

6. Appendix

6.1 Boolean algebra

George Boole (1815 - 1864), English mathematician. Boolean algebra is a mathematical structure $\mathcal{B} = (B, \cup, \cap, \neg)$ consisting of a set B and two binary operations called *union* (\cup) and *intersection* (\cap) and one unitary operation called *complementation* (\neg). The system which originally inspired this collection of laws is the algebra of sets with the familiar operations of set union and intersection.

The following relations¹ hold true:

1. Closure:

- (i) The union of two elements in B yields a unique element in B .
 $a, b \in B \rightarrow (a \cup b) \in B$
- (ii) The intersection of two elements in B yields a unique element in B .
 $a, b \in B \rightarrow (a \cap b) \in B$

2. Commutativity: $\forall a, b \in B$:

- (i) $a \cup b = b \cup a$
- (ii) $a \cap b = b \cap a$

3. Associativity: $\forall a, b, c \in B$:

- (i) $(a \cup b) \cup c = a \cup (b \cup c)$
- (ii) $(a \cap b) \cap c = a \cap (b \cap c)$

4. Distributivity: $\forall a, b, c \in B$:

- (i) $a \cap (b \cup c) = (a \cap b) \cup (a \cap c)$
- (ii) $a \cup (b \cap c) = (a \cup b) \cap (a \cup c)$

5. The idempotent laws: $\forall a \in B$

- (i) $a \cup a = a$
- (ii) $a \cap a = a$

6. Identity elements 0 and 1:

- (i) In B there is the unique element 0 with the following properties:
 $a \cup 0 = a$ and $a \cap 0 = 0 \forall a \in B$.
 0 is the identity element with respect to union.
- (ii) In B there is the unique element 1 with the following properties:
 $a \cup 1 = 1$ and $a \cap 1 = a \forall a \in B$.
 1 is the identity element with respect to intersection.

Remark: If you consider the ordinary union and intersection of sets the 0-element corresponds to the empty set and the 1-element corresponds to the whole set.

¹ We do not speak of axioms because some of relations are redundant.

7. Complementation: $\forall a \in B$ there exists a unique element \bar{a} such that

$$(i) \quad a \cup \bar{a} = 1$$

$$(ii) \quad a \cap \bar{a} = 0.$$

\bar{a} is called the *complement* of a . The elements $a, b \in B$ obey the DeMorgan laws:

$$(iii) \quad \overline{a \cup b} = \bar{a} \cap \bar{b}$$

$$(iv) \quad \overline{a \cap b} = \bar{a} \cup \bar{b}$$

Law of involution: $\forall a \in B$

$$(v) \quad \overline{\bar{a}} = a$$

Principle of duality: The substitution

$$(\cup, \cap, 0, 1) \rightarrow (\cap, \cup, 1, 0)$$

transforms true expressions of the Boolean algebra into true expressions.

Proof: All laws listed above obey the principle of duality. Law 7(v) is selfdual.

Exercise 6.1.1. ()**

Show that the structure

$$\mathcal{B}_{tf} = (B = \{true, false\}, AND, (inclusive)OR, NOT)$$

defines a Boolean algebra. Show that *XOR* can be expressed in terms of *AND*, *OR* and *NOT*. Why is

$$\mathcal{N} = (B = \{true, false\}, AND, XOR, NOT) (XOR = \text{exclusive or})$$

not a Boolean algebra?

Exercise 6.1.2. (*)

Consider the set $B = \{0, 1 \in \mathbb{N}\}$ and the operations addition modulo 2 (+) and multiplication (\cdot). Show: this structure obeys the laws of Boolean algebra if complementation is appropriately defined (how?).

Exercise 6.1.3. ()**

Prove that for all elements a and b in the set B of a Boolean algebra $(B, \cup, \cap, \bar{\cdot})$:

$$(a \cap b) \cup (a \cap \bar{b}) = a$$

Exercise 6.1.4. (*)

Consider the set of integers and the operations addition (+) and multiplication (\cdot). Show that this structure is not a Boolean algebra.

6.2 FHP: After some algebra one finds ...

In this appendix the Lagrange multipliers of the equilibrium distributions for the FHP-I and the HPP model will be calculated (compare Subsection 3.2.5). For vanishing flow velocity the occupation numbers equal each other

$$\mathbf{u} = 0 \implies N_i = \frac{\rho}{b} = d \quad (6.2.1)$$

(b number of cells per node, $b = 6$ for FHP-I, $b = 4$ for HPP; d density per cell) and therefore

$$N_i(\rho, \mathbf{0}) = \frac{1}{1 + \exp[h(\rho, \mathbf{0})]} = d \quad (6.2.2)$$

and

$$\mathbf{q}(\rho, \mathbf{0}) = 0. \quad (6.2.3)$$

Because of invariance of the occupation numbers under the parity transform

$$\mathbf{u} \rightarrow -\mathbf{u}, \quad \mathbf{c}_i \rightarrow -\mathbf{c}_i \quad (6.2.4)$$

it follows that

$$h(\rho, -\mathbf{u}) = h(\rho, \mathbf{u}), \quad (6.2.5)$$

and

$$\mathbf{q}(\rho, -\mathbf{u}) = -\mathbf{q}(\rho, \mathbf{u}). \quad (6.2.6)$$

The Lagrange multipliers h and \mathbf{q} will be expanded up to second order in \mathbf{u} :

$$h(\rho, \mathbf{u}) = h_0(\rho) + h_2(\rho)\mathbf{u}^2 + \mathcal{O}(\mathbf{u}^4) \quad (6.2.7)$$

$$\mathbf{q}(\rho, \mathbf{u}) = q_1(\rho)\mathbf{u} + \mathcal{O}(\mathbf{u}^3). \quad (6.2.8)$$

All other low order terms vanish because of the parity constraints. It is remarkable that h_2 and q_1 are scalars instead of tensors of rank 2. This fact is a consequence of the isotropy of lattice tensors (compare Section 3.3) of rank 2.

The expansions (6.2.7) and (6.2.8) will be inserted into the Fermi-Dirac distribution (3.2.28). Then the distribution is expanded in a Taylor series with respect to \mathbf{u} at $\mathbf{u} = 0$ up to second order.

$$\begin{aligned} N_i(\mathbf{u}) &= N_i(\mathbf{u} = \mathbf{0}) + \frac{\partial N_i}{\partial u} \cdot \mathbf{u} + \frac{\partial N_i}{\partial v} \cdot v \\ &\quad + \frac{1}{2} \frac{\partial^2 N_i}{\partial u^2} \cdot \mathbf{u}^2 + \frac{\partial^2 N_i}{\partial u \partial v} \cdot \mathbf{u} \cdot v + \frac{1}{2} \frac{\partial^2 N_i}{\partial v^2} \cdot v^2 + \mathcal{O}(\mathbf{u}^3), \end{aligned}$$

$$\begin{aligned}
N_i(\mathbf{u}) &= \frac{1}{1 + \exp[x(\mathbf{u})]}, \\
x(\mathbf{u}) &= h_0 + h_2 \mathbf{u}^2 + q_1 \mathbf{u} c_i, \\
x(\mathbf{0}) &= h_0, \\
N_i(h_0) &= \frac{1}{(1 + \exp[h_0])} = d,
\end{aligned}$$

→

$$\begin{aligned}
\exp[h_0] &= \frac{1-d}{d}, \\
h_0 &= \ln \frac{1-d}{d} \\
\frac{\partial N_i}{\partial u_\alpha} &= \frac{\partial N_i}{\partial x} \cdot \frac{\partial x}{\partial u_\alpha} \xrightarrow[\mathbf{u}=0]{} d(d-1)q_1 c_{i\alpha}, \\
\frac{\partial N_i}{\partial x} &= -\frac{\exp[x]}{(1 + \exp[x])^2} \xrightarrow[\mathbf{u}=0]{} \frac{d-1}{d} d^2 = d(d-1) \\
\frac{\partial x}{\partial u_\alpha} &= 2h_2 u_\alpha + q_1 c_{i\alpha} \rightarrow q_1 c_{i\alpha}, \\
\frac{\partial^2 N_i}{\partial u_\alpha^2} &= \frac{\partial}{\partial u_\alpha} \left[\frac{\partial N_i}{\partial x} \cdot \frac{\partial x}{\partial u_\alpha} \right] \\
&= \frac{\partial^2 N_i}{\partial x \partial u_\alpha} \cdot \frac{\partial x}{\partial u_\alpha} + \frac{\partial N_i}{\partial x} \cdot \frac{\partial^2 x}{\partial u_\alpha^2} \\
&= \frac{\partial^2 N_i}{\partial x^2} \cdot \left(\frac{\partial x}{\partial u_\alpha} \right)^2 + \frac{\partial N_i}{\partial x} \frac{\partial^2 x}{\partial u_\alpha^2} \\
&\rightarrow d(d-1)(2d-1)q_1^2 c_{i\alpha}^2 + d(d-1)2h_2, \\
\frac{\partial^2 N_i}{\partial x^2} &= -\frac{\exp[x](1 + \exp[x])^2 - \exp[x] \cdot 2(1 + \exp[x]) \exp[x]}{(1 + \exp[x])^4} \\
&= \frac{\exp[x](\exp[x] - 1)}{(1 + \exp[x])^3} \\
&\rightarrow \frac{1-d}{d} \left(\frac{1-d}{d} - 1 \right) d^3 = d(d-1)(2d-1), \\
\frac{\partial^2 x}{\partial u_\alpha^2} &= 2h_2.
\end{aligned}$$

For $\alpha \neq \beta$:

$$\begin{aligned}
\frac{\partial^2 N_i}{\partial u_\alpha \partial u_\beta} &= \frac{\partial}{\partial u_\beta} \left[\frac{\partial N_i}{\partial x} \cdot \frac{\partial x}{\partial u_\alpha} \right] \\
&= \frac{\partial^2 N_i}{\partial x \partial u_\beta} \cdot \frac{\partial x}{\partial u_\alpha} + \frac{\partial N_i}{\partial x} \cdot \frac{\partial^2 x}{\partial u_\alpha \partial u_\beta}
\end{aligned}$$

$$\begin{aligned}
&= \frac{\partial^2 N_i}{\partial x^2} \cdot \frac{\partial x}{\partial u_\alpha} \cdot \frac{\partial x}{\partial u_\beta} + \frac{\partial N_i}{\partial x} \cdot \frac{\partial^2 x}{\partial u_\alpha \partial u_\beta} \\
&\rightarrow d(d-1)(2d-1)q_1^2 c_{i\alpha} c_{i\beta}, \\
\frac{\partial^2 x}{\partial u_\alpha \partial u_\beta} &= 0,
\end{aligned}$$

$$\begin{aligned}
N_i(\mathbf{u}) &= d + d(d-1)q_1 \mathbf{c}_i \cdot \mathbf{u} \\
&+ \frac{1}{2}d(d-1)(2d-1)q_1^2 c_{i\alpha}^2 u_\alpha^2 + d(d-1)h_2 \mathbf{u}^2. \quad (6.2.9)
\end{aligned}$$

At this point the coefficients h_2 and q_1 are not known yet. The expression for N_i , however, looks much simpler now: a polynomial instead of a rational function with an exponential function in the denominator. Next insert the N_i according to eq. (6.2.9) into the definitions of mass and momentum density and use the moments relations (3.2.3 - 3.2.5):

$$\begin{aligned}
\rho &= \sum_i N_i \\
&= \underbrace{\sum_i d}_{=\rho} + \underbrace{\sum_i d(d-1)q_1 \mathbf{c}_i \cdot \mathbf{u}}_{=0} \\
&+ \underbrace{\sum_i \frac{1}{2}d(d-1)(2d-1)q_1^2 c_{i\alpha}^2 u_\alpha^2}_{=\frac{1}{2}3d(d-1)(2d-1)q_1^2 \mathbf{u}^2} \\
&+ \underbrace{\sum_i d(d-1)h_2 \mathbf{u}^2}_{=6d(d-1)h_2 \mathbf{u}^2}.
\end{aligned}$$

From this a relation between h_2 and q_1 follows:

$$\begin{aligned}
h_2 &= \frac{1}{4}(1-2d)q_1^2, \\
\rho \mathbf{u} &= \sum_i N_i \mathbf{c}_i \\
&= \underbrace{\sum_i d \mathbf{c}_i}_{=0} + \underbrace{\sum_i d(d-1)q_1 (\mathbf{c}_i \cdot \mathbf{u}) \mathbf{c}_i}_{=3d(d-1)q_1 \mathbf{u}}
\end{aligned}$$

$$\begin{aligned}
& + \underbrace{\sum_i \frac{1}{2} d(d-1)(2d-1) q_1^2 c_{i\alpha}^2 u_\alpha^2 \mathbf{c}_i}_{=0} \\
& + \underbrace{\sum_i d(d-1) h_2 \mathbf{u}^2 \mathbf{c}_i}_{=0},
\end{aligned}$$

$$\begin{aligned}
q_1 &= \frac{2}{d-1}, \\
h_2 &= \frac{1-2d}{(d-1)^2}, \\
N_i(\mathbf{u}) &= d + 2d \mathbf{c}_i \cdot \mathbf{u} + 2d \frac{1-2d}{1-d} c_{i\alpha}^2 u_\alpha^2 - d \frac{1-2d}{1-d} \mathbf{u}^2 \\
&= \frac{\rho}{6} + \frac{\rho}{3} \mathbf{c}_i \cdot \mathbf{u} + \rho G(\rho) Q_{i\alpha\beta} u_\alpha u_\beta,
\end{aligned}$$

with

$$G(\rho) = \frac{1}{3} \frac{6-2\rho}{6-\rho} \quad \text{and} \quad Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - \frac{1}{2} \delta_{\alpha\beta}.$$

6.3 Coding of the collision operator of FHP-II and FHP-III in C

```

/* collision with 1 rest particle (FHP-II) 17.5.89 dwg */

for(ix=0; ix < IXM; ix++) {
for(iy=0; iy < IYM; iy++) {

/* i's -> register a,...,f */

    a = i1[ix][iy];
    b = i2[ix][iy];
    c = i3[ix][iy];
    d = i4[ix][iy];
    e = i5[ix][iy];
    f = i6[ix][iy];
    r = rest[ix][iy];

/* three body collision <-> 0,1 (bits) alternating
   <-> triple = 1 */

    triple = (a^b)&(b^c)&(c^d)&(d^e)&(e^f);

/* two-body collision
   <-> particles in cells a (b,c) and d (e,f)
       no particles in other cells
   <-> db1 (db2,db3) = 1 */

    db1 = (a&d&~(b|c|e|f));
    db2 = (b&e&~(a|c|d|f));
    db3 = (c&f&~(a|b|d|e));

/* rest particle and 1 particle */

    ra = (r&a&~(b|c|d|e|f));
    rb = (r&b&~(a|c|d|e|f));
    rc = (r&c&~(a|b|d|e|f));
    rd = (r&d&~(a|b|c|e|f));
    re = (r&e&~(a|b|c|d|f));
    rf = (r&f&~(a|b|c|d|e));

/* no rest particle and 2 particles (i,i+2) */

```



```

ra2 = (f&b&~(r|a|c|d|e));
rb2 = (a&c&~(r|b|d|e|f));
rc2 = (b&d&~(r|a|c|e|f));
rd2 = (c&e&~(r|a|b|d|f));
re2 = (d&f&~(r|a|b|c|e));
rf2 = (e&a&~(r|b|c|d|f));

/* change a and d
   <-> three-body collision triple=1
       or two-body collision db1=1
       or two-body collision db2=1 and eps=1   (- rotation)
       or two-body collision db3=1 and noeps=1 (+ rotation)
   <-> chad=1                                     */

eps = irn[ix][iy];          /* random bits */
noeps = ~eps;

cha=(triple|db1|(eps&db2)|(noeps&db3)|ra|rb|rf|ra2|rb2|rf2);
chd=(triple|db1|(eps&db2)|(noeps&db3)|rd|rc|re|rd2|rc2|re2);
chb=(triple|db2|(eps&db3)|(noeps&db1)|rb|ra|rc|rb2|ra2|rc2);
che=(triple|db2|(eps&db3)|(noeps&db1)|re|rd|rf|re2|rd2|rf2);
chc=(triple|db3|(eps&db1)|(noeps&db2)|rc|rb|rd|rc2|rb2|rd2);
chf=(triple|db3|(eps&db1)|(noeps&db2)|rf|ra|re|rf2|ra2|re2);
chr=(ra|rb|rc|rd|re|rf|ra2|rb2|rc2|rd2|re2|rf2);

/* change: a = a ^ chad */

k1[ix][iy] = i1[ix][iy]^cha;
k2[ix][iy] = i2[ix][iy]^chb;
k3[ix][iy] = i3[ix][iy]^chc;
k4[ix][iy] = i4[ix][iy]^chd;
k5[ix][iy] = i5[ix][iy]^che;
k6[ix][iy] = i6[ix][iy]^chf;
rest[ix][iy] ^= chr;

/* collision finished (except at the boundaries) */
}}
```

```

/*
i=====i
i
i      c o l l i s i o n      FHP-III      i
i      -----      i
i
i ( two, three and four body collisions)      i
i  162 bit-operations      i
i=====i

collision with 1 rest particle (FHP-III)
24.6.91 Armin Vogeler      */

    for(ix=0; ix < IXM; ix++)
        for(iy=0; iy < IYM; iy++) {

a = i1[ix][iy];
b = i2[ix][iy];
c = i3[ix][iy];
d = i4[ix][iy];
e = i5[ix][iy];
f = i6[ix][iy];
r = rest[ix][iy];
s = sb[ix][iy];
eps = irn[ix][iy];

ns = ~s;      /* no solid bit */
h1 = a&c&e;      /* 3 particles a,c,e */
h2 = b&d&f;      /* 3 particles b,d,f */
h3 = a^c^e;      /* 1 or 3 particles in a,c,e */
h4 = b^d^f;      /* 1 or 3 particles in b,d,f */
h5 = a|c|e;      /* at least 1 particle in a,c,e */
h6 = b|d|f;      /* at least 1 particle in b,d,f */
/* 0 particles in a,c,e or!! in b,d,f and no solid */
h0 = ns&(h5^h6);
/* 2 particles in a,c,e or b,d,f and no solid */
z1 = ns&((~h3&h5)^(~h4&h6));

/* three-body collisions */

```

```

c3 = (h1^h2)&h0;

/* head-on collisions with spectator */

c2s = z1&((a&d)^(b&e)^(c&f));

/* two- and four-body collisions */

c24 = ns&((f^a)|(a^b))&(~((f^c)|(a^d)|(b^e)));

/* rest particle and 1 particle collisions */

r1 = r&((h3&~h1)^(h4&~h2))&h0;

/* no rest particle and 2 particles collisions */

r2 = z1&h0&~r;

/* no s,c24, r1, r2 and c2s collision */
no = ~(c24|r1|r2|c2s)&ns;
le = c24&eps;      /* c24 collision and left rotation */
ri = c24&~eps;     /* c24 collision and right rotation */

/* change bitfield: */

/*|---| |-----| |-----| |-----| |-----| |-----|*/
/*|  | |         | |  |----| |  |         | |  |----| |  |  */
k1[ix][iy]
=(s&d)|(ri&b^le&f)|(no&(a^c3))|(b&f&r2)|((b^f)&r1)|(~d&c2s);
k2[ix][iy]
=(s&e)|(ri&c^le&a)|(no&(b^c3))|(a&c&r2)|((a^c)&r1)|(~e&c2s);
k3[ix][iy]
=(s&f)|(ri&d^le&b)|(no&(c^c3))|(b&d&r2)|((b^d)&r1)|(~f&c2s);
k4[ix][iy]
=(s&a)|(ri&e^le&c)|(no&(d^c3))|(c&e&r2)|((c^e)&r1)|(~a&c2s);
k5[ix][iy]
=(s&b)|(ri&f^le&d)|(no&(e^c3))|(d&f&r2)|((d^f)&r1)|(~b&c2s);
k6[ix][iy]
=(s&c)|(ri&a^le&e)|(no&(f^c3))|(e&a&r2)|((e^a)&r1)|(~c&c2s);
krest[ix][iy] = r^(r1|r2); }

/*----- end of collision ----- */

```

6.4 Thermal LBM: derivation of the coefficients

Constraints from the definitions of mass and momentum.

Mass:

$$\rho = \sum_i F_i^{eq} = A_0 + 6(A_1 + A_2) + (3C_1 + 12C_2 + D_0 + 6D_1 + 6D_2) \mathbf{u}^2$$

→ constraints 1 and 2

$$3C_1 + 12C_2 + D_0 + 6D_1 + 6D_2 = 0 \quad (6.4.1)$$

$$A_0 + 6(A_1 + A_2) = \rho \quad (6.4.2)$$

Momentum:

$$\mathbf{j} = \sum_i \mathbf{c}_i F_i^{eq} = \mathbf{u} \left[3B_1 + 12B_2 + \left(\frac{9}{4}E_1 + 36E_2 + 3G_1 + 12G_2 \right) \mathbf{u}^2 \right]$$

→ constraints 3 and 4

$$3B_1 + 12B_2 = \rho \quad (6.4.3)$$

$$\frac{9}{4}E_1 + 36E_2 + 3G_1 + 12G_2 = 0 \quad (6.4.4)$$

Conservation of mass, momentum, and energy.

The expansions (5.2.25) will be substituted into the conservation equations for mass, momentum and energy

$$0 = \sum_i \begin{pmatrix} 1 \\ \mathbf{c}_i \\ \mathbf{c}_i^2/2 \end{pmatrix} [F_i(\mathbf{x} + \mathbf{c}_i, t + 1) - F_i(\mathbf{x}, t)]$$

which lead to

$$\begin{aligned} 0 &\stackrel{(5.2.25)}{=} \sum_i \begin{pmatrix} 1 \\ c_{i\alpha} \\ c_{i\alpha}c_{i\alpha}/2 \end{pmatrix} \left[F_i(\mathbf{x}, t) + \partial_t F_i + c_{i\beta} \partial_{x_\beta} F_i + \frac{1}{2} \partial_t \partial_t F_i \right. \\ &\quad \left. + \frac{1}{2} \partial_{x_\beta} \partial_{x_\gamma} c_{i\beta} c_{i\gamma} F_i + c_{i\beta} \partial_t \partial_{x_\beta} F_i + \mathcal{O}(\partial^3 F_i) - F_i(\mathbf{x}, t) \right] \\ &= \sum_i \begin{pmatrix} 1 \\ c_{i\alpha} \\ c_{i\alpha}c_{i\alpha}/2 \end{pmatrix} \left[\epsilon \partial_t^{(1)} F_i^{(0)} + \epsilon^2 \partial_t^{(1)} F_i^{(1)} + \epsilon^2 \partial_t^{(2)} F_i^{(0)} \right. \\ &\quad \left. + c_{i\beta} \epsilon \partial_{x_\beta}^{(1)} F_i^{(0)} + c_{i\beta} \epsilon^2 \partial_{x_\beta}^{(1)} F_i^{(1)} + \frac{1}{2} \epsilon^2 \partial_t^{(1)} \partial_t^{(1)} F_i^{(0)} \right. \\ &\quad \left. + \frac{1}{2} \epsilon^2 \partial_{x_\beta}^{(1)} \partial_{x_\gamma}^{(1)} c_{i\beta} c_{i\gamma} F_i^{(0)} + c_{i\beta} \epsilon^2 \partial_t^{(1)} \partial_{x_\beta}^{(1)} F_i^{(0)} + \mathcal{O}(\epsilon^3) \right] \end{aligned}$$

and finally sorted according to orders in ϵ

$$\begin{aligned}
0 = & \sum_i \begin{pmatrix} 1 \\ c_{i\alpha} \\ c_{i\alpha}c_{i\alpha}/2 \end{pmatrix} \left\{ \epsilon \left[\partial_t^{(1)} F_i^{(0)} + c_{i\beta} \partial_{x_\beta}^{(1)} F_i^{(0)} \right] \right. \\
& + \epsilon^2 \left[\partial_t^{(1)} F_i^{(1)} + \partial_t^{(2)} F_i^{(0)} + c_{i\beta} \partial_{x_\beta}^{(1)} F_i^{(1)} + \frac{1}{2} \partial_t^{(1)} \partial_t^{(1)} F_i^{(0)} \right. \\
& \left. \left. + \frac{1}{2} \partial_{x_\beta}^{(1)} \partial_{x_\gamma}^{(1)} c_{i\beta} c_{i\gamma} F_i^{(0)} + c_{i\beta} \partial_{x_\beta}^{(1)} \partial_t^{(1)} F_i^{(0)} \right] + \mathcal{O}(\epsilon^3) \right\} \quad (6.4.5)
\end{aligned}$$

Terms of first order in ϵ : mass.

To first order in ϵ eq. (6.4.5) yields:

$$0 = \sum_i \left[\partial_t^{(1)} F_i^{(0)} + c_{i\alpha} \partial_{x_\alpha}^{(1)} F_i^{(0)} \right]$$

or

$$\partial_t^{(1)} \rho + \partial_{x_\alpha}^{(1)} j_\alpha = 0 \quad (\text{continuity equation}), \quad (6.4.6)$$

\rightarrow no further constraints from mass conservation.

Terms of first order in ϵ : momentum.

$$\begin{aligned}
0 &= \sum_i \left[c_{i\alpha} \partial_t^{(1)} F_i^{(0)} + \partial_{x_\beta}^{(1)} c_{i\alpha} c_{i\beta} F_i^{(0)} \right] \\
0 &= \partial_t^{(1)} (\rho u_\alpha) + \partial_{x_\beta}^{(1)} P_{\alpha\beta}^{(0)}. \quad (6.4.7)
\end{aligned}$$

whereby

$$P_{\alpha\beta}^{(0)} := \sum_i c_{i\alpha} c_{i\beta} F_i^{(0)}$$

is the momentum flux tensor with components

$$\begin{aligned}
P_{xx}^{(0)} &= 3A_1 + 12A_2 + \left(\frac{3}{4}C_1 + 12C_2 \right) (3u^2 + v^2) + (3D_1 + 12D_2)u^2 \\
&= 3A_1 + 12A_2 + \left(\frac{9}{4}C_1 + 36C_2 + 3D_1 + 12D_2 \right) u^2 \\
&\quad + \left(\frac{3}{4}C_1 + 12C_2 + 3D_1 + 12D_2 \right) v^2
\end{aligned}$$

$$P_{xy}^{(0)} = \left(\frac{3}{2}C_1 + 24C_2 \right) uv = P_{yx}^{(0)} \quad (6.4.8)$$

$$\begin{aligned} P_{yy}^{(0)} &= 3A_1 + 12A_2 + \left(\frac{3}{4}C_1 + 12C_2 \right) (u^2 + 3v^2) + (3D_1 + 12D_2) u^2 \\ &= 3A_1 + 12A_2 + \left(\frac{3}{4}C_1 + 12C_2 + 3D_1 + 12D_2 \right) u^2 \\ &\quad + \left(\frac{9}{4}C_1 + 36C_2 + 3D_1 + 12D_2 \right) v^2 \end{aligned}$$

The momentum flux tensor should yield

$$P_{\alpha\beta}^{(0)} = \rho u_\alpha u_\beta + p \delta_{\alpha\beta} = \rho \begin{pmatrix} u^2 & uv \\ uv & v^2 \end{pmatrix} + p \delta_{\alpha\beta}. \quad (6.4.9)$$

Comparison of (6.4.8) and (6.4.9) leads to:

$$\begin{aligned} 3A_1 + 12A_2 &= p \\ \frac{9}{4}C_1 + 36C_2 + 3D_1 + 12D_2 &= \rho \\ \frac{3}{4}C_1 + 12C_2 + 3D_1 + 12D_2 &= 0 \\ \frac{3}{2}C_1 + 24C_2 &= \rho. \end{aligned}$$

This results in the three independent constraints 5 to 7:

$$3A_1 + 12A_2 = p \quad (6.4.10)$$

$$\frac{3}{2}C_1 + 24C_2 = \rho \quad (6.4.11)$$

and

$$6D_1 + 24D_2 = -\rho \quad (6.4.12)$$

The first order terms of the moment equation lead to the Euler equation

$$\begin{aligned} &\underbrace{=}_{(6.4.6)} \rho \partial_t^{(1)} u_\alpha - u_\alpha \partial_{x_\beta}^{(1)} (\rho u_\beta) \\ &= \rho \partial_t^{(1)} u_\alpha + u_\alpha \partial_t^{(1)} \rho \\ \partial_t^{(1)} (\rho u_\alpha) &= \\ &= -\partial_{x_\beta}^{(1)} P_{\alpha\beta}^{(0)} \\ &\underbrace{=}_{(6.4.9)} -\partial_{x_\beta}^{(1)} (\rho u_\alpha u_\beta + p \delta_{\alpha\beta}) \\ &= -\rho u_\beta \partial_{x_\beta}^{(1)} u_\alpha - u_\alpha \partial_{x_\beta}^{(1)} (\rho u_\beta) - \partial_{x_\alpha}^{(1)} p \quad (6.4.13) \end{aligned}$$

and therefore

$$\rho \partial_t^{(1)} u_\alpha = -\rho u_\beta \partial_{x_\beta}^{(1)} u_\alpha - \partial_{x_\alpha}^{(1)} p \quad (6.4.14)$$

Terms of first order in ϵ : energy.

$$\begin{aligned} 0 &= \frac{1}{2} \sum_i \left[\partial_t^{(1)} c_{i\alpha} c_{i\alpha} F_i^{(0)} + \partial_{x_\beta}^{(1)} c_{i\alpha} c_{i\alpha} c_{i\beta} F_i^{(0)} \right] \\ \frac{1}{2} \partial_t^{(1)} \sum_i c_{i\alpha} c_{i\alpha} F_i^{(0)} &= \frac{1}{2} \partial_t^{(1)} P_{\alpha\alpha}^{(0)} = \partial_t^{(1)} \left[\underbrace{\frac{1}{2} \rho u_\alpha u_\alpha}_{= \rho \varepsilon_K} + \underbrace{p}_{= \rho \varepsilon_I} \right] \end{aligned}$$

where p is to be identified with the internal energy, i.e. $p = \rho \varepsilon_I$, and $\frac{1}{2} \rho u_\alpha u_\alpha$ is the kinetic energy.

$$\begin{aligned} &\frac{1}{2} \partial_{x_\beta}^{(1)} \sum_i c_{i\alpha} c_{i\alpha} c_{i\beta} F_i^{(0)} \\ &= \partial_{x_\beta}^{(1)} \left[\underbrace{\left(\frac{3}{2} B_1 + 24 B_2 \right) u_\beta}_{=: f_1(\rho, \varepsilon_I)} + \underbrace{\left(\frac{9}{8} E_1 + 72 E_2 + \frac{3}{2} G_1 + 24 G_2 \right) u_\alpha u_\alpha u_\beta}_{=: f_2(\rho, \varepsilon_I)} \right] \\ &= \partial_{x_\beta}^{(1)} [f_1(\rho, \varepsilon_I) u_\beta + f_2(\rho, \varepsilon_I) u_\alpha u_\alpha u_\beta] \quad (6.4.15) \end{aligned}$$

and thus

$$\partial_t^{(1)} (\rho \varepsilon_K + \rho \varepsilon_I) = -\partial_{x_\beta}^{(1)} [f_1(\rho, \varepsilon) u_\beta + f_2(\rho, \varepsilon) u_\alpha u_\alpha u_\beta] \quad (6.4.16)$$

$$\begin{aligned} \partial_t^{(1)} (\rho \varepsilon_K) &= \partial_t^{(1)} \left(\frac{1}{2} \rho u_\alpha u_\alpha \right) \\ &= \frac{1}{2} u_\alpha \partial_t^{(1)} (\rho u_\alpha) + \frac{1}{2} \rho u_\alpha \partial_t^{(1)} u_\alpha \\ &\stackrel{(6.4.13), (6.4.14)}{=} -\frac{1}{2} u_\alpha [\rho u_\beta \partial_{x_\beta}^{(1)} u_\alpha + u_\alpha \partial_{x_\beta}^{(1)} (\rho u_\beta) + \partial_{x_\alpha}^{(1)} p] \\ &\quad + \rho u_\beta \partial_{x_\beta}^{(1)} u_\alpha + \partial_{x_\alpha}^{(1)} p \\ &= -\rho u_\alpha u_\beta \partial_{x_\beta}^{(1)} u_\alpha - u_\alpha \partial_{x_\alpha}^{(1)} p \\ &\quad - \frac{1}{2} u_\alpha u_\alpha \partial_{x_\beta}^{(1)} (\rho u_\beta) \quad (6.4.17) \end{aligned}$$

$$\begin{aligned}
\rho \partial_t^{(1)} \varepsilon_I &= \partial_t^{(1)} (\rho \varepsilon_I) - \varepsilon_I \partial_t^{(1)} \rho \\
&\stackrel{(6.4.6), (6.4.16)}{=} -\partial_t^{(1)} (\rho \varepsilon_K) - \partial_{x_\alpha}^{(1)} [f_1 u_\alpha + f_2 u_\alpha u_\beta u_\beta] + \varepsilon_I \partial_{x_\alpha}^{(1)} (\rho u_\alpha) \\
&\stackrel{(6.4.17)}{=} \rho u_\alpha u_\beta \partial_{x_\beta}^{(1)} u_\alpha + u_\alpha \partial_{x_\alpha}^{(1)} p + \frac{1}{2} u_\alpha u_\alpha \partial_{x_\beta}^{(1)} (\rho u_\beta) \\
&\quad - \partial_{x_\alpha}^{(1)} [f_1 u_\alpha + f_2 u_\alpha u_\beta u_\beta] + \varepsilon_I \partial_{x_\alpha}^{(1)} (\rho u_\alpha). \quad (6.4.18)
\end{aligned}$$

Substitution of $p = \rho \varepsilon_I$ and expansion of all terms leads to

$$\begin{aligned}
\rho \partial_t^{(1)} \varepsilon_I &= \underbrace{\rho u_\alpha u_\beta \partial_{x_\beta}^{(1)} u_\alpha}_{(1)} + \underbrace{\rho u_\alpha \partial_{x_\alpha}^{(1)} \varepsilon_I}_{(2)} + \underbrace{u_\alpha \varepsilon_I \partial_{x_\alpha}^{(1)} \rho}_{(3)} \\
&\quad + \underbrace{\frac{1}{2} \rho u_\beta u_\beta \partial_{x_\alpha}^{(1)} u_\alpha}_{(4)} + \underbrace{\frac{1}{2} u_\alpha u_\beta u_\beta \partial_{x_\alpha}^{(1)} \rho}_{(5)} \\
&\quad - \underbrace{f_1 \partial_{x_\alpha}^{(1)} u_\alpha}_{(6)} - \underbrace{u_\alpha \partial_{x_\alpha}^{(1)} f_1}_{(7)} \\
&\quad - \underbrace{u_\alpha u_\beta u_\beta \partial_{x_\alpha}^{(1)} f_2}_{(8)} - \underbrace{f_2 u_\beta u_\beta \partial_{x_\alpha}^{(1)} u_\alpha}_{(9)} - \underbrace{2 f_2 u_\alpha u_\beta \partial_{x_\alpha}^{(1)} u_\beta}_{(10)} \\
&\quad + \underbrace{\rho \varepsilon_I \partial_{x_\alpha}^{(1)} u_\alpha}_{(11)} + \underbrace{u_\alpha \varepsilon_I \partial_{x_\alpha}^{(1)} \rho}_{(12)} \quad (6.4.19)
\end{aligned}$$

which should yield

$$\rho \partial_t^{(1)} \varepsilon_I = - \underbrace{\rho u_\alpha \partial_{x_\alpha}^{(1)} \varepsilon_I}_{(13)} - \underbrace{\rho \varepsilon_I \partial_{x_\alpha}^{(1)} u_\alpha}_{(14)} \quad (6.4.20)$$

Terms (1) and (10), (4) and (9), and (5) and (8) cancel each other when $f_2 = \rho/2$. The sum (2) + (3) + (7) + (12) gives (13) when $f_1 = 2\rho \varepsilon_I$. Finally, (6) + (11) gives (14). Thus we obtain the constraints 8 and 9:

$$\frac{3}{2} B_1 + 24 B_2 = 2\rho \varepsilon_I (= f_1) \quad (6.4.21)$$

$$\frac{9}{8}E_1 + 72E_2 + \frac{3}{2}G_1 + 24G_2 = \frac{\rho}{2} (= f_2) \quad (6.4.22)$$

Calculation of the coefficients.

B_1 and B_2 are constrained by (6.4.3) and (6.4.21)

$$3B_1 + 12B_2 = \rho$$

$$\frac{3}{2}B_1 + 24B_2 = 2\rho\varepsilon_I$$

which lead to the unique solution

$$B_1 = \frac{4}{9}\rho(1 - \varepsilon_I) \quad (6.4.23)$$

$$B_2 = \frac{\rho}{36}(4\varepsilon_I - 1). \quad (6.4.24)$$

A_1 and A_2 are constrained only by (6.4.2) and (6.4.10) and A_0 only by (6.4.2):

$$A_0 + 6A_1 + 6A_2 = \rho$$

$$3A_1 + 12A_2 = p (= \rho\varepsilon_I).$$

In order to obtain a unique solution one may require (compare a similar constraint in Section 5.4, Eq. 5.4.4) that $A_1/B_1 = A_2/B_2$. This leads to

$$A_0 = \rho(1 - \frac{5}{2}\varepsilon_I + 2\varepsilon_I^2), \quad A_1 = \rho\frac{4}{9}(\varepsilon_I - \varepsilon_I^2), \quad A_2 = \rho\frac{1}{36}(-\varepsilon_I + 4\varepsilon_I^2),$$

e.g. the expressions given by Alexander et al. (1993).

The C_ν and D_ν are constrained by (6.4.1), (6.4.11), and (6.4.12):

$$3C_1 + 12C_2 + D_0 + 6D_1 + 6D_2 = 0$$

$$\frac{3}{2}C_1 + 24C_2 = \rho$$

and

$$6D_1 + 24D_2 = -\rho.$$

The choice of Alexander et al. is consistent with these constraints.

E_ν and G_ν are constrained by (6.4.4) and (6.4.22):

$$\frac{9}{4}E_1 + 36E_2 + 3G_1 + 12G_2 = 0$$

$$\frac{9}{8}E_1 + 72E_2 + \frac{3}{2}G_1 + 24G_2 = \frac{\rho}{2}.$$

Alexander et al. (1993) have chosen $G_1 = 0 = G_2$. Then E_1 and E_2 are uniquely given by

$$E_1 = -\frac{4}{27}\rho \quad (6.4.25)$$

$$E_2 = \frac{\rho}{108} \quad (6.4.26)$$

6.5 Schläfli symbols

Regular polytopes can be characterized by Schläfli² symbols instead of listing, for example, the coordinates of the whole set of vertices. Coxeter (1963, p.126/7) defines a polytope “as a finite convex³ region of n -dimensional space enclosed by a finite number of hyperplanes”. A polytope is characterized by its ensemble of *vertices*. Two-dimensional polytopes are called *polygons*. Three-dimensional polytopes are called *polyhedra*. The part of the polytope that lies in one of the hyperplanes is called a *cell* (each cell is a $(n - 1)$ -dimensional polytope; example: consider the cube where the cells are squares). The cells of polyhedra are called *faces*; they are polygons bounded by *edges* or *sides*. Edges join nearest-neighbor vertices. Thus a four-dimensional polytope Π_4 has solid cells Π_3 , plane faces Π_2 (separating two cells), edges Π_1 , and vertices Π_0 .

A polygon with p vertices is said to be *regular* if it is both *equilateral* (all sides are equal) and *equiangular* (all angles between nearest neighbor vertices are equal). If $p > 3$ a polygons can be equilateral without being equiangular (a rhomb, for example), or vice versa (a rectangle). Regular polygons are denoted by $\{p\}$ (the Schläfli symbol = number of vertices put in cranked brackets); thus $\{3\}$ is an equilateral triangle, $\{4\}$ is a square, $\{5\}$ is a regular pentagon, and so on.

A polyhedron is said to be *regular* if its faces are regular and equal, while its vertices are all surrounded alike. If its faces are $\{p\}$'s (i.e. regular polygons), q surrounding each vertex, the polyhedron is denoted by the Schläfli symbol $\{p, q\}$. In three dimensions there exist only five regular polyhedra, namely the Platonic solids (compare Section 3.4). Consider, for instance, the cube. The faces are squares (4 edges) and each vertex is surrounded by 3 faces. Accordingly the cube is denoted by the Schläfli symbol $\{4, 3\}$. The Schläfli symbols for the other Platonic solids read: tetrahedron $\{3, 3\}$, octahedron $\{3, 4\}$, dodecahedron $\{5, 3\}$, icosahedron $\{3, 5\}$. Please note that the dual polytope to $\{p, q\}$ has the Schläfli symbol $\{q, p\}$.

A polytope Π_n ($n > 2$) is said to be *regular* if its cells are regular and there is a regular *vertex figure*⁴ at every vertex (‘regular surrounded’). It can be shown that as a consequence of this definition all cells are equal ($\{p, q\}$ for $n = 4$) and the vertex figures are all equal ($\{q, r\}$ for $n = 4$). A regular polytope Π_4 is denoted by the Schläfli symbol $\{p, q, r\}$ where the cells are $\{p, q\}$ and r is the number of cells that surround an edge. The three regular polytopes in four dimensions

² After the Swiss mathematician Ludwig Schläfli (1814-95).

³ “A region is said to be **convex** if it contains the whole of the segment joining every pair of its points.” (Coxeter, 1963, p.126)

⁴ “If the mid-points of all the edges that emanate from a given vertex O of Π_n lie in one hyperplane ..., then these mid-points are the vertices of an $(n - 1)$ -dimensional polytope called the *vertex figure* of Π_n at O .” (Coxeter, 1963, p. 128)

$$\{3, 3, 3\}, \quad \{3, 3, 4\}, \quad \{4, 3, 3\}, \quad (6.5.1)$$

are bounded by tetrahedrons ($\{3, 3\}$) or cubes ($\{4, 3\}$). $\Pi_4 = \{4, 3, 3\}$ is the hypercube (not FCHC!). Similarly, a regular polytope Π_5 whose cells are $\{p, q, r\}$ must have vertex figures $\{q, r, s\}$, and thus will be denoted by

$$\Pi_5 = \{p, q, r, s\}. \quad (6.5.2)$$

It can be shown (Coxeter, 1963) that the parameters of the Schläfli for regular polyhedra are constrained by “Schläfli’s criterion” which reads

$$\frac{1}{p} + \frac{1}{q} > \frac{1}{2} \quad \text{for} \quad \{p, q\} \quad (6.5.3)$$

and

$$\sin \frac{\pi}{p} \sin \frac{\pi}{r} > \sin \frac{\pi}{q} \quad \text{for} \quad \{p, q, r\}. \quad (6.5.4)$$

This and $p, q, r \geq 3$ leads to

$$\{3, 3\}, \quad \{3, 4\}, \quad \{4, 3\}, \quad \{3, 5\}, \quad \{5, 3\} \quad (6.5.5)$$

and

$$\{3, 3, 3\}, \quad \{3, 3, 4\}, \quad \{4, 3, 3\}, \quad \{3, 4, 3\}, \quad \{3, 3, 5\}, \quad \{5, 3, 3\}. \quad (6.5.6)$$

$\{3, 4, 3\}$ is the face-centered hypercube (FCHC). Since Schläfli’s criterion is merely a *necessary* condition, it remains to be proved that the corresponding polytopes actually exist (this can be very laboriously!; result: all above mentioned polytopes exist).

Further reading: Rothman and Zaleski (1997, p. 265-270).

6.6 Notation, symbols and abbreviations

General remarks:

Latin indices refer to the lattice vectors and run from 0 or 1 to l where l is the number of non-vanishing lattice velocities.

Greek indices assign the cartesian components of vectors and therefore run from 1 to D where D is the dimension.

If not otherwise stated (Einstein's) summation convention is used, i.e. summation is performed over repeated indices ($n_i \mathbf{c}_i = \sum_{i=1}^l n_i \mathbf{c}_i$). No summation will be done over primed indices ($n_{j'} v_{j'} \neq \sum_{j'=1}^l n_{j'} v_{j'}$).

Table 6.6.1. Notation (miscellaneous symbols)

Symbol	Meaning
∇	nabla operator
∂	partial derivative
$\&$	AND (Boolean operator)
$ $	OR (inclusive or; Boolean operator)
\wedge	XOR (exclusive or; Boolean operator)
\sim	NOT (Boolean operator)
\cup	union (Boolean algebra)
\cap	intersection (Boolean algebra)
$-$	complementation (Boolean algebra)
\circ	composition (of two elements; group theory)

Table 6.6.2. Notation (Latin letters)

Symbol	Meaning
A	Lagrange multiplier
$A(s \rightarrow s')$	transition probability
$A_{ss'}$	transition matrix
$A_\nu, B_\nu \dots$	free parameters of equilibrium distributions
$a_i^{(t)}$	state of cell i at time t
\mathcal{B}	Boolean algebra
B	Lagrange multiplier
b	number of lattice velocities ('bits')
\mathcal{C}	collision operator
C	number of corners
\mathbf{c}_i	lattice vectors, lattice velocities
$c_{i\alpha}$	cartesian component of the i th lattice velocity
c_s	speed of sound
c_v	heat capacity at constant volume
D	(spatial) dimension
$DkQb$	lattice notation (k =dimension, b =number of lattice velocities)
d	density per cell
\mathcal{E}	evolution operator
E	number of edges
E_A	Ekman number
\mathcal{F}	operator that interchanges particles and holes
\mathbf{F}	body force
F	number of faces
F_m	distribution functions
f	Coriolis parameter
f_0	Coriolis parameter at φ_0
\mathcal{G}	isometric group
$G_{\alpha_1\alpha_2\dots\alpha_n}$	generalized lattice tensor of rank n
$G(\rho)$	g-factor (breaking Galilean invariance)
$g(\rho)$	$= G(\rho)/2$; g-factor (breaking Galilean invariance)
g	group element
H	Boltzmann's H ($= -$ entropy)
H_i	Zanetti invariants
h	Lagrange multiplier
\mathcal{I}	identity operator
$I(P)$	measure of information
$J(f)$	collision operator (BGK)
$J(a, b)$	Jacobi operator
\mathbf{j}	momentum density
K_n	Knudsen number
k	number of states (CA)
k_B	Boltzmann constant
k_s	friction coefficient

Table 6.6.3. Notation (Latin letters; continued)

Symbol	Meaning
\mathcal{L}	a lattice
L	characteristic length scale
$L_{\alpha_1\alpha_2\ldots\alpha_n}$	lattice tensor of rank n
M_a	Mach number
\mathbb{N}	the set of natural numbers (integers)
\mathbb{N}_0	the set of non-negative integers
N_i	mean occupation number (real variable)
n_i	occupation number (Boolean variable)
$\mathcal{O}(\epsilon^2)$	on the order of ϵ^2
$O_{\alpha\beta}$	orthogonal transformation matrix
P	discrete probability distribution
P	kinematic pressure
$P_{\alpha\beta}$	momentum flux tensor
p	pressure
p_i	probabilities
Q	set of possible automata states
$Q(f, f)$	collision integral
$Q_{i\alpha\beta}$	Q-tensors (FHP)
q	(vectorial) Lagrange multiplier
\mathbb{R}	the set of real numbers
Re	Reynolds number
$Re_{e,g}$	grid Reynolds number
Ro	Rossby number
r	range (CA)
r_j	cartesian coordinates of nodes
\mathcal{S}	streaming (propagation) operator
S	entropy
T	temperature
$T_{\alpha\beta\gamma\delta}^{(\text{MA})}$	momentum advection tensor (MAT)
$T_{x,y}$	components of the wind stress
t	time
U	characteristic speed
$\mathbf{u} = (u, v, w)$	velocity
W_M	Munk scale
W_i	global equilibrium distributions
w_i	weights (generalized lattice tensors)
$\mathbf{x} = (x, y, z)$	cartesian coordinates
\mathbb{Z}_k	residue class (integers modulo k)
Z	discrete set

Table 6.6.4. Notation (Greek letters)

Symbol	Meaning
β	gradient of the Coriolis parameter
Γ	phase space
Δ_1	collision function
Δt	time step
Δx	spatial step size
$\delta_{\alpha\beta}$	Kronecker symbol
$\delta_{\alpha\beta\gamma\delta}$	generalized Kronecker symbol
ϵ	expansion parameter
$\epsilon_{\alpha\beta\gamma}$	Levi-Civita symbol
ε_I	internal energy density
ε_K	kinetic energy density
θ	$= k_B T$ temperature in energy units
κ	diffusion coefficient
κ	magnitude of wave number
λ	mean free path
ν	shear viscosity
ξ	bulk viscosity
ξ	random Boolean variable
ρ	mass density
σ	collision cross section
τ	collision time
ψ	stream function
ψ_n	collision invariants
Ω	set of events
Ω	angular velocity of the Earth
Ω_i	collision operator
ω	SOR or viscosity parameter

Table 6.6.5. Abbreviations

Acronym	Meaning
BC	boundary conditions
BGK	Bhatnagar, Gross, Krook
CA	cellular automata
EFD	explicit finite difference
FCHC	face-centered hypercube
FHP	Frisch, Hasslacher, Pomeau
HPP	Hardy, Pazzis, Pomeau
LBM	lattice Boltzmann model
LBGK	lattice BGK models
LGCA	lattice-gas cellular automata
MD	molecular dynamics
ODE	ordinary differential equation
PCLBM	pressure corrected lattice Boltzmann model
PDE	partial differential equation
PI	pair interaction
MSC	multi-spin coding
NSE	Navier-Stokes equation
q.e.d.	quot erat demonstrandum
SOR	successive over-relaxation