Design and Validation of a Large-Eddy Simulation Methodology for Compressible shock-free flows on Unstructured Meshes

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Abstract. The objective of the present work is to develop a large-eddy simulation methodology (LES) for complex wall-bounded flows, and to apply it to an unstructured flow solver for compressible shock-free flows, called *Argo*. This solver is basically designed for Euler or Reynolds averaged Navier-Stokes (RANS) simulations, so that the modifications required for this code to perform well for LES applications are explained. A first issue is the numerical dissipation introduced by standard upwind schemes in order to stabilize the convective term discretization. This artificial dissipation indeed interacts strongly with subgrid scale (SGS) model. The proposed solution is to resort to a pure central scheme that is naturally stable through the conservation of the discrete kinetic energy. Another issue is the choice of a SGS model that is compatible with the geometrical complexity and a parallel unstructured code. The LES methodology is then validated on a turbulent channel flow at $Re_\tau = 395$. Furthermore, results are compared with a structured fourth-order incompressible flow solver using the same SGS model, in order to investigate the influence of truncation errors. Finally, a LES of the unsteady turbulent flow past a sphere in the subcritical regime is performed.

Key words: LES, unstructured meshes, sphere, channel flow, compressible flow.

1. Introduction

We are interested in simulating high Reynolds number flows around complex geometries. For this purpose, we have developed a parallel implicit solver for three-dimensional compressible flows on unstructured tetrahedral meshes. The method uses an edge-based hybrid finite volume and finite element discretization. It blends an upwind scheme for the convective fluxes based on Roe's approximate Riemann solver and a piecewise linear reconstruction of the flow variables in each control volume, with a P1 finite element Galerkin approximation of the diffusive fluxes. This second-order accurate numerical scheme, which is representative of most numerical schemes used on unstructured meshes, was designed for Euler and RANS simulations, and therefore performs well for this type of flows. Since large-eddy simulations have proved to perform better than RANS for complex phenomena like turbulent

mixing and separated flows, the objective is this paper is to present the issues related to the development and implementation of the modifications required by such a standard code for unstructured meshes to perform properly for LES applications. A first issue is the effect of the numerical dissipation of standard RANS-based upwind schemes. It is well-known that this numerical dissipation competes and often overwhelms the effect of the subgrid scale model (SGS). This interaction must be properly controlled. For unsteady simulations, this artificial damping removes discrete kinetic energy on dynamically important scales of the flow. Said otherwise, the numerical dissipation mechanism interferes in the balance between the production of turbulence and its dissipation at the smallest resolved length scales. A possible solution is to implement central schemes. Stability is then enforced using central schemes that conserve the discrete kinetic energy. Following the work by Mahesh and al. [7], we have implemented an extension to compressible shock-free flows of their kinetic energy conserving scheme (initially developed for incompressible flows on unstructured meshes).
The second issue is the choice of a subgrid scale (SGS) model compatible with LES in complex geometries. Among the properties presented by the different SGS models, the following properties are retained. First, the SGS model has to model properly the energy transfer from the resolved scales to the subgrid ones through the subgrid dissipation. Second, the eddy-viscosity has to present the correct near-wall behavior, $\nu_t \sim y^{+3}$. Third, it is necessary to handle properly complex geometries, characterized by the lack of homogeneous flow directions or by complex meshes (as unstructured grids). Considering these criteria, the Wall Adapting Local Eddy viscosity (WALE) of Nicoud et al. [9] is an attractive solution.
To address the issues outlined above, the remainder of this paper is organized as follows. In the following section, Section 2., the LES methodology is developed. First, the implementation of a kinetic energy conserving scheme in the context of LES on complex unstructured meshes is discussed. Second, the choice of the WALE model is briefly explained along with its main limitation. The next section, Section 3., is devoted to the validation of the methodology using LES of a turbulent channel flow at a Re_τ of 395. The baseline grid is a structured mesh where volume elements are divided into tetrahedra. This enables to compare our results with a fourth-order structured incompressible flow solver using the same SGS model. The influence of truncation errors can then be investigated properly. The methodology is also applied for the LES of the flow past a sphere at a Reynolds number of $10,000$, see Section 4. Finally, concluding remarks are offered.

2. LES methodology

2.1. Discretization aspects

In order to avoid the interaction of a numerical dissipation with the SGS model, a central scheme is selected. Stability is then enforced by implementing a central scheme that conserves the discrete kinetic energy. In the present unstructured code, an extension to compressible shock-free flows of the kinetic energy conserving scheme of Mahesh et al. [7] (initially designed for incompressible flows on unstructured meshes) has been developed. Theoretical developments can be found in Georges et al. [3].

Although stable, the kinetic energy conserving schemes are prone to truncation errors. As the scheme is central, these errors turn out to be *dispersion* errors. This concept highlights the incorrect advection of high wavenumbers which can lead to spurious oscillations in marginally resolved simulations. This behavior is increased in the presence of mesh inhomogeneities such as a mesh stretch [6], as the truncation errors are more important there. In turbulent parts of the simulation, where the SGS model is expected to be active, the eddy-viscosity dissipation maintains the effective resolution to a certain level. However, it is not proved that the eddy-viscosity can prevent the formation of spurious oscillations in regions of mesh discontinuities. Furthermore, in non-turbulent parts of the simulation domain, the simulation can also be marginally resolved. In these regions, ν_t is expected to be inactive so that no dissipation process is present to inhibit the spurious oscillations. As a conclusion, a controlled amount of artificial dissipation sometimes has to be accepted in order to filter out the spurious numerical noise. The major challenge is that this dissipation process has to remain low enough to leave the energy cascade essentially unaffected. To increase accuracy, a *mass matrix* for the evaluation of the time derivative terms can also be implemented. The implementation of a P1 Galerkin finite element mass matrix as well as a controlled amount of numerical dissipation in form of a ∇^4 *hyperdiffusion* is introduced and discussed in Georges et al [3].

2.2. Modeling aspects

The WALE model of Nicoud et al. [9] is an interesting SGS model for LES in complex geometries. This model presents the good near-wall behavior, $\nu_t \sim y^{+3}$, without the use of a dynamic procedure nor a damping function (like the well-known Van Driest function). In fact, it is well-recognized that the use of the dynamic procedure in complex geometries (without any homogeneous flow direction) is not obvious. Furthermore, using damping functions, each volume node has to known its y^+ distance to the closest wall. This is by essence a *global* process. On the contrary, the WALE model is based on *local* quantities so that its implementation in a parallel unstructured code is straightforward. The main drawback of the WALE model is that the model is dissipative on well-resolved scales of the flow, and in laminar vortex cores. A possible solution to this problem is to perform a flow scale discrimination where the eddy-viscosity ν_t is evaluated on a high-pass filtered velocity field [9, 11]. This model, termed filtered WALE model, is not investigated here as the implementation of proper filters on unstructured meshes is not obvious [5].

3. LES of the turbulent channel flow at Re_τ of 395

In order to validate the present methodology, LES of a turbulent channel flow at $Re_\tau = 395$ is performed. Results will be compared to the DNS of Moser et al. [8]. The geometry is a channel composed of two plates separated by a distance 2δ. The wall-normal direction is y, where $y = 0$ is the center of the channel. The streamwise and spanwise directions, x and z respectively, are periodic. As in the DNS of Moser et al. [8], the computational box is defined as

$$L_x = 2\pi\delta, \quad L_y = 2\delta \quad \text{and} \quad L_z = \pi\delta, \tag{1}$$

where L_x, L_y and L_z are the dimensions in the x, y and z directions respectively. The grid is structured, uniform in the x and z directions, and stretched using a hyperbolic-tangent function [4] in the y wall-normal direction. Volume elements are further divided into tetrahedra. The number of grid points is

$$N_x = 64, \quad N_y = 48 \quad \text{and} \quad N_z = 64, \tag{2}$$

in the x, y and z directions respectively, leading to the following resolution in term of wall-units,

$$\Delta x^+ = \frac{\Delta x \, u_\tau}{\nu} \simeq 38, \quad \Delta z^+ = \frac{\Delta z \, u_\tau}{\nu} \simeq 26, \tag{3}$$

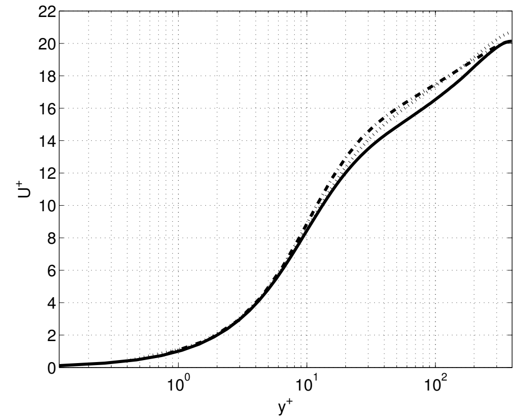
for the periodic directions, and

$$\Delta y^+_{min} = \frac{\Delta y_{min} \, u_\tau}{\nu} \simeq 0.8, \quad \Delta y^+_{max} = \frac{\Delta y_{max} \, u_\tau}{\nu} \simeq 50, \tag{4}$$

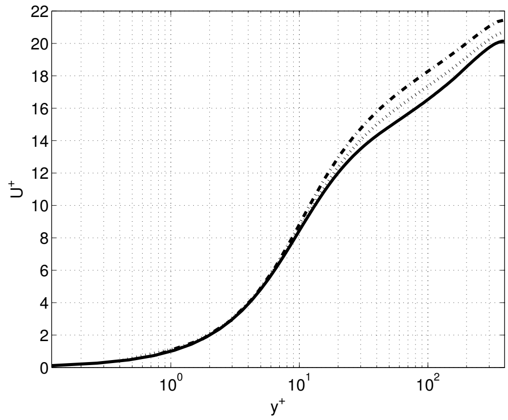
for the stretched wall-normal direction. Δx, Δz here refers to the uniform grid spacing in x and z, Δy_{min} and Δy_{max} are the minimum wall-normal grid spacing located near the wall and the maximum wall-normal grid spacing in center of the channel, respectively. Finally, u_τ is the friction velocity.

Simulations are performed using the unstructured Argo code with the kinetic energy conserving scheme and the WALE model (with a constant C_w of 0.5, relevant for this low Reynolds application [9]). The influence of the mass matrix is also investigated. In the present application, the numerical dissipation in form of a ∇^4 hyperdiffusion is not introduced as the mesh is regular : no numerical noise filtering procedure is required. As the grid is structured, it enables to compare the results with a high-order accurate incompressible flow solver, initially developed at the UCL, using the same SGS model and grid. This code is equipped with the fourth-order kinetic energy conserving finite differences of Vasilyev [10] in the skew-symmetric form. In this way, the influence of truncation errors can be properly investigated.

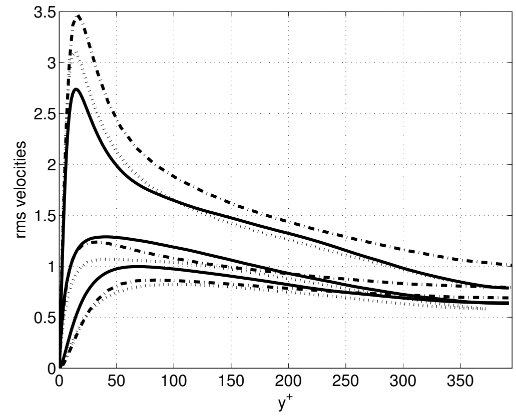
A first conclusion is simply to notice that the kinetic energy conserving scheme gives stable solutions without any additional numerical dissipation. This is the case with and without mass matrix, even though the discrete kinetic energy is not strictly conserved using a mass matrix. The central scheme without mass matrix gives a mean velocity profile, U^+, is close agreement with the fourth-order structured code, see Fig 1(a). Nevertheless, as expected, the unstructured code is less accurate in terms of rms velocities, Fig. 1(c), especially in the streamwise directions where a large overshoot of u'^+ is reported. A major discrepancy is also present for each rms velocity in the center of the channel. In term of resolved shear stress, Fig. 1(e), the solution quality of both codes is comparable. The use of a mass matrix impairs slightly the U^+ profile, see Fig. 1(b), but increases drastically the velocity fluctuations, Figs. 1(d) and 1(f) : overshoots are reduced significantly and the agreement is better in the center of the channel. The present test case leads us to conclude that the LES methodology for unstructured meshes performs pretty well, the mass matrix increasing the solution quality significantly.



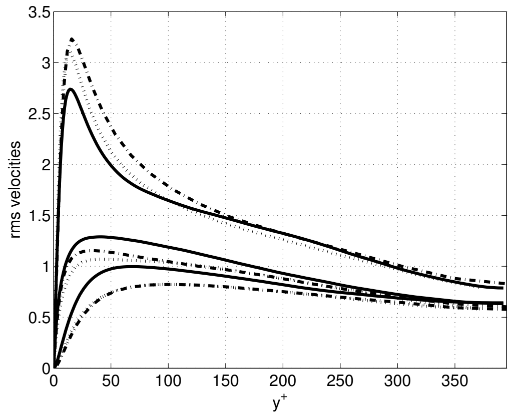
(a) U^+ (lumped)



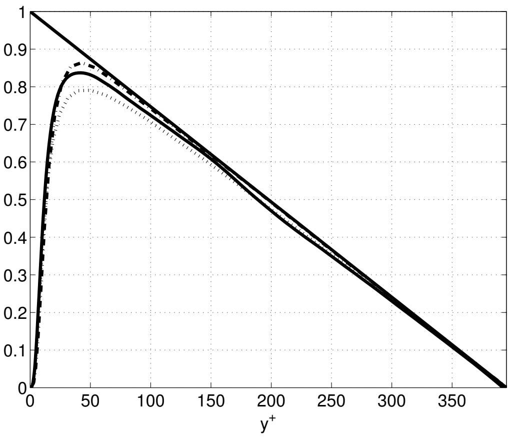
(b) U^+ (mass matrix)



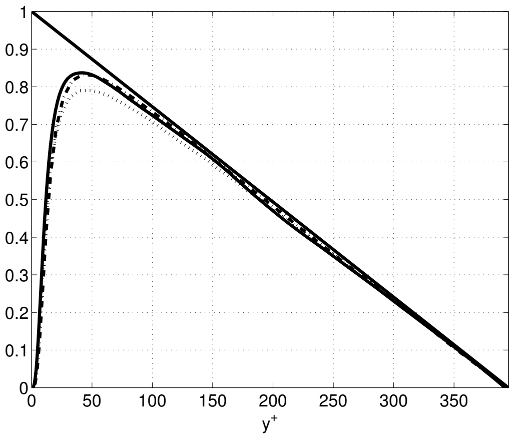
(c) rms velocities (lumped)



(d) rms velocities (mass matrix)



(e) resolved shear stress (lumped)



(f) resolved shear stress (mass matrix)

*Figure 1***:** Turbulent channel flow LES at $Re_\tau = 395$: LES using the WALE SGS model for the unstructured flow solver (dash-dotted line) without (left figures) and with mass-matrix (right figures), the fourth-order structured code (dotted line) and DNS of Moser et al. [8] (solid line). Reported values are the mean streamwise velocity, U^+, the rms velocities, u'^+ (top curve), v'^+ (bottom curve) and w'^{rms} (center curve), and the resolved shear-stress.

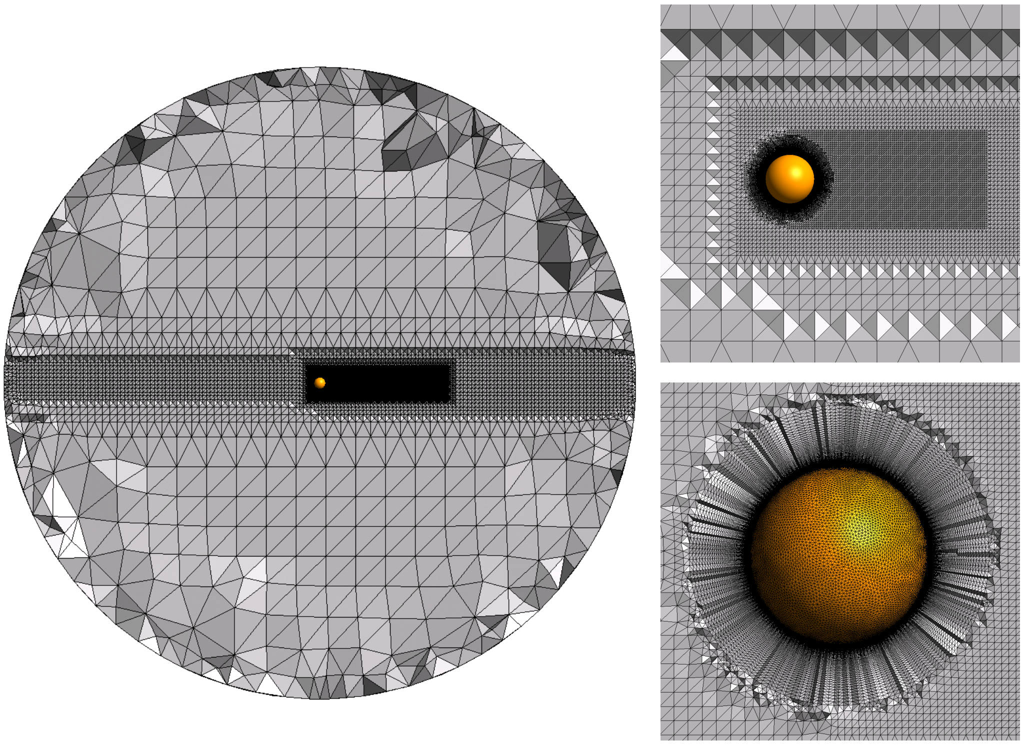


Figure 2: Anisotropic boundary layer and isotropic wake meshes for the flow past a sphere at Re = 10,000

4. LES of the subcritical turbulent flow past a sphere at $Re = 10,000$

The simulation of the unsteady flow past a sphere at a Reynolds number of 10,000 (based on the free stream velocity U_∞ and the sphere diameter D) is considered here. At such a Reynolds number, the flow is in the subcritical regime. This means that the boundary layers in the separation region are laminar, the transition to turbulence occurs further downstream in the separated shear layers (by way of the Kelvin-Helmholtz instabilities), and the wake is turbulent. Given the Reynolds number, it is impossible to afford a DNS with an unstructured solver so that major flow properties must be captured with a large eddy simulation. This rather academic problem is well documented in the scientific literature [1, 2, 12]. While most references assume an incompressible flow formulation, a compressible flow solver is used in the present work. The Mach number is therefore taken low enough to neglect the compressible effects, and large enough to prevent the nonlinear system of equations to be too stiff. Numerical experiments show that $M_\infty = 0.1$ is an acceptable value.

The mesh used for the simulation contains 1.2×10^6 nodes and 6.6×10^6 tetrahedra (see Fig. 2). It captures properly the boundary layers since its wall normal spacing is such that $y_{min}/\delta \sim 0.04$ and its growing factor is equal to 1.06. The physical time-step adopted for the simulation is equal to $0.04D/U_\infty$ and is similar to the value given in [1, 2]. Three LES simulations using the WALE model [9] are performed with the following schemes: (1) the kinetic energy conserving scheme, (2) the kinetic energy conserving scheme where the volume integrals are evaluated with a mass matrix, and (3) the second scheme supplemented by a ∇^4 hyperdiffusion term to ensure a

Table 1: Main characteristics of the flow past a sphere at Re = 10,000

	C_D	$C_{D\tau}/C_D$	φ_s	Str
LES #1	0.399	8.6%	85 – 88	0.2
LES #2	0.387	8.7%	84 – 86	–
LES #3	0.394	8.7%	84 – 87	0.2
Constantinescu et al. [1, 2] (LES)	0.393	$\sim$ 8.5%	84 – 86	0.195
Constantinescu et al. [1, 2] (DES)	0.397	$\sim$ 8.5%	84 – 87	0.200
Yun et al. [12] (LES)	0.393	–	90	0.17

smooth variation of the solution (as the mesh presents strong inhomogeneities).
The flow structure is analyzed using the λ_2 visualization method, see Figs 3. As expected, the wake is irregular and presents a wide range of scales. For the kinetic-energy conserving scheme without mass matrix, the wake and the boundary layer are surrounded by a spurious numerical noise (see Fig. 3(a)). By adding a mass matrix, this noise is reduced significantly (see Fig. 3(b)) even though there are still some issues in regions corresponding to highly skewed mesh elements (where truncation errors are important). As shown in Fig. 3(c), the scheme supplemented with a ∇^4 hyperdiffusion produces smooth vortical structures. Finally, Fig. 3(d) shows the detrimental effect on the vortex structures of the competition between the numerical dissipation introduced by a typical second-order upwind scheme and the subgrid scale model.
Table 1 reports the averaged drag coefficient C_D, the friction forces contribution to the total drag $C_{D\tau}/C_D$, the separation angle φ_s on the sphere measured from the stagnation point, the low-frequency Strouhal number Str associated to the large-scale instability of the wake, and compares these values to those obtained by Constantinescu and Squires [1, 2] (using a LES equipped with a dynamic Smagorinsky model and a detached eddy simulation, DES) and by Yun et al. [12] (using a LES). For all three simulations, a good agreement is obtained. It is again interesting to note that the pure central scheme is still stable adding a mass matrix. Nevertheless, unsteady flow statistics like the Strouhal number here cannot be captured. The desired physical behavior is retrieved by adding a small artificial diffusion. Notice that the time averaged lift coefficient C_L is not reported because it is equal to zero. Let's also mention that the high-frequency Strouhal number associated to the small-scale instability of the separating shear layer is not captured by the present simulations.

5. Concluding remarks

A LES methodology for complex wall-bounded flows using unstructured meshes was presented. First, the discretization is based on a kinetic energy conserving central discretization of the convective fluxes. This enables to reach stability without the use of an additional numerical dissipation process, as upwinding. Nevertheless, in regions of mesh irregularities where truncation errors are important, it is sometimes needed to add a controlled amount of numerical dissipation in order to filter out the possible numerical noise (in marginally resolved simulations). The selected artificial dissipation is here a ∇^4 hyperdiffusion with an incompressible scaling [3]. In order to increase the accuracy of the time derivative terms, a mass matrix is also implemented. Second, the WALE model [9] turns out to be an attractive model for LES of complex geometries using a parallel unstructured code. The methodology was first validated on the LES of a turbulent channel flow at Re_τ of 395. Results were also compared to a fourth-order accurate structured incompressible flow solver using the same SGS model and grid. The present methodology performed pretty well and it was found that the mass matrix had a beneficial effect on the flow statistics, especially in term of turbulent fluctuations. The mesh being highly regular, the hyperdiffusion term was not required. Nevertheless, as a future work, it would be very interesting to perform the channel flow benchmark using this term in order to check the interaction of this artificial dissipation and the SGS model. Finally, the LES of the unsteady flow past a sphere in the subcritical regime was performed. The implementation of a mass matrix increases the solution quality even though the low-frequency Strouhal number was not properly captured. This is possibly due to small discrete energy injections resulting from the mass matrix. Best results were indeed obtained using the kinetic energy central scheme supplemented by a mass matrix and a hyperdiffusion. Computed results were then in pretty good agreement with the references [1, 2, 12].

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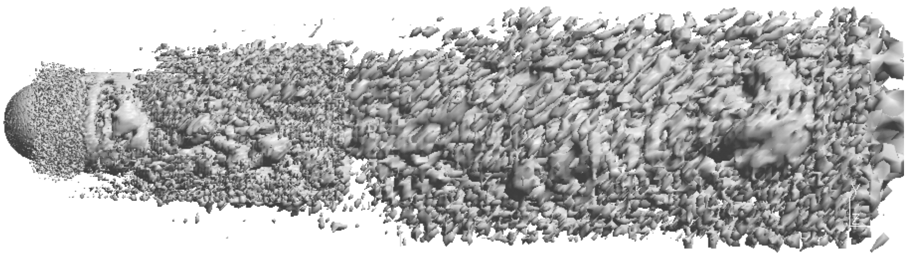
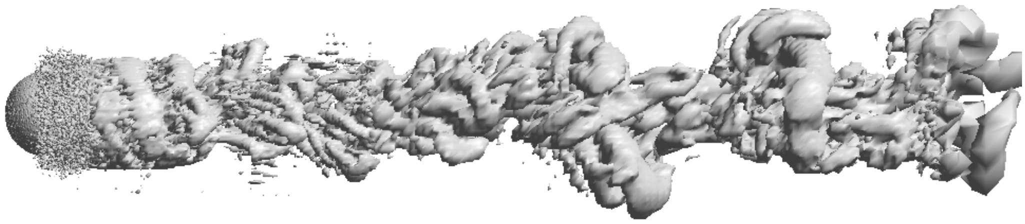
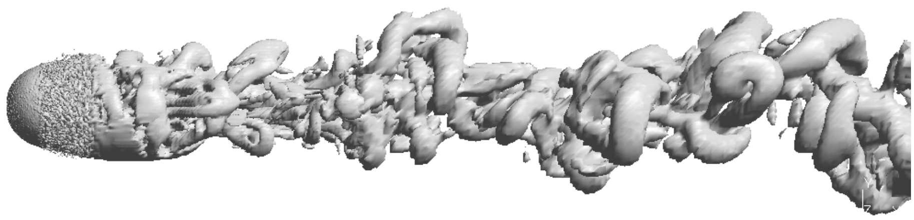


(a) K-energy conserving central scheme



(b) K-energy conserving central scheme with mass matrix



(c) K-energy conserving central scheme with mass matrix and hyperdiffusion

(d) Upwind Roe scheme with linear reconstruction

Figure 3: Vortical structures of the flow past a sphere at Re = 10,000 detected using the λ_2 criterion.