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Global kinetic energy conservation with unstructured meshes

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SUMMARY

Conserving kinetic energy is essential in Large Eddy Simulation (LES) in order that subgrid scale modelling (SGS) is not hidden by numerical errors. High-order schemes, which are not available for unstructured grids, are sufficient but not a necessary condition for energy conservation. The problem addressed here is directly ensuring energy conservation through a careful discretization of the momentum and mass equations, and it is shown that this can be achieved with a low-order scheme for unstructured grids. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: large eddy simulation; finite volume–finite element method; unstructured mesh; global energy conservation, unsteady Navier–Stokes

1. INTRODUCTION

It can be shown that 'classical' collocated arrangements using the traditional convection schemes do not conserve kinetic energy. The well-known structured discretization 'fully staggered' [1] with a proper choice for time advancing scheme conserves the global kinetic energy. This discretization is only applicable to simple geometries and has been recently extended to an unstructured formulation by Perot [2].

The present work deals with the discretization of unsteady Navier–Stokes equations for incompressible flows. The derivation of the kinetic energy equation is usually not verified in a discrete sense. Actually, continuous formulas such as $\mathrm{div}(pV) = p\cdot\mathrm{div}(V) + V\cdot\mathrm{grad}(p)$, where p and V stand, respectively, for the pressure and the velocity field are not true in a discrete sense. Perot [2] recently proposed a discretization using triangular or tetrahedral elements which conserve global kinetic energy by using the normal components of the velocity located at the centre of faces and the pressure at the circumcentre. However, applications in the latter paper were limited to 2D laminar flows. The present work proposes a somewhat different discretization with more pressure nodes and using the Cartesian components of the velocity. The pressure is located at the cell vertex and at the centre of gravity of the elements, while the velocity is at the centre of the faces, retaining a collocation of all three components

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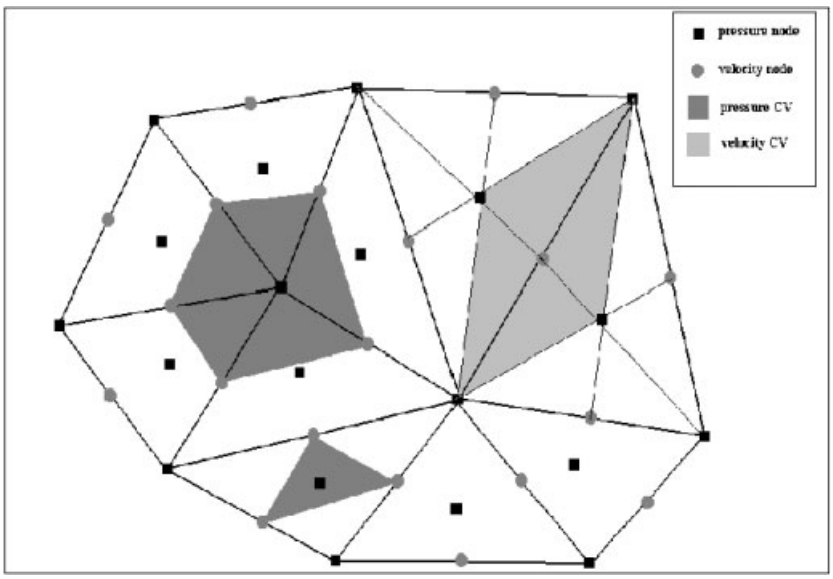

Figure 1. *P1NCP1B* discretization.

(see Figure 1). A finite volume–finite element method is used, whereby the principle of shape functions is introduced into the finite volume method [3].

2. DISCRETIZATION

The equations solved are the Navier–Stokes equations for an incompressible flow using the rotational form for the convective term and for the time being setting aside viscous terms:

$$\begin{aligned} &\frac{\partial V}{\partial t} + \mathrm{rot}(V) \wedge V + \mathrm{grad}\left(\frac{V^2}{2}\right) = -\mathrm{grad}(p) \\ &\mathrm{div}(V) = 0 \end{aligned} \tag{1}$$

The discretization is based on triangular (resp. tetrahedral) in 2D (resp. in 3D). The velocity is linear over the elements (*P1 non-conform*). The pressure is $P1$ over the internal diamond elements obtained by joining in 2D (resp. in 3D) two nodes (resp. three nodes) and the centre of gravity (see Figure 1). This is equivalent to adding the bubble *min* to the classical $P1$ element in a finite element approach. The pressure element is then called *P1 Bubble*. Thus, the velocity–pressure discretization is called *P1-non-conform-P1-Bubble* (or *P1NC-P1B*) using a finite element nomenclature. The control volumes of the velocity and the pressure are shown in Figure 1.

2.1. The momentum equations

By integrating the momentum equations over a velocity control volume Ω_i, one obtains

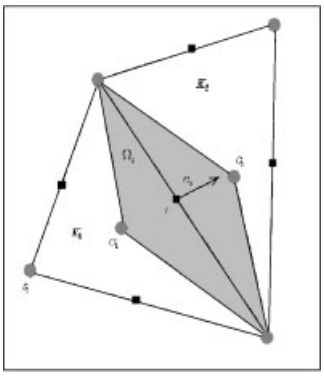

Figure 2. Velocity control volume.

$$\int_{\Omega_i} \frac{\partial V}{\partial t}\,\mathrm{d}\Omega + \int_{\Omega_i} [\mathrm{rot}(V) \wedge V]\,\mathrm{d}\Omega = -\int_{\Omega_i} \mathrm{grad}\left(p + \frac{V^2}{2}\right)\mathrm{d}\Omega \tag{2}$$

where Ω_i is the diamond control volume enclosing the common surface between primary cells K_1 and K_2 (see Figure 2).

For simplicity, $\frac{1}{2}V^2$ is introduced in the pressure term.

Using operators formalism, one can write Equation (2) as

$$\frac{\partial M(V)_i}{\partial t} + R(V)_i = -B(p)_i \tag{3}$$

where M stands for the mass operator, R the rotational part of the convection operator and B the gradient operator estimated through the velocity control volume.[†]

The mass operator: The velocity field is assumed constant over Ω_i. This is equivalent to a mass lumping:

$$M(V)_i = \int_{\Omega_i} V\,\mathrm{d}\Omega \approx V_i\,\mathrm{mes}(\Omega_i) \tag{4}$$

where mes is the surface of the element in 2D and its volume in 3D.

The rotational operator: V is, respectively, linear over $\Omega_i \cap K_1$ and $\Omega_i \cap K_2$ (see Figure 2). Thus, rot(V) is constant over K_1 and K_2 separately. The velocity on the R.H.S. of the vector product is assumed constant over Ω_i

$$R(V)_i = \frac{\mathrm{mes}(\Omega_i)}{d+1}\,[\mathrm{rot}(V)_{K_1} + \mathrm{rot}(V)_{K_2}] \wedge V_i \tag{5}$$

where d stands for the dimension.

The pressure gradient: The pressure gradient is constant over $\Omega_i \cap K_1$ and $\Omega_i \cap K_2$. One obtains

[†]Although diffusion is not described here, it is noting that the finite volume formulation using the shape function interpolation, leads to the same diffusion matrix as the standard finite element method [3].

$$B(p)_i = \frac{1}{d}(p_{G_2} - p_{G_1})n_i - \frac{1}{d(d+1)} \sum_{s_j \in \Omega_i} p_{s_j} n_j \tag{6}$$

where G_1 and G_2 are the centres of gravity of K_1 and K_2, s_j are the vertices which belong to Ω_i and n_j the opposite normal vectors of these vertices (see Figure 2).

2.2. The continuity equation

The continuity equation is integrated over the pressure CVs. There are two different control volumes, those linked to a vertex (Γ_{s_j}) and those linked to a centre of gravity (Γ_{G_j}).

B^{T} stands for the divergence operator. The following formulas are given in 2D:

$$B^{\mathrm{T}}(V)_{G_j} = \int_{\Gamma_{G_j}} \mathrm{div}(V)\,\mathrm{d}\Omega = \int_{\partial\Gamma_{G_j}} V \cdot n = -\frac{1}{4}\left(\sum_{i \in K_j} V_i n_i\right) \tag{7}$$

where n_i is the external normal of the face i.

$$B^{\mathrm{T}}(V)_{s_j} = \int_{\Gamma_{s_j}} \mathrm{div}(V)\,\mathrm{d}\Omega = \int_{\partial\Gamma_{s_j}} V \cdot n = \frac{1}{4} \sum_{s_j \in K_l} (V_1^l + V_2^l) n_{s_j}^l \tag{8}$$

where V_1^l and V_2^l are the velocities located at the faces which contain the vertex s_j and $n_{s_j}^l$ is the opposite external normal of the node s_j in the element K_l. The external normals used in the equations are not normalized.

The divergence operator written in such a way is not exactly the transpose of the pressure gradient operator. Taking the exact transpose of the pressure gradient for the discrete divergence operator does not affect the divergence constraint on the velocity over the pressure control volumes. This is done to obtain a symmetric matrix for the projection step (*Poisson equation*) and makes it easier to solve with iterative methods like the conjugate gradient.

2.3. The time-advancing scheme

The choice presented here is based on the concept of conserving kinetic energy. We use a centred scheme (second order) in time by mixing the Crank–Nicolson interpolation and the Adams–Bashforth extrapolation. t^n stands for the discrete time and $\Delta t = t^{n+1} - t^n$ for the time step. One needs to estimate the discrete equation at $t^{n+1/2}$.

The time derivative:

$$\frac{\partial M(V)_i^{n+1/2}}{\partial t} \approx \mathrm{mes}(\Omega_i)\,\frac{V_i^{n+1} - V_i^n}{\Delta t} \tag{9}$$

The rotational operator:

$$R^{n+1/2}(V)_i = \frac{\mathrm{mes}(\Omega_i)}{d+1}\,[\mathrm{rot}^{n+1/2}(V)_{K_1} + \mathrm{rot}^{n+1/2}(V)_{K_2}] \wedge V_i^{n+1/2} \tag{10}$$

$$\mathrm{rot}^{n+1/2}(V)_{K_i} = \tfrac{3}{2}\,\mathrm{rot}^n(V)_{K_i} - \tfrac{1}{2}\,\mathrm{rot}^{n-1}(V)_{K_i} \tag{11}$$

$$V_i^{n+1/2} = \frac{V_i^{n+1} + V_i^n}{2} \tag{12}$$

This choice is unusual. The implicit term in the rotational operator is a part of the transporting velocity whereas usually it is the transported velocity which is implicit (i.e. $V\nabla V$ is usually discretised as $(V^n\nabla)\cdot V^{n+1}$).

The pressure: The pressure is fully implicit. Coupling velocity and pressure is introduced via a projection method with a fix-point algorithm (inner iterations on the system).

3. CONSERVATION OF KINETIC ENERGY

3.1. Conservation in a continuous sense

The scalar product of the velocity and the momentum equations yields to the kinetic energy equation of evolution:

$$\frac{\partial V^2/2}{\partial t} = \mathrm{div}\left(\left[-\frac{V^2}{2} - p\right]V\right) \tag{13}$$

This is obtained by using formulas such as

$$\mathrm{div}(pV) = p\cdot\mathrm{div}(V) + V\cdot\mathrm{grad}(p) \tag{14}$$

If Ω is the total domain and $\partial\Omega$ its border, by integrating Equation (13), one obtains

$$\frac{\partial}{\partial t}\int_\Omega \frac{V^2}{2}\,\mathrm{d}\Omega = \int_{\partial\Omega} -\left[\frac{V^2}{2} + p\right](V\cdot n)\,\mathrm{d}\omega \tag{15}$$

This is the relation we want to obtain in a discrete sense.

3.2. Conservation in a discrete sense

The choices we have made allow us to conserve the kinetic energy and to obtain an equivalent of Equation (15) in a discrete sense. The kinetic energy is defined as $E_c = \sum_K \int_K \frac{1}{2} V^2\,\mathrm{d}K$.

As V is linear over the element K and located at the centre of the faces, the kinetic energy can be approximated by (the formula is exact in 2D):

$$\int_K \frac{1}{2} V^2\,\mathrm{d}K = \frac{\mathrm{mes}(K)}{2(d+1)} \sum_{i\in K} V_i\cdot V_i \tag{16}$$

The scalar product of the velocity with each operator is detailed below:

The mass operator:

$$V_i^{n+1/2}\cdot\frac{\partial M(V)_i^{n+1/2}}{\partial t} = \mathrm{mes}(\Omega_i)\,\frac{(V_i^{n+1})^2 - (V_i^n)^2}{2\Delta t} = \int_{\Omega_i}\frac{\partial(V^2/2)}{\partial t}\,\mathrm{d}\Omega \tag{17}$$

The sum over the whole domain gives exactly the time derivative of E_c.

The rotational operator: The rotational operator is orthogonal to the velocity in a discrete sense. Thus, the scalar product vanishes.

$$V_i^{n+1/2} \cdot R(V)_i^{n+1/2} = 0 \tag{18}$$

The pressure gradient: The scalar product of the velocity and the pressure gradient yields to a discrete formula such as (14).

The sum over the whole domain gives in 2D

$$\sum_i V_i \cdot B(p)_i = \frac{1}{3} \sum_K \sum_{l \in K} V_l \cdot \int_{K \in \Omega_l} \nabla p = \sum_{G_j} -2 p_{G_j} \int_{\Gamma_{G_j}} \mathrm{div}(V) - \frac{2}{3} \sum_{s_j} p_{s_j} \int_{\Gamma_{s_j}} \mathrm{div}(V) + \text{border terms} \tag{19}$$

The border terms are products of p and V. This formula looks like Equation (14). As the velocity field is divergence free, one can write

$$\sum_i V_i \cdot B(p)_i = \text{border terms} \tag{20}$$

An attractive feature of standard finite volume schemes, is that they conserve momentum on any grid. The new scheme focuses on energy, and it seems the previous property has been lost (even on a 2D grid it is difficult to simplify). But since in the discrete sense the rotational or convective formulation are equivalent, it is expected that for fine enough meshes, momentum will be conserved as in the finite difference limit. More precisely, in the LES framework, momentum of the large-scale structures should be conserved. While for smaller scales, standard schemes introduce a systematic energy error (numerical dissipation), it is possible that in the new scheme, momentum conservation error scale occur randomly and cancel during the statistical processing.

The scheme proposed in this article will be named either the rotational form—fully implicit or *Conservative Algorithm for Kinetic Energy* (CAKE).

4. NUMERICAL TESTS

Two test-cases have been used, a 2D case with the Taylor–Green vortices and a 3D one with the *Homogeneous Isotropic Turbulence* (*HIT*).

4.1. Taylor–Green vortices

The velocity field is initialized by (see Figure 3):

$$u(t=0,x,y) = -\sin(kx)\cos(ky)$$
$$v(t=0,x,y) = \cos(kx)\sin(ky)$$

This field should remain unchanged over time in the absence of viscosity. Two different meshes have been used, one obtained via a structured mesh (squares divided in two triangles)

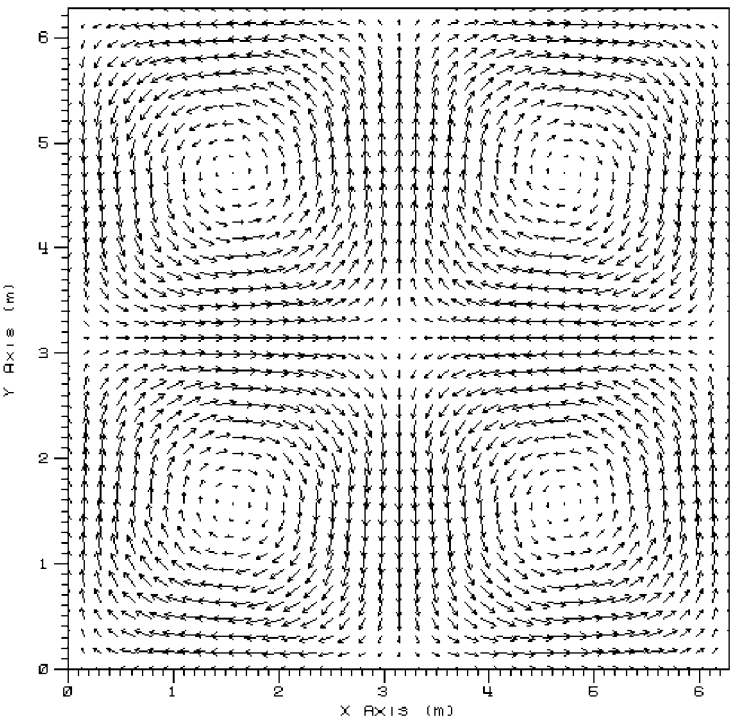

Figure 3. Velocity field—Taylor–Green.

and a fully unstructured one (Figure 4). E_c is calculated at the end of each time step (several time steps have been used). The global kinetic energy is exactly conserved (see Figure 5).

4.2. HIT

This test case is based on a realistic spectrum of the kinetic energy. The domain is a cube $(2\pi)^3$. The velocity field is initialized via FFTs using the spectrum given by

$$E(k, t=0) = Ak^8 \mathrm{e}^{-4(k/k_i)^2} \tag{21}$$

where k stands for the wave numbers in the spectral space.

The meshes are obtained by dividing the cube in n^3 cubes, each one divided in six tetrahedra. We used the meshes obtained with $n = 16$ and 32.

Various values of time steps have been used up to a CFL equal to 3. The fix-point algorithm converged with less than six iterations for each time step, which is reasonable [4].

It is shown in Figures 6 and 7 that our scheme conserves the global kinetic energy. The results of CAKE (or fully implicit with the rotational form) are compared with several numerical schemes. Figure 6 compares CAKE to the numerical schemes which do not conserve kinetic energy at all such as the centred scheme (using the divergence form for the convective term) with a second-order Runge–Kutta time advancing scheme, the alternant Mac Cormack scheme or the rotational form using an Euler explicit scheme. Figure 7 compares CAKE to

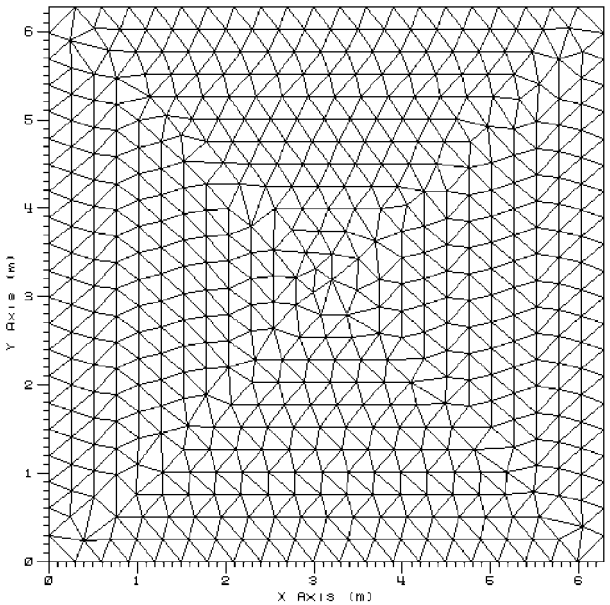

Figure 4. Unstructured mesh—Taylor–Green.

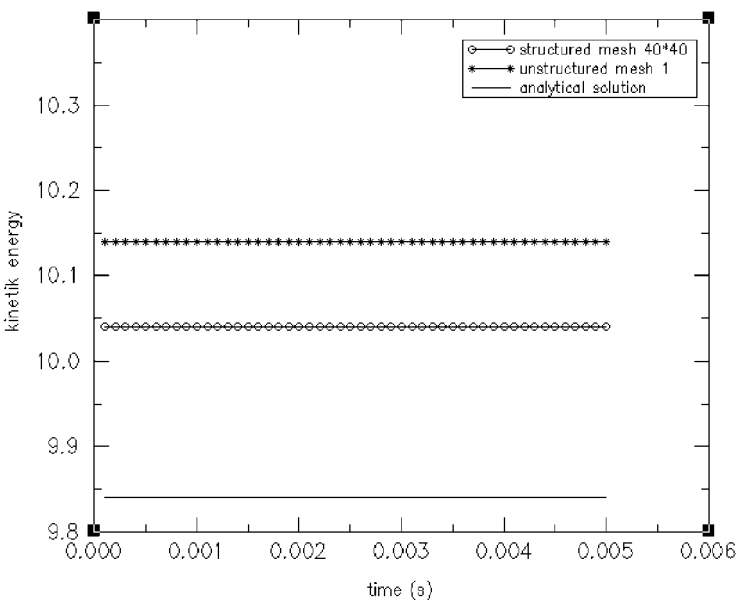

Figure 5. Kinetic energy evolution—Taylor–Green.

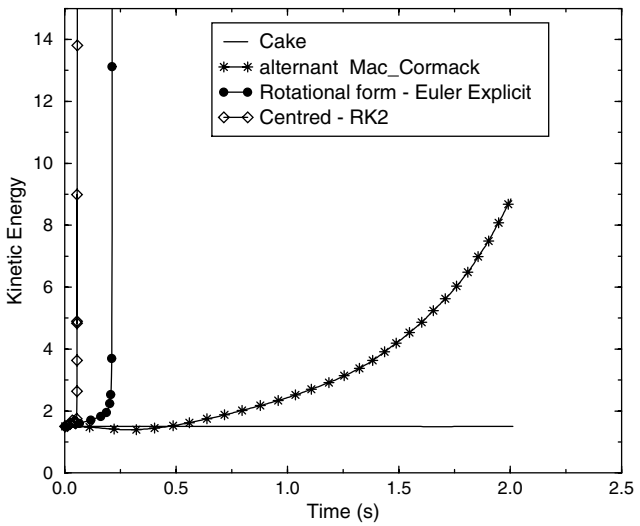

Figure 6. Kinetic energy evolution 1—HIT.

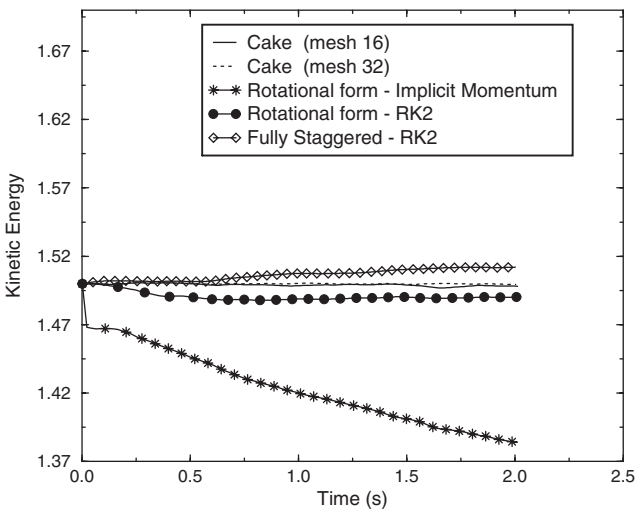

Figure 7. Kinetic energy evolution 2—HIT.

other schemes that are satisfactory concerning the conservation property such as 'the fully staggered with a third-order Runge–Kutta scheme' and other variants of the discretization used in this work. These schemes could be interesting if the CPU time is too high in some other cases. The discretization proposed in the present work is the only one which conserves exactly the kinetic energy.

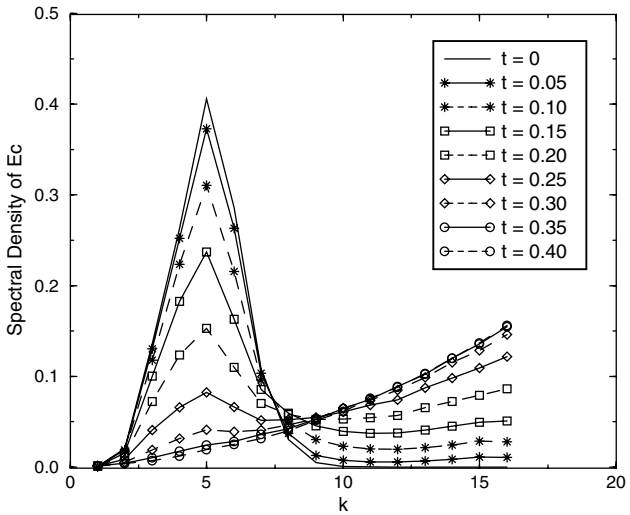

Figure 8. Energy spectrum evolution for CAKE.

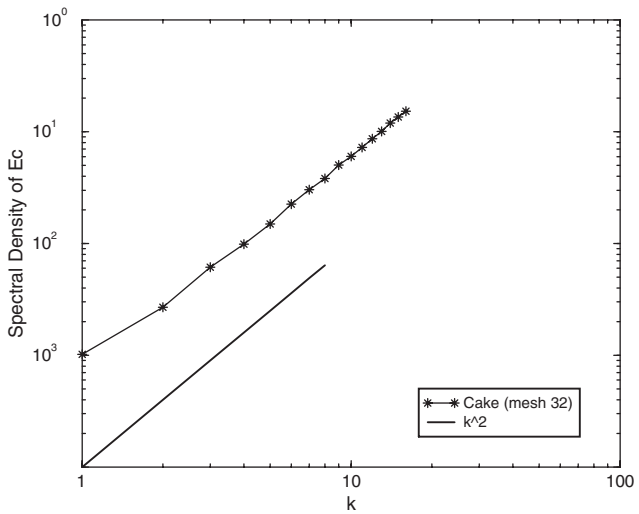

Figure 9. Spectrum behaviour for CAKE.

The time evolution of the spectrum (Figure 8) is shown at different time steps and proves that the kinetic energy of the large eddies (small wave numbers) is progressively transferred to small eddies (high wave numbers). The last spectrum is shown in Figure 9. It is proportional to the square of the wave length, which is a theoretical result, but rarely verified computationally (equipartion of the spectral density of the kinetic energy).

5. CONCLUSION

A proper choice of variable arrangements, discrete operators and time-advancing scheme allowed us to reach the challenging aim of conserving global kinetic energy on unstructured grids for the non-viscous part of the momentum equations.

Two test-cases have been carried out successfully. The Taylor–Green vortices (2D) and the HIT (3D). Both of them proved that the scheme developed in this work conserves the global kinetic energy even with high Courant numbers and the 3D case allowed us to compare this scheme to other 'classical' schemes and to verify a physical result, the final stage of the density spectrum of kinetic energy without any viscosity is proportional to the square of the wave number.

The diffusion operator has been tested with the Taylor–Green vortices test-case and is of second order. It will be used to compute real LES with the Smagorinsky subgrid scale model. The diffusion operator is the only one responsible for the dissipation of kinetic energy. The analysis of the dissipation due to this operator will be done in future to verify if it leads to the expected dissipation in the kinetic energy equation.

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