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Lagrangian Particle Approach to Large Eddy Simulations of Hydrodynamic Turbulence

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The flux of energy from large to small scales in hydrodynamic turbulence controls the dissipation of energy at a given scale in the fluid. An accurate parametrization of this flux is a prerequisite in order to devise reliable methods to simulate turbulent flows without resolving all the scales of motion. This problem is discussed in the context of a particle method based on the Smooth Particles Hydrodynamics algorithm. Motivated by the von Karman–Howarth–Kolmogorov exact relation for the energy flux, and by Lagrangian dynamics considerations we postulate an energy transfer term which is quadratic in the velocity and formally time reversal invariant. The numerical simulation of the model however is observed to spontaneously break the time reversal symmetry, demonstrating that the proposed term acts on average as the desired eddy damping.

KEY WORDS: Hydrodynamic turbulence; lagrangian particles; numerical simulations; time reversibility.

Hydrodynamic turbulence in 3 dimensions is characterized by a nonlinear flux of energy from large to small scales, which gives rise to the celebrated "energy cascade."[1, 2] The exact Kolmogorov equation:

$$\frac{d}{dx}\langle \Delta u(x)^3 \rangle = -\frac{4}{5}\epsilon + 6\nu \frac{d^2}{dx^2}\langle \Delta u(x)^2 \rangle \tag{1}$$

relates the average rate of energy dissipation, or the energy flux ε to the moments of the longitudinal velocity difference $\Delta u(x)$. Remarkably, in the

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limit where the viscosity ν goes to zero, or equivalently, when the Reynolds number becomes infinitely large, the dissipation becomes independent of viscosity.[2] The existence of a mean energy flux in highly turbulent flows is thus well understood. Providing a reliable description of the *instantaneous* energy transfer and of its fluctuations remains however a challenging problem. This difficulty has serious practical consequences. Indeed, with the present computer technology, it is still effectively impossible to resolve adequately all the scales of motion for most problems of practical importance. Because the large scale features of the flow only are of interest, a truncated description, where the smallest scales of the motion are parametrized in some adequate fashion, is expected to be sufficient. However, it has proven rather difficult to truncate reliably the smallest scales of the motion and to parametrize the energy flux below the resolved length. So far, the attempts to devise such a numerical scheme, known as Large Eddy Simulations (LES),[3] have been mostly restricted to the Eulerian representation of the equations of motion. The lagrangian point of view is also very appealing in this context.[4]

In this note, we consider the possibility of using particle simulations to parametrize the energy transfer, and its application to effectively simulate turbulent flows. Much insight has been recently gained in the problem of passive scalar mixing by analyzing the motion of individual lagrangian particles.[5, 6] Similar ideas have been used to understand the fluctuations of the turbulent velocity field itself.[7–9] In particular, it has been shown that the local energy flux at scale R can be parametrized by using the knowledge of the position $\mathbf{r}_i$ and the velocities $\mathbf{v}_i$ of a cloud of lagrangian particles. The constructions[8] involves the mean moment of inertia tensor g, the mean velocity V, and the mean velocity gradient tensor M, defined by:

$$g_{ab} \equiv \overline{(r^i - r^0)_a\,(r^i - r^0)_b}; \quad \mathbf{V} \equiv \overline{\mathbf{v}^i}; \quad M_{ab} \equiv \sum_c g^{-1}_{ac} \overline{(r^i - r^0)_c\,(v^i - V)_b} \tag{2}$$

(the overbar represents an average over the particles of the cloud). The energy flux can be parametrized by: $\alpha\,\mathrm{tr}(gM^2M^\dagger)$, where α is a weakly dependent function of scale, of order 1 ($1 \lesssim \alpha$).

Simulating a flow by using particles can be done by considering a gas of elementary molecules, which reproduce the dynamics of the fluid only at scales much larger than the mean free path.[10, 11] Here, we rather try to use directly the fluid dynamics equations, expressed in lagrangian terms. The Smooth Particle Hydrodynamics (SPH) method[12] provides a convenient framework to perform such calculations. SPH is based on interpolation from discrete particles, characterized by their masses m_i, positions $\mathbf{r}_i$, and velocities $\mathbf{v}_i$, see Fig. 1, and obeying the equations of motion for fluid particles:

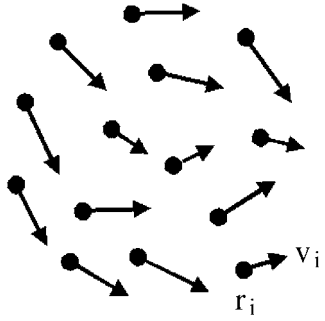

Fig. 1. Representation of the gas of particles. A set of particles, characterized by their masses m_i, their positions $\mathbf{r}_i$, and their velocities $\mathbf{v}_i$, evolving according to the equations of motion Eqs. (3) and (4). The pressure field and the gradients are contructed with the help of a kernel function $W(\mathbf{x}, h)$ of spatial extent h.

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i \tag{3}$$

$$\frac{d\mathbf{v}_i}{dt} = -\frac{\nabla p_i}{\rho_i} + \mathbf{f}_i + \mathbf{D}_i \tag{4}$$

where ∇p_i is the pressure gradient, $\mathbf{f}_i$ an external forcing term, and $\mathbf{D}_i$ an energy flux term discussed below. We consider here a weakly compressible case, where pressure p is related to density ρ by $p = \frac{1}{\gamma}\rho^{\gamma}$. For consistency, the velocities are required to remain small compared to the velocity of sound: $|\mathbf{v}_i| \ll \sqrt{\frac{dp}{d\rho}}$. Quantities such as the density ρ_i, or the pressure gradient, are computed by interpolation. To this end, a positive kernel $W(\mathbf{x}, h)$, with a spatial extend of order h in the variable $\mathbf{x}$, and normalized by $\int W(\mathbf{x}, h)\, dx = 1$, is introduced. For isotropy reasons, we restrict ourselves to the case where W depends only on the norm of $\mathbf{x}^2$. A convenient example is the gaussian kernel: $W(\mathbf{x}, h) = \frac{1}{(\sqrt{\pi}h)^3} \exp -(\mathbf{x}^2/h^2)$. The density $\rho(\mathbf{r})$ is defined by:

$$\rho(\mathbf{r}) = \sum_j m_j W(\mathbf{r} - \mathbf{r}_j, h) \tag{5}$$

and, in general, the interpolation of a field A, whose value A_j is known at each of the lagrangian particle j, is defined by:

$$A(\mathbf{r}) = \sum_j \frac{m_j}{\rho_j} A_j W((\mathbf{r} - \mathbf{r}_j), h) \tag{6}$$

where $\rho_j \equiv \rho(\mathbf{r}_j)$. Gradients are computed directly by differentiating Eq. (6) with respect to $\mathbf{r}$. For explicit calculations, it is convenient to use:[12]

$$\frac{\nabla p_i}{\rho_i} = \sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \nabla_i W_{ij} \tag{7}$$

where $W_{ij} \equiv W((\mathbf{r}_i - \mathbf{r}_j), h)$ and $\nabla_i W_{ij} \equiv \nabla W((\mathbf{r} - \mathbf{r}_j), h)|_{\mathbf{r}=\mathbf{r}_i}$. In the following, we will use the notation $\mathbf{r}_{ij} \equiv (\mathbf{r}_i - \mathbf{r}_j)$ and $\mathbf{v}_{ij} \equiv (\mathbf{v}_i - \mathbf{v}_j)$.

In the absence of forcing and energy transfer ($\mathbf{f}_i = \mathbf{D}_i = 0$), the resulting system of equations can be derived from a lagrangian. The dynamics resulting from SPH approximates the usual hydrodynamics. In particular, it leads to conservation properties for the linear and angular momentum. In the limit where particles get very close to one another, circulation conservation is recovered.[13]

The smoothing length h is the smallest scale unaffected by the smoothing. The SPH method does not attempt to describe faithfully the motion at scales smaller than h, since it resorts to an averaging. This approach is particularly appropriate for the coarse-grained description of turbulence we are interested in. The key requirement is to provide a consistent energy flux at the smallest resolved scale h.

Various schemes have been proposed to approximate molecular viscous dissipation.[12, 14] Here, we are rather interested in modelling the energy transfer occuring at the smallest resolved length, in a situation where scales smaller than h are not properly taken into account. In order to represent the nonlinear energy flux term, and inspired by previous work,[8] we postulate the following form for the energy transfer term $\mathbf{D}_i$:

$$\mathbf{D}_i = -\nu_t \sum_j m_j \left(\frac{1}{\rho_i} + \frac{1}{\rho_j} \right) \frac{dW_{ij}}{dt} \mathbf{v}_{ij} \tag{8}$$

$$= -\nu_t \sum_j m_j \left(\frac{1}{\rho_i} + \frac{1}{\rho_j} \right) \mathscr{W}'_{ij} (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}) \, \mathbf{v}_{ij} \tag{9}$$

To write the second equality, we simply assumed that $W(\mathbf{x}, h)$ is a function of $u \equiv \mathbf{x}^2$, and we use the notation $\mathscr{W}'_{ij} \equiv \partial_u W(u, h)|_{u=\mathbf{r}_{ij}^2}$. The parameter ν_t is dimensionless. The energy transfer term is quadratic in the velocity field $\mathbf{v}$. The change $t \to -t$, $\mathbf{r} \to \mathbf{r}$, and $\mathbf{v} \to -\mathbf{v}$ leaves $\mathbf{D}$ invariant. As a consequence, in the absence of any other viscous dissipation term, the equations of motion are time reversal invariant. A spontaneous symmetry breaking must occur so that $\mathbf{D}$ can act as a genuine dissipation.

The evolution equation for the kinetic energy, $E = \frac{1}{2} \sum_i m_i \mathbf{v}_i^2$, is:

$$\frac{dE}{dt} = -\nu_t \sum_i \sum_j m_i m_j \left(\frac{1}{\rho_i} + \frac{1}{\rho_j} \right) \mathscr{W}'_{ij} (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}) \, \mathbf{v}_{ij}^2 \tag{10}$$

In the case where W is a gaussian, $\mathscr{W}'(\mathbf{x}, h) = -\frac{1}{h^2} W(\mathbf{x}, h)$, the expression above becomes:

$$\frac{dE}{dt} = +\frac{v_t}{h^2} \sum_i \sum_j m_i m_j W_{ij} \left(\frac{1}{\rho_i} + \frac{1}{\rho_j} \right) (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})\, \mathbf{v}_{ij}^2 \tag{11}$$

Thus, for particles with the same mass ($m_i = m$), the equation for the mean kinetic energy reads:

$$\frac{1}{2} \frac{d\langle v^2 \rangle}{dt} = \frac{v_t}{h^2} \langle (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})\, \mathbf{v}_{ij}^2 \rangle \tag{12}$$

where $\langle \cdots \rangle$ denotes an average over all particles. For more general kernel functions, with the mild assumption that W is a decreasing functions of $\mathbf{x}^2$, Eq. (12) still provides a convenient estimate of the energy dissipation. Equation (12) is very reminiscent of the Kolmogorov equation, Eq. (1). For an incompressible turbulent velocity field, with a $2/3$ scaling exponent ($\Delta u(x)^2 \propto x^{2/3}$), one has:

$$\langle (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})\, \mathbf{v}_{ij}^2 \rangle = -\tfrac{20}{9} \varepsilon \mathbf{r}_{ij}^2 \tag{13}$$

Comparing Eqs. (12) and (13), one deduces that the parameter v_t should be of order 1 for consistency.

The forcing term $\mathbf{f}_i$ is assumed to act at the largest spatial scale; it feeds kinetic energy into the system.

To test these ideas, we have integrated numerically the SPH equations, Eqs. (3) and (4). The algorithm is based on the code kindly provided to us by Morris.[15] The density, as well as the right hand side of the Eq. (4) are estimated by a sum over neighbouring particles, Eqs. (5) and (7), which involves of order N^2 operations for N particles. To reduce the corresponding prohibitively large CPU cost, we use kernel functions with a compact support, typically a quintic spline function, and we partition space in boxes, making sure that two particles contributing to the sums in Eqs. (5) and (7) are located either in the same box, or in two adjacent boxes. This reduces the computational cost to order N. In the present calculation, we use periodic boundary conditions, with a domain size L. The forcing is a superposition of Fourier modes at wavenumbers $\mathbf{k} = \pm \frac{2\pi}{L} \hat{\mathbf{e}}_i$, where $\hat{\mathbf{e}}_i$ are the unit vectors in the three directions of space. Particles are initialized on a lattice of mesh 1. With these conventions, the total number of particles is L^3. A typical value of h is $h \sim 1.5$ (the number of particles in the sums in Eqs. (5) and (7) of order of 380). The equations of motion are integrated by a modified predictor corrector algorithm, second order in time. The time step is determined dynamically to ensure that the scheme is stable. With

the parameters of the forcing chosen, the velocity remained on average small compared to the velocity of sound, c ($\langle \mathbf{v}^2 \rangle^{1/2} \sim 0.1$; whereas $c \sim 1$). The maximum value of $|\mathbf{v}|$ became on occasions comparable to the sound velocity.

A number of simulations of the gas of lagrangian particles have been performed. In the absence of a forcing term ($\mathbf{f} = 0$), the initial condition was chosen to be a superposition of Fourier modes at low wave numbers, with random coefficients. The energy transfer term $\langle (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})\, \mathbf{v}_{ij}^2 \rangle$ is a function of time, which satisfies: $\langle (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})\, \mathbf{v}_{ij}^2 \rangle|_{t=0} = 0$. The particle average energy transfer is found to be negative, with occasionally positive values. We thus observe time reversal symmetry breaking, so the energy transfer term acts on average as a dissipation.

When the forcing is present ($\mathbf{f} \neq 0$), we observe that the energy flux term is negative, without reaching positive values. Although the energy transfer dissipates, we found that it cannot by itself control the evolution of the particle ensemble. At long times, we observed degradation of the solution which manifests itself in particular as growth of the velocity divergence $\langle (\nabla \cdot \mathbf{v})^2 \rangle$. We interpret this effect as resulting from a slow growth of correlations between the geometry of the distorted lattice and the velocity field.[8]

To avoid this problem, we periodically re-interpolated, using the kernel W (see Eq. (6)) the velocity field onto a regular lattice. In practice, re-interpolating the solution every ~ 100 time steps, which corresponds here to $\sim 1/10$ of the eddy turn over time $L/\langle \mathbf{v}^2 \rangle^{1/2}$, was found sufficient to prevent the degradation of the flow, at the cost of a moderate amount of extra dissipation. With this procedure, the solution remained well behaved for as long as we have been able to check.

Again, the main observation is that the energy flux term $\langle (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})\, \mathbf{v}_{ij}^2 \rangle$ spontaneously becomes negative. A typical recording of this quantity as a function of time is shown in Fig. 2, as well as the corresponding record of $\langle \mathbf{v}_i^2 \rangle$. The system goes through large fluctuations of integral quantities, yet, the energy transfer remains always negative. The system thus spontaneously breaks the time invariance symmetry, a non trivial result. Similarly, we observe that the skewness of the longitudinal velocity difference $S_3(x) = \langle \Delta u(x)^3 \rangle / \langle \Delta u(x)^2 \rangle^{3/2}$ is observed to decay towards a negative value for $x \lesssim h$.

The spectrum of the solution remains close to the $k^{-5/3}$ Kolmogorov spectrum at large scales, see Fig. 3. Although this is an encouraging sign, more work remains to be done to show that the solution of the model correctly reproduces the large scale features of a true turbulent flow. To proceed, one needs to understand, among other things, the relation between the energy flux observed in the model and the large scale properties of the

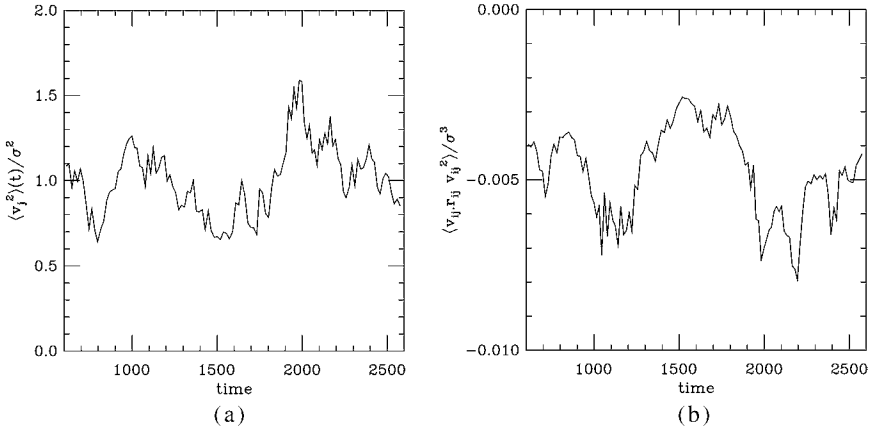

Fig. 2. The mean value of the averaged kinetic energy per particle $\langle \mathbf{v}^2 \rangle$ (a), and of the dissipation rate $\langle (\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})\, \mathbf{v}_{ij}^2 \rangle$ (b), as a function of time. The eddy damping term is observed to be definite positive, thus leading to a genuine energy dissipation. The parameters of the simulations are $\nu_t = 1$, $\gamma = 9$. In this simulation, the effective eddy damping is responsible for half of the total energy dissipation. The rest of the dissipation comes from the discrete remeshing of the solution, every 80 time steps.

flow.[16] In practice one also needs to assess the convergence of the methods, and the corresponding computational effort.

Finally, it is interesting to discuss the properties of the gas of lagrangian particles considered in this article in relation with other systems, described by dissipative, time-reversible evolution equations.

In the context of LES, the "non-linear" and the "similarity" models of energy transfer lead to quadradic dissipation terms, and to equations that

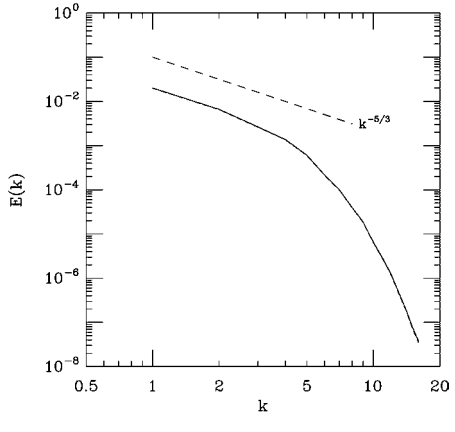

Fig. 3. An example of the energy spectrum of the solution.

are time-reversal invariant. Interestingly, it is observed, see ref. 3 and references therein, that these quadratic terms are not enough to properly dissipate energy, and that a term that explicitely breaks the time symmetry must be added to correctly dissipate energy. This is in a way similar to the situation we have discussed here, since the smoothing acts irreversibly on the system. We emphasize however that in our case, the spontaneous symmetry breaking occurs even in the absence of explicit symmetry breaking.

From a theoretical point of view, important results have been obtained concerning fluctuations in dissipative time-reversible systems.[17] These ideas might possibly apply to hydrodynamic turbulence,[18] as they have been demonstrated to apply to other physical systems.[19] Analyzing the properties of our gas of particles from this point of view should lead to new insight.

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