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Lattice-Boltzmann / Finite-Difference Hybrid Simulation of Transonic Flow

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A lattice-Boltzmann / finite-difference hybrid method has been developed for transonic flow. In the method, we introduce an interaction force to reduce the speed of sound so that high Mach number flows can be simulated. In this model, the conservation of mass and momentum is represented by a lattice-Boltzmann model while the energy dynamics is described by a finite difference scheme. It has been a challenge problem for a long time to couple between a complete energy equation and a lattice-Boltzmann model. The proposed hybrid scheme has been used to simulate flows past a wedge and flows past an airfoil. The results are consistent with theoretic or experimental results.

I. Introduction

In recent years, the lattice Boltzmann method has been developed as an alternative method of Computational Fluid Dynamics.[1–3] This method originates from kinetic theory[4,5] and has several advantages in modeling micro-flows,[6,7] flows in complex geometries[8,9] and multiphase flows.[10,11] In addition, the explicit and local interaction makes it easy for parallel realizations in large scale simulations. The utilization of lattice-Boltzmann has been focused on incompressible flow since the deviations of the many lattice-Boltzmann model are proportional to the square of Mach numbers. Recently, the effort to recover the Navier-Stokes equations of compressible flow has become successful for flows with medium Mach numbers near one using the Hermite polynomials as the expansion basis.[12–14] In the early development the equilibrium distribution function is chosen to be a small-Mach number expansion containing a few coefficients. This approach has achieved great success for the continuity and momentum equations. The effort of recovering the energy equation[15–17] has met some difficulties due to numerical instability.[18,19] There are some models that aim to simulate Euler equations.[20–22] The two-dimensional Navier-Stokes equations are recovered by the finite difference LB method with a small time step.[22] In this paper we present a lattice-Boltzmann / finite-difference hybrid method that can recover the complete Navier-Stokes equations of supersonic flow. The proposed hybrid model does not significantly altering the conventional lattice-Boltzmann algorithm so that its advantages are reserved.

A lattice Boltzmann equation with the single-relaxation-time (BGK[23]) collision model can be written as:[24,25]

$$f_i(\mathbf{x}+\boldsymbol{\xi}_i\Delta t, t+\Delta t) \quad = \quad f'_i(\mathbf{x},\mathbf{t}) \tag{1}$$

where usually $\Delta t = 1$, and the post-collision distribution function is:

$$f'_i(\mathbf{x},\mathbf{t}) = f_i(\mathbf{x},t) - \frac{1}{\tau}\left[f_i(\mathbf{x},\mathbf{t}) - f_i^{(eq)}(\mathbf{x},\mathbf{t})\right], \tag{2}$$

where $\{\boldsymbol{\xi}_i, i=1,b\}$ are discrete velocities. The equilibrium distribution up to the fifth order of Hermit polynomial is:[13]

$$\begin{aligned}
f_i^{(eq)} &= w_i\rho\{1+\boldsymbol{\xi}_{i\alpha}u_\alpha + \frac{1}{2}[(\boldsymbol{\xi}_{i\alpha}u_{i\alpha})^2 - u^2] + \frac{\theta-1}{2}(\boldsymbol{\xi}_i^2 - D) + \frac{\boldsymbol{\xi}_{i\alpha}u_\alpha}{6}[(\boldsymbol{\xi}_{i\alpha}u_{i\alpha})^2 - 3u^2] \\
&+ \frac{\theta-1}{2}(\boldsymbol{\xi}_{i\alpha}u_\alpha)(\boldsymbol{\xi}_a^2 - D - 2) + \frac{1}{24}[(\boldsymbol{\xi}_{i\alpha}u_\alpha)^4 - 6(\boldsymbol{\xi}_{i\alpha}u_\alpha)^2u^2 + 3u^4] \\
&+ \frac{\theta-1}{4}[(\boldsymbol{\xi}_i^2 - D - 2)((\boldsymbol{\xi}_{i\alpha}u_\alpha)^2 - u^2) - 2(\boldsymbol{\xi}_{i\alpha}u_\alpha)^2] + \frac{(\theta-1)^2}{8}[\boldsymbol{\xi}_a^4 - 2(D+2)\boldsymbol{\xi}_a^2 + D(D+2)]
\end{aligned}$$

$$
\begin{aligned}
&+ \quad \frac{u_\alpha}{120}[(\boldsymbol{\xi}_{i\alpha}u_\alpha)^4 - 10(\boldsymbol{\xi}_{i\alpha}u_\alpha)^2u^2 + 15u^4] + \frac{\theta-1}{12}u_\alpha[(\boldsymbol{\xi}_i^2 - D - 4)((\boldsymbol{\xi}_{i\alpha}u_\alpha)^2 - u^2) - 2(\boldsymbol{\xi}_{i\alpha}u_\alpha)^2] \\
&+ \quad \frac{(\theta-1)^2}{8}u_\alpha[\boldsymbol{\xi}_a^4 - 2(D+2)\boldsymbol{\xi}_a^2 + (D+2)(D+4)]\}. \qquad (3)
\end{aligned}
$$

where the Greek subscripts α denotes the spatial directions in Cartesian coordinates and D is the spatial dimension. In a pure lattice-Boltzmann model, the density ρ, fluid velocity $\boldsymbol{u}$, and temperature θ are determined by the moments of f_i.

$$\rho = m\Sigma_i f_i, \qquad (4)$$

$$\rho\boldsymbol{u} = m\Sigma_i f_i \boldsymbol{\xi}_i. \qquad (5)$$

$$\rho\epsilon = \frac{m}{2}\Sigma_i f_i|\boldsymbol{\xi} - \boldsymbol{u}|^2, \qquad (6)$$

where

$$\rho\epsilon = \frac{d}{2}\theta. \qquad (7)$$

It has been shown that the Navier-Stokes equations including the energy equation for a monatomic gas have been completely recovered[13,14] by the 120-state lattice-Boltzmann model. The 39-state model also recoveres the Navier-Stokes equations except that the heat diffusivity is not Galilean invariant.

The numerical tests show that these updated 39-state and 120-state models are stable for flow with medium Mach numbers that are close to one. However, it also becomes unstable for flows with higher Mach number flows. An approximate criteria for a lattice-Boltzmann model to be stable can be obtained by the positivity of the equilibrium distribution function. Fig. 1 shows the zero points of different orders of equilibrium distribution functions in the constant temperature $\theta = 1$. In the figure, u is the amplitude of the fluid velocity, s is the amplitude of particle velocity and α is the angle between fluid velocity and the particle velocity. The discrete velocities used in the lattice-Boltzmann model are distributed in a subspace of σ near $\sigma = 0$ in many directions. In another word, the angle α can be arbitrary values. The maximum value of discrete velocity varies with models. The higher the order of the equilibrium distribution function is, the larger the maximum value of discrete velocity is. In the 39$-$state model, the maximum amplitude of discrete velocity is $3\sqrt{1.5}$. If the $4th$ order equilibrium distribution function is used, the maximum fluid velocity that makes the equilibrium distribution function positive is about 0.9. From the figure, it also clear that the use of the higher order of the equilibrium distribution function add the positive region very little. Therefore, it is fare to say that the maximum velocity that these lattice-Bolztamnn model can achieve is about $u_{max} = 0.9$. Considering the speed of sound for a monatomic gas is $c_s = \sqrt{5/3} = 1.29$, the maximum Mach number that these lattice-Boltzamnn model can handle is

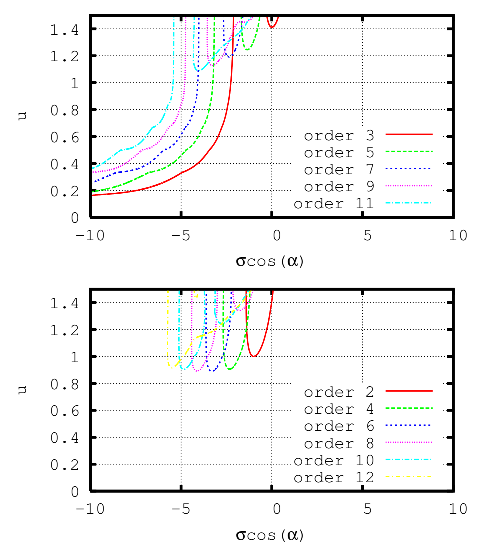

Figure 1. The zero points of different orders of equilibrium distribution functions in the constant temperature $\theta = 1$. The vertical axis is for the amplitude of the fluid velocity, the horizontal axis is for the product of σ and $cos(\alpha)$. Here σ is the amplitude of the particle velocity and α is the angle between the fluid velocity and the particle velocity.

$$Ma_{max} = 0.7. \qquad (8)$$

It is also numerically validated that the up limit of Mach number of the current updated lattice-Boltzamnn model is consistent with the above estimation based on the positivity of the equilibrium distribution.

Since the cap of allowed velocity is fixed, it is nature for one to think about reducing the speed of sound in order to simulate high Mach number flows. It is also well known that an interact force can change the speed of sound which was demonstrated in a lattice-Boltzamnn multiphase model.[26] Unfortunately, an introduced force breaks the conservation of energy in the lattice-Boltzamnn model. A separate energy equation is needed. The hybrid model that using a separate energy equation has been practiced for a long time for incompressible flows.[3] In incompressible flow, it is enough for most applications to use an incomplete energy equation that ignores the work done by pressure compressing fluid and the viscous heating. In order to simulate Mach number flows, a complete energy equation is needed.

How to couple between a complete energy equation and the lattice-Boltzmann model has been an open problem for a long time. The main challenge is to get a stable hybrid scheme without significantly altering the conventional lattice-Boltzmann algorithm so that its advantages are retained. Fortunately, a stable hybrid method has been developed by us. In the following sections the interaction force, the hybrid method and some validations are going to be presented. It worth to point out that such a hybrid scheme also has several other advantages over the pure lattice-Boltzmann method. First, it is easy to include a variable ratio of specific heats. Although this has been realized recently in a pure lattice-Boltzamnn frame by introducing an internal state which needs more memory,[27] the hybrid method still has better computational efficiency. Second, it is easy for the hybrid method to include a variable Prantal number. This was realized for low Mach number flow in a pure lattice-Boltzmann frame by including multi relaxation time.[28] Third, the hybrid method provides a possibility to simulate energy conserving thermodynamic non-ideal gas flows with multiple phases.[29] So far, there is no pure lattice-Boltzamnn multiphase model that conserves the energy.

II. Hybrid Method

II.A. Reduction of Speed of Sound by Interaction Force

In order to reduce the speed of sound, the following interaction force F_g has been introduced to the lattice-Boltzmann model Eqs. (1, 2, 3).

$$\begin{aligned} F_g &= -\bigtriangledown \Psi \\ &= G(|\mathrm{e}_i|)\sum_i \Psi(\mathrm{x}+\mathrm{e}_i)\mathrm{e}_i, \qquad (9) \\ \Psi &= -\frac{g}{2}\rho\theta. \qquad (10) \end{aligned}$$

where the function $G(\cdot)$ decides the accuracy of the derivative and constant g determines the strength of the force. Because of this interaction force, the equation of state changes to

$$\begin{aligned} p &= \rho\theta + \Psi \\ &= \rho R\theta, \qquad (11) \end{aligned}$$

where the gas constant R is decided by g:

$$R = \left(1 - \frac{g}{2}\right) \qquad (12)$$

If a correct energy equation (described in the following section) is included, the speed of sound becomes

$$c_s = \sqrt{\gamma R\theta}, \qquad (13)$$

where γ is the ratio of specific heats. Therefore, the speed of sound can be adjusted by the parameter g.

II.B. Conservation Equation of Energy

A complete conservation equation of energy in terms of temperature θ can be written as:

$$\partial_t\theta + u_\alpha\partial_\alpha\theta = \frac{1}{\rho c_p}\frac{dp}{dt} - \frac{1}{\rho c_p}\partial_\alpha q_\alpha + \frac{\Phi}{\rho c_p}, \qquad (14)$$

where the pressure p and the heat flux $\mathbf{q}$ are

$$\begin{aligned} p &= \rho R\theta, \qquad (15) \\ q_\alpha &= -\rho c_p \kappa \partial_\alpha \theta, \qquad (16) \end{aligned}$$

and the dissipation function Φ, the strain rate tensor $\mathbf{e}$ and the viscous stress tensor τ are

$$\begin{aligned}
\Phi &= e_{\alpha\beta}\tau_{\alpha\beta} \\
&= 2\rho\nu\sum_{\alpha,\beta}(e_{\alpha\beta} - \frac{1}{D}\delta_{\alpha\beta}\partial_\gamma u_\gamma)^2 + \rho\eta(\partial_\gamma u_\gamma)^2,
\end{aligned} \tag{17}$$

$$e_{\alpha\beta} = \frac{1}{2}\partial_\alpha u_\beta + \partial_\beta u_\alpha, \tag{18}$$

$$\tau_{\alpha\beta} = 2\rho\nu(e_{\alpha\beta} - \frac{1}{D}\delta_{\alpha\beta}\partial_\gamma u_\gamma) + \rho\eta\delta_{\alpha\beta}\partial_\gamma u_\gamma. \tag{19}$$

Here c_p is the specific heat at constant pressure and κ is the heat diffusivity. The shear viscosity ν and bulk viscosity η are given by the lattice-Boltzmann equations (see the following section).

It seems that a hybrid modeling can be realized by solving the above energy equation with the lattice-Bolztamnn equation trivially. However, although a great effort has been made, no explicit difference scheme of the above equation has been found to result in stable solutions when it is coupled with the lattice-Boltzmann model. Fortunately, it is found by us that much better stability can be achieved by solving the equation of the entropy. It can be derived from Eq.(14) the entropy S satisfies the following equation:

$$\partial_t S + u_\alpha\partial_\alpha S = -\frac{1}{\rho\theta}\partial_\alpha q_\alpha + \frac{\Phi}{\rho\theta}. \tag{20}$$

Here the entropy S is defined by the density and the temperature

$$S = c_v ln\left(\frac{\theta}{\rho^{\gamma-1}}\right). \tag{21}$$

where c_v is the specific heat at constant volume. The differential equation of S, Eq. 20, has been solved in several different deference schemes that depend on different treatments of the convection term which including the Lax-Wendroff scheme, the upwind scheme, the upwind-central Mixing Scheme. These different deference schemes gives almost the same results for several test simulations. The results in the following numerical simulations are presented for the Lax-Wendroff scheme.

II.C. Conservation Equations of Density and Momentum

The conservation equations of density and momentum have been derived using Chapman-Enskog expansion from the lattice-Boltzamnn equation Eq. (1, 2, 3) and the conservation equation of energy Eq. (20). They completely recover the density and momentum equation of a polyatomic gas:

$$\partial_t\rho + \partial_\alpha(\rho u_\alpha) = 0, \tag{22}$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) + \partial_\beta P_{\alpha\beta} = 0, \tag{23}$$

where the pressure tensor

$$P_{\alpha\beta} = p\delta_{\alpha\beta} - \tau_{\alpha\beta}. \tag{24}$$

The shear viscosity ν and the bulk viscosity η are given by:

$$\nu = \left(\tau - \frac{1}{2}\right)\theta\Delta t, \tag{25}$$

$$\eta = \frac{2S\nu}{D(D+S)}. \tag{26}$$

II.D. Fractional Lattice-Boltzmann Scheme and Modified $5th$ Order Equilibrium Distribution Function

The hybrid method is stable for integer and fractional lattice-Boltzamnn schemes although it is more stable with the fractional version. The fractional model[30] also avoids the non neighboring particle convection caused by the 39-states model that employs discrete velocities with several speeds. The following results are obtained using a fractional version of the 39-state model.

A modified $5th$ order equilibrium distribution function is constructed by $4th$ order plus 0.722 times $5th$ order term of the hermit polynomial expansion of the equilibrium distribution function. This modified $5th$ order equilibrium distribution function is positive for fluid velocity $u < 1.2$ when 39-state model is used. The original $5th$ order distribution needs $u < 0.9$ to have positivity. In the following of this report, the $5th$ order equilibrium distribution refers this modified one and this modified $5th$ order equilibrium distribution function is usually employed except otherwise indicated.

II.E. Simulation of Sound Wave

The simulations of sound wave have been used to test the speed of sound, the decay rate of the sound wave and the Galilean invariance of the hybrid model. The waves propagating in x-direction and then in diagonal direction have been simulated. The speed of sound is very well predicted by the hybrid model and is Galilean invariant for parameters $g = 0$ to 1.8, $\nu = 0.5$ to 0.05 and $u_0 \leq 1.2$. The decay rate is well predicated and is Galilean invariant in the smaller parameter space $g = 0$ to 1.8, $\nu = 0.5$ to 0.05 and $u_0 \leq 1.0$ when $4th$ order equilibrium distribution function is used. The $5th$ order equilibrium distribution may result in a velocity-dependent decay rate. The $5th$ order improves the stability of the hybrid model for high velocity closed to 1.2.

II.F. Artificial Viscosity and Simulation of Sod Solution

It is well known that an artificial viscosity is needed when the shock wave is designed to be captured automatically by a difference scheme. It is also well know that a conservation form of differential equation should be solved to get better solutions across shock waves. Here, the equation of entropy is chosen to be solved because it forms a stable hybrid scheme combined with the lattice-Boltzmann equations although it is not a conservation form equation. Since it is not a conservation form, the artificial viscosity is more important in order to get a correct jump of entropy across a shock. In another word, the bigger viscosity is needed to make the shock more smooth. In order to add an artificial bulk viscosity, the following viscous heating term needs to be added to the energy equation:

$$\Phi = \rho\eta_{art}(\partial_\gamma u_\gamma)^2 \tag{27}$$

and the following viscous force needs to be added to the lattice-Boltzmann equation:

$$F_{diss,\alpha} = \partial_\alpha[\rho\eta_{art}\partial_\gamma u_\gamma(\mathbf{x}, t)]. \tag{28}$$

Here an artificial viscosity that is proportional to the pressure gradient has been chosen

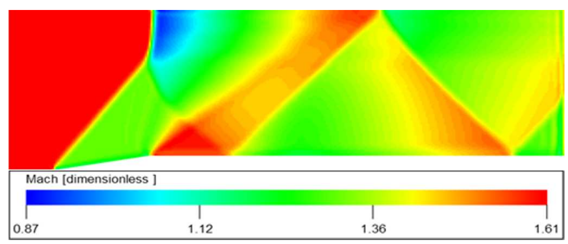

Figure 2. Distributions of pressure for Mach 1.8 flow past a 15° wedge. Here $\gamma = 1.4$, $\nu = 0.0054$, $Pr = 0.667$, $R = 0.25$. The simulation employs 300x100 grids. The size of each grid is $\Delta x = r$.

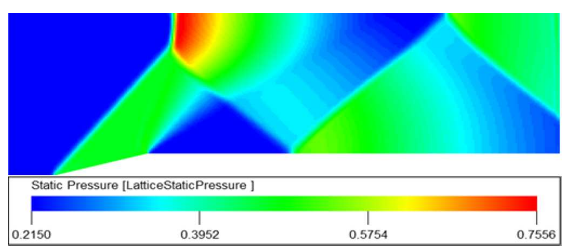

Figure 3. Mach number profile for Mach 1.6 flow past a 10° wedge. Here $\gamma = 1.4$, $\nu = 0.0054$, $Pr = 0.667$, $R = 0.16$. The simulation employs 300x100 grids. The size of each grid is $\Delta x = r$.

$$\eta_{art} \quad = \quad a_1(R, \gamma)\rho\sum_{i=1}^{d}\frac{|p_{i+1} - p_{i-1}|}{p_{i+1} + p_{i-1}}, \tag{29}$$

where the value of coefficient function $a_1(R, \gamma)$ depends on the accuracy requirement. Generally speaking, the bigger the a_1 is, the better accuracy the solution gets. The function $a_1(R, \gamma)$ has been determined by requiring that the numerical results has about 5% accuracy. In the process to find $a_1(R, \Gamma)$, it has been assumed that

$$a_1(R, \gamma) = a_2(\gamma)a_3(R) \tag{30}$$

Here $a_2(\gamma)$ is determined by a series of numerical simulations of Sod solution with $R = 0.25$ and different γ.

$$a_2(\gamma) = (1 + 0.155s), \tag{31}$$

where s is the internal degree of molecule:

$$s = \frac{2}{\gamma - 1} - D. \tag{32}$$

Then $a_3(R)$ is determined by a series of numerical simulations of Sod solution with $\gamma = 1.4$ and different R.

$$a_3(\gamma) = -0.94 + 61.1R - 88.3R^{1.5} + 36R^2. \tag{33}$$

III. Simulation of Flow Past A Forward Facing Step

The hybrid method has been used to simulate the flow past a wedge in a two dimensional wind tunnel or a channel. The channel width is 1 length unit and the length is 3 times of the width. The step is placed in the bottom-right corner of the channel. The wedge is placed between 0.25 and 0.75 length units from the inlet. The incoming flow is uniform and unidirectional flow with certain Mach number and fixed temperature $\theta_0 = 1$ and density $\rho_0 = 1$. The spectacle boundary condition is applied to all wall boundaries. This boundary condition represents a frictionless and adiabatic wall. The fluid is a perfect gas with $\gamma = 1.4$. Initially the channel is filled with the perfect gas with the the incoming Mach number, density 1, temperature 1. Figure 2 presents the pressure distribution for Mach 1.8 flow past a 15° wedge. The inclined shock and its interaction with walls are nicely captured. The angle between the shock and the bottom wall has been determined from the numerical results as 51°. It is consistent with the theoretic value 51.4°.[31] Figure 3 is for Mach 1.6 flow past a 10° wedge. The angle obtained from numerical results is 53.5° which is close to the theoretic value 51.5°. The hybrid method also has been used to simulate Mach 3 flow past a forward facing step in a two dimensional wind tunnel.[32,33] The results are close to the one obtained by a kinetic scheme.[33]

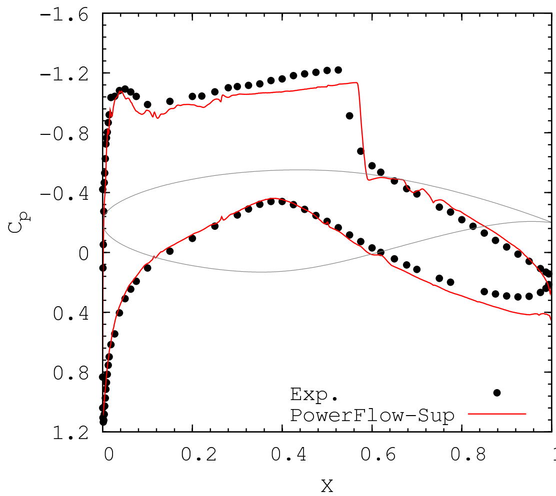

Figure 4. Pressure coefficients on the airfoil. The coordinate is normalized by the chord C of the airfoil.

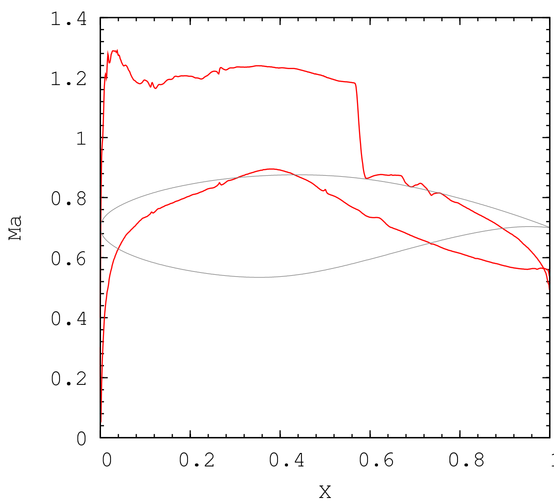

Figure 5. Mach number profile on the airfoil. The coordinate is normalized by the chord C of the airfoil.

IV. Simulation of RAE 2822 transonic airfoil

We studied the transonic flow around a RAE 2822.[34] The incoming flow is an uniform flow with Mach number 7.29. The angle of attack is 2.31. The frictionless and adiabatic wall boundary conditions are used to simulate the high Reynolds number flow. In our simulation the Reynolds number $Re = 10^5$ and no turbulent model is employed. In the experiments the $Re = 6.5 \times 10^6$ and flow is turbulent. In figure 4 the pressure coefficients obtained from the hybrid simulation are plotted against the experimental data.[35] The agreement between two results indicates the treatment of boundary is a good approximation for such kind of unseparated high Reynolds number flow. A variable grids have employed in the simulation. The finest grids are around the surface of the airfoil. In this simulation, 768 cells has been used across the chord.

Figure 5 plots the Mach number profile on the surface of the airfoil. It is evident both high supersonic and subsonic flows are both present. Figure 6 shows the contours of pressure. The shock wave can be well identified by the dense contours.

V. Conclusion

The proposed lattice-Boltzamnn / finite-difference hybrid method recovers the the complete Navier-Stokes equations of a compressible thermal gas with an adjustable speed of sound. The adjustable sound of speed is realized by adding an interaction force to the lattice-Bolzmann equation. The introduced force breaks conservation of energy in the lattice-Boltzamnn model. The conservation of energy is recovered by a separate differential energy equation. It is found that numerically solving an energy equation in terms of entropy results in much better stability. The supersonic flow past a wedge in a two dimension wind tunnel and transonic flow past a RAE 2822 airfoil have been correctly simulated by the proposed hybrid method.

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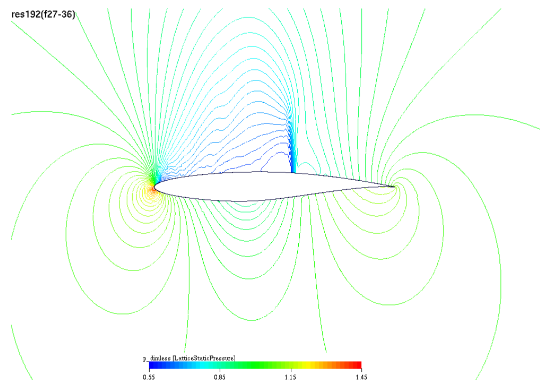

Figure 6. The pressure contours for the RAE 2822 transonic flow. The pressure is normalized by the far filed pressure.

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