Reynolds Number Scaling of Cellular-Automaton Hydrodynamics

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We argue that the computational requirements for presently envisaged cellular-automaton simulations of continuum fluid dynamics are much more severe than for solution of the continuum equations.

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It has recently been suggested[1,2] that cellular automata (CAs) [defined as discretely and locally linked, finite- (and few-) state machines] may be an effective way to compute complex fluid flows. These automata have the advantage that they may be simply and perhaps inexpensively constructed with use of specially designed parallel hardware. With suitable interaction rules, it has been argued,[1,2] the space-time average kinetic behavior of the CA system follows the incompressible Navier-Stokes dynamical equations. While the Navier-Stokes equations for continuum fluids can be calculated efficiently on parallel-architecture machines, it is probably easier to make efficient use of the parallel architecture with CAs. In this Letter, we wish to point out that there are some considerations that require resolution before these methods can be considered to be a viable alternative to traditional continuum mechanical methods for high–Reynolds-number fluid dynamics.

Let us compare the resolution and work requirements for a CA simulation of a high–Reynolds-number flow with those of direct numerical solution of the incompressible Navier-Stokes equations. It is well known[3,4] that, at Reynolds number N_{Re}, the Kolmogorov and Batchelor-Kraichnan theories of three- and two-dimensional equilibrium range dynamics, respectively, predict that the range of excited scales is of order $N_{\mathrm{Re}}^{3/4}$ and $N_{\mathrm{Re}}^{1/2}$ and the computational work required to calculate a significant time in the evolution of large-scale flow structures is of order N_{Re}^{3} and $N_{\mathrm{Re}}^{3/2}$ in three and two dimensions, respectively.

The suggested evolution rules for CAs to reproduce hydrodynamic behavior are based on conservation laws of mass, momentum, and energy. Dissipation is modeled through the thermalization of coherent hydrodynamic modes. Therefore, the lattice resolution of the CA calculation must be much finer than that of the hydrodynamic simulation, the latter requiring the retention of only those degrees of freedom describing motions on scales of the dissipation range or larger. Thus, the lattice spacing a must be smaller than the dissipation scale η in the turbulent fluid.

We now discuss some conditions that CA models should satisfy to describe high–Reynolds-number fluid flows. We present three successively more restrictive arguments that show that η/a must grow rapidly with Reynolds number.

Signal-to-noise ratio.—The hydrodynamic velocity in the CA simulation is calculated by subdividing the computational domain into cells with linear dimensions $\gg a$, averaging over the CAs within a (finite) cell, and smoothing (filtering) the resulting (noisy) velocity field. Thus, the hydrodynamic velocity at a point x is the (space-time) filtered velocity of the CAs in the cell C_x centered at x, $v_H(x)=\langle v(x)\rangle$, where the local velocity in C_x is

$$v(x)=\frac{1}{n}\sum_{i\in C_x} v_i, \tag{1}$$

where n is the number of occupied sites i within the cell. We assume that the possible velocity values at an occupied CA site are $v_i=\pm v_{\mathrm{th}}$ where v_{th} is the constant (thermal) velocity over the CA grid. At low Mach numbers, $v_H \ll v_{\mathrm{th}}$. In this case, the fluctuations in $v(x)$ are of order $n^{-1/2}v_{\mathrm{th}}$. In order that the hydrodynamic velocity found in this way may be a good representation of the continuum hydrodynamics, it is necessary that the noise $n^{-1/2}v_{\mathrm{th}}$ be small compared to the smallest significant hydrodynamic velocity. The smallest significant hydrodynamic velocity is the eddy velocity on scales of order of the dissipation scale η. In three dimensions, $\eta=O((\epsilon/\nu^3)^{-1/4})$ and the eddy velocity on the scale of η is $v_\eta=O((\epsilon\nu)^{1/4})$. Here ν is the viscosity and ϵ is the turbulent energy dissipation rate per unit mass. Thus, we require that the number of CA sites n within a cell of size η be at least

$$n \gg v_{\mathrm{th}}^2/(\epsilon\nu)^{1/2}. \tag{2}$$

Since $\epsilon=O(U^3/L)$ where U is the large-scale rms fluctuating velocity and L is the associated large-scale length of these velocity fluctuations, we find that $n \gg N_{\mathrm{Re}}^{1/2}M^2$, where $N_{\mathrm{Re}}=UL/\nu$ is the Reynolds number and $M=U/v_{\mathrm{th}}$ is the Mach number.[5] Since the number of cells of size η within a three-dimensional turbulent eddy of size L scales as $N_{\mathrm{Re}}^{9/4}$, the overall number of CA sites must increase at least as $N_{\mathrm{Re}}^{11/4}/M^2$.

Since the effective evolution time of the fluid system is L/U, while the time step on the CA lattice is a/v_{th}, it follows that the CA simulation requires at least L/aM steps in time. Since the computational work for each site update is of order 1, it follows that the CA simulation requires at least of order $(N_{Re}/M)^{11/3}$ work.

In summary, the above signal-to-noise considerations suggest the following lower-bound estimates for the computer storage S and work W for CA simulations of high–Reynolds number, low–Mach-number flows (where, for reference, we include the corresponding estimates for the continuum Navier-Stokes equations): for CA (2D),

$$S = N_{Re}^{3/2}/M^2, \quad W = N_{Re}^{9/4}/M^4;$$

for Navier-Stokes (2D),[6]

$$S = N_{Re}, \quad W = N_{Re}^{3/2};$$

for CA (3D),

$$S = N_{Re}^{11/4}/M^2, \quad W = (N_{Re}/M)^{11/3};$$

for Navier-Stokes (3D),[7]

$$S = N_{Re}^{9/4}, \quad W = N_{Re}^3.$$

Upper bound for the Reynolds number.—A more stringent condition on the Reynolds-number dependence of the minimal number of lattice sites in a CA simulation of hydrodynamics is found as follows. If the discrete velocity of the CAs is $\pm v_{th}$ (again, the thermal velocity or sound speed on the CA lattice) and the lattice spacing is a, then the kinematic viscosity ν on the lattice is at least of order va. For the CA to give a self-consistent hydrodynamic simulation, the viscosity determined on the "molecular" level must equal the viscosity governing the dissipation of the hydrodynamic modes. Thus the Reynolds number of the simulated fluid can be at most UL/ν or ML/a. Since the number N of CA sites in the lattice is of order $(L/a)^d$, where d is the dimension of space, we obtain the result that N must be at least of order $(N_{Re}/M)^d$. As above, the CA simulation of the flow requires at least L/aM steps in time. It follows that the CA simulation requires at least of order $(N_{Re}/M)^d$ memory and of order N_{Re}^{d+1}/M^{d+2} work.

These estimates for storage S and work W based on lower bounds for the effective viscosity on the lattice are of order

$$S = (N_{Re}/M)^2, \quad W = N_{Re}^3/M^4$$

for CA (2D),

$$S = N_{Re}, \quad W = N_{Re}^{3/2}$$

for Navier-Stokes (2D);

$$S = (N_{Re}/M)^3, \quad W = N_{Re}^4/M^5$$

for CA (3D);

$$S = N_{Re}^{9/4}, \quad W = N_{Re}^3$$

for Navier-Stokes (3D).

Hydrodynamic fluctuations.—The CA system will yield a self-consistent continuum hydrodynamic description only if the thermal energy fluctuations on hydrodynamic spatial scales are small compared to the energy of the hydrodynamic modes on corresponding length scales. If the "mass" of an occupied CA site is m, its energy is $d/2m v_{th}^2$ in d space dimensions. Then the fluctuation in total thermal energy over a cell with n occupied CAs is $\sqrt{n}\, m v_{th}^2$. (We note that in a CA with velocity states $\pm v_{th}$, energy fluctuations are proportional to density fluctuations.) The corresponding hydrodynamic energy within a cell of size η is $\rho\eta^3 v_H^2$, where v_H is the hydrodynamic velocity and ρ is the hydrodynamic density. In three dimensions, the dissipation scale is η and the associated hydrodynamic velocity is v_η. Also, the relation between m and ρ is $nm = \rho\eta^3$. Thus, for thermal fluctuations to be small, we must require that $n >> N_{Re}/M^4$. In two dimensions, the corresponding result is $n >> N_{Re}^2/M^4$.

This argument shows that the storage and work required for a self-consistent hydrodynamic description using CAs is of order

$$S = N_{Re}^3/M^4, \quad W = N_{Re}^{9/2}/M^7$$

for CA (2D),

$$S = N_{Re}, \quad W = N_{Re}^{3/2}$$

for Navier-Stokes (2D);

$$S = N_{Re}^{13/4}/M^4, \quad W = N_{Re}^{13/3}/M^{19/3}$$

for CA (3D),

$$S = N_{Re}^{9/4}, \quad W = N_{Re}^3$$

for Navier-Stokes (3D).

The CA models approximate fluids that are by their nature necessarily compressible. This means that an equation of state for pressure is needed. However, self-consistency requires that thermodynamic pressure fluctuations over dissipation scales be small. This latter condition leads to results identical to those just obtained by use of energy estimates. Indeed, it is known[8] that the rms thermodynamic pressure fluctuations in a volume η^3 are $(\rho kTc^2/\eta^3)^{1/2}$, where T is the temperature of the fluid and c is the sound speed. But the hydrodynamic pressure fluctuations over length scales of order η are of order $\rho(\epsilon\nu)^{1/2}$. Since $kT = m v_{th}^2$ and $c \approx v_{th}$, the previously given estimates apply.

We believe that these pessimistic estimates for high Reynolds numbers and low Mach numbers must be overcome before CAs can be an effective modeling tool for complex fluid flows. This can, in principle, be

done by averaging over the shortest scales $a << \eta$ in order to reduce the number of degrees of freedom.[9] However, it seems that this renormalization can be useful (in the context of local, few-bit, parallel computations) only if it does not generate nonlocal, complex interactions in the set of basic rules defining CAs. Unfortunately, we do not now understand why this kind of "turbulence transport" modeling should be either easier or more successful on the CA lattice than for the continuum equations or for molecular dynamics.

While the above estimates for CA simulations of turbulence are quite pessimistic, there may be cases in which CA simulations of turbulence may be effective. In a turbulent boundary layer, the local Reynolds number is $O(1)$ in the viscous sublayer and is modest within the buffer layer. A CA model could be effective in these regions in the modeling of turbulent burst formation and evolution. However, this application requires the development of three-dimensional CA models and suitable techniques to match the outer regions of the flow.

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[2]J. Salem and S. Wolfram, to be published.

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[5]Notice that the Mach number is bounded in CA simulations of fluid dynamics. With allowed velocities of $\pm v_{th}$, $M \leq O(1)$, the upper limit being achieved when the CAs exhibit pure streaming, nonhydrodynamic motion.

[6]The Batchelor-Kraichnan theory suggests that there may be logarithmic corrections to these estimates.

[7]Intermittency effects may slightly change these estimates.

[8]L. D. Landau and E. M. Lifschitz, *Fluid Mechanics* (Pergamon, London, 1959), p. 529.

[9]A kind of renormalization using "pseudovertices" is suggested in Ref. 1. The idea is to introduce vertices on subhydrodynamic scales that are not kept track of explicitly. If this idea can be successfully implemented, it would reduce the computational storage requirements given above but apparently not the computational work. We are grateful to C. H. Bennett for this comment.