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A New Computer Method of Solving Dynamic Equations under Externally Applied Deformations

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Numerical analysis can be a powerful method to get insight into nonlinear dynamical response against externally applied deformations in many physical systems. If such dynamics is described in terms of space-time dependent partial differential equations, we propose to integrate them in an appropriately deformed space. As a representative example, let us consider fluids under shear flow. Together with analytic work,[1] computer studies of shear flow effects have also been made on the basis of time-dependent Ginzburg-Landau models in the presence of a velocity field $\boldsymbol{v}$.[2] These studies aim to examine phase transitions and rheology in the presence of shear flow. However, there are some difficulties in numerically integrating such dynamic equations. First, due to the convection term, numerical data violate translational invariance. Second, because of the lack of the usual periodic boundary condition, we cannot use the FFT (fast Fourier transform) scheme. As a result it is difficult to take into account the hydrodynamic interaction. The aim here is to propose a new efficient method of externally applying deformations to dynamic equations in continuous media. It has already been applied to a complex problem of highly viscous polymer solutions in shear flow,[3] where there is no explanation of the method itself. We believe that it is applicable to a wide range of dynamic models including usual hydrodynamic equations.

Taking the x axis in the average flow direction and the y axis in the velocity gradient direction, we start with the simplest equation,

$$\frac{\partial}{\partial t}\phi = -\dot{\gamma}(t)y\frac{\partial}{\partial x}\phi - \nabla^2\left[\tau - \nabla^2 + \phi^2\right]\phi, \qquad (1)$$

where $\dot{\gamma}$ is the shear rate and τ represents the reduced temperature measured from the critical value. We neglect the velocity field fluctuations around the average flow and the random noise term on the right hand side, though they may easily be included in our scheme. The space $\boldsymbol{r}$, time t, and composition ϕ are made dimensionless appropriately. Hereafter $\dot{\gamma}(t)$ may be an arbitrary function of t. The usual Euler scheme is to integrate (1) as

$$\phi(\boldsymbol{r}, t+\Delta t) = \phi(\boldsymbol{r}, t) - \Delta t(\dot{\gamma}(t)y)(\partial\phi/\partial x) + \cdots, \qquad (2)$$

where Δt is a small time increment. Note that the second term linearly depends on y and the translational invariance is violated. To attain reliable integration $L\dot{\gamma}\Delta t$ must be very small, where L is the system size. However, if L is large and $\dot{\gamma}$ is not small, large scale heterogeneities inevitably develop in the y direction at long times.

To improve this situation we rewrite (1) in terms of new deformed space coordinates $\boldsymbol{r}' = (x', y', z')$ defined by

$$x' = x - \gamma(t)y, \qquad y' = y, \qquad z' = z, \qquad (3)$$

where $\gamma(t)$ is the strain rate,

$$\gamma(t) = \int_0^t \mathrm{d}t_1\dot{\gamma}(t_1). \qquad (4)$$

We simply have $\gamma = \dot{\gamma}t$ if $\dot{\gamma}$ is stationary. Then, by writing $\phi(\boldsymbol{r}, t) = \hat{\phi}(\boldsymbol{r}', t)$, (1) is rewritten as

$$\frac{\partial}{\partial t}\hat{\phi} = \hat{\boldsymbol{\nabla}}^2\left[\tau - \hat{\boldsymbol{\nabla}}^2 + \hat{\phi}^2\right]\hat{\phi} \qquad (5)$$

where

$$\hat{\boldsymbol{\nabla}} = (\partial/\partial x', \partial/\partial y' - \gamma\partial/\partial x', \partial/\partial z'), \qquad (6)$$

so that the deformed Laplacian is

$$\hat{\boldsymbol{\nabla}}^2 = (\partial/\partial x')^2 + (\partial/\partial y' - \gamma\partial/\partial x')^2 + (\partial/\partial z')^2. \qquad (7)$$

Remarkably (5) is invariant with respect to the uniform translation $\boldsymbol{r}' \to \boldsymbol{r}' + \boldsymbol{a}$ by a constant vector $\boldsymbol{a}$. Therefore, we solve (5) on a square lattice fixed in the deformed space as

$$\hat{\phi}(\boldsymbol{r}', t+\Delta t) = \hat{\phi}(\boldsymbol{r}', t) - \Delta t[(\partial\hat{\phi}/\partial t)(\boldsymbol{r}', t)], \qquad (8)$$

imposing the periodic boundary condition,

$$\hat{\phi}(x', y', z', t) = \hat{\phi}(x'+L, y', z', t)$$
$$= \hat{\phi}(x', y'+L, z', t) = \hat{\phi}(x', y', z'+L, t), \qquad (9)$$

in all the directions, where the system linear dimension L is assumed to be common in the x', y', z' axes. In the original reference frame (9) implies

$$\phi(x, y+L, z, t) = \phi(x - \gamma L, y, z, t), \qquad (10)$$

which has indeed been used in the previous simulations.[2] It corresponds to the Lee-Edwards boundary condition widely use in molecular dynamics simulations.[4,5] Of course, when data are displayed in figures, we invert the affine transformation as $\boldsymbol{r}' \to \boldsymbol{r}$ to obtain $\phi(\boldsymbol{r}, t)$.

We note that the Euler scheme of solving (5) becomes unstable for large $|\gamma|$ because $\hat{\boldsymbol{\nabla}}^2 \sim (\gamma\partial/\partial x')^2$ as $|\gamma| \to \infty$. This breakdown occurs for steady shear and may be avoided for oscillatory shear by choosing sufficiently small Δt. However, it can be overcome even for steady shear if we follow the following steps. (i) First, (5) is solved in the deformed reference frame in the time region $0 < t < 1/\dot{\gamma}$. (ii) Second, we stop the integration at $t = 1/\dot{\gamma}$. The data $\hat{\phi}(\boldsymbol{r}', 1/\dot{\gamma})$ in the deformed reference frame are then transformed into the data $\phi(\boldsymbol{r}, 1/\dot{\gamma})$ in the original reference frame using $x' = x - y, y' = y, z' = z$ at $\gamma = 1$. (iii) Third, we restart the integration by using the above $\phi(\boldsymbol{r}, 1/\dot{\gamma})$ as the initial value. The strain after the reset is given by

$$\gamma(t) = \dot{\gamma}t - 1. \tag{11}$$

(iv) We repeat the above steps at $t = n/\dot{\gamma}$ with $n = 2, 3, \cdots$. The strain $\gamma(t)$ is set equal to zero at each reset.

The merits of our method are as follows.

(i) Our scheme is perfectly invariant with respect to the shift of the origin of the reference frame and is stable even for very large $\dot{\gamma}$ and at long times.

(ii) We may use the FFT method in the deformed space because of the periodic boundary condition (9). The gradient operator (6) is replaced by a deformed wave vector (multiplied by i),

$$\mathrm{i}\hat{\boldsymbol{k}} = (\mathrm{i}k_x, \mathrm{i}k_y - \gamma \mathrm{i}k_x, \mathrm{i}k_z). \tag{12}$$

The structure factor may readily be calculated. Moreover, we may easily take into account the velocity field fluctuations (or the so-called hydrodynamic interaction) in the deformed space (which is neglected in (1) for simplicity). This is because the velocity field deviation $\delta\hat{\boldsymbol{v}}(\boldsymbol{r}', t) = \boldsymbol{v}(\boldsymbol{r}, t) - \dot{\gamma}y\boldsymbol{e}_x$ may be assumed to satisfy the periodic boundary condition in the deformed space. For example, in near-critical fluids, neglecting the acceleration (the Stokes or Kawasaki approximation) yields[6]

$$\eta_0 \hat{\boldsymbol{\nabla}}^2 \delta\hat{\boldsymbol{v}}(\boldsymbol{r}', t) = \left[\phi \hat{\boldsymbol{\nabla}} \frac{\delta}{\delta\phi} F\right]_\perp . \tag{13}$$

Here η_0 is the viscosity and $[\cdots]_\perp$ denotes taking the transverse part (or the orthogonal part to $\hat{\boldsymbol{k}}$ in the deformed Fourier space).

We note that our recent work of shear-induced phase separation[3] has been carried out using the method in this paper. It involves the velocity field fluctuation calculated using the FFT method in the deformed space. It demonstrates efficiency and stability of our method in complex situations over long times at large shear. Our method also enables us to examine three dimensional phase separation in a fluid binary mixture in shear flow.[1] In particular, we may examine break-up and coagulation of droplets in shear flow[7] in the Ginzburg-Landau scheme. Generally, we may take into account the hydrodynamic interaction in various complex fluids such as polymer solutions, block copolymers, and amphiphilic systems using the FFT method in the deformed space.

Finally we discuss possible extensions of our idea. (i) We may generally treat a flow field which has a homogeneous velocity gradient tensor $\overleftrightarrow{D}(t)$ defined by

$$\langle \boldsymbol{v} \rangle = \overleftrightarrow{D}(t) \cdot \boldsymbol{r}, \tag{14}$$

which includes shear, elongational, and rotational flows as special cases.[8] For this flow, if the system extends to infinity and in a steady state, the equal-time correlation function has the translational invariance and the structure factor is well-defined. An affine deformation $\boldsymbol{r}' = \overleftrightarrow{K}(t) \cdot \boldsymbol{r}$ (a generalization of (3)) is then needed, where $\overleftrightarrow{K}(t)$ is the deformation tensor obtained from

$$\frac{\partial}{\partial t}\overleftrightarrow{K}(t) = -\overleftrightarrow{D}(t) \cdot \overleftrightarrow{K}(t). \tag{15}$$

(ii) In the shear flow case we have assumed the periodic boundary condition (9) because we are interested in the bulk properties of sheared fluids. Another important category of problems is constituted by time-dependent volume change of fluids and solids enclosed by boundary walls. As an illustration let us assume that the system dimension $L(t)$ in the x axis is uniaxially changed in an arbitrary manner. The affine deformation needed is then

$$x' = \lambda(t)x, \qquad y' = y, \qquad z' = z. \tag{16}$$

Because we solve the equations on a fixed lattice in the deformed space, the system dimension L_0 in the deformed space should be fixed, so

$$\lambda(t) = L_0/L(t). \tag{17}$$

In the dynamic equations we replace $\partial/\partial t$ by $\partial/\partial t + [\partial \log(\lambda)/\partial t]x'\partial/\partial x'$ and $\partial/\partial x$ by $\lambda\partial/\partial x'$. If the boundary at $x = L(t)$ is rigid, the boundary velocity at $x' = L_0$ in the deformed space is along the x' axis and is $\partial L(t)/\partial t$. With these transformations we may generate acoustic waves (including shock waves) in systems described in continuous media. This method may be used to investigate anomalous behavior of the bulk viscosity in various fluids and solids with slowly relaxing internal structures.

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Note added in proof—After this paper has been accepted, I have been informed of a similar method of solving the Navier-Stokes equation in the presence of uniform shear.[9,10] I thank Professor S. Toh for showing his work.