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Kinetically reduced local Navier-Stokes equations: An alternative approach to hydrodynamics

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An alternative approach, the kinetically reduced local Navier-Stokes (KRLNS) equations for the grand potential and the momentum, is proposed for the simulation of low Mach number flows. The Taylor-Green vortex flow is considered in the KRLNS framework, and compared to the results of the direct numerical simulation of the incompressible Navier-Stokes equations. The excellent agreement between the KRLNS equations and the incompressible nonlocal Navier-Stokes equations for this nontrivial time-dependent flow indicates that the former is a viable alternative for computational fluid dynamics at low Mach numbers.

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The notion of incompressible flow usually refers to a situation where a characteristic flow speed u is small compared to the speed of sound c_s, and the Mach number $\mathrm{Ma}=u/c_s$ is small. Then, the simplest characterization of the degree of "molecularity" is the Knudsen number $\mathrm{Kn}\sim\lambda/H$, the ratio of the mean free path of molecules λ, and the characteristic scale H of variation of hydrodynamic fields (density, momentum, and energy). When $\mathrm{Kn}\lesssim 10^{-3}$, one considers the hydrodynamic limit, where molecularity reduces to a specific set of transport coefficients (viscosity, thermal conductivity, etc.) for each molecular model. If, in addition, the Mach number is small, one enjoys incompressible hydrodynamics with the ordering $\mathrm{Kn}\ll\mathrm{Ma}\ll 1$, and the flow can be characterized solely by the ratio

$$\mathrm{Re}=\frac{\mathrm{Ma}}{\mathrm{Kn}}, \tag{1}$$

which is one of the definitions of the Reynolds number.

Computational fluid dynamics (CFD) of flows at small Mach number has been traditionally based on the mechanical description of the incompressible fluid, the classical incompressible Navier-Stokes (INS) equations,

$$\partial_t u_\alpha + u_\beta\partial_\beta u_\alpha + \partial_\alpha P = \frac{1}{\mathrm{Re}}\partial_\beta\partial_\beta u_\alpha, \quad \partial_\alpha u_\alpha = 0, \tag{2}$$

where $\boldsymbol{u}$ is the fluid velocity, P the pressure, and Re the Reynolds number, which characterizes the relative strength of the viscous and inertial forces [1]. The pressure in (2) is not an independent thermodynamic variable, and must be determined so that it satisfies the incompressibility condition. Thus, in order to obtain the pressure at a point, one has to solve the Poisson equation

$$\partial_\beta\partial_\beta P = -(\partial_\beta u_\alpha)(\partial_\alpha u_\beta) \tag{3}$$

in the domain, and the relationship between the pressure and the velocity becomes highly nonlocal. The physical meaning of (3) is that in a system with infinitely fast sound propagation, any pressure (and thus density) disturbance induced by the flow is instantaneously propagated into the whole domain.

This "elliptic problem" is arguably the most severe obstacle for developing numerical methods for CFD. Therefore, in the recent past, alternative physical models of incompressibility have been explored based on a more local (thermodynamic) picture. To date, the most successful approach is the lattice Boltzmann method (LBM) [2]. The LBM models are derived from the Boltzmann equation under the assumption of a low Mach number [3,4], and provide a viable alternative for CFD methods for practical applications [5]. However, certain features pertinent to the LBM (the relatively large number of fields and the restriction to uniform grids) impose limitations that so far persist in spite of numerous attempts.

Recently, an alternative thermodynamic description of incompressible fluid flows was introduced in [6]. It was found that the grand potential in the Euler coordinate system is the proper thermodynamic variable to study the onset of incompressibility. The starting point in [6] was the set of compressible (local) Navier-Stokes equations for the density ρ, the momentum density $\boldsymbol{m}=\rho\boldsymbol{u}$, and the negative of the grand potential $\mathcal{G}$,

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$$\mathcal{G} = P - \frac{m^2}{2\rho}. \tag{4}$$

Here, P is the (local) thermodynamic pressure measured in a comoving (Lagrange) coordinate system. It was shown that, after the acoustic (density) mode is damped out on the short time and length scales,

$$t_a \sim \sqrt{\mathrm{Kn}}\mathrm{Ma}T, \quad l_a \sim \sqrt{\mathrm{Kn}}L, \tag{5}$$

respectively, where L is a characteristic flow length scale, and T is the flow time scale, one arrives at a coupled system of equations for the nondimensional momentum density $\boldsymbol{j} = \boldsymbol{m}/(\bar{\rho}U_0)$, where $\bar{\rho}U_0$ is a characteristic momentum (known from the initial or boundary conditions), and the nondimensional grand potential density $\Theta = \mathcal{G}/(\bar{\rho}U_0^2)$. In these kinetically reduced local Navier-Stokes (KRLNS) equations, the fast dynamics of the grand potential becomes singularly coupled to the slow dynamics of momentum, and the incompressible Navier-Stokes equations are the quasistationary solution of the KRLNS equations at small Mach number.

In this paper, we demonstrate that the KRLNS equations [6] are capable of providing an alternative, local-in-space framework for computational fluid dynamics. We report an extensive simulation of the classical three-dimensional Taylor-Green vortex flow [7] both in the KRLNS equation framework, and in the classical incompressible Navier-Stokes setting using the spectral element method [8]. Excellent agreement between the two approaches is observed. Moreover, the quasicompressible nature of the KRLNS equations is quantified in this flow as nonrandom oscillations of the divergence of the velocity field on the Mach number scale. Implications of this quasicompressibility as well as possible ways to increase the simulation time step are also discussed as areas in which further work is needed.

We consider a simplified version of the KRLNS equations that contain the terms required to reconstruct the incompressible Navier-Stokes equations as the quasistationary approximation. The simplification is achieved following two steps.

(1) The equation for the dimensionless grand potential density Θ [Eq. (10) in Ref. [6]] is a diffusion equation with a source term that depends solely on the dimensionless momentum $\boldsymbol{j}$,

$$\partial_t\Theta - \sqrt{\mathrm{Kn}}\frac{\gamma}{\mathrm{Pr}}\partial_\alpha\partial_\alpha\Theta = -\frac{1}{\mathrm{Ma}}\partial_\alpha j_\alpha + F(\boldsymbol{j}), \tag{6}$$

where γ is the adiabatic exponent, Pr is the Prandtl number, and F is the nonlinear part of the source term,

$$F = \mathrm{Ma}\partial_\alpha\left(\frac{j_\alpha j^2}{2}\right) + \sqrt{\mathrm{Kn}}\left[\left(\frac{\gamma}{\mathrm{Pr}} - 1\right)\partial_\alpha\partial_\alpha\frac{j^2}{2} + (\partial_\alpha j_\beta)(\partial_\alpha j_\beta)\right.$$
$$+ \left.\frac{\partial P}{\partial T}\bigg|_p \frac{1}{2C_V}(\partial_\alpha j_\beta + \partial_\beta j_\alpha)(\partial_\alpha j_\beta + \partial_\beta j_\alpha)\right.$$
$$\left. - \left(1 + \lambda - \frac{2}{D}\right)\partial_\beta(j_\beta\partial_\alpha j_\alpha)\right]. \tag{7}$$

In the following, we neglect the nonlinear term F, and retain only the leading order source term, $\mathrm{Ma}^{-1}\partial_\alpha j_\alpha$, $\mathrm{Ma} \ll 1$, responsible for maintaining incompressibility. As was explained in Ref. [6], the use of the grand potential is crucial in the KRLNS equations since any other choice of the thermodynamic function (e.g., of the entropy S) would immediately result in the presence of an advection term $j_\alpha\partial_\alpha S$, and in nontrivial coupling to the momentum equation. Finally, although not necessarily, we shall also set $\mathrm{Pr} = \gamma$.

(2) The momentum equation [Eq. (10) in Ref. [6]] reads

$$\partial_t j_\alpha = -\mathrm{Ma}j_\alpha\partial_\beta j_\beta - \mathrm{Ma}j_\beta\partial_\beta j_\alpha - \mathrm{Ma}\partial_\alpha\left(\Theta + \frac{j^2}{2}\right)$$
$$+ \sqrt{\mathrm{Kn}}\left(1 + \lambda - \frac{2}{D}\right)\partial_\alpha\partial_\beta j_\beta + \sqrt{\mathrm{Kn}}\partial_\beta\partial_\beta j_\alpha, \tag{8}$$

where λ is the ratio of bulk viscosity to shear viscosity. In (8) we shall neglect the bulk viscosity term, which is proportional to the divergence, $\sim\sqrt{\mathrm{Kn}}\partial_\alpha\partial_\beta j_\beta$, as compared to the first term in the right-hand side, $-\mathrm{Ma}j_\alpha\partial_\beta j_\beta$. This is consistent with the assumption $\mathrm{Kn} \ll \mathrm{Ma}$ under which the KRLNS equations were derived. Eventually, both these terms could be neglected because we expect (this has been confirmed by the simulations below) that the divergence itself is of the order Ma. However, we shall retain the first term in the right-hand side of (8) in order to achieve a conservation law form of the momentum equation, which is more convenient from the numerical perspective. The same approach is routinely applied in the numerical simulation of low-Mach-number hydrodynamics [8].

With these simplifications, the KRLNS equations are written as

$$\partial_t j_\alpha = -\mathrm{Ma}\partial_\beta\left[j_\alpha j_\beta + \delta_{\alpha\beta}\left(\Theta + \frac{j^2}{2}\right)\right] + \sqrt{\mathrm{Kn}}\partial_\beta\partial_\beta j_\alpha,$$
$$\partial_t\Theta = -\frac{1}{\mathrm{Ma}}\partial_\alpha j_\alpha + \sqrt{\mathrm{Kn}}\partial_\beta\partial_\beta\Theta. \tag{9}$$

The KRLNS equations (9) are valid for $\mathrm{Kn} \ll \mathrm{Ma} \ll 1$, on scales larger than the acoustic (5). They can be considered as a simplified computational model of the complete equations, derived in [6]. Note that these simplifications retain the basic physical properties of the equations approaching incompressibility. Loosely speaking, (9) is what survives from the compressible Navier-Stokes equations just before incompressibility sets in. Indeed, the time derivative of Θ becomes singularly perturbed as the Mach number tends to zero, and we recover the incompressibility condition $\partial_\alpha j_\alpha = 0$ as the quasistationary solution of the system (9). This solution, when substituted in the momentum equation, recovers the INS equation (2) with the usual accuracy of $O(\mathrm{Ma}^2)$. The dissipation terms (proportional to $\sqrt{\mathrm{Kn}}$) cannot be neglected in the equation for the grand potential (9). We hasten to add that this is at crucial variance with the artificial compressibility method [9], where one considers an artificial singularly perturbed dynamic equation for the pressure.

Now, the KRLNS equations (9) are a parametric family of hydrodynamic systems (parametrized by the values of Ma and Kn), which we study numerically and compare with the solution of the incompressible Navier-Stokes equations (2).

Both the INS and the KRLNS equations were discretized using the spectral element method [8]. The temporal discretization is based on a second-order mixed explicit-implicit operator splitting formulation [10,11]. The message passing interface (MPI) based parallel code runs with good scalability on a number of different platforms [12].

The KRLNS equations (9) are first transformed into a new set of variables $\Theta' = \mathrm{Ma}\Theta$ and $u_\alpha = j_\alpha/\bar{\rho}$, with $\bar{\rho}$ being constant. In order to compare the results from the INS and the KRLNS equations, the time scale (t_{NS}) in the incompressible Navier-Stokes equations (2) is related to the time scale of the KRLNS equations (t_{KRLNS}) as follows:

$$t_{\mathrm{KRLNS}} = \mathrm{Ma}\ t_{\mathrm{NS}}. \tag{10}$$

On the other hand, the Reynolds number Re in the Navier-Stokes equations (2) is related to the parameters Ma and Kn in the KRLNS equations (9) according to Eq. (1).

We consider the classical three-dimensional Taylor-Green vortex flow, and compare the results from the numerical solution of the rescaled KRLNS equations with the results from the direct numerical simulation of the incompressible Navier-Stokes equations (2). This flow has the property that, at large Re, the enstropy shows a rapid increase due to vortex stretching followed by a monotonic decay due to dissipation; on the other hand, the total energy of the flow decreases monotonically for all Re. Various discretizations were employed, with a total of 512 spectral elements and number of collocation points ranging from seven to 15 in each direction in the interior of each element. In rescaled time (10), the restriction on the time step was the same in the two methods; this means that the time step used in the solution of the KRLNS equations was always Ma times smaller than the INS one, i.e., $\delta t_{\mathrm{KRLNS}} = \mathrm{Ma}\ \delta t_{\mathrm{NS}}$. No other parameter matching between the KRLNS and INS equations was involved.

Snapshots of the isosurfaces of the vorticity component, $\omega_x = \partial_y w - \partial_z v = -5$, where v and w are the velocities in the y and z directions, respectively, for the KRLNS equations at the time of maximum enstrophy for Re=1000 are presented in Fig. 1. The general structure of the flow as well as all pertinent details agree very well in the two approaches at all computed Reynolds number, and only the KRLNS results are shown.

Figure 2 shows the time development of the total enstrophy $\Omega = \int \omega^2 d\boldsymbol{x}$ for both approaches at various Reynolds numbers. It can be observed that the maximum value of the total enstrophy as well as the nondimensional time where it occurs increase with Re. As can be observed from the figure, the resulting time variation of the enstrophy for both the INS and the KRLNS equations agree very well with each other.

It is important to note that the KRLNS equations are quasicompressible, that is, the incompressibility condition $\partial_\alpha j_\alpha = 0$ is valid only in the limit $\mathrm{Ma} \to 0$. The dynamics of the divergence, $\partial_\alpha j_\alpha$, show a rapidly fluctuating pattern with a characteristic frequency $\sim \mathrm{Ma}^{-1}$ around the specified value of Ma (see Fig. 3, where Ma=0.01 and the divergence fluctuates at the 10^{-2} level); the expanded inset clearly shows the nonrandom high-frequency fluctuations of the divergence.

The dependence of the amplitude and the variance of these fluctuations on the Mach number is presented in Fig. 4.

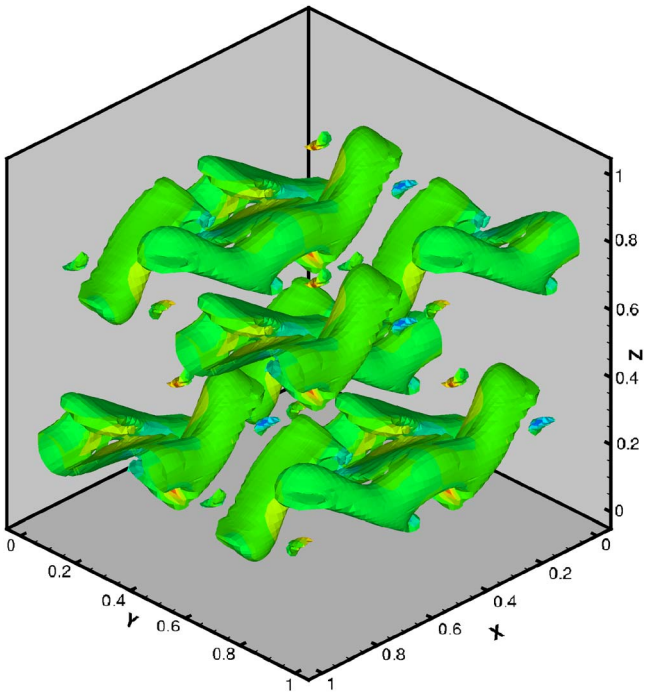

FIG. 1. (Color online) Isosurfaces of $\omega_x = -5$ at the time of maximum enstrophy in the Taylor-Green flow simulation at Re = 1000 computed with the KRLNS equations.

It is quite remarkable that both the average value as well as the variance of the divergence scale linearly with Mach number. While in most of the simulations presented here we have used $\mathrm{Ma} = 10^{-2}$, it was found that results for the energy and enstrophy (the quantities of primary interest in incompressible flow simulations) agree with the incompressible Navier-Stokes simulation up to $\mathrm{Ma} \sim 0.1$, the value typically used in lattice Boltzmann simulations.

To conclude, we have shown that the KRLNS equations (9) provide an alternative physical description of incom-

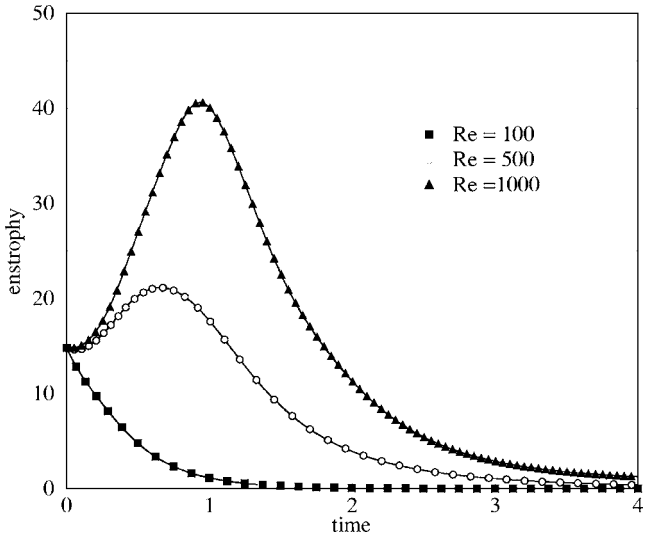

FIG. 2. Time history of total enstrophy for Re=100, 500, and 1000. Symbol: KRLNS equations. Line: INS equations. Time is measured in the Navier-Stokes units.

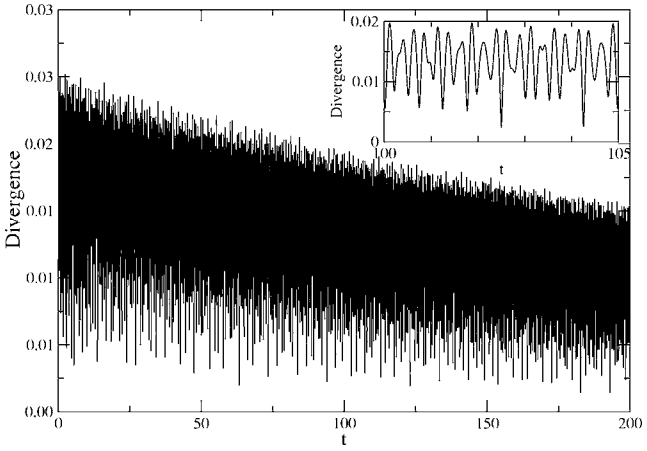

FIG. 3. Time history of the divergence $\partial_\alpha j_\alpha$ at Ma=0.01, Kn $=10^{-5}$ (Re=1000).

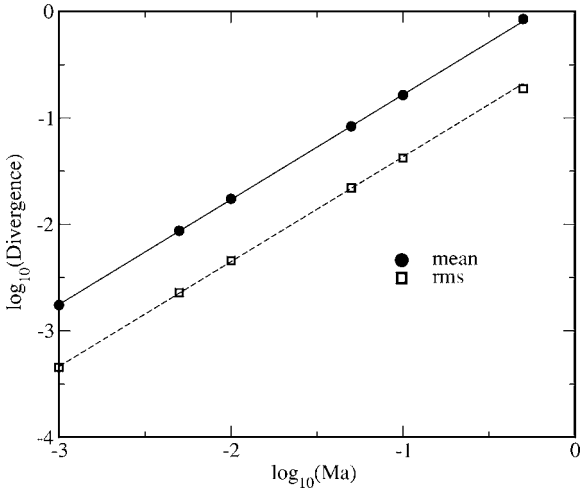

FIG. 4. Dependence of the mean (filled circles) and of the root mean square (open squares) of the fluctuations of the divergence on the value of the Mach number in Taylor-Green vortex flow as predicted by the KRLNS equations. Lines are to guide the eye.

pressible flows. The attractive feature of these equations is their locality, i.e., no elliptic pressure equation needs to be solved. The KRLNS equations should be considered therefore as an analog of the lattice Boltzmann models of incompressible flows. Unlike the latter, the number of fields in KRLNS equations is only four, and the equations are amenable to standard discretization procedures. On the other hand, the locality in any physical model of incompressible flows has to be traded against the significant decrease of the time step as compared to Navier-Stokes solvers [see Eq. (10)]. For example, using a Ma=0.1 will result in a reduction of the time step for the KRLNS equations of ten times compared to the time step which can be used for the solution of the INS. Due to the locality of the KRLNS solver, however, one avoids the solution of a pressure Poisson equation which can carry a significant computational cost.

It is worth mentioning here that no attempt was made to optimize the time step, which was taken simply as in (10) (i.e., Mach number times smaller that of the INS solver). It is expected that precisely the scaling of order Ma, shown in Fig. 4, which includes the time scale of variation of the divergence, can be exploited by appropriate numerical schemes (e.g., projective integration [13]), which will allow a significant increase of the time step in the solution of the KRLNS equations. This means that, even though the explicit time step is more severely restricted, at low Mach numbers, it is likely that due to more pronounced scale separation, more substantial computational savings can be achieved at lower Ma.

On the other hand, the smoothing effect of the dissipation term in the equation for the grand potential is crucial: its neglect leads to unstable schemes, which may require the use of time steps much smaller than (10). This particular term, which is derived by rigorous asymptotic analysis of the compressible Navier-Stokes equations [6], is the main difference of the physical model (9) from artificial compressibility models.

Our further studies will be focused on devising ways to filter out the rapid fluctuations in order to increase the time step. We are also investigating the proper treatment of boundary conditions for the KRLNS equations in the presence of walls as well as inflow-outflow boundaries.

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[1] L. D. Landau and E. M. Lifshitz, *Fluid Mechanics* (Pergamon Press, Oxford, 1987).
[2] F. Higuera, S. Succi, and R. Benzi, Europhys. Lett. **9**, 345 (1989).
[3] X. Shan and X. He, Phys. Rev. Lett. **80**, 65 (1998).
[4] S. Ansumali and I. V. Karlin, Phys. Rev. Lett. **95**, 260605 (2005).
[5] H. Chen, S. Kandasamy, S. Orszag, R. Shock, S. Succi, and V. Yakhot, Science **301**, 633 (2003).
[6] S. Ansumali, I. V. Karlin, and H. C. Öttinger, Phys. Rev. Lett. **94**, 080602 (2005).
[7] G. I. Taylor and A. E. Green, Proc. R. Soc. London, Ser. A **158**, 499 (1937).
[8] M. O. Deville, P. F. Fischer, and E. H. Mund, *High-Order Methods for Incompressible Fluid Flow* (Cambridge University Press, New York, 2002).
[9] A. J. Chorin, J. Comput. Phys. **2**, 12 (1967).
[10] G. Karniadakis, M. Israeli, and S. Orszag, J. Comput. Phys. **97**, 414 (1991).
[11] A. Tomboulides, M. Israeli, and G. Karniadakis, J. Sci. Comput. **4**, 291 (1989).
[12] P. Fischer and H. Tufo, *Parallel Computational Fluid Dynamics: Towards Teraflops, Optimization and Novel Formulations* (North-Holland, Amsterdam, 2000), pp. 17–26.
[13] C. Gear and I. Kevrekidis, J. Comput. Phys. **187**(1), 95 (2003).