipole expansions and of a hierarchical subdivision of space (i.e. "fast tree codes"). However, even with the fast tree codes, the velocity evaluation remains rather expensive, limiting the number of vortex elements to the order of a few million, even when using parallel version of the fast tree codes (such as that developed by Salmon, Warren and Winckelmans).

Vortex methods combining Lagrangian and Eulerian fields, and making use of fast grid solvers, also exist: the so-called vortex-in-cell (VIC) methods. Yet, in their classical formalism, they do not allow the use of a compact grid while still correctly satisfying the open domain condition. One of the main achievements of the present work is precisely to develop a VIC method with compact grid and with true open domain condition (see Chapter 1).

Besides the numerical method, some CFD problems require physical modelling to be properly captured. At low Reynolds number, the evolution of the flow can be correctly computed and resolved, without any model: it is known as Direct Numerical Simulation (DNS) of the Navier-Stokes equations. However, in many practical situations (i.e. that have an industrial interest), the problems are most often at high Reynolds numbers. These flows are generally turbulent containing a wide range of length scales, from the largest "coherent structures" to the smallest "dissipation scales". The grid used in the simulations is often not able to capture the smallest scales; the Navier-Stokes equations need then to be completed with a subgrid scale (SGS) model, that correctly dissipates the energy at the smallest captured scales, to take into account the effect of the uncaptured scales: it is known as Large-Eddy Simulation (LES).

The aim of this thesis is to develop a vortex method that efficiently combines two existing vortex methods by taking the advantages of each one. It is thus the continuation of the work by Winckelmans, Ploumhans and Daeninck, but also by Koumoutsakos, Cottet and Poncet. To give further sturdiness to the method, a detailed study of some existing SGS models for LES is also fulfilled. This part is mainly related to the work by Winckelmans and Jeanmart.

Some preliminaries

As the main objective of the thesis is to efficiently simulate unbounded convection-dominated unsteady flows, vortex element methods (VEM) rapidly comes up as a good choice. As already mentioned, VEM are well-suited to simulations of incompressible flows using particles that convect the vorticity information. The

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main assets of VEM are a negligible numerical dispersion and a negligible numerical dissipation. The Navier-Stokes equations for incompressible flow, here in the vorticity-velocity formulation, are given by

$$\frac{D\omega}{Dt} = \nabla \cdot (\mathbf{u}\omega) + \nu \nabla^2 \omega \quad (1)$$

where $\mathbf{u}(\mathbf{x}, t)$ is the velocity field, ν is the kinematic viscosity and $\omega = \nabla \times \mathbf{u}$ is the vorticity. The velocity can be expressed as

$$\mathbf{u} = \nabla \times \psi + \mathbf{U}_\infty \quad (2)$$

where ψ is the associated stream function, related to ω by the Poisson equation,

$$\nabla^2 \psi = -\omega, \quad (3)$$

and $\mathbf{U}_\infty$ a freestream velocity. In VEM, the vorticity field is discretized using a set of N vortex particles of position $\mathbf{x}(t)$ and of strength $\alpha(t) = \int \omega d\mathbf{x}$. Two approaches are classically used for solving the Poisson equation (3):

- The Biot-Savart approach: the Poisson equation is solved using the Green's function approach. The unbounded domain is thus taken into account implicitly. In its simple formulation, the computational cost is $\mathcal{O}(N^2)$. When a Fast Multipole (FM) solver is used, the computational cost is reduced to $\mathcal{O}(N \log N)$.
- The Vortex-in-cell (VIC) approach: the Poisson equation is solved on a grid. Using this approach requires to impose boundary conditions or to assume periodicity. In its classical formalism, the unbounded domain is thus not taken into account implicitly. The grid has to be taken much larger than the vorticity field to impose a far field analytical solution or, in the case of periodicity, to reduce the influence of the periodic images. The computational cost of such grid solvers is $\mathcal{O}(M \log M)$, where M is the number of grid points.

Both solvers are $\mathcal{O}(N \log N)$ but fast grid solvers are much faster than fast multipole solvers, they however require boundary conditions. The idea at the base of this thesis is to combine these two approaches by taking the advantages of each one and, eventually, to obtain an efficient algorithm to solve incompressible flows in open domain. The efficient combination, here called VIC-FM, is illustrated in Fig. 1. The main idea is to use a compact grid, that tightly includes the vorticity

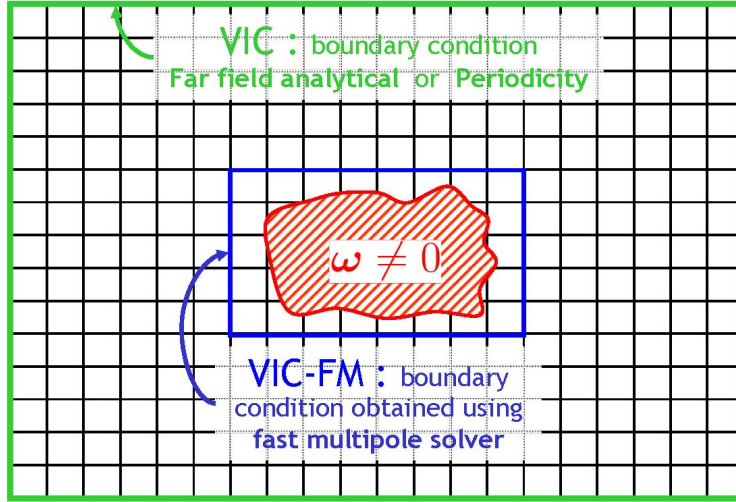


Figure 1: Illustration of the efficient combination developed within the present thesis.

field, on which the Poisson equation is solved using a fast grid solver, and where the exact boundary conditions are obtained using the FM solver. The major interest of this combination is its computational efficiency: compared to the FM solver used alone, the VIC-FM combination is 15 to 20 times faster. Moreover, the VIC-FM method is easily parallelized using the Parallel Fast Multipole (PFM) solver. The computational domain is then decomposed in several subdomains, one subdomain per processor. The boundary conditions on each subdomain are obtained using the PFM solver, which has a global view of the entire vorticity field. The Poisson equation can then be solved locally on each processor. The resulting VIC-PFM method also leads to a very good computational efficiency and a good speedup performance.

The second major advantage of the present combination is the possibility to run LES at high Reynolds number. Indeed, as a part of the operations are done in a Eulerian way, all the existing SGS models used in classical Eulerian codes, including the recent "multiscale" models, can be easily implemented. In such models, we use the fact that the complete LES field, i.e. the field that contains all the wavenumbers captured by the LES, can be decomposed into a large scale field (a field containing only the low to medium wavenumbers captured by the LES) and into a small scale

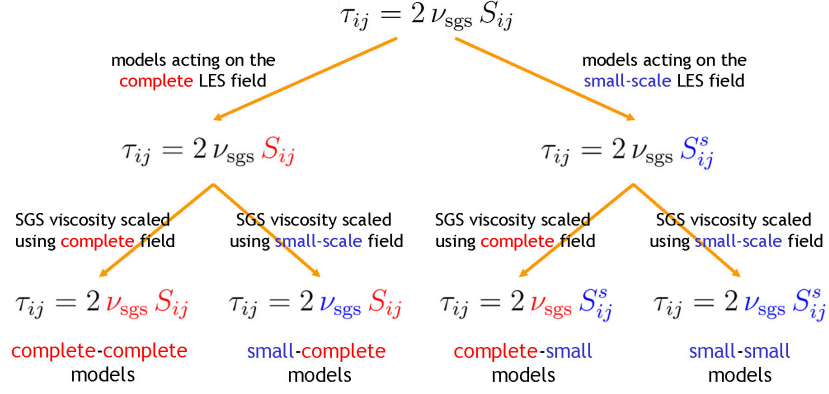


Figure 2: Illustration of the global classification of the SGS models studied within the present thesis.

field (a field containing only the highest wavenumbers captured by the LES, i.e. the smallest scales). For a given complete field f , we have: $f = \bar{f} + f^s$ with $\bar{f}$ the large scale field and f^s the small scale field. Depending the type of SGS model used, the LES equations are then:

$$\frac{D\mathbf{u}}{Dt} + \nabla P = \nu \nabla^2 \mathbf{u} + \nabla \cdot (2\nu_{sgs} \mathbf{S}) \quad (4)$$

$$\frac{D\mathbf{u}}{Dt} + \nabla P = \nu \nabla^2 \mathbf{u} + \nabla \cdot (2\nu_{sgs} \mathbf{S}^s) \quad (5)$$

or equivalently, in the vorticity-velocity formulation:

$$\frac{D\boldsymbol{\omega}}{Dt} - \nabla \cdot (\mathbf{u} \boldsymbol{\omega}) = \nu \nabla^2 \boldsymbol{\omega} + \nabla \cdot (2\nu_{sgs} \mathbf{Q}) \quad (6)$$

$$\frac{D\boldsymbol{\omega}}{Dt} - \nabla \cdot (\mathbf{u} \boldsymbol{\omega}) = \nu \nabla^2 \boldsymbol{\omega} + \nabla \cdot (2\nu_{sgs} \mathbf{Q}^s) \quad (7)$$

with $S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ and $Q_{ij} = \frac{1}{2} \left(\frac{\partial \omega_i}{\partial x_j} + \frac{\partial \omega_j}{\partial x_i} \right)$ ($\mathbf{S}^s$ and $\mathbf{Q}^s$ are computed in the same way but using $\mathbf{u}^s$ and $\boldsymbol{\omega}^s$ respectively). Eqs. (4) and (6) are used with the models that act on the complete LES field. In Fig. 2, which presents a global classification of the SGS models studied here, they are classified in the left branch of the tree. Eqs. (5) and (7) are used with the models that act on the small scale LES field (classified in the right branch of the tree). The idea is here to apply the diffusion operator mainly on the highest wavenumbers, and thus on the smallest scales (i.e. where it is needed). Behind this first classification, in each case, the

SGS viscosity ν_{sgs} can also be computed using either the complete LES field or the small scale LES field. The SGS models can thus be classified among four classes, as shown in Fig. 2. A part of this thesis is devoted to the study of the capabilities and the behavior of such SGS models for LES at high Reynolds number.

Outline

The outline of the thesis is as follows:

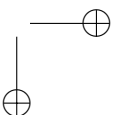
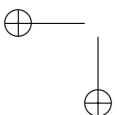
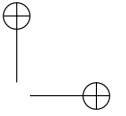
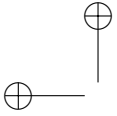
- *Chapter 1: Combining the VIC and PFM methods for efficient domain decomposition simulations.* We present a new combination of vortex-in-cell (VIC) and parallel fast multipole (PFM) methods which allows to efficiently simulate, in parallel, unbounded and half-unbounded vortical flows. This present "VIC-PFM" method permits to work on a compact domain, itself decomposed in several subdomains, that tightly contains the vorticity field. The Poisson equation is solved without requiring any iteration, as the exact boundary conditions are obtained, on each subdomain, using the PFM method. It leads to an efficient method in terms of memory requirements and computational efficiency. The VIC-PFM method is also implemented with one periodic direction and two unbounded directions. The method is validated on a vortex ring at moderate and high Reynolds numbers. The cases of flows above a viscous flat ground can also be taken into account. The case of a two vortex system in ground effect is also simulated. Finally, a space-developing simulation of an aircraft vortex wake in ground effect is also presented, using the space-developing version of the VIC-PFM method.
- *Chapter 2: Multiscale subgrid models for LES of instabilities and turbulence in wake vortex systems.* We study the capabilities of different SGS models, including the recent "multiscale" models, for LES of complex wake vortex dynamics using the VIC-PFM method. More specifically, we consider the multiscale dynamics developing in a counter-rotating four vortex system, that evolves from a simple state to a turbulent state. The various SGS models are tested and compared on this complex and transitional flow. Comparisons are also made with results obtained using a pseudo-spectral method.
- *Chapter 3: Scaling and asymptotic high Reynolds number behavior of multi-scale subgrid models.* We investigate the capabilities of different SGS models for LES, used either in a VIC method or in a pseudo-spectral method, and

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their applicability to the simulation of decaying homogeneous isotropic turbulence (HIT) in the limit of very high Reynolds number (i.e. simulations where the molecular viscosity dissipation is negligible compared to the SGS dissipation). We compare and obtain the asymptotic spectral behavior of each model in the limit of large grids. We are then able to emphasize the global behavior of these SGS models. A previous detailed analysis is also performed to provide the scale-dependence of each model coefficient in the viscous range of turbulence and, then, in the limit of very high Reynolds number.

- *Chapter 4: Counter-rotating four vortex system.* We present a part of the results obtained within a European research project concerning temporal and spatial developing simulations, using the VIC-PFM method, of a counter-rotating four vortex system. Several comparisons are also made with the temporal development results obtained using a pseudo-spectral method. This system undergoes 3-D instabilities more rapidly than what is observed in a two vortex system. A proper assessment of the efficiency of these rapidly growing instabilities as a means for wake alleviation requires to follow the dynamics of the vortices over a significant period of time. These results show the capability of the VIC-PFM method to simulate a complex "real-life" problem: here the quantitative study of the vortex system decay.
- *Chapter 5: Turbulent round jet.* The last application of the space-developing version of the VIC-PFM method is concerned with the LES of a turbulent round jet at a high (yet still moderate) Reynolds number. As it is one of the most commonly studied shear flows, the numerical solution can be compared to both the theoretical and the experimental results found in the literature. The qualitative and quantitative agreements are very good, confirming the potential (efficiency and accuracy) of the present method.



Chapter 1

Combining the VIC and PFM methods for efficient domain decomposition simulations

The content of this chapter was submitted in April 2007 and accepted for publication in August 2007 as an article entitled *Combining the vortex-in-cell and parallel fast multipole methods for efficient domain decomposition simulations*, on invitation by one of the editors of the Journal of Computational Physics for a special issue on "LES, Vortex Methods and Dynamical Systems" honoring the career of Prof. A. Leonard of CALTECH (professor emeritus). The authors are R. Cocle, G. Winckelmans and G. Daeninck. The article is here mainly reproduced as it was submitted.

A part of this work is also published as an article entitled *Vortex methods and their application to trailing wake vortex simulations*, *Comptes-Rendus Physique*, special issue on "Aircraft trailing vortices", Elsevier, Académie des Sciences, Paris, Vol. 6, No. 4-5, 467-486, 2005. The authors are G. Winckelmans, R. Cocle, L. Dufresne and R. Capart.

Historically, the method presented here was first implemented in 2-D to validate the concept. The interested reader can find in Appendix C an illustration of the 2-D VIC-FM method applied to the study of a zero circulation vortex. As explained in the introduction, the method was then developed in 3-D, first with a sequential

version, then with a parallel version. The content of this chapter is only related to the parallel version.

Abstract

A new combination of vortex-in-cell and parallel fast multipole methods is presented which allows to efficiently simulate, in parallel, unbounded and half-unbounded vortical flows (flows with one flat wall). In the classical vortex-in-cell (VIC) method, the grid used to solve the Poisson equation is typically taken much larger than the vorticity field region, so as to be able to impose suitable far field boundary conditions and thus approximate the truly unbounded (or half-unbounded) flow; an alternative is to assume periodicity. This approach leads to a solution that depends on the global grid size and, for large problems, to unmanageable memory and CPU requirements. The idea exploited here is to work on a domain that contains tightly the vorticity field and that can be decomposed in several subdomains on which the exact boundary conditions are obtained using the parallel fast multipole (PFM) method. This amounts to solving a 3-D Poisson equation without requiring any iteration between the subdomains (e.g. no Schwarz iteration required): this is so because the PFM method has a global view of the entire vorticity field and satisfies the far-field condition. The solution obtained by this VIC-PFM combination then corresponds to the simulation of a truly unbounded (or half-unbounded) flow. It requests far less memory and leads to a far better computational efficiency compared to simulations done using either (1) the VIC method alone, or (2) the vortex particle method with PFM solver alone. 3-D unbounded flow validation results are presented: instability, non linear evolution and decay of a vortex ring (first at a moderate Reynolds number using the sequential version of the method, then at a high Reynolds number using the parallel version); instability and non-linear evolution of a two vortex system in ground effect. Finally, a space-developing simulation of an aircraft vortex wake in ground effect is also presented.

Keywords: vortex methods, parallel fast multipole method, vortex-in-cell method, particle methods, lagrangian methods, incompressible flows, unsteady flows, unbounded flows, wall-bounded flows.

1.1 Introduction

The method developed here is a combination of the parallel fast multipole (PFM) method and of the vortex-in-cell (VIC) method that allows to efficiently simulate, in 2-D and in 3-D, incompressible unsteady flows that are unbounded or half-unbounded.

Vortex particle methods are based on the vorticity-velocity formulation of the Navier-Stokes equations and on the fact that, for incompressible flows, it is sufficient to follow the evolution of the vorticity field, the velocity field being recovered from the vorticity. See, e.g., Cottet and Koumoutsakos [16], Winckelmans [82] for global reviews. The Lagrangian treatment of the convection term leads to methods with negligible dispersion error. It also eliminates the CFL stability constraint; however, there is still an accuracy constraint that limits the relative rotation of vortex particles ($|\omega| \Delta t$ must remain moderate). Vortex methods also have good energy conservation properties. These two qualities (negligible dissipation and negligible dispersion) make vortex methods suitable candidates for direct numerical simulation (DNS) and/or large-eddy simulation (LES) of complex convection dominated flows.

When using the vorticity-velocity formulation of the incompressible Navier-Stokes equations, one needs to solve a Poisson equation for the streamfunction. Two different approaches are commonly used:

- *Lagrangian vortex method*: the Poisson equation is solved using the unbounded Green's function approach (Biot-Savart). The unbounded domain is thus taken into account implicitly. Thanks to PFM methods (Greengard and Rokhlin [29], Barnes and Hut [6]), one is able to obtain, both in 2-D and in 3-D, the streamfunction (and thus the velocity, its gradient, etc.) with an $\mathcal{O}(N \log N)$ computational cost, where N is the number of particles. Those approaches make use of outer multipole expansions (i.e., expansions representing the field outside of a ball). There are also implementations that make use of both inner and outer expansions, allowing to reduce the cost to $\mathcal{O}(N)$. Our parallel 3-D implementation is based on an oct-tree and outer expansions; it also uses active error control based on tight error bounds, allowing to minimize the computational cost required to obtain the field with an error that is uniformly bounded in space at a prescribed level (the error tolerance being an input to the code): see Salmon and Warren [66], Salmon *et al.* [67], Ploumhans *et al.* [59, 61]. Another parallel 3-D implementation

is that by Krasny *et al.* [47].

- *Vortex-in-cell method*: in such hybrid Lagrangian-Eulerian methods, the Poisson equation is solved on a grid, see Christiansen [11], Cottet *et al.* [18, 19], Ould-Salihi *et al.* [56]. This is done using fast Poisson solvers. Those also have a computational cost $\mathcal{O}(M \log M)$, where M is the number of grid points, but are considerably faster than the PFM methods. However, boundary conditions are required. Hence, for unbounded (or half-unbounded) flows problems, the grid must be taken much larger than the vorticity field region, so that approximate far field boundary conditions can be used. In some cases, one assumes periodicity: this too calls for a large grid. In both cases, the obtained solution is dependent on the global grid size, and so are the computational memory and cost requirements. In other implementations, a slightly modified Schwarz alternating algorithm can be used: an iterative method to obtain consistent boundary conditions on each subdomains and that avoids solving a boundary integral problem while still retaining good convergence properties [3, 56]. Nevertheless, it results that the VIC approach used "alone" is not really appropriate for unbounded flows, as it does not retain the ability of vortex methods to exactly satisfy the far-field condition.

The present "VIC-PFM" method constitutes a combination of these two approaches. It uses the "smallest" possible domain (i.e. the "smallest" grid): one that tightly contains the vorticity region. In parallel, this domain is further decomposed by splitting it into several subdomains, with one subdomain per processor. The boundary conditions required on the sides of these subgrids are obtained "exactly" by using the PFM method, which has a global view of the entire vorticity field. The Poisson equation is then solved on each subgrid, i.e. locally on each processor, and the combination of all subgrid solutions still provides the solution of a truly unbounded flow. Moreover, from a computational point of view, the efficiency of this method is better than that obtained using a pure PFM method, while benefiting from the powerful parallelization of the fast multipole algorithm. As the grid can be taken compact, it is also better than that obtained using a pure VIC method (when the grid is taken large enough to properly approximate an unbounded domain). The present VIC-PFM methodology is here also extended to unbounded flows with one periodic direction (e.g., useful for simulations of aircraft vortex wakes) and also to half-unbounded flows: those with a flat wall (e.g. simulations of aircraft wakes vortices in ground effect). A last variant, used to

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perform space-developing simulations (thus, simulations with inflow and outflow boundary conditions), is also implemented and is here illustrated on simulating a space-developing aircraft vortex wake in ground effect.

1.2 The VIC-PFM method

The VIC-PFM approach will be explained for the 3-D case only; the 2-D method can easily be deduced from it (and was also implemented). In this section, we first present the basic equations. Then, we explain the VIC-PFM methodology by presenting a global time step. Finally, we describe some essential "tools" used to ensure the method's accuracy/efficiency or required for some specific applications.

1.2.1 Basic equations

Let us first recall the vorticity-velocity formulation for the incompressible Navier-Stokes equations :

$$\frac{D\boldsymbol{\omega}}{Dt} = \nabla \cdot (\mathbf{u}\boldsymbol{\omega}) + \nu \nabla^2 \boldsymbol{\omega} \quad (1.1)$$

where $\mathbf{u}(\mathbf{x}, t)$ is the velocity field, ν is the kinematic viscosity, and $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the vorticity field. In 2-D, $\boldsymbol{\omega} = \omega \hat{e}_z$ and there is no stretching term ($\nabla \cdot (\mathbf{u}\boldsymbol{\omega}) = 0$). The flow being incompressible, the velocity can be expressed as

$$\mathbf{u} = \nabla \times \boldsymbol{\psi} + \mathbf{U}_\infty \quad (1.2)$$

where $\boldsymbol{\psi}$ is the associated stream function, related to $\boldsymbol{\omega}$ by the Poisson equation,

$$\nabla^2 \boldsymbol{\psi} = -\boldsymbol{\omega} , \quad (1.3)$$

and $\mathbf{U}_\infty$ a freestream velocity.

In vortex methods, the vorticity field is discretized using a set of N Lagrangian particles, see Leonard [43] and global presentations in Leonard [44], Cottet and Koumoutsakos [16], and Winckelmans [82]. Here, we use the Gaussian function as regularization, so that the regularized particle vorticity field is:

$$\boldsymbol{\omega}_\sigma(\mathbf{x}, t) = \sum_{p=1}^N \frac{1}{(\sqrt{2\pi} \sigma_p)^3} \exp\left(-\frac{1}{2} \frac{|\mathbf{x} - \mathbf{x}_p|^2}{\sigma_p^2}\right) \boldsymbol{\alpha}_p \quad (1.4)$$

where $\mathbf{x}_p$ is the position of particle p and $\boldsymbol{\alpha}_p = \int \boldsymbol{\omega} d\mathbf{x} = \omega_p h_p^3$ is the particle's strength (with h_p the local grid size). The vector streamfunction, $\boldsymbol{\psi}_\sigma$, on the sides of the grid of each subdomain is thus obtained using the PFM method. To ensure

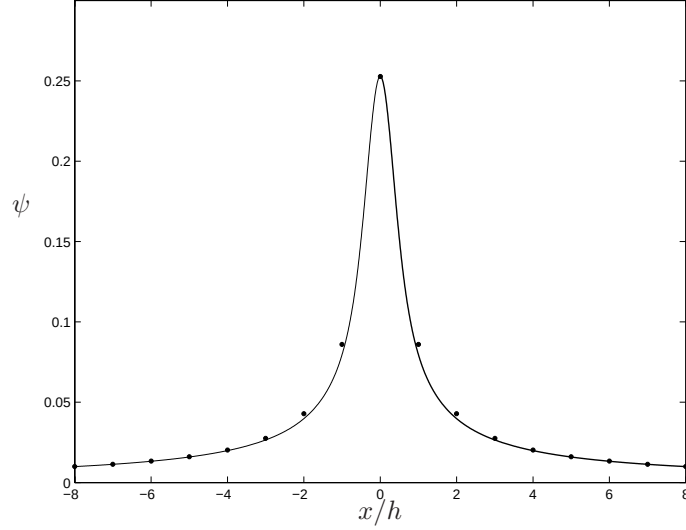


Figure 1.1: The streamfunction obtained for a unit vorticity strength α_0 placed at $x = 0$: ψ_h obtained using the grid solver (dot) and ψ_σ obtained using the PFM method (solid).

a good agreement between the grid solver and the PFM solver, the core size σ_p of the regularized particles has to be chosen such that $\psi_\sigma = \psi_h$ (where ψ_h is the streamfunction obtained using the grid Poisson solver). In Fig. 1.1, we show the value of ψ_h obtained with the grid solver for a unit vorticity strength α_0 placed at $x = 0$. In the multipole method, for the direct interactions, the streamfunction is obtained as:

$$\psi_\sigma(\mathbf{x}, t) = \frac{1}{4\pi} \sum_p \operatorname{erf} \left(\frac{1}{\sqrt{2}} \frac{|\mathbf{x} - \mathbf{x}_p|}{\sigma_p} \right) \alpha_p. \quad (1.5)$$

We can then determine the proper σ_p that leads to the same regularization as the “intrinsic” regularization of the Poisson grid solver, which is due to the finite differences schemes used in those solvers. With the FishPack Poisson solver used here, we find $\sigma_p = 0.251 h_p$. The resulting ψ_σ is shown in Fig. 1.1. We observe that the two curves, ψ_σ and ψ_h , are indeed in good agreement, which ensures the continuity of the streamfunction obtained with the Lagrangian field (i.e. the particles used in the PFM method) and with the Eulerian field (i.e. the field as seen by the grid used in the VIC method).

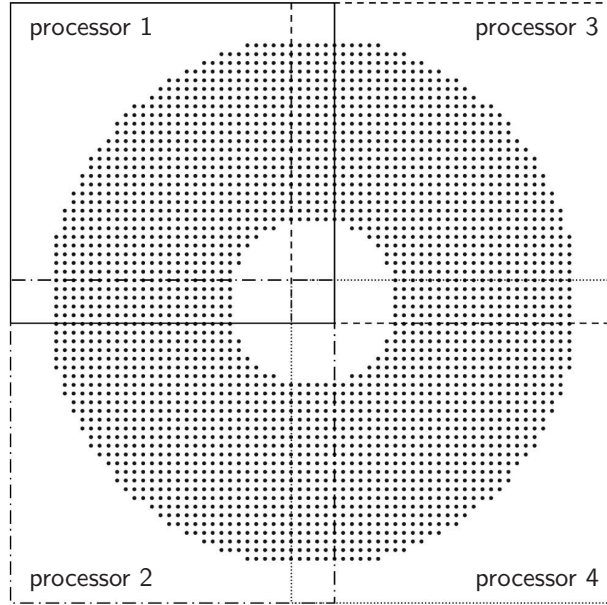


Figure 1.2: Example of domain decomposition for a vorticity field shared between 4 processors. For proper interpolation reasons, an overlapping between the subdomains is required.

1.2.2 Global time step

We now explain the VIC-PFM methodology. We consider the case with uniform grid (of grid size h); the case with non-uniform grid was also considered but the results are not presented here. The initial information is a set of particles of position $\mathbf{x}_p$ and strength α_p which represents the complete vorticity field. Depending on the number of processors p used, the spatial domain defined by the particles, chosen so that it tightly includes the vorticity field, is split equally into several intervals in each direction (p_x intervals in the x -direction and equivalently, p_y and p_z for the others two directions) so that $p_x \times p_y \times p_z = p$ subdomains are created and allotted to the p processors. This is illustrated in Fig. 1.2, using a 2-D example to make it easier. For interpolation reasons that will be explained later, an overlapping between the subdomains is required (minimum $2h$). The particles are then distributed among the processors (i.e. the subdomains) depending on their positions. To prevent

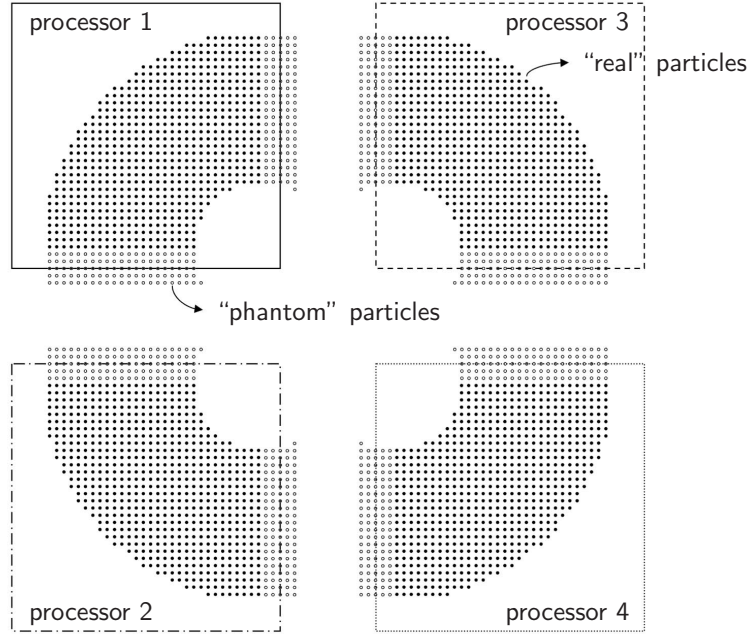


Figure 1.3: Example of distribution of vortex particles between the processors. The “real” particles ($\bullet$) are those which represent the vorticity field in the physical part of each subdomain. Some of these particles, the “phantom” particles ($\circ$), are repeated between the processors.

useless communications, some particles are repeated on several processors: we call them the “phantom” particles, in opposition to the “real” particles that are only present in one processor. Fig. 1.3 illustrates this distribution. We observe that the particles located inside the overlapping region are repeated between the different subdomains. It is also the case for the particles located up to a distance of $2h$ outside the grid limits. We will explain below, in the detailed time step explanation, how these “phantom” particles are useful during the interpolation/redistribution steps.

We also recall that, in Lagrangian methods, particle redistribution is an essential operation to ensure a good representation of the vorticity field and thus maintain the accuracy of the simulation as time proceeds. A particle redistribution is thus done every few time steps (e.g., typically 5, see [59, 61]). When it is time to do a particle redistribution before the time step, one first creates a new set of particles

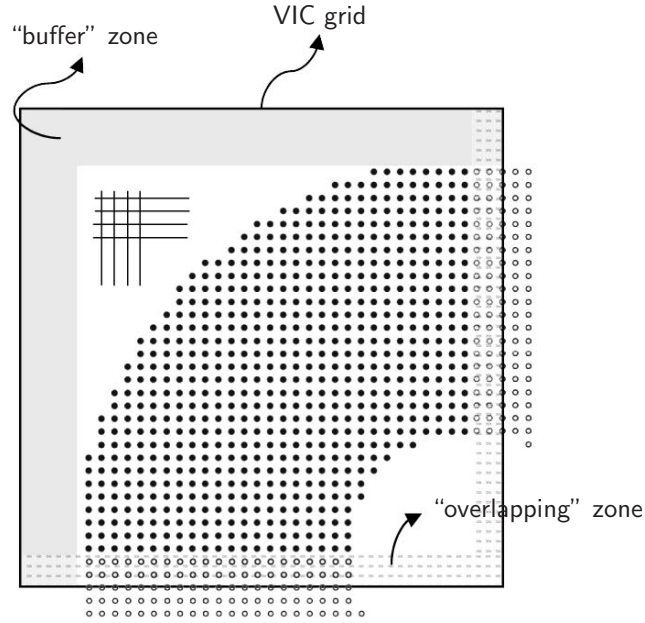


Figure 1.4: Illustration of the Lagrangian and Eulerian "configuration" inside a processor.

on a regular lattice: here based on the VIC grid. This is done using the M'_4 high order interpolation/redistribution scheme (see Section 1.2.3), which preserves the moments of order zero, one and two of the vorticity field (corresponding, respectively, to the total vorticity $\Omega = \int \omega \, dx$, the linear impulse $\mathbf{I} = \frac{1}{2} \int \mathbf{x} \times \omega \, dx$, and the angular impulse $\mathbf{A} = -\frac{1}{2} \int |\mathbf{x}|^2 \omega \, dx$). In case no particle redistribution is done before the time step, the particles are not on a regular lattice, yet they are not much distorted.

In either case, at the beginning of the time step, each processor has a set of particles ("real" and "phantom") of position $\mathbf{x}_p$ and strength α_p . The time step in each subdomain is then as follows:

1. Create the subgrid used to solve the Poisson equation (resulting from the spatial subdivision of the global vorticity field). It is chosen so that it tightly includes the vorticity field defined by the "real" particles domain. In practice, as shown in Fig. 1.4, a "buffer" zone of a few h (typically $5h$) is added in

the "open domain" directions to ensure that the VIC grid is not changed too often. As already mentioned, an "overlapping" zone is also added on all "subdomain-interfaces".

2. Interpolate the particle's strengths onto the grid, to obtain the vorticity field ω on the grid. The M'_4 high order interpolation scheme is used (see Section 1.2.3). As the stencil width of this scheme is $4h$, one notes the utility of the "phantom" particles, located in the region $2h$ outside of the grid limits, to properly obtain the interpolated vorticity field everywhere on the grid.
3. Obtain the Dirichlet boundary conditions for ψ on the sides of the VIC grid, using the PFM method. The oct-tree and outer multipole expansions are computed using the set of grid points (i.e. the grid's strength previously interpolated) located in the "real" subdomain of each processor.
4. Solve, locally on each processor, the Poisson equation $\nabla^2 \psi = -\omega$ on the VIC grid using a fast Poisson solver (e.g., public domain libraries, such as Fishpack [1] and Mudpack [2]). The solver uses the grid with ψ provided on the boundaries and with $-\omega$ known inside. It returns the ψ field on the grid. In 3-D, the Poisson solver is called three times (as ω and ψ are vector fields).
5. Evaluate the velocity field, $\mathbf{u}$, from ψ , using finite differences (here second order, decentered on the boundaries and centered elsewhere).
6. Evaluate the evolution (without convection) of the vorticity field on the grid, $d\omega/dt = \nabla_h \cdot (\mathbf{u} \omega) + \nu \nabla_h^2 \omega$:
 - The diffusion term, $\nu \nabla_h^2 \omega$, is here evaluated using a second order scheme using the 27 points of a cube (in 2-D, the 9 points of a square), see Appendix A. These "isotropic" schemes have the advantage that their truncation error is independent of the local grid orientation (as opposed to the classical "cross" schemes).
 - The stretching term, $\nabla_h \cdot (\mathbf{u} \omega)$, is also evaluated on the grid using finite differences (also second order, decentered on the boundaries and

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centered elsewhere). It is interesting to note that using the conservative form of the stretching term ($\nabla \cdot (\mathbf{u} \omega)$) leads to better results (i.e., moments, energy and zero vorticity divergence conservation) than using the non-conservative form ($(\nabla \mathbf{u}) \cdot \omega$).

At this stage, the fields $\mathbf{u}$ and $d\alpha/dt = h^3 d\omega/dt$ are known at each grid point. It remains to "send back" the information (i.e. $\mathbf{u}$ and $d\alpha/dt$) to the "real" particles and update their position and strength. The "phantom" particles are here deleted as they are no longer useful.

7. Update, still locally on each processor, the "real" particles' position and strength:

- In the case particle redistribution has been done prior to the time step, the particles are aligned with the grid. So, no interpolation is needed: $\mathbf{u}$ and $d\alpha/dt$ are simply copied from the grid points to the corresponding particles. We then use the second order Runge-Kutta scheme (i.e., Euler as first step predictor and trapezoidal rule as second step corrector), as we do not have the information at the previous time step. The Euler predictor is

$$\begin{aligned} \mathbf{x}_p^{n+1,*} &= \mathbf{x}_p^n + \Delta t \mathbf{u}_p(\mathbf{x}_p^n, \alpha_p^n) \\ \alpha_p^{n+1,*} &= \alpha_p^n + \Delta t \frac{d\alpha_p}{dt}(\mathbf{x}_p^n, \alpha_p^n) \end{aligned}$$

The trapezoidal rule corrector first requires redoing steps (1) to (6). Moreover, as the particles are no longer aligned with the grid, the grid fields $\mathbf{u}$ and $d\omega/dt$ are interpolated from the grid to the particles (using again M'_4). We see here the interest of the minimum $2h$ overlapping zone that permits to correctly interpolate the information from the grid to the particles located at the border of the "real" subdomain. After that, the correction step is as follows :

$$\begin{aligned} \mathbf{x}_p^{n+1} &= \mathbf{x}_p^n + \frac{1}{2} \Delta t (\mathbf{u}_p(\mathbf{x}_p^n, \alpha_p^n) + \mathbf{u}_p(\mathbf{x}_p^{n+1,*}, \alpha_p^{n+1,*})) \\ \alpha_p^{n+1} &= \alpha_p^n + \frac{1}{2} \Delta t \left(\frac{d\alpha_p}{dt}(\mathbf{x}_p^n, \alpha_p^n) + \frac{d\alpha_p}{dt}(\mathbf{x}_p^{n+1,*}, \alpha_p^{n+1,*}) \right) \end{aligned}$$

- In the case particle redistribution has not been done prior to the time step, $\mathbf{u}$ and $d\omega/dt$ are interpolated from the grid, as for the second substep of the Runge-Kutta scheme. Now, as we have the information from the previous time step, we use second order two-step schemes. For $d\alpha/dt$, we use Adams-Bashforth. For particle convection, we use Leap-Frog:

$$\begin{aligned}\mathbf{x}_p^{n+1} &= \mathbf{x}_p^{n-1} + 2\Delta t \mathbf{u}_p(\mathbf{x}_p^n, \alpha_p^n) \\ \alpha_p^{n+1} &= \alpha_p^n + \frac{1}{2}\Delta t \left(3\frac{d\alpha_p}{dt}(\mathbf{x}_p^n, \alpha_p^n) - \frac{d\alpha_p}{dt}(\mathbf{x}_p^{n-1}, \alpha_p^{n-1}) \right)\end{aligned}$$

8. Finally, the particles are distributed among the processors according to their new position. If the vorticity field has grown and/or moved, the computational VIC domain and its subdomains limits are redefined.

It is interesting to note that communications are needed only twice per time step: when the boundary conditions are determined using the PFM method (3) and during the particles distribution (8). It leads to a good speedup, in fact nearly the same as the speedup of the PFM method used alone but, as we will see, with a better global computational time.

We should also mention that, in order to limit the number of particles, a "cut" is done every time step. This operation consists in removing the particles having a strength weaker than a fraction of the maximum strength present in the flow. In the case where strong stretching occurs, the maximum strength can rapidly grows up (and thus leading to a too important cut). In that case, the maximum strength taken into account is the maximum strength of the initial condition. Typically, the limit of the cut is taken as $10^{-5} \|\alpha\|_{max}$. To ensure the total vorticity conservation, the sum of the "cut" vorticity is uniformly distributed to the remaining particles.

1.2.3 Particle redistribution/interpolation scheme

As already mentioned, Lagrangian methods require particle redistribution, see [16, 82]. It is an essential operation to maintain a good overlap of the particle regularization functions, and thus maintain a good representation of the vorticity field. In the VIC-PFM method, as we continuously go between the particles and the grid, we also need a good quality scheme to bring the particles information to the grid, and the grid information to the particles. The scheme chosen is the M'_4 scheme (the Λ_3 scheme was also studied but, in 3-D, some noise was noticed, see

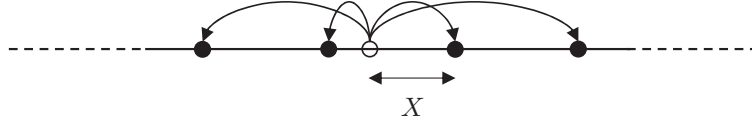


Figure 1.5: Illustration of the stencil width of the M'_4 redistribution/interpolation scheme.

also [16]). In 1-D, the M'_4 scheme, illustrated in Fig. 1.5, is as follows :

$$M'_4(X) = \begin{cases} \frac{1}{2}(2 - 5X^2 + 3X^3) & \text{if } 0 \leq X \leq 1 \\ \frac{1}{2}(1 - X)(2 - X)^2 & \text{if } 1 < X \leq 2 \\ 0 & \text{otherwise} \end{cases}$$

where X is the distance between the particle and the grid node, normalized by h . The fraction of the particle information which is attributed to the grid node (or conversely) is given by $M'_4(X)$. In 2-D and 3-D, one uses tensor products.

The M'_4 scheme is continuous and so is its first derivative. It is a second order scheme: it conserves Ω , $\mathbf{I}$ and $\mathbf{A}$. Of course, the use of such scheme introduces some dissipation. One can show that, on average, it acts as a hyper-viscosity. For a $h/2$ shift between particle positions and grid (which represents the worst situation), it corresponds to a hyper-viscosity operator discretized to second order and with effective $\nu^{(2)}\Delta t$ equal to $3h^4/128$. Considering all possible shifts statistically, the net hyper-viscosity obtained is only a fraction of that.

1.2.4 Projection scheme used to maintain zero vorticity divergence

In 3-D, vortex particle methods do not guarantee that the divergence of the vorticity field remains zero in long-time simulations and/or in under-resolved simulations. In the VIC method (thus also in the VIC-PFM method), a good way to prevent any possible bad behavior consists in regularly re-projecting the vorticity field onto a divergence free basis (Cottet and Poncet [19], Poncet [62]):

$$\omega^{new} = \omega - \nabla_h F \quad (1.6)$$

where F is obtained by solving

$$\nabla_h^2 F = \nabla_h \cdot \omega \quad (1.7)$$

on the grid using, again, the efficient Poisson solver, with Dirichlet boundary condition $F = 0$. This operation is done as soon as the vorticity divergence $\nabla_h \cdot \omega$ is seen to exceed a prescribed value, and when the particles are on a regular lattice (i.e., after a redistribution). The new vorticity field is such that $\nabla_h \cdot \omega^{new} = 0$ and the particle strengths are reset to $\alpha^{new} = \omega^{new} h^3$. This operation provides an efficient and essentially non-diffusive "relaxation" scheme, which allows for simulations at high Reynolds number and for arbitrarily long times.

1.2.5 Subgrid-scale modelling for LES

The aim of this new VIC-PFM method is also to be able to simulate complex 3-D flows at high Reynolds number, thus also using Large-Eddy Simulation (LES) approaches. In this case, only the most energetic scales are captured and the effect of the subgrid-scales (SGS) on the captured scales is modelled.

The capabilities of different SGS models for LES, here implemented in the VIC method, have been investigated in [13, 17, 31, 35, 37, 73, 80]. Their applicability to the simulation of decaying homogeneous isotropic turbulence (HIT) was also tested in [14]. In [13], various SGS models were tested and compared on a more complex and transitional flow: the multiscale dynamics developing in a counter-rotating four-vortex system that evolves from a simple state to a turbulent state. Here, we use a simplified version of the regularized variational multiscale model (here called RVM), where the diffusion, using an effective eddy viscosity ν_{sgs} , operates solely on the high frequency part of the LES vorticity field. In the vorticity-velocity formulation, this gives:

$$\frac{D\omega}{Dt} = \nabla \cdot (\mathbf{u}\omega) + \nu \nabla^2 \omega + \nabla \cdot (\nu_{sgs} (\nabla \omega^s + (\nabla \omega^s)^T)) , \quad (1.8)$$

with ω^s the "small scale" vorticity field and $\nu_{sgs} = C_R^{(n)} \Delta^2 (2 S_{ij} S_{ij})^{1/2}$. The rhs of Eq.(1.8) is discretized as presented in Appendix A. Here the small-scale fields are obtained using a compact (stencil 3) tensor-product explicit discrete filter which is iterated n times to produce an order $2n$ filter [35, 37, 80].

In some simulations, done prior to the RVM model, we also performed LES using a simple "hyper-viscosity" SGS dissipation model. It was also first chosen for its simplicity of implementation and its computational efficiency. The LES equations are then taken as:

$$\frac{D\omega}{Dt} = \nabla \cdot (\mathbf{u}\omega) + \nu \nabla^2 \omega - \frac{C}{T_0} (h^2 \nabla^2)^2 \omega \quad (1.9)$$

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with T_0 a global time scale and C a coefficient. The $(h^2 \nabla_h^2)^2$ operator is evaluated by applying twice the discrete Laplacian of Appendix A.

The global and spectral behavior of these models, as well as others, are discussed in detail in [14, 37]. The present brief presentation is sufficient for the examples of VIC-PFM applications presented here.

1.2.6 Beyond purely open domain flows

There is a large class of purely open-domain flows which can be solved efficiently using the VIC-PFM method as such. We here describe how the method can be extended to further address problems with one periodic direction, problems bounded by a ground, or problems evolving jointly in space and time (space-developing flows).

Case of flows with one periodic direction

As we will illustrate in Section 1.4.2 using an aircraft vortex wake simulation, the VIC-PFM method is also implemented with one periodic direction. This allows to determine the ψ field on the four faces of the grid corresponding to the unbounded directions.

When the code is used on a single processor or when the domain is not split in the periodic direction, the Poisson solver used (here FishPack [1]) is able to take into account one direction with periodic condition and the two others with Dirichlet conditions. A fast and optimal way to determine the ψ field is illustrated in Fig. 1.6. To determine the ψ field at a point P , one has to compute the influence of the main box Ω (i.e. the computational domain) and also of a series of equivalent boxes repeated periodically on both sides of the main box. We use the fact that the influence of the box Ω_{left} on the point P is exactly the same as the influence of the main box Ω on the point P_{right} , and conversely; and so on for all points on both sides of Ω . In this way, the ψ field at P can be computed by summing the contributions of Ω on P , P_{left} and P_{right} . Only the multipole expansions for the computational domain Ω are required. Experience has shown that taking 50 image points on each side provides a well converged solution (i.e. a periodic solution). Compared with the non-periodic case, this periodic evaluation has an additional computational cost of only about 25%. It is thus still very acceptable.

In the parallel case (i.e. when the domain Ω is itself split in the periodic direction in various subdomains), the Poisson equation is solved in two steps to

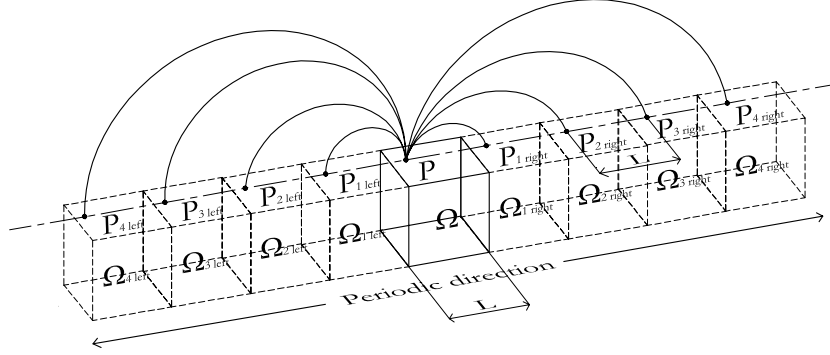


Figure 1.6: Illustration of the PFM method used to compute flows with one periodic direction. The ψ field at P is obtained by summing the contributions of Ω on the “shifted” points.

ensure a perfect continuity between each subdomain:

$$\begin{cases} \nabla^2 \bar{\psi} = -\bar{\omega} \\ \nabla^2 \psi' = -\omega' \end{cases}$$

where $\bar{\omega}$ is the 2-D vorticity “base flow” field (i.e. the vorticity field space averaged in the periodic direction) and $\omega' = \omega - \bar{\omega}$. The base flow is first evaluated on the grid and is used to obtain the boundary conditions $\bar{\psi}$ required to solve the first Poisson equation. Then, the ω' field is evaluated and is used to obtain the related ψ' boundary condition to solve the second Poisson equation. The total streamfunction ψ is then simply the sum of $\bar{\psi}$ and ψ' .

In that way, we impose that each processor in the periodic direction “sees” exactly the same base flow field. Without such procedure, we have noticed, in long-time simulations, the possible apparition of some small discontinuities at the subdomain interfaces. This behavior is due to the method used to compute the periodic boundary conditions. Indeed, even if 50 image points are sufficient to have a well converged periodic solution, it doesn’t guarantee that the solution obtained on the ends of the periodic domain are exactly the same, the multipole summations being not exactly equivalent. Imposing the same base flow field all over the periodic domain avoids this problem and leads to a continuous periodic solution.

Case of flows in semi-open domains

As we have already mentioned, the PFM method is ideal to take into account boundary conditions for open domain flows, also those with one periodic direction. However, in some cases (e.g. flows bounded by a ground, space-developing simulations with inflow and outflow, etc.), we also may want to impose:

- *A no-through flow plane*: this is used for bounded flows where we need to enforce the no-through flow condition. For that, we symmetrize the vorticity field with respect to the plane (here written for a $x - y$ plane located at $z = 0$):

$$\begin{cases} \omega_n(x, y, -z) &= \omega_n(x, y, z) \\ \omega_t(x, y, -z) &= -\omega_t(x, y, z), \end{cases}$$

where ω_n and ω_t are respectively the normal component and the tangential components of the vorticity field. This leads to $u_n(x, y, 0) = 0$.

- *A through flow plane*¹: this is used for outflow where the tangential velocity is enforced to zero. This is also done by enforcing symmetries on the flow. It leads to the following constraints on the vorticity field (also written for a $x - y$ plane located at $z = 0$):

$$\begin{cases} \omega_n(x, y, -z) &= -\omega_n(x, y, z) \\ \omega_t(x, y, -z) &= \omega_t(x, y, z). \end{cases}$$

This leads to $u_t(x, y, 0) = 0$.

In practice, we don't have to build the symmetrized vorticity field explicitly: when one evaluates, using the PFM method, the ψ field at a point $\mathbf{x}$ (for the boundary conditions) induced by the vorticity field, one also makes evaluations at symmetric locations and adds it to the first contribution, changing adequately the sign of each component.

In order to simulate a flow above a viscous ground, we also need to enforce a zero slip velocity at the wall. It is done in two steps. First, we use the "no-through flow" symmetrization to enforce a zero normal velocity over the whole ground plane. After the Poisson equation has been solved, there is however still

¹The through flow plane condition is useful as outflow condition for space-developing simulations where the normal velocity is dominant (e.g. a jet flow as illustrated in Chapter 5). In opposition, the no-through flow plane (i.e., equivalent to a slip plane) will be used when the tangential velocities are dominant.

a spurious slip velocity, $\mathbf{u}_{\text{slip}}$, at the wall. The second step is then to enforce the no-slip by emitting a vorticity flux at the wall:

$$\nu \frac{\partial \omega}{\partial \mathbf{n}} = \frac{\Delta \gamma}{\Delta t}, \quad \Delta \gamma = 2 \mathbf{u}_{\text{slip}}. \quad (1.10)$$

Since the ground is flat, there is no need to solve numerically a boundary integral equation for the panel strengths: the solution is trivially obtained as $\Delta \gamma = 2 \mathbf{u}_{\text{slip}}$. This flux must be emitted during a time Δt , see [16, 40, 61, 82]. As this operation is done on the VIC grid, we have square panels of strength $\Delta \gamma$ and size $h \times h$. We here consider that the ground is located on the XY plane and that the panels diffuse towards the positive Z direction. The "amount" of strength diffused, from one panel, to a grid point located at $(x, y, z > 0)$, during a time Δt , is given by:

$$\Delta \alpha = \int_0^{\Delta t} \frac{d\alpha}{dt} dt \quad (1.11)$$

with

$$\frac{d\alpha}{dt}(x, y, z) = \int_{x-h/2}^{x+h/2} \int_{y-h/2}^{y+h/2} \int_{z-h_l/2}^{z+h/2} \frac{d\omega}{dt} dz dy dx \quad (1.12)$$

$$= \frac{\Delta \gamma}{\Delta t} \left([\text{erfc}(u)]_{(z+h/2)/\sqrt{4\nu t}}^{(z-h_l/2)/\sqrt{4\nu t}} \right) \quad (1.13)$$

$$\left(\sqrt{4\nu t} \frac{1}{2} \left([\text{ierfc}(u)]_{(x-h)/\sqrt{4\nu t}}^{x/\sqrt{4\nu t}} - [\text{ierfc}(u)]_{x/\sqrt{4\nu t}}^{(x+h)/\sqrt{4\nu t}} \right) \right)$$

$$\left(\sqrt{4\nu t} \frac{1}{2} \left([\text{ierfc}(u)]_{(y-h)/\sqrt{4\nu t}}^{y/\sqrt{4\nu t}} - [\text{ierfc}(u)]_{y/\sqrt{4\nu t}}^{(y+h)/\sqrt{4\nu t}} \right) \right)$$

where $\text{ierfc}(u) = \int_u^\infty \text{erfc}(v) dv = \frac{1}{\sqrt{\pi}} \exp(-u^2) - u \text{erfc}(u)$. Notice that $h_l/2 = h$ for the "first layer" of grid points (i.e. located at $z = h$) and $h_l/2 = h/2$ otherwise. The time integral in Eq. (1.11) is evaluated numerically using a Gauss quadrature (4 points). The vorticity is generally distributed on a "region" of size $7h \times 7h \times 4h$ centered on the panel, so that we ensure that the whole panel strength is distributed. As this operation is done on the grid, most of the terms of Eq. (1.13) can be precomputed for all panels. The no-slip condition is enforced at each time step, just after step (6).

When the divergence is reset to zero, using the projection scheme presented before, the boundary conditions for the resolution of the Poisson equation also need to be changed. At the wall, we impose Neumann boundary conditions, $\partial F / \partial n = 0$, so that the normal vorticity remains zero: $\omega_z^{\text{new}} = \omega_z - \partial F / \partial z = \omega_z = 0$.

1.2. The VIC-PFM method

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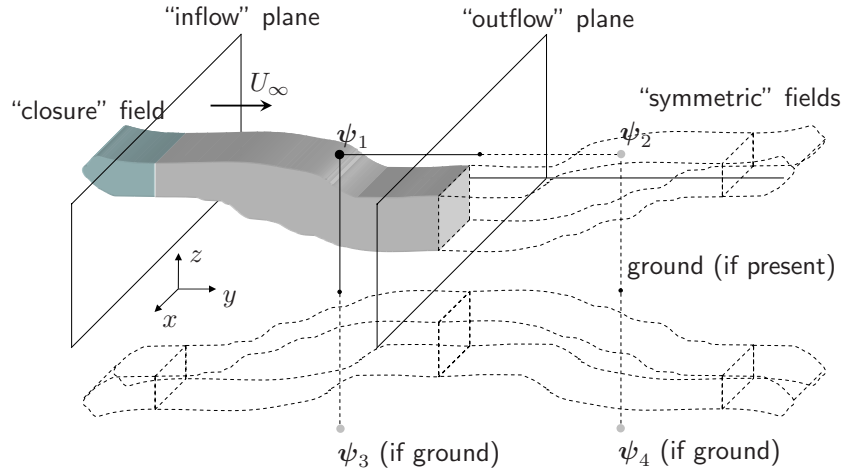


Figure 1.7: Illustration of the configuration used for space-developing simulations using the VIC-PFM method.

Case of space-developing simulations

The setup for space developing simulations is presented in Fig. 1.7. It essentially consists on an inflow condition that dynamically evolves in space and time, due to the vorticity and the induced velocity of an added potential flow ϕ (and maybe time dependent).

In order to "close" the problem, a fixed vorticity field is added in front of the inflow plane to close the vortex lines coming from the "main" vorticity domain. The injection of the entry condition is ensured by buffer particles, located in front of the entry plane and convected with the velocity computed on the inflow plane. As soon as their position is inside the main vorticity domain, they become "real" particles. As we do not want to keep the vortex wake particles "forever", an outflow boundary condition is also used; it is imposed by enforcing symmetries on the flow.

When the boundary conditions are obtained using the PFM method, the set of particles representing the fixed vorticity field is used, in addition to the particles from the main vorticity domain. Then, the symmetrizations previously presented are used to impose the correct outflow conditions and/or the presence of a ground, as shown in Fig. 1.7. The choice of the outflow conditions is dictated by the vorticity field. If the normal component of the vorticity distribution is dominating (e.g. an aircraft wake vortex system), the "no-through flow" condition is used. It means that the normal velocity obtained from the Poisson equation is set to

Table 1.1: *Efficiency analysis: CPU times (computations ran on one Intel Pentium IV processor at 2.4 GHz) and memory requirements (based on the storage of $\mathbf{u}$, ψ and ω in double precision) for the hybrid VIC-PFM method, the PFM method alone, and the periodic VIC method alone (for three grids).*

	VIC-PFM	PFM	VIC (1)	VIC (2)	VIC (3)
L/D	1.66	—	1.66	2.28	3.20
H/D	0.64	—	0.64	1.28	1.92
Grid size	166×166 $\times 64$	— —	166×166 $\times 64$	228×228 $\times 128$	320×320 $\times 192$
CPU times	55.0 s.	926.0 s.	12.5 s.	24.7 s.	72.0 s.
Mem. req.	172 MB	52 MB	120 MB	456 MB	1350 MB

zero, and thus that the total normal velocity on the outflow plane is equal to the velocity of the added potential flow. Conversely, if the tangential components of the vorticity distribution is dominating (e.g. a shear layer flow, or a jet flow), the "through flow" condition is used. The velocity field on the outflow plane is then purely normal (unless the added potential flow also has a tangential component).

1.3 Efficiency analysis of the VIC-PFM method

The aim of this section is to analyse the CPU time cost and the memory requirements for the VIC-PFM method, as compared to the PFM method alone (which also solves the unbounded flow case) and to the VIC method alone (which here solves a periodic flow problem). To make the comparison, we consider a generic flow : a vortex ring of centerline radius R , of Gaussian vorticity distribution as in Eq. (1.20), and of core size $\sigma_0/R = 0.21$. The discretization is $h/R = 0.02$, the number of particles is $\sim 7.8 \cdot 10^5$ and the VIC-PFM grid is $166 \times 166 \times 64$ ($\sim 1.8 \cdot 10^6$ grid points).

Table 1.1 provides, for one time step, the computational times and the memory requirements obtained using the different methods, running on one processor. For the periodic VIC method alone, three different grid sizes are considered: they are illustrated in Fig. 1.8.

1.3. Efficiency analysis of the VIC-PFM method

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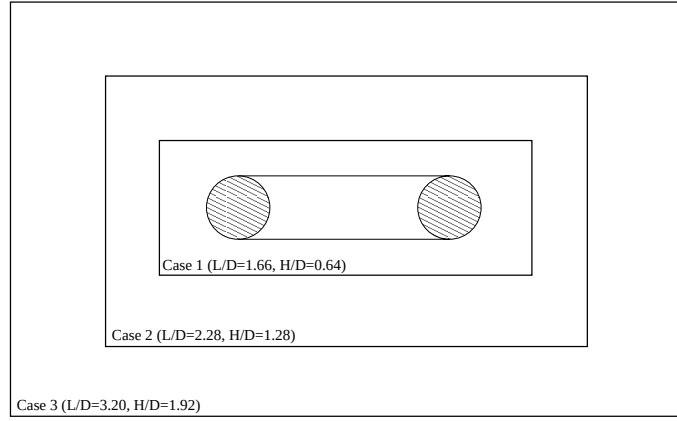


Figure 1.8: Illustration of the three grids used for the periodic VIC method in the efficiency analysis.

First, one notices that the VIC-PFM method is 17 times faster than the PFM method alone. We clearly see the interest to combine the two methods. Both solvers are $C * \mathcal{O}(N \log(N))$, but the Poisson solver used in the VIC method has a much smaller C than the PFM method. As we use the PFM method only for obtaining ψ at the boundary grid points, we are able to save a lot of CPU time and finally obtain a large factor (17) between the two methods.

It is interesting to measure where the computational time is spent in this hybrid method: roughly half of the time is devoted to the determination of the proper ψ boundary conditions using the PFM method, a quarter is devoted to the grid Poisson solver, and a quarter to the interpolation operations between the particles and the grid; the other operations (finite differences for velocity, stretching term, particles distribution among the processors, etc.) have a negligible cost.

We also compare with the VIC method alone, assuming periodic conditions. One clearly sees, in Fig. 1.8, that the Cases 1 and 2 are still very far from representing a vortex ring in unbounded space. Case 3 could be considered as closer to an unbounded flow, but the memory requirements then become very large.

Another interesting point is the speedup performance of the VIC-PFM implementation. Two cases are illustrated to distinguish the gain obtained with two different scalings: the weak scaling, where the problem size is doubled when the number of processors is doubled, and the strong scaling, where the problem size is held fixed. When a $\mathcal{O}(N)$ method is used, a perfect parallelization would lead

to a speedup equal to the number of processors. Here, the method is the combination of two $\mathcal{O}(N \log(N))$ methods, the best speedup that can be obtained is thus not as good. In [18], the computational cost of the VIC method is fitted with $\mathcal{O}(N^a)$, where $a \approx [1.10 - 1.15]$. In the range of N classically used (i.e. $N \in [10^4 - 10^8]$), both writings are essentially equivalent: $\mathcal{O}(N \log(N)) \approx \mathcal{O}(N^a)$ for $a \approx [1.11 - 1.15]$. Here, we used the $\mathcal{O}(N \log(N))$ fit.

1.3.1 Weak scaling

For the weak scaling, the computational time using one processor and p processors are respectively:

$$T_1 = C_P 6 N^{2/3} \log(rN) + C_V N \log(N) \quad (1.14)$$

$$T_p = C_P 6 N^{2/3} \log(prN) + C_V N \log(N) \quad (1.15)$$

where C_P and C_V are the coefficients related to the PFM method and to the VIC method, r is a "filling" coefficient that gives the ratio between the number of particles and the number of grid points (typically $r \approx 0.5$) and N is the number of grid points, here with a grid assumed of cubical shape. The first term in the rhs of Eq. (1.15) is the cost of the boundary conditions computed on the 6 faces of the grid (composed of $N^{2/3}$ grid points) using the prN particles. The second term is the cost of the Poisson equation resolution: for the weak scaling, it remains constant with the number of processors. The best reachable speedup is then given by:

$$\begin{aligned} S_{max}(p) &= p \frac{T_1}{T_p} \\ &= p \frac{1}{1 + \frac{\log(p)}{\log(r) + \left(1 + \frac{N^{1/3}}{6(C_P/C_V)}\right) \log(N)}} \end{aligned} \quad (1.16)$$

The curve is shown in Fig. 1.9 and is compared with the speedup effectively obtained with a simulation on a single domain size of $N = 1.2 \cdot 10^6$, $r \approx 0.5$ and with $C_P/C_V = 100$. This last value is deduced from sequential simulations and is in good agreement with [18]. The speedup obtained is good: even with 128 processors and more than 150 million grid points, the efficiency is still very acceptable: $\epsilon(p) = S(p)/S_{max}(p) \approx 0.63$.

1.3. Efficiency analysis of the VIC-PFM method

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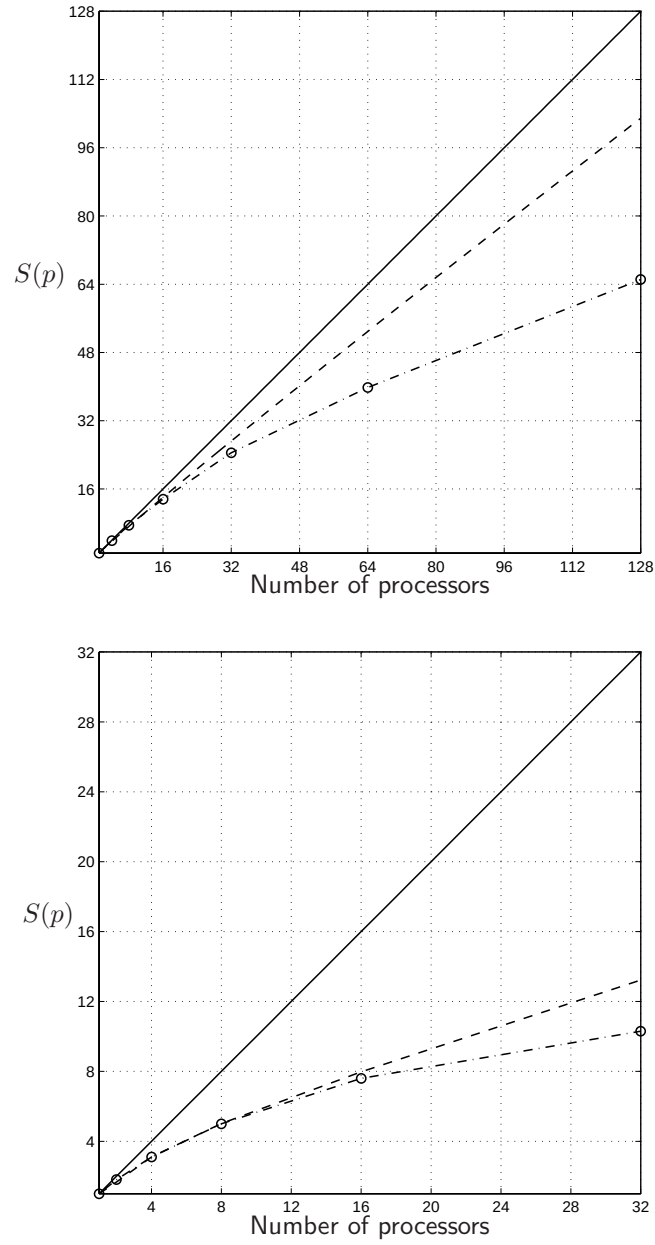


Figure 1.9: Speedup performance for the weak scaling (top) and for the strong scaling (bottom): the perfect parallelization of a $\mathcal{O}(N)$ method with N the number of computational elements (solid), the best reachable parallelization of a VIC-PFM method (dashed) and the speedup obtained with our code (dash-dot).

1.3.2 Strong scaling

For the strong scaling, the computational time using one processor and p processors are here respectively:

$$T_1 = C_P 6 N^{2/3} \log(rN) + C_V N \log(N) \quad (1.17)$$

$$T_p = C_P A(p) N^{2/3} \log(rN) + C_V \frac{N}{p} \log\left(\frac{N}{p}\right) \quad (1.18)$$

where $A(p)$ is the coefficient taking into account the variation of the number of grid points where the boundary conditions have to be computed (depending on the number of processors used). Again, the first term in the rhs of Eq. (1.18) is the computational cost related to the boundary conditions evaluated using the rN particles. The second term is the cost of the Poisson equation resolution. Here, the grid is split between the p processors and becomes smaller when p increases. The best reachable speedup is then given by:

$$\begin{aligned} S(p) &= \frac{T_1}{T_p} \\ &= \frac{(C_P/C_V) 6 \log(rN) + N^{1/3} \log(N)}{(C_P/C_V) A(p) \log(rN) + \frac{N^{1/3}}{p} \log\left(\frac{N}{p}\right)} \end{aligned} \quad (1.19)$$

The curve is illustrated in Fig. 1.9. The real speedup is here obtained using a simulation with $N = 4.8 \cdot 10^6$ and $r \approx 0.5$. We observe that, up to 16 processors, both speedup curves collapse very well. With 32 processors, the real curve saturates because the grid allocated to each processor becomes too small: no significant further gain can then still be obtained.

We can finally conclude that the coupling of the PFM and VIC methods provides an efficient algorithm for truly unbounded flow problems, with good computational efficiency and much acceptable memory requirements.

1.4 Validations and illustrations

1.4.1 Instability of vortex rings at moderate and high Reynolds numbers

The first application we consider is the instability of vortex rings. Fig. 1.10 shows a visualization of a vortex ring in water at $Re \approx 2000$. The objective is not to carry a detailed study on vortex rings instabilities, but to show that the VIC-PFM

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method is competitive for this type of flow because of its Lagrangian framework (low dispersion) and its unbounded domain capacity. We first examine a configuration that was previously studied by Shariff, Verzicco and Orlandi [71]: a vortex ring at moderate Reynolds number, where we examine the most amplified waves and their growth rate. Here, we will also simulate the complete non-linear phase, up to the saturation of the instabilities, and also capture the following global decay. The second case is far more challenging: a much thinner vortex ring and at higher Reynolds number. We will also examine the most amplified waves, their growth rate and compare them to those predicted using Saffman's theory.

The initial azimuthal vorticity distributions are Gaussian, function of the distance to the ring centerline:

$$\omega_\theta = \frac{\Gamma_0}{\pi\sigma_0^2} \exp(-s^2/\sigma_0^2) \quad (1.20)$$

with $s^2 = z^2 + (r - R)^2$, Γ_0 the initial circulation, σ_0 the initial core size, and R the ring radius. The time scale used for normalization is taken as $t_0 = R^2/\Gamma_0$. This distribution does not constitute a steady solution, but for core rotation frequencies not small compared to the growth rate, this unsteadiness will act as an intrinsic forcing on the instability waves (Shariff *et al.* [70, 71]). The initial perturbation is done by displacing the vortex lines radially, from their unperturbed position r to their perturbed r_{pert} , as follows:

$$r_{pert}(\theta) = r(1 + \epsilon g(\theta)) \quad (1.21)$$

where $g(\theta)$ is a sum of Fourier modes (with unit amplitudes and random phases) and ϵ is the perturbation amplitude. To maintain the zero divergence of the vorticity field after applying the perturbation, ω_θ and ω_r are realigned along the perturbed vortex lines.

The first vortex ring studied has a $\sigma_0/R = 0.4131$ and is perturbed on the 24 first modes with an amplitude $\epsilon = 0.0002$; the Reynolds number is $Re = \Gamma_0/\nu = 5500$ (corresponding to Case 1 in Shariff *et al.* [71]). The discretization is $h/R = 0.040$ and the time step used is $\Delta\tau = \Delta t/t_0 = 0.05$. To be able to better capture the turbulent decay phase, we add some hyper-viscosity SGS dissipation (with $C = 2.5 \cdot 10^{-2}$). Without such LES model, one cannot go much further than $\tau = 80$. We also use the projection scheme described in Section 1.2.4.

The simulation was carried out for 4700 time steps and took ~ 64 hours on a single Pentium IV at 2.4 GHz. The number of particles goes from $\sim 3.6 \cdot 10^5$ up to $\sim 1.0 \cdot 10^6$, and the number of grid points grows from $\sim 9.0 \cdot 10^5$ to $\sim 4.4 \cdot 10^6$. At

$\tau = 100$, a part of the distant wake left by the vortex ring was removed, to be able to continue the simulation on a single processor. Because of the very low energy level of this far wake, the flow around the vortex ring is not affected by this cut.

Before presenting the results, we provide definitions regarding the characterization of the instabilities and the evaluation of the energy diagnostics. Formulating the velocity field in cylindrical coordinates, we can write

$$\mathbf{u}(r, \theta, z, t) = \sum_{n=-N_\theta/2}^{N_\theta/2} \hat{\mathbf{u}}(r, n, z, t) e^{i n \theta}, \quad (1.22)$$

with N_θ the number of azimuthal grid points; a similar development applies to ψ and ω . The azimuthal Fourier transform of $\mathbf{u}$ is given by

$$\hat{\mathbf{u}}(r, n, z, t) = \frac{1}{2\pi} \int_0^{2\pi} \mathbf{u}(r, \theta, z, t) e^{-i n \theta} d\theta. \quad (1.23)$$

The azimuthal modal energy E_n is accordingly defined by

$$E_n(t) = \frac{1}{2} \iint \hat{\mathbf{u}} \cdot \hat{\mathbf{u}}^* r dr dz = \frac{1}{4} \iint [\hat{\psi} \cdot \hat{\omega}^* + \hat{\omega} \cdot \hat{\psi}^*] r dr dz, \quad (1.24)$$

with superscript $*$ denoting the complex conjugate. Using the symmetry ($E_n = E_{-n}$), we consider only the modes with $n \geq 0$. Accordingly, the modal energy becomes

$$E_n(t) = \iint \hat{\mathbf{u}} \cdot \hat{\mathbf{u}}^* r dr dz = \frac{1}{2} \iint [\hat{\psi} \cdot \hat{\omega}^* + \hat{\omega} \cdot \hat{\psi}^*] r dr dz. \quad (1.25)$$

The total energy is then

$$E(t) = \sum_{n=0}^{N_\theta/2} E_n(t). \quad (1.26)$$

Fig. 1.11 shows the evolution of the modal energies E_n . One can observe different phases : the transient phase for $\tau \leq 25$; the linear phase, when linearly fastest growing eigenmodes begin to dominate over transients ($25 \leq \tau \leq 80$); the non-linear stage, when highest wavenumber modes begin to grow more rapidly than the first eigenmodes ($80 \leq \tau \leq 150$); the saturation which occurs at $\tau \approx 150$; and finally, the global decay for $\tau \geq 150$. The most amplified modes during the linear phase are $n = 6$, $n = 7$, and, a little less, $n = 8$. Shariff *et al.* found the $n = 5$, $n = 6$ and $n = 7$ modes. In our simulation, the $n = 7$ mode is dominant whereas it was the $n = 6$ in Shariff's simulation. But, if we compare the growth rates, $\alpha_n = 1/(2E_n)(dE_n/dt)$, evaluated at $\tau = 45$, we obtain very similar values. These are illustrated in Fig. 1.11 (a). We obtain a growth rate equal to

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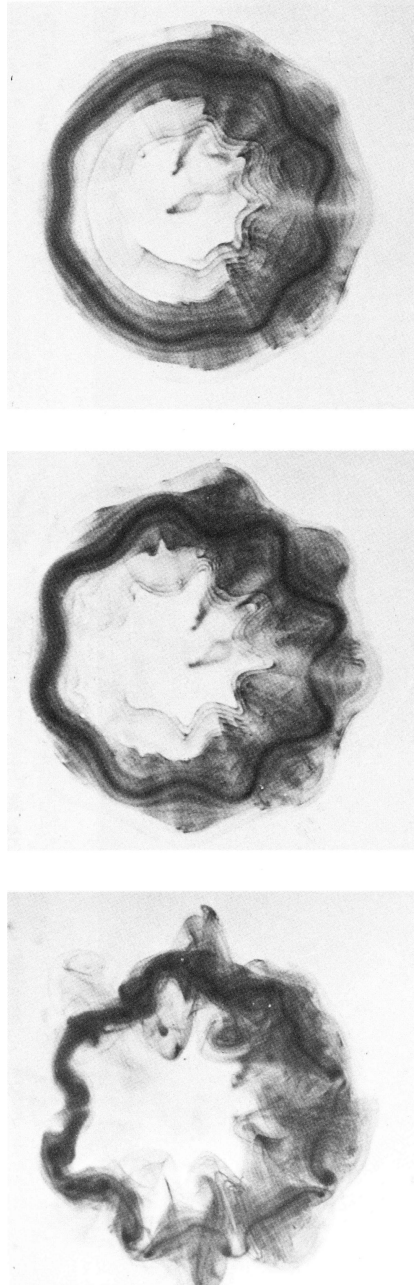


Figure 1.10: *Growth of waves on a vortex ring at $Re \approx 2000$: the sequence shows eight waves growing on a laminar vortex ring in water (reproduced from Van Dyke [75]).*

~ 0.08 for the $n = 6$ and $n = 7$ modes (with a small preference for $n = 7$), which is the same value as Shariff found (with a small dominance for the $n = 6$ mode). The small difference observed could be due to the periodic condition in the z -direction in Shariff's simulation, contrary to the unbounded domain condition here. Indeed, his box size in this direction was equal to $6R$; but, at $\tau = 45$, the ring has travelled over $8R$. The ring has then entered in contact with his own wake, which is dominated by the $n = 6$ mode. This could explain why the $n = 6$ mode was a little more present in Shariff's simulation than in ours.

Fig. 1.11 (b) provides the growth rates during the non-linear phase at $\tau = 100$. One observes that $n = 1$ and $n = 2$ modes are significantly amplified (as also observed by Shariff). One also sees that the next most non-linearly amplified waves are $n = 12$ and $n = 13$: the harmonics of the most linearly amplified modes, as also observed by Shariff. The next most amplified wave is $n = 19$, which is close to the second harmonic.

Fig. 1.12 (a) and (b) show isocontours of $\omega_z t_0$ in the plane of maximum $\|\omega\|$ during the linear stage ($\tau = 70$), and at the early non-linear stage ($\tau = 100$). One sees that distinct patterns emerge. The $n = 6$ and $n = 7$ waves are clearly dominant and have the signature of second radial mode (i.e. three layers arranged radially), also consistent with flow visualization experiments. Fig. 1.12 (c) to (f) also give isocontours of $\omega_z t_0$ (levels have changed) but for longer times, during the non-linear phase and after the saturation. One observes the rapid growth of axial vorticity, and for (c) and (d), the loss of well structured patterns : the "turbulent" phase, with strong decay. Fig. 1.13 provides the front and side three-dimensional views of the ring evolution for the same times as in Fig. 1.12. One first observes the distortion of the isosurfaces due to the linear instability, then the more complex flow resulting from the non-linear evolution. At $\tau = 175$, we also see an ejection of hairpin vortices into the wake: this behavior was observed in experiments by Schneider [69], Auerbach [4] and Weigand and Gharib [77].

For the second case, we choose a much thinner vortex ring. The initial core size is here set to $\sigma_0/R = 0.2$. The ring is also perturbed on the first 24 azimuthal modes, with an amplitude $\epsilon/R = 0.0001$. The Reynolds number is also increased to $Re = 25000$. The discretization is quite fine, $h/R = 0.010$, and the time step is $\Delta\tau = \Delta t/t_0 = 0.01$. To be able to also capture the turbulence and the turbulent decay phase, we add a SGS model: we here use the advanced RVM model presented in Section 1.2.5, which is guaranteed not to dissipate in the well-resolved flow region.

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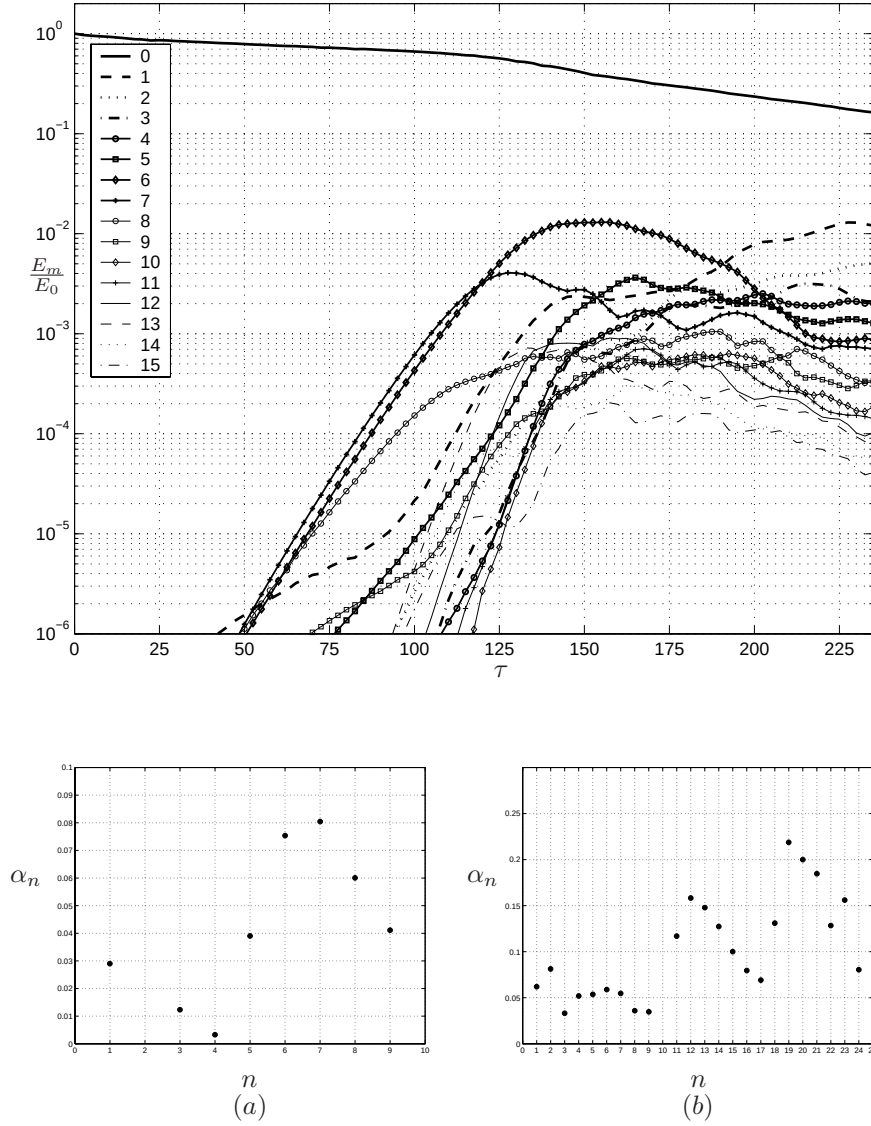


Figure 1.11: Vortex ring at $Re = 5500$. Top: evolution of the modal energies, for modes 0 to 15. Bottom: growth rates for the modal energy at $\tau = 45$ (a) and $\tau = 100$ (b). The modes which still have an oscillatory behavior are not shown.

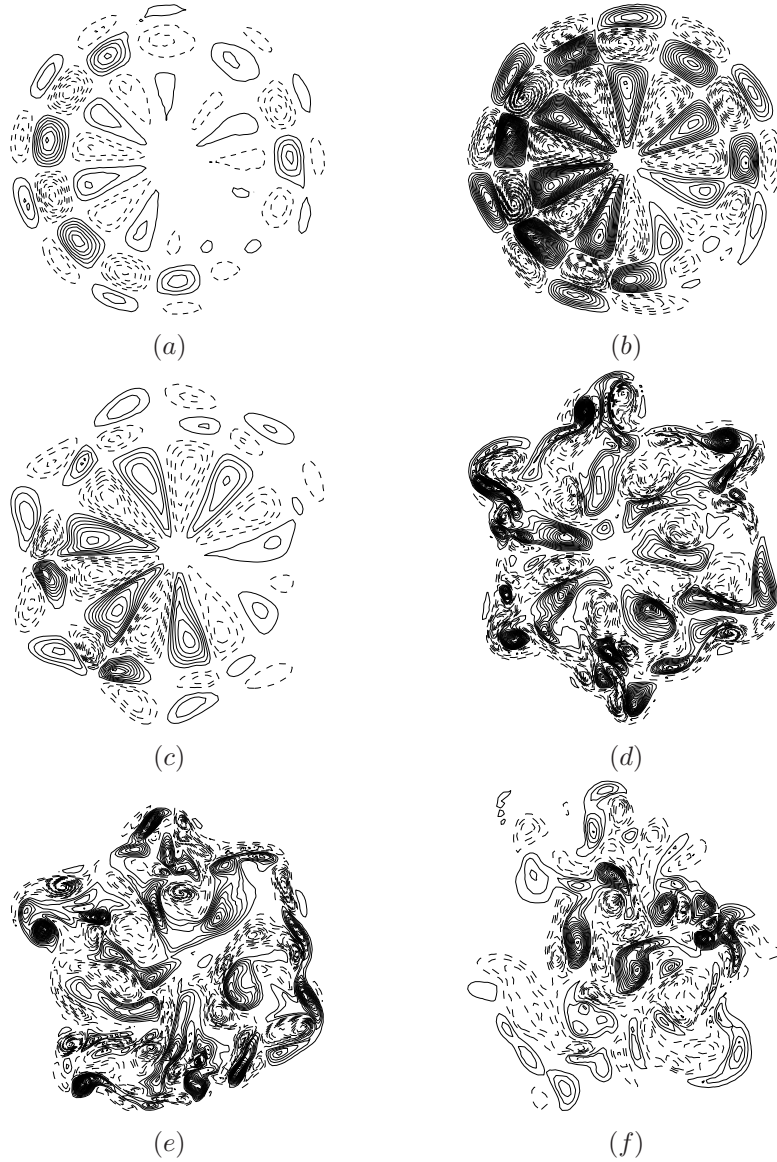


Figure 1.12: Vortex ring at $Re = 5500$: isocontours of $\omega_z t_0$ in the plane of maximum $\|\omega\|$. Dashed and dotted lines represent positive and negative values, respectively. Levels are first by step of 0.02: (a) $\tau = 70$ (linear stage), (b) $\tau = 100$ (beginning of the non-linear stage). Levels are then by step of 0.08: (c) $\tau = 115$ (non-linear stage), (d) $\tau = 130$ (saturation), (e) $\tau = 175$ and (f) $\tau = 220$: ("turbulent" and decay phase).

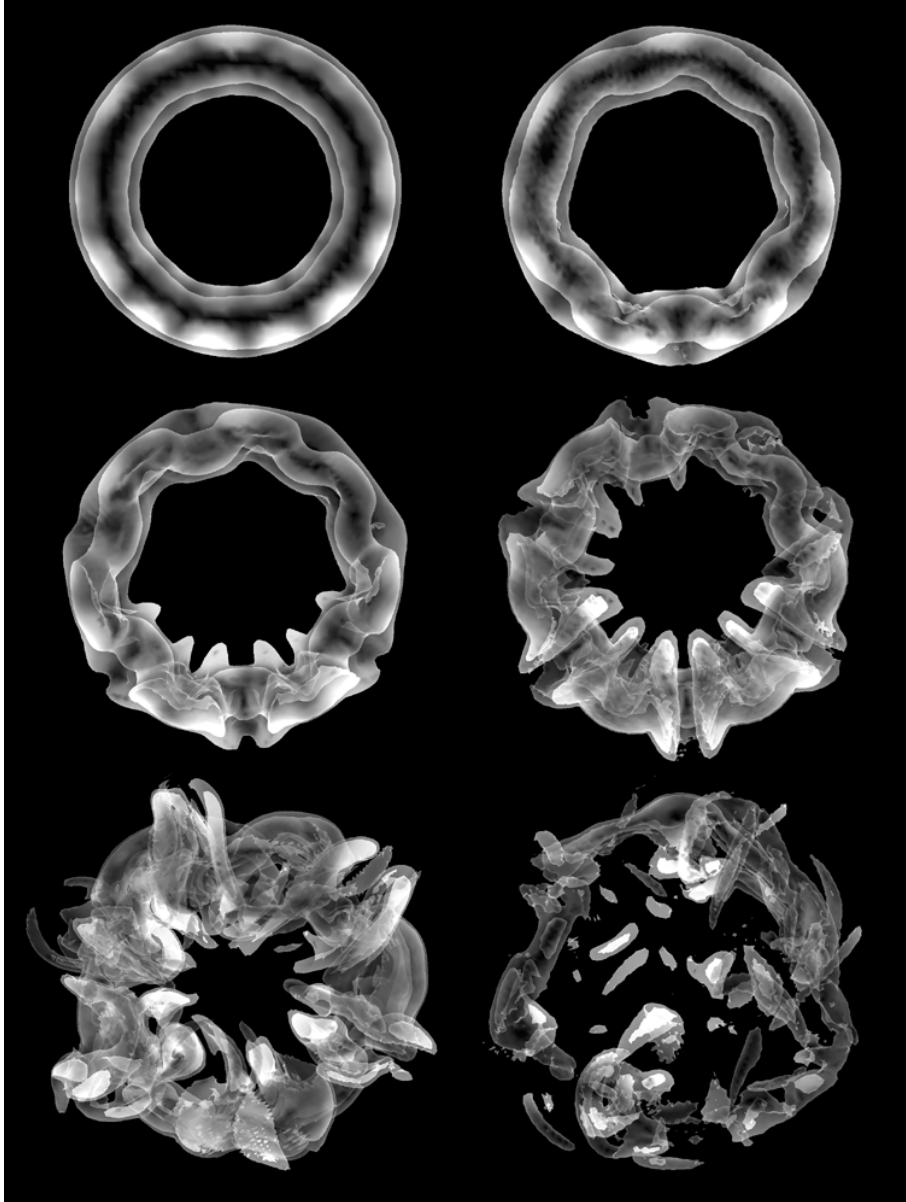


Figure 1.13: Vortex ring at $Re = 5500$: 3-D front view of the instabilities. Two isosurfaces of vorticity shown : $\|\omega\|t_0 = 1.0$ (opaque) and $\|\omega\|t_0 = 0.686$ (semi-transparent). The grey scale is proportional to ω_z . Times shown are: $\tau = 70$, $\tau = 100$, $\tau = 115$, $\tau = 130$, $\tau = 175$ and $\tau = 220$.



Figure 1.13: Vortex ring at $Re = 5500$: 3-D side view of the instabilities. The same isosurfaces of vorticity are shown.

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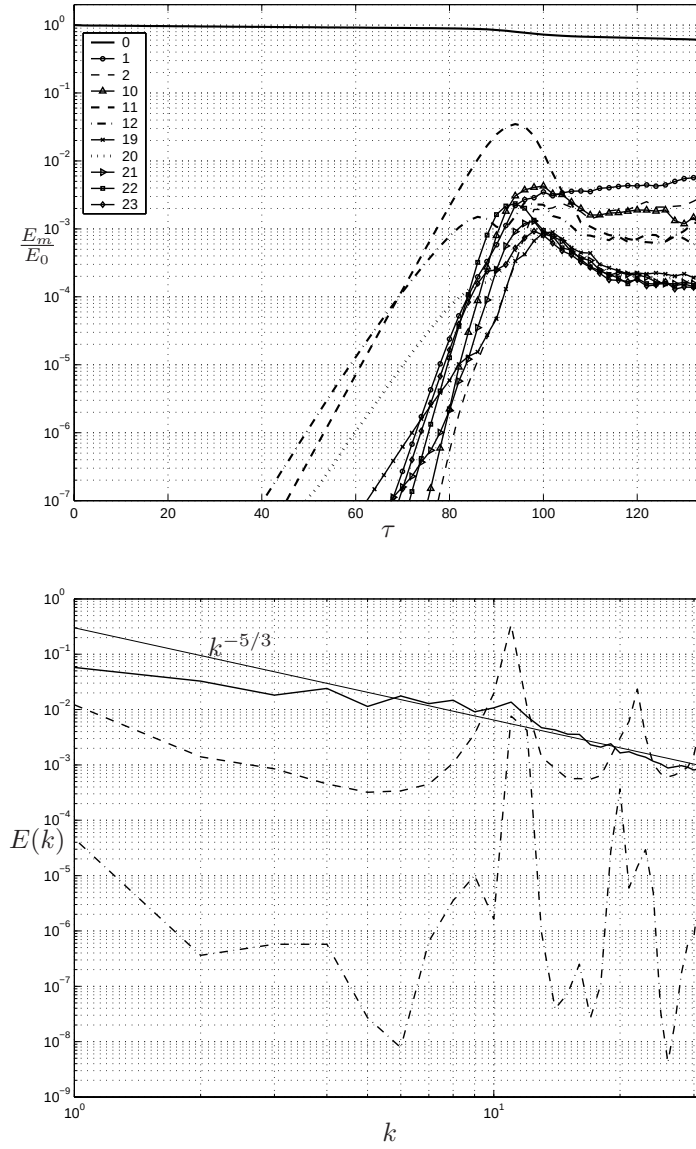


Figure 1.14: Thin vortex ring at $Re = 25000$. Top: evolution of the modal energies, for modes in the range 0 to 23. Bottom: energy spectrum at $\tau = 76$ (dash-dotted), $\tau = 92$ (dashed) and $\tau = 134$ (solid).

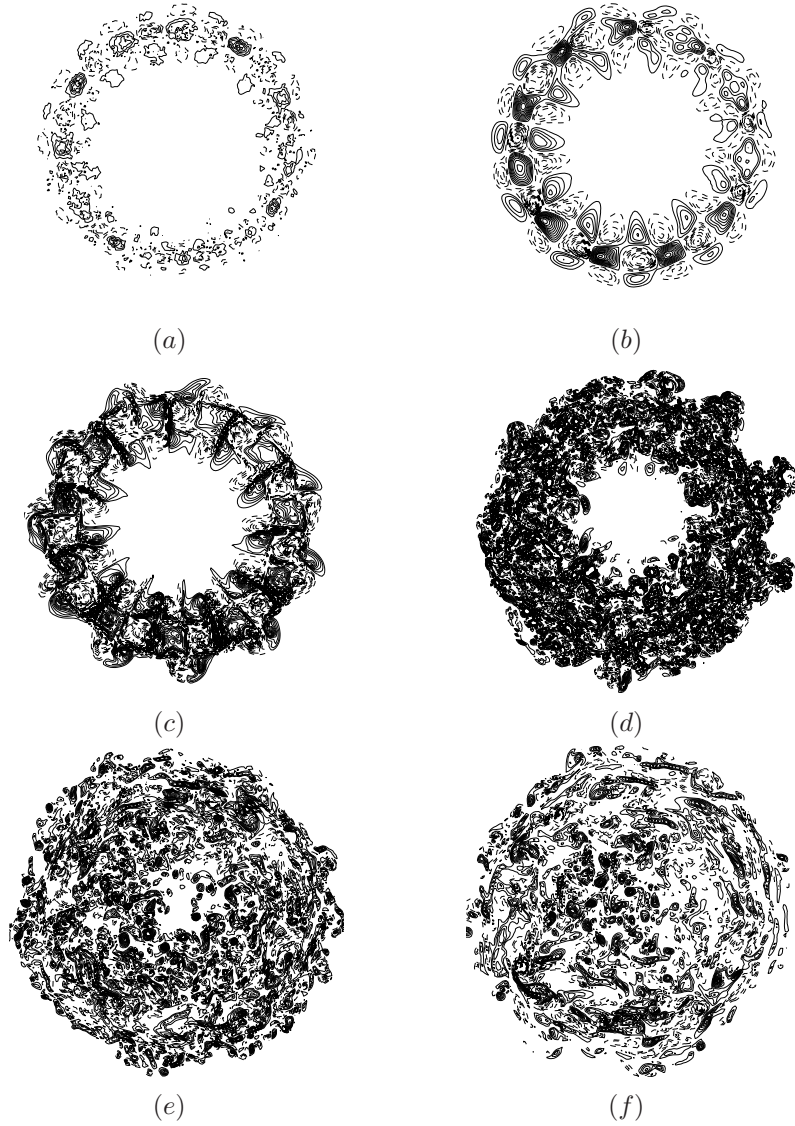


Figure 1.15: Thin vortex ring at $Re = 25000$: isocontours of $\omega_z t_0$ in the plane of maximum $\|\omega\|$. Dashed and dotted lines represent positive and negative values, respectively. Levels are first by step of 0.02: (a) $\tau = 50$ (linear stage), levels are then by step of 0.16, (b) $\tau = 76$ (beginning of the non-linear stage). Levels are finally by step of 0.64: (c) $\tau = 92$ (saturation), (d) $\tau = 102$ (decay phase), (e) $\tau = 112$ and (f) $\tau = 134$ (turbulent and decay phase).

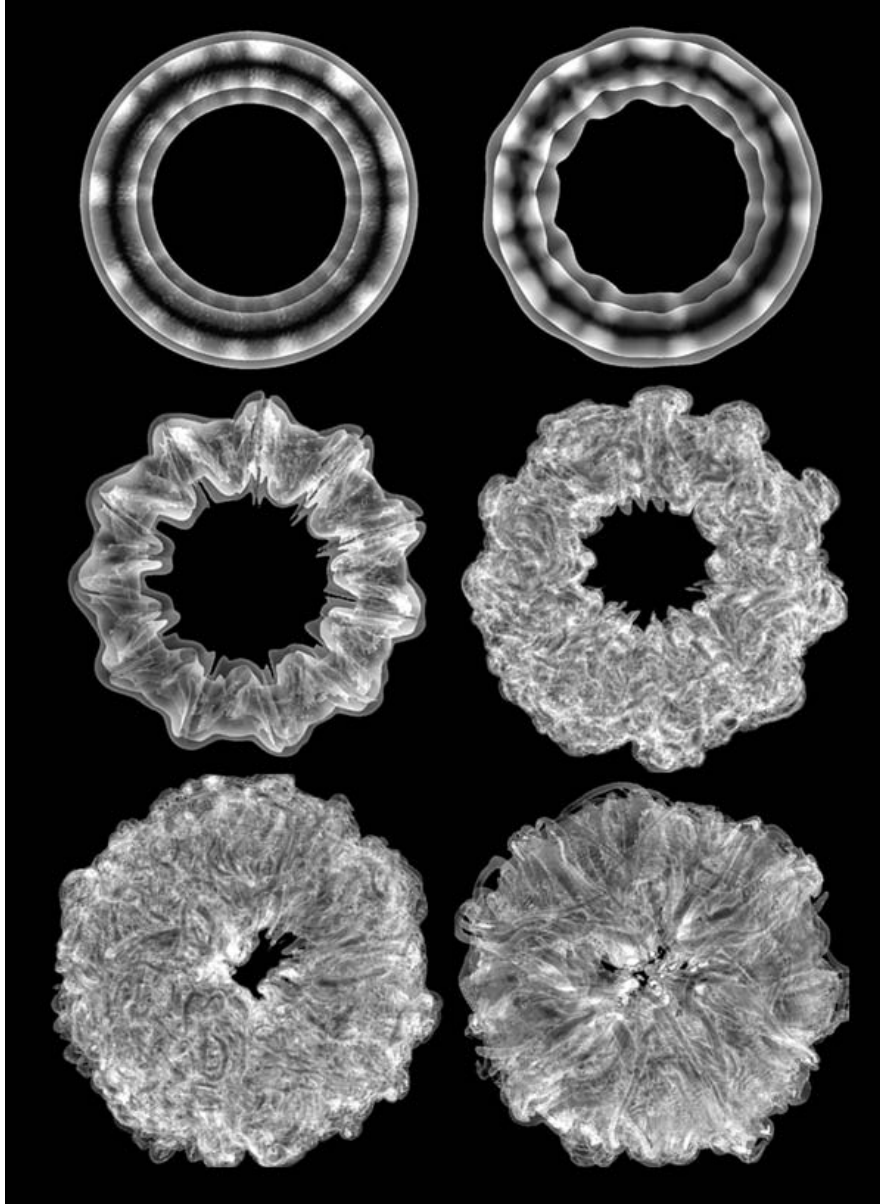


Figure 1.16: Thin vortex ring at $Re = 25000$: 3-D front view of the instabilities. Two isosurfaces of vorticity shown : $\|\omega\|t_0 = 3.0$ (opaque) and $\|\omega\|t_0 = 1.0$ (semi-transparent). The grey scale is proportional to ω_z . Times shown are: $\tau = 50$, $\tau = 76$, $\tau = 92$, $\tau = 102$, $\tau = 112$ and $\tau = 134$.

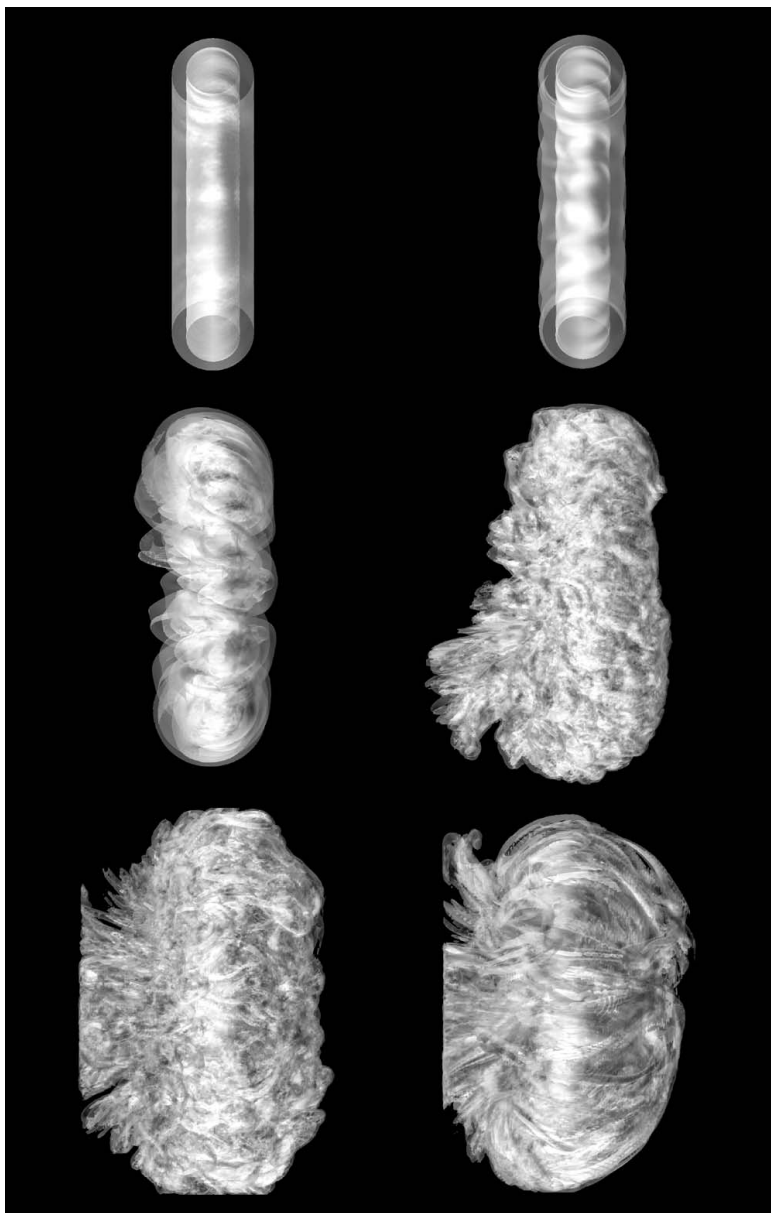


Figure 1.16: Thin vortex ring at $Re = 25000$: 3-D side view of the instabilities. The same isosurfaces of vorticity are shown.

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The simulation was carried out for 13500 time steps and took 250 hours on 9 Opteron at 2.6 GHz. The number of vortex particles grew from 5.5 million to 10 million, and the number of grid points grew from 12 million to 24 million. We see in such case the interest to use a compact grid: the same simulation using the VIC method with periodic boundary conditions and using a grid size corresponding to Case 3 of Fig. 1.8, would lead to more than 240 million grid points and still would not represent well an unbounded flow. Another interesting comparison can be made with the vortex ring simulation done by M. Bergdorf, P. Koumoutsakos and A. Leonard (private communication, submitted 2007) using the VIC method with periodic boundary conditions and $h/R = 0.014$: the grid was $L/D = 2.8$ and $H/D = 11.2$ (as $H = 4L$, it indeed better represents an unbounded flow) and it required $400 \times 400 \times 1600 = 256$ million grid points.

Fig. 1.14 shows the evolution of the modal energies E_n . The same behavior as for the first case is observed. The most amplified mode during the linear phase is here the mode 11. We can compare this result with the most unstable mode expected using Saffman's theory:

$$n(t) = \frac{2.51}{1.12091 s(t)/R} \quad \text{with} \quad s^2(t) = \sigma_0^2 + 4\nu t . \quad (1.27)$$

For $t \in [0; 40]$ (i.e. during the linear phase), $n(t) \in [10.4; 11.2]$ which is exactly the most unstable mode obtained numerically. Fig. 1.14 illustrates the energy spectrum at three times. We here also see the most unstable mode $n = 11$ and the next most non-linearly amplified mode, its first harmonic $n = 22$. We observe that, for the last time, the spectra has a fair $k^{-5/3}$ behavior, arguing that we tend to a fully turbulent decaying flow.

Fig. 1.15 shows isocontours of $\omega_z t_0$ in the plane of maximum $\|\omega\|$ during the linear stage ($\tau = 50$), the early non-linear stage ($\tau = 76$), at the saturation ($\tau = 92$), during the decay phase ($\tau = 102$) and when the flow becomes fully turbulent ($\tau = 112$ and $\tau = 134$). Fig. 1.16 provides the front and side three-dimensional views of the vortex ring evolution, shown at half the grid resolution. The different phases are also well observed.

1.4.2 Two vortex system in ground effect

As an illustration of periodic and half-unbounded flows, we present a DNS of a two vortex system in ground effect at moderate Reynolds number. The thorough understanding of aircraft wake dynamic is largely studied in several research programs, especially in order to reduce the separation standards while maintaining or

increasing the safety level during landing and take-off phases. The far wake of an aircraft is mainly constituted of two counter-rotating vortices (of circulation Γ_0 and separated by b_0). This event can be hazardous, especially near the ground. A follower aircraft entering such wake could experience a strong rolling moment. Harvey and Perry [30] performed first experimental tests of a wing in ground effect where they observed the well-known rebound of the vortices due to the separation of the boundary layer created on the no-slip wall. Later, Barker and Crow [5] also observed experimentally the rebound phenomenon. Several numerical studies, in 2-D, were also performed by Peace and Riley [58], confirmed analytically by Saffman [65] and Orlandi [54]. Luton and Ragab [48] showed, using 3-D numerical simulations at low Reynolds number, that the interaction between a two vortex system and a viscous ground leads to a complex three-dimensional flow due to the appearance of short-wavelength instabilities (i.e. Widnall instabilities) on the secondary vortices. Here, we performed a similar simulation but at a higher (yet still moderate) Reynolds number, to obtain a stronger interaction between the secondary and primary vortices compared with [48].

The problem is taken periodic in x and of large extent $L_x = 4b_0$. Initially, the vortices are algebraic vortices:

$$\omega_x(r) = \frac{\Gamma_0}{\pi} \frac{\sigma^2}{(r^2 + \sigma^2)^2} \quad (1.28)$$

with Γ_0 the total circulation and with a small core size $\sigma/b_0 = 0.05$. The dimensionless time is defined as $\tau = t/t_0$ with $t_0 = b_0/V_0$ (based on the descent velocity of a vortex pair away from the ground: $V_0 = \Gamma_0/(2\pi b_0)$). They are separated by a distance b_0 and are placed at height $h_0 = b_0$. The discretization is $h/L_x = 1/256$. The simulation is a DNS at $Re = \Gamma_0/\nu = 5000$, still low enough to avoid the use of a SGS model. The run was performed on 16 Opteron 2.6 GHz, 8 in the periodic direction and 2 in the spanwise direction.

Fig. 1.17 shows a view of the solution at different times. One sees that secondary vortices emanate from the ground because of the detachment of the boundary layer and are responsible for the rebound of the main vortices. During their orbital movement, short-wave (elliptic) instabilities develop on these secondary vortices. The non-linear interactions of these unstable modes and their saturation lead to a strong interaction with the main vortices, then to a complex 3-D flow and eventually, to the turbulent decay of the main vortices. Fig. 1.18 shows, at the same times, the space averaged vorticity for the right half plane. We observe more precisely the detachment of the boundary layer, the resulting orbital movement



Figure 1.17: Two vortex system in ground effect at $Re = 5000$: two isosurfaces of vorticity are shown (for one periodicity length): $\|\omega\|b_0^2/\Gamma_0 = 10.0$ (opaque) and 1.0 (semi-transparent). The grey scale is proportional to ω_x . Times shown are: $\tau = 0.08$; $\tau = 1.6$ (secondary vortices emanate from the ground); $\tau = 2.9$ (short-wave instabilities visible on the secondary vortices); $\tau = 3.5$ and $\tau = 4.2$ (strong interactions between the vortices); $\tau = 6.1$ ("turbulent" and decay phase).

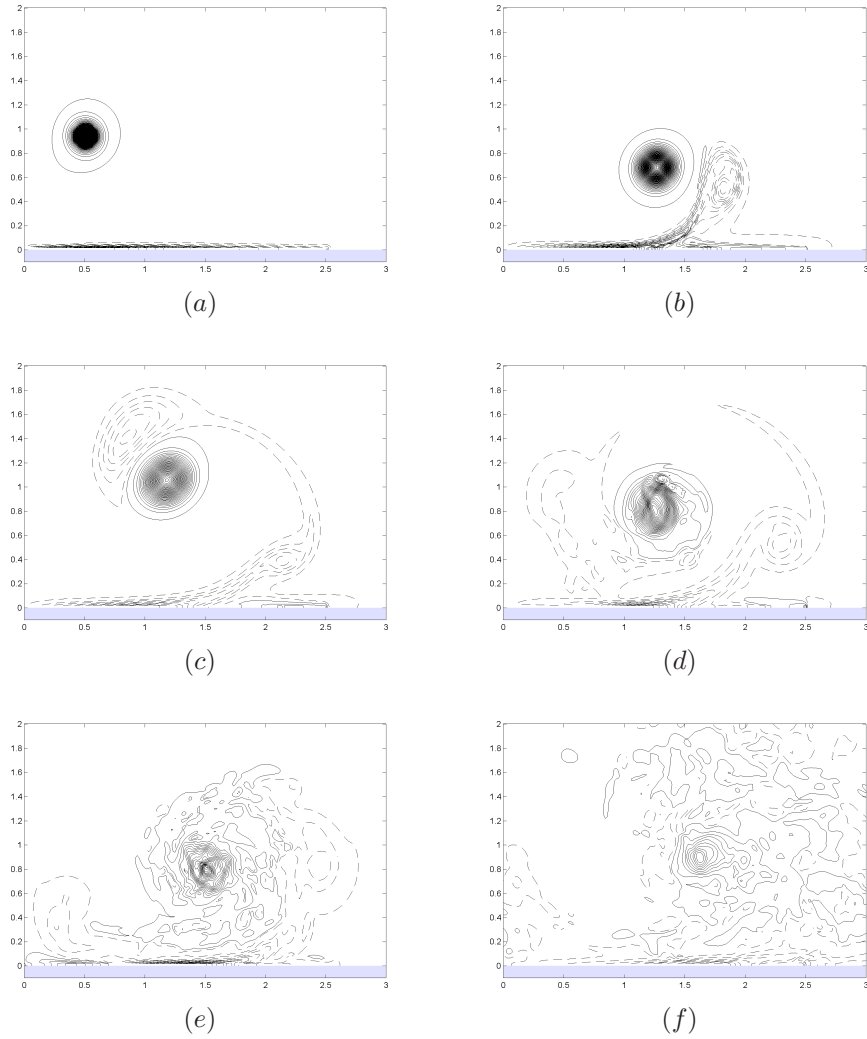


Figure 1.18: Two vortex system in ground effect at $Re = 5000$: isocontours of longitudinally averaged vorticity $\omega_x t_0$ for the right half plane. Dashed and dotted lines represent positive and negative values, respectively. Levels are by step of 0.8π . The figures are shown at the same times as in Fig. 1.17.

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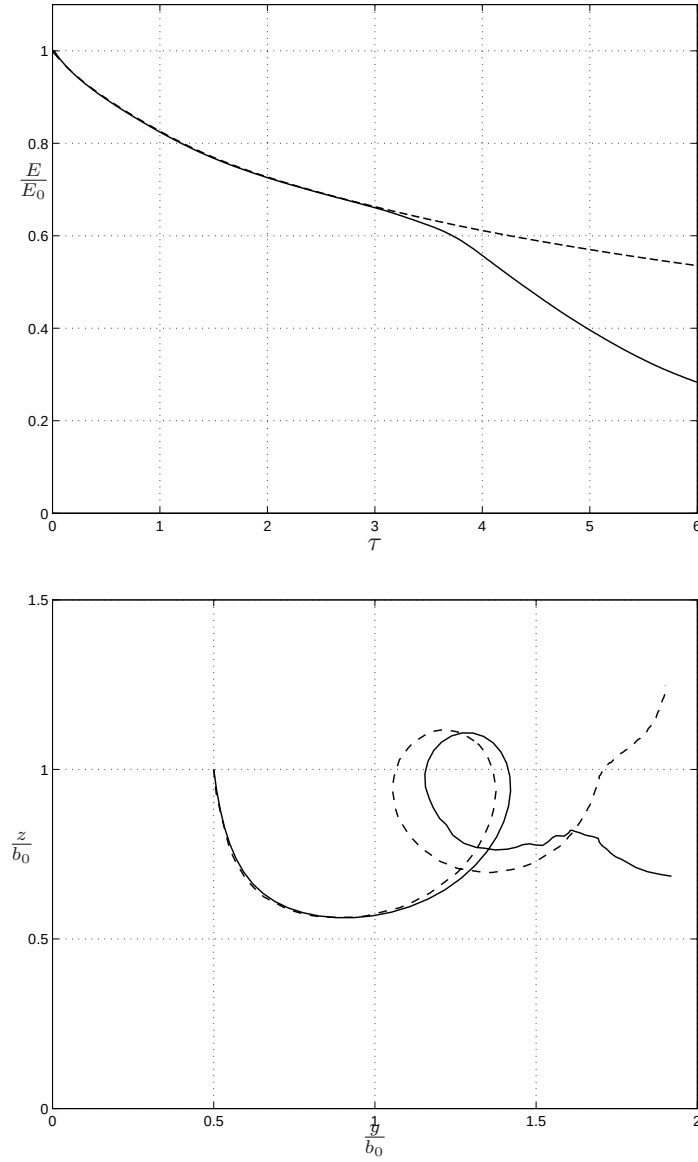


Figure 1.19: Two vortex system in ground effect at $Re = 5000$. Top: total energy evolution using the VIC-PFM method (solid) and using a 2-D FD method with spanwise periodicity (dashed). Bottom: trajectory of the primary vortex.

and, eventually, the turbulent vortex system.

We also compare our results to the solution obtained using a 2-D finite differences (FD) method that is energy conserving: it is thus a good reference to further validate our results. In this code, the computational box is also periodic in the spanwise direction: the box size was thus taken large "enough" ($L_y = 8b_0$) to mitigate the effect of the periodic images. The domain in the wall normal direction is taken as $L_z = 3b_0$ and a slip condition is used on top. The discretization is $h/b_0 = 0.004$ (thus $N_y = 2000$ and $N_z = 750$).

Fig. 1.19 shows the energy evolution. The curves compare quite well before the saturation of the secondary vortex instability (i.e., before the flow becomes 3-D). Fig. 1.19 also compares the trajectories of the center of the main vortices (defined as the maximum of the averaged axial vorticity in the 3-D case, and as the maximum vorticity in the 2-D case). Even during the essentially 2-D phase, a difference is observed, due to the artificial confinement effects in the FD code: it leads to a slightly different displacement of the vortices (i.e., a different "rebound"). We see again the usefulness of an open domain simulation performed by the VIC-PFM combination.

1.4.3 Space-developing wake behind an elliptically loaded wing in ground effect

The last illustration of application is the case of a space-developing (SD) wake generated by an elliptically loaded wing in ground effect at a moderate (yet significant) Reynolds number ($\Gamma_0/\nu = 10000$), and using LES. One important feature, that is not present in the previous time-developing (TD) simulations is the fact that the SD wake induces an axial velocity defect in the vortices. It therefore also exhibits an earlier and more violent transition to turbulence than the TD simulations. The SD configuration further differs from the TD case by the fact that the vortex tubes describe a spiralling motion. This feature is also suspected to trigger some kind of vortex meandering.

We consider the wake generated by an elliptically loaded wing of span b . The initial vortex sheet produced by the wing is as follows: its circulation per unit length is $\gamma(y) = -\frac{d\Gamma}{dy}(y)$ with

$$\Gamma(y) = \Gamma_0 \left(1 - \left(\frac{y}{b/2} \right)^2 \right)^{1/2}.$$

In reality, $\Gamma(y)$ is slightly modified to take into account the ground effect using

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a modified "lifting line" theory, but we do not enter into the details here. This singular vortex sheet is then regularized in order to produce a regular vorticity field. For this, we use convolution with a Gaussian:

$$\omega_\sigma(y, z) = \frac{1}{2\pi\sigma^2} \int_{-b/2}^{b/2} \exp\left(-\frac{(y-y')^2 + (z-h_0)^2}{2\sigma^2}\right) \gamma(y') dy' \quad (1.29)$$

where h_0 is the distance to the ground and σ is the regularization parameter. We here used $\sigma/b = 0.02$. The regularized vorticity field is then further discretized using particles put on multiple layers.

The height of the wing flying above the ground is $h_0/b = 0.25$. Fig. 1.20 shows a snapshot of the spatially developing flow when established. The effective computational domain extends between the inflow and outflow planes. The flight velocity, U_∞ , was here taken lower than that of a realistic case: U_∞/V_0 is about 4 times lower than it should (where $V_0 = \Gamma_0/(2\pi b_0)$ and $b_0 = (\pi/4)b$). That choice limits the computational requirements in the longitudinal direction. A more realistic case would require a four times longer domain. The SD simulation presented here is thus to be taken as a "proof of concept" of what the VIC-PFM method can do. The resolution used is $h/b = 0.01$. The time step was $\Delta t/t_0 = 5 \cdot 10^{-4}$, with $t_0 = b_0/V_0$. The number of particles reached about 14 million and the size of the grid was $L_x/b = 12.5$, $L_y/b = 4$ and $L_z/b = 1.1$ (thus $N_x = 1250$, $N_y = 400$ and $N_z = 110$ for a total of 55 million grid points).

Compared to TD simulations, the computation has here to be carried on for a sufficiently long time for the flow to reach its regime state (i.e., its statistical equilibrium). Indeed, the flow being initialized using a spatially uniform wake, at least a complete flow through time, $t = L_x/U_\infty$, is required to "evacuate" this initial condition. A visualization of the space developing simulation showed that the flow had reached a well established regime after about 1.6 flow through times. Once this regime state was attained, the flow was computed further, to attain statistical convergence of the time averaged fields of interest at different x/b stations (not shown). The complete simulation ran 10^4 time steps.

We see, in Fig. 1.20, the global spiraling motion of the wake vortices. The secondary vortex interacts with the primary vortex before having performed a complete revolution around it. The interaction is initiated by a medium wave instability that propagates on the secondary vortex. There is also some kind of vortex "meandering" of the secondary vortex, seen when examining time sequences (not shown here). Fig. 1.21 provides zooms of the flow in the mid wake and in the far wake: this also illustrates the good resolution quality of this simulation. It shows how the sec-



Figure 1.20: 3-D Space developing LES of wake vortices behind an elliptically loaded wing in ground effect: isosurfaces of vorticity norm, $||\omega|| t_0 = 80$ (opaque) and 25 (semi-transparent), colored by the longitudinal component of vorticity, when the flow has reached it's regime. Top and side views.

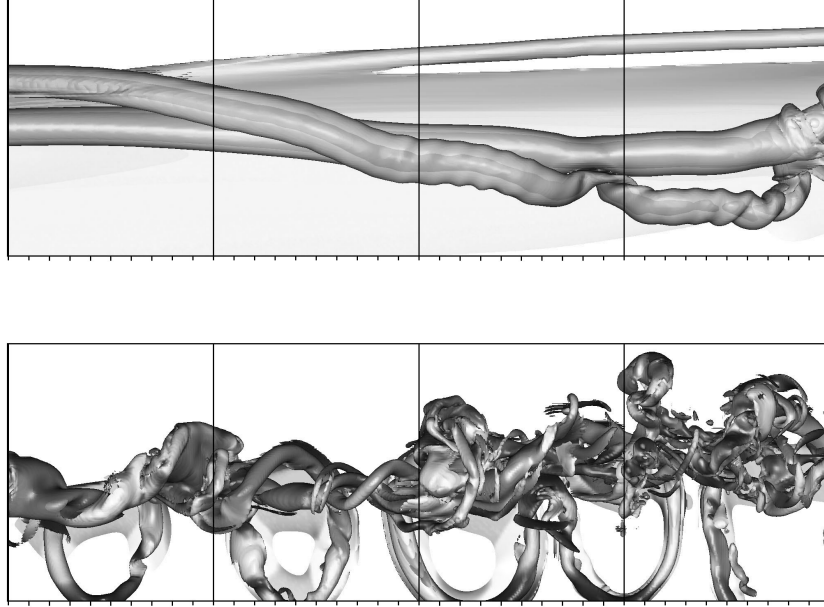


Figure 1.21: 3-D Space developing LES: top view, here shown at full resolution, of the regions $x/b = [4, 8]$ and $[8, 12]$ at an arbitrary time once in regime.

ondary vortex partially reconnects with the primary one through a complex spiraling motion. Due to this interaction, the primary vortex appears to “burst” into two or even three helical vortices which then further “break down” into small-scales. This simulation, and its detailed analysis (not shown), is part of the European project FAR-Wake.

1.5 Conclusions

We have presented a new approach, the VIC-PFM method, that efficiently combines a vortex-in-cell (VIC) method and a parallel fast multipole (PFM) method. It allows to efficiently simulate unbounded or half-unbounded flows, by using the advantages of each method: the efficiency of grid Poisson solvers used in VIC methods, and the implicit unbounded domain condition of PFM methods. As the open-domain boundary conditions are obtained correctly using the PFM method,

it avoids any iterative method and it permits to use a computational domain (i.e., the VIC grid) as compact as the vorticity field, leading to much smaller memory requirements.

For large problems, the method was further parallelized. The grid is then split into several subdomains, each subgrid being allotted to one processor. The continuity between the subdomains is ensured by the PFM method, that always has a global view of the entire vorticity field.

The VIC-PFM is able to simulate complex flows, also turbulent flows using Large-Eddy Simulation (LES) approaches. Different SGS models were also implemented. An efficient relaxation scheme was also implemented (following Cottet and Poncet [19]): it enforces that the vorticity field remains divergence free at all times, which significantly enhances the accuracy and robustness of the method.

Various applications were presented and some compared with other methods and/or existing results. The VIC-PFM method shows its efficiency and its ability to simulate complex and turbulent unbounded flows, as shown by the simulation of a thin vortex ring at high Reynolds number. The VIC-PFM method was also implemented with one periodic direction and was here illustrated on the simulation of a two vortex system in ground effect. A space-developing simulation was also presented, for the longitudinal development, in ground effect, of the vortex wake emitted by an elliptically loaded wing.

1.6 Acknowledgements

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Chapter 2

Multiscale subgrid models for LES of instabilities and turbulence in wake vortex systems

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Abstract

This paper investigates the capabilities of different subgrid scale (SGS) models, including the recent "multiscale" models, for large-eddy simulation (LES), here in a vortex-in-cell (VIC) method, of complex wake vortex dynamics. More specifically, we here consider the multiscale dynamics developing in a counter-rotating four vortex system, that evolves from a simple state to a turbulent state. The various SGS models are tested and compared on this complex and transitional flow. Compar-

isons are also made with results obtained using a pseudo-spectral method. Energy diagnostics (global and modal) and spectra are provided and used to support the comparisons. A discussion on the applicability of the various models to LES of complex wake vortex flows is made. The multiscale models are seen to be the most appropriate.

2.1 Introduction

The present investigation is concerned with LES of complex and transitional flows at very high Reynolds number, in aircraft wake vortex systems and involving multiscale instabilities. The flow problem considered here provides potential for rapid changes in flow topology as well as for the generation of small scale structures and turbulence, through the strong interaction between counter-rotating vortices. To simulate such high Reynolds number flows, one needs LES models that are inactive during the initial, well-resolved, phase of the dynamics, and become active only when the strong interactions between the vortices create small scales.

We here consider the dynamics of a longitudinally periodic counter-rotating four vortex system and we investigate different SGS models. More specifically, two types of SGS effective viscosity models are investigated: 1) models acting on the complete LES field, $\tau_{ij} = 2\nu_{\text{sgs}} S_{ij}$: the Smagorinsky (SMAG) model, the "small-complete" Filtered Structure Function (FSF) model, the "small-complete" version of the Smagorinsky model (SMAG2) and the Wall-Adapting Local Eddy-viscosity (WALE) model; 2) models acting on a small-scale LES field, $\tau_{ij} = 2\nu_{\text{sgs}} S_{ij}^s$: the "complete-small" Regularized Variational Multiscale (RVM) model, the "small-small" Regularized Variational Multiscale (RVM2) model and the "small-small" Filtered Structure Function (FSF2) model.

The notation "small/complete - small/complete" means that ν_{sgs} is computed from the small-scale or the complete LES field, and that the diffusion operator acts on the small-scale or the complete LES field. A simulation is also carried out using a low order hyper-viscosity (HV) SGS model, thus also pushing the SGS dissipation towards the smallest scales. Comparisons are also made with results obtained using a Fourier-based pseudo-spectral method (see Appendix D) with a high order k^8 hyper-viscosity SGS model.

The numerical method and the SGS models are first presented briefly. The definition of the flow problem is presented next, together with some definitions for the energy diagnostics. We then show results on the global evolution of the vortex

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system, followed by the more formal comparison between the different models. A discussion on the applicability of the different models to complex wake vortex flows, transitional and turbulent, concludes the paper.

2.2 Numerical method

We here consider LES of incompressible vortex flows, using an effective SGS viscosity ν_{sgs} and in the vorticity-velocity formulation of the Navier-Stokes equations. Depending if the LES model acts on the complete LES field or on the small-scale LES field, the equations are respectively:

$$\frac{D\boldsymbol{\omega}}{Dt} = \nabla \cdot (\mathbf{u}\boldsymbol{\omega}) + \nu \nabla^2 \boldsymbol{\omega} + \nabla \cdot (\nu_{\text{sgs}} (\nabla \boldsymbol{\omega} + (\nabla \boldsymbol{\omega})^T)) , \quad (2.1)$$

$$\frac{D\boldsymbol{\omega}}{Dt} = \nabla \cdot (\mathbf{u}\boldsymbol{\omega}) + \nu \nabla^2 \boldsymbol{\omega} + \nabla \cdot (\nu_{\text{sgs}} (\nabla \boldsymbol{\omega}^s + (\nabla \boldsymbol{\omega}^s)^T)) , \quad (2.2)$$

in which $\boldsymbol{\omega} = \nabla \times \mathbf{u}$. As the problems of interest are at very high Reynolds number and in unbounded domain, we here furthermore restrict ourselves to LES where the molecular viscosity ν is set to zero. The numerical solution of (2.1) or (2.2) is obtained following the vortex-in-cell (VIC) approach, see [16, 19, 82]. The vorticity field is constructed from a sum of regularized vortex particles:

$$\boldsymbol{\omega}_\sigma(\mathbf{x}, t) = \sum_p \alpha_p(t) \frac{1}{(\sqrt{\pi} \sigma)^3} \exp\left(-\frac{|\mathbf{x} - \mathbf{x}_p(t)|^2}{\sigma^2}\right) ,$$

with $\alpha_p = \int \boldsymbol{\omega} d\mathbf{x} = \boldsymbol{\omega}_p h^3$ the strength of particle p , $\mathbf{x}_p$ its position, h the discretization size (grid size, also used for particle redistribution), and σ the regularization parameter. Interpolations between particles and grid, as well as particle redistribution, are all done using the M'_4 scheme. The vector streamfunction $\boldsymbol{\psi}$ is obtained by solving the Poisson equation $\nabla^2 \boldsymbol{\psi} = -\boldsymbol{\omega}$ on the grid, using 2nd order finite differences (FD). The velocity field (needed for convection and stretching) is then obtained from $\mathbf{u} = \nabla \times \boldsymbol{\psi}$, also using FD. The convective part (i.e., the lhs of (2.1) or (2.2)) is done using the Lagrangian approach: $D\mathbf{x}_p/Dt = \mathbf{u}(\mathbf{x}_p)$; this ensures good convection (i.e., negligible dispersion errors). The time variation of the particle strengths (i.e., the rhs of (2.1) or (2.2) including both the vorticity stretching and the dissipation terms) is evaluated on the grid using FD. The global time marching procedure is carried out using the Leap Frog scheme for the convection and the Adams-Bashford scheme for the diffusion. Finally, the intrinsic divergence-free character of the vorticity field is maintained by a proper projection of the discrete vorticity field (which also requires solving a Poisson equation).

Particular to our VIC implementation is the treatment of the boundary conditions on the grid, required for solving the Poisson equation. The boundary conditions for ψ are here obtained using the Green's function approach, via a Parallel Fast Multipole (PFM) method [12, 79, 82]. The unbounded domain condition can then be ensured accurately while using a small grid: a grid only as large as the vorticity field itself. This allows for very significant reduction of the computational cost. Furthermore, the method can be parallelized, using the domain decomposition method: the PFM code, which has a global view of the whole field, is used to obtain the proper boundary conditions on each subdomain [79, 82]. Such VIC-PFM combination amounts to a very efficient parallelized Poisson solver: one without iteration between the subdomains.

2.2.1 SGS models investigated

Concerning the LES modelling, we investigated two approaches: ν_{sgs} computed using the complete LES field or using the small-scale LES field. When (2.1) is used, we refer to the first approach as "complete-complete" and to the second as "small-complete". Equivalently, when (2.2) is used, the notation used is: "complete-small" for the first approach and "small-small" for the second. For all models, the LES cut-off length Δ is taken equal to the grid size h (here uniform).

We begin with the models used in (2.1). The Smagorinsky (SMAG) model is the most common "complete-complete" model:

$$\nu_{\text{sgs}} = C_S \Delta^2 (2 S_{ij} S_{ij})^{1/2}, \quad (2.3)$$

where S_{ij} is the strain rate tensor: $S_{ij} = \frac{1}{2}(g_{ij} + g_{ji})$ with $g_{ij} = \partial u_i / \partial x_j$. The coefficient C_S was set to its theoretical value in isotropic turbulence at high Reynolds number: $C_S = (0.3)^3 = 0.027$.

We also recall that, for flow with homogeneous directions (isotropic turbulence, channel flow), the coefficient can also be obtained dynamically, using the "dynamic procedure" [27, 28]: this is then the "dynamic" version of the Smagorinsky model. In fact, any model can be made dynamic (e.g., a dynamic mixed model as in [81]). Notice that the dynamic procedure does not change the spectral behavior of the Smagorinsky model: it remains a "complete-complete" model. Moreover, unless one uses ad hoc "clipping", the dynamic procedure is not usable for flows without homogeneous directions, such as the flows investigated here. Thus, the present paper investigates SGS models from the point of view of their spectral behavior; recognizing that any model can be made dynamic.

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A second model considered here is the FSF model [23] (a "small-complete" model). Here, the subgrid viscosity is related to the "filtered structure function" $F_2^{s(n)}$:

$$\nu_{\text{sgs}} = C_F^{(n)} \Delta \sqrt{F_2^{s(n)}}, \quad (2.4)$$

where

$$F_2^{s(n)} = \left\langle \|\mathbf{u}^{s(n)}(\mathbf{x} + \mathbf{x}') - \mathbf{u}^{s(n)}(\mathbf{x})\|^2 \right\rangle_{|\mathbf{x}'| = \Delta}. \quad (2.5)$$

Numerically, this is evaluated using the nearest neighbors ($3^3 = 27$) values. The small-scale field $\mathbf{u}^{s(n)}$ is here obtained as in [23] (also for the FSF2 model below) by application (n times) of the 2nd order FD Laplacian:

$$\mathbf{u}^{s(n)} = \left(-\frac{\Delta^2}{4} \nabla^2 \right)^n \mathbf{u}. \quad (2.6)$$

The present results were obtained using the coefficients $C_F^{(n)}$ as proposed in [23], see Table 2.1. The model has already been shown to capture well the transition to turbulent flow that results from the growth of instabilities in wake vortex simulations [42].

A third model is the SMAG2 model (also a "small-complete" model):

$$\nu_{\text{sgs}} = C_{S_2}^{(n)} \Delta^2 (2 S_{ij}^s S_{ij}^s)^{1/2}, \quad (2.7)$$

where S_{ij}^s is the strain rate tensor of the small-scale field. The small-scale field is here obtained (and also for all models presented after, except FSF2) using the compact (stencil 3) tensor-product discrete filter, and that is iterated n times to produce a order $2n$ filter [35, 80]:

$$\begin{aligned} \mathbf{u}^{s(n)} &= \mathbf{u} - \bar{\mathbf{u}}^{(n)} \\ \bar{\mathbf{u}}^{(n)} &= \left[\left(I - (-\delta_x^2/4)^n \right) \left(I - (-\delta_y^2/4)^n \right) \left(I - (-\delta_z^2/4)^n \right) \right] \mathbf{u} \end{aligned} \quad (2.8)$$

where $\delta_x^2 f_{i,j,k} = f_{i+1,j,k} - 2f_{i,j,k} + f_{i-1,j,k}$, etc. In Fourier space, the filtered field is

$$\begin{aligned} \bar{\mathbf{u}}^{(n)}(\mathbf{k}) &= G^{(n)}(k_x h_x) G^{(n)}(k_y h_y) G^{(n)}(k_z h_z) \mathbf{u}(\mathbf{k}) \\ &= (1 - \sin^{2n}(k_x h_x/2)) (1 - \sin^{2n}(k_y h_y/2)) \\ &\quad (1 - \sin^{2n}(k_z h_z/2)) \mathbf{u}(\mathbf{k}). \end{aligned} \quad (2.9)$$

The model was used with the coefficients given in Table 2.1. The coefficient $C_{S_2}^{(1)}$ was fixed using, as for the RVM models (see the explanation below), the same ratio

between the SGS viscosity computed with a small-scale field and with a complete field: $1.88/1.60 = 1.18$ which gives $C_{S_2}^{(1)} = 1.18 C_S$. The coefficients for $n > 1$ are computed so that each operator $G^{(n)}$ has the same value as $G^{(1)}$ at the medium wavenumber¹, $k = k_c/2 = \pi/(2h)$: $1 - \sin^{2n}(\alpha^{(n)}\pi/4) = G^{(n)}(\alpha^{(n)}\pi/2) = G^{(1)}(\pi/2) = 1 - \sin^2(\pi/4) = 1/2$. One obtains $\alpha^{(2)} = 1.27$ and $\alpha^{(3)} = 1.40$.

A last model is the WALE model [53]:

$$\nu_{\text{sgs}} = C_W \Delta^2 \frac{(\mathcal{S}_{ij}^d \mathcal{S}_{ij}^d)^{3/2}}{(\mathcal{S}_{ij} \mathcal{S}_{ij})^{5/2} + (\mathcal{S}_{ij}^d \mathcal{S}_{ij}^d)^{5/4}}, \quad (2.10)$$

where $\mathcal{S}_{ij}^d$ is the traceless part of the square of the velocity gradient tensor:

$$\mathcal{S}_{ij} = \frac{1}{2} (g_{ik} g_{kj} + g_{jk} g_{ki}) = S_{ik} S_{kj} + \Omega_{ik} \Omega_{kj}, \quad \mathcal{S}_{ij}^d = \mathcal{S}_{ij} - \frac{1}{3} S_{kk} \delta_{ij}, \quad (2.11)$$

where $\Omega_{ij} = \frac{1}{2} (g_{ij} - g_{ji})$ is the rotation rate tensor. The coefficient C_W was set from isotropic turbulence to $C_W = (0.5)^2 = 0.25$. The term $\mathcal{S}_{ij}^d \mathcal{S}_{ij}^d$ has been shown to be a good detector of turbulence. In pure shear (e.g. next to a wall), the model gives a zero ν_{sgs} ; in turbulent channel flow, ν_{sgs} has the proper near-wall behavior. In pure rotation however, ν_{sgs} is found to be proportional to the vorticity ($\nu_{\text{sgs}} = C_W \Delta^2 (2/3)^{1/4} |\omega|/2$); it is thus maximum in the center of a vortex : a non-desirable feature in our applications, as we wish to capture the development and growth of inviscid unstable modes while preserving the vortex cores as much as possible.

We now present the models used in (2.2) where the SGS viscosity is applied on the small-scale vorticity field (ω^s), here obtained using (2.8) acting on ω . The first "complete-small" model is the "regularized" version, here using discrete filters, of the "variational multiscale" model (VM) of [31, 32]. The VM model used by Hughes *et al.* is a "large-small" model as the viscosity is computed using the large-scale LES field (i.e. using $\bar{\mathbf{u}}$). Here, it is simply the Smagorinsky model but acting on the small-scale field, it is thus a "complete-small" model. It was first proposed and tested, in isotropic turbulence, by [80] who called it the "regularized variational multiscale" (RVM) model. It was then tested by [35, 37] in channel flow

¹This choice is dictated by a simple arithmetic proportion related to the order of the filters used. When a higher order filter is used, the wavenumber corresponding to $G^{(n)} = 1/2$ is shifted to the right. The part of the small-scale field is thus reduced when n increases. The idea was here to increase the model coefficient proportionally to this shift. Another choice would be to increase it proportionally to the integral of the filter. However, the results presented in Chapter 3 will confirm that this simple choice provides a good preliminary estimation of the model coefficients when a higher order filter is used.

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and using the dynamic procedure: thus a dynamic RVM model. The RVM model was then further proposed and tested by [76] and also by [73, 74]. The theoretical (for isotropic turbulence) model coefficients $C_R^{(n)}$ are given in Table 2.1. $C_R^{(1)}$ is obtained knowing that $|S|^2 \simeq |\bar{S}|^2 + |S^s|^2$ and using the values proposed in [31], with sharp Fourier cutoff applied at the medium wavenumber. This choice is justified as the discrete $n = 1$ filter is symmetrical with respect to the medium wavenumber: $G^{(1)}(\pi/2) = 1/2$. From the "large-small" and "small-small" models coefficients used by Hughes *et al.* ($2.62 C_S$ and $1.64 C_S$ respectively), we can deduce that $|S^s|/|\bar{S}| \simeq 2.62/1.64 = 1.60$. It leads, using the previous relation, to $|S|/|\bar{S}| \simeq 1.88$ and thus $|S|/|S^s| \simeq 1.88/1.60 = 1.18$. Finally, this gives $C_R^{(1)} \simeq (2.62/1.88) C_S = 1.39 C_S$.

The second model is the regularized version (RVM2) of the "small-small" variational multiscale (VM2) model of [31, 32]. It was proposed and evaluated by [76] and [73, 74]:

$$\nu_{\text{sgs}} = C_R^{(n)} \Delta^2 (2 S_{ij}^s S_{ij}^s)^{1/2}. \quad (2.12)$$

The coefficients $C_{R_2}^{(n)}$ are given in Table 2.1 and are computed from the $C_{R_2}^{(1)}$ given in [31]. The VM and RVM models (also their VM2 and RVM2 counterparts) have been tested, with good success, on homogenous isotropic turbulence and on channel flow. Here, we want to test their ability to simulate complex (transitional and turbulent) vortex flows.

The last "small-small" model considered is the FSF2 model [74]:

$$\nu_{\text{sgs}} = C_{F_2}^{(n)} \Delta \sqrt{F_2^{s(n)}}, \quad (2.13)$$

where the coefficients $C_{F_2}^{(n)}$ are given in Table 2.1. The coefficient $C_{F_2}^{(1)}$ was determined from $C_F^{(1)}$, using the same ratio as between a SGS viscosity acting on a small-scale field (RVM) and on a complete field (SMAG): it gives $C_{F_2}^{(1)} = 1.39 C_F^{(1)}$. $C_{F_2}^{(2)}$ and $C_{F_2}^{(3)}$ are obtained, in the same way, from $C_F^{(2)}$ and $C_F^{(3)}$ respectively.

In addition to the eddy-viscosity models, we also investigated simple (uniform) hyper-viscosity models. With the VIC-PFM methodology, we used

$$\frac{D\omega}{Dt} = \nabla \cdot (\mathbf{u}\omega) - \nu_{\text{hv}} \nabla^4 \omega \quad (2.14)$$

where ∇^4 was evaluated by two applications of the FD Laplacian and where the hyper-viscosity was taken as $\nu_{\text{hv}} = C_4 \Delta^4 / T_0$ with T_0 the global time scale. With the parallel pseudo-spectral code (velocity based), used for comparisons, we used a high order k^8 hyper-viscosity model:

$$\frac{D\mathbf{u}}{Dt} = -\nabla P - \nu_{\text{hv}} \nabla^8 \mathbf{u} \quad (2.15)$$

Table 2.1: Coefficients values for the different SGS models, depending on the order of the filter used. The values in boldface are determined from theory or are taken as proposed in the literature (notice that, as previously computed, $\alpha^{(2)} = 1.27$ and $\alpha^{(3)} = 1.40$).

	C_S	C_{S_2}	C_F	C_W	C_R	C_{R_2}	C_{F_2}
$n = 0$	(0.3)³	—	—	(0.5)²	—	—	—
$n = 1$	—	$1.18 C_S$	0.080	—	$1.39 C_S$	1.64 C_S	1.39 0.080
$n = 2$	—	$\alpha^{(2)} 1.18 C_S$	0.069	—	$\alpha^{(2)} 1.39 C_S$	$\alpha^{(2)} 1.64 C_S$	$\alpha^{(2)} 1.39$ 0.069
$n = 3$	—	$\alpha^{(3)} 1.18 C_S$	0.054	—	$\alpha^{(3)} 1.39 C_S$	$\alpha^{(3)} 1.64 C_S$	$\alpha^{(3)} 1.39$ 0.054

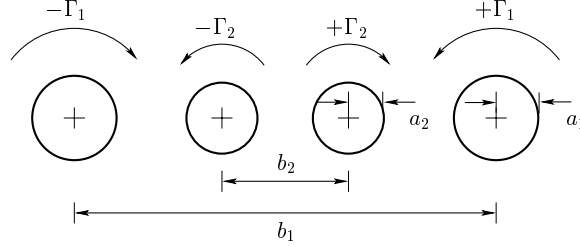


Figure 2.1: Schematic transversal view of a four vortex system in counter-rotating configuration.

with $\nu_{\text{hv}} = C_8 \Delta^8 / T_0$. The dealiasing is done using a phase shift procedure [10, 9], and the time marching is carried out using a 3rd order Runge-Kutta scheme. In a spectral method, such high order term is easily done. Even higher order terms ($\nabla^{16} \mathbf{u}$) have been used before in the simulation of turbulent flows [7, 8].

2.3 Simulation results

2.3.1 Definition of the problem

The base flow condition consists of a four vortex system with two pairs of counter-rotating vortices, see Fig. 2.1. The outer principal vortices are characterized by their circulation Γ_1 , their core size radius a_1 , and their inner spacing b_1 . The inner secondary pair is characterized by Γ_2 , a_2 and b_2 . Normalization of the dimensional quantities can be made using the natural reference scales: $b_0 = (\Gamma_1 b_1 + \Gamma_2 b_2) / \Gamma_0$ with $\Gamma_0 = \Gamma_1 + \Gamma_2$, $V_0 = \Gamma_0 / (2\pi b_0)$ and $T_0 = b_0 / V_0$. In what follows, all quantities will be written in dimensionless form (for instance, $\tau = t / T_0$).

The results were obtained considering the case where $\Gamma_2 / \Gamma_1 = -0.3$, $b_2 / b_1 = 0.3$, $a_1 / b_1 = 0.075$, and $a_2 / a_1 = 2/3$. This configuration was shown to develop rapidly growing instabilities [26, 79]. This configuration provides a challenging simulation problem with rapid change in flow topology, generation of small scale structures and, finally, turbulence. Simpler configurations, as the co-rotating vortex pair, have been studied by Crouch [20] (a simulation was also performed in [79]). The counter-rotating configuration creates more rapid instabilities, strong interactions between vortices of opposite sign and different strength, and turbulence; it constitutes a good configuration to test the ability of SGS models in LES

of complex (transitional and turbulent) vortex flows. Notice that such flow also develops short wavelength (elliptic type) instabilities (see Widnall [78]) and long wavelength (Crow type) instabilities. See also reviews by Spalart [72] and Jacquin et al. [34].

The longitudinal vorticity distribution of each vortex is here taken as:

$$\omega_x = \frac{\Gamma}{\pi} \frac{a^2}{(r^2 + a^2)^2}, \quad (2.16)$$

with $r^2 = (y - y_0)^2 + (z - z_0)^2$, r being the distance to the vortex centerline of coordinates $\{y_0, z_0\}$.

2.3.2 Longitudinal modal energy

Before presenting the comparisons between the results, we provide definitions regarding the characterization of the instabilities and the evaluation of the energy diagnostics. Taking into account the periodicity in the longitudinal direction, we write, for the velocity field,

$$\mathbf{u}(x, y, z, t) = \sum_{m=-N_x/2}^{N_x/2} \hat{\mathbf{u}}(k_x, y, z, t) e^{ik_x x} \quad \text{with} \quad k_x = m \frac{2\pi}{L_x}, \quad (2.17)$$

with N_x the number of grid points; a similar development applies to ψ and ω . The longitudinal Fourier transform of $\mathbf{u}$ is given by

$$\hat{\mathbf{u}}(k_x, y, z, t) = \frac{1}{L_x} \int_0^{L_x} \mathbf{u}(x, y, z, t) e^{-ik_x x} dx. \quad (2.18)$$

The longitudinal modal energy E_m (for a given domain length L_x , we make use of the modal index integer m instead of the wavenumber k_x) is accordingly defined by

$$E_m(t) = \frac{L_x}{2} \iint \hat{\mathbf{u}} \cdot \hat{\mathbf{u}}^* dydz = \frac{L_x}{4} \iint [\hat{\psi} \cdot \hat{\omega}^* + \hat{\omega} \cdot \hat{\psi}^*] dydz, \quad (2.19)$$

with superscript $*$ denoting the complex conjugate. Using the symmetry ($E_m = E_{-m}$), we consider only the modes with $m \geq 0$. Accordingly, the modal energy becomes

$$E_m(t) = L_x \iint \hat{\mathbf{u}} \cdot \hat{\mathbf{u}}^* dydz = \frac{L_x}{2} \iint [\hat{\psi} \cdot \hat{\omega}^* + \hat{\omega} \cdot \hat{\psi}^*] dydz. \quad (2.20)$$

The total energy is then

$$E = \sum_{m=0}^{N/2} E_m. \quad (2.21)$$

2.3.3 Global evolution

The global evolution of the four vortex system is illustrated in Fig. 2.2. The length of the domain was set to $L_x/b_0 = 8.53$ to allow for the simultaneous development of one long wavelength "Crow" type instability, in addition to the medium and short wavelength instabilities. As the secondary vortices orbit around the primary ones, the fastest growing medium wavelength instability strongly distorts the secondary vortices to form "Omega-loops", as also observed experimentally [55]. Furthermore, as the vortices come into contact, and only partially reconnect (they cannot fully reconnect as they have different circulation), a significant amount of small scale structures is being produced, eventually leading to a turbulent flow.

These results were obtained using VIC-PFM for 5800 time steps in 65 hours on 48 Xeon processors. The VIC grid grew from $720 \times 128 \times 64$ to $720 \times 310 \times 312$ points and the number of vortex particles from 3.3 to 18 millions. The low order hyper-viscosity SGS model was used (Eq. 2.14, and using $C_4 = 6.8$). This run was done so as to compare with one carried using the spectral code, and using a high order k^8 hyper-viscosity SGS model (Eq. 2.15, and using $C_8 = 3.5$). It was then later verified that the hyper-viscosity SGS models are not as performant as the multiscale models (see next section). The results presented here are thus for assessment of instability growth and global evolution.

We show, in Fig. 2.3, the evolution of the modal energies E_m of the base flow ($m = 0$) as well those for the most unstable short ($m = 77$, elliptic instability), medium ($m = 9$, Omega-loops), and long ($m = 1$, Crow instability) modes; the values have been normalized by the initial base flow energy $E_{m=0}(\tau = 0)$ (noted E_0). The values obtained using the spectral code are also shown for comparison. Assuming an exponential growth (i.e., $E_m \propto \exp(2\sigma_m\tau)$) for the early (linear) phase of the dynamics, we obtain, for both simulations, $\sigma_1 \approx 26$, $\sigma_9 \approx 15$ and $\sigma_{77} \approx 15$. Notice that both runs are not affected by the SGS model so long as there are no small scales produced: thus up to $\tau \approx 1$. The small differences in the time at which the unstable modes start to grow comes from the slightly different initial, low amplitude, random perturbation. The evolution of both the total and the base flow energies is shown in Fig. 2.4. The agreement between the energy evolutions is seen as quite good.

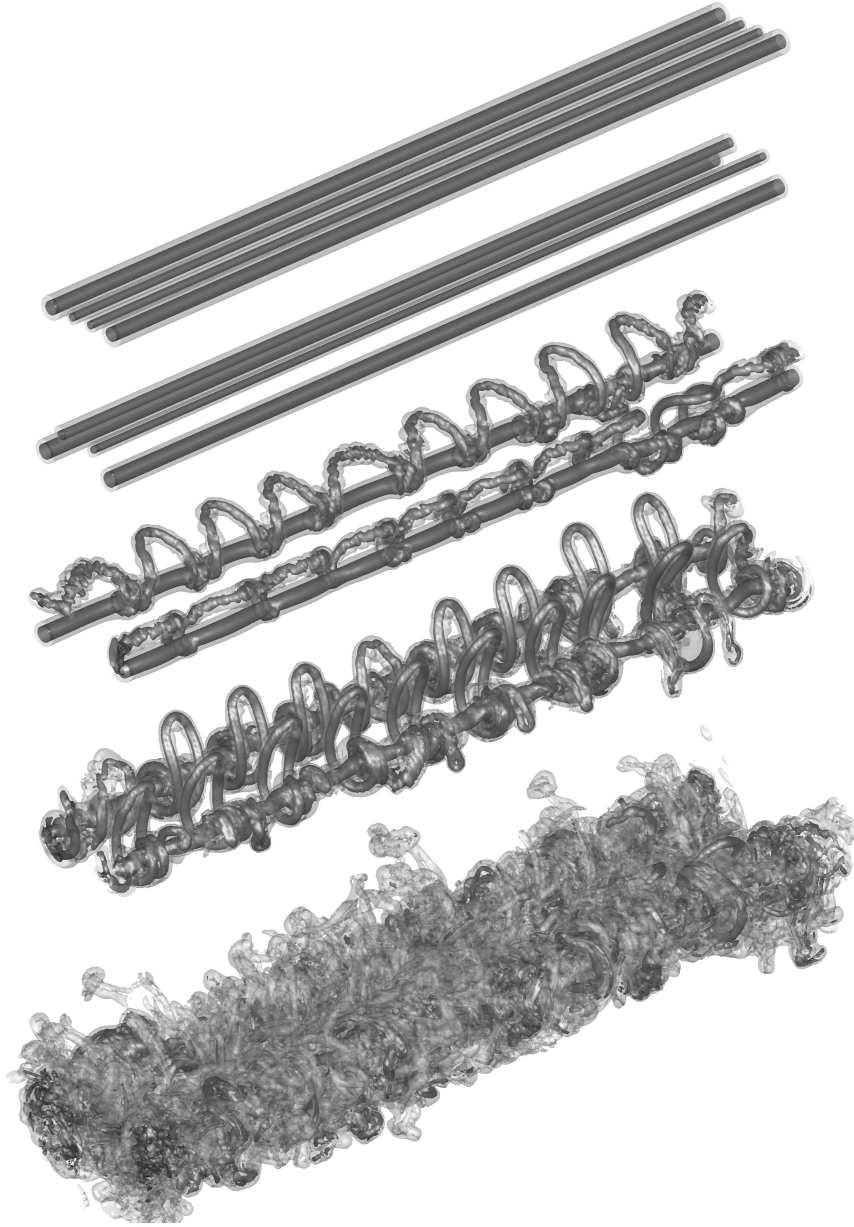


Figure 2.2: Evolution of the four vortex system as obtained using the VIC-PFM method with hyper-viscosity model. Iso-surfaces shown are $|\omega|b_1^2/\Gamma_1 = 10$ (high opacity) and 2 (low opacity). Times shown are $\tau = 0.0, 0.52, 1.06, 1.16$ and 1.58 .

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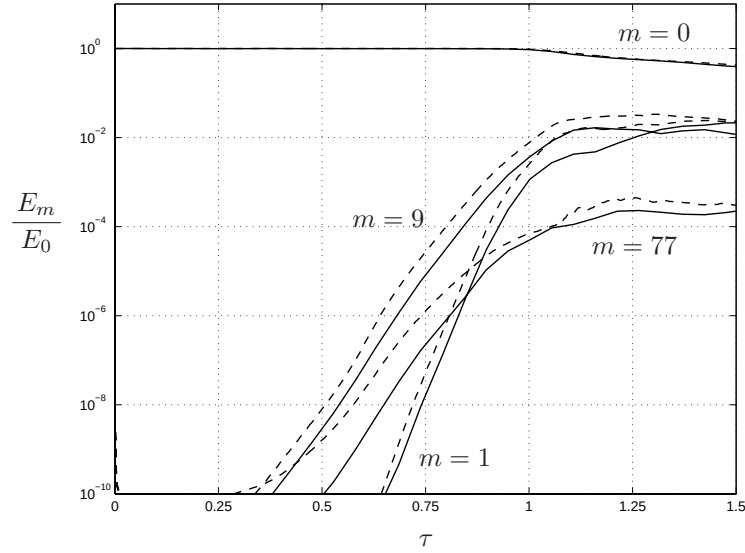


Figure 2.3: Evolution of the modal energy E_m for the base flow mode $m = 0$, the equivalent long wavelength Crow mode ($m = 1$), the most unstable medium ($m = 9$) and short ($m = 77$) wavelength modes; VIC-PFM (solid) and spectral (dash).

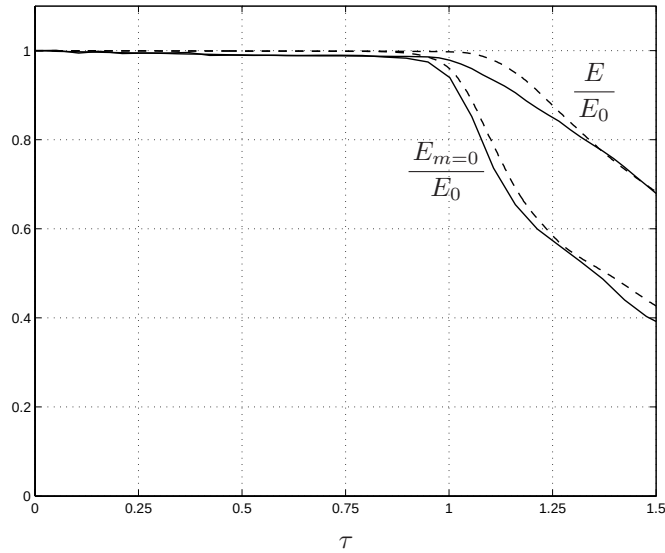


Figure 2.4: Evolution of the total energy E and of the base flow energy $E_{m=0}$: VIC-PFM (solid) and spectral (dash).

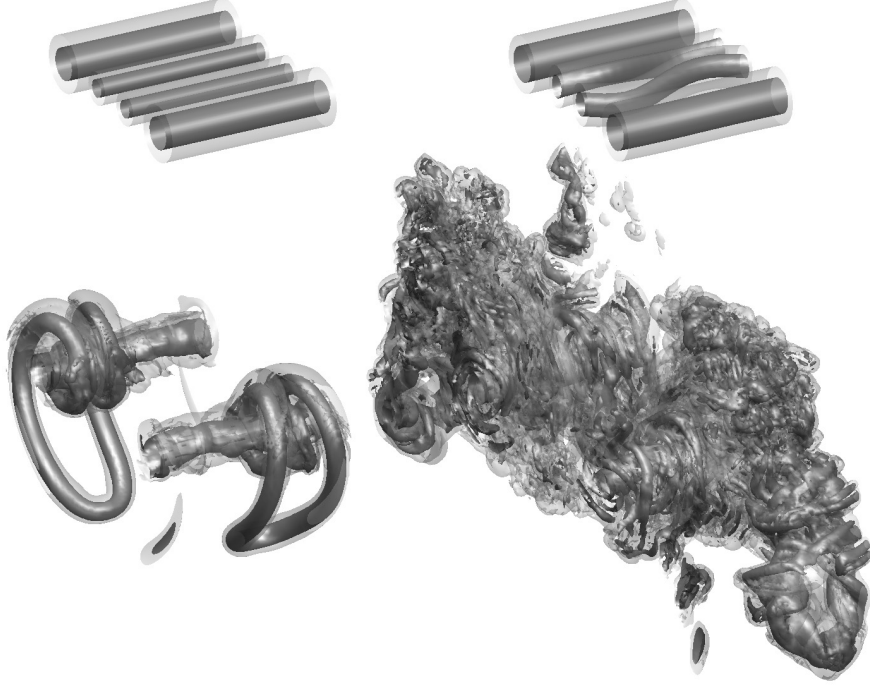


Figure 2.5: Evolution of the four vortex system obtained using the VIC-PFM method with the RVM model. Iso-surfaces shown are $|\omega|b_1^2/\Gamma_1 = 10$ (high opacity) and 2 (low opacity). Times shown are $\tau = 0.0, 0.61, 0.79$ and 1.05.

2.3.4 Comparison of the SGS models

Due to the high computational cost of the simulations above, the detailed comparison of the SGS models was carried out on a computational domain corresponding to one single medium wavelength instability: $L_x/b_0 = 0.76$. To further standardize the evolution of the vortex system, the same structured low amplitude perturbation of the fundamental mode $m = 1$ (i.e., $\lambda/b_0 = 0.76$) was used for all cases. The evolution of this short four vortex system, obtained using the VIC-PFM method with the RVM model ($n = 3$), is shown in Fig. 2.5.

In Fig. 2.6, we show the evolution of the modal energies (base flow, perturbed mode and its first harmonic) for various SGS models. The modal energy values have been renormalized by the initial base flow energy E_0 . For all models, we obtain the same growth rate values $\sigma_1 \approx 14$ (similar to $\sigma_9 \approx 15$ for the long domain simulation) and $\sigma_2 \approx 27$. When reaching the nonlinear phase and saturation,

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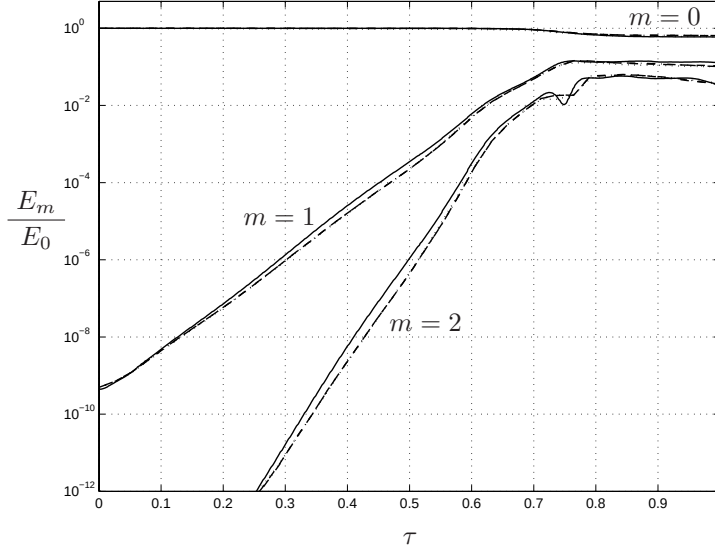


Figure 2.6: Evolution of the modal energy E_m for the base flow mode $m = 0$, the perturbed mode $m = 1$ and its first harmonic $m = 2$: SMAG (dot), RVM (dash-dot), FSF (dash), and spectral method with k^8 hyper-viscosity (solid). Results with the other multiscale models (not shown) are similar to RVM.

small differences are seen to occur, but the overall modal energy behavior remains similar.

In Fig. 2.7, we show the evolution of both the total and the base flow energies. Before the instability significantly develops, the flow remains essentially 2-D and both E and $E_{m=0}$ remain nearly equal. When the flow becomes 3-D, the difference between the two curves becomes apparent. As the simulations are done without ν , one would expect energy conservation as long as there are no strong interactions between the primary and secondary vortices. As expected, the Smagorinsky model produces significant effective dissipation. If we associate its energy decrease between $\tau = 0$ and 0.6 to an effective Reynolds number (using $dE/dt = -2\nu_{\text{eff}}\mathcal{E}$, in which $\mathcal{E} = \frac{1}{2} \int |\omega|^2 dV$ is the enstrophy), we obtain $Re = \Gamma_0/\nu_{\text{eff}} \approx 10^4$: indeed quite low (recall that a vortex at $Re = \Gamma_0/\nu = 5 \cdot 10^3$ is already quite diffusive and is easily computed using DNS, as in [82]). The results obtained using the WALE model are even worse: this is due to its high dissipation in vortex flows. The SMAG and the WALE models are clearly not acceptable for LES of high Reynolds number vortex flows. On the contrary, the multiscale models (RVM, RVM2, FSF,

FSF2, SMAG2) all perform quite well: good energy conservation up to the time of strong vortex interactions, and then roughly same energy decay of the turbulent flow. The low order HV model also produces good results, yet not as good as those obtained using the multiscale models. For the final simulation time shown ($\tau = 1$), the multiscale models lead to about the same energy: $E/E_0 \approx 0.83$. The results shown are all $n = 3$; but even $n = 1$ produces results far superior to SMAG or WALE models.

Finally, we also consider the spectral behavior of the models, see Fig. 2.8 which provides the spectrum of the turbulent flow (at $\tau = 1.05$). We confirm the good behavior of the multiscale models, best using the available wavenumbers of the LES grid: they preserve the low to medium wavenumbers (inertial range) while providing dissipation at the high wavenumbers. The SMAG and WALE models dissipate at all wavenumbers, thus significantly altering the inertial range dynamics of the LES.

As a last observation, we note that the energy decay during the turbulent phase of the flow is essentially independent of the SGS model details, as long as the model is "good" and thus does not affect the large to medium scale dynamics (here of order of the Omega-loops). In turbulence, it is indeed the dynamics of those scales that determine the dissipation rate.

2.4 Conclusions

We have considered LES of transitional flows involving multiscale instabilities developing in complex vortex systems and with small cores (as typical of aircraft wake vortices). First, it is essential that the numerical method used be of high quality: energy conserving (in absence of viscosity and SGS modelling) and with negligible dispersion; the VIC-PFM method and the spectral method are such quality methods. Second, it is also most important that the SGS model be active only during the complex phases of the flow (here, the strong interactions between the opposite sign vortices, leading to partial reconnection, generation of small scales and turbulence), while remaining inactive during the "gentle" phases. The SMAG and the WALE models are not able to achieve that. The multiscale models (RVM, RVM2, FSF, FSF2, SMAG2) achieve that naturally: the effect of the model remains negligible as long as there is no significant energy content in the high wavenumbers of the LES field. Hyper-viscosity models also do that; yet they do not perform as well: they tend to over-dissipate at the high wavenumbers.

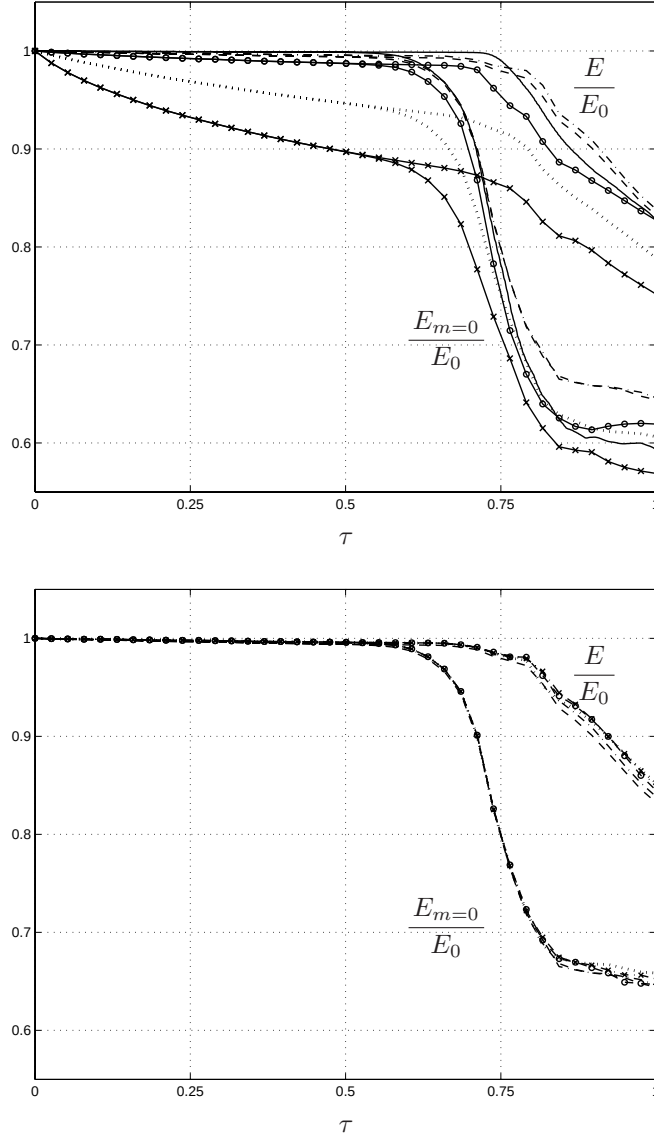


Figure 2.7: Evolution of the total energy E and of the base flow energy $E_{m=0}$. Top: SMAG (dot), RVM (dash-dot), FSF (dash), WALE (solid with crosses), low order HV (solid with circles) and spectral method with k^8 hyper-viscosity (solid). Bottom: SMAG2 (dot), RVM (dash-dot), RVM2 (dash-dot with crosses), FSF (dash) and FSF2 (dash with circles).

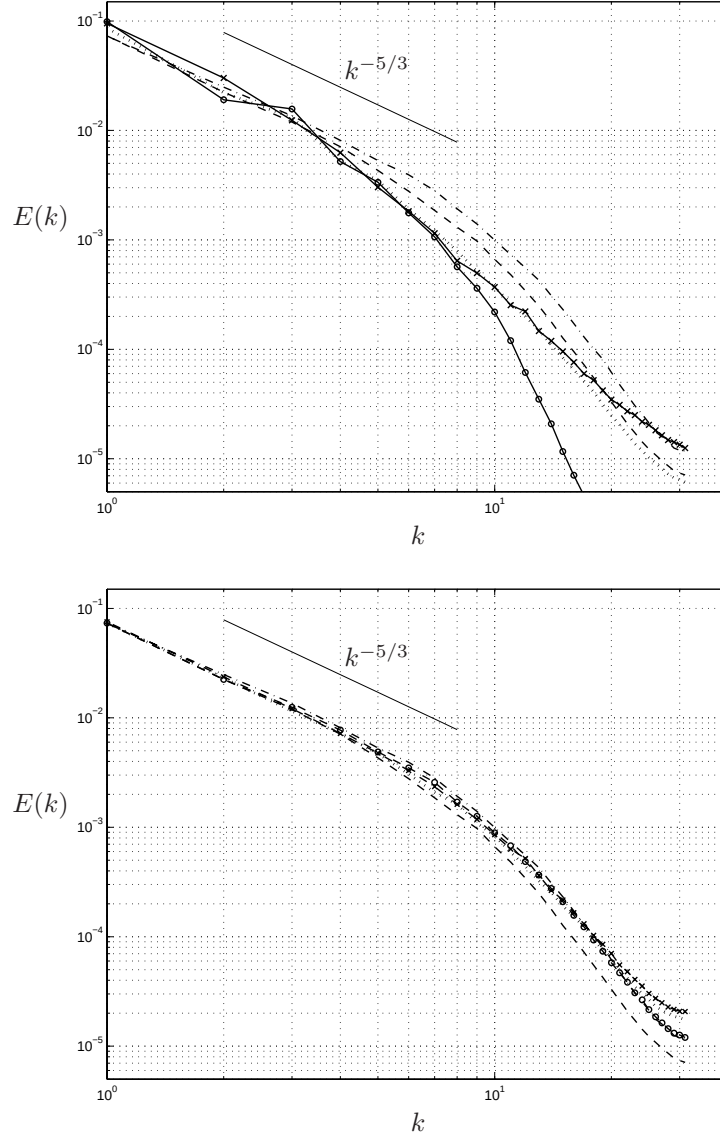


Figure 2.8: Energy spectrum at $\tau = 1.05$. Top: SMAG (dot), RVM (dash-dot), FSF (dash), WALE (solid with crosses) and low order HV (solid with circles). Bottom: SMAG2 (dot), RVM (dash-dot), RVM2 (dash-dot with crosses), FSF (dash) and FSF2 (dash with circles).

2.4. Conclusions

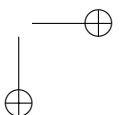
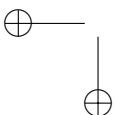
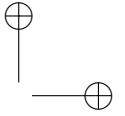
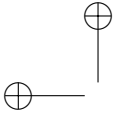
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From a computational point of view, there are some differences in the CPU cost between the models. The "small-small" models (RVM2 and FSF2, here with $n = 3$) are about 40% more expensive than the basic SMAG model: this is so because we here need to filter twice (filter $\mathbf{u}$ and $\boldsymbol{\omega}$). The "small-complete" and "complete-small" models (RVM, FSF, SMAG2) are about 25% more expensive.

For LES of complex (transitional and/or turbulent) vortex flows, and using FD methods (thus also VIC; other validations being currently performed using a fourth-order FD code in the velocity-pressure formulation), the multiscale SGS models come out as good choices. They are easily implemented (here using iteration of efficient, tensor product, stencil-3 discrete filters) and they have a good spectral behavior: they preserve the low to medium wavenumbers while they provide the SGS dissipation at the high wavenumbers.

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Chapter 3

Scaling and asymptotic high Reynolds number behavior of multiscale subgrid models.

The content of this chapter is being submitted for publication in *Physics of Fluids* as an article entitled *Scaling and asymptotic high Reynolds number behavior of multiscale subgrid models*. The authors are R. Cocle, L. Bricteux and G. Winckelmans. The article is here reproduced as it will be submitted.

A part of this work was also published in a conference proceeding with a peer review and is entitled *Investigation of multiscale subgrid models in homogeneous isotropic turbulence at high Reynolds number*, at the 7th National Congress on Theoretical and Applied Mechanics NC-TAM2006 in May 2006. The authors are R. Cocle and G. Winckelmans.

Abstract

This paper investigates the capabilities of different subgrid scale (SGS) models for large-eddy simulation (LES), used either in a vortex-in-cell (VIC) method or in a pseudo-spectral method, and their applicability to the simulation of decaying homogeneous isotropic turbulence (HIT) in the limit of very high Reynolds number

(i.e. simulations where the molecular viscosity dissipation is negligible compared to the SGS dissipation). This study is done using different grid resolutions (128^3 , 256^3 and 512^3) to compare and obtain the asymptotic spectral behavior of each model in the limit of large grids. We are then able to emphasize the global behavior of those SGS models, not necessarily observable in "small" LES (i.e. in LES at moderate Reynolds number and using smaller mesh resolutions). This analyze requires to use the correct coefficient value for each model investigated, but, except for specific SGS models, these model coefficients cannot be fully determined theoretically and thus needs to be further validated numerically on a flow with "a priori" known behavior. So, a detailed analysis first provides the scale-dependence of each model coefficient in the viscous range of turbulence and then, in the limit of very high Reynolds number. More specifically, we consider LES of decaying HIT using several "smaller" mesh resolutions (48^3 , 64^3 , 128^3 LES compared to a 256^3 DNS). Those results lead to a proper fit which can then be further used to correctly determine the different model coefficients essential for the study of the asymptotic behavior at high Reynolds number. For each simulation presented in this paper, energy (global and spectra), enstrophy and dissipation rate evolutions are provided and used to support the quantitative comparisons.

Keywords: Large-eddy simulation, subgrid-scale modelling, multiscale modelling, high Reynolds number flows, asymptotic spectral behavior, effective viscosity, hyper-viscosity, scale-dependent model coefficients, decaying homogeneous isotropic turbulence, Lagrangian methods, vortex particle method, vortex-in-cell method, spectral method.

3.1 Introduction

The present investigation is concerned with LES of decaying HIT, using here two codes (a vortex-in-cell (VIC) method and a pseudo-spectral method), to study the asymptotic spectral behavior of various subgrid-scale (SGS) models, as well as the scale-dependence of the associated coefficient. With the Smagorinsky model at large Reynolds number and for LES cutting into the inertial range (i.e. when $\Delta/\eta \geq 20$, with Δ the LES cut-off length and η the Kolmogorov scale), the coefficient can be determined theoretically as $C_S \simeq (0.3)^3 = 0.027$. Meneveau *et al.* [49] have shown that, when the cut falls outside of the inertial range (i.e. inside part of the viscous dissipation range), the coefficient becomes dependent on

3.2. Equations and numerical method

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the ratio Δ/η . They found, using the von Karman and Pao spectrum, the relation $C_S = C_S(\Delta/\eta)$. Here, we first find an equivalent relation for the coefficient of each SGS model investigated. It then further leads to properly determine the asymptotic coefficient value when the SGS model is used in LES with $\Delta/\eta \gg 20$. The aim is then to numerically obtain the asymptotic behavior of each SGS model in the limit of very high Reynolds number LES: LES on a large grid and where the energy dissipation is solely ensured by the SGS model.

Two types of SGS effective viscosity models are investigated:

- *Type I* models: models acting on the complete LES field. The SGS stress is then modelled using $\tau_{ij} = 2\nu_{\text{sgs}} S_{ij}$ where S_{ij} is the strain rate tensor: $S_{ij} = \frac{1}{2}(g_{ij} + g_{ji})$ with $g_{ij} = \partial u_i / \partial x_j$. Such models are the Smagorinsky (SMAG) model, the "small-complete" Filtered Structure Function (FSF) model and the "small-complete" version of the Smagorinsky model (SMAG2);
- *Type II* models: models acting on the "small-scale" LES field. The SGS stress is then modelled using $\tau_{ij} = 2\nu_{\text{sgs}} S_{ij}^s$ with S_{ij}^s the strain rate tensor of the small scale field. Such models are the "complete-small" Regularized Variational Multiscale (RVM) model, the "small-small" Regularized Variational Multiscale (RVM2) model and the "small-small" Filtered Structure Function (FSF2) model.

The notation "small/complete - small/complete" means that ν_{sgs} is computed from the small-scale or the complete LES field, and that the diffusion operator acts on the small-scale or the complete LES field. Thus the *Type I* models are the "x-complete" models and the *Type II* models are the "x-small" models.

3.2 Equations and numerical method

We here consider LES of incompressible flows, thus $\nabla \cdot \mathbf{u} = 0$. For LES in the velocity-pressure formulation (as done in the pseudo-spectral code), the LES equations are, respectively for *Type I* and *Type II* models;

$$\begin{aligned} \frac{D\mathbf{u}}{Dt} + \nabla P &= \nabla \cdot (2(\nu + \nu_{\text{sgs}}) \mathbf{S}) \\ &= \nu \nabla^2 \mathbf{u} + \nabla \cdot (2\nu_{\text{sgs}} \mathbf{S}) \end{aligned} \quad (3.1)$$

$$\begin{aligned} \frac{D\mathbf{u}}{Dt} + \nabla P &= \nabla \cdot (2\nu \mathbf{S}) + \nabla \cdot (2\nu_{\text{sgs}} \mathbf{S}^s) \\ &= \nu \nabla^2 \mathbf{u} + \nabla \cdot (2\nu_{\text{sgs}} \mathbf{S}^s) \end{aligned} \quad (3.2)$$

in which $P = p/\rho$ is the reduced pressure and $\nu = \mu/\rho$ is the kinematic viscosity. P is obtained by solving a Poisson equation so as to ensure the reprojection, at every time step, of the velocity field onto a divergence free field. For LES in the vorticity-velocity formulation (as used here in the vortex-in-cell (VIC) code), and defining $Q_{ij} = \frac{1}{2} \left(\frac{\partial \omega_i}{\partial x_j} + \frac{\partial \omega_j}{\partial x_i} \right)$, the LES equations are, respectively,

$$\begin{aligned} \frac{D\boldsymbol{\omega}}{Dt} - \nabla \cdot (\mathbf{u}\boldsymbol{\omega}) &= \nabla \cdot (2(\nu + \nu_{\text{sgs}}) \mathbf{Q}) \\ &= \nu \nabla^2 \boldsymbol{\omega} + \nabla \cdot (2\nu_{\text{sgs}} \mathbf{Q}) \end{aligned} \quad (3.3)$$

$$\begin{aligned} \frac{D\boldsymbol{\omega}}{Dt} - \nabla \cdot (\mathbf{u}\boldsymbol{\omega}) &= \nabla \cdot (2\nu \mathbf{Q}) + \nabla \cdot (2\nu_{\text{sgs}} \mathbf{Q}^s) \\ &= \nu \nabla^2 \boldsymbol{\omega} + \nabla \cdot (2\nu_{\text{sgs}} \mathbf{Q}^s) \end{aligned} \quad (3.4)$$

in which $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ and $\boldsymbol{\omega}^s = (\nabla \times \mathbf{u})^s$, and thus $\nabla \cdot \boldsymbol{\omega} = 0$ and $\nabla \cdot \boldsymbol{\omega}^s = 0$. The vortex stretching term is here written as $\nabla \cdot (\mathbf{u}\boldsymbol{\omega})$. The numerical solution of (3.3) or (3.4) is obtained following the vortex-in-cell (VIC) approach: see [16, 82] for a detailed presentation. In VIC, the vorticity field is represented by "vortex particles" of position $\mathbf{x}_p$ and of strength $\alpha_p = \int \boldsymbol{\omega} d\mathbf{x} = \boldsymbol{\omega}_p h^3$ where h is the discretization size (grid size, also used for particle redistribution). Interpolations between particles and grid, as well as particle redistribution, are all done using high order interpolation schemes (here the M'_4 scheme). The vector streamfunction $\boldsymbol{\psi}$ is obtained by solving the Poisson equation $\nabla^2 \boldsymbol{\psi} = -\boldsymbol{\omega}$ on the grid, using a fast Poisson solver (here FishPack). The velocity field (needed for convection and stretching) is then obtained from $\mathbf{u} = \nabla \times \boldsymbol{\psi}$, using 4th order finite differences (FD). The convective part is computed using the Lagrangian approach: $d\mathbf{x}_p/dt = \mathbf{u}(\mathbf{x}_p)$; this ensures that the structures of a turbulent flow are properly convected (i.e., negligible dispersion errors). The time variation of the particle strengths (i.e., both the vorticity stretching and the dissipation terms) is evaluated on the grid, using FD. The global time marching procedure is here carried out using the Leap Frog scheme for the Lagrangian convection part and the Adams-Bashforth scheme for the Eulerian parts (stretching and dissipation terms). Finally, the divergence-free character of the vorticity field is maintained by proper reprojection of the discrete vorticity field (which also requires solving a Poisson equation). The present VIC method has very good energy conservation (i.e., negligible numerical dissipation) and negligible dispersion. It constitutes a high quality method suitable for LES, and thus for the present investigations (see also [42] for comparison of VIC and pseudo-spectral solvers in HIT).

3.3 SGS models investigated

Concerning the SGS viscosity modelling, we investigate the same models as in Section 2.2.1 (except the WALE model as we have no wall). The discussion about each coefficient associated to these SGS models is done in the next section (the coefficient values presented in Table 2.1 are thus no longer used here; yet they will be compared with the values obtained with the scale-dependence study performed in the next section).

3.4 Simulation results

The coefficient of each SGS model is generally determined from a theoretical analysis, based on a given spectrum corresponding to an HIT at large Reynolds number (e.g. the von Karman and Pao spectrum). The main assumption is then that the LES cutoff Δ fall inside a well-defined and large inertial range. For instance Lilly [45, 46] provided the relationship between the Smagorinsky constant C_S and the Kolmogorov constant C_K :

$$C_S = \frac{1}{\pi^2} \left(\frac{2}{3 C_K} \right)^{3/2}.$$

If we use the Kolmogorov constant $C_K = 1.6$, this gives $C_S = 0.027$. However, in more general LES of flows where the Reynolds number is moderate and/or the grid resolution is relatively good, the LES cutoff Δ could fall inside a poorly-defined "inertial range" or inside the viscous dissipation range. Typically, this will occur in LES with $\Delta/\eta < 20$ with $\eta = (\nu^3/\epsilon)^{1/4}$ the Kolmogorov scale. Then, the coefficient value of each model needs to be adapted so as to provide the proper dissipation rate. To find the scale dependence of each SGS model coefficient, as was done in detail by Meneveau [49] for the Smagorinsky model, first theoretically and then applied using a spectral method, we first consider LES of decaying HIT using several mesh resolutions (i.e. several ratios Δ/η). The comparison with the reference DNS then permits to determine the scale-dependence of the coefficients. Furthermore, and to really test the ability of the SGS model in more "challenging" LES (and also further validate the model coefficient value found from the first study), LES at very high Reynolds number are carried, thus LES where the molecular dissipation is very small, and thus negligible, compared to the SGS dissipation. Such LES are done by using a large enough grid (at least

128³) and by running the code with ν equal to zero: thus only the SGS model dissipates energy.

3.4.1 LES at moderate Reynolds number: scale-dependence investigation

The reference data is a 256³ DNS [81] started using a field with given spectra and random phases, that evolved into turbulence. The initial condition of the LES ($t = 0$) is taken from the DNS at the time where the turbulence is well established. From that time, the DNS covers a usable window of Re_λ from 90 to 60. At $t = 0$, the "inertial" range corresponds to $k \approx [19 - 25]$. The DNS is then restricted to 48³, 64³ and 128³ LES, corresponding to $\Delta/\eta = 13.6$, 10.3 and 5.2 respectively. As it is moderate Reynolds number turbulence, the molecular viscosity dissipation is never negligible. It also does not permit to obtain larger Δ/η (a 32³ would here not be pertinent as it corresponds to "cut" the spectrum before the inertial range).

In the following, the model coefficients are determined so as to have the correct resolved enstrophy evolution (i.e. the same as the truncated DNS) during the early times of the simulation. This choice is found to lead to the best energy evolution. Fig. 3.1 shows, for a 48³ LES using the RVM model, the enstrophy evolution and the energy spectra at $t = 3.33$ for different values of C_R . It is verified that the best spectral behavior is obtained when the coefficient corresponds to that providing the best enstrophy evolution. It is here illustrated with the RVM model, but the same conclusion can be made for all other models; thus, we do not show them.

Figs. 3.2 provides, for 48³ LES and using the *Type I* models, the energy evolution and the dissipation evolution, respectively. We observe that these models give very similar results: they are too dissipative during the early times of the simulation. The decay of the enstrophy is presented in Fig. 3.3. The SMAG and FSF models deviate significantly from the DNS data. The SMAG2 model is slightly more accurate; yet the difference with the DNS is still important. Fig. 3.3 shows the energy spectra. We observe that the *Type I* models are clearly too dissipative at the large to medium scales and not dissipative enough at the small scales. As they act on the complete LES field, as a viscosity model, the shape of their dissipation spectrum cannot properly approximate the exact SGS dissipation spectrum (see also [37]). As the coefficient is correctly chosen in each case, the fact that ν_{sgs} is computed using the complete LES field or using the small-scale LES field does not, in the present case of HIT, change significantly the results. Hence we do not show results with ν_{sgs} computed using the small-scale field. The conclusion is

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different for simulations of transitional flows (i.e. that evolve from a simple state to a turbulent state): for instance see [13] where the "small-complete" models are verified to be much better: this is because they are inactive during the initial, well-resolved, phases of the flow (as ν_{sgs} is then negligible) and become active only when the flow locally creates small scales. In any case, the results presented here in HIT confirm that the dissipation of those *Type I* models is too large at the medium scales.

48^3 LES using the *Type II* models is investigated next. The energy evolution and the dissipation evolution are presented in Fig. 3.4. Those models are seen to produce results that coincide well with the DNS data, and for the entire simulation time. This is especially true for the RVM model where the field has been filtered three times (i.e. $n = 3$). As the initial condition of our LES is obtained from a truncated DNS (computed using the pseudo-spectral method), we do not ascribe much significance to the small difference of dissipation at the very early times of the simulation. We have also verified that it is due to a "transitional" period, where the smallest resolved scales are particularly damped by the SGS model. The enstrophy evolution, illustrated in Fig. 3.5, further confirms the good behavior of these models; and here too, the RVM model with $n = 3$ is seen to produce the best result: it follows almost exactly the DNS curve. The energy spectra are presented in Fig. 3.5. With only one iteration of the filter ($n = 1$), all *Type II* models produce similar results: also a better behavior compared to the *Type I* models, even if the dissipation is still too large in the range $k \approx [8 - 16]$. This behavior can be improved by using higher order filtering (i.e. $n > 1$). This is clearly observed in the spectrum obtained using the RVM model with $n = 3$: it produces a spectrum nearly the same as the one of the truncated DNS. Similar results can be obtained with the others *Type II* models (also using higher order filtering). Hence, we choose to only present the results obtained using the RVM model. Note that it is also the simplest to implement (the application of the discrete operations required to obtain the high order filter is most easily performed).

Finally, less challenging LES have also been performed, on 64^3 and 128^3 grids, and for each SGS models, in order to obtain the coefficient variation as function of Δ/η . The detailed results (evolution of energy, dissipation, and enstrophy; obtained spectra) are not shown here as they lead to the same conclusions as those for the most challenging 48^3 LES. The *Type II* models still come out as the better choice, as their resulting dissipation is located at the smallest scales where it is most required. For each 64^3 and 128^3 LES, we determined the coefficient value

to obtain, as for the 48^3 , the best enstrophy evolution. Fig. 3.6 is then an important figure (and one of the main output of this first investigation): it provides the scale-dependence of the obtained coefficient for each SGS model investigated. It gives the ratio C/C_∞ as function of Δ/η where C_∞ stands for the asymptotic value (provided in Table 3.1): that for LES with $\Delta/\eta \gg 20$. Recall that the asymptotic coefficient of the SMAG model is the only well known value (i.e. $C_{S_\infty} = 0.027$). We also observed that, choosing adequately the asymptotic value for the other models, one obtains a very similar curve for each model. The solid curve plotted on Fig. 3.6 is a proper fit given by:

$$\log_{10} \left(\frac{C}{C_\infty} \right) = -a e^{-b\Delta/\eta} . \quad (3.5)$$

with $a = 10.0$ and $b = 0.30$.

The scale-dependence of the coefficients value found is similar to that found by Meneveau [49] who obtained theoretically the scale-dependence of the SMAG coefficient using a von Karman and Pao spectrum. The shape of our fit is inspired from a proper fit found by Meneveau and given by: $\log_{10} \left(\frac{C}{C_\infty} \right) = -a Re_\Delta^{-b}$, with $Re_\Delta = \Delta^2 |\mathbf{S}|/\nu$, $a = 3.23$ and $b = 0.92$. For small Δ/η , our curve, obtained by actual LES runs, drops faster. Meneveau also observed some differences between the theoretical behavior and the required coefficients from spectral LES, mainly due to the differences between the von Karman and Pao spectrum and the actual LES obtained spectrum.

The asymptotic coefficients obtained in Table 3.1 can also be compared with those cited in the literature. In [31], Hughes *et al.* used $C_S = 0.010$ in a spectral method on a 64^3 LES of decaying HIT based on 256^3 DNS (in fact the same database as that used here). Using Eq. (3.5), we find $C_S = 0.0095$, thus very close. In [49], for $\Delta/\eta = 10.5$ (corresponding here to the 64^3 LES), Meneveau *et al.* announce a "true coefficient" obtained numerically from dissipation balance as $C_S \approx 0.01$, thus also very close to our value, while his theoretical curve predicts $C_S \approx 0.02$. For the FSF model, we obtain, as asymptotic value for $\Delta/\eta \gg 20$, $C_F^{(1)} = 0.078$: to be compared with Ducros *et al.* [23] who found, from a theoretical analysis assuming a LES where the cut is falling well in an inertial range, $C_F^{(1)} = 0.080$.

For the RVM model, Jeanmart *et al.* [37] found $C_R^{(1)} = 0.021$ using a spectral code on 48^3 LES of the same decaying HIT. Using our fit, one finds $C_R^{(1)} = 0.024$: also very close. The difference is mainly because, in [37], they choose the coefficient so that the dissipation rate at $t = 0$ is the same as the DNS, whereas, here, we

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Table 3.1: Asymptotic value of the coefficient for each model investigated. The asymptotic values are obtained from the best fit based on the LES runs, and using $\Delta/\eta \gg 20$.

C_S	0.027
$C_{S_2}^{(1)}$	0.045
$C_F^{(1)}$	0.078
$C_R^{(1)}$	0.036
$C_R^{(3)}$	0.060
$C_{R_2}^{(1)}$	0.066
$C_{F_2}^{(1)}$	0.110

chose to impose the correct enstrophy evolution. This leads to a slightly larger dissipation rate (as shown in Fig. 3.4), and so to a slightly larger coefficient. In [13], we also propose, as asymptotic value based on some theoretical argument, $C_R^{(1)} = 1.39 C_S = 0.038$: this too compares well with $C_R^{(1)} = 0.036$ of Table 3.1.

For the RVM2 model, Hughes *et al.* [31] obtain theoretically the relation $C_{R_2} = (1.28)^2 C_S = 1.64 C_S$. Numerically, using a pseudo-spectral code, they show that the "best" value for C_S would lie between $(0.1)^2$ and $(0.2)^2$, but closer to $(0.1)^2$, which then leads to $C_{R_2} \approx 0.02$. When one uses Eq. (3.5), one find $C_{R_2} = 0.023$. The slightly higher value can be explained because the SGS viscosity is here obtained using a velocity field computed using high order FD. Due to the truncation errors, the highest wavenumbers are damped and the norm of the strain rate tensor based on the small-scale field is smaller (i.e. also the ν_{sgs}); thus, the coefficient needs to be taken larger to ensure the same dissipation rate.

For the FSF2 model, we propose in [13], the asymptotic value of $C_{F_2}^{(1)} = 1.39 C_F^{(1)} = 0.111$: also in very good agreement with the value in Table 3.1.

We conclude that the asymptotic coefficients obtained in the present investigation and reported in Table 3.1 are indeed close to what can best be obtained by simulation. The fit of Eq. (3.5) also allows to obtain the proper coefficient value depending on the ratio Δ/η , for all the models. Both those results (asymptotic value and fit for coefficient variation) constitute an important outcome of this work.

3.4.2 LES at very high Reynolds number: asymptotic spectral behavior investigation

Now that the asymptotic value of the coefficient is determined for each model, we investigate LES of decaying HIT in the limit of very high Reynolds number (i.e. simulations where $\Delta/\eta \gg 20$ and thus where the molecular viscosity dissipation is truly negligible compared to the SGS dissipation). The LES grid is taken large enough (see later) and LES is run with ν set to zero: hence, only the SGS model dissipates energy.

The initial condition is build following the algorithm described by Rogallo in [64]. This initial field is isotropic, divergence free and has a given spectrum. We describe in Appendix B the way to build it.

This initial field then evolved using LES. For the investigations using the vortex-in-cell (VIC) code, the following SGS models are used: SMAG, FSF (with $n = 1$) and RVM (with $n = 1$ and $n = 3$); RVM2 and FSF2, and using the asymptotic coefficient value previously obtained (see Table 3.1). For the sake of comparison, simulations were also carried out using a dealised pseudo-spectral method. The models investigated are the SMAG model, the RVM2 (with $n = 3$) model and also a high order (k^{16}) hyper-viscosity (HV) model.

From grid turbulence experiments (e.g., Comte-Bellot and Corrsin [15]) and from theory, we know that, after the transient required to obtain a "statistically converged turbulence", the kinetic energy evolves as a power law:

$$\frac{E(t)}{E_0} = \left(\frac{t}{t_0} \right)^{-p} \quad (3.6)$$

where the value of the decay exponent p is found between 1.15 and 1.45 in the literature. Mohamed and LaRue [51] suggest that a good value is $p = 1.30$. Fig. 3.7 shows the energy evolution, using a 128^3 grid (both with the VIC code and the pseudo-spectral code). We find, for the RVM model ($n = 1$ and $n = 3$), that the obtained exponent is $p \approx 1.38$. Thus well into the range of admissible values. The other *Type II* models (i.e. RVM2 and FSF2) give the same energy decay exponent as the RVM model. The same results hold when using the spectral code with the RVM2 model, and even with the HV model (the exponent is then found as $p \approx 1.37$).

A significant difference is noticed with the *Type I* models (here the SMAG, FSF and SMAG2 models) that act on the whole field. As they produce spectra that are not as good as the one produced by the *Type II* models, this also influences the

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obtained p value: we obtain $p = 1.49$ for the SMAG model (equivalently for both codes) and $p = 1.45$ for the FSF model (also for the SMAG2 model, not shown). Clearly, the 1.49 value obtained with the "complete-complete" model (SMAG) is out of acceptable range. That obtained with the "small-complete" models (FSF and SMAG2) is at the border of the acceptable range: already better but still not as good as the *Type II* models that act on the small-scale field (RVM, RVM2, FSF2).

Fig. 3.8 shows the influence of the model coefficient value (here RVM) on the energy evolution and on the corresponding spectra. With a too small coefficient, the obtained p exponent obtained remains the same but the energy is then slightly larger due to an accumulation of energy at the smallest scales, as observed on the spectrum. Using a too large coefficient, the SGS model becomes too active at the medium and large scales of the flow and leads to a larger value of $p = 1.49$. We here observe the interest of having determined the proper coefficient values before doing this study. We are now able to further focus on the spectral behavior of the models and also investigate the asymptotic behavior of the models when performing LES on larger and larger grids.

Fig. 3.9 shows the obtained energy spectra for 128^3 grid (also time-averaged between $t = 10$ and 40, when the turbulence is statistically converged). To better highlight the inertial range in the spectra, we also show the compensated energy spectra on Fig. 3.10. We observe that the *Type II* models (with $n = 3$) provide the broader inertial range (i.e., the range with the $k^{-5/3}$ behavior). The width of this captured inertial range decreases with the order of the filter used to compute the small-scale fields (compare RVM with $n = 1$ to RVM with $n = 3$). In opposition, the FSF and the SMAG models do not exhibit any inertial range on such 128^3 grid. In any case, all spectra are clearly altered by a "bump-like" behavior at the medium wavenumbers, though to a much lesser extent for the *Type II* models using high order ($n = 3$) filters. This non-physical energy accumulation is present because the shape of the dissipation spectra of the SGS models is never exactly the required one. The behavior is improved when the *Type II* models are used (especially with high order filters); yet it does not prevent this "bottleneck" effect in the energy cascade. As they act only at the small scales (in opposition with the *Type I* models), their influence on the large scales is reduced and allows to capture a true $k^{-5/3}$ inertial range. This conclusion is also valid for the spectrum obtained when using the HV model: it provides an inertial range as broad as the *Type II* models with $n = 3$ but the energy "bump" is more pronounced. This result

compares well with [41] who shows the presence of the "bottleneck" effect in the energy spectra when a hyper-viscous dissipation is used.

An argument that could explain the presence of this bottleneck is that a LES is always locally under-resolved with respect to its own SGS viscosity. We can illustrate this concept using the SMAG model. Consider first the cell Péclet number based on the SGS viscosity:

$$Pe_h = \frac{|S| h^2}{\nu_{\text{sgs}}} = \frac{1}{C_S} = \frac{1}{0.027} \approx 37.$$

We observe that its value is too high to meet the quality criterion of a locally well-resolved simulation. We can also evaluate the $k_{\text{max}} \eta_{\text{sgs}}$ criterion based on a pseudo Kolmogorov length scale η_{sgs} . The SGS dissipation is then:

$$\epsilon_{\text{sgs}} = \langle 2 \nu_{\text{sgs}} S_{ij} S_{ij} \rangle = C_S h^2 \langle (2 S_{ij} S_{ij})^{3/2} \rangle$$

leading to

$$\eta_{\text{sgs}} = \left(\frac{\nu_{\text{sgs}}^3}{\epsilon_{\text{sgs}}} \right)^{1/4} = \left(\frac{C_S^3 h^6 \langle (2 S_{ij} S_{ij})^{3/2} \rangle}{C_S h^2 \langle (2 S_{ij} S_{ij})^{3/2} \rangle} \right)^{1/4} \approx (C_S^2 h^4)^{1/4} \approx 0.16 h$$

and

$$k_{\text{max}} \eta_{\text{sgs}} = \frac{\pi}{h} 0.16 h \approx 0.50 < 1.50.$$

We confirm that the obtained value for this criterion is too small to consider a well-resolved computation. It thus leads to a local energy accumulation due to the under-resolution, as observed in the previous spectra. If we impose a classical well-resolved criterion of $k_{\text{max}} \eta_{\text{sgs}} = 1.50$, we have to take a SMAG coefficient greater than $9 C_S$. In Fig. 3.11, we show that with a higher coefficient value ($C_S = 0.27$), the obtained spectra is indeed similar to a low Reynolds number DNS. As a consequence, no inertial range can be observed.

Finally, we investigate the asymptotic behavior of the models when performing LES on larger and larger grids, see Fig. 3.12. We consider the SMAG model, the RVM2 model ($n = 3$) and the HV model and we compare the shape of the spectra obtained using the spectral code and higher resolution (128^3 and 256^3 , and even 512^3). As in the previous results, we show the unequivocal presence of the "bump-like" behavior. As expected, the $k^{-5/3}$ inertial range becomes broader as the grid is taken larger. Such LES has indeed reached its "asymptotic behavior", with self-similar obtained spectra: going to an even finer grid will produce an even larger $k^{-5/3}$ inertial range followed by the same bump part; this is verified by running the

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HV model on a 512^3 grid. On Fig. 3.12, we also illustrate that each model produces its own energy spectrum in the dissipation range and that the bump part conserves the same shape when going from 128^3 to 512^3 grid. Indeed, if we decompose the energy spectrum in the following way,

$$E(k, t) \approx E_0(t) k^{-5/3} \tilde{E}(k/k_{max})$$

we can observe that $\tilde{E}(k/k_{max})$ preserves its shape whatever the time or the LES resolution. We also observe that, for the RVM2 model and the HV model, the width of the captured inertial range is, in each case, appreciably smaller than the number of modes computed. For the 128^3 , the inertial range extends on $k \approx [2-8]$, for the 256^3 it grows to $k \approx [2-20]$ and $k \approx [2-40]$ for the 512^3 . In opposition, the SMAG model, even with the 256^3 resolution, is not able to capture any inertial range.

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We first analyzed, for LES and using a VIC method, the scale-dependence of the coefficients used in different SGS models: *Type I* models that act on the complete LES field (SMAG, FSF, SMAG2) and *Type II* models that act on the small-scale LES field (RVM, RVM2 and FSF2). In all cases, it is essential that the numerical method used be of high quality: energy conserving (in absence of viscosity and SGS modelling) and with negligible dispersion; the VIC method is such a quality method, as shown throughout this paper with the several comparisons of the results with those obtained using a pseudo-spectral code. This analysis led to a proper fit $C(\Delta/\eta)$ for each SGS model. It permits to determine "a priori", for a LES with a given mesh size, the best coefficient value that has to be used to ensure the best energy evolution and spectral behavior. The coefficients obtained are also in good accordance with those found in the literature.

Second, we considered LES of decaying HIT in the limit of high Reynolds number, i.e., when the SGS model dissipation is much greater than the molecular viscosity dissipation. To validate the quality of our conclusions, this analysis was done using two different numerical methods: the VIC method and a pseudo-spectral method. This analysis showed the superiority of the *Type II* models acting on the small scales field since they are able to capture a significant inertial range, as illustrated in many results, even if they clearly suffer from the presence of a "bump-like behavior" in their spectra. This behavior is also observed with the HV model;

in this case, the bump is even more pronounced while also keeping a significant inertial range. The results obtained with these models are also in good agreement with the grid turbulence experiments found in the literature from the point of view of global dissipation rate. The *Type I* models that act on the complete LES field also have the non-physical "bump-like" behavior; moreover they cannot reproduce any inertial range, they also do not predict the correct global dissipation rate.

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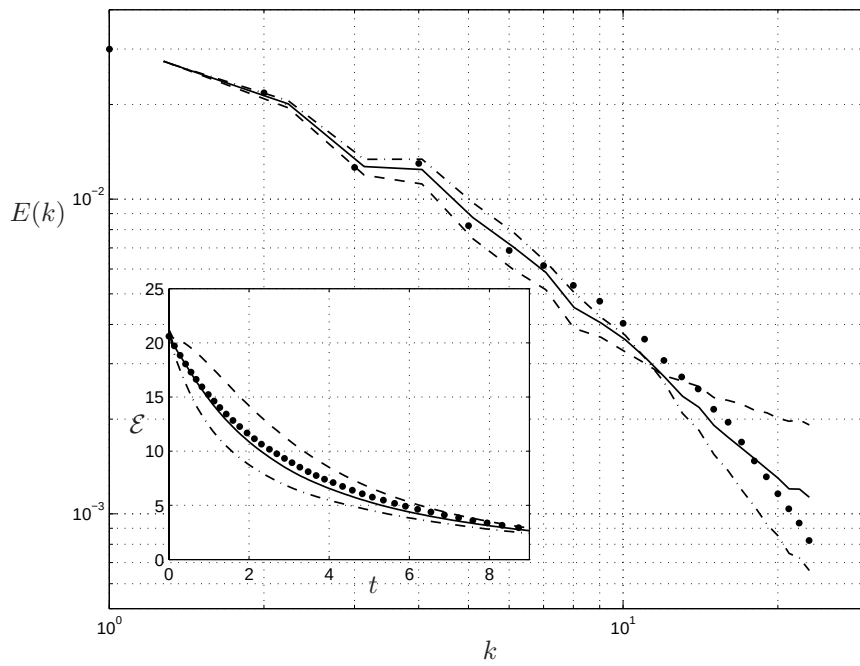


Figure 3.1: 48^3 LES at moderate Reynolds number: Energy spectra using the RVM model at $t = 3.33$: $C_R = 0.024$ (solid), $C_R = 0.010$ (dash), $C_R = 0.040$ (dash-dot) and truncated 256^3 DNS (bullets). Insert: enstrophy evolution for each coefficient value.

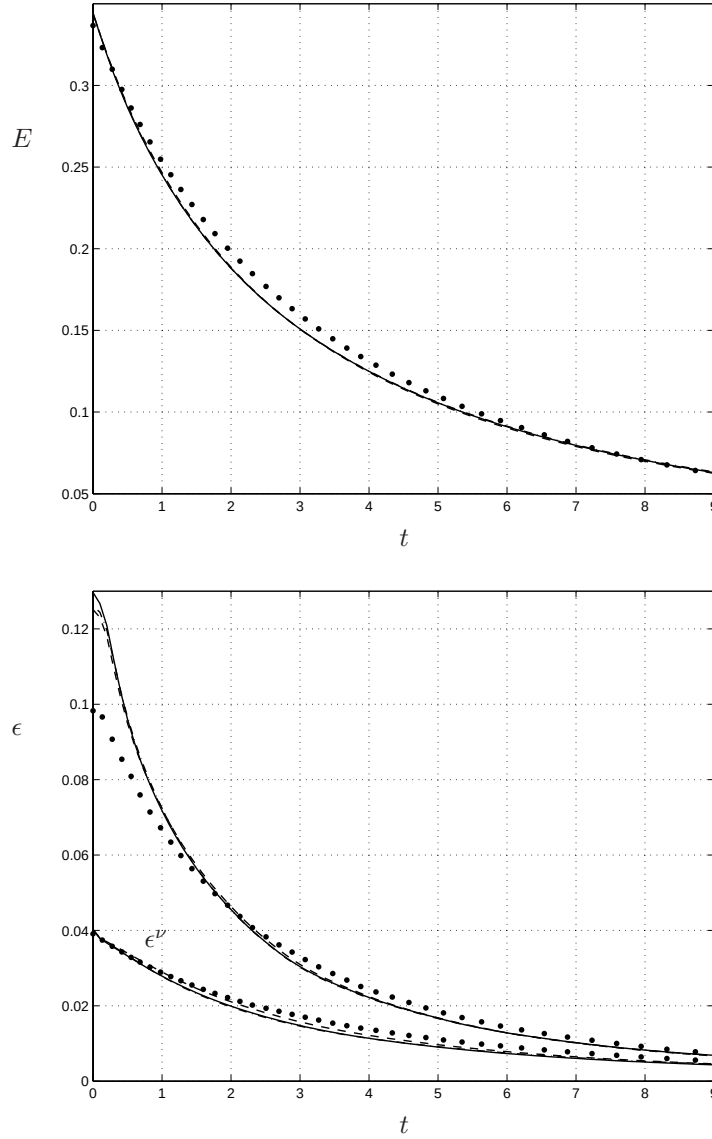


Figure 3.2: 48^3 LES at moderate Reynolds number using Type I models: Evolution of the energy (top) and the dissipation $\epsilon = \epsilon^\nu + \epsilon^{sgs}$ (bottom): SMAG (solid), SMAG2 with $n = 1$ (dash), FSF with $n = 1$ (dash-dot) and truncated 256^3 DNS (bullets).

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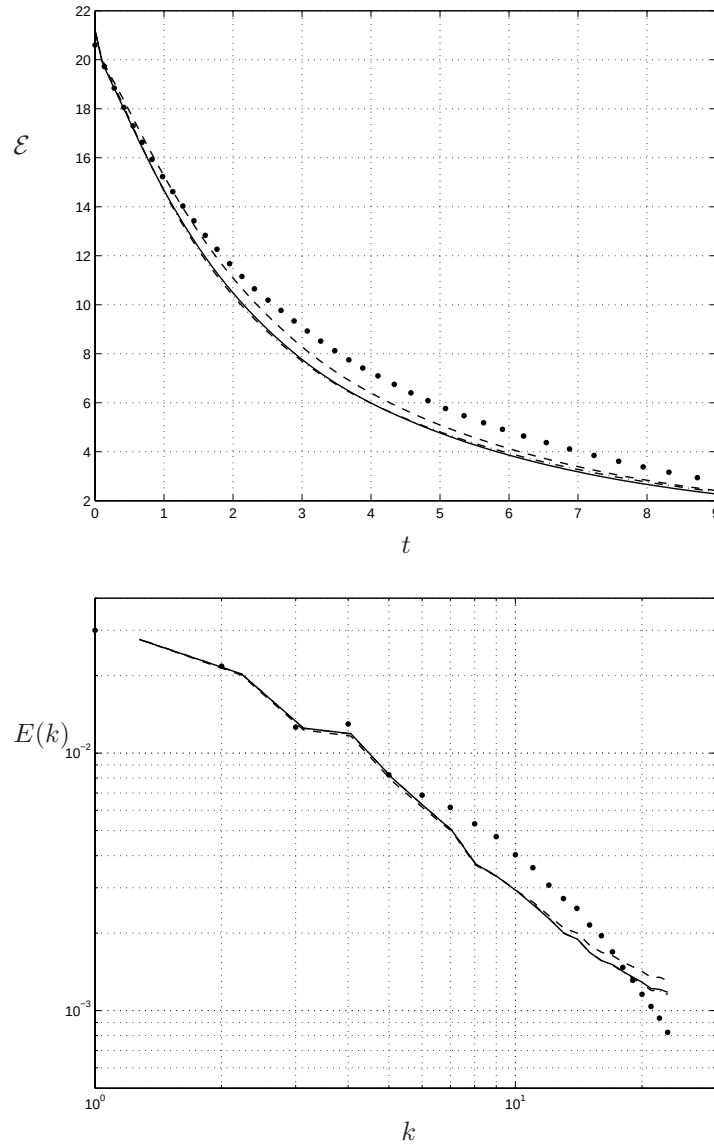


Figure 3.3: 48^3 LES at moderate Reynolds number using Type I models: Evolution of the entrophy (top) and energy spectra at $t = 3.33$ (bottom): SMAG (solid), SMAG2 with $n = 1$ (dash), FSF with $n = 1$ (dash-dot) and truncated 256^3 DNS (bullets).

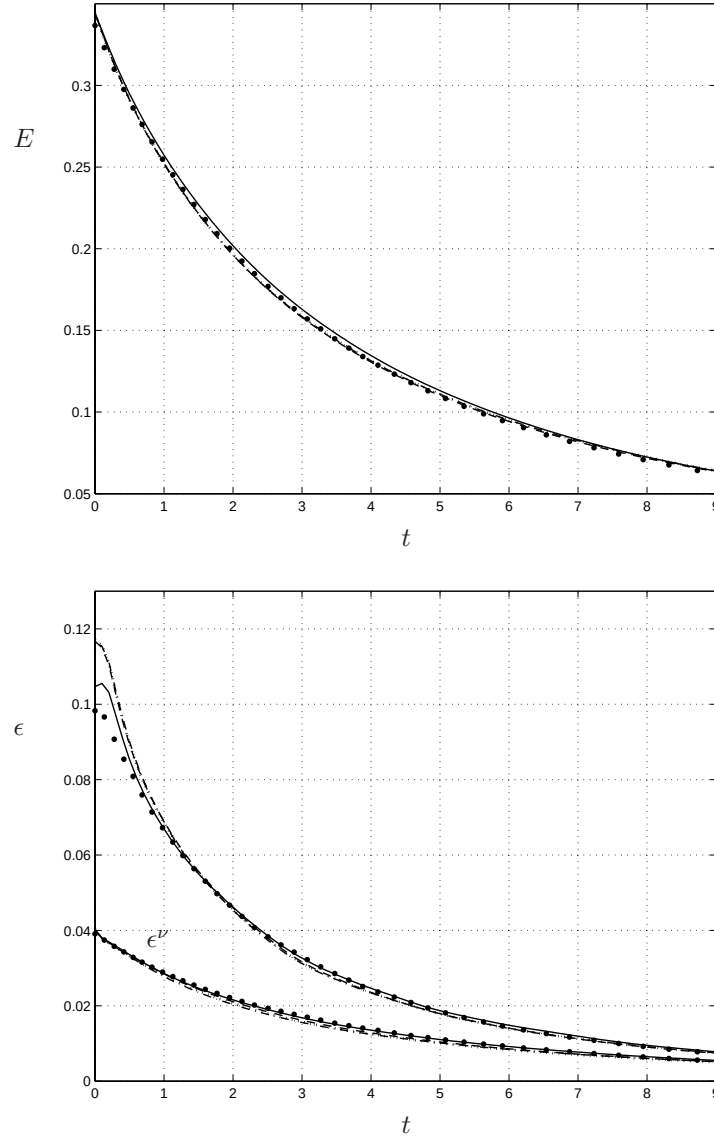


Figure 3.4: 48^3 LES at moderate Reynolds number using Type II models: Evolution of the energy (top) and the dissipation $\epsilon = \epsilon^\nu + \epsilon^{sgs}$ (bottom): RVM with $n = 1$ (dot), RVM2 with $n = 1$ (dash), FSF2 with $n = 1$ (dash-dot), RVM with $n = 3$ (solid) and truncated 256^3 DNS (bullets).

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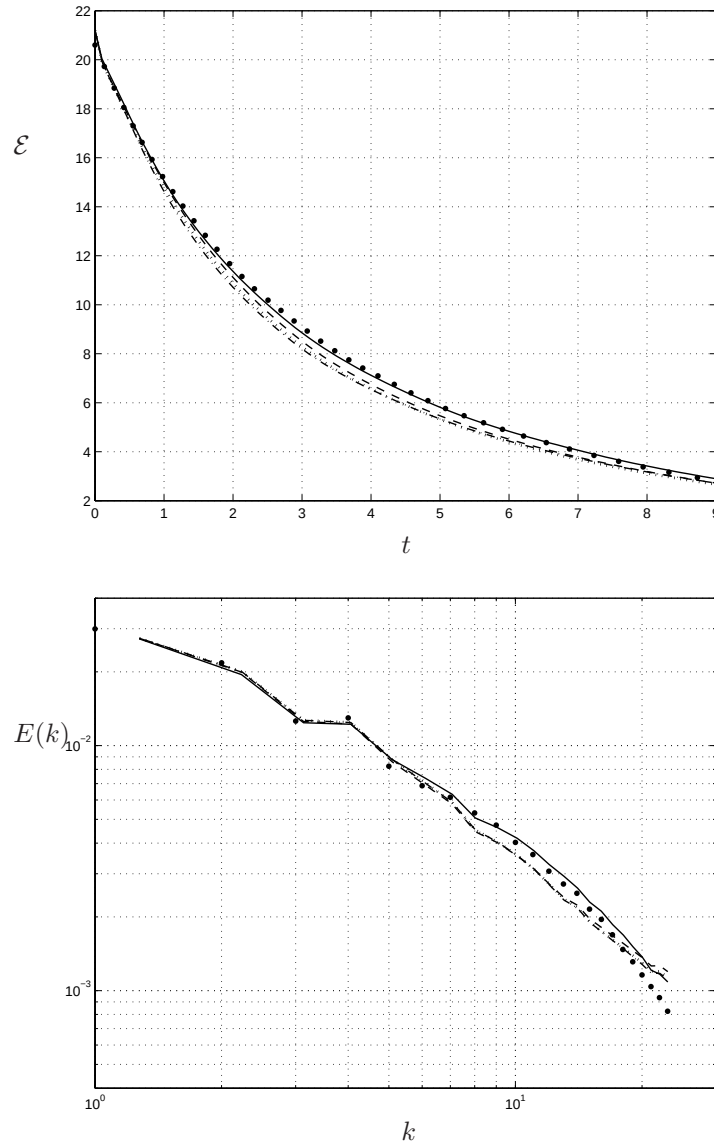


Figure 3.5: 48^3 LES at moderate Reynolds number using Type II models: Evolution of the enstrophy (top) and energy spectra at $t = 3.33$ (bottom): RVM with $n = 1$ (dot), RVM2 with $n = 1$ (dash), FSF2 with $n = 1$ (dash-dot), RVM with $n = 3$ (solid) and truncated 256^3 DNS (bullets).

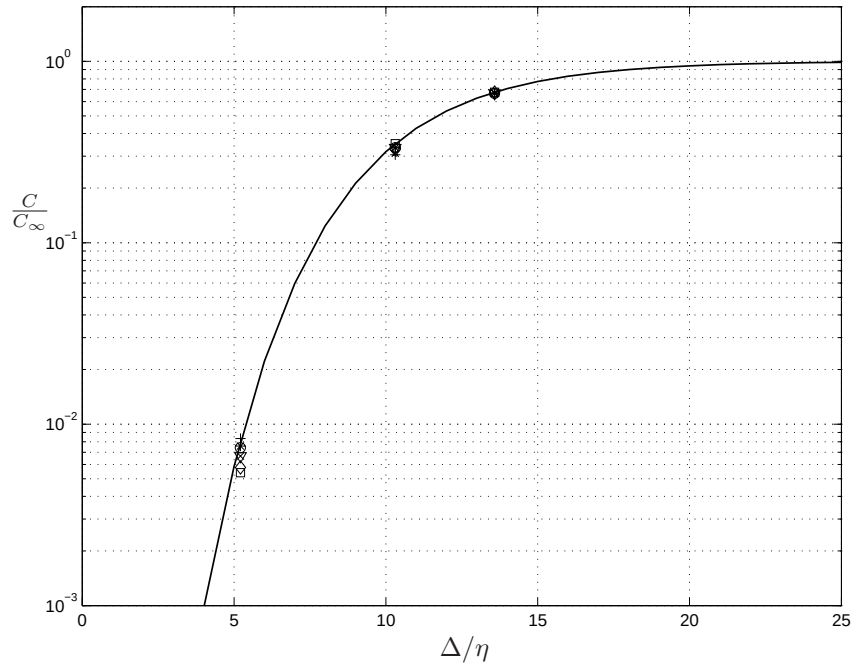


Figure 3.6: SGS model coefficients obtained from 48^3 , 64^3 and 128^3 LES of 256^3 DNS: SMAG (circle), SMAG2 with $n = 1$ (cross), RVM with $n = 1$ (plus), RVM2 with $n = 1$ (star), FSF with $n = 1$ (square), FSF2 with $n = 1$ (diamond), RVM with $n = 3$ (triangle) and the proper fit of Eq. (3.5) (solid)

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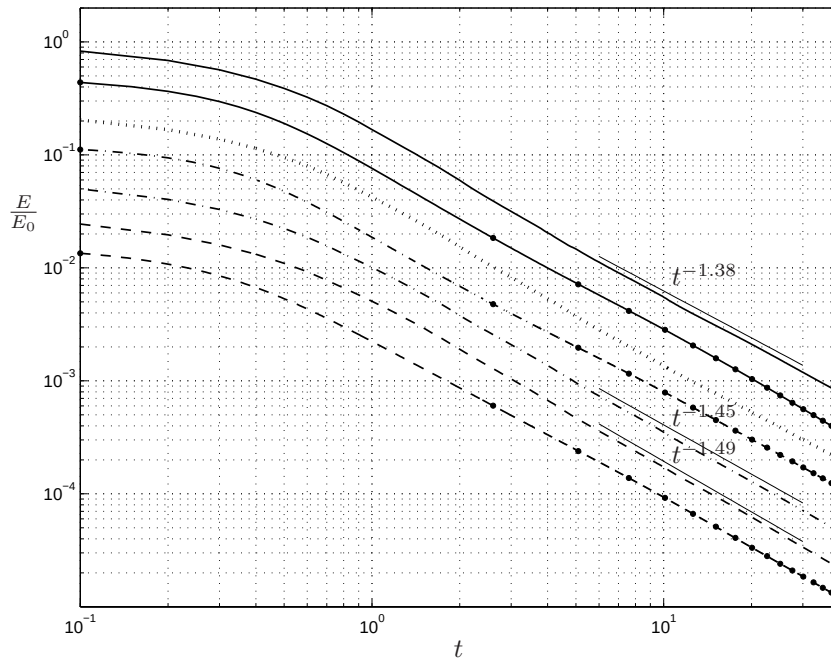


Figure 3.7: 128^3 LES at very high Reynolds number: Evolution of the energy (the curves are shifted vertically by 0.5 to better distinguish them): 1) using the VIC method: SMAG (dash), FSF with $n = 1$ (dash-dot), RVM with $n = 1$ (dot) and RVM with $n = 3$ (solid); 2) using the pseudo-spectral method: SMAG (dash with bullets), HV (dash-dot with bullets) and RVM2 with $n = 3$ (solid with bullets).

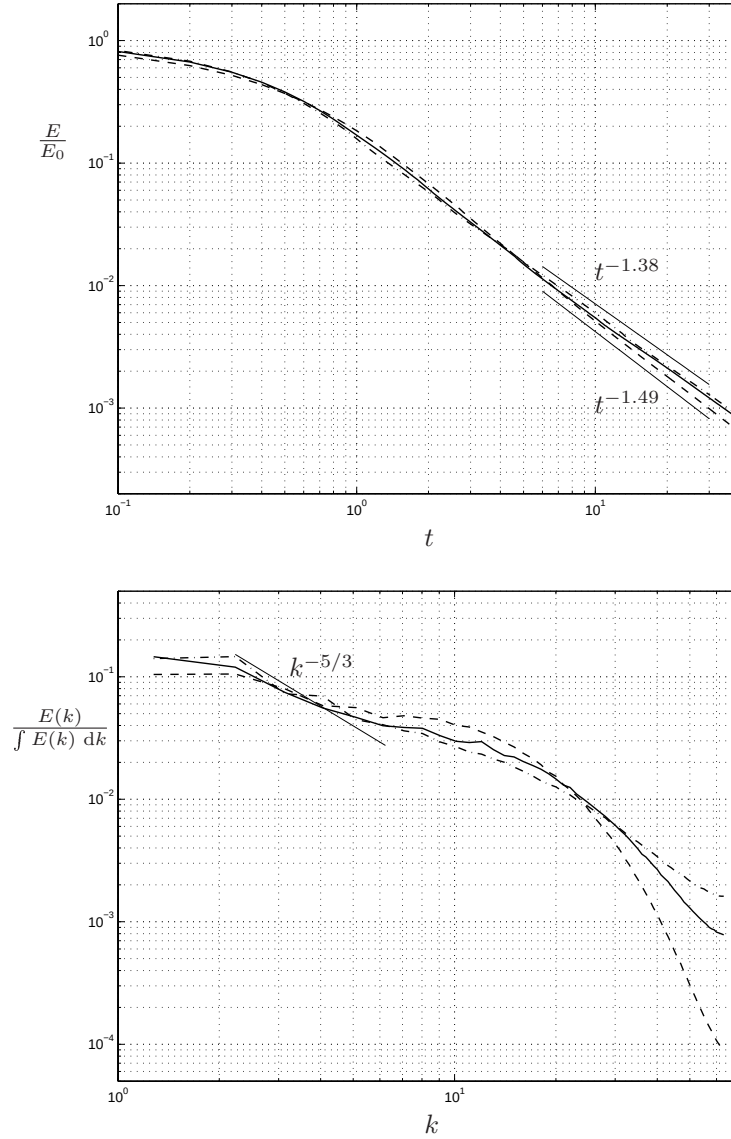


Figure 3.8: 128^3 LES at very high Reynolds number: Evolution of the energy (top) and the normalized energy spectra at $t = 20$ (bottom) using the VIC method with the RVM model ($n = 1$): $C = C_R = 0.036$ (solid), $C = 5C_R$ (dash) and $C = C_R/5$ (dash-dot).

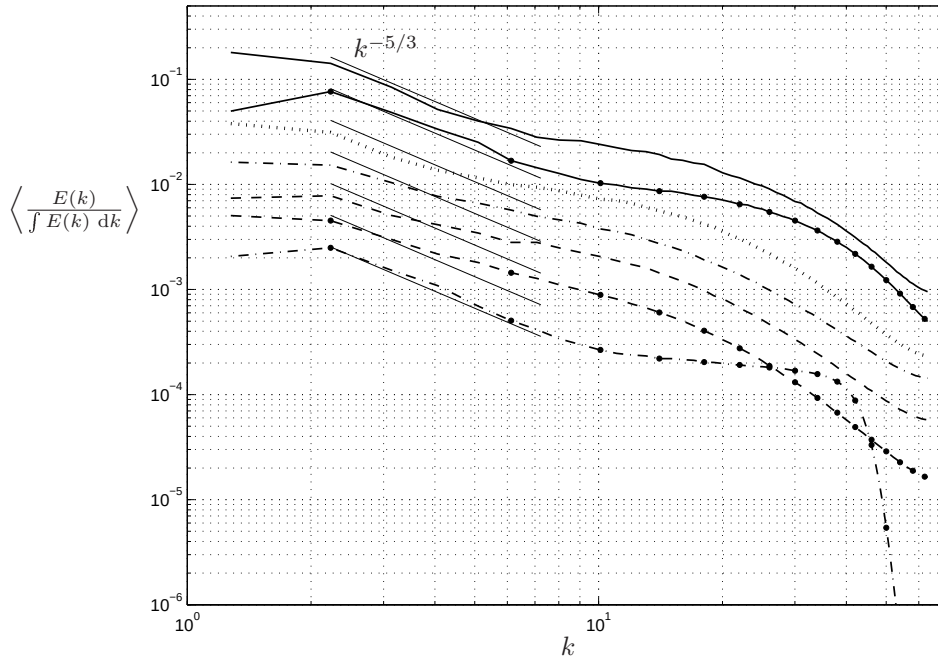


Figure 3.9: 128^3 LES at very high Reynolds number: normalized energy spectra (also time-averaged between $t = 10$ and 40 ; the curves are shifted vertically by 0.5 to better distinguish them): 1) using the VIC method: SMAG (dash), FSF (dash-dot), RVM with $n = 1$ (dot) and RVM with $n = 3$ (solid); 2) using the pseudo-spectral method: SMAG (dash with bullets), HV (dash-dot with bullets) and RVM2 with $n = 3$ (solid with bullets).

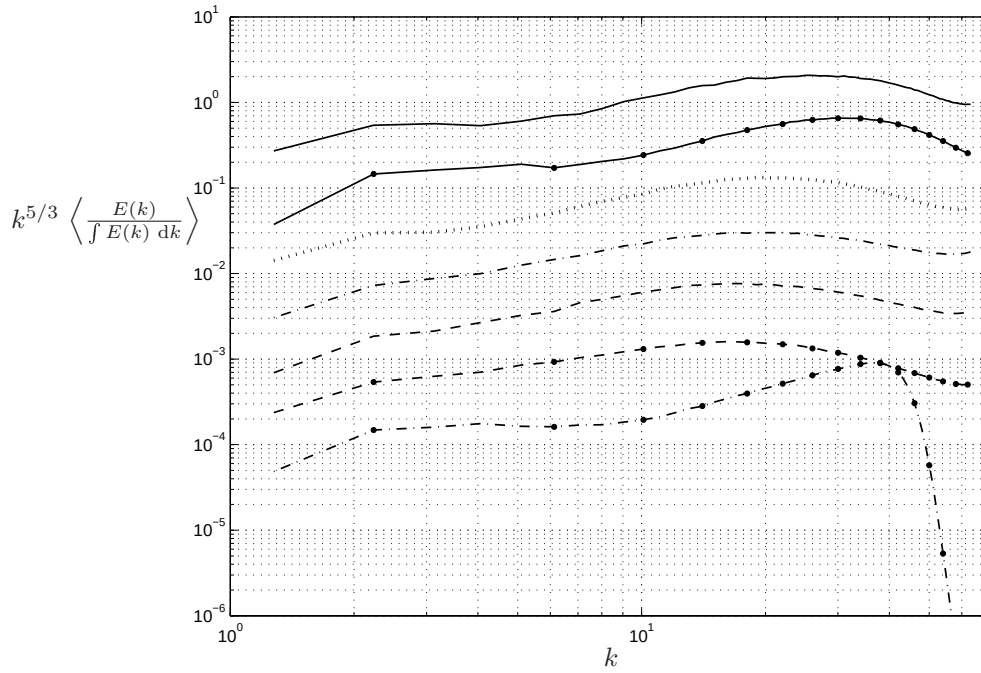


Figure 3.10: 128^3 LES at very high Reynolds number: compensated and normalized energy spectra (also time-averaged between $t = 10$ and 40 ; the curves are shifted vertically by 0.5 to better distinguish them): 1) using the VIC method: SMAG (dash), FSF (dash-dot), RVM with $n = 1$ (dot) and RVM with $n = 3$ (solid); 2) using the pseudo-spectral method: SMAG (dash with bullets), HV (dash-dot with bullets) and RVM2 with $n = 3$ (solid with bullets).

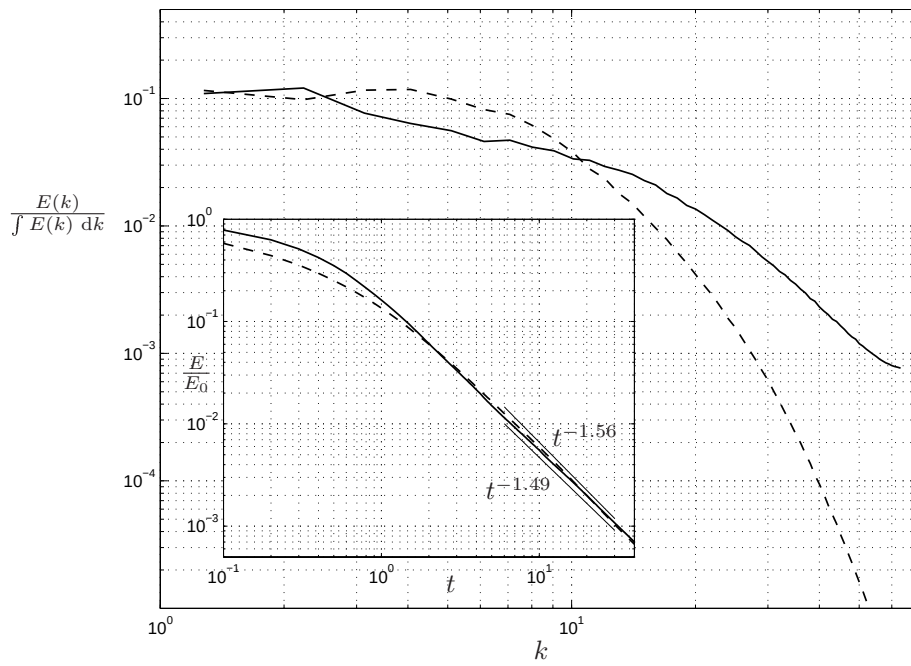


Figure 3.11: 128^3 LES at very high Reynolds number: normalized energy spectra at $t = 20$ using the VIC method with the SMAG model: $C_S = 0.027$ (solid) and $C_S = 0.27$ (dash). Insert: dimensionless energy evolution for both coefficient value.

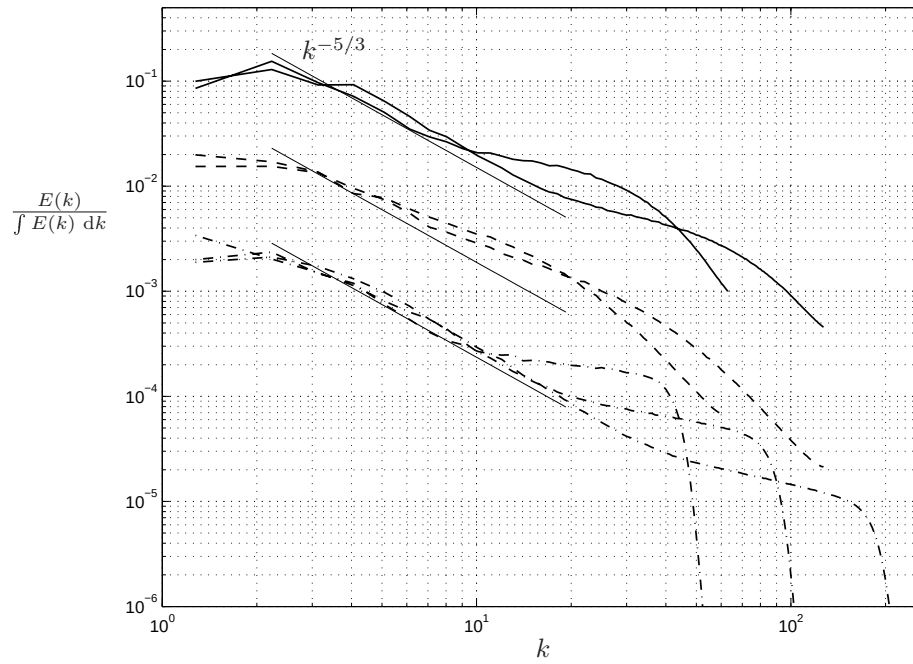


Figure 3.12: LES at very high Reynolds number: Asymptotic behavior of the normalized energy spectra when using larger grids (pseudo-spectral method at $t = 20$; the curves are shifted vertically by 0.125 to better distinguish them): RVM2 with $n = 3$ on 128^3 and 256^3 grids (solid), SMAG on 128^3 and 256^3 grids (dash), HV on 128^3 , 256^3 and 512^3 grids (dash-dot).

3.5. Conclusions

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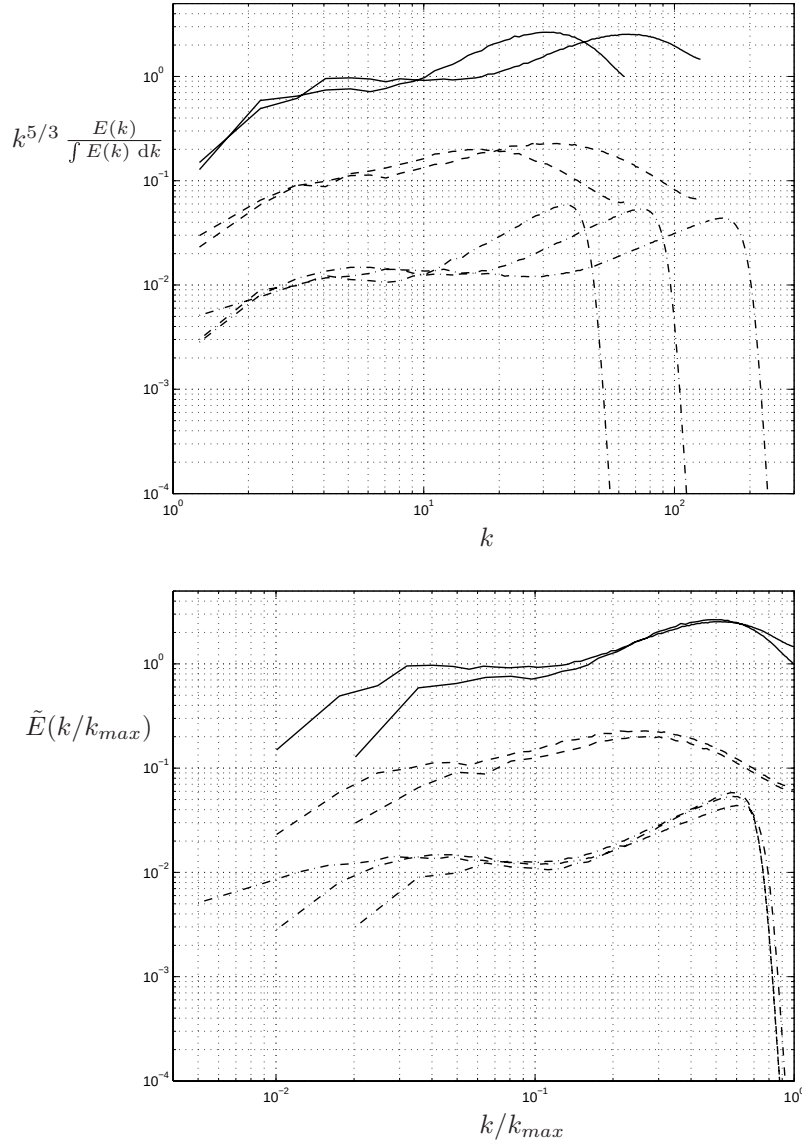
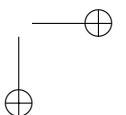
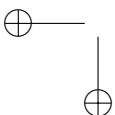
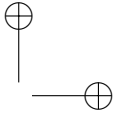
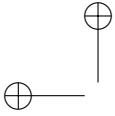


Figure 3.13: LES at very high Reynolds number: Asymptotic behavior of the compensated and normalized energy spectra when using larger grids (top) and illustration of the shape similarity in the dissipation range (bottom) (pseudo-spectral method at $t = 20$; the curves are shifted vertically by 0.125 to better distinguish them): RVM2 with $n = 3$ on 128^3 and 256^3 grids (solid), SMAG on 128^3 and 256^3 grids (dash), HV on 128^3 , 256^3 and 512^3 grids (dash-dot).



Chapter 4

Counter-rotating four vortex system

A part of the following results was obtained within the AWIATOR project leading to an article entitled *Large-eddy simulation of wake vortex flows at very high Reynolds numbers: a comparison of different methodologies*, to be submitted to *Aerosp. Sci. Tech.* in 2007. The authors are L. Dufresne, R. Baumann, T. Gerz, G. Winckelmans, H. Moet, R. Capart, R. Cogle and L. Nybelen.

A part of this section was also written within the FAR-Wake project as a technical report entitled *Numerical simulations of counter-rotating four vortex systems*, European project AST4-CT-2005-012238, Report TR1.2.2-2, January, 2007. The authors are O. Desenfans, T. Lonfils, G. Daeninck, R. Cogle, L. Bricteux, L. Dufresne and G. Winckelmans.

4.1 Introduction

This chapter presents the results of temporal and spatial developing simulations of counter-rotating four vortex system (4VS). It is known that 4VS undergo 3-D instabilities more rapidly than what is observed in 2VS, with their more standard long or short wavelength instabilities. A proper assessment of the efficiency of these rapidly growing instabilities as a means for wake alleviation requires to follow

the dynamics of the vortices over a significant period of time. Instabilities need to develop far into the nonlinear regime before the resulting interactions between the vortices can lead to a significant decay of the vortex system.

The chapter is divided in three parts. In the first one, we redefine the reference scales and the diagnostics used to make quantitative comparisons between the results. In the next section, we present the results of a time-developing DNS simulation performed at a low Reynolds number and on a small longitudinal extent. In the last section, we analyze the results of time-developing (TD) and space-developing (SD) LES simulations performed at very high Reynolds number and on a large longitudinal extent.

4.2 Definition and diagnostics

The global definition of the 4VS was already given in Chapter 2. One of the analysis performed within the FAR-Wake project was to analyze the influence of the Γ_2/Γ_1 ratio on the dynamics of the 4VS. This imposes to redefine the reference scales used, to allow comparisons between the different cases. They are thus slightly different from those used within the AWIATOR project and in Chapter 2.

The reference length is here b_1 and is set constant. We also set $b_2 = 0.3 b_1$. This means that we set the geometry. All systems have the same lift. When $\Gamma_2 \rightarrow 0$, we obtain the "reference" two-vortex system (2VS) with circulation Γ_0^* and spacing $b_0^* = b_1$. This system also defines the reference velocity scale $V_0^* = \Gamma_0^*/(2\pi b_0^*)$ and the reference time scale $t_0^* = b_0^*/V_0^* = 2\pi (b_0^*)^2/\Gamma_0^*$. All quantities in this chapter will be written in dimensionless form using these references scales.

The 4VS total half plane circulation is

$$\Gamma_0 = \Gamma_1 + \Gamma_2 \quad (4.1)$$

The "equivalent" 2VS (as used in Chapter 2, and thus not the reference 2VS) is the system with circulation Γ_0 and spacing b_0 (spacing between vorticity centroids) of same lift, obtained from

$$\Gamma_0 b_0 = \Gamma_1 b_1 + \Gamma_2 b_2 \quad (4.2)$$

and thus

$$b_0 = \frac{(\Gamma_1 b_1 + \Gamma_2 b_2)}{\Gamma_0} . \quad (4.3)$$

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Table 4.1: Useful numbers related to the references scales for different cases $\frac{\Gamma_2}{\Gamma_1}$.

$\frac{\Gamma_2}{\Gamma_1}$	$\frac{\Gamma_0}{\Gamma_1}$	$\frac{\Gamma_0^*}{\Gamma_1}$	$\frac{\Gamma_0}{\Gamma_0^*} = \frac{b_0^*}{b_0} = \frac{b_1}{b_0}$	$\frac{b_1 V_0^*}{\Gamma_1}$	$\frac{\Gamma_1 t_0^*}{b_1^2}$
0	1	1	1	0.1592	6.283
-0.10	0.90	0.970	0.9278	0.1544	6.478
-0.15	0.85	0.955	0.8901	0.1520	6.579
-0.20	0.80	0.940	0.8511	0.1496	6.684
-0.25	0.75	0.925	0.8108	0.1472	6.793
-0.30	0.70	0.910	0.7692	0.1448	6.905

This system defines the velocity $V_0 = \Gamma_0/(2\pi b_0)$ and the time $t_0 = b_0/V_0 = 2\pi b_0^2/\Gamma_0$. Because all systems have the same lift, we have

$$\Gamma_0 b_0 = \Gamma_1 b_1 + \Gamma_2 b_2 = \Gamma_0^* b_0^* = \Gamma_0^* b_1 \quad (4.4)$$

We thus obtain

$$\frac{\Gamma_0}{\Gamma_1} = \left(1 + \frac{\Gamma_2}{\Gamma_1}\right) \quad (4.5)$$

$$\frac{\Gamma_0^*}{\Gamma_1} = \left(1 + \frac{\Gamma_2 b_2}{\Gamma_1 b_1}\right) \quad (4.6)$$

and thus also

$$\frac{\Gamma_0}{\Gamma_0^*} = \frac{b_0^*}{b_0} = \frac{b_1}{b_0} = \frac{\left(1 + \frac{\Gamma_2}{\Gamma_1}\right)}{\left(1 + \frac{\Gamma_2 b_2}{\Gamma_1 b_1}\right)}. \quad (4.7)$$

Note that the reference time t_0^* is easily related to:

$$\frac{t_0^*}{t_0} = \left(\frac{b_0^*}{b_0}\right)^2 \frac{\Gamma_0}{\Gamma_0^*} = \left(\frac{b_0^*}{b_0}\right)^3 = \left(\frac{\Gamma_0}{\Gamma_0^*}\right)^3 \quad (4.8)$$

Table 4.1 provides the numbers for different cases Γ_2/Γ_1 (within the FAR-Wake project, the $\Gamma_2/\Gamma_1 = -0.1$, -0.2 and -0.3 cases were investigated, here we limit our investigation to the $\Gamma_2/\Gamma_1 = -0.3$ case). As previously discussed in Chapter 2, the core size radii are set to $a_1/b_1 = 0.075$ and $a_2/a_1 = 2/3$.

After making some qualitative analysis of the 4VS dynamics based on averaged 2-D and 3-D visualizations, quantitative comparisons between the results will be done by considering energy diagnostics, instabilities and vortex characterization.

The energy diagnostics and instabilities characterizations were already presented in Section 2.3.2. For the vortex characterization, we consider only the diagnostics on the longitudinally averaged vorticity fields. For the 3-D vorticity vector field $\omega(\mathbf{x}, t)$, we write, following our previous convention,

$$\tilde{\omega}(\tilde{\mathbf{x}}, t) = \frac{1}{L_x} \int_0^{L_x} \omega(\mathbf{x}, t) dx . \quad (4.9)$$

In what follows, we limit our discussion to the behavior of the right-hand side (or rhs) part of the averaged wake vortex system, i.e., for the half y - z plane with $y \geq 0$. The first quantity we examine is the half-plane total circulation

$$\tilde{\Gamma}_0 = \iint_{y \geq 0} \tilde{\omega}_x(y, z) dydz . \quad (4.10)$$

for the rhs plane $y \geq 0$. A similar definition can be applied to region where $y \leq 0$ and which is identified as the left-hand side (or lhs) plane. The averaged half-plane circulation $\tilde{\Gamma}_0$ is to remain constant unless there is a net exchange of vorticity between the two half planes.

The second integral quantity we consider is the positive vorticity circulation

$$\tilde{\Gamma}_1 = \iint_{y \geq 0} \tilde{\omega}_x^+(y, z) dydz , \quad (4.11)$$

where

$$\tilde{\omega}_x^+ = \begin{cases} \tilde{\omega}_x & \text{if } \tilde{\omega}_x > 0 , \\ 0 & \text{if } \tilde{\omega}_x \leq 0 . \end{cases}$$

and which initially corresponds to the primary vortex circulation Γ_1 .

With these two definitions, the ratio $\tilde{\Gamma}_1/\tilde{\Gamma}_0$ can be seen as a measure of the efficiency of the merging of both primary and secondary vortices. In the limit $\tilde{\Gamma}_1/\tilde{\Gamma}_0 \rightarrow 1$, we end up with a complete homogenization of the half-plane (longitudinal) vorticity. Following again these definitions, the value of $\tilde{\Gamma}_0$ gives a measure of the vorticity exchange between the lhs and rhs half planes. As long as there is no mid-plane ($y = 0$) vorticity exchange, $\tilde{\Gamma}_0$ is conserved.

Another important quantity that will be considered for the characterization of the individual vortices is the maximum of the circulation profile:

$$\tilde{\Gamma}_{max} = \max [\tilde{\Gamma}(r)] . \quad (4.12)$$

This quantity is a good indicator of the total circulation contained in the primary vortex. To evaluate $\tilde{\Gamma}_{max}$, the vortex circulation profile is needed. It is determined using

$$\tilde{\Gamma}^+(r) = \int_0^{2\pi} \int_0^r \tilde{\omega}_x^+(r', \theta) r' dr' d\theta \quad (4.13)$$

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where the integration radius is taken from the centroid of the positive vorticity field that are naturally determined by

$$y_c = \frac{1}{\tilde{\Gamma}_1} \int \int_{y \geq 0} y \tilde{\omega}_x^+(y, z) dy dz \text{ and } z_c = \frac{1}{\tilde{\Gamma}_1} \int \int_{y \geq 0} z \tilde{\omega}_x^+(y, z) dy dz . \quad (4.14)$$

Knowing the circulation profile, we can then evaluate the vortex induced tangential velocity using

$$\tilde{u}_\theta = \frac{\tilde{\Gamma}^+(r)}{2 \pi r} . \quad (4.15)$$

The determination of the "effective vortex core radius" r_c naturally follows as the point of maximum azimuthal velocity, i.e. the point r such that:

$$\tilde{u}_\theta(r_c) = \max [\tilde{u}_\theta(r)] . \quad (4.16)$$

The evolution of the structure of the main vortex can be measured in a more global manner by considering the partial radial averaging of the circulation defined by

$$\tilde{\Gamma}_{avg} = \frac{1}{b/6} \int_{b/12}^{b/4} \tilde{\Gamma}^+(r) dr , \quad (4.17)$$

in which b represents the span of the reference wing. This average circulation is often referred to as Γ_{5-15} , assuming a reference wingspan of 60 meters. Here, we assume that the case of the reference 2VS has an elliptical loading. We thus have $b_0^* = b_1 = \frac{\pi}{4} b$: this value can be considered typical of the vortex spacing behind a commercial aircraft. The use of the $\tilde{\Gamma}^+$ profile furthermore provides a conservative upper-bound diagnostics because it only accounts for single sign (positive) instead of total vorticity.

The last averaged circulation diagnostics relates to the rolling moment that would be exerted on a simple elliptically loaded wing making a centered and instantaneous encounter with the main vortex. The resulting rolling moment, in this particular situation, is determined from the anti-symmetric modification of the effective angle of attack of the encountering wing due to the vertical velocity induced by the encountered vortex. Applying this approach to our main (positive) vortex, we write the equivalent rolling moment coefficient $\tilde{C}_R$ as

$$\tilde{C}_R = \frac{4}{\pi} \int_0^1 \tilde{\Gamma}^+(\xi) \sqrt{1 - \xi^2} d\xi , \quad (4.18)$$

in which $\xi = r/(b/2)$. Here too, the use of $\tilde{\Gamma}^+$ provides an admittedly conservative estimate of the diagnostics in terms of vortex hazard assessment as it neglects the

contribution of negative vorticity coming from the secondary vortex; in terms of purely quantitative comparisons between the different data sets, it provides another integral measure of the vorticity field. One may further note that if $\tilde{\Gamma}_{avg}$ can be considered as partial or local averaging of the vortex circulation, then $\tilde{C}_R$ can be viewed as a weighted average circulation of the vortex.

4.3 DNS at moderate Reynolds number

4.3.1 Time-developing simulation

In this section, we present the results of a time-developing DNS simulation performed at a low Reynolds number and on a small longitudinal extent. The objective was here to make a preliminary investigation of the most unstable medium-wavelength instabilities for wake systems with counter-rotating vortices. It was shown theoretically by Fabre *et al.* [26] that this system is very unstable to medium-wavelength instabilities developing on the secondary vortices. This was confirmed experimentally by Ortega *et al.* [55], for a case with slightly different parameters from those used here.

Initially, the centerline of the vortices are perturbed in the spanwise direction using a sine function with a wavenumber equal to the most unstable mode ($k_m = 2\pi/\lambda_m = 6.39/b_1$) and with a displacement amplitude $\epsilon/b_1 = 10^{-6}$. The length of the computational box is chosen equal to the most unstable wavelength: $L_x = 0.983 b_1$.

The results are compared with the solutions obtained using a pseudo-spectral code with dealiasing (L. Dufresne). Of course, in this code, the computational box is periodic in the three directions. To simulate the unbounded flow in the y and z directions, the box size was taken large in these two directions. The same discretization was used (i.e., same h) in both methods. For the spectral method, the box size was $64h \times 320h \times 192h$. The spectral method is energy conserving and has zero dispersion; it is thus a good reference to make quantitative comparisons with the VIC-PFM method.

The simulation was done at $Re = \Gamma_0/\nu = 3500$. The time step was $\Delta t/t_0 \approx 3.3 \cdot 10^{-4}$, the simulation was carried out for 4000 time steps and took ~ 55 hours on one Pentium IV CPU at 2.4 GHz. Fig. 4.1 provides a view of the solution at several times. One clearly observes the development of the medium wavelength instabilities on the secondary vortices (the so called " Ω loops"), which then leads,

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after viscous interaction with the primary vortices and partial reconnection (partial because the vortex circulations are different), to a complex three-dimensional flow.

Fig. 4.2 shows the total kinetic energy and the kinetic energy of the base flow (mode $k_x = 0$, thus the 2-D flow corresponding to the longitudinal average of the 3-D flow) computed using the VIC-PFM code and using the spectral code. The results are very similar, although, for $t/t_0 > 0.8$, the VIC-PFM energy curve is a little above the spectral curve: partially due to a too small dissipation during the strong interactions (i.e. when the mesh Reynolds number $Re_h = \|\omega\|_{max} h^2/\nu$ becomes too large to respect the criteria of a well-resolved DNS), but also because of the different boundary conditions. The difference between the total kinetic energy and the kinetic energy of the base flow is a good quantitative representation of the three-dimensionality of the flow. Here, one can observe that, before the strong viscous interaction between the vortices, the flow is laminar (energy decay solely due to core spreading of the vortex tubes); it becomes more complex (i.e., "turbulent") after the strong interaction between the primary and secondary vortices. Fig. 4.2 shows the evolution of the modal kinetic energy E_{k_x} for the base flow ($k_x = 0$), the perturbation mode $k_x = k_m$ and its two first harmonics using the VIC-PFM method and using the spectral method. Again, one can see that the growth rates of each mode compare well between the two methods, and that the saturation of the instability, which occurs at time $t/t_0 \approx 0.8$, is also the same for both methods.

4.4 LES at very high Reynolds number

4.4.1 Time-developing simulation

In this section, we present additional results of the TD LES simulations presented in Section 2.3 and performed using both the VIC-PFM method and the pseudo-spectral (PS) method. We are here more interested about the physical behavior of the 4VS at very high Reynolds, than about the capabilities of the SGS model used.

Global wake dynamics. Figure 4.5 presents the evolution of the wake topology evolution of the 4VS computed using the VIC-PFM method and the PS method. The solutions are shown for various dimensionless times. The visualizations show two isosurfaces of the constant vorticity modulus and are made using a coarser grid (one visualization point for every two computational points, in all three directions).

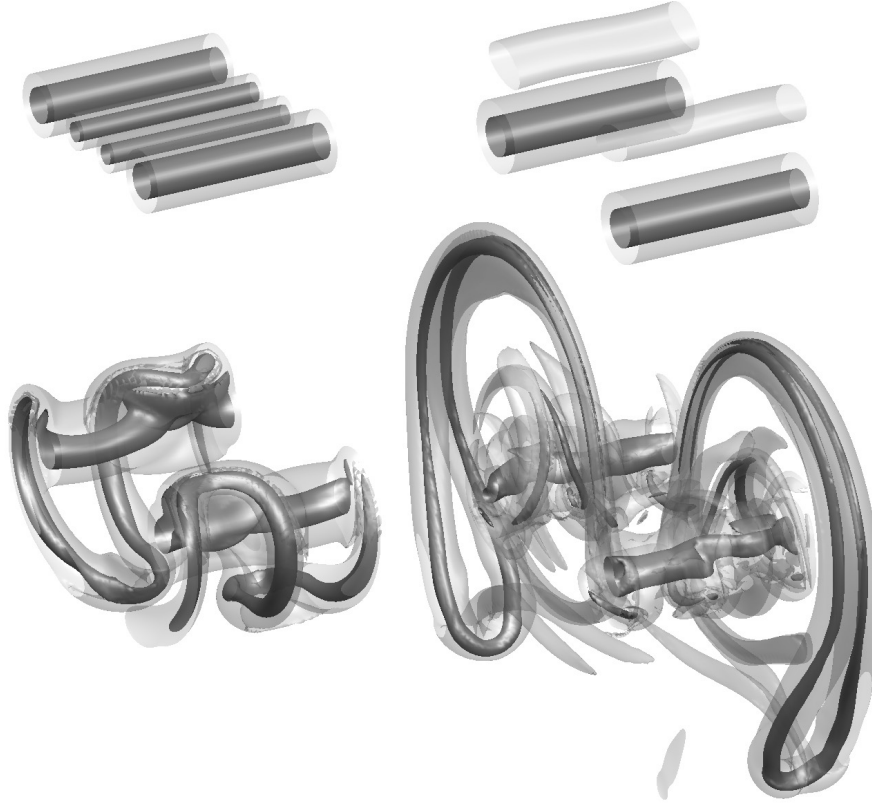


Figure 4.1: Counter-rotating four vortex system at $Re = 3500$ illustrated for one computational periodicity length. Two isosurfaces of vorticity are shown : $\|\omega\|b_1^2/\Gamma_1 = 10.0$ (opaque) and 2.0 (semi-transparent). The grey scale is proportional to the axial vorticity ω_x . Times shown are: $t/t_0 = 0.0$, the initial condition; $t/t_0 = 0.47$, the medium wavelength instability is already visible; $t/t_0 = 0.79$, beginning of the strong interaction between the vortices (the Ω loops are clearly visible); $t/t_0 = 1.10$, after partial viscous reconnection (small scales are seen, as well as further stretching of the secondary loops).

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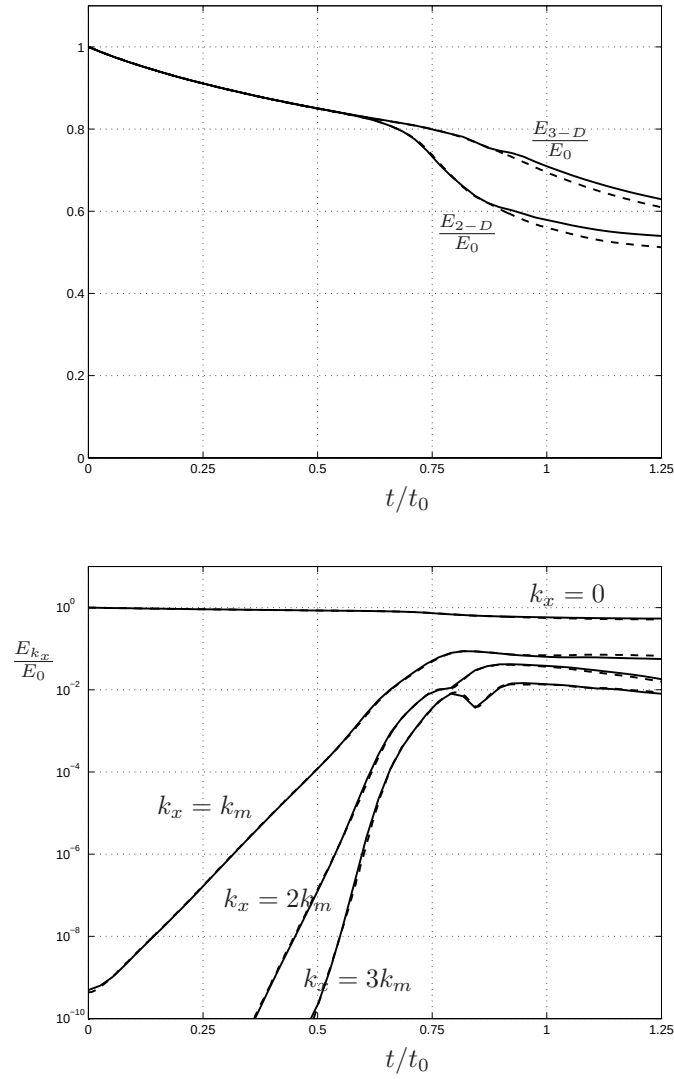


Figure 4.2: Counter-rotating four vortex system at $Re = 3500$: energy of the 3-D flow and energy of the 2-D (y, z) base flow (top) and modal kinetic energy evolution (bottom) using the VIC-PFM method (solid) and using the spectral method (by L. Dufresne, dashed).

What can be seen in Figure 4.5 is that, for both methods, the secondary vortices achieve one complete revolution around the primary ones before the instabilities become developed enough to be observed. Once they are visible, the instabilities expand quickly and the secondary vortices eventually interact with the primary ones. The interaction between the secondary and the primary vortices occurs slightly sooner in the VIC-PFM simulation, due to the initial random perturbation which is not exactly the same in the two cases.

As previously shown with the modal energy analysis presented in Section 2.3.2, one can clearly see, in Figure 4.5, that at least two types of instabilities appear: medium wavelength instabilities ($\lambda/b_1 = \mathcal{O}(1)$) which mainly develop in anti-symmetrical " Ω -loops" and short wavelength core instabilities ($\lambda/b_1 = \mathcal{O}(0.1)$), also called elliptic instabilities. This is more clearly shown in Figure 4.6 which exposes top and side views of the 4VS (using the VIC-PFM method) for different times during the phase of instability development. One can see that there is a competition between the medium wave instabilities and the short wave instabilities (see at $\tau = 2.20$). Looking further in time, at $\tau = 2.32$, it can be concluded that the medium wave instabilities finally win (this is confirmed by the modal energy analysis) and preferentially develop in anti-symmetrical " Ω -loops".

Figure 4.7 shows a comparison, at different times, of the averaged vorticity fields $\tilde{\omega}_x$ using both methods. The non zero vorticity modulus $|\tilde{\omega}|$ regions are shown and are colored according to the sign of $\tilde{\omega}_x$: red for $\tilde{\omega}_x > 0$, blue for $\tilde{\omega}_x < 0$, and white for $\tilde{\omega}_x = 0$. As observed in the 3-D visualizations (Figures 4.5 and 4.6), one sees that the secondary vortices remain essentially 2-D over one complete orbit. The averaged vorticity in the secondary vortices then rapidly decreases when the instabilities develop significantly and when the secondary vortices partially reconnect with the primary ones. Indeed, since they do not have the same circulation ($\Gamma_2 \neq \Gamma_1$), the reconnection cannot fully occur: it is a partial reconnection, which itself can only happen by producing small scales (turbulence) and also significant "vortex bursting" events (which themselves also produce small scales, see also [25]). One can also already observe that the periodic boundary conditions imposed with the PS method clearly influence the global position of the vortices. At $\tau = 1.62$, using the VIC-PFM, the primary vortices are located at $z/b_0^* \approx -1.2$ while they are located at $z/b_0^* \approx -1.0$ using the PS method. The difference still grows up for longer time as one can observe for $\tau > 2.50$.

The trajectories obtained with both methods are superimposed in Figure 4.8. As was concluded from the previous 2-D views, the averaged trajectories are not exactly

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the same; nevertheless the global "orbital" movement is similar. One can note that the loops made by the secondary vortices around the primary ones are similar in the spanwise direction but have not the right descent velocity. This difference with the spectral method was also observed with vortex filament simulation results where true "open domain" boundary conditions in the transverse directions are also imposed (as in the VIC-PFM method), in opposition to the periodic boundary conditions where the vortex dynamics are affected by the "image" vortices.

Circulations analysis. The averaged circulation profiles $\tilde{\Gamma}^+(r)$ (Eq. (4.13)) are shown in Figure 4.9 for various times. As expected, for both methods, the averaged circulation profiles (centered on the primary vortex) are very similar. From the time evolution of the circulation profile, one can see that the primary vortex is initially almost not affected by the secondary vortex (up to $\tau \simeq 2.20$). After this initial phase, the secondary vortices start to interact with the primary ones. Due to these interactions, the circulation profiles become flatter and the maximum values decrease. The system has essentially become turbulent and the opposite sign vorticity has mixed with the primary vorticity.

Figure 4.10 shows the averaged azimuthal velocity profiles for various time. One can observe that the profiles obtained with the VIC-PFM method slightly decrease during the initial phase of the flow (up to $\tau = 2.20$) whereas the PS method better conserves the profiles. It indicates that, at such very high Reynolds number, the VIC-PFM method tends to be slightly more diffusive than the spectral method. This is confirmed with Figure 4.11 where one observes that the main vortex characteristic radius r_c obtained using the VIC-PFM method slightly grows during the "laminar" phase of the flow. After the interaction between the primary and secondary vortices, the velocity profiles becomes rapidly flatter and the characteristic radius also quickly grows.

The half-plane total circulation $\tilde{\Gamma}_0$, the half-plane positive circulation $\tilde{\Gamma}_1$, the maximum of the circulation profile $\tilde{\Gamma}_{max}$ and the average circulation $\tilde{\Gamma}_{5-15}$ are shown in Figure 4.12. This figure highlights clearly what has been concluded from Figure 4.9: there is no interaction between the primary and the secondary vortices for $\tau \lesssim 2.20$, leading to a conservation of $\tilde{\Gamma}_0$, $\tilde{\Gamma}_1^+$ and $\tilde{\Gamma}_{5-15}$. This constant circulation phase is followed by a complex transition phase, when the secondary vortices interact with the primary ones with partial (i.e., incomplete) reconnection, vortex bursting, generation of small scales and of turbulence. Finally, after those complex interactions ($\tau \simeq 3.5$), the 4VS becomes a decaying 2VS (see Figure

4.7). The same behavior is observed for the evolution of the rolling moment in Figure 4.13. The curve is very similar to that of $\tilde{\Gamma}_{5-15}$. Thanks to the strong interaction, the rolling moment, and so the dangerousness, rapidly decreased to attain $\sim 50\%$ of its initial value at $\tau \approx 3.5$.

4.4.2 Space-developing simulation

This section is dedicated to the space-developing simulation. Such simulation was also performed in the FAR-Wake subtask 3.1.2 entitled “Spatially-evolving wakes” (see Daeninck *et al.* [22]). We first describe how the 4VS is defined for a space-developing simulation and how the simulation is configured. Then, we present and analyze the results.

Wake definition and simulation configuration

The counter-rotating 4VS studied with the space-developing method is the same as in the previous section. The quantities Γ_0 , b_0 as well as all the reference scales Γ_0^* , b_0^* , and t_0^* are identically defined.

In order to “close” the problem, an inflow and an outflow boundary conditions are used. The inflow condition is imposed by an “artificial” lifting line shedding a vortex sheet and computed such that it generates the desired 4VS. The wake vortex sheet then dynamically evolves, in space and time, due to its own induced velocity and to the velocity induced by the lifting line itself. The outflow boundary condition is imposed by enforcing the no-through flow symmetry on the flow. This ensures that the normal component of vorticity is conserved through the outflow plane and thus allows for a natural outflow condition for wake vortices (see Section 1.2.6).

Figure 4.3 shows a schematic of the spatially developing domain. The effective computational domain for the VIC-PFM method extends between the inflow and outflow plane ($L_x/b_0 = 15.4$). In the transverse directions, the grid size is always adapted automatically to the region where the vorticity is non zero. When computing the boundary conditions with the PFM method, the lifting line vorticity, the inflow vortex sheet and the symmetrized vorticity outflow field are all taken into account. The resulting velocity field thus corresponds to a true open domain calculation of a lifting line and its wake. As was done for the time-developing LES simulations, a quasi-Euler formulation is used, by setting $\nu = 0$. This is thus LES at “very high” (and undefined) Reynolds number. The choice of the wing lift coefficient $C_L = L/(\frac{1}{2}\rho U_\infty^2 S)$ is essential, as it has a direct effect on the spatial

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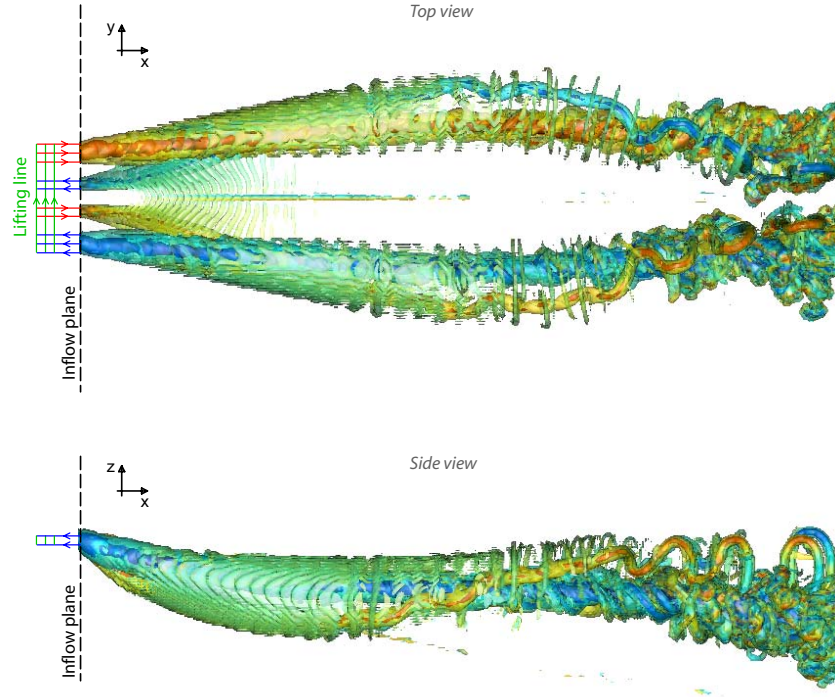


Figure 4.3: Schematic of a part of the spatially developing domain. The lifting line (green) and the initial vortex sheet (red and blue) are located next to the inflow plane.

development of the wake: it basically determines the computational requirements of the longitudinally developing simulation. We will now establish how the C_L value has been set.

The lift is related to $\Gamma_0 b_0$ by :

$$L = \rho U_\infty \int_{-b/2}^{b/2} \Gamma(y) dy = \rho U_\infty \Gamma_0 b_0 \quad (4.19)$$

Remembering that the wing aspect ratio is $A_r = b^2/S$ with b the wing span, we obtain the lift coefficient as

$$C_L = 2 \frac{\Gamma_0 b_0}{U_\infty S} = 2 \frac{\Gamma_0}{U_\infty} \frac{b_0}{b} \frac{A_r}{b}. \quad (4.20)$$

The case of the reference 2VS (Γ_0^* and $b_0^* = b_1$) is assumed to have an elliptical

loading. We thus have that $b_1 = \frac{\pi}{4} b$. This leads to

$$C_L = \frac{\pi^2}{8} \frac{\Gamma_0}{U_\infty} \frac{b_0}{b_1} \frac{A_r}{b_1} = \frac{\pi^2}{8} \frac{\Gamma_0}{\Gamma_1} \frac{b_0}{b_1} \frac{\Gamma_1}{U_\infty} \frac{A_r}{b_1}. \quad (4.21)$$

For the present 4VS with $\frac{\Gamma_2}{\Gamma_1} = -0.3$, we have $\frac{b_0}{b_1} = 1.3$ and $\frac{\Gamma_0}{\Gamma_1} = 0.7$, and thus

$$\begin{aligned} C_L &= 1.123 \frac{\Gamma_1}{U_\infty} \frac{A_r}{b_1} \\ \frac{U_\infty C_L}{A_r} &= 1.123 \frac{\Gamma_1}{b_1}. \end{aligned}$$

The present simulation was done using a very high, and unrealistic, value of $C_L/A_r = 1.35$. The ratio U_∞/V_0^* is thus too low compared to realistic wings (with, say, $C_L/A_r \simeq 0.15 - 0.2$). The high value of C_L/A_r is taken so as to limit the extent of the computational domain required for attaining sufficiently high values of $(L_x/U_\infty)/t_0^*$, thus sufficient development of the 4VS into a fully developed and turbulent 2VS. The extent of the computational domain was set to $L_x/b_1 = 20.0$. We stress that such simulation is to be taken as a proof of concept of what is possible to do in space-developing simulation as of today.

Such a lift coefficient reduces the characteristic distance (i.e., the distance traveled by the wing for the vortex wake to descend by one vortex spacing b_0) to $d_0 = U_\infty t_0 \simeq 9.75 b_0$. The extent of the present computational domain, $L_x/b_1 = 20.0$ and thus $L_x/b_0 \simeq 15.4$, is chosen to be larger than this distance. This case requires about 111 million grid points! A more realistic case, with $C_L/A_r \simeq 0.2$ for example, would require a seven times longer domain (if one wants to reach the same characteristic time in the wake) and thus a seven times larger computational grid!

We used the same spacial resolution as the time-developing calculation $h/b_1 = 1/64 \simeq 1.563 \times 10^{-2}$, thus $h/b_0 \simeq 1.2 \times 10^{-2}$, and it is also uniform in all directions. The time step for the simulation was set to $\Delta t/t_0^* = 7.24 \times 10^{-4}$. The particles were redistributed every 4 time steps. When the established regime was attained, the number of particles was about 26 million and the size of the VIC grid was $L_x/b_1 = 20.0$, $L_y/b_1 = 4.375$ and $L_z/b_1 = 4.845$ (thus $N_x = 1280$, $N_y = 280$ and $N_z = 310$ for a total of 111 million grid points).

Compared to the time-developing simulations, the computation must here be carried on for sufficiently long times for the flow to reach it's regime state (i.e., its statistical equilibrium). Indeed, the flow is initialized with a spatially uniform

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wake. At least one complete flow through time, L_x/U_∞ , (i.e., the time for the flow to completely traverse the computational domain) is required to "evacuate" this initial condition. A visualization of the temporal development of the space-developing simulation showed that the flow had reached a well established regime at $t/t_0^* = 4.34$ (thus after about 1.24 flow through times). Once this regime state is attained, the flow has to be computed further, to attain statistical convergence of the time averaged fields of interest. The averaged fields were considered sufficiently converged at $t/t_0^* = 7.24$ after initialization (i.e., statistics were gathered over $2.9 t_0^*$). The complete simulation required 10,000 time steps.

Contrary to what was done for the time-developing simulations, no explicit perturbation was added. Nevertheless, the discrete procedure used to shed the wake vorticity at the inflow plane introduces some perturbation (at a still fairly low level): this suffices to excite the unstable modes.

Simulation results

The results obtained with the space-developing simulation are presented in this section. These results will be compared (when possible) with the corresponding results of the time-developing simulation performed previously.

Global wake dynamics. Figure 4.14 presents a time sequence of flow snapshots, using two vorticity modulus isosurfaces, $|\omega| t_0^* = 20\pi$ (high opacity) and $|\omega| t_0^* = 4\pi$ (low opacity). They illustrate the wake topology development, from the simulation beginning until the 4VS has reached it's regime.

The three-dimensional dynamics is clearly quite different compared to the corresponding TD case. First, one can observe that the lifting line induces a negative vertical velocity that moves the 4VS down. One can also observe a global spiraling motion of the wake vortices. Finally, one can see that the secondary vortices interact with the primary ones much sooner: before having performed a complete revolution around them. The interaction is initiated by a medium wave instability that propagates on the secondary vortex. This is better illustrated by the time sequence of top and side view shown in Figure 4.15. One can also see that the statistical equilibrium is reached at $t/t_0^* = 4.34$, since the flow topology does not further evolve at later times.

Averaged wake dynamics. Figure 4.16 presents a comparison of SD and TD vorticity contours shown at comparable times. For the space-developing simulation,

the vorticity field corresponds to the longitudinal component of the time averaged vorticity field in distinctive planes behind the lifting line; τ is defined based on the distance in the wake: $\tau = (x/U_\infty)/t_0^*$ (see Figure 4.4). For the time-developing case, the vorticity field is shown at the corresponding times $\tau = t/t_0^*$.

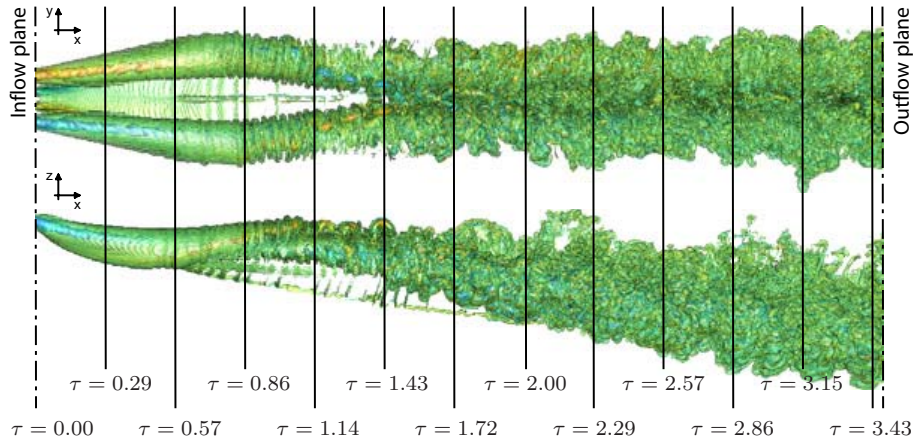


Figure 4.4: Space-developing LES. Top and side view of vorticity modulus isosurfaces, $|\omega| t_0^* = 20\pi$ (high opacity) and 4π (low opacity), colored by the longitudinal vorticity component when the flow has reached its regime state. The locations of the time averaging planes used in Figures 4.16 and 4.18 are also shown. The outflow plane corresponds to $\tau = 3.49$.

As can be seen from these results, the dynamics is essentially identical for time-developing and space-developing simulations up to $\tau \simeq 0.86$. A closer look at $\tau = 0.57$ (0.57 for the SD and 0.58 for the TD) shows that interactions between the secondary vortices and the primary ones have already begun in the SD case: the secondary vorticity is already rolled up in the primary vorticity and the secondary vortices are already stretched. One can also clearly observe the effect of the lifting line in the SD simulation: the 4VS is shifted down by its induced velocity.

After that time, for the SD case, secondary vortices interact with the primary ones (from $\tau = 1.14$ to $\tau = 1.43$), leading quickly to a turbulent flow state ($\tau \geq 2.57$). As seen in the previous section, the TD secondary vortices interact much later (after one complete revolution) with the primary ones.

Figure 4.17 shows the trajectories of the primary vortex centers. Comparing the SD trajectories with the TD ones (Figure 4.8), we observe that the SD trajectories are somewhat vertically stretched. Looking at the altitude of the most outside

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point of the trajectories (which corresponds to the moment when the secondary vortices have achieved a complete orbit), it is seen that the vortices have a higher downward velocity. This is due to the downwash velocity induced by the lifting line itself in the near wake region.

Axial flow component. An essential feature of the spatial developing flow, that was not discussed so far, is the presence of an axial flow component in the wake vortices. The fact that the roll-up of the vortex sheet occurs in a spiraling manner (instead of parallel vortex lines) introduces a significant tangential vorticity component in the rolled-up vortices. The axial flow corresponds to a velocity deficit in the rolled-up wake vortices. In a simplified and global manner, the result can be seen as the combination of a vortex and an axial jet. The time averaged axial velocity for the SD case is shown in Figure 4.18.

The parameter that determines the type of instabilities that occur in a vortex-jet configuration is related to the swirl number, the ratio between the maximum axial velocity and the maximum tangential velocity:

$$S = \frac{u_{\theta, \max}}{u_{x, \max}}.$$

Here, we obtain $S \approx 1.7$ at $\tau = 0$ and $S \approx 0.6$ at $\tau \approx 1.0$. These low values of the swirl number indicate that the vortices have a relatively strong jet component and will thus be more unstable than in the TD configuration (that has no axial jet). However, we must stress that the strength of the axial velocity component is directly related to the ratio C_L/A_r : a realistic configuration (i.e., $C_L/A_r \simeq 0.2$) will exhibit an axial velocity component about seven times lower than the current configuration ($C_L/A_r = 1.35$). The swirl number will be increased in the same proportion, thus reducing the gap between the temporal and spatial simulations.

Again, the results of the present SD simulations are to be considered with caution: they show interesting trends and differences between TD and SD simulations but they suffer from too low U_∞/V_0^* .

Evolution of diagnostics. Another interesting view of the vortex system is obtained when considering the energy of the averaged 2-D velocity fields (longitudinally space averaged in the TD case and time averaged in the SD case). The time evolution of the cross-plane kinetic energy (i.e., only the transverse components of the velocity) is shown in Figure 4.19. The results are very much in line with

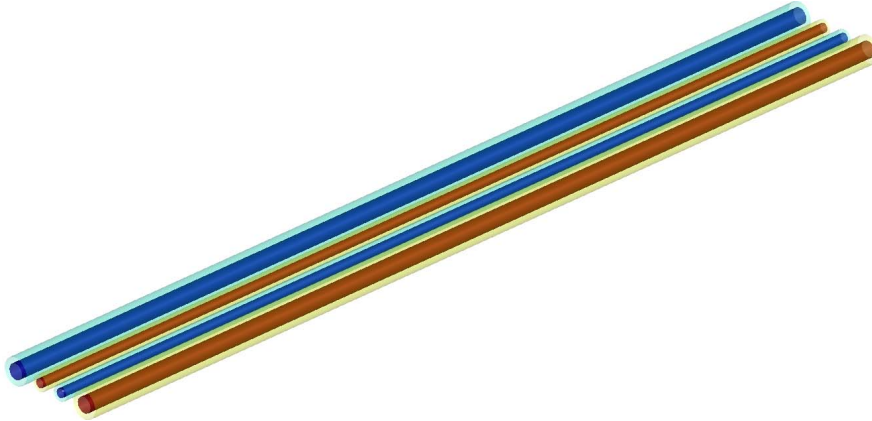
the previous observation. Again, these results show that the SD case transitions to turbulence earlier and thus that the energy decay mechanism is significantly fastened.

4.5 Conclusions

The conclusion of the time-developing LES is that this 4VS configuration lead to high instabilities growth rates, to fast and violent interactions between the secondary and the primary vortices, to fast transition to turbulence, and thus to a turbulent 2VS. The time evolution of the circulation profile and the energy analysis confirmed that, in terms of decay mechanism, the case $\Gamma_2/\Gamma_1 = -0.3$ is very efficient, even if sorely achievable in a "realistic" case. The $\Gamma_2/\Gamma_1 = -0.2$ case was also studied and compared within the FAR-Wake project, and it was shown that it remains also a very efficient means for wake alleviation, compared to a 2VS.

Realizing the space-developing simulation highlighted the difficulties to perform more realistic simulations than the time-developing ones. The computation cost of realistic simulations is unaffordable so far. Nevertheless, assuming a too large C_L/A_r ratio (thus a too low U_∞/V_0^* ratio), we are able to perform a very interesting simulation, pointing out the trends and differences between time and space-developing approaches. Among these, one will retain the axial velocity component of the SD simulation. The second important difference is that the SD case secondary vortices interact earlier with the primary ones than the TD case secondary vortices, leading to an earlier transition to turbulence in the SD case. However, this has to be moderated by the fact that the random perturbations added on the initial field in the TD simulation were of very little amplitude. With a higher value of perturbations, the instabilities would develop faster, leading to quicker interactions between the primary and the secondary vortices.

VIC-PFM, $\tau = 0.00$



PS, $\tau = 0.00$

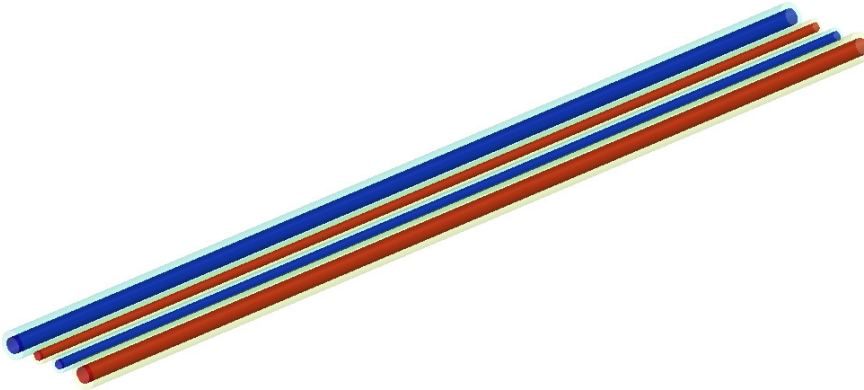
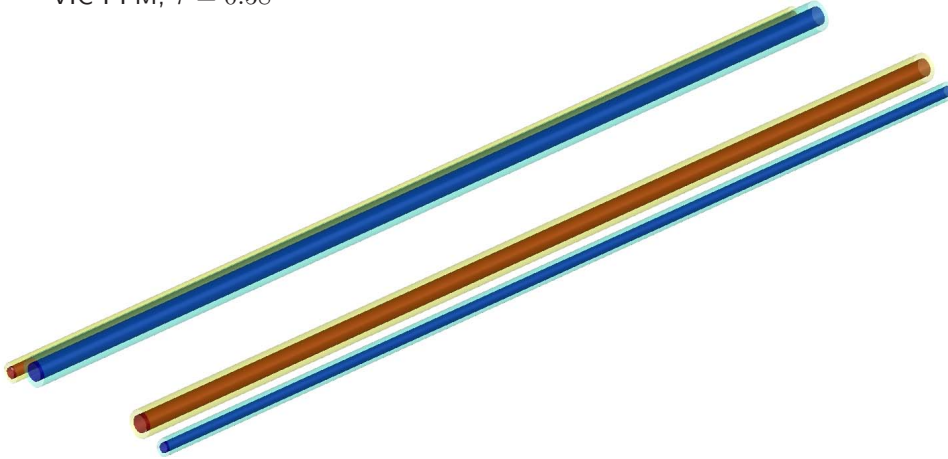


Figure 4.5: Time-developing LES. Time sequence of vorticity modulus isosurfaces, $|\omega|_{t_0^*} = 20\pi$ (high opacity) and 4π (low opacity), colored by the longitudinal component of vorticity.

VIC-PFM, $\tau = 0.58$



PS, $\tau = 0.55$

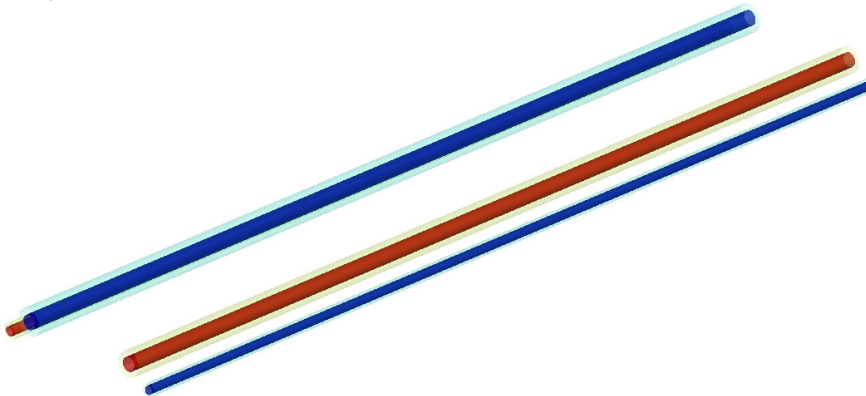
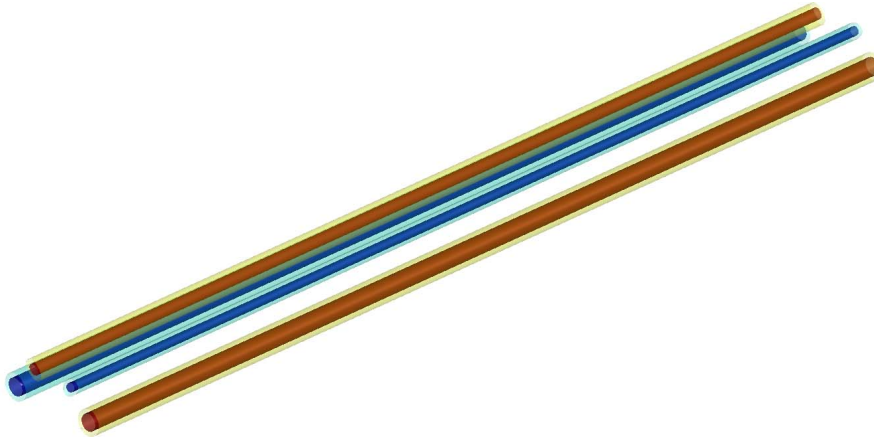


Figure 4.5: [Cont'd].

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VIC-PFM, $\tau = 1.15$



PS, $\tau = 1.11$

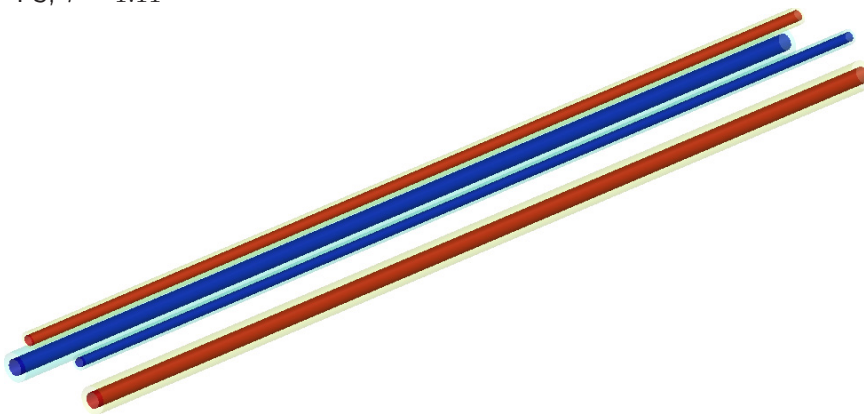
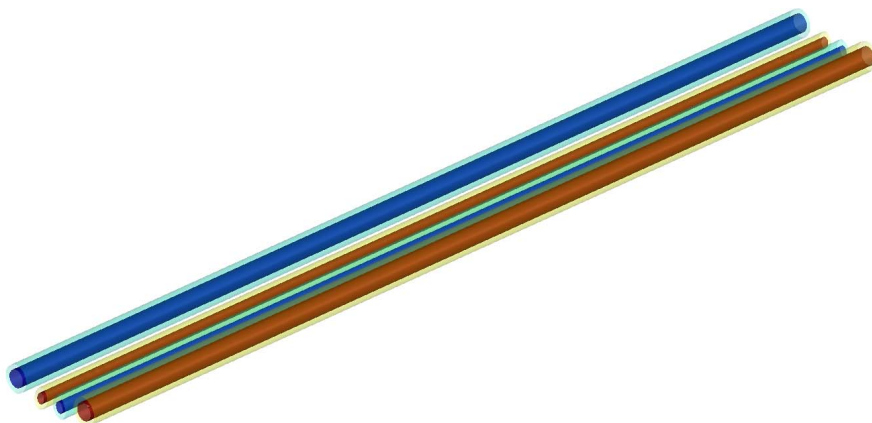


Figure 4.5: *[Cont'd].*

VIC-PFM, $\tau = 1.39$



PS, $\tau = 1.37$

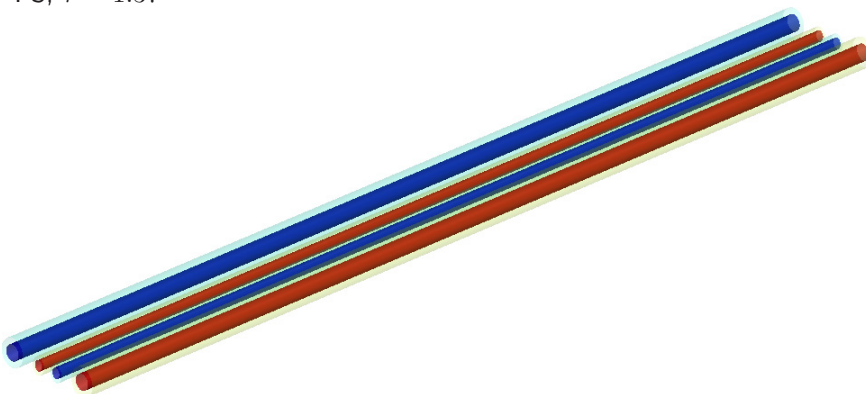
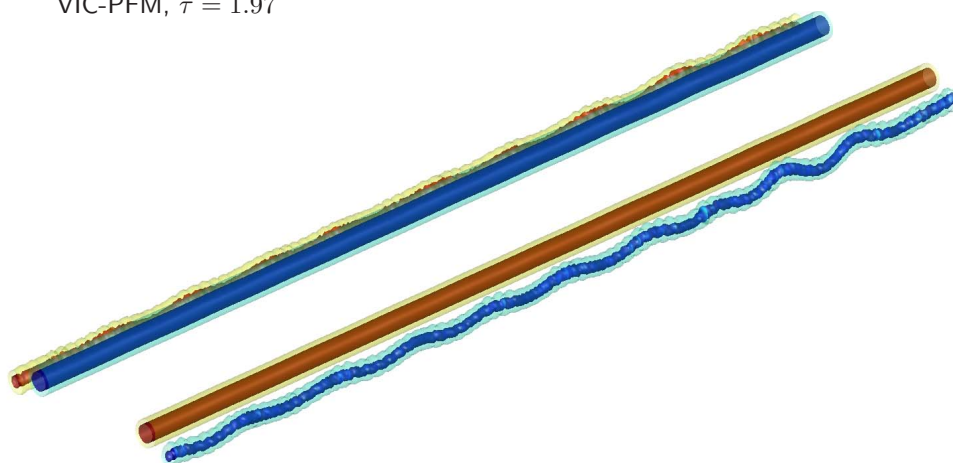


Figure 4.5: [Cont'd].

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VIC-PFM, $\tau = 1.97$



PS, $\tau = 1.92$

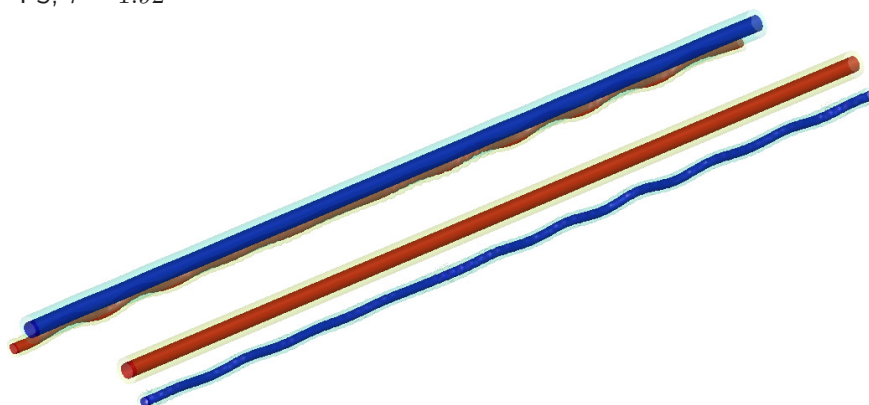
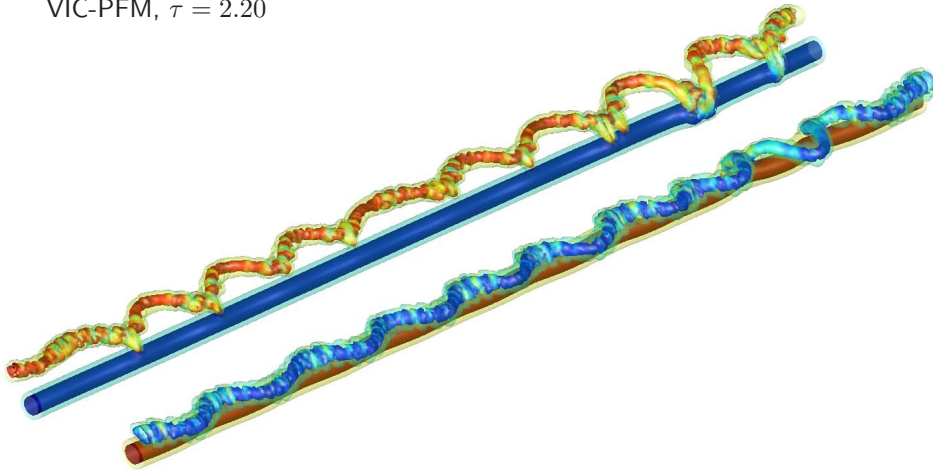


Figure 4.5: [Cont'd].

VIC-PFM, $\tau = 2.20$



PS, $\tau = 2.19$

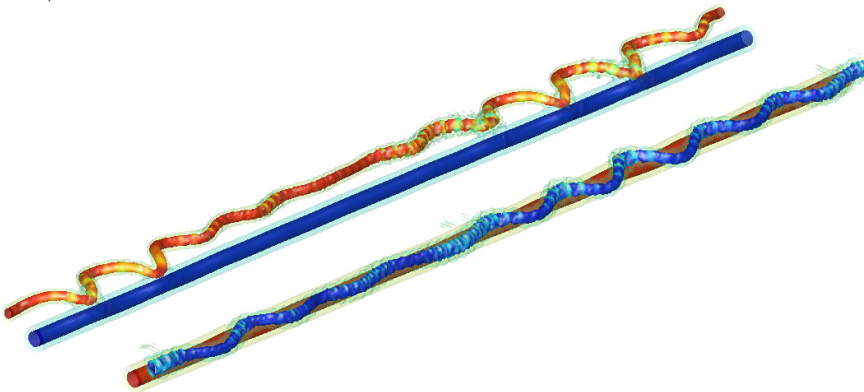
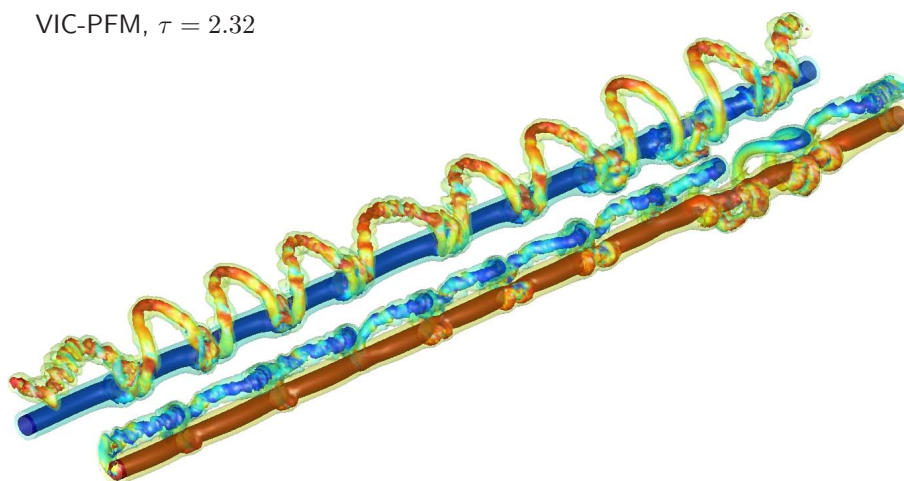


Figure 4.5: [Cont'd].

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VIC-PFM, $\tau = 2.32$



PS, $\tau = 2.35$

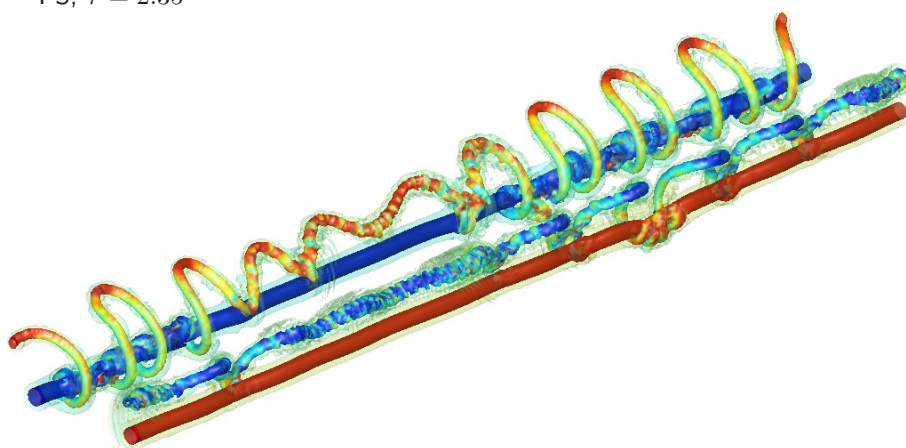
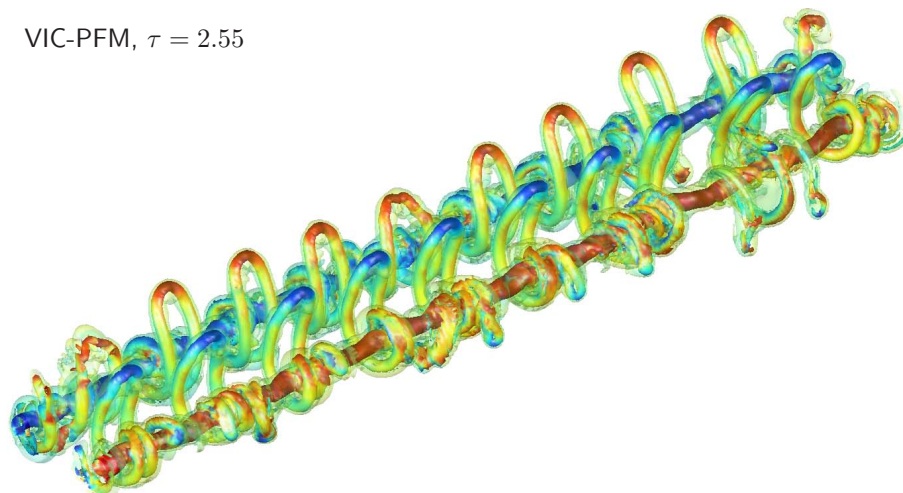


Figure 4.5: [Cont'd].

VIC-PFM, $\tau = 2.55$



PS, $\tau = 2.52$

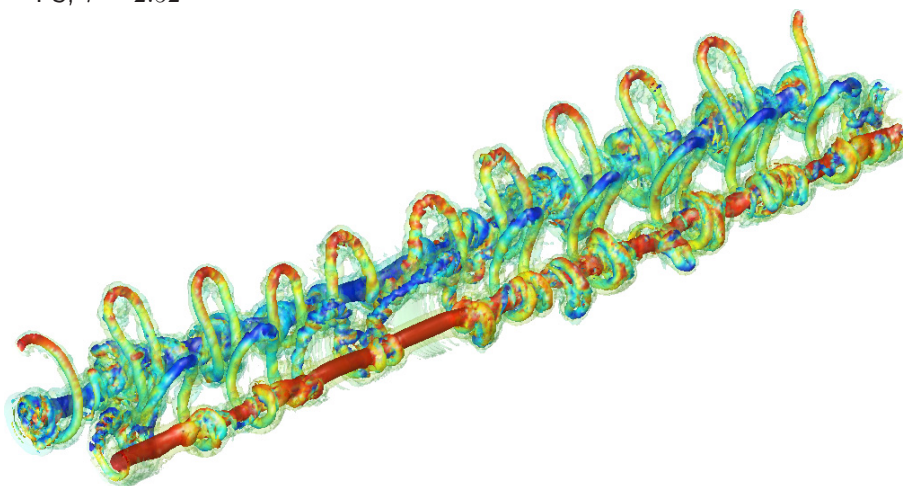
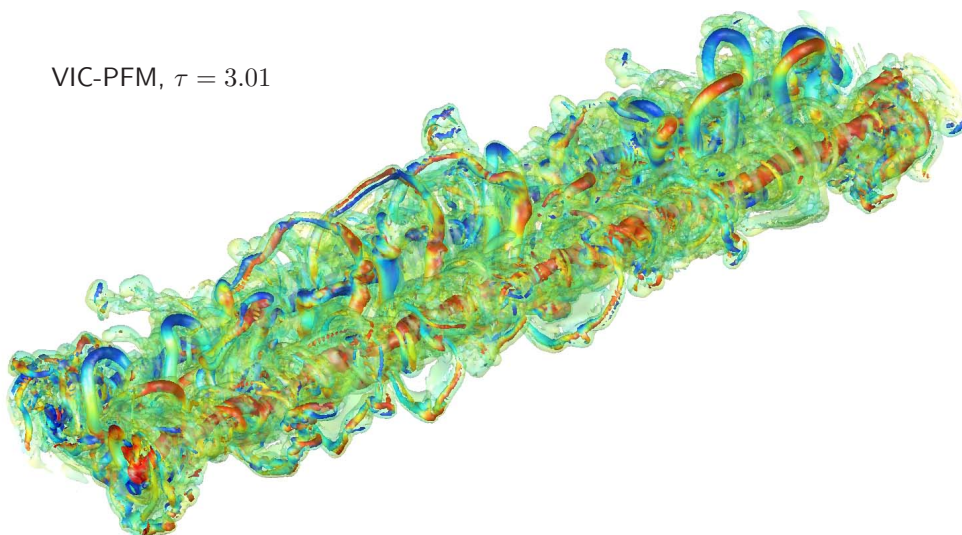


Figure 4.5: [Cont'd].

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VIC-PFM, $\tau = 3.01$



PS, $\tau = 2.93$

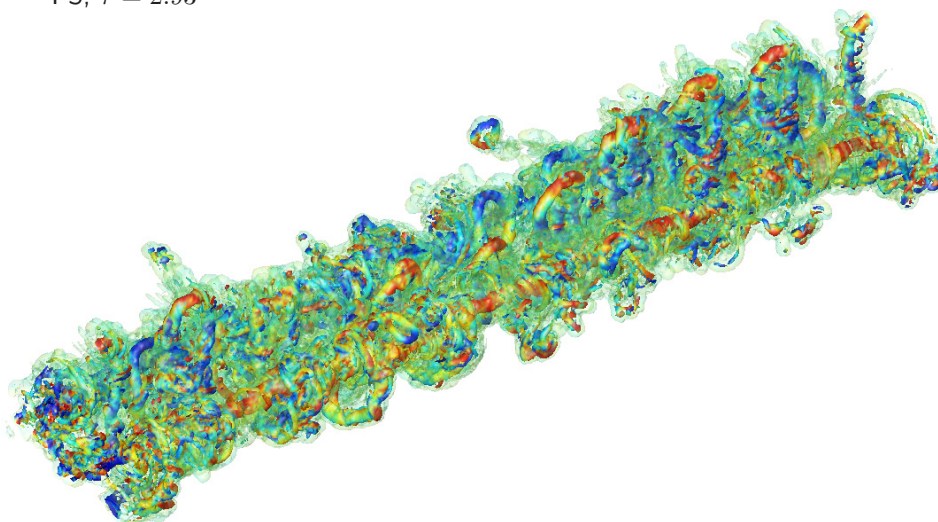
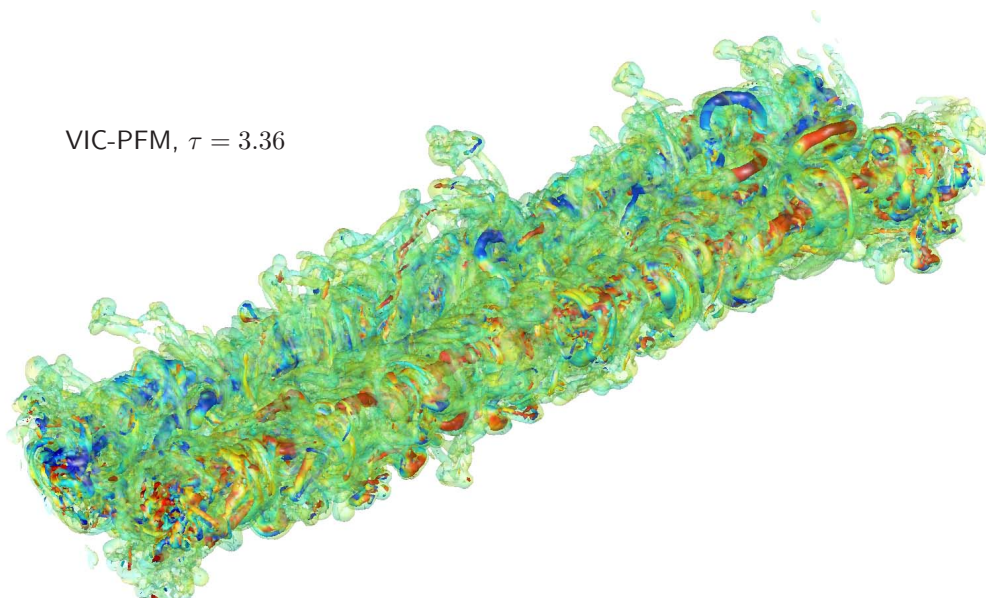


Figure 4.5: [Cont'd].

VIC-PFM, $\tau = 3.36$



PS, $\tau = 3.39$

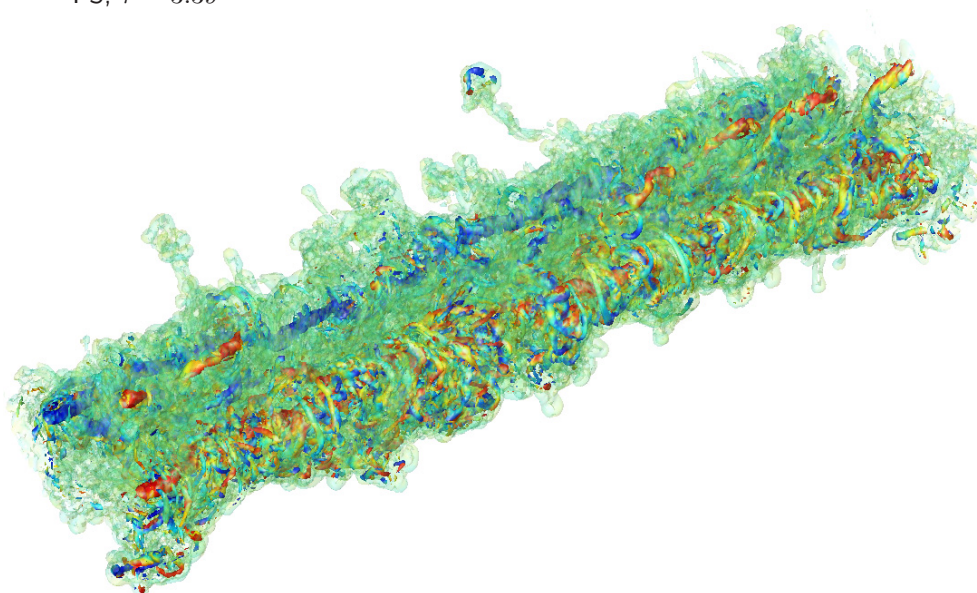


Figure 4.5: [Cont'd].

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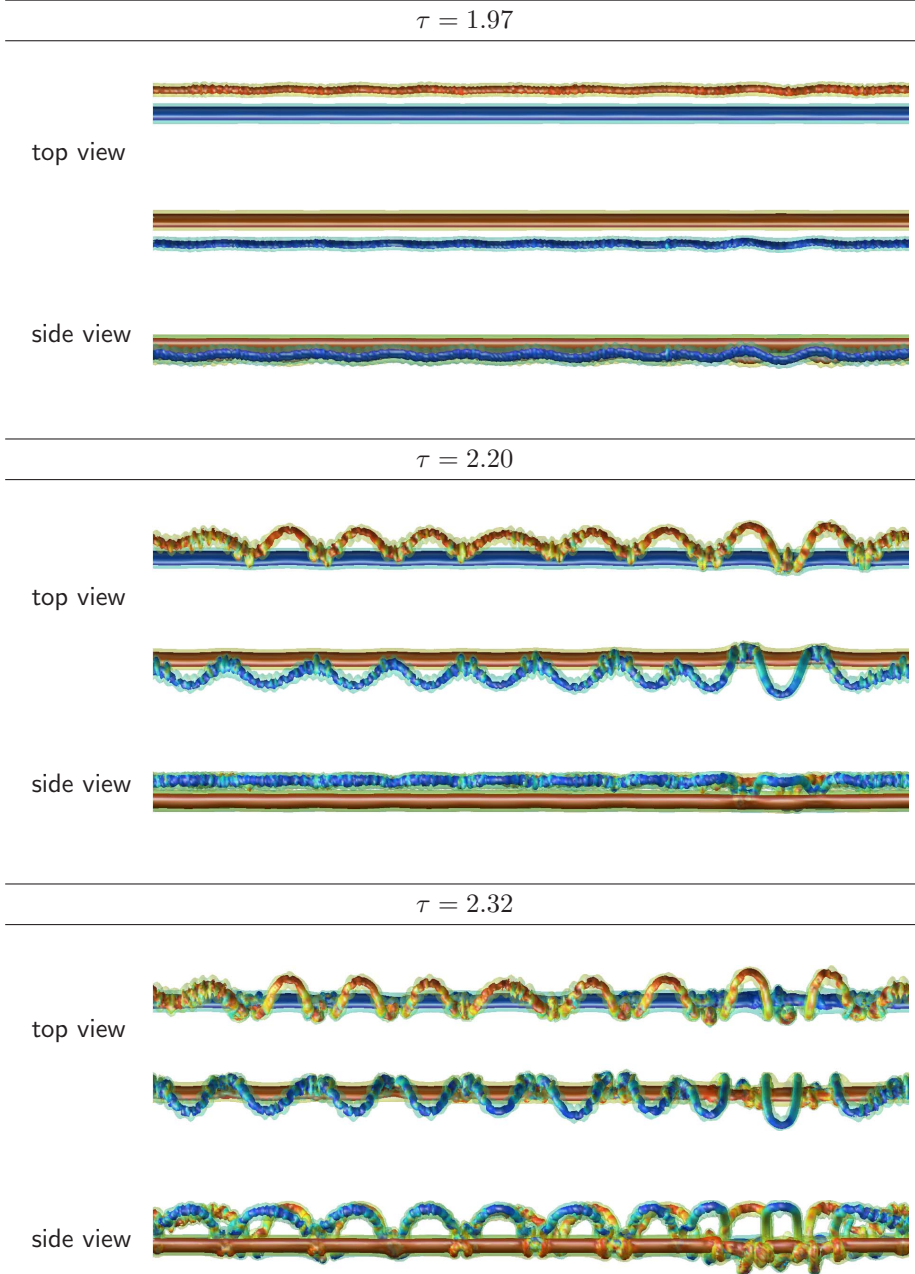


Figure 4.6: Time-developing LES using the VIC-PFM method. Time sequence of top and side views of vorticity modulus isosurfaces, $|\omega| t_0^* = 20\pi$ (high opacity) and 4π (low opacity), colored by the longitudinal vorticity component.

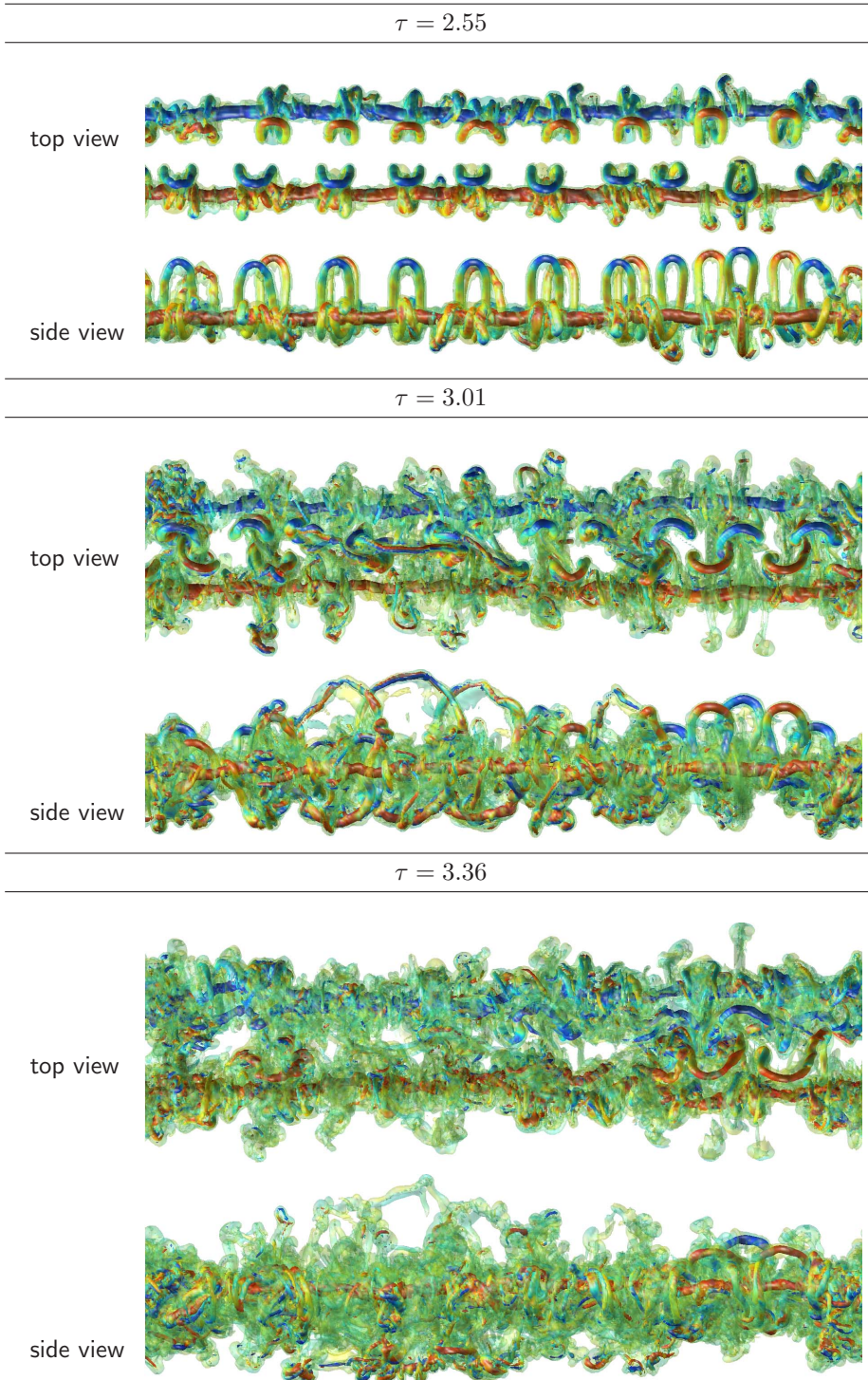


Figure 4.6: [Cont'd].

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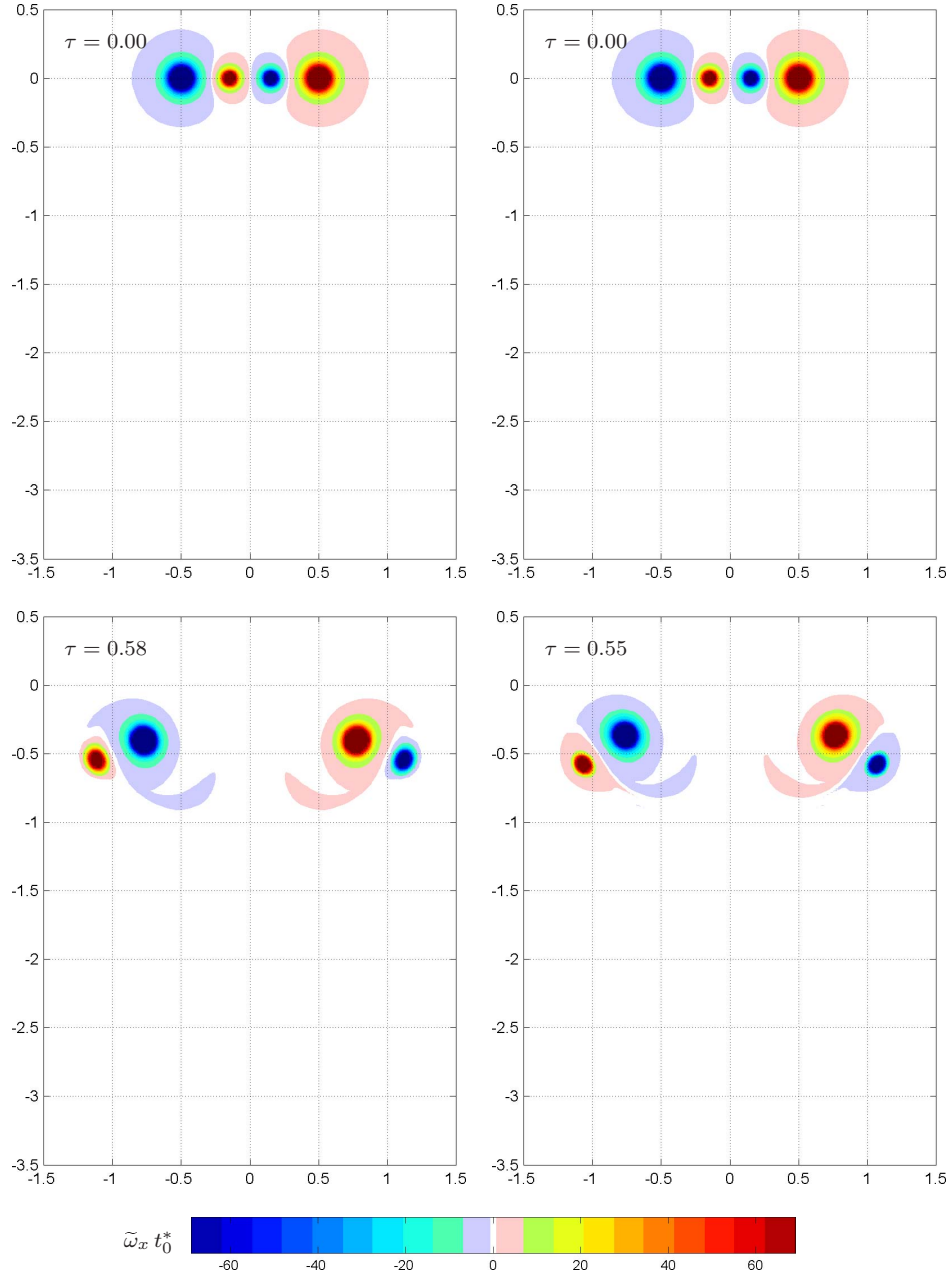


Figure 4.7: Time-developing LES. Evolution of the longitudinally averaged vorticity field $\tilde{\omega}_x t_0^*$ using the VIC-PFM method (left) and using the PS method (right). Fields are shown approximately at the same dimensionless time τ . The y and z axes are dimensionless (using b_0^*).

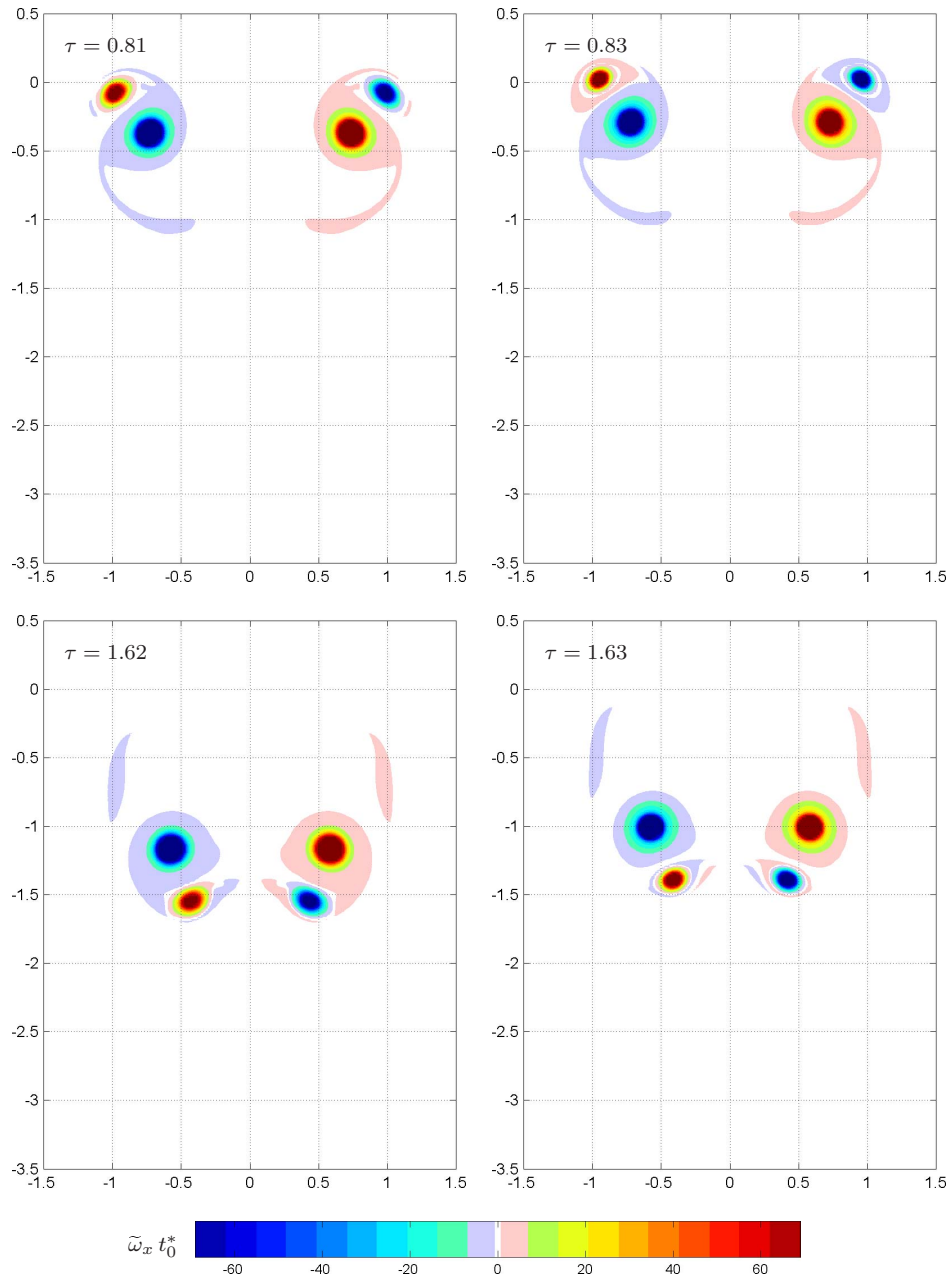


Figure 4.7: [Cont'd].

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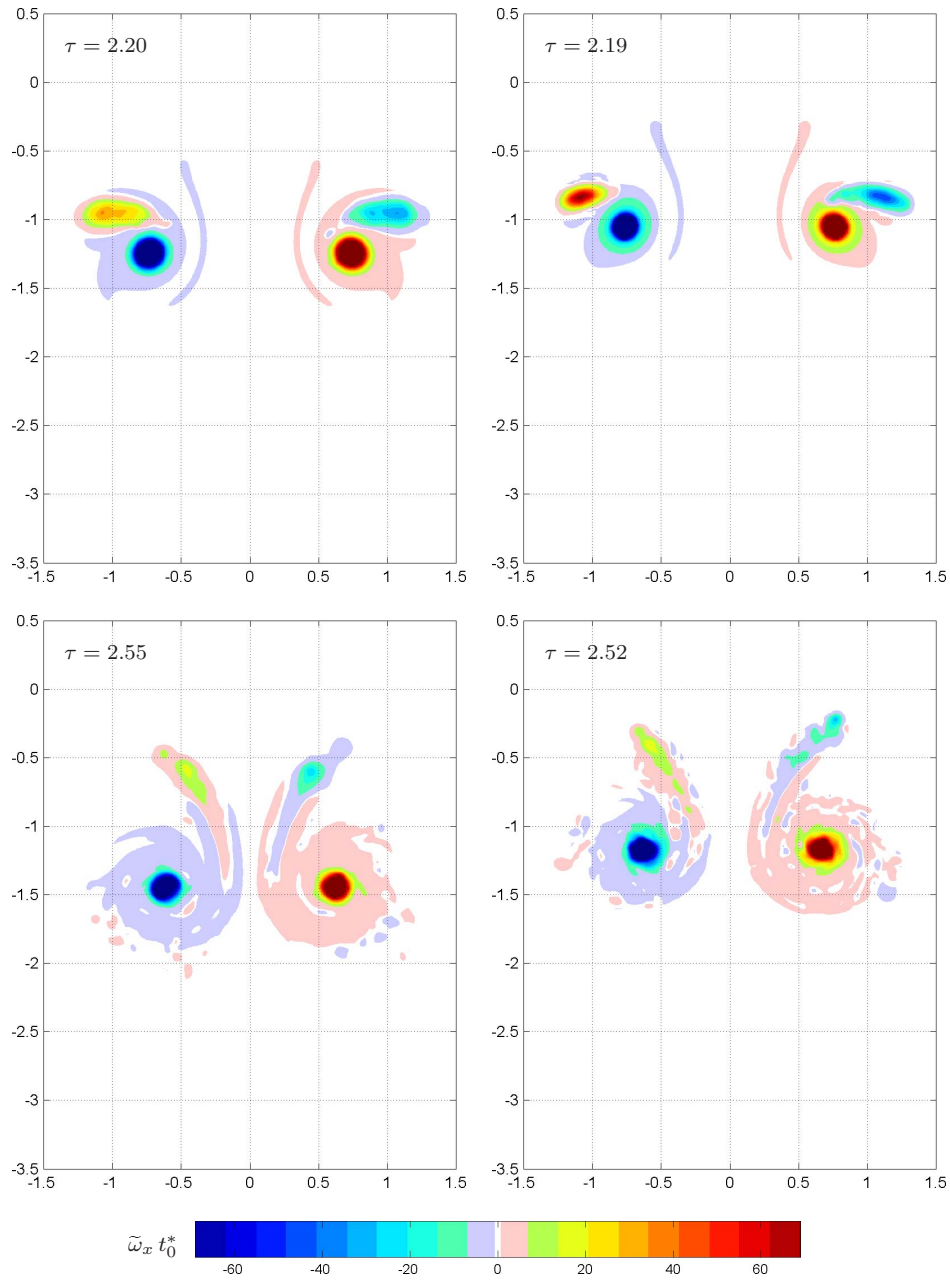


Figure 4.7: [Cont'd].

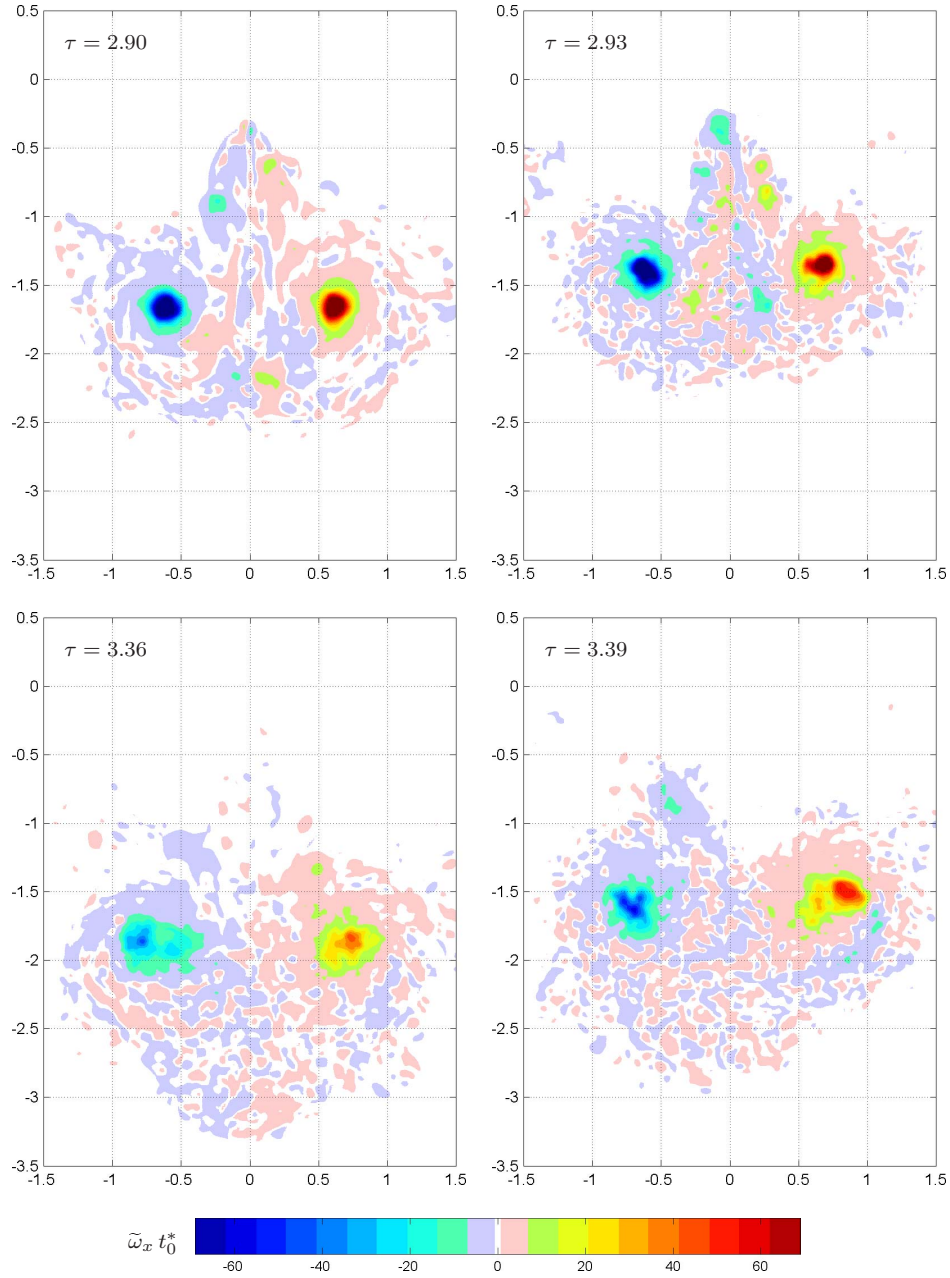


Figure 4.7: [Cont'd].

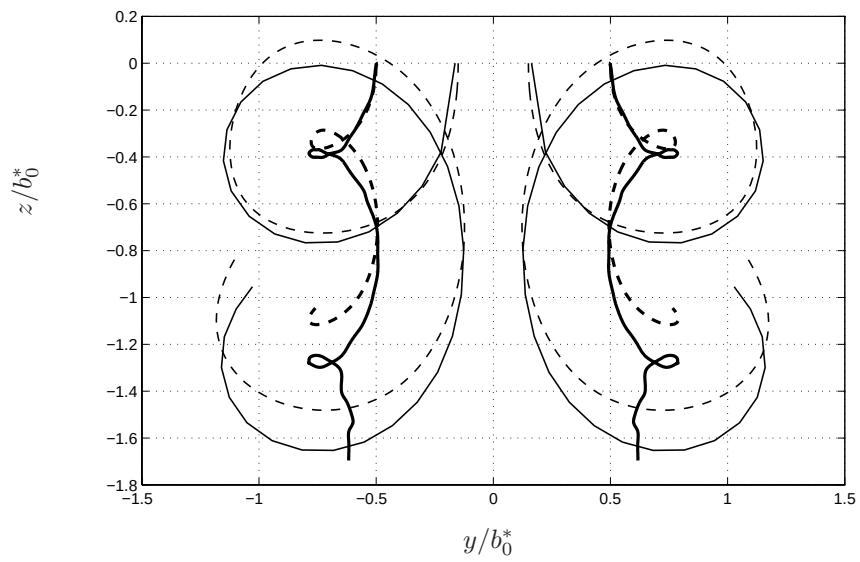


Figure 4.8: Time-developing LES. Trajectories of the primary vortices (thick line) and of the secondary vortices (thin line) up to reconnection: using the VIC-PFM method (solid line) and using the PS method (dashed line).

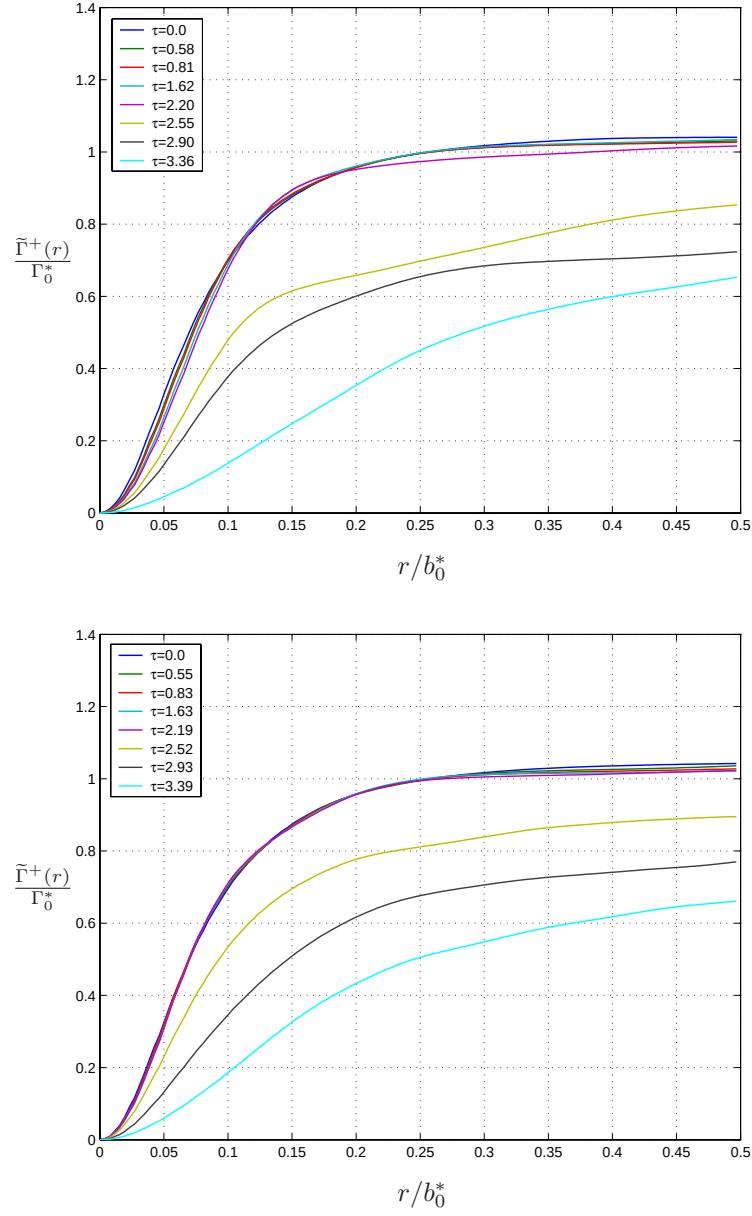


Figure 4.9: Time-developing LES. Longitudinally averaged circulation profiles, $\tilde{\Gamma}^+(r)$, for various dimensionless times: using the VIC-PFM method (top) and using the PS method (bottom).

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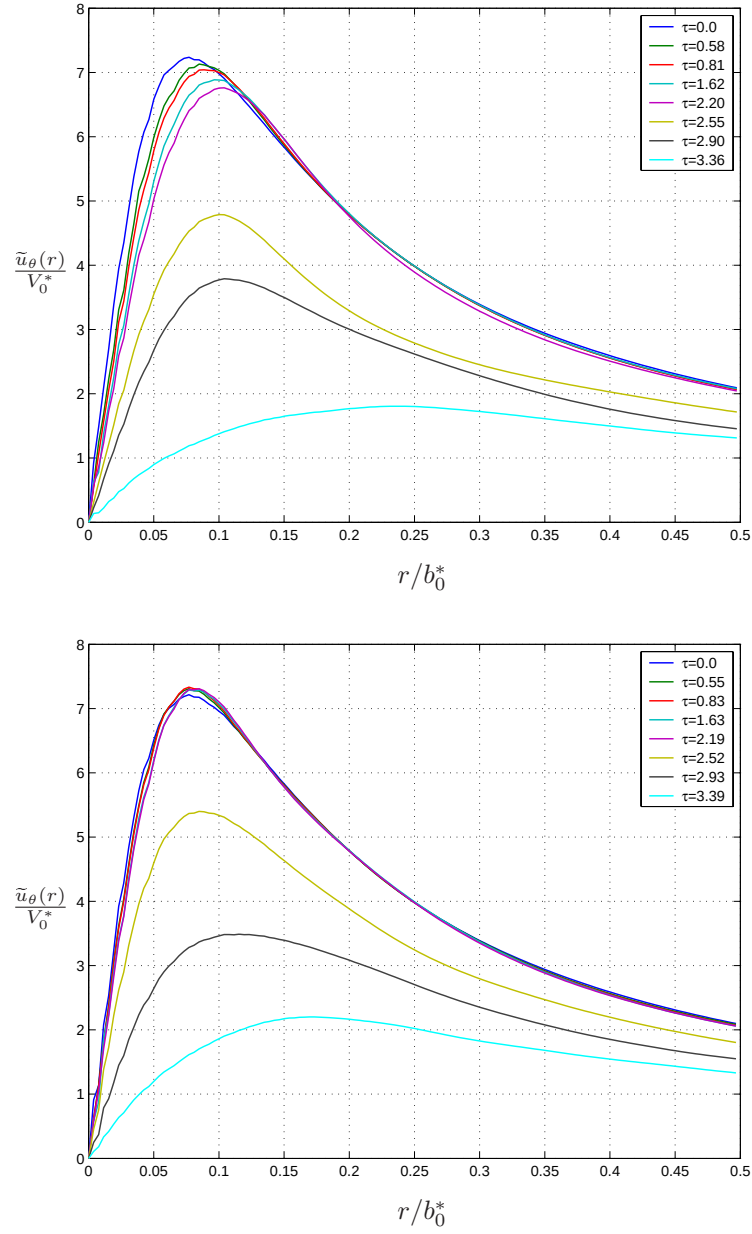


Figure 4.10: Time-developing LES. Longitudinally averaged azimuthal velocity profiles, $\tilde{u}_\theta(r)$, for various dimensionless times: using the VIC-PFM method (top) and using the PS method (bottom).

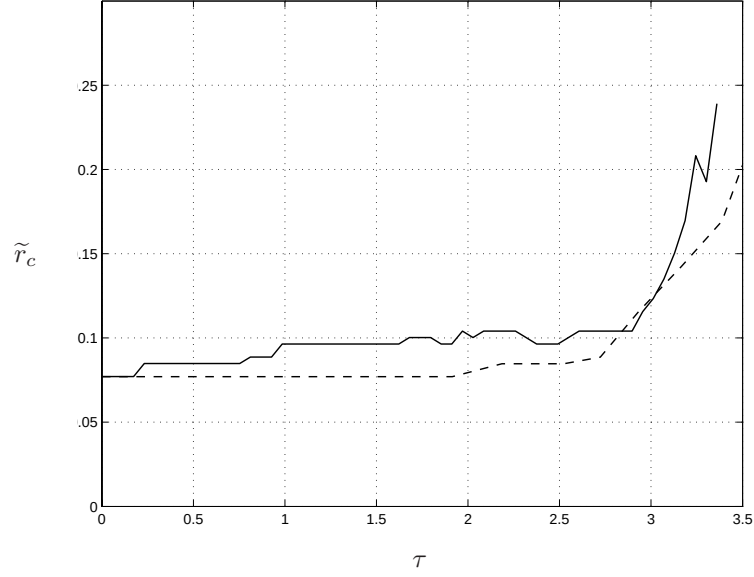


Figure 4.11: Time-developing LES. Evolution of the main vortex characteristic radius $\tilde{r}_c$: using the VIC-PFM method (solid) and using the PS method (dashed).

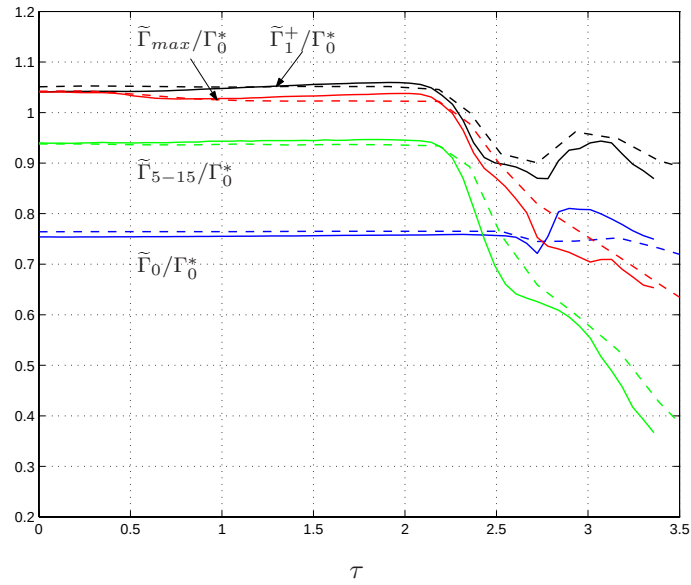


Figure 4.12: Time-developing LES. Evolution of $\tilde{\Gamma}_0/\Gamma_0^*$ (blue), $\tilde{\Gamma}_1^+/\Gamma_0^*$ (black), $\tilde{\Gamma}_{max}/\Gamma_0^*$ (red) and $\tilde{\Gamma}_{5-15}/\Gamma_0^*$ (green): using the VIC-PFM method (solid) and using the PS method (dashed).

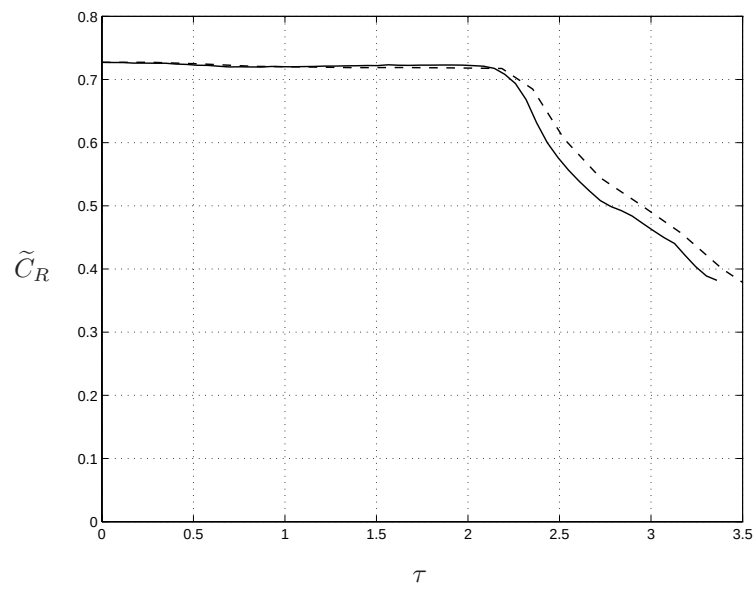


Figure 4.13: Time-developing LES. Evolution of the main vortex induced rolling moment coefficient $\tilde{C}_R$: using the VIC-PFM method (solid) and using the PS method (dashed).

$t/t_0^* = 0.00$

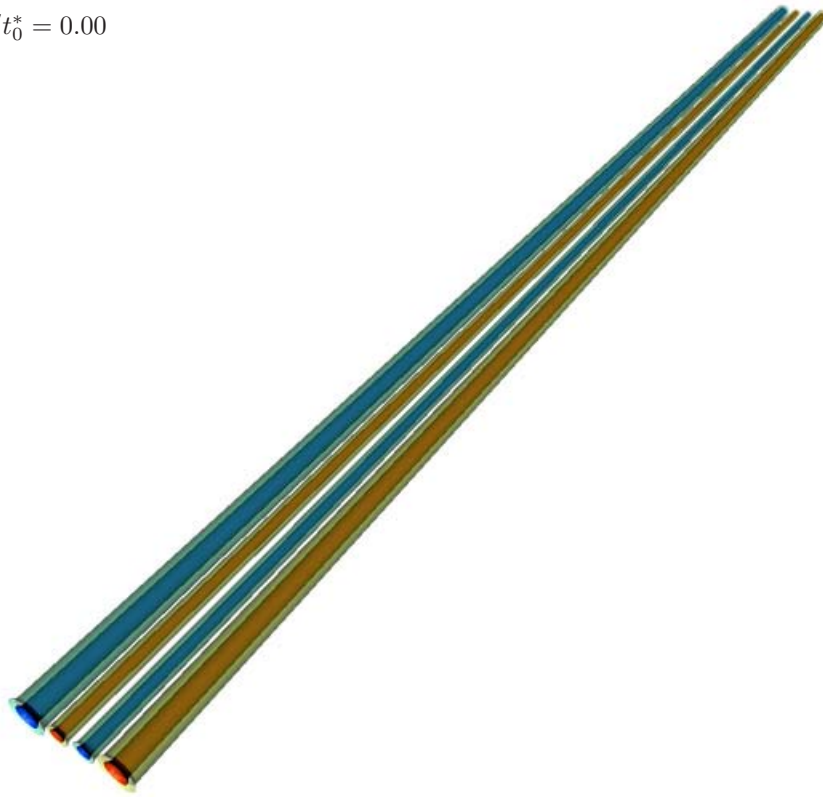


Figure 4.14: *Space-developing LES. Time sequence perspective view of vorticity modulus isosurfaces, $|\omega| t_0^* = 20\pi$ (high opacity) and 4π (low opacity), colored by the longitudinal vorticity component.*

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$$t/t_0^* = 0.72$$



Figure 4.14: [Cont'd].

$$t/t_0^* = 1.45$$



Figure 4.14: [Cont'd].

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$$t/t_0^* = 2.17$$



Figure 4.14: [Cont'd].

$t/t_0^* = 2.90$

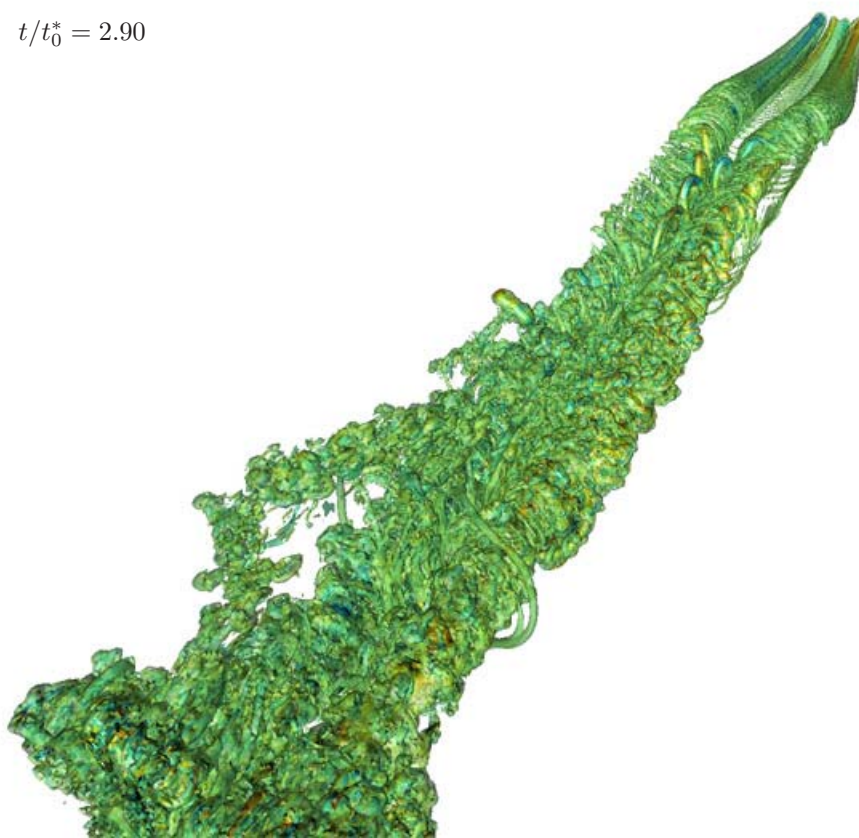


Figure 4.14: [Cont'd].

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$$t/t_0^* = 4.34$$

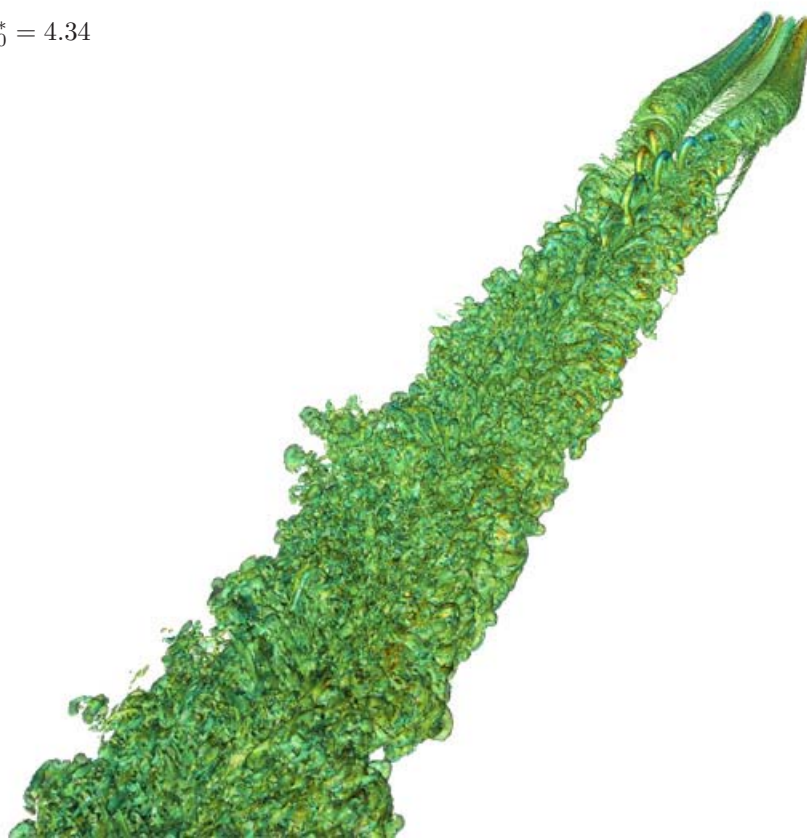


Figure 4.14: *[Cont'd].*

$$t/t_0^* = 7.24$$



Figure 4.14: [Cont'd].

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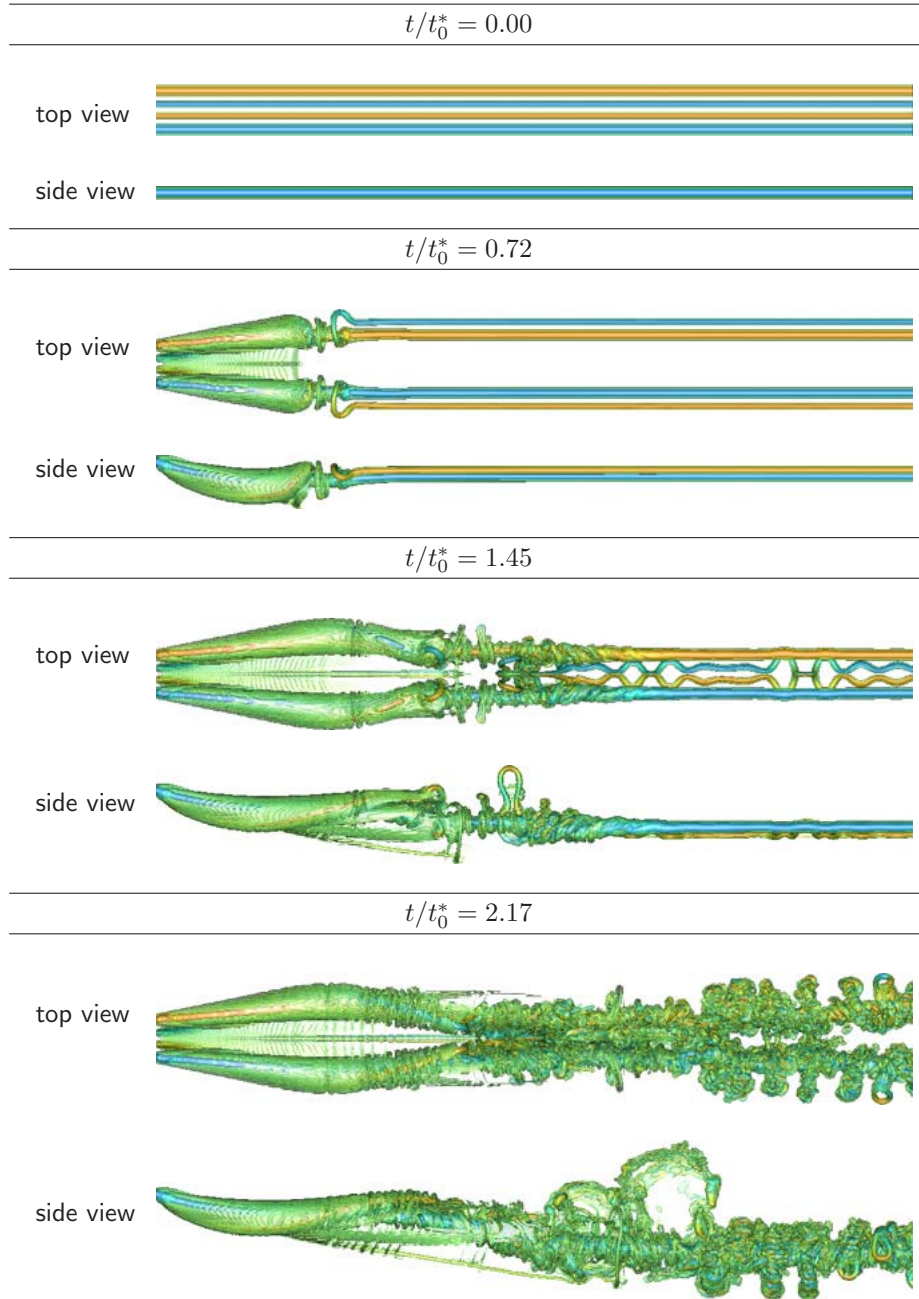
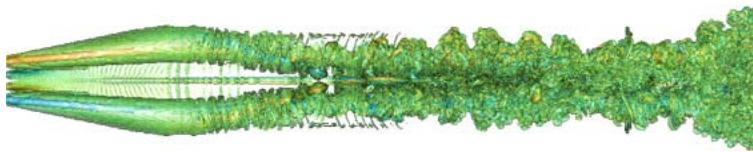


Figure 4.15: Space-developing LES. Time sequence (top and side views) of vorticity modulus isosurfaces, $|\omega| t_0^* = 20\pi$ (high opacity) and 4π (low opacity), colored by the longitudinal vorticity component.

$$t/t_0^* = 2.90$$

top view

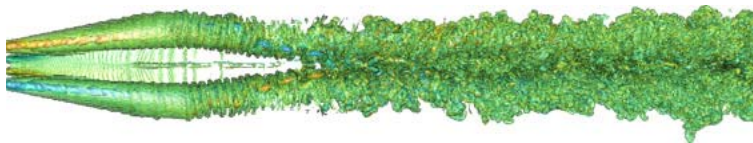


side view

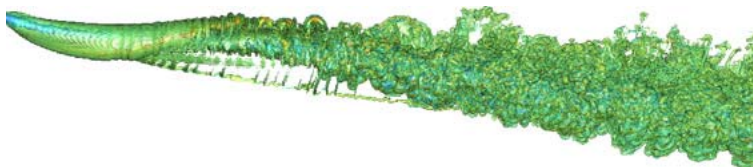


$$t/t_0^* = 5.07$$

top view

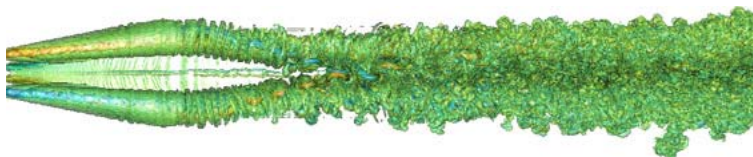


side view



$$t/t_0^* = 7.24$$

top view



side view

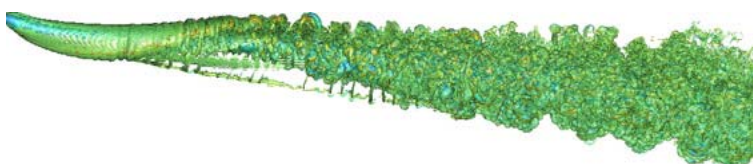


Figure 4.15: [Cont'd].

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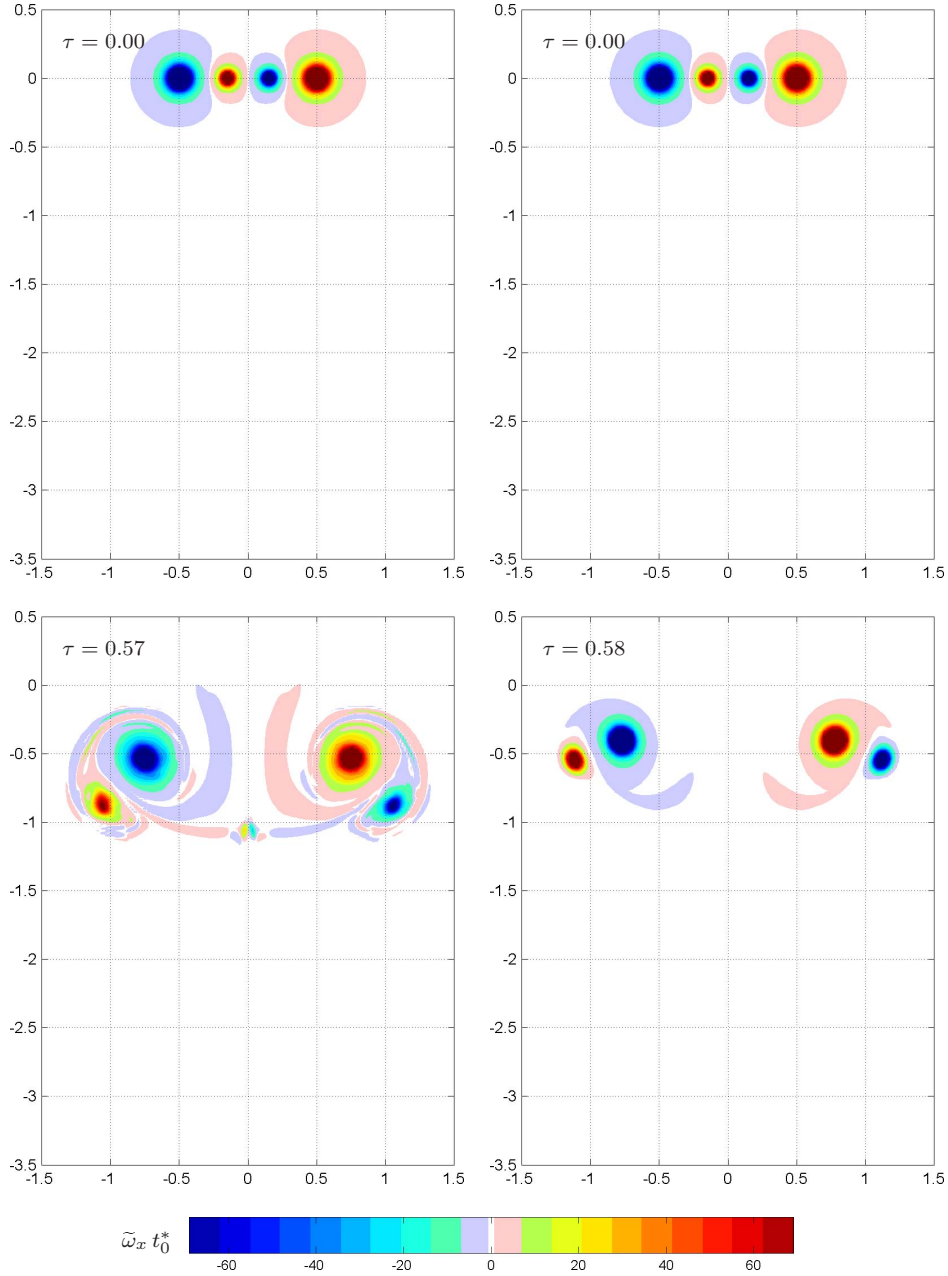


Figure 4.16: Time averaged vorticity contours of space-developing results on the left and time-developing results on the right using the VIC-PFM method. Vorticity fields are shown for distinctive slices during the roll-up for the SD case, $\tau = (x/U_\infty)/t_0^*$ and at different times, $\tau = t/t_0^*$ for the TD case.

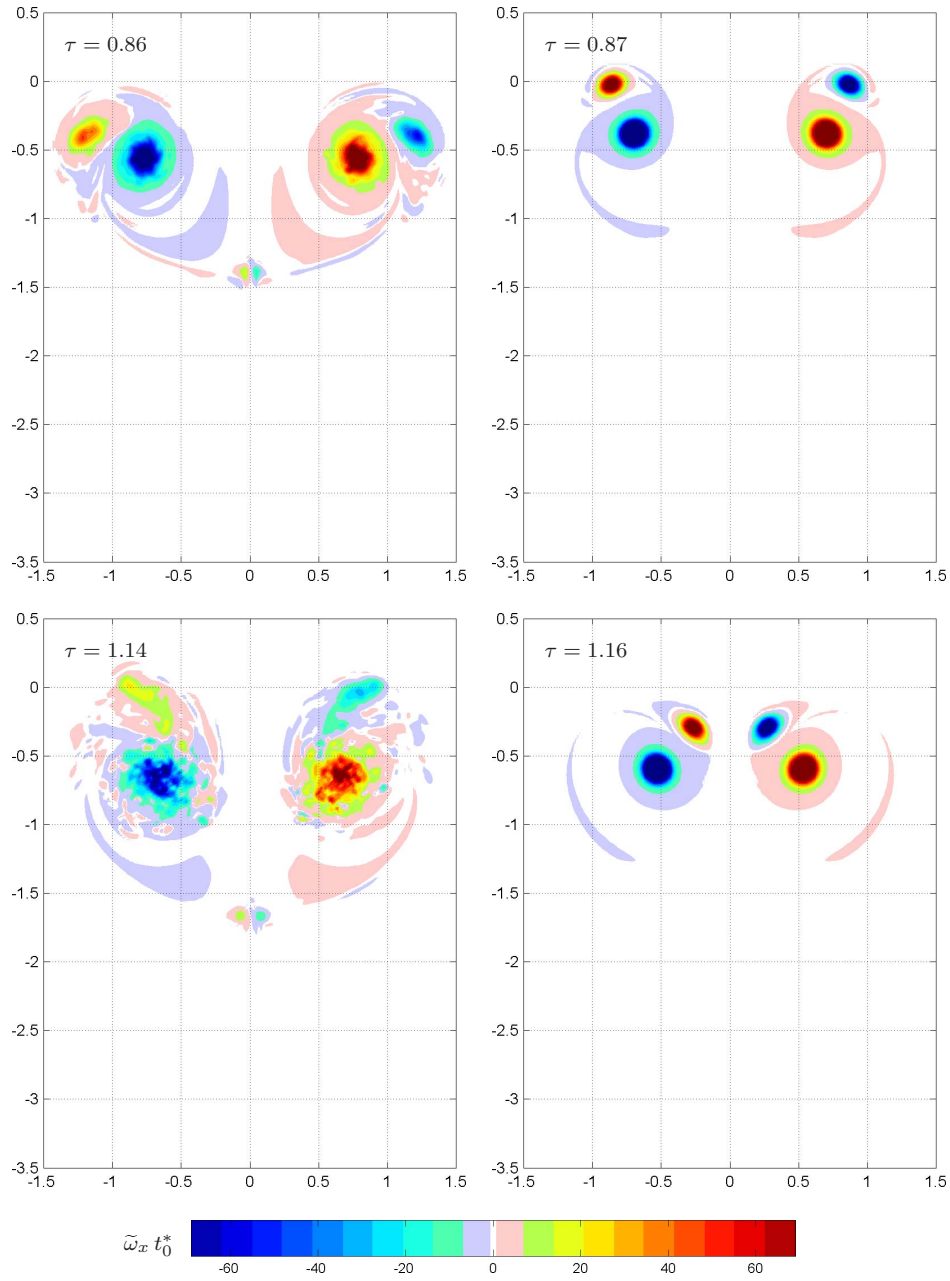


Figure 4.16: [Cont'd].

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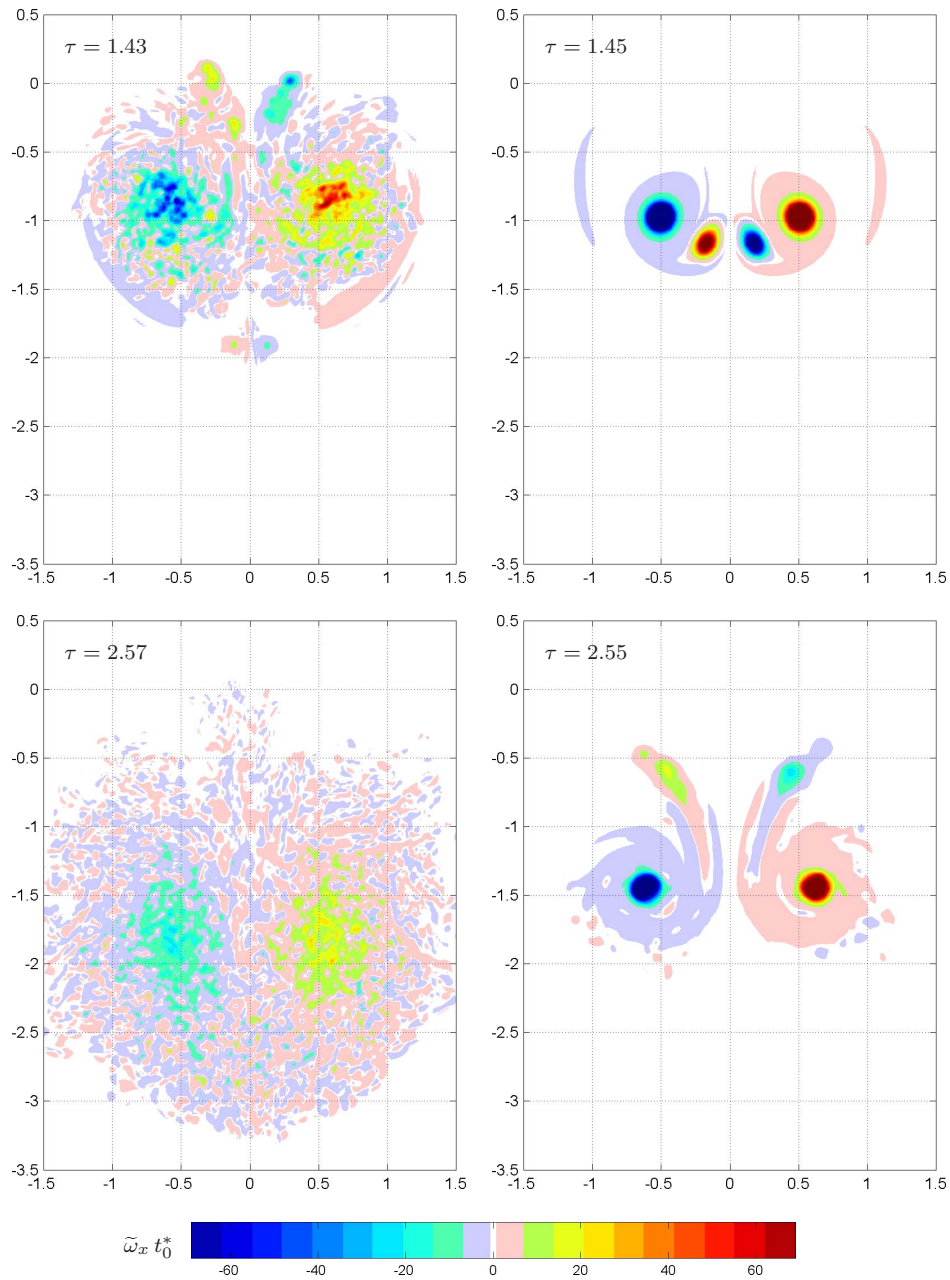


Figure 4.16: [Cont'd].

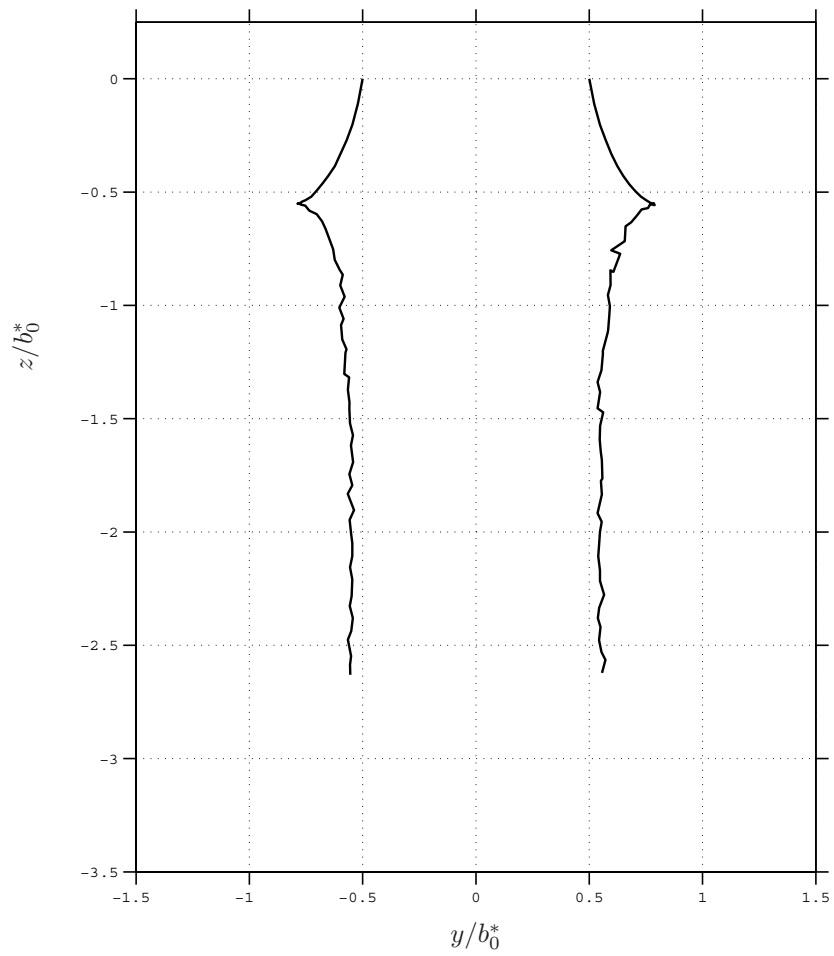


Figure 4.17: Space-developing LES. Trajectories of the primary vortices.

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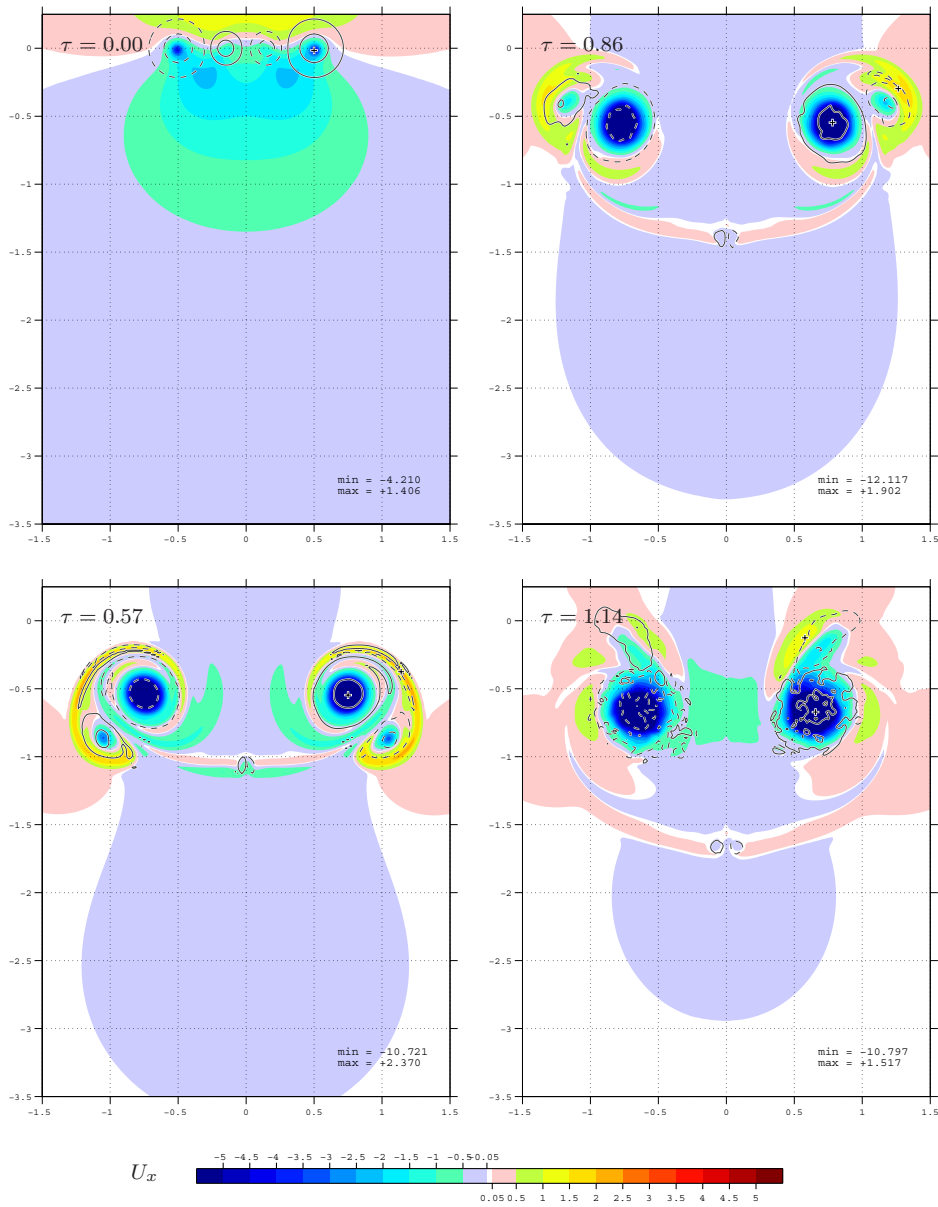


Figure 4.18: Space-developing LES. Time averaged axial velocity contours, $\frac{u_x}{V_0^*}$, shown for distinctive slices, $\tau = (x/U_\infty)/t_0^*$, during the roll-up.

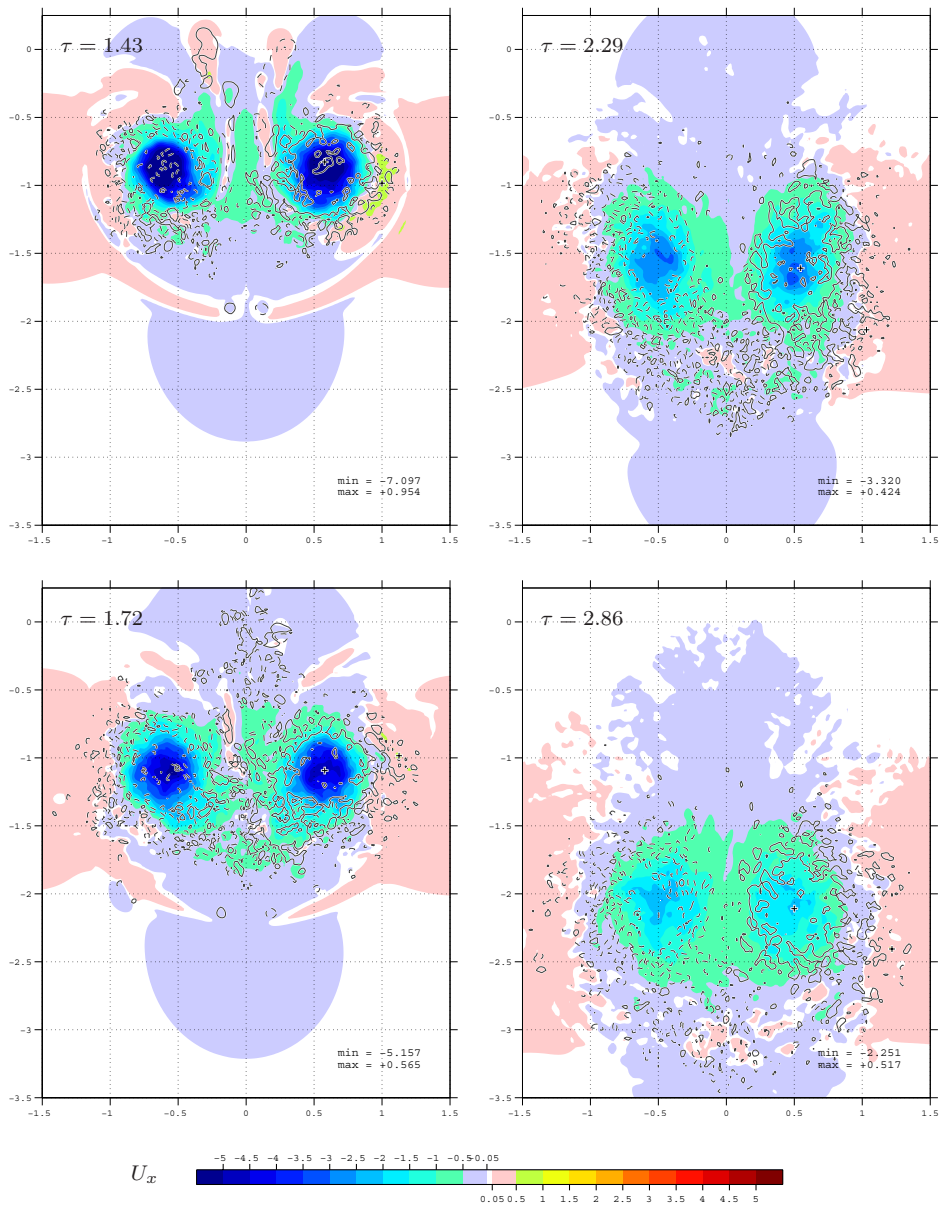


Figure 4.18: [Cont'd].

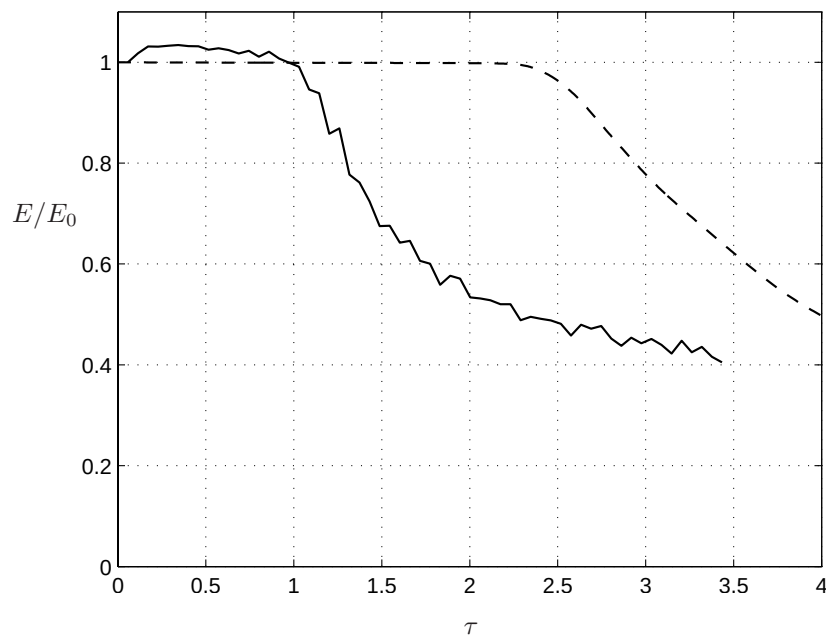
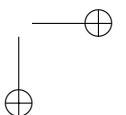
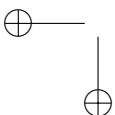
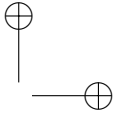
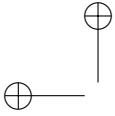


Figure 4.19: Evolution of the kinetic energy for the time averaged space-developing LES (solid line) and for the space averaged time-developing LES (dashed line).



Chapter 5

Turbulent round jet

5.1 Introduction

The present investigation is concerned with the LES of a turbulent round jet at high (yet still moderate) Reynolds number. The round jet flow is one of the most commonly studied free shear flows, together with wakes and mixing layers [63]. It constitutes a suitable application of the space-developing VIC-PFM method as the simulation is in a free space, without walls or periodic boundary conditions. The inflow condition, a flat-topped circular velocity profile, evolves in space and time, and becomes turbulent due to instabilities developing because of the important velocity gradients. We here examine various pertinent diagnostics, and we compare them with experimental and/or theoretical results.

5.2 Definition

The fluid flows through a nozzle of diameter $D = 2R$ into an ambient fluid, at rest at infinity. The inflow radial velocity profile is taken as:

$$U(r) = \frac{1}{2} U_J \left[1 - \tanh \left(\frac{1}{4} \frac{R}{\Theta} \left(\frac{r}{R} - \frac{R}{r} \right) \right) \right] \quad (5.1)$$

where U_J is the jet core velocity and Θ is the momentum thickness of the jet shear layer. This profile has been used by several authors; it models the jet flow quite well, as shown by Moore [52]. The present simulation is done using $R/\Theta = 10$. Michalke and Herman [50] have shown that this value corresponds to the most unstable jet velocity profile.



Figure 5.1: Round jet at $Re = 10000$: 3-D view at $t/t_0 = 495$. One isosurface of vorticity is shown ($\|\omega\|t_0 = 0.2$) at half the grid resolution.



Figure 5.2: Round jet at $Re = 10000$: 3-D view at $t/t_0 = 495$. One isosurface of $\lambda_2 = 0$ is shown at half the grid resolution.

The turbulent flow is statistically stationary and axisymmetric. The time-averaged statistics thus only depend on the axial and radial coordinates (x and r). The jet is completely defined by U_J , D and ν that are gathered in the Reynolds number $Re = U_J D / \nu$. Here, we choose $Re = 10^4$.

The extent of the computational box is $L_x/R = 50.0$ and the discretization is $h/R = 0.075$. The time step used is $\Delta t/t_0 = 0.03$, with $t_0 = R/U_J$ the time scale used for normalization. As the flow rapidly becomes turbulent, we need to add a SGS model. Here, we use the RVM model with $n = 1$ and $C_R = 0.036$. As for the space-developing simulation of the 4VS presented in the previous section, the computation has to be carried on for sufficiently long times for the flow to reach its regime state. As we will see, the jet core velocity evolves as $1/x$: the time required for the flow to completely traverse the computational domain is thus quite large. The simulation was carried out for ~ 16600 time steps (corresponding to $t/t_0 = 500$) and took 350 hours on 24 Opteron processors at 2.6 GHz. All the statistics presented in the next section are computed within the time interval $t/t_0 = [300 - 500]$, corresponding to the time when the regime is established. At this point, the number of particles was about 18 million and the number of grid points was 110 million.

5.3 Simulation results

Fig. 5.1 shows a 3-D view, at half the grid resolution, of the round jet at $t/t_0 = 495$. The linear spreading of the jet core is clearly visible. The flow is turbulent and contains small-scale structures. Fig. 5.3 shows a zoom in the jet, at full grid resolution, to better illustrate the complexity and the large range of scales captured by the simulation. Fig. 5.4 shows an experimental visualization of a turbulent jet (in water) at $Re \approx 2300$. It can be compared with Fig. 5.5 that shows a snapshot of the vorticity field in the plane $y = 0$. Even if the view obtained with laser induced fluorescence is not equivalent to the vorticity field, we can observe the strong similarity between the experimental and numerical results. The smallest scales, in the experimental case, are clearly larger, because of the lower Reynolds number, than in our simulation. The transition distance (from the laminar to the turbulent flow) is in turn similar. Fig. 5.6 also shows snapshots of the vorticity field: the first three views are shown during the transition phase (i.e. before the regime is attained). We clearly observe the "front" progression of the jet. The next three views are taken during the established regime. The spreading of the jet is also well

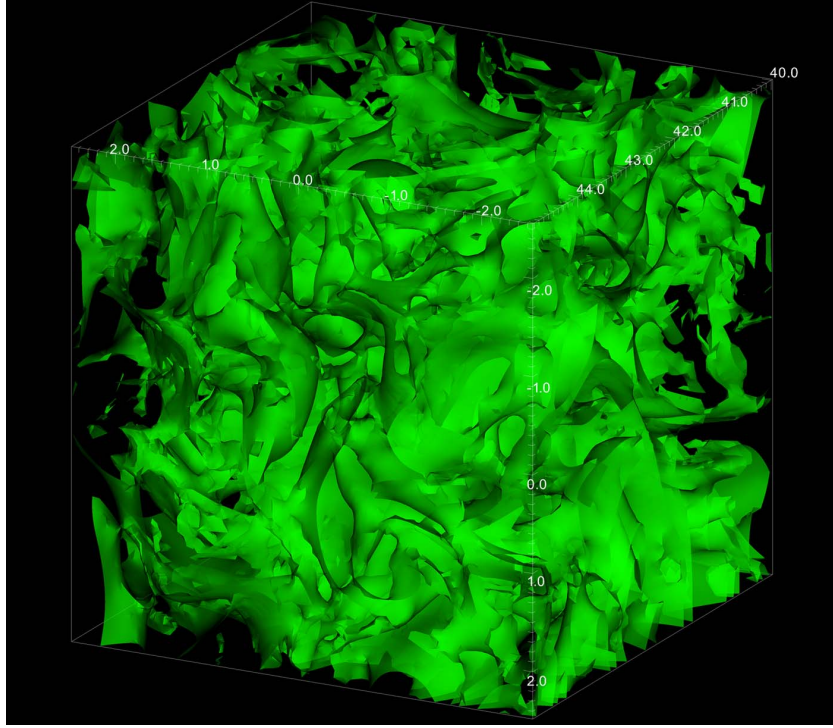


Figure 5.3: Round jet at $Re = 10000$: zoom on a region of the jet at $t/t_0 = 495$. The volume shown is $([40\ 45]; [-2.5\ 2.5]; [-2.5\ 2.5])$. One isosurface of vorticity is shown ($\|\omega\|_{t_0} = 0.2$) at full grid resolution.

observed; so is the formation of vortex rings in the development region: these are due to the Kelvin-Helmoltz instabilities appearing in the circular shear layer. The resulting rings are unstable and rapidly transition to fully developed turbulence.

We now focus on the time-averaged velocity fields and velocity fluctuations fields. They are obtained by time averaging of the instantaneous velocity fields every $\Delta t/t_0 = 1.5$, between $t/t_0 = [300-500]$ (leading to 135 samples). Moreover, we take advantage of the flow axisymmetry and we also perform spatial averaging in the azimuthal direction. This is done every $\Delta\theta = 2\pi/100$. The averaging was thus done using 13500 samples, leading to well converged results.

Fig. 5.7 shows the radial profiles of the mean axial velocity $\langle U_x(x, r, \theta) \rangle$ (which is independent of θ as the averaging is also made in the azimuthal direction) at three locations x/R after the development region. We observe that, when the axial distance increases, the jet simultaneously decays and spreads. Nevertheless, the

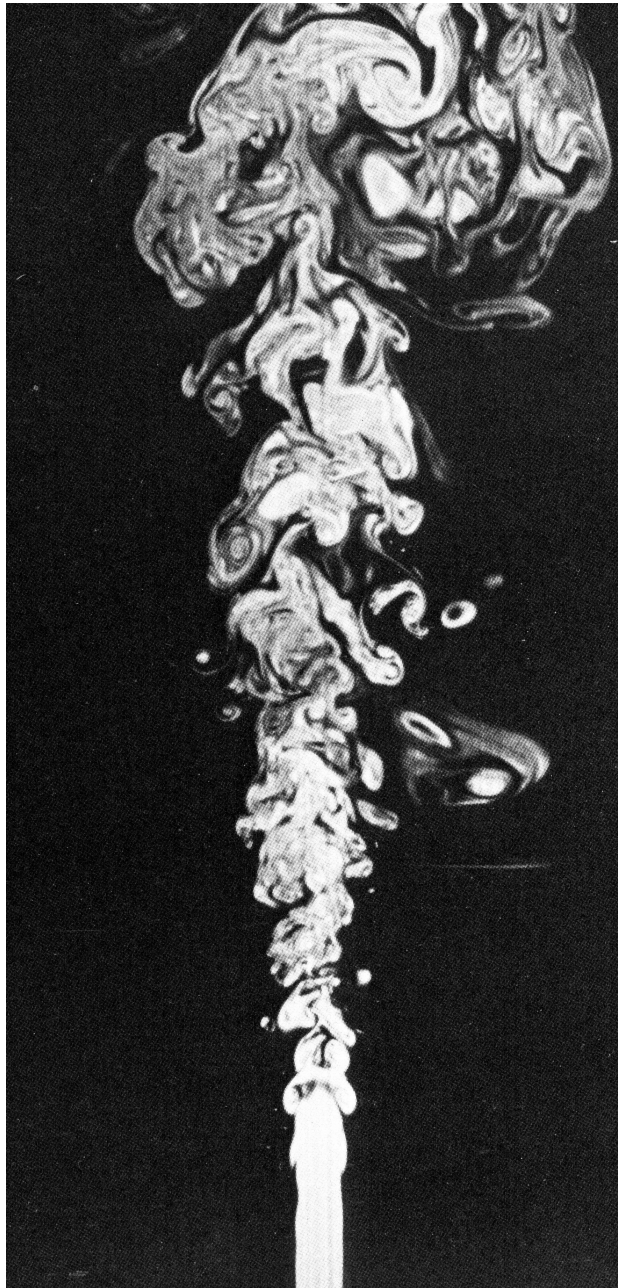


Figure 5.4: *Jet in water at $Re \approx 2300$: Laser induced fluorescence shows the concentration of jet fluid in one cross plane (reproduced from Van Dyke [75]).*

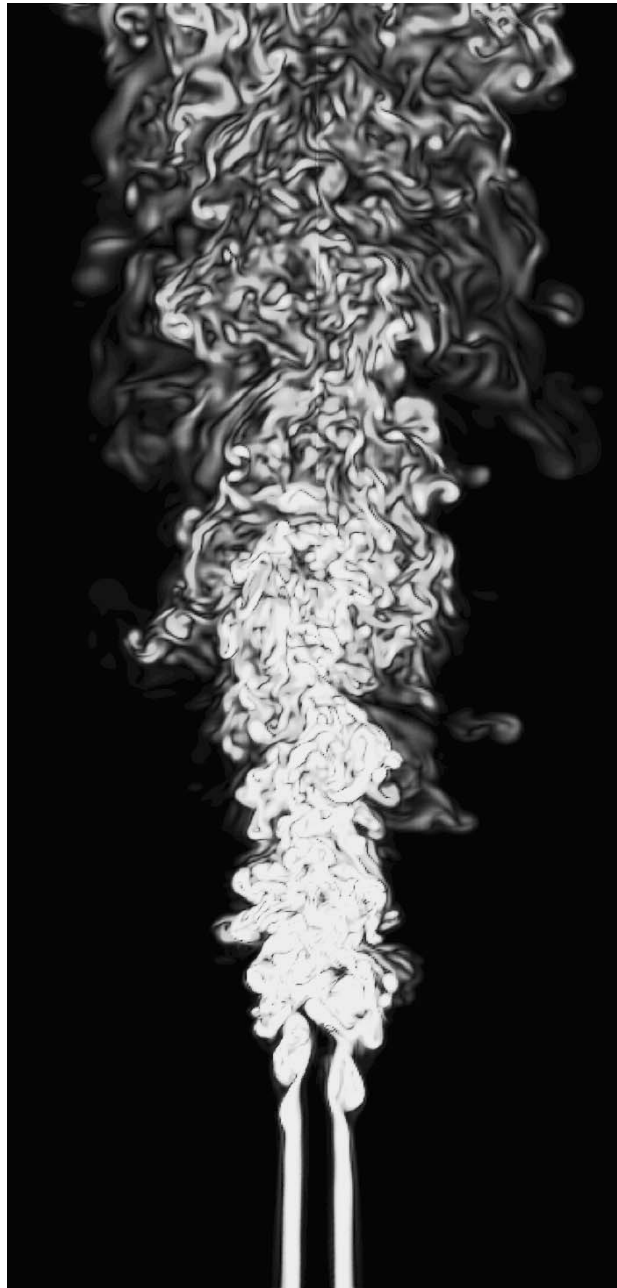


Figure 5.5: *Round jet at $Re = 10000$: view of the vorticity field in the plane $y = 0$ at $t/t_0 = 450$.*

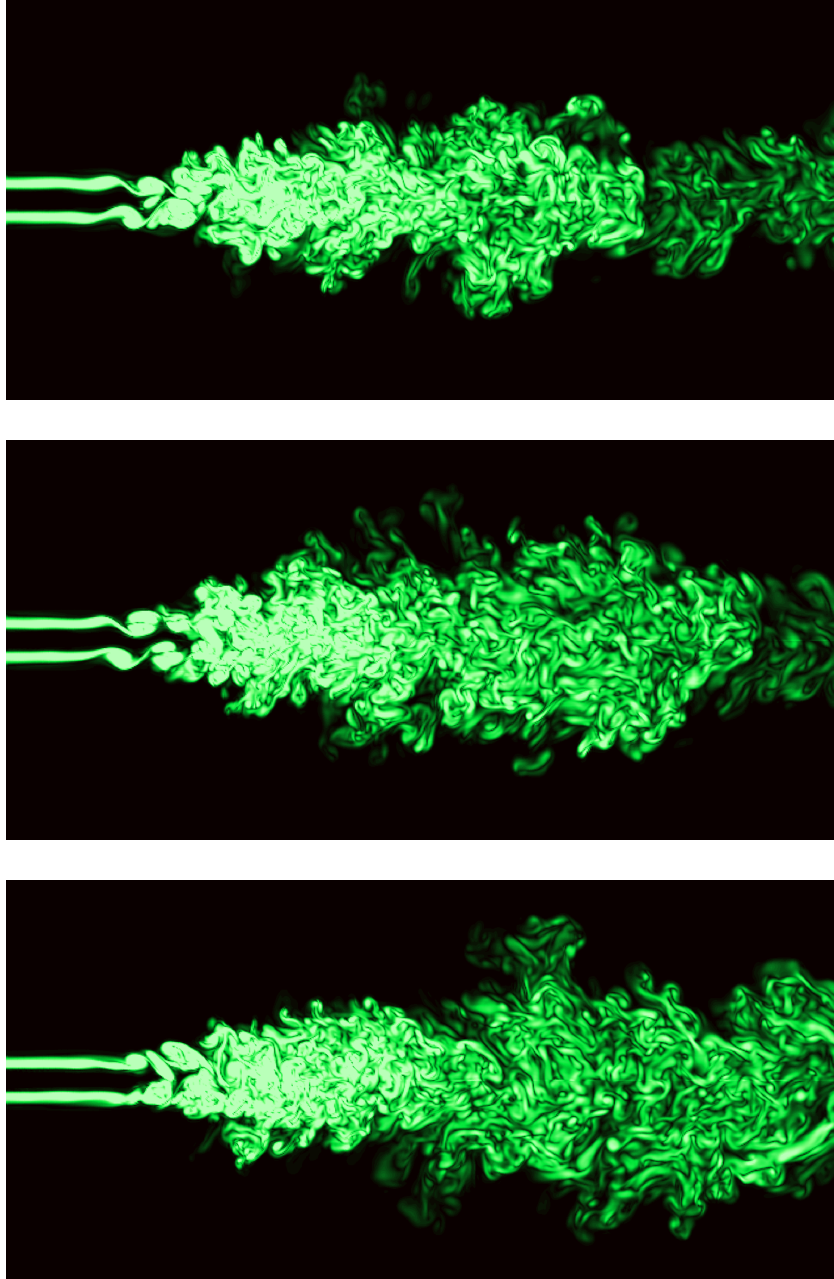


Figure 5.6: Round jet at $Re = 10000$: view of the vorticity field in the plane $y = 0$, before the regime is attained: $t/t_0 = 150$ (top), $t/t_0 = 195$ (center) and $t/t_0 = 240$ (bottom).

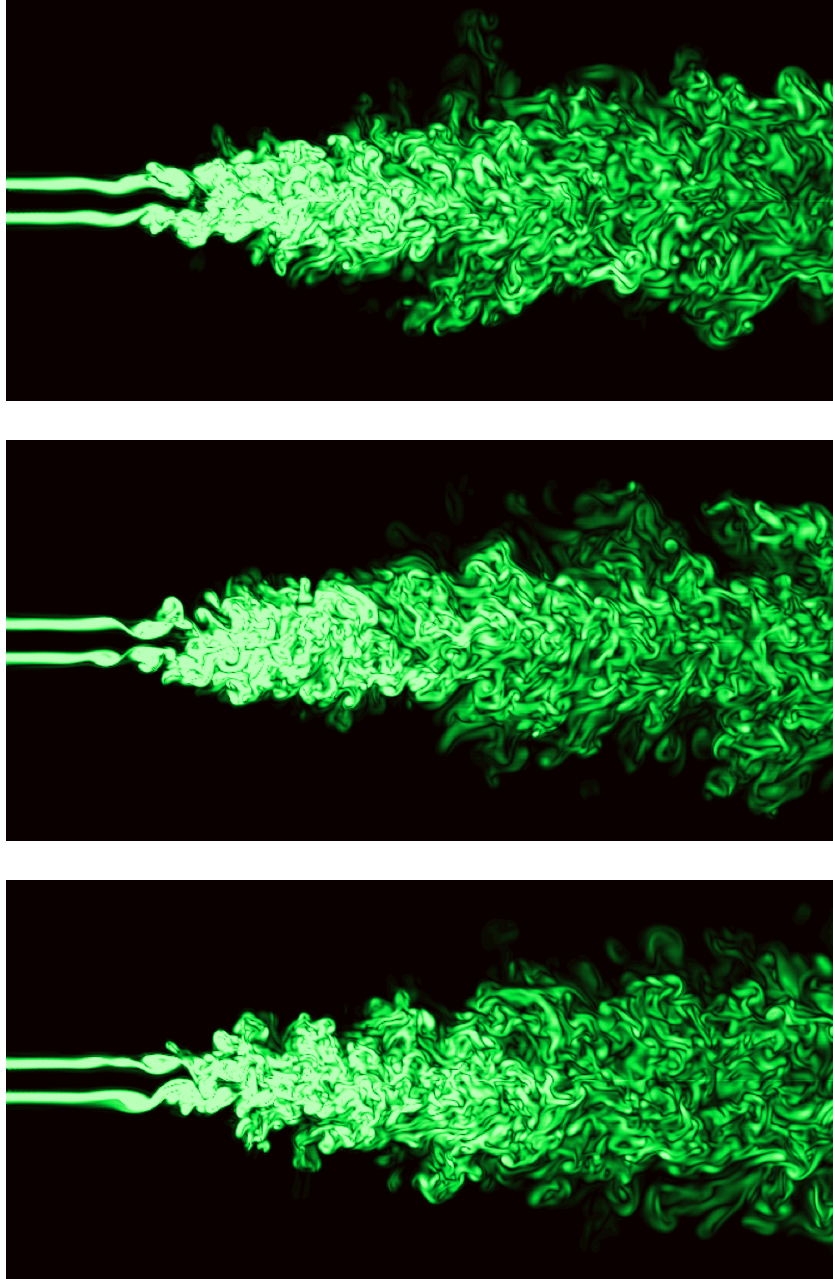


Figure 5.6: Round jet at $Re = 10000$: view of the vorticity field in the plane $y = 0$ when the regime is attained: $t/t_0 = 300$ (top), $t/t_0 = 375$ (center) and $t/t_0 = 457.5$ (bottom).

shape of these profiles appears to remain identical. Defining the centerline velocity as

$$U_0(x) \equiv \langle U_x(x, 0, 0) \rangle, \quad (5.2)$$

and the jet's half-width $r_{1/2}(x)$ such that

$$\langle U_x(x, r_{1/2}(x), 0) \rangle = \frac{1}{2} U_0(x), \quad (5.3)$$

the velocity profiles can be plotted using these two scales, instead of U_J and R [63]. Fig. 5.7 shows the resulting curves. We observe that they now collapse fairly well on a single curve: the so-called self-similar velocity profile. Note that, in our simulation, we cannot use the velocity field up to the end of the computational domain, because of the approximate outflow condition imposed at $x/R = 50.0$. As it will be confirmed with the next results, the self-similar region here extends from $x/R \simeq 15$ to $x/R \simeq 34$. Usually, for an unperturbed jet, the self-similar region starts later. To reduce the developing region, we here slightly perturbed the inflow condition so as to enhance the transition to turbulence. Indeed, a computational domain twice as long would lead to a number of grid points at least eight times larger (considering that the jet spreads linearly), leading to a currently unaffordable domain of 1 billion grid points.

Fig. 5.8 provides the axial velocity profiles, now also averaged inside the self-similar region: our best "self-similar axial velocity profile". Fig. 5.8 also provides the radial velocity profile (note that, due to the slenderness of this flow, $\langle U_r \rangle$ is much smaller than U_0 , by a factor of ~ 50). These two curves are seen to be in very good agreement with the experimental LDA data of Hussein *et al.* [33]. We have also observed that taking a larger self-similar region (up to $x/R \simeq 40$) leads to an axial velocity profile that is slightly flatter in the center of the jet compared with the experimental data. This behavior is due to the outflow boundary condition that tends to slightly "block" the flow. A significant part of the computational domain has thus to be neglected for the statistics.

We now examine the axial variation of scales. Fig. 5.9 shows the evolution of $U_J/U_0(x)$ with the axial distance x/D . We observe that, in the self-similar region, the evolution is mainly linear. The straight line shown in the figure is obtained by least mean square fit of the data in the self-similar region. It is usually expressed as,

$$\frac{U_0(x)}{U_J} = \frac{B}{(x - x_0)/D}, \quad (5.4)$$

where B is a constant [63]. Fig. 5.9 also shows the axial evolution of $r_{1/2}(x)/R$.

5.3. Simulation results

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Table 5.1: The spreading rate S and the velocity decay B obtained from several experimental data [63] and from the present LES.

	Panchapakesan and Lumley	Hussein <i>et al.</i> , hot-wire data	Hussein <i>et al.</i> , laser-Doppler data	present LES (VIC-PFM)
Re	11000	95500	95500	10000
S	0.096	0.102	0.094	0.103
B	6.06	5.9	5.8	5.5

In the self-similar region, the jet spreads linearly:

$$S = \frac{d}{dx} r_{1/2}(x) . \quad (5.5)$$

Table 5.1 provides the spreading rate S and the velocity decay B obtained from several experimental data. The values here obtained are in good agreement with these data, and especially for the spreading rate value. Neglecting the "Towsend" term, the continuity equation

$$\frac{\partial \langle U_x \rangle}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (r \langle U_r \rangle) = 0 \quad (5.6)$$

can also be written function of the spreading rate S

$$S \xi \frac{d}{d\xi} (\xi f(\xi)) = \frac{d}{d\xi} (\xi h(\xi)) \quad (5.7)$$

with $f(\xi) = \langle U_x \rangle / U_0$, $h(\xi) = \langle U_r \rangle / U_0$ and $\xi = r / r_{1/2}$. Fig. 5.10 shows the radial velocity profile obtained by integration of Eq. (5.7) and using the S value obtained. Both curves collapse rather well even if a small difference is observed for the largest value attained.

Finally, Fig. 5.11 shows another statistic on the mean velocity field, the axial variation of the mass flow rate:

$$\dot{m}(x) = 2\pi\rho \int_0^\infty \langle U_x \rangle r dr . \quad (5.8)$$

It too grows linearly with x . Once more, we observe that the outflow condition influences the flow before $x/R \approx 38$.

The next interesting statistics are the fluctuating velocity components, more specifically the Reynolds stress components. As for the mean values ($\langle U_x \rangle$ and $\langle U_r \rangle$), the Reynolds stresses ($\langle u_x'^2 \rangle$, $\langle u_r'^2 \rangle$, $\langle u_\theta'^2 \rangle$ and $\langle u_x' u_r' \rangle$) are also self-similar.

The components $\langle u'_x u'_\theta \rangle$ and $\langle u'_r u'_\theta \rangle$ are zero because of the circumferential symmetry (these diagnostics are here also used as criteria to confirm well converged statistics). Fig. 5.12 provides the self-similar profiles. The curves are in good agreement with the profiles obtained by Hussein *et al.* [33]. As expected, the $\langle u'^2_r \rangle$ and $\langle u'^2_\theta \rangle$ curves collapse well and start at a value included between $[0.04 - 0.05]$. The $\langle u'_x u'_r \rangle$ profile has the correct shape with a maximum value of ~ 0.02 at $r/r_{1/2} \approx 0.6$, which also fits very well with Hussein's data. The maximum value of $\langle u'^2_x \rangle$ is slightly lower than that obtained by Hussein: 0.07 instead of 0.08.

Fig. 5.12 also shows the ratio of the r.m.s. axial velocity fluctuations to the velocity. It was shown [33] that this value increases with $\xi = r/r_{1/2}$ without bound. On the centerline, it has the value of about 0.25. This result is also well observed here. We also consider the r.m.s. axial velocity on the centerline

$$u'_0(x) \equiv \langle u'^2_x \rangle_{r=0}^{1/2}. \quad (5.9)$$

Panchapakesan and Lumley [57] showed that, in the self-similar region, $u'_0(x)/U_0(x)$ tends to a constant value of approximately 0.25. Fig. 5.13 provides the value obtained numerically. In the self-similar region, we obtain 0.248, thus also close to the experimental value.

Fig. 5.14 shows the normalized turbulent viscosity profile, defined as

$$\hat{\nu}_T = \frac{\nu_T}{U_0 r_{1/2}} \quad (5.10)$$

with

$$\langle u'_x u'_r \rangle = -\nu_T \frac{\partial \langle U_x \rangle}{\partial r}. \quad (5.11)$$

In the center of the jet, the experimental data of Hussein show a mean value of 0.03 and, for $\xi > 1$, it decreases up to ~ 0.01 at $\xi = 2$. Here, some oscillations are observed in the center, and for larger ξ , the values collapse rather well. The oscillations are essentially due to the numerical difficulty to compute the ratio between the numerator $\langle u'_x u'_r \rangle$ and the denominator $\frac{\partial \langle U_x \rangle}{\partial r}$ that both tend to zero when $\xi \rightarrow 0$. If we take the assumption of a uniform turbulent viscosity to overcome the closure problem, the axial momentum equation becomes

$$\langle U_x \rangle \frac{\partial \langle U_x \rangle}{\partial x} + \langle U_r \rangle \frac{\partial \langle U_x \rangle}{\partial r} = \frac{\nu_T}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \langle U_x \rangle}{\partial r} \right). \quad (5.12)$$

The solution of Eq. (5.12), together with Eq. (5.6), was first obtained by Schlichting [68] and is given by

$$f(\xi) = \frac{1}{(1 + (\sqrt{2} - 1)\xi^2)^2}. \quad (5.13)$$

5.3. Simulation results

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Fig. 5.15 compares this profile with the present profile and we observe that, in the center, our profile collapses very well. For $\xi > 1$, the comparison with the experimental data of Hussein shows that the analytic profile is not valid. This is so because the assumption of a constant turbulent viscosity in this region is not correct, as it has to decrease with ξ .

The last diagnostic is concerned with the relative magnitude of the shear stress, presented using the ratio $\langle u'_x u'_r \rangle / \langle k \rangle$ with

$$\langle k \rangle \equiv \frac{1}{2} \langle u_i u_i \rangle \quad (5.14)$$

the turbulent kinetic energy. Fig. 5.16 shows the obtained profiles. The curve has a flat central portion with a value around 0.3, also confirmed by the experimental data.

Fig. 5.17 provides the axial and radial velocity fields. We notice that the radial velocity is still important at the lateral domain boundary, indicating that the ambient fluid is indeed entrained into the jet. This is confirmed in Fig. 5.22 giving the axial and radial velocity profiles along the x axis. Again, it confirms the importance of having the correct boundary conditions. If periodic boundary conditions were used, the jet would be rapidly confined (as the radial velocity would be zero on the boundaries) leading to an incorrect spreading rate S and velocity decay B . The same would occur if using slip conditions.

Figs. 5.18 to 5.20 show the velocity fluctuations fields. Up to $x/R \approx 5$, the flow remains laminar. The most important fluctuations are observed between $x/R \approx 5$ and 20. Figs. 5.19 and 5.24 also show the good similarity between the radial and azimuthal velocity fluctuations. Fig. 5.20 shows the cross-correlation fluctuations $\frac{\langle u'_x u'_\theta \rangle}{U_j^2}$ and $\frac{\langle u'_r u'_\theta \rangle}{U_j^2}$, that should be zero if the turbulence statistics are converged: it is here well verified. Finally, Fig. 5.21 provides the turbulent kinetic energy.

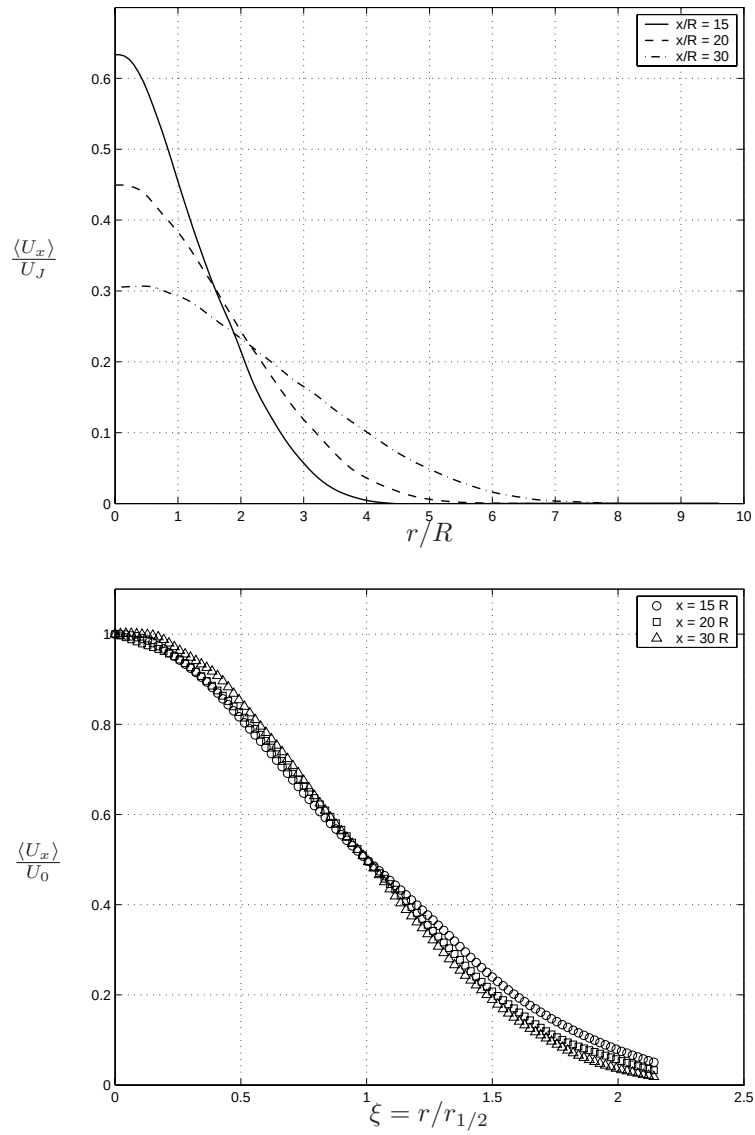


Figure 5.7: Round jet at $Re = 10000$: radial profiles of the axial velocity at three locations x/R , made dimensionless using U_J and R (top), and using $U_0(x)$ and $r_{1/2}(x)$ (bottom).

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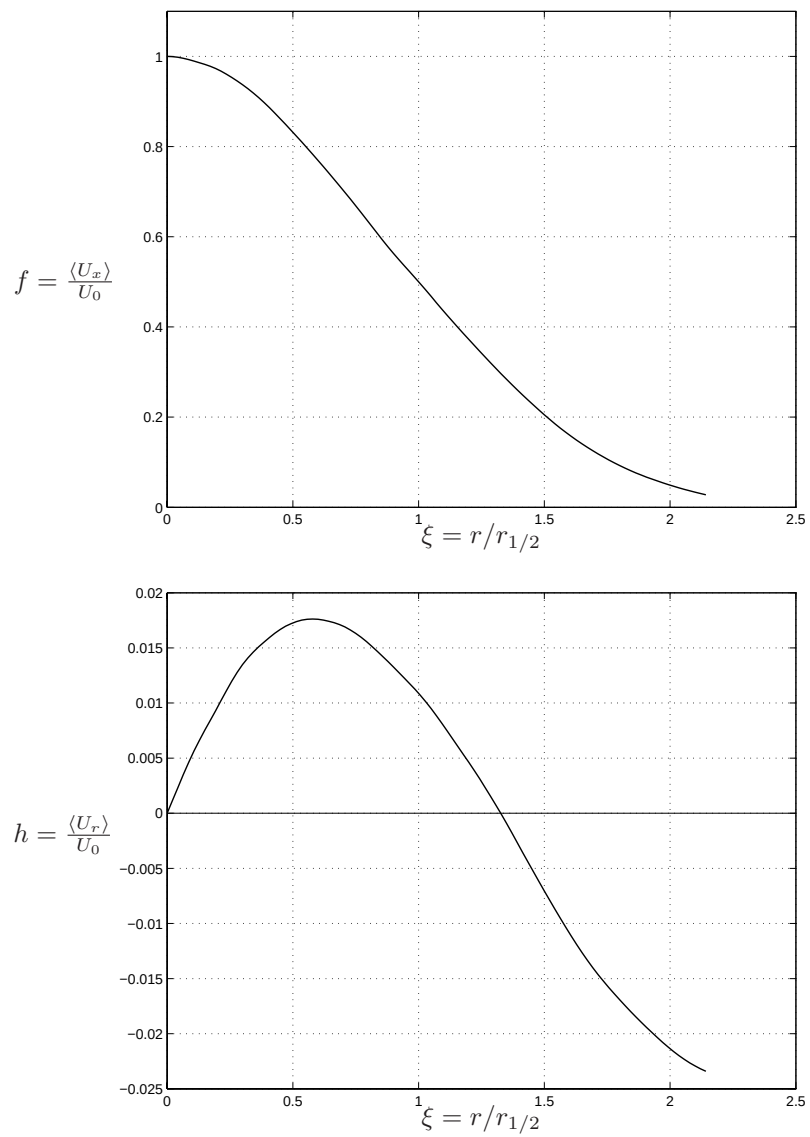


Figure 5.8: Round jet at $Re = 10000$: self-similar profiles of the axial velocity (top) and of the radial velocity (bottom).

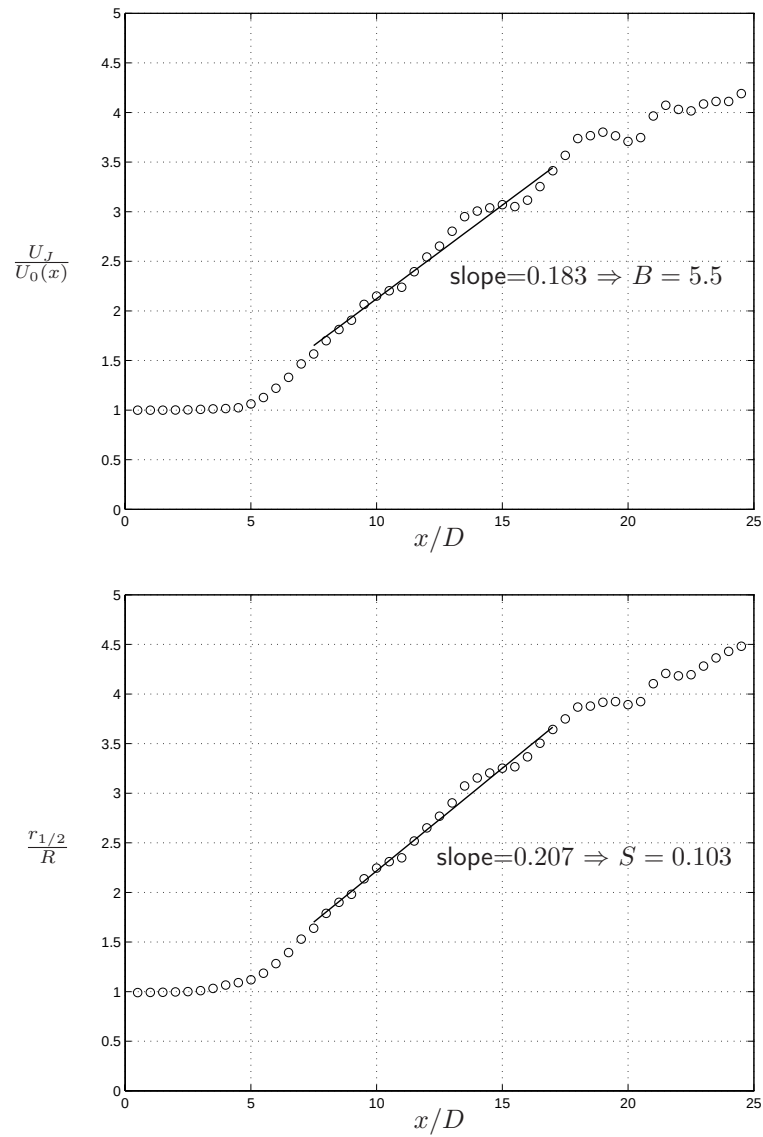


Figure 5.9: Round jet at $Re = 10000$: variation, with axial distance, of the centerline velocity (top) and of the jet's half-width (bottom).

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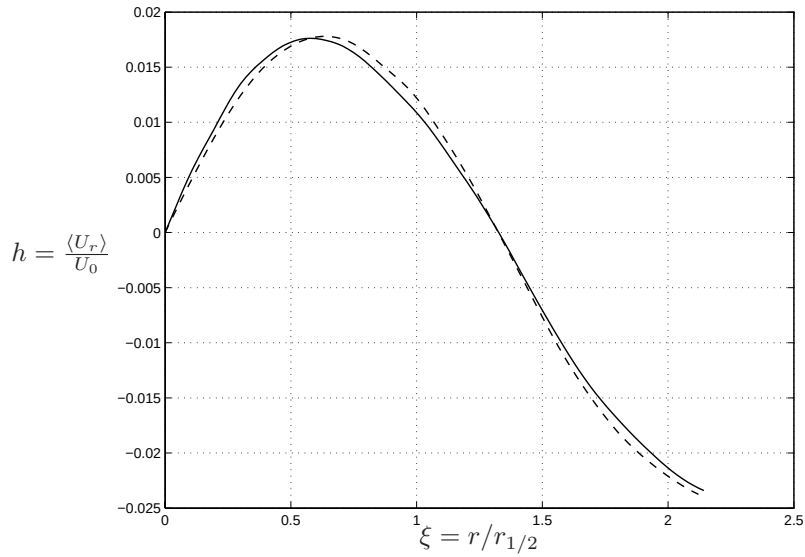


Figure 5.10: Round jet at $Re = 10000$: self-similar profiles of the radial velocity; direct computation (solid) and using the continuity equation (dash).

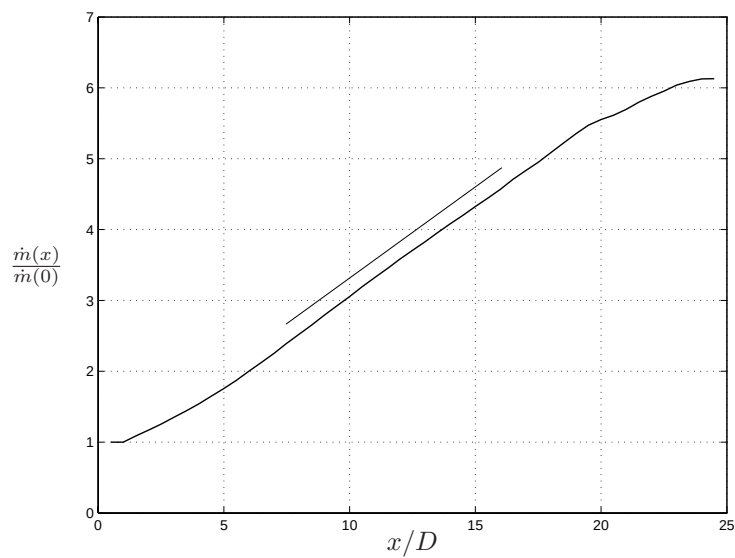


Figure 5.11: Round jet at $Re = 10000$: variation, with axial distance, of the mass flow rate.

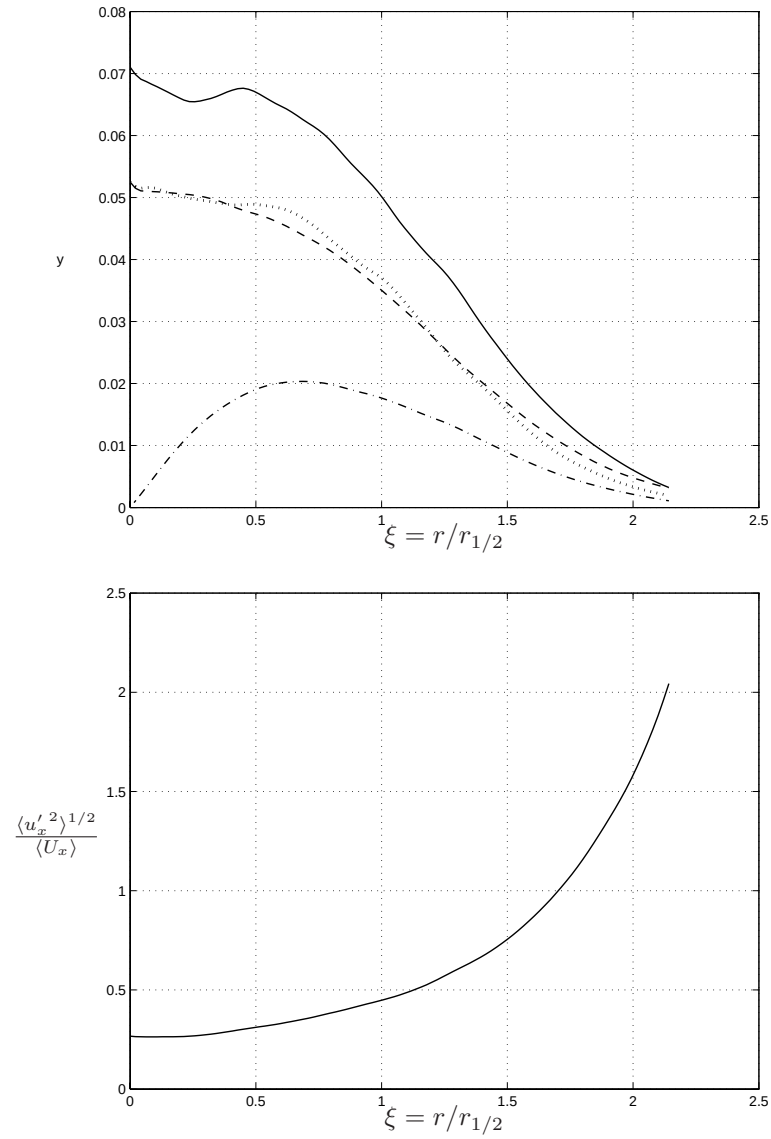


Figure 5.12: Round jet at $Re = 10000$: self-similar profiles of the turbulence intensities (Reynolds stresses) (top) and of the ratio of "r.m.s. velocity fluctuations to velocity" (bottom).

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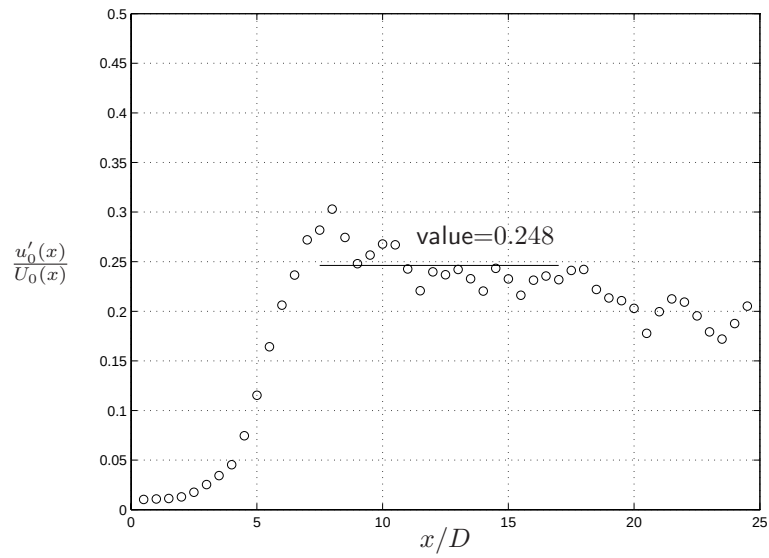


Figure 5.13: Round jet at $Re = 10000$: variation, with axial distance, of the centerline r.m.s. velocity.

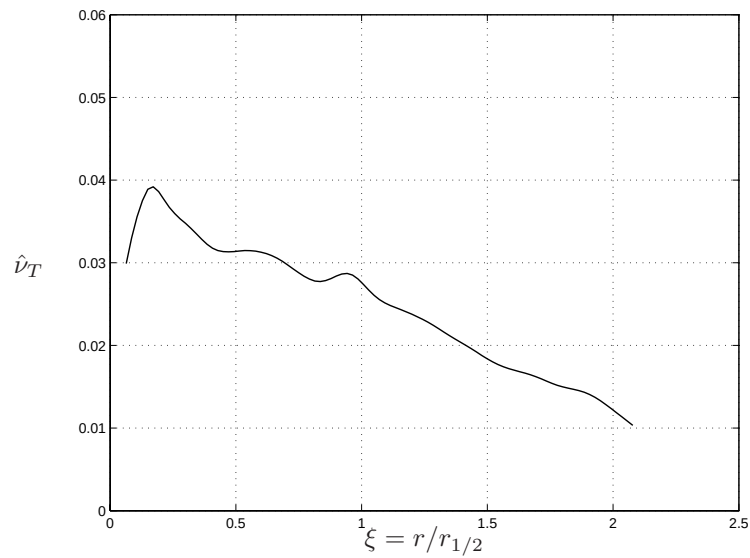


Figure 5.14: Round jet at $Re = 10000$: normalized turbulent viscosity.

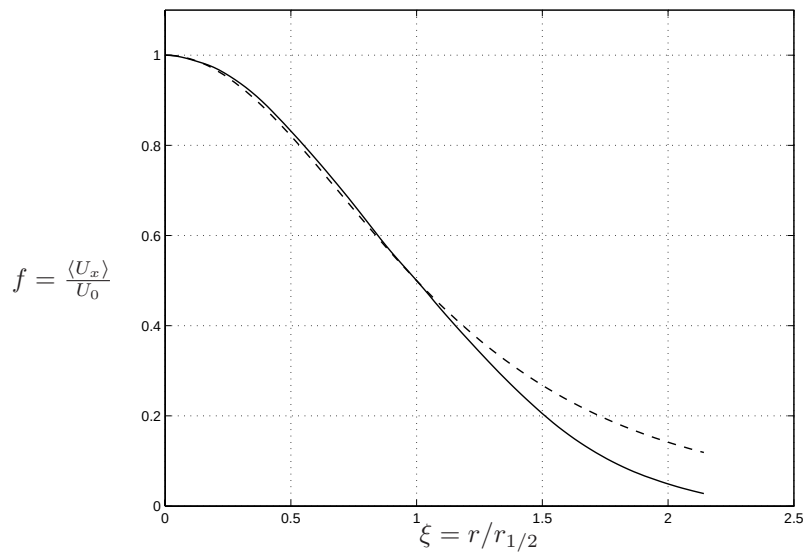


Figure 5.15: Round jet at $Re = 10000$: self-similar profiles of the axial velocity; direct computation (solid) and using the uniform turbulent viscosity solution (dash).

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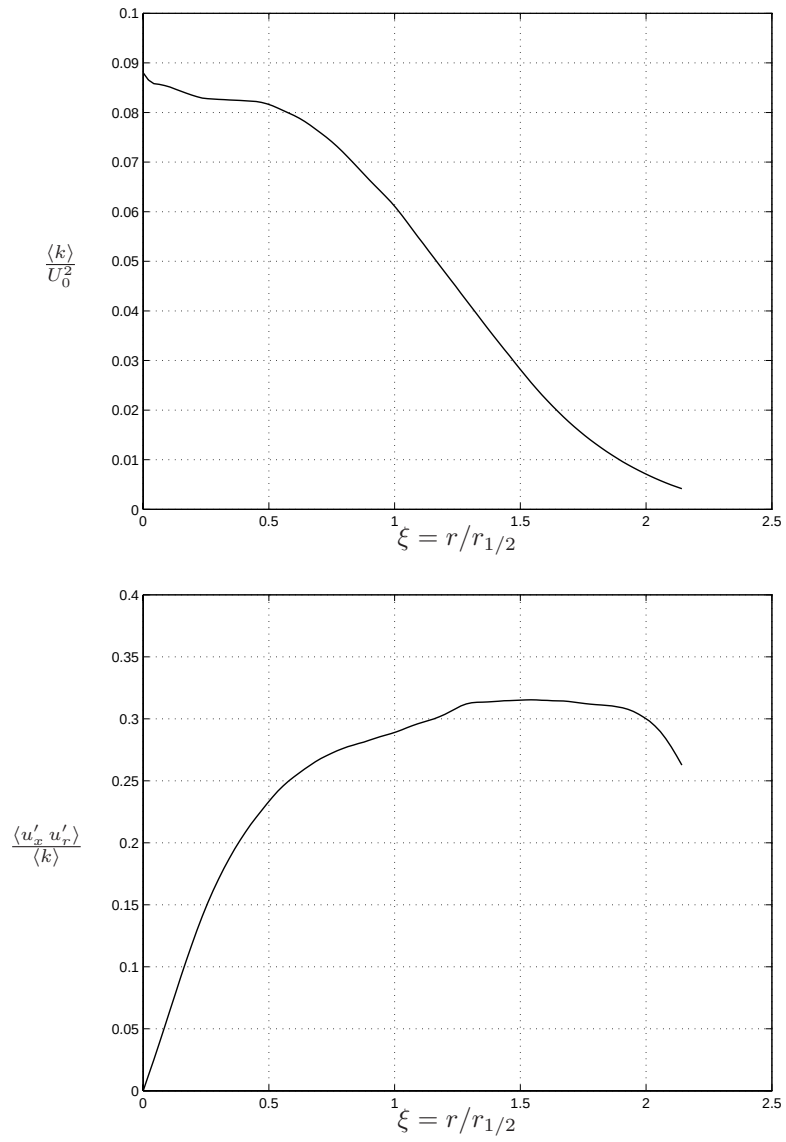


Figure 5.16: Round jet at $Re = 10000$: self-similar profiles of the turbulent kinetic energy (top) and of the shear stress (bottom).

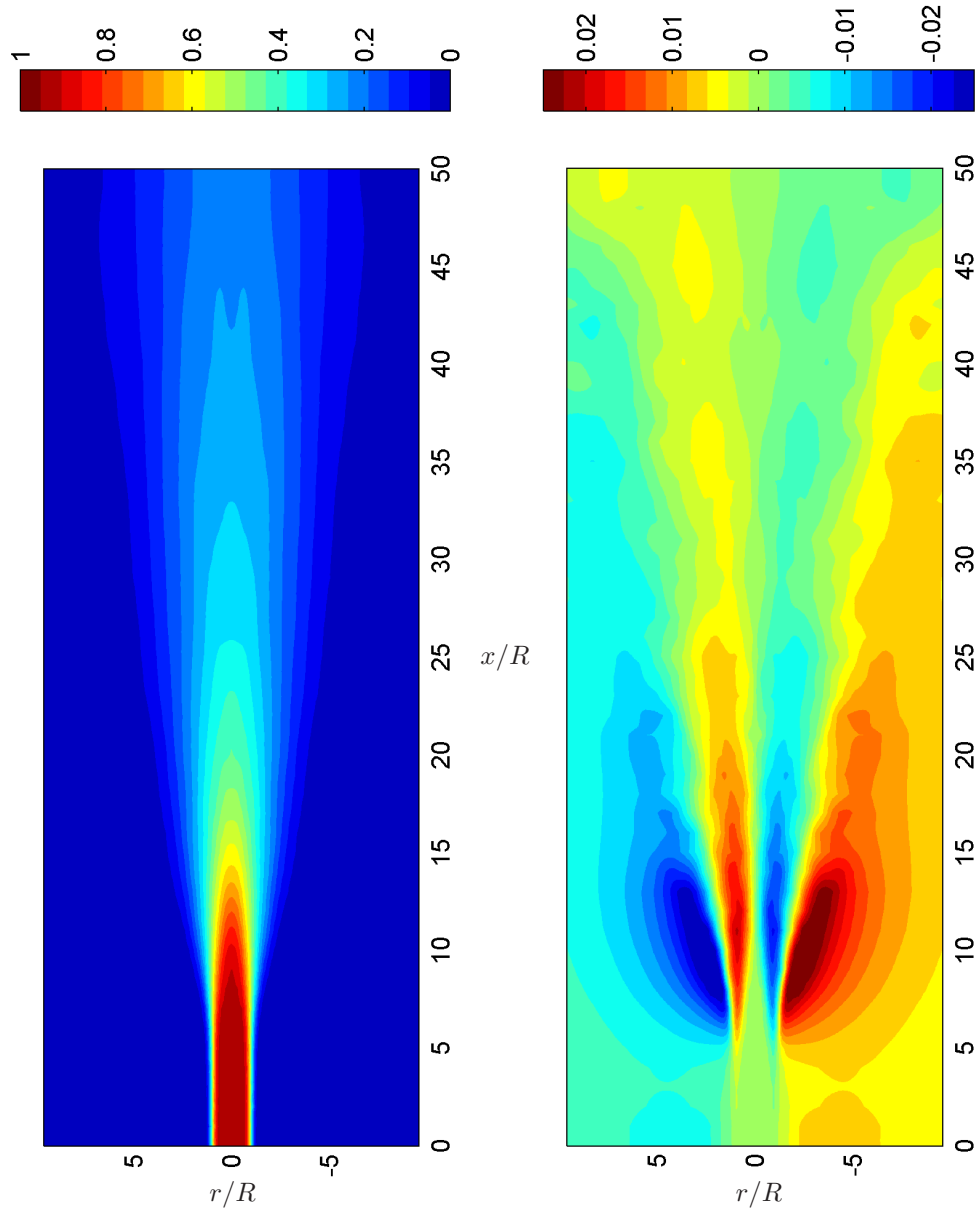


Figure 5.17: Round jet at $Re = 10000$: axial velocity field, $\langle U_x \rangle / U_J$ (left), and radial velocity field, $\langle U_r \rangle / U_J$ (right).

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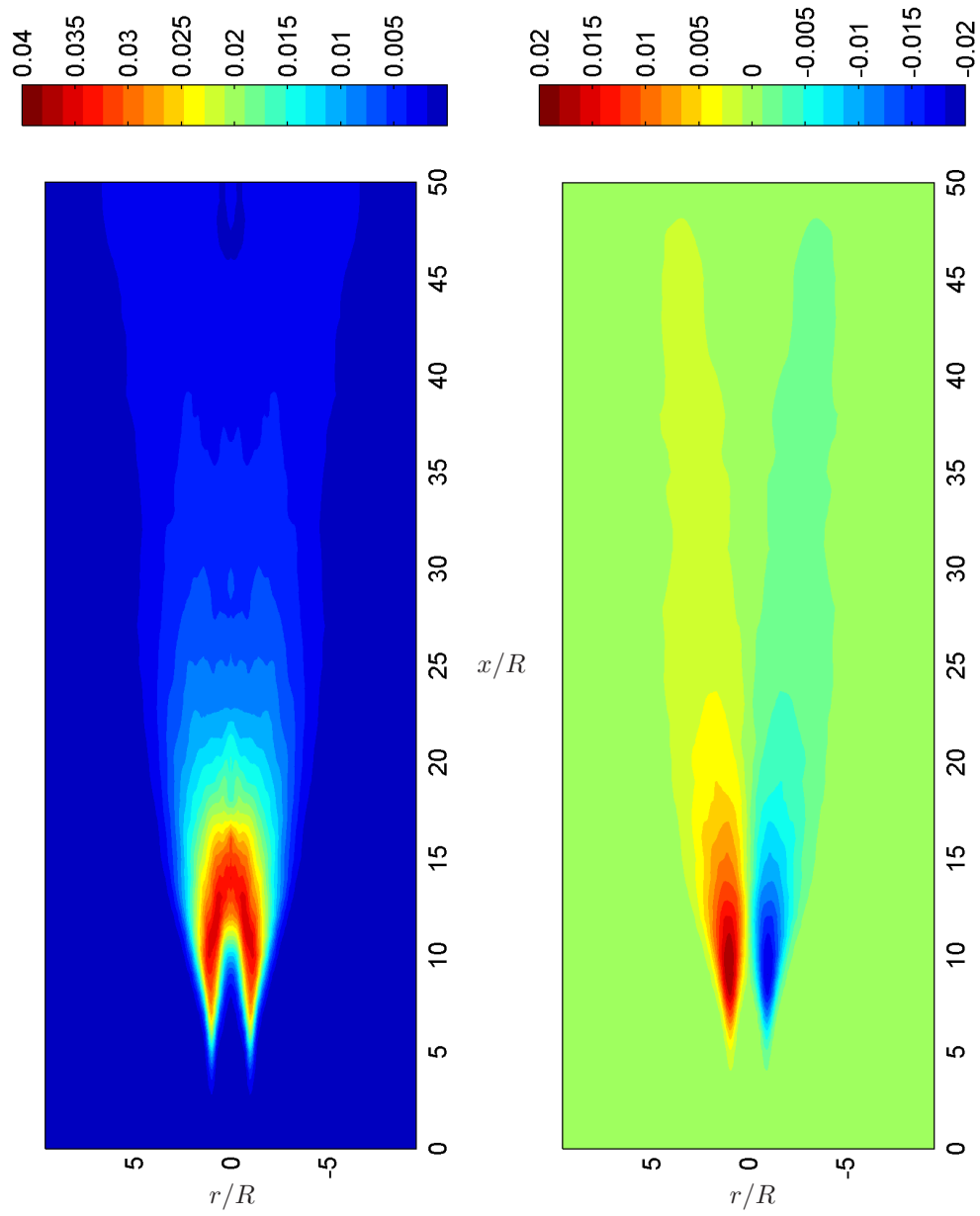


Figure 5.18: Round jet at $Re = 10000$: axial velocity fluctuations, $\frac{\langle u'_x u'_x \rangle}{U_j^2}$ (left) and cross-correlation velocity fluctuations, $\frac{\langle u'_x u'_r \rangle}{U_j^2}$ (right).

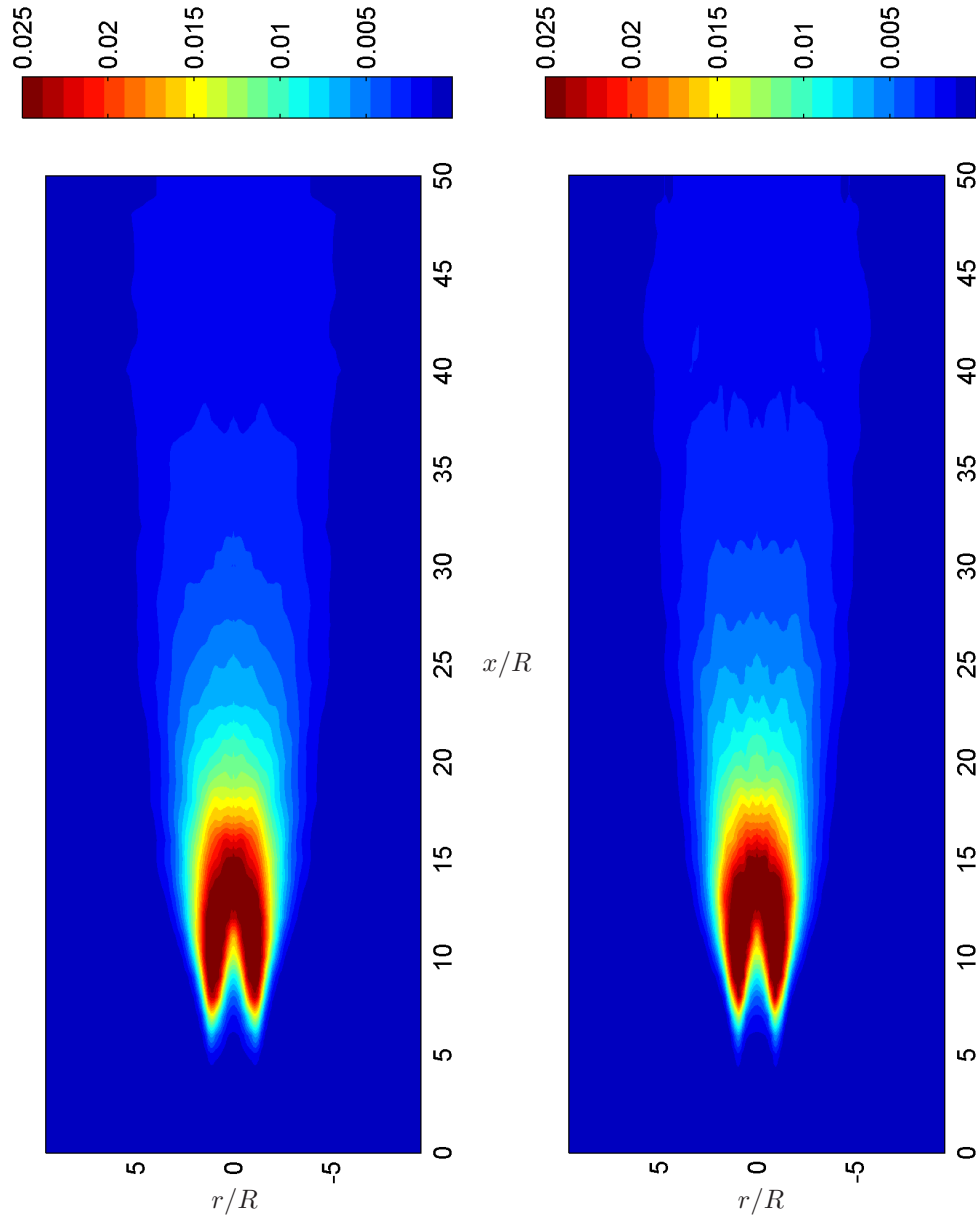


Figure 5.19: Round jet at $Re = 10000$: radial velocity fluctuations, $\frac{\langle u'_r u'_r \rangle}{U_j^2}$ (left), and azimuthal velocity fluctuations, $\frac{\langle u'_\theta u'_\theta \rangle}{U_j^2}$ (right).

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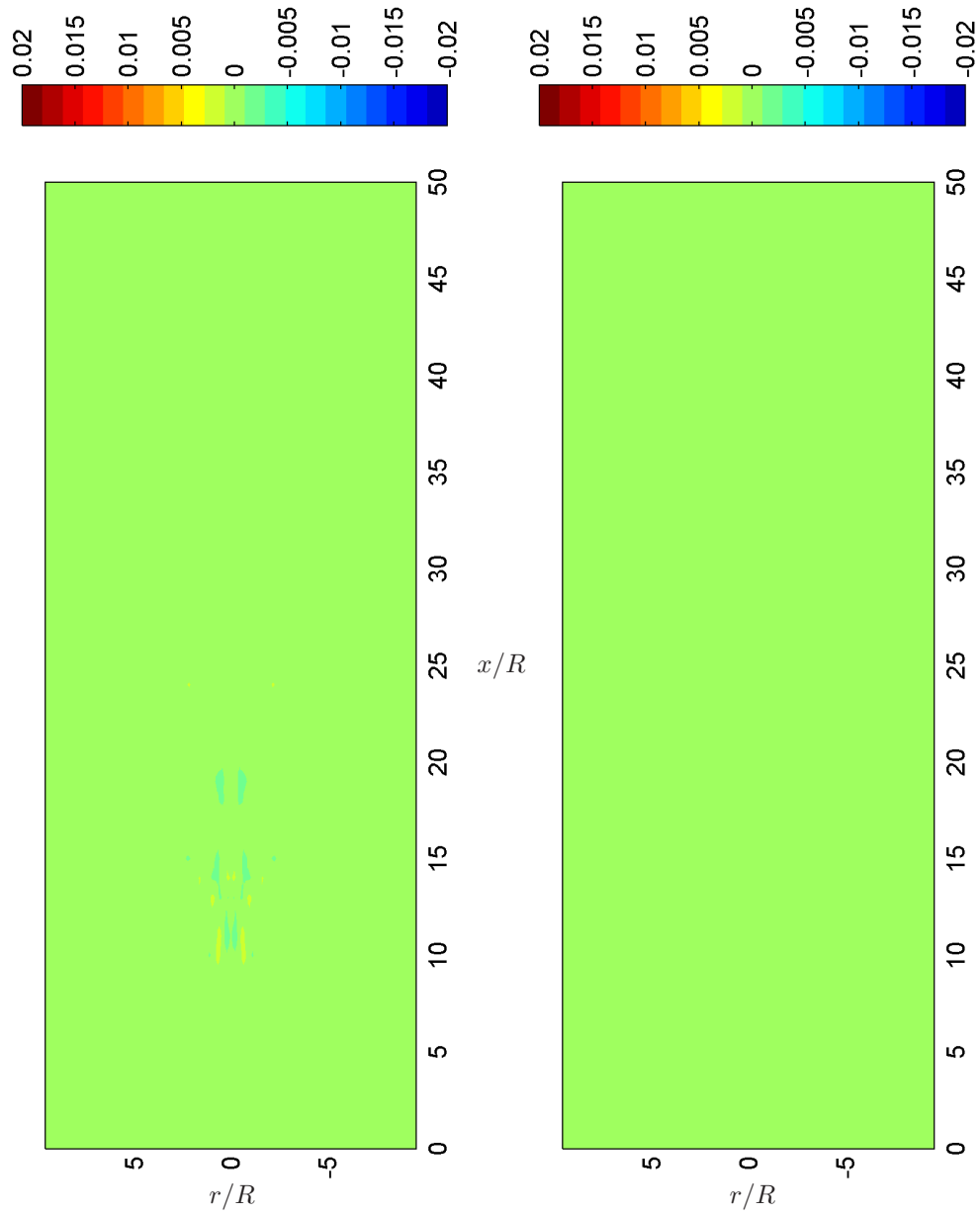


Figure 5.20: Round jet at $Re = 10000$: cross-correlation velocity fluctuations, $\frac{\langle u'_x u'_x \rangle}{U_j^2}$ (left), and $\frac{\langle u'_r u'_r \rangle}{U_j^2}$ (right).

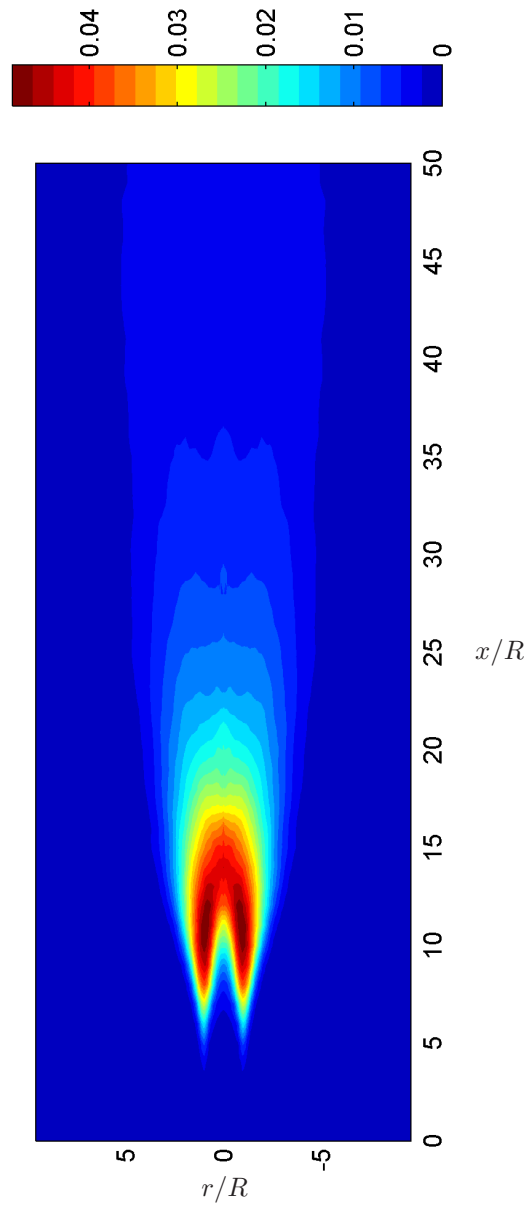


Figure 5.21: Round jet at $Re = 10000$: turbulent kinetic energy $\frac{\langle k \rangle}{U_j^2}$.

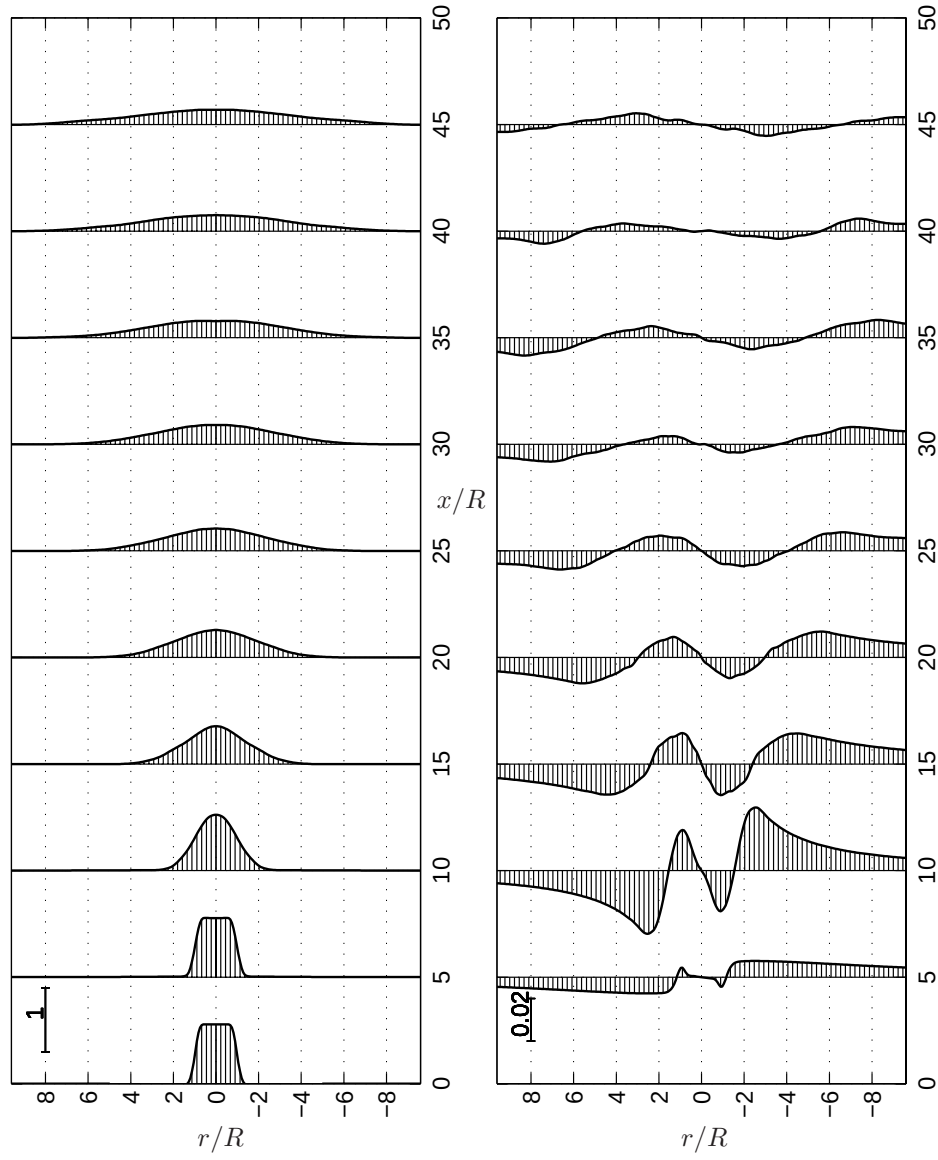


Figure 5.22: Round jet at $Re = 10000$: profiles of axial velocity, $\frac{\langle U_x \rangle}{U_J}$ (left), and of radial velocity profiles, $\frac{\langle U_r \rangle}{U_J}$ (right).

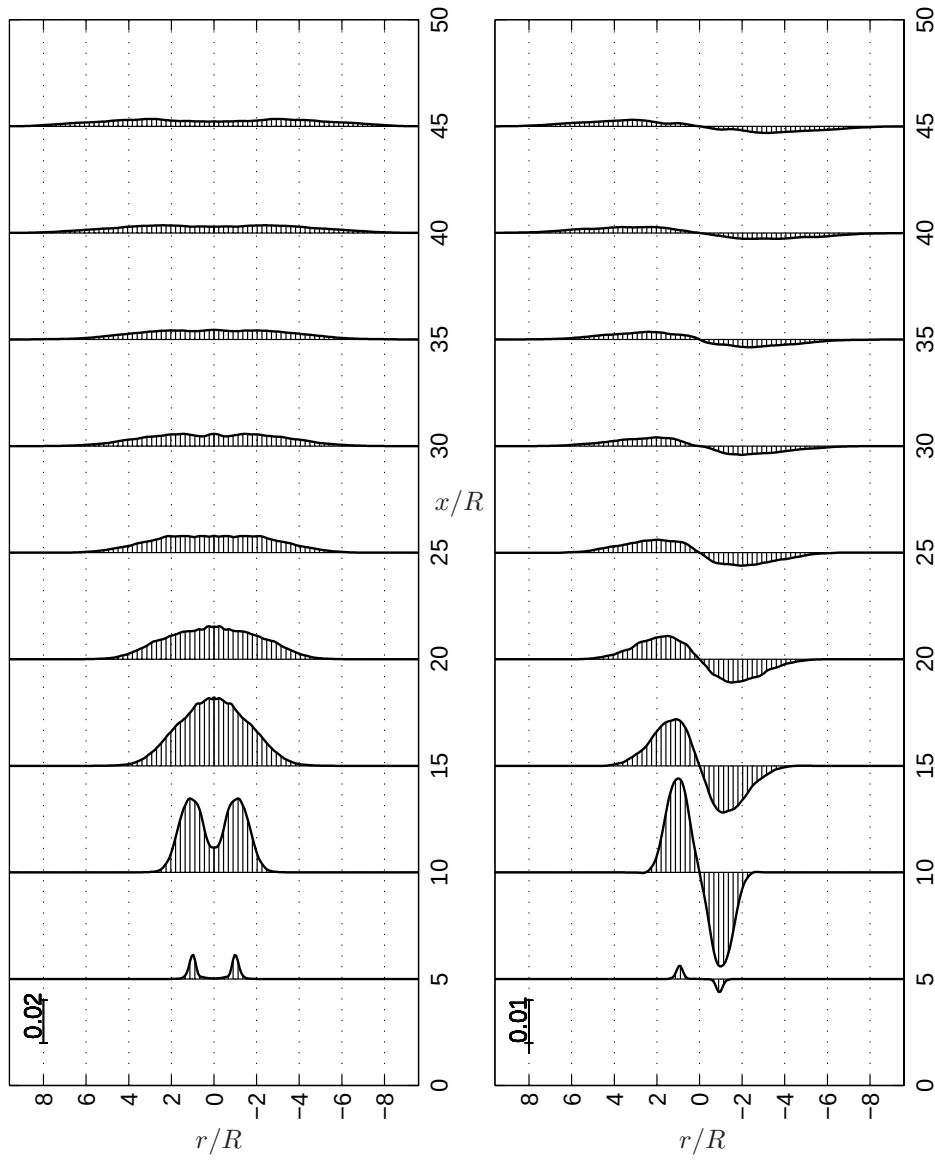


Figure 5.23: Round jet at $Re = 10000$: profiles of axial velocity fluctuations, $\frac{\langle u'_x u'_x \rangle}{U_J^2}$ (left), and of cross-correlation velocity fluctuations, $\frac{\langle u'_x u'_r \rangle}{U_J^2}$ (right).

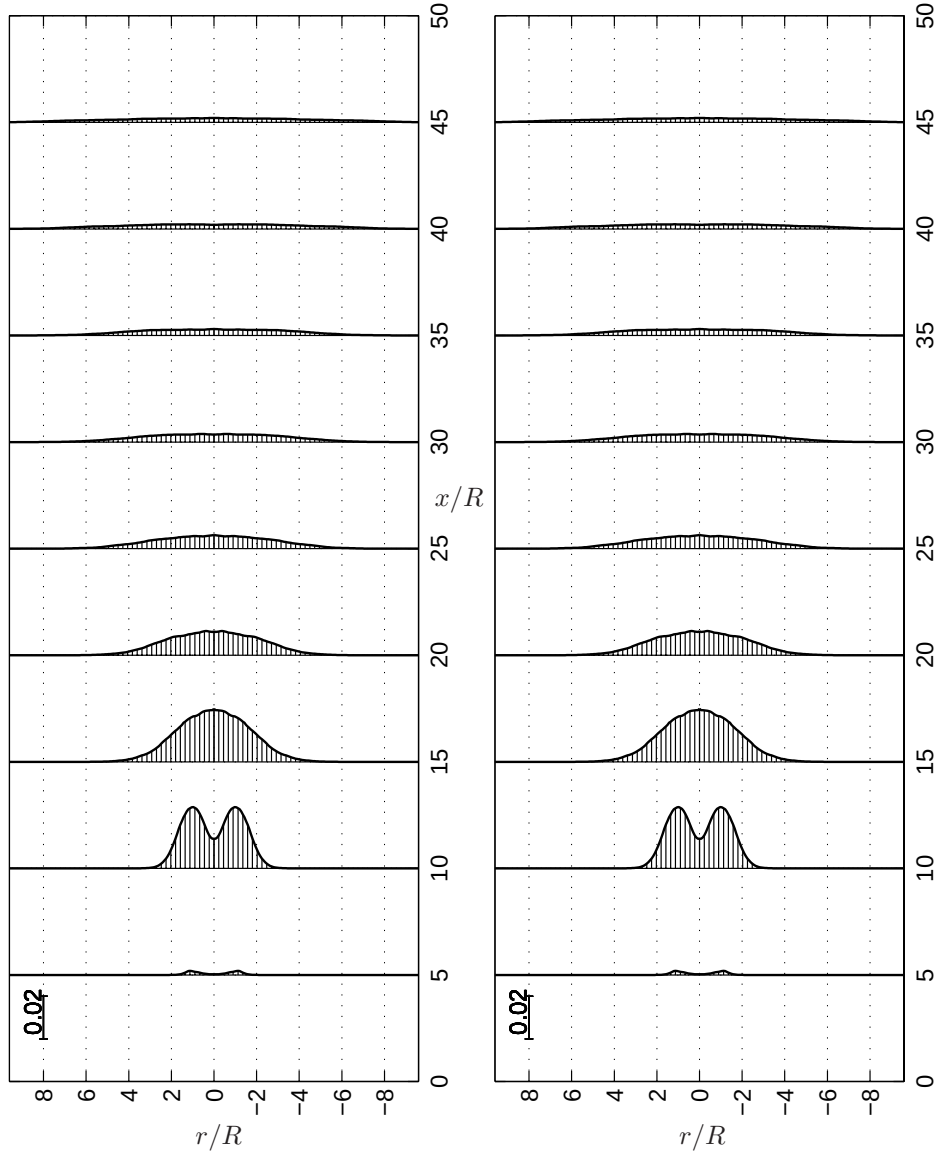


Figure 5.24: Round jet at $Re = 10000$: profiles of radial velocity fluctuations, $\frac{\langle u_r' u_r' \rangle}{U_J^2}$ (left), and of azimuthal velocity fluctuations, $\frac{\langle u_\theta' u_\theta' \rangle}{U_J^2}$ (right).

Conclusions

This thesis was concerned with the simulation of high Reynolds number, three-dimensional, incompressible flows in open domain. At the beginning of this work, the existing numerical "tools" in vortex methods were the following:

- The parallel fast multipole (PFM) method: an efficient algorithm able to compute the velocity field from the vorticity field in $\mathcal{O}(N \log(N))$ operations. Its Lagrangian framework and its ability to correctly satisfy the open domain condition makes the vortex method based on the PFM solver very appropriate for the kind of open domain flows considered here. However, its computational cost rapidly becomes too large when considering high Reynolds number flows computed on large domains.
- The vortex-in-cell (VIC) method: an efficient algorithm that combines Lagrangian and Eulerian methods. As it uses fast Poisson grid solvers, its computational efficiency is better than for the PFM method solver. Unfortunately, in its classical formulation, it cannot handle open domain.

The main objective of this thesis was to develop a new vortex method that efficiently combines these two existing methods. This development was achieved and validated through many steps:

- A 2-D version of the method was first implemented to validate the concept. It was successfully tested on a zero circulation vortex flow (see Appendix C). The results were compared, from a qualitative and quantitative point of view, with the results obtained using the vortex method with solver based solely

on fast multipole method.

- A 3-D parallel version was then developed, based on a preliminary sequential version. It led to address some interesting issues such as: ensure the continuity between the PFM solver and the VIC grid solver, the choice of a good quality redistribution/interpolation scheme and the implementation of a projection scheme to maintain the zero vorticity divergence. The parallel and sequential versions were validated on a well-known 3-D unbounded flow: the vortex ring, first at moderate Reynolds number, and then at high Reynolds number. The instability, non linear evolution and decay of the vortex ring were analyzed and compared with the theory and/or with the results found in the literature.
- The 3-D parallel version was also implemented with one periodic direction and two unbounded directions. As an example, this version is very useful for the simulation of aircraft vortex wakes. Various applications were mainly performed within two European Research projects (AWIATOR and FAR-Wake). The results were compared with those of other numerical methods also showing the quality and efficiency of the VIC-PFM method.
- The ability to treat a realistic viscous flat ground was also added. The scheme to enforce the no-slip boundary condition is essentially the same as the procedure developed by Ploumhans *et al.* [61]. It permits to simulate aircraft vortex wakes in ground effect. The results were compared with simulations achieved using a 4th order finite differences code and were in very good accordance.
- The last methodological development was the implementation of a space-developing version. We were then able to simulate the evolution, in space and time, of an inflow condition. It also requests to impose some symmetries on the flow, as also used in the case with a flat ground. This version permits to compute space-developing aircraft vortex wakes. Some comparisons were made with the time-developing simulations and highlighted some specific behaviors absent in the time-developing cases. The method was also applied

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to the simulation of a turbulent round jet at high Reynolds number. The results were in very good agreement with the theory and with the experimental results found in the literature.

- Aside from the numerical method developments, the use of subgrid-scale (SGS) models for large-eddy simulations (LES) was rapidly required. Various SGS models were implemented and compared between themselves on a complex and transitional flow: a counter-rotating four vortex system. The first objective was to find SGS models that are active only during the complex and turbulent phases of the flow, and inactive otherwise. The coefficients included in the formulation of such models were first determined from theory or were taken as proposed in the literature.
- A more complete study of the asymptotic behavior of the various SGS models was then performed on homogeneous isotropic turbulence (HIT) at high Reynolds number. To be able to make quantitative comparisons with existing results, the VIC code with periodic conditions was also implemented. A proper fit of the scale-dependence of the coefficients used in the various SGS models was obtained and was in good accordance with what it is found in the literature. This analysis also showed the asymptotic spectral behavior of such models by comparing the shape of the obtained spectra. The superiority of the models acting on the small scales was highlighted even if their behavior is still not perfect.

As already mentioned, this thesis took advantage of all the work and research achieved during the last decade by Pr. G. Winckelmans and his colleagues or Ph.D. students (P. Ploumhans [60], H. Jeanmart [36] and G. Daeninck [21]). The present VIC-PFM method constitutes an important step in the evolution of vortex methods, but many future developments still have to be done. The method is certainly very efficient for complex, turbulent, unbounded (or half-unbounded) flows. Yet it now remains to transfer some recent developments made in the frame of "pure" Lagrangian methods for bluff-body flows. More specifically:

- The coupling of the VIC-PFM method with an Eulerian grid based solver treating the near-wall region. The concept was already developed by Daen-

inck [21], in 2-D, and using the fast multipole method alone. The idea is to replace the fast multipole method with the present VIC-PFM method. It would permit an important benefit in computational cost and the possibility to extend the concept to 3-D.

- The implementation of hierarchically refined grids within the VIC-PFM method. This approach, developed by Daeninck in 3-D [21], allows to arbitrarily refine the particle resolution where the flow physics require it, using hierarchically refined grids.
- A hybrid RANS-LES approach: coupling of a finite volume method with unstructured grid and RANS/LES approach for the flow around complex bluff-bodies (as developed at CENAERO) and of the VIC-PFM method for LES in the wake region.

The future of vortex methods is thus very promising. All we have to do is "just" to keep working...

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Appendix A

Laplacian schemes that are less sensitive to grid orientation

We here present the 2-D and 3-D "isotropic" Laplacian schemes for which the performance is less dependant of the local grid orientation than the classical "cross" scheme.

We begin with the 2-D case, see Fig. A.1. We search the coefficients a , b and c to use in

$$\begin{aligned} (\nabla^2 \omega)_{i,j} \approx \frac{1}{h^2} [& a (\omega_{i-1,j+1} + \omega_{i+1,j+1} + \omega_{i-1,j-1} + \omega_{i+1,j-1}) \\ & + b (\omega_{i,j+1} + \omega_{i,j-1} + \omega_{i+1,j} + \omega_{i-1,j}) \\ & + c (\omega_{i,j})] \end{aligned} \quad (\text{A.1})$$

under the constraint that the truncation error is independent of orientation. We ask that the numerical Laplacian has the form :

$$(\nabla_h^2 \omega)_{i,j} = (\nabla^2 \omega)_{i,j} + \mathcal{C} h^2 (\nabla^2 (\nabla^2 \omega))_{i,j} + \mathcal{O}(h^4). \quad (\text{A.2})$$

Expressing $\omega_{i+1,j}$, etc. using Taylor series, and replacing their expressions in Eq. (A.1), the constraint Eq. (A.2) leads to a system for a , b and c :

$$\begin{cases} 4a + 2b = 2 \\ 4a + 4b + c = 0 \\ 24a - 2(4a + 2b) = 0 \end{cases}$$

which gives $a = 1/6$, $b = 4/6$ and $c = -20/6$. Replacing these values in Eq. (A.2), one obtains :

$$(\nabla_h^2 \omega)_{i,j} = \left(\nabla^2 \left(\omega + \frac{h^2}{12} \nabla^2 \omega \right) \right)_{i,j} + \mathcal{O}(h^4) \quad (\text{A.3})$$

The leading truncation error term is thus $(h^2/12) (\nabla^4 \omega)_{i,j}$ which is not sensitive to the orientation of the grid with relation to the solution. This is not the case for the usual cross scheme. The fact that the scheme also uses the corner points makes it less sensitive to the grid orientation.

The same development can be done in 3-D, see Fig. A.1. We have to determine the constants a , b , c and d to use in

$$\begin{aligned} (\nabla^2 \omega)_{i,j,k} \approx \frac{1}{h^2} [& a (\omega_{i+1,j+1,k+1} + \omega_{i+1,j+1,k-1} + \omega_{i+1,j-1,k+1} + \dots) \\ & + b (\omega_{i+1,j+1,k} + \omega_{i+1,j-1,k} + \omega_{i-1,j+1,k} + \dots) \\ & + c (\omega_{i-1,j,k} + \omega_{i+1,j,k} + \omega_{i,j-1,k} + \dots) \\ & + d (\omega_{i,j,k})] \end{aligned} \quad (\text{A.4})$$

under the constraint that :

$$(\nabla_h^2 \omega)_{i,j,k} = (\nabla^2 \omega)_{i,j,k} + \mathcal{C} h^2 (\nabla^2 (\nabla^2 \omega))_{i,j,k} + \mathcal{O}(h^4) \quad (\text{A.5})$$

Again, using Taylor series, one obtains a system of three equations for the four unknowns :

$$\begin{cases} 8a + 8b + 2c = 2 \\ 8a + 12b + 6c + d = 0 \\ 48a + 24b - 2(8a + 8b + 2c) = 0 \end{cases}$$

Thus, contrary to the 2-D case, there is a family of such schemes. The one we choose is such that we recover the $h^2/12$ factor as in 2-D : $a = 2/30$, $b = 1/30$, $c = 18/30$ and $d = -136/30$. Using these values, the truncation error term is as in 2-D :

$$(\nabla_h^2 \omega)_{i,j,k} = \left(\nabla^2 \left(\omega + \frac{h^2}{12} \nabla^2 \omega \right) \right)_{i,j,k} + \mathcal{O}(h^4) \quad (\text{A.6})$$

For LES, the *Type II* models (rhs of Eq.(3.4)) are programmed as follows:

$$\begin{aligned} h^2 \nabla \cdot (\nu^{\text{sgs}} (\nabla_h \omega^s + (\nabla_h \omega^s)^T)) = & \frac{2}{30} \left[\frac{(\nu_{i+1,j+1,k+1}^{\text{sgs}} + \nu_{i,j,k}^{\text{sgs}})}{2} (\omega_{i+1,j+1,k+1}^s - \omega_{i,j,k}^s) + \dots \right] + \\ & \frac{1}{30} [\dots] + \frac{18}{30} [\dots] . \end{aligned} \quad (\text{A.7})$$

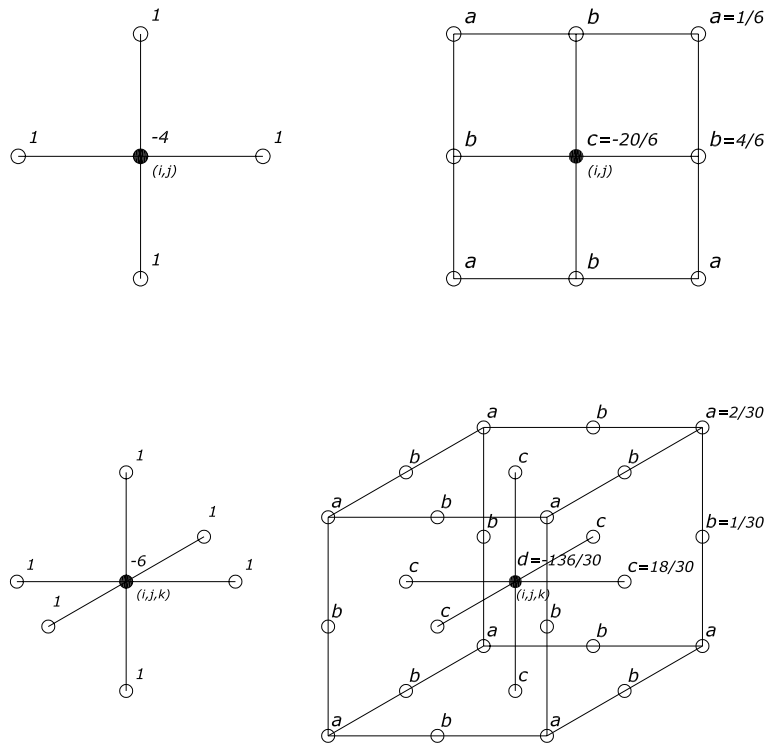
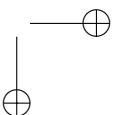
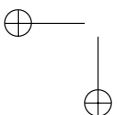
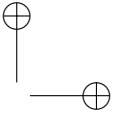
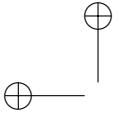


Figure A.1: Illustration of 2-D and 3-D second order Laplacian schemes: the "cross" schemes (left), and the "isotropic" schemes (right).



Appendix B

Description of the initial HIT field

The velocity field in the spectral domain, $\widehat{\mathbf{u}} = \widehat{u}_1 \mathbf{e}_1 + \widehat{u}_2 \mathbf{e}_2 + \widehat{u}_3 \mathbf{e}_3$, is built in the following way :

$$\begin{aligned}\widehat{u}_1 &= \left(\frac{\alpha k k_2 + \beta k k_3}{k (k_1^2 + k_2^2)^{1/2}} \right) , \\ \widehat{u}_2 &= \left(\frac{\beta k_2 k_3 - \alpha k k_1}{k (k_1^2 + k_2^2)^{1/2}} \right) , \\ \widehat{u}_3 &= \left(\frac{-\beta (k_1^2 + k_2^2)^{1/2}}{k} \right)\end{aligned}\tag{B.1}$$

where

$$\begin{aligned}k &= (k_1^2 + k_2^2 + k_3^2)^{1/2} , \\ \alpha &= \left(\frac{E(k)}{4\pi k^2} \right)^{1/2} \exp(i\theta_1) \cos(\phi) , \\ \beta &= \left(\frac{E(k)}{4\pi k^2} \right)^{1/2} \exp(i\theta_2) \sin(\phi)\end{aligned}$$

where θ_1 , θ_2 and ϕ are uniformly distributed random numbers on the interval $[0, 2\pi]$. The spectrum is taken as

$$E(k) = \frac{a k^4 \exp(-b k^{1.1})}{(q^4 p^4)^p}\tag{B.2}$$

Here we used $a = 2.74$, $b = 0.0278$, $q = 3.33$ and $p = 1.23$. The shape of this spectrum (Eq. B.2) does not correspond to HIT as it has no well-defined $k^{-5/3}$ inertial range. However, it grows like k^4 at small scales which is consistent with turbulence without net momentum, and it decays exponentially at high wavenumbers to mimic a dissipation range. In any case, the precise definition of this initial spectrum is not important here, as it quickly evolves to a statistically converged turbulence spectrum.

Appendix C

A 2-D zero circulation vortex

In this appendix, we illustrate the implementation of the 2-D VIC-FM method by applying it to the study of a zero circulation vortex. This is a circular vortex patch whose vorticity profile was given and studied by Kloosterziel and Carnevale [38] and by Dufresne and Dumas [24]. Laboratory experiments, which have applications in quasi-geostrophic fluid dynamics, were also done by Kloosterziel and Van Heijst [39].

The initial vorticity and corresponding velocity profiles are taken as:

$$\frac{\omega(r)}{\omega_0} = \left(\frac{1}{2} \alpha \left(\frac{r}{r_c} \right)^\alpha - 1 \right) e^{-\left(\frac{r}{r_c} \right)^\alpha} \quad (\text{C.1})$$

$$\frac{u_\theta(r)}{\omega_0 r_c} = -\frac{1}{2} \left(\frac{r}{r_c} \right) e^{-\left(\frac{r}{r_c} \right)^\alpha} \quad (\text{C.2})$$

These profiles define an axisymmetric flow with a negative vorticity core surrounded by a positive vorticity annulus, and with zero net circulation. When α is sufficiently large, the problem can be seen as a negative near top-hat vortex surrounded by a positive annulus, thus leading to an axisymmetric shear layer. Fig. C.1 shows the vorticity and velocity profiles for different α values.

The time and length scales used for normalization are defined by $1/\omega_0$, and by the velocity profile "crossing point" r_c . The dimensionless time is thus $\tau = t\omega_0$, while the Reynolds number is defined $Re = \omega_0 r_c^2/\nu$.

Here, we will limit our study to the $\alpha = 7$ case. For $\alpha > 3$, Kloosterziel and Carnevale [38] have shown that the vortex is unstable to perturbations with various azimuthal wavenumbers: this is essentially the instability of a shear layer.

A random perturbation can therefore initiate the simultaneous growth of several modes with different azimuthal wavenumbers. For $\alpha = 7$, the most unstable modes are $k_\theta = 2, 3$ and 4, with maximum growth rate for $k_\theta = 3$.

The first simulation was done at $Re = 10^4$ and using a perturbation with azimuthal wavenumber $k_\theta = 3$. The grid discretization was $h/r_c = 0.01$ and the time step was $\Delta\tau = 0.1$. Fig. C.2 shows the isocontours of vorticity for different τ . In Fig. C.2(a), the growth of a wavenumber 3 instability is already visible. In Fig. C.2(c), the core has become triangular, with three satellites around it and thin vorticity filaments. In Fig. C.2(d) and (e), the triangular vortex system rotates about the center, reaching a stable configuration while slowly diffusing. The grid size goes from 316×316 at $\tau = 0$ to 405×411 at the end of the simulation and the number of particles goes from ~ 69000 up to ~ 112000 for a total CPU time of ~ 100 minutes (on one AMD Athlon processor at 1.8GHz).

As mentioned before, this problem has zero net circulation. It however has non-zero angular impulse $A = -\frac{1}{2} \int |\mathbf{x}|^2 \omega \, d\mathbf{x}$. As the angular impulse A evolves according to $\frac{dA}{dt} = -2\nu\Omega$, it must here be conserved even for viscous flow (as $\Omega = 0$). Fig. C.3 provides the angular impulse evolution; it is indeed well conserved during the whole run. The kinetic energy ($E = \frac{1}{2} \int \mathbf{u} \cdot \mathbf{u} \, d\mathbf{x} = \frac{1}{2} \int \psi \omega \, d\mathbf{x}$) and the enstrophy ($\mathcal{E} = \frac{1}{2} \int \omega \omega \, d\mathbf{x}$) evolutions are reported on Fig. C.4. We also report, on Fig. C.4(b), an enstrophy curve obtained from the energy evolution according to: $\frac{dE}{dt} = -2\nu\mathcal{E}$. Although one can observe some small oscillations, also due to the poor precision on the time derivative of the energy, the evolutions compare quite well.

To further validate our results, Fig. C.5 shows the kinetic energy evolution and the enstrophy evolution obtained from two simulations: the one done using the hybrid VIC-FM method, and another one done using the FM method alone. One sees that the curves compare very well; this further confirms the accuracy and validity of the present hybrid method.

The second simulation was done using a random azimuthal perturbation, also at $Re = 10^4$. The grid discretization and the time step were the same as in the first simulation. Again, Fig. C.6 shows the isocontours of vorticity for different τ . Fig. C.6(a) shows the vorticity distribution at $\tau = 25$ and one can see that it is still mainly circular. At $\tau = 40$ (Fig. C.6(b)), the growth of a wavenumber-4 instability is visible. The core becomes square in shape and four satellites are formed. The square being here not perfectly symmetrical, another mode-2 instability emerges. The four satellites then fuse together, two by two, to form a more complex system,

see Fig. C.6(c)). That system elongates (Fig. C.6(d)) and breaks up into two parts. The resulting flow is quite complex, with some dipole structures (Fig. C.6(e) and (f)). In this simulation, the grid size grew from 316×316 to 1200×608 with a final number of particles of ~ 216000 and a total CPU time of ~ 140 minutes (on one AMD Athlon processor at 1.8GHz). We further see the interest of the VIC-FM method: it also allows to continuously adjust the grid size and shape as the vorticity field evolves. To solve the same problem using the VIC method alone, the grid would have to be taken much larger and thus lead to too large memory requirements and CPU time.

Fig. C.7 and C.8 illustrate, respectively, the angular impulse, the energy and the enstrophy evolutions for this second, more demanding, simulation. In spite of the complexity present in this flow, we see that the angular impulse is almost as well conserved as in the much easier "triangular" case; there is however some little variation at the end of the run. As to the enstrophy curve evaluated from the time derivative of the energy, it is more irregular, which is also indicative of some under-resolution.

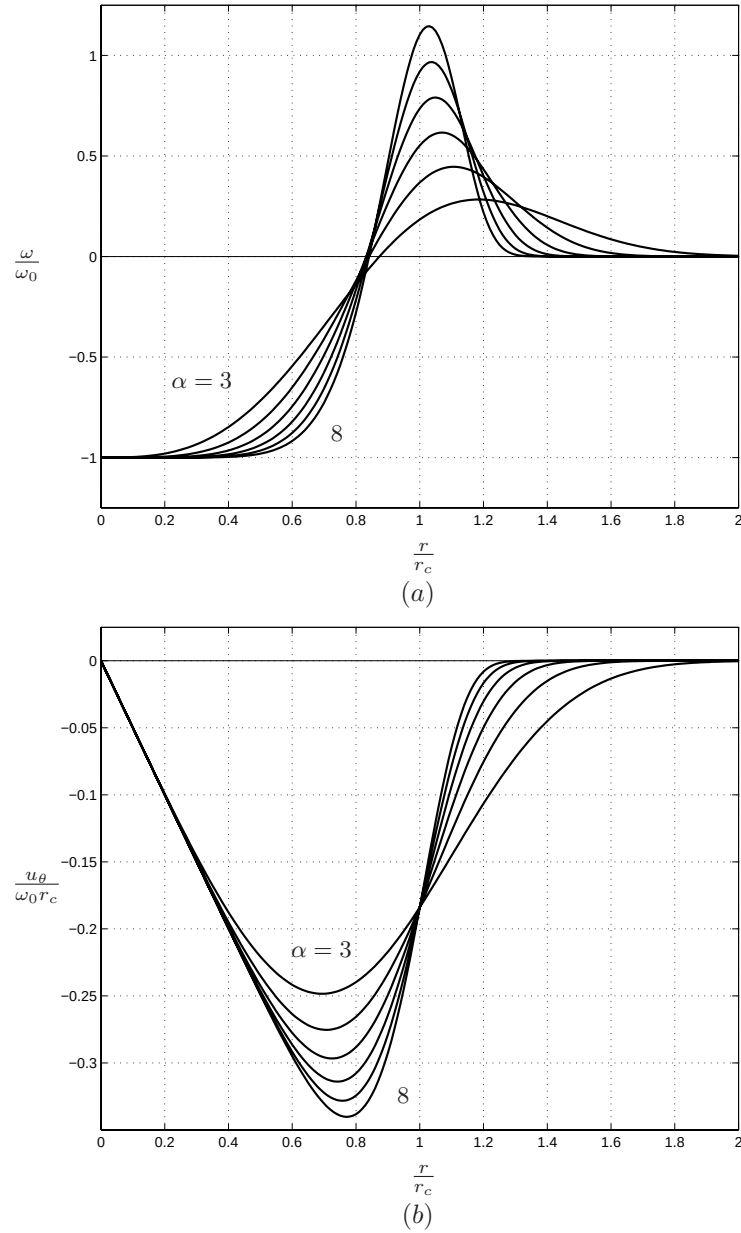


Figure C.1: Zero circulation vortex: (a) vorticity and (b) velocity profiles. The curves are plotted for every unitary value of α between 3 and 8.

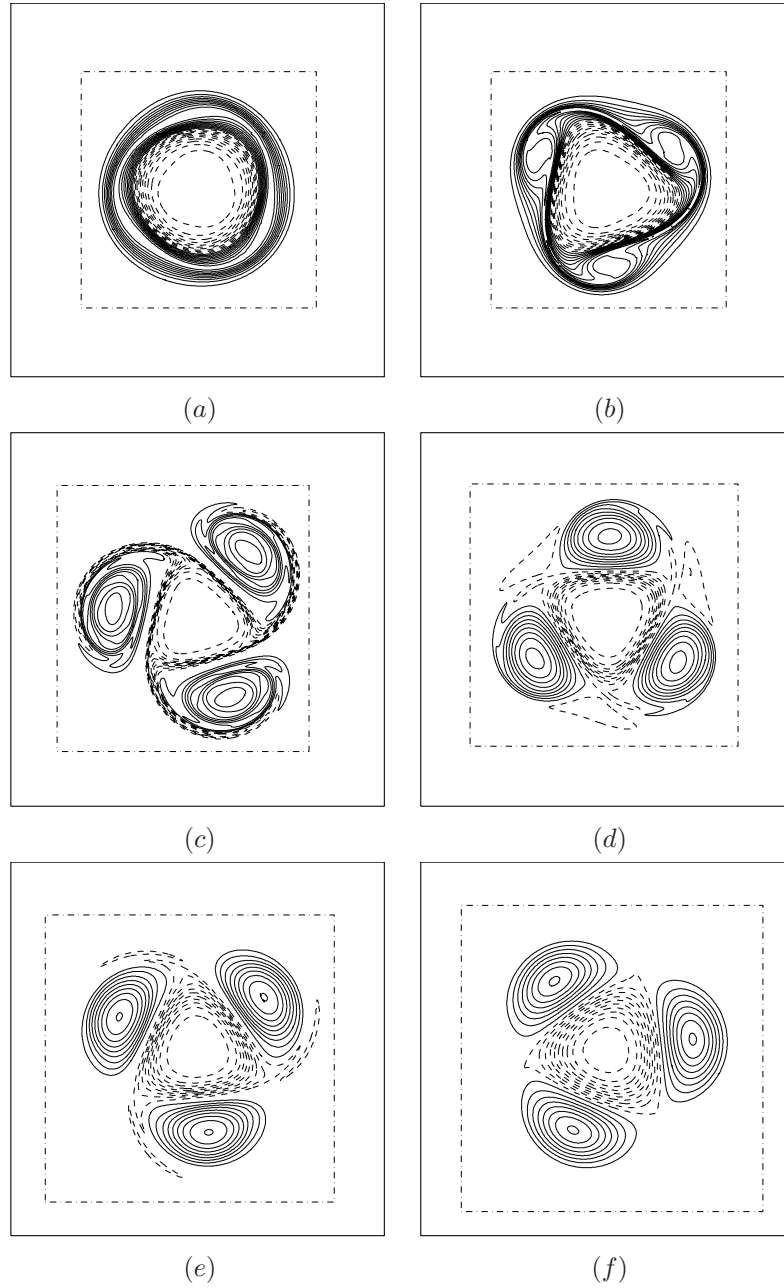


Figure C.2: Zero circulation vortex at $Re = 10^4$ and with mode-3 perturbation: isocontours of vorticity. Dashed and dotted lines represent positive and negative values, respectively. (a) $\tau = 8$, (b) $\tau = 15$, (c) $\tau = 30$, (d) $\tau = 45$, (e) $\tau = 75$, (f) $\tau = 150$. Levels are by step of 0.1.

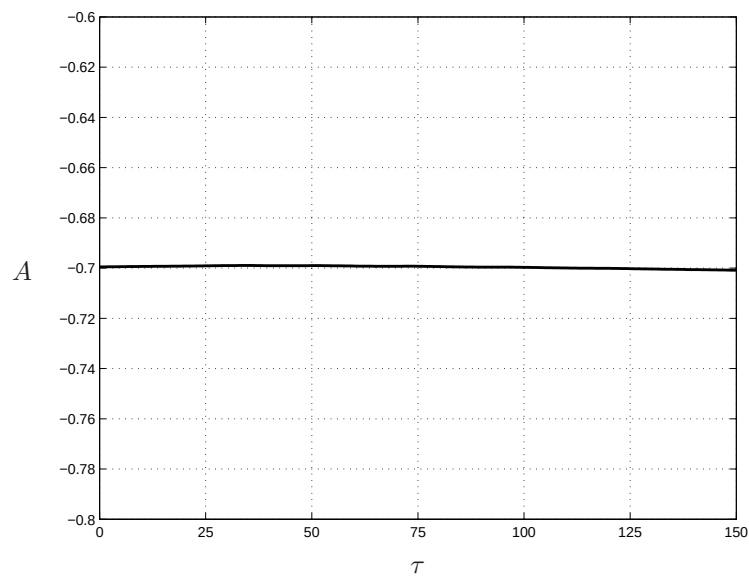


Figure C.3: Zero circulation vortex at $Re = 10^4$ and with mode-3 perturbation: angular impulse evolution.

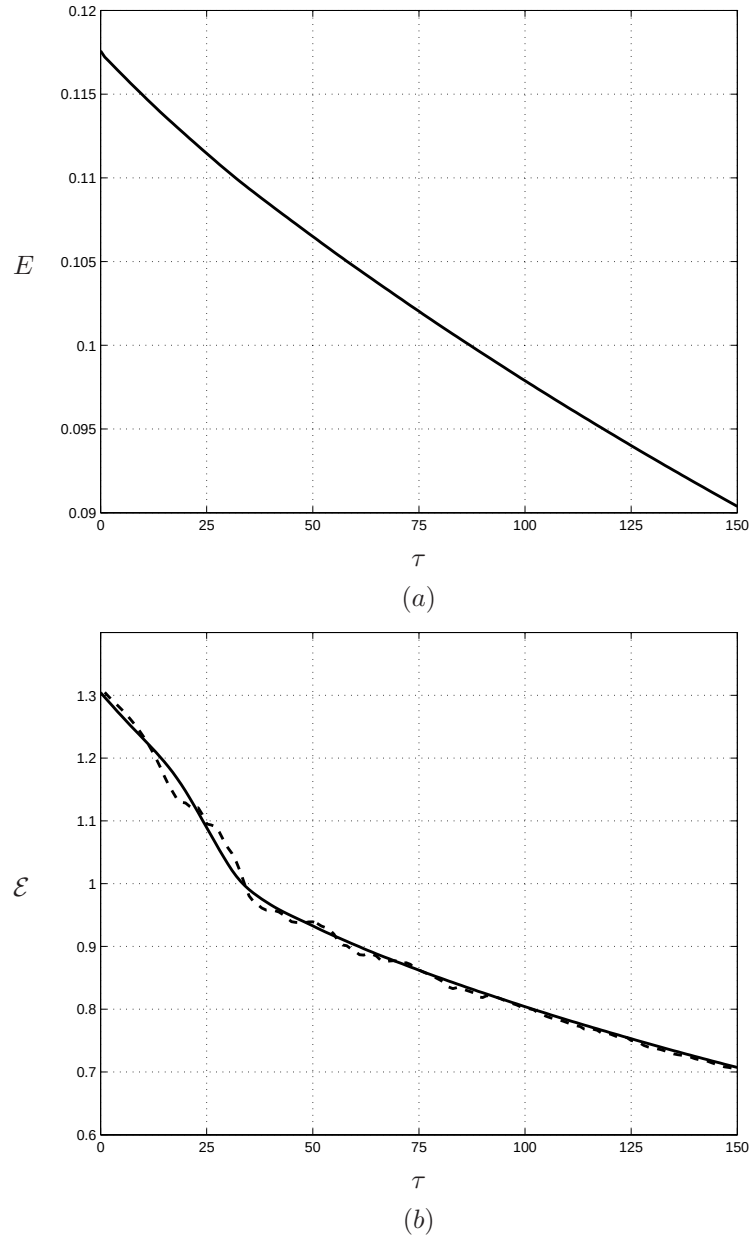


Figure C.4: Zero circulation vortex at $Re = 10^4$ and with mode-3 perturbation: (a) energy evolution, (b) enstrophy evolution (solid) and that evaluated from the time derivative of the energy (dashed).

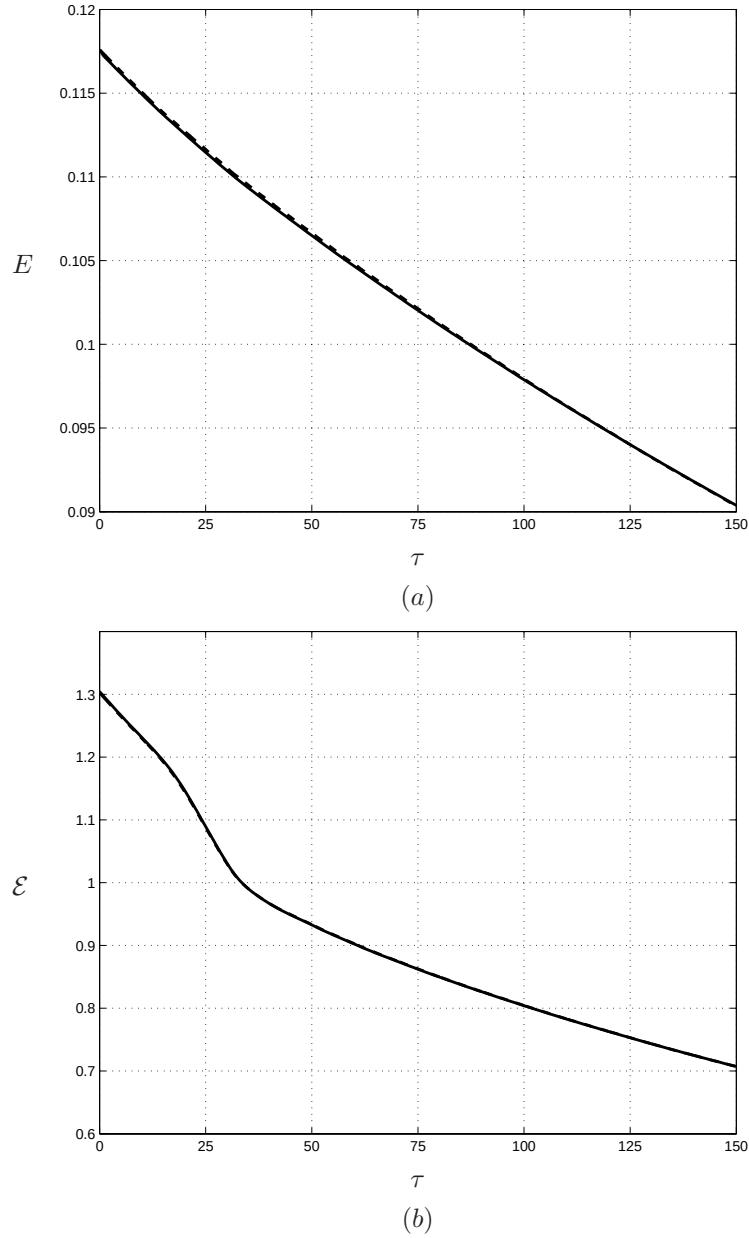


Figure C.5: Zero circulation vortex at $Re = 10^4$ and with mode-3 perturbation: comparison between the simulations done using the hybrid VIC-FM method (solid) and using the FM method alone (dashed): (a) energy evolution, (b) enstrophy evolution.

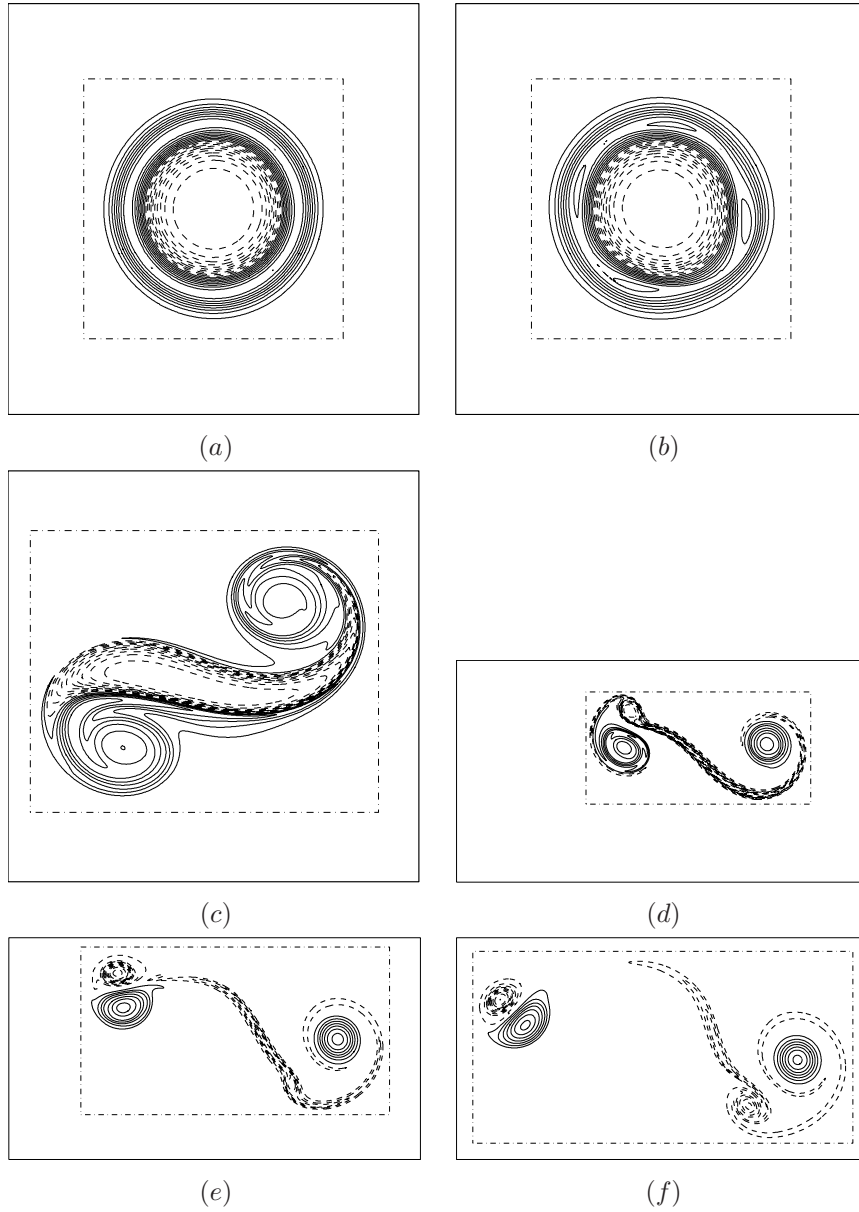


Figure C.6: Zero circulation vortex at $Re = 10^4$ and with random perturbation: isocontours of vorticity. Dashed and dotted lines represent positive and negative values, respectively. (a) $\tau = 25$, (b) $\tau = 40$, (c) $\tau = 65$, (d) $\tau = 90$, (e) $\tau = 120$, (f) $\tau = 150$ (there is a change of scale by a factor of 2.6 between figure (c) and (d)). Levels are by step of 0.1.

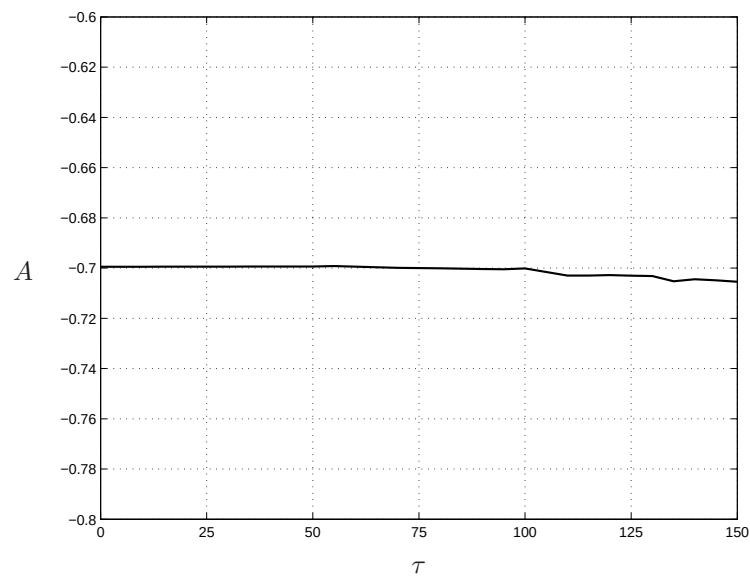


Figure C.7: Zero circulation vortex at $Re = 10^4$ and with random perturbation: angular impulse evolution.

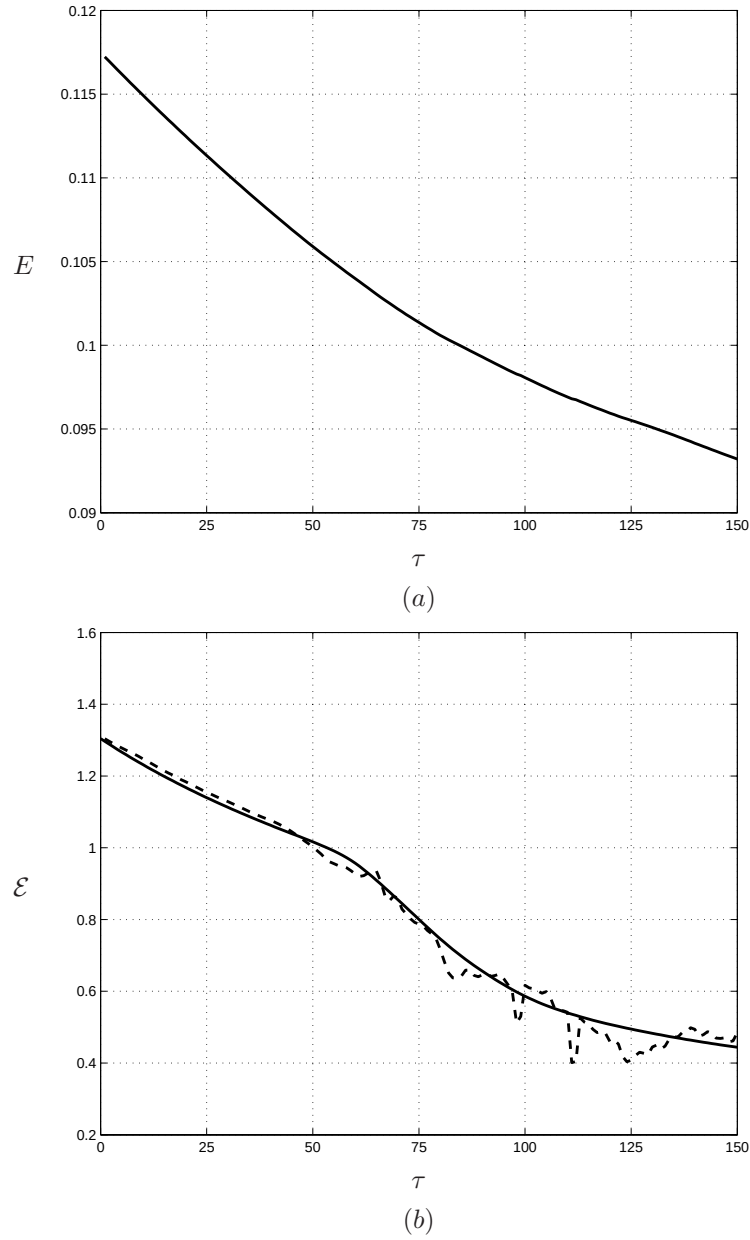
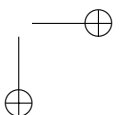
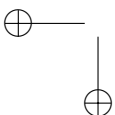
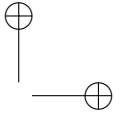
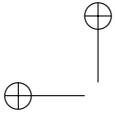


Figure C.8: Zero circulation vortex at $Re = 10^4$ and with random perturbation: (a) energy evolution, (b) enstrophy evolution (solid) and enstrophy evaluated from the time derivative of the energy (dashed).



Appendix D

The pseudo-spectral method

We here briefly present the pseudo-spectral (PS) methodology often used to make validations and/or comparisons with the VIC-PFM method. It solves the conservative formulation of the incompressible Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla P + \nabla \cdot \mathcal{T} , \quad (\text{D.1})$$

together with the incompressibility constraint

$$\nabla \cdot \mathbf{u} = 0 . \quad (\text{D.2})$$

The divergence of the effective stress tensor $\mathcal{T}$ is formulated such that

$$\nabla \cdot \mathcal{T} = \nu \nabla^2 \mathbf{u} - \nu_{\text{hv}} \nabla^m \mathbf{u} , \quad (\text{D.3})$$

with $\nu_{\text{hv}} = C h^m / t_0$ where C is a constant ($C = 0$ in the case of a DNS), t_0 is a global time scale and h is the grid size. Thus, the LES modeling is done using a high order hyper-viscosity dissipation [7].

The numerical solution of Eqs. (D.1) and (D.2) is sought using a standard Fourier-Galerkin projection in all three Cartesian directions [9, 10]. The spectral approximation of the velocity vector $\mathbf{u}$ is symbolically written such that

$$\mathbf{u}(\mathbf{x}, t) = \sum_{\mathbf{k}} \hat{\mathbf{u}}(\mathbf{k}, t) \exp(i \mathbf{k} \cdot \mathbf{x}) , \quad (\text{D.4})$$

where $\mathbf{x} = \{x, y, z\}$ and $\mathbf{k} = \{k_x, k_y, k_z\}$, with $k_x = n 2\pi / L_x$ and so on; the “ $\hat{}$ ” notation is used to identify Fourier transforms. The time integration of Eq. (D.1) is carried out in spectral space using an integrating-factor technique in

which: (a) the dissipation terms are integrated analytically and therefore exactly, and (b) the convective terms are marched explicitly using a 3rd order Runge-Kutta scheme. The incompressibility condition is imposed exactly by an appropriate projection of the velocity field onto a divergence-free space (in fact solving the Poisson equation for the pressure in the spectral space). The nonlinear term is evaluated using a pseudo-spectral algorithm and dealiasing is done using a phase shift procedure [10]. It may also be noted that the hyper-viscosity formulation used here provides a subgrid scale dissipation term that comes at no extra computational cost when compared to the standard DNS formulation.