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On Direct and Adjoint Lattice Boltzmann Equations

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Our communication will be divided into two parts. In the first part, we show that it is possible to formulate the lattice Boltzmann equation with a small time step Δt and an associated space scale Δx. Thus a Taylor expansion establish macroscopic fluid equations as a formal limit. In a second part of our contribution, we summarize recent results obtained conjointly with M. Bouzidi, P. Lallemand and M. Tekitek [1] on data assimilation.

We denote by x a node of the lattice, by θ_j the spatial direction of the neighbour number j, by $x - \Delta x\, \theta_j$ the space location of this neighbour, by $f_j(x, n\, \Delta t)$ the number of particles located at the position x at discrete time $n\Delta t$ and going from position $x - \Delta x\, \theta_j$ towards the position x during one time step. We first have to take into consideration the collision step $f \longmapsto f^* \equiv C(f, \sigma)$. This step is nonlinear, local in space and is parameterized by the choice of the equilibrium state and by the time scales of relaxation (represented here with the notation σ). Then the advection step $f^* \longmapsto A \bullet f^*$ is linear but couples the node x with his neighbours. The lattice Boltzmann equation takes the compact form

$$f_j(x, (n+1)\, \Delta t) = f_j^*(x - \Delta x\, \theta_j\,, n\, \Delta t) \equiv (A \bullet C(f, \sigma))(x\,, n\, \Delta t)\,. \qquad (1)$$

When both Δx and Δt tend towards zero with a fixed "lattice velocity" $\lambda \equiv \frac{\Delta x}{\Delta t}$, we can expand both terms of relation (1) at the first order accuracy and recover the Euler equations of gas dynamics. Then we expand those expressions at the second order of accuracy and recover the Navier-Stokes equations with a new version of the so-called "Chapman-Enskog" discrete expansion. Note that we have not used the classical asumption proposed by D'Humières [2].

We suppose now that we have observed some quantities $\psi(x_k, t)$ at the particular position x_k of the lattice and during all the values t of time, with $0 \leq t \leq T$. We suppose that these quantities are *a priori* equal to a given function $\varphi(\bullet)$ of the variables $f(x_k, t)$. We suppose also that some parameters σ of the lattice Boltzmann equation are free to be ajusted. We wish to minimize the quadratic error between the values $\varphi(f(x_k, t))$ given by the model and the observed values $\psi(x_k, t)$.

We introduce an "error cost function"

$$(2) \qquad J(\sigma) \,\equiv\, \frac{1}{2} \sum_k \sum_{t=0}^{t=T-\Delta t} \mid \varphi(f(x_k,\, t)) \,-\, \psi(x_k,\, t) \mid^2$$

that we wish to minimize under the constraint that the variable f is solution of the lattice Boltzmann dynamics. We use classical methods of optimal control (see *e.g.* [3]) and we introduce the so-called "adjoint state" $p(x,\, t)$ and the Lagrangian function

$$(3) \qquad \mathcal{L} \,\equiv\, J(\sigma) \,+\, \sum_x \sum_{t=0}^{t=T-\Delta t} \big(p(x, t+\Delta t) \,,\, f(x, t+\Delta t) \,-\, (A \bullet C(f,\, \sigma))(x\,,\, t) \big) \,.$$

We choice the dynamics of the adjoint state according to the backward linearized equation also called "adjoint lattice Boltzmann equation" :

$$(4) \qquad p(x,t) \,=\, \mathrm{d}C^{\mathrm{t}} \bullet A^{\mathrm{t}} \bullet p(x, t+\Delta t) \,-\, \sum_k \delta(x - x_k)\, (\varphi(f(x_k,\, t)) \,-\, \psi(x_k,\, t))\, \frac{\partial \varphi}{\partial f}$$

associated with the "terminal condition"

$$(5) \qquad p(x,T) \,=\, 0\,.$$

Thus it is simple to establish that the gradient $\frac{\partial J}{\partial \sigma}$ of the cost function relatively to the parameter σ can be obtained according to te relation

$$(6) \qquad \frac{\partial J}{\partial \sigma} \,=\, - \sum_{t=0}^{t=T-\Delta t} \big(p(x, t+\Delta t) \,,\, A \bullet \frac{\partial C}{\partial \sigma}(f,\, \sigma) \big) \,.$$

A gradient-like algorithm, parameterized by a strictly positive parameter ρ

$$(7) \qquad \sigma^{\mathrm{new}} \,=\, \sigma \,-\, \rho \, \frac{\partial J}{\partial \sigma}$$

allows to fit progressively the unknown parameters. We will present preliminary results for linearized fluid dynamics and a first test case for nonlinear dynamics.

Références

[1] Tekitek M., M. Bouzidi, F. Dubois, P. Lallemand, "Adjoint Lattice Boltzmann Equation for Parameter Identification", to appear, *Computers and Fluids*, 2005.

[2] D'Humières D., "Generalized Lattice-Boltzmann Equations", in *Rarefied Gas Dynamics : Theory and Simulations*, vol. 159 of *AIAA Progress in Astronautics and Astronautics*, p. 450-458, 1992.

[3] Lions J.L., *Contrôle optimal de systèmes gouvernés par des équations aux dérivées partielles*, Dunod, Paris, 1968.

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