Euler-characteristic boundary conditions for lattice Boltzmann methods

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Outline

1. Introduction

2. Euler-characteristic boundary conditions for LB

3. Results

4. Conclusions
# Table of contents

1. Introduction

2. Euler-characteristic boundary conditions for LB

3. Results

4. Conclusions
Motivation: open boundaries

- Open boundary conditions (constant pressure, far-field environment)
- Non-reflecting open boundaries
Motivation: examples

- **Microcantilever**: fluid-structure interaction where small pressure perturbations modify the behavior.
- **Industrial boiler**: flames generate pressure waves which have influence on the combustion.
Review of solutions

- Zero-gradient boundary conditions at outlet (Incompressible!?)
  - [Yu et al. (2005)]
  - [Yang’s Thesis (2007)]

- Non-reflecting boundary conditions (thermodynamical consistency?)
  - Absorbing layers [Ricot et al. (2008), Tekitek et al. (2008), da Silva (2007)]
  - Characteristic BC [Kam et al. (2007), Dehee (2008)] (without details of the implementation)
Table of contents

1 Introduction

2 Euler-characteristic boundary conditions for LB

3 Results

4 Conclusions
Lattice Boltzmann method

LBM with **MRT** collision operator

\[ f(x_i + e_i \delta t, t + \delta t) - f(x_i, t) = -M^{-1} S [m(x_i, t) - m^{eq}(x_i, t)] \]

**Transformation matrix** \( D2Q9 \)

\[
\begin{pmatrix}
\rho \\
e \\
\epsilon \\
jx \\
qx \\
jy \\
qy \\
p_{xx} \\
p_{xy}
\end{pmatrix}
= \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 \\
4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 \\
0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 \\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 \\
0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 \\
\end{pmatrix}
\begin{pmatrix}
f_0 \\
f_1 \\
f_2 \\
f_3 \\
f_4 \\
f_5 \\
f_6 \\
f_7 \\
f_8
\end{pmatrix}
\]

**Relaxation matrix**

- **MRT**: \( S = diag(0, s_e, s_\epsilon, 0, s_q, 0, s_q, s_\nu, s_\nu) \) → related to transport properties
- **SRT**: \( \tau = 1/s_\nu \rightarrow \) viscosity (and stability)
- **TRT**: \( s_\nu = s_e = s_\epsilon, s_q \)
UBB – velocity bounce-back

**APPROACH:** reflection rule + Dirichlet BC (+ correction)

\[
f_{\alpha}(x_f, t + 1) = \tilde{f}_{\alpha}(x_f, t) - 2f_{\alpha}^{eq^-}(x_b, \hat{t})
\]

where:

\[
f_{\alpha}^{eq^-} = \omega_{\alpha} \rho_0 c_s^{-2} (e_\alpha \cdot u)
\]

is the anti-symmetric part of the \( f_{\alpha}^{eq} \)
**PAB – pressure anti-bounce-back**

**APPROACH: reflection rule + Dirichlet BC + correction**

\[ f_\alpha(x_f, t + 1) = -\tilde{f}_\alpha(x_f, t) + 2f^{eq+}_\alpha(x_b, \hat{t}) + (2 - s_v) (f^+_\alpha(x_f, t) - f^{eq+}_\alpha(x_f, t)) \]

where:

\[ f^{eq+}_\alpha = \omega_\alpha \rho + \frac{1}{2} \omega_\alpha \rho_0 c_s^{-4} [(e_\alpha \cdot u)^2 - c_s^2 (u \cdot u)] \]

\[ f^+_\alpha = \frac{1}{2} (f_\alpha + f_\bar{\alpha}) \]

are the symmetric part of \( f^{eq}_\alpha \) and \( f_\alpha \).
Objective

To find the \( \rho \) or \( u_i \) to set the Dirichlet boundary condition in the open boundary, extracting the pressure-wave reflection component. Based on [Poinsot and Lelle (1992)]

Solving in the boundary the 2D Euler equations in \( x \)-direction:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} &= 0 \\
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} &= 0 \\
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} &= 0 \\
\frac{\partial \rho E}{\partial t} + \frac{\partial [u(\rho E + p)]}{\partial x} &= 0
\end{align*}
\]

Eigenvalues!
LODI with wave amplitudes

Wave amplitudes: (isothermal! → \( p = c_s^2 \rho \))

\[
L = \begin{pmatrix}
L_1 \\
L_2 \\
L_3 \\
L_4 \\
\end{pmatrix}
= \begin{pmatrix}
(u - c_s) \left( \frac{\partial p}{\partial x} - \rho c_s \frac{\partial u}{\partial x} \right) \\
u \frac{\partial v}{\partial x} \\
u \left( c_s^2 \frac{\partial p}{\partial x} - \frac{\partial p}{\partial x} \right) \\
(u + c_s) \left( \frac{\partial p}{\partial x} + \rho c_s \frac{\partial u}{\partial x} \right)
\end{pmatrix}
\]

LODI equation using L (without the energy equation):

\[
\frac{\partial \rho}{\partial t} + \frac{1}{2c_s^2} (L_4 + L_1) + \frac{1}{c_s^2} L_3 = 0
\]

\[
\frac{\partial u}{\partial t} + \frac{1}{2\rho c_s} (L_4 - L_1) = 0
\]

\[
\frac{\partial v}{\partial t} + L_2 = 0
\]
Equilibrium distribution functions

Modified $m_{\alpha}^{eq}$ at the boundary: ($\kappa \rightarrow$ heat capacity ratio)

\[
e^{eq} = -2(2 - \kappa)\rho + \rho_0(u^2 + v^2)
\]
\[
e^{eq} = \rho + \rho_0(u^2 + v^2)
\]
\[
q_x^{eq} = -\rho_0u
\]
\[
q_y^{eq} = -\rho_0v
\]
\[
p_{xx}^{eq} = \rho_0(u^2 - v^2)
\]
\[
p_{xy}^{eq} = \rho_0uv
\]

In the continuum limit:

- Speed of sound $\rightarrow c_s = \sqrt{\kappa RT} = \sqrt{\frac{\kappa}{\rho}}$
- Viscosity $\rightarrow \nu = \frac{1}{3} \left( \frac{1}{s_v} - \frac{1}{2} \right)$
- Bulk viscosity $\rightarrow \zeta = \frac{2-\kappa}{6} \left( \frac{1}{s_e} - \frac{1}{2} \right)$
Implementation

Approach: UBB or PAB with computed $\rho$ and $u_i$ from LODI

LODI discretization (OUTLET–PAB)

\[
\rho(\hat{t}) \approx \rho(\hat{t} - 1) - \frac{\delta t}{2c_s^2} (L_4(\hat{t} - 1) + L_1(\hat{t} - 1)) - \frac{1}{c_s^2} L_3(\hat{t} - 1)
\]

\[
u(\hat{t}) \approx \nu(\hat{t} - 1) - \frac{\delta t}{2\rho c_s} (L_4(\hat{t} - 1) - L_1(\hat{t} - 1))
\]

\[
v(\hat{t}) \approx v(\hat{t} - 1) - \delta t L_2(\hat{t} - 1)
\]

Models for $L_{\text{in}}$

\[
L_1(x_b, \hat{t} - 1) = k_1 (p(x_b, \hat{t} - 1) - p_b)
\]

where:

\[
k_1 = \sigma_1 (1 - Ma^2) \frac{c_s}{L}
\]
Table of contents

1 Introduction

2 Euler-characteristic boundary conditions for LB

3 Results

4 Conclusions
Results I: 1D wave

(a) equilibrium distribution functions
(b) inlet: UBB; outlet: PAB
(c) characteristic boundary conditions (CBC)
(d) CBC with corrections
Results II: reflection ratio

- Evaluate performance of two parameters:
  - bulk viscosity in the fluid domain ($s_e$)
  - heat capacity ratio in the boundary ($\kappa$)
Laminar channel

CBC: (i) avoids pressure reflection + (ii) allows mass conservation (well-posedness of BC)
Results IV: unsteady simulation

- Flow around a square cylinder
- UBB-PAB: resonance has effects on the solution
- CBC is the solution
Results IV: unsteady simulation

**UBB-PAB**

- Time steps: 25000, 50000, 75000, 100000
- Cd

- Frequency
- FFT(Cd)

**CBC**

- Time steps: 93000, 96000, 99000
- Cd

- Frequency
- FFT(Cd)
# Table of contents

1. Introduction

2. Euler-characteristic boundary conditions for LB

3. Results

4. Conclusions
Conclusions

- No previous implementation description of CBC for LB (isothermal)
- Characteristic boundary conditions:
  - Presented for 2D open boundaries with Dirichlet conditions
  - Direct application for: 3D, walls and Neumann conditions
  - Reduction of the interaction up to 99%

- Key points:
  1. NSCBC by Poinset and Lele (1992)
Bibliography