Contents

1 Streaming Step

During the streaming step, distributions are propagated into the neighbour cells in the corresponding direction. There are several ways to implement the streaming step in memory. The simplest approach is the A-B streaming pattern, which uses two distribution fields. Distributions are read from old locations in field A and written into new locations in field B. This doubles memory consumption.

To prevent the second field, it is necessary to find an algorithm that always writes data into the same locations where it read from. One of such algorithms is the A-A streaming, which combines streaming and collision steps together and alters between odd and even timesteps.

There is also another way that does not require altering between odd and even timesteps presented in [4], called Periodic Shift.

1.1 Periodic Shift Streaming

Article [4] presents the algorithm "Periodic Shift" (PS). This algorithm requires the "Structure of Arrays" (SoA) organization so that each distribution array $\underline{f_q}$ is saved separately in a continous block of memory. Instead of physically writing data into new positions during the streaming step, it uses periodic shifting of the memory index, independent for each distribution.

1.1.1 Basic idea

Before formalizing the algorithm, let's illustrate the idea on a D2Q9 scheme (Figure 1):

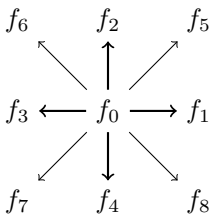

Figure 1: D2Q9 scheme

Consider a field with 3 rows and 4 columns with cells labelled using row-major indexing as shown in Figure 2:

0	1	2	3
4	5	6	7
8	9	10	11

Figure 2: D2Q9 field with cell labels

During streaming, values of each distribution array $\underline{f_q}$ move through the field in the direciton given by the velocity set. This means, after streaming, in cell $\overline{2}$ we want to find the original value of f_1 from cell 1, original value of f_2 from cell 6, etc. Values f_4, f_7, f_8 are unknown ("?") in cell 2 and need to be filled by a boundary condition. Table 1 shows, for every cell and every distribution f_q, from where the value was streamed.

cell i	0	1	2	3	4	5	6	7	8	9	10	11
f_q	**In cell i, where was the value of f_q streamed from?**											
f_0	0	1	2	3	4	5	6	7	8	9	10	11
f_1	?	0	1	2	?	4	5	6	?	8	9	10
f_2	4	5	6	7	8	9	10	11	?	?	?	?
f_3	1	2	3	?	5	6	7	?	9	10	11	?
f_4	?	?	?	?	0	1	2	3	4	5	6	7
f_5	?	4	5	6	?	8	9	10	?	?	?	?
f_6	5	6	7	?	9	10	11	?	?	?	?	?
f_7	?	?	?	?	1	2	3	?	5	6	7	?
f_8	?	?	?	?	?	0	1	2	?	4	5	6

Table 1: Streaming map

Taking a look at Table 1, it seems that the cells always stay ordered. During streaming, they are all just shifted by a constant, which is different for every distribution. This is used by the PS algorithm.

1.1.2 Full PS algorithm

Let's now consider a 3 dimensional case, using the $D3Q27$ scheme with the following velocity set (Table 2):

Table 2: D3Q27 velocity set

	f_0	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	f_{10}	f_{11}	f_{12}	f_{13}	f_{14}	f_{15}	f_{16}	f_{17}	f_{18}	f_{19}	f_{20}	f_{21}	f_{22}	f_{23}	f_{24}	f_{25}	f_{26}
c_x	0	1	−1	0	0	0	0	1	−1	1	−1	−1	1	0	0	−1	1	0	0	−1	1	−1	1	1	−1	−1	1
c_y	0	0	0	0	0	−1	1	0	0	0	0	−1	1	1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1
c_z	0	0	0	−1	1	0	0	−1	1	1	−1	0	0	−1	1	0	0	1	−1	−1	1	1	−1	−1	1	−1	1
w	$\frac{8}{27}$	$\frac{2}{27}$	$\frac{2}{27}$	$\frac{2}{27}$	$\frac{2}{27}$	$\frac{2}{27}$	$\frac{2}{27}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{54}$	$\frac{1}{216}$	$\frac{1}{216}$	$\frac{1}{216}$	$\frac{1}{216}$	$\frac{1}{216}$	$\frac{1}{216}$	$\frac{1}{216}$	$\frac{1}{216}$

The field will be block-shaped, sized $N = N_x \cdot N_y \cdot N_z$. Cells will be indexed i, j, k to represent x, y, z position and the 3-dimensional index will be mapped onto 1D index idx as

$$idx(i, j, k) = k \cdot (N_x \cdot N_y) + j \cdot N_x + i \tag{1.1}$$

The index idx determines placement of data for each distribution array of length N in memory. To read distribution f_1 in cell i, j, k we call $f_1 = \underline{f_1}[idx(i, j, k)]$.

During the streaming step, distributions should flow into neighbour cells in directions determined by the velocity set.

A distribution value located at $idx(i, j, k)$ after streaming was placed at $idx(i - c_x, j - c_y, k - c_z)$ before streaming. This gives, independently for each $\underline{f_q}$,

$$\begin{gathered} idx(i - c_x, j - c_y, k - c_z) \\ = \\ (k - c_z) \cdot (N_x \cdot N_y) + (j - c_y) \cdot N_x + (i - c_x) \\ = \\ k \cdot (N_x \cdot N_y) + j \cdot N_x + i - [c_z \cdot (N_x \cdot N_y) + c_y \cdot N_x + c_x] \\ = \\ idx(i, j, k) - s_q \end{gathered} \tag{1.2}$$

where the s_q term is constant and only depends on q (index of the distribution):

$$s_q = c_z \cdot (N_x \cdot N_y) + c_y \cdot N_x + c_x \tag{1.3}$$

For t streaming steps,

$$idx(i - tc_x, j - tc_y, k - tc_z) = idx(i, j, k) - ts_q \tag{1.4}$$

Instead of moving the data, it is possible to just read and write it into its original location everytime it is accessed. This can be formalized by making the index idx a function of iteration number t:

$$idx(i,j,k,t) = idx(i,j,k) - ts_q \tag{1.5}$$

To avoid negative indexes or indexes higher than N, just do

$$idx(i,j,k,t) = ((idx(i,j,k) - ts_q) \mod N + N) \mod N \tag{1.6}$$

Note that this makes all distributions that enter the field from the boundaries invalid, but these would have to be fixed by boundary conditions anyway.

When implemented, this results in by 27 parts coalescent memory access during the collision step. There is only a single large jump of the pointer per every distribution array. There is no memory access during the streaming step, except for some implementation of the index shifter. There is no second field required, and there is no difference between odd and even iterations.

2 Boundary Conditions

2.1 Moment based boundary conditions

Moment based boundary conditions in 3 dimensions are investigated in [3], [2]. The idea is to approximate raw moments as their Maxwell-Boltzman equilibrium and use those in a system of equations to calculate the unknown distributions. The equilibriums are calculated from ρ, u_x, u_y and u_z. It is required that those 4 quantities are known a priori by prescribing them at the inlet or outlet or by using some relations to calculate them. Examples of how this can be done for particular inlet or outlet type is shown further below.

One advantage of using moment based boundary conditions is locality [3]. Once ρ, u_x, u_y, u_z are known, it is only necessary to work with information from a single cell.

Another advantage is that the prescribed quantities have clearer physical meaning compared to some other options, where part of what is used to define the distribution functions is somewhat artificial [3].

The specific formulation of equations depends on type and orientation of the cell. A face cell is a cell that does not have neighbours in one direction. A edge cell does not have neighbours in two directions. A corner cell misses neighbours in three directions. A general approach to the derivation process is needed to handle all different kinds of cells [2].

The procedure presented below can be generalized and can be used to automatically generate code for all different cell types. For example, let's consider an edge cell with outer normal $(0, 1, -1)$ (so it has neighbours in X direction but misses neighbours in positive Y and negative Z). After streaming, the distributions with $c_y = -1$ and $c_z = 1$ are unknown. Let's put all known distributions into a vector $\underline{f_k}$ and unknown distributions into $\underline{f_u}$ as displayed in Table 3.

Table 3: Known and unknown distributions for a cell with $(0, 1, -1)$ outer normal

Known distributions	$\underline{f_k} = (f_0, f_1, f_2, f_3, f_6, f_7, f_{10}, f_{12}, f_{13}, f_{15}, f_{19}, f_{22})^T$
Unknown distributions	$\underline{f_u} = (f_4, f_5, f_8, f_9, f_{11}, f_{14}, f_{16}, f_{17}, f_{18}, f_{20}, f_{21}, f_{23}, f_{24}, f_{25}, f_{26})^T$

Raw moments are a product of both known and unknown distributions. They can be defined as [1]

$$m_{abc} = \sum_i f_i c_{xi}^a c_{yi}^b c_{zi}^c \tag{2.1}$$

Resulting expressions for moments up to 4th order as a product of $\underline{f_k}$ and $\underline{f_u}$ are displayed in Table 4.

Table 4: Moments for a cell with $(0, 1, -1)$ outer normal

Moment	**Known distributions**	**Unknown distributions**
m_{000}	$\underline{f_k} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$
m_{100}	$\underline{f_k} \cdot (\ 0,\ 1, -1,\ 0,\ 0,\ 1, -1,\ 1,\ 0, -1, -1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0, -1,\ 1, -1,\ 0,\ 1,\ 0,\ 0,\ 1, -1,\ 1, -1, -1,\ 1)^T$
m_{010}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0, -1,\ 0,\ 0, -1, -1, -1,\ 1, -1, -1, -1, -1,\ 1, -1,\ 1)^T$
m_{001}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0, -1,\ 0, -1, -1,\ 0, -1,\ 0, -1, -1)^T$	$\underline{f_u} \cdot (\ 1,\ 0,\ 1,\ 1,\ 0,\ 1,\ 0,\ 1, -1,\ 1,\ 1, -1,\ 1, -1,\ 1)^T$
m_{200}	$\underline{f_k} \cdot (\ 0,\ 1,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 0,\ 1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 1,\ 1,\ 1,\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$
m_{020}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$
m_{002}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 0,\ 1,\ 0,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 1,\ 0,\ 1,\ 1,\ 0,\ 1,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$
m_{011}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 0, -1, -1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 0,\ 1,\ 1, -1, -1,\ 1,\ 1,\ 1,\ 1)^T$
m_{101}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 1,\ 0,\ 0,\ 0,\ 1, -1)^T$	$\underline{f_u} \cdot (\ 0,\ 0, -1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1, -1, -1, -1,\ 1,\ 1)^T$
m_{110}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0, -1, -1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 1,\ 0, -1,\ 0,\ 0, -1,\ 1, -1, -1,\ 1,\ 1)^T$
m_{111}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1, -1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 1,\ 1, -1, -1,\ 1)^T$
m_{210}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0, -1,\ 0, -1,\ 0,\ 0, -1, -1, -1,\ 1, -1,\ 1)^T$
m_{201}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0, -1, -1,\ 0,\ 0,\ 0, -1, -1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 1, -1,\ 1, -1,\ 1)^T$
m_{120}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0, -1, -1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0, -1,\ 0,\ 1,\ 0,\ 0,\ 1, -1,\ 1, -1, -1,\ 1)^T$
m_{021}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 0, -1, -1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1, -1,\ 1,\ 1, -1,\ 1, -1,\ 1)^T$
m_{102}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1, -1,\ 0,\ 0,\ 0, -1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0, -1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1, -1,\ 1, -1, -1,\ 1)^T$
m_{012}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 0,\ 1, -1, -1, -1, -1,\ 1, -1,\ 1)^T$
m_{022}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$
m_{202}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 1,\ 0,\ 0,\ 0,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$
m_{220}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$
m_{211}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, -1, -1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, -1, -1,\ 1,\ 1,\ 1,\ 1)^T$
m_{121}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1, -1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1, -1, -1, -1,\ 1,\ 1)^T$
m_{112}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0, -1,\ 1, -1, -1,\ 1,\ 1)^T$

There are 15 unknown distributions, so it is necessary to find 15 independent equations. Despite there are 23 moments, some of the combinations of unknown distributions would result in linearly dependent equations. It is necessary to choose such moments where the groups of unknown distributions are independent. Firstly, all unique distribution groups and corresponding moments are displayed in Table 5.

Table 5: Unique unknown distribution groups for a cell with $(0, 1, -1)$ outer normal

Unique unknown distribution group	**Moments**
$\underline{f_u} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{000}
$\underline{f_u} \cdot (\ 0,\ 0,-1,\ 1,-1,\ 0,\ 1,\ 0,\ 0,\ 1,-1,\ 1,-1,-1,\ 1)^T$	m_{100}
$\underline{f_u} \cdot (\ 0,-1,\ 0,\ 0,-1,-1,-1,\ 1,-1,-1,-1,-1,\ 1,-1,\ 1)^T$	m_{010}
$\underline{f_u} \cdot (\ 1,\ 0,\ 1,\ 1,\ 0,\ 1,\ 0,\ 1,-1,\ 1,\ 1,-1,\ 1,-1,\ 1)^T$	m_{001}
$\underline{f_u} \cdot (\ 0,\ 0,\ 1,\ 1,\ 1,\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{200}
$\underline{f_u} \cdot (\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{020}
$\underline{f_u} \cdot (\ 1,\ 0,\ 1,\ 1,\ 0,\ 1,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{002}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,-1,\ 0,\ 1,\ 1,-1,-1,\ 1,\ 1,\ 1,\ 1)^T$	m_{011}
$\underline{f_u} \cdot (\ 0,\ 0,-1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,-1,-1,-1,\ 1,\ 1)^T$	m_{101}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,-1,\ 0,\ 0,-1,\ 1,-1,-1,\ 1,\ 1)^T$	m_{110}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,-1,\ 1,\ 1,-1,-1,\ 1)^T$	m_{111}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,-1,\ 0,-1,\ 0,\ 0,-1,-1,-1,\ 1,-1,\ 1)^T$	m_{210}
$\underline{f_u} \cdot (\ 0,\ 0,\ 1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 1,-1,\ 1,-1,\ 1)^T$	m_{201}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,-1,\ 0,\ 1,\ 0,\ 0,\ 1,-1,\ 1,-1,-1,\ 1)^T$	m_{120}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,-1,\ 1,\ 1,-1,\ 1,-1,\ 1)^T$	m_{021}
$\underline{f_u} \cdot (\ 0,\ 0,-1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,-1,\ 1,-1,-1,\ 1)^T$	m_{102}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,-1,\ 0,\ 1,-1,-1,-1,-1,\ 1,-1,\ 1)^T$	m_{012}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{022}
$\underline{f_u} \cdot (\ 0,\ 0,\ 1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{202}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{220}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,-1,-1,\ 1,\ 1,\ 1,\ 1)^T$	m_{211}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,-1,-1,-1,\ 1,\ 1)^T$	m_{121}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,-1,\ 1,-1,-1,\ 1,\ 1)^T$	m_{112}

As shown in Table 5, in this case, there are actually 23 unique distribution groups. In other configurations, some moments can share the same unknown group. See example of a face cell with outer normal $(0, 0, -1)$ in Table 6:

Table 6: Unique unknown distribution groups for a cell with $(0, 0, -1)$ outer normal

Unique unknown distribution group	**Moments**
$\underline{f_u} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{000}, m_{001}, m_{002}
$\underline{f_u} \cdot (\ 0,-1,\ 1,\ 0,\ 0,\ 1,-1,-1,\ 1)^T$	m_{100}, m_{101}, m_{102}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,-1,\ 1,-1,-1,\ 1,\ 1)^T$	m_{010}, m_{011}, m_{012}
$\underline{f_u} \cdot (\ 0,\ 1,\ 1,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1)^T$	m_{200}, m_{201}, m_{202}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T$	m_{020}, m_{021}, m_{022}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,-1,\ 1,-1,\ 1)^T$	m_{110}, m_{111}, m_{112}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,-1,-1,\ 1,\ 1)^T$	m_{210}, m_{211}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,-1,-1,\ 1)^T$	m_{120}, m_{121}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ 1,\ 1,\ 1)^T$	m_{220}

Returning back to our case of an outer normal $(0, 1, -1)$, it is now necessary to choose such moments from Table 5 so that the corresponding groups are linearly independent. It is also suggested to preferably select lower order moments that have clearer physical meaning [3]. Such selection of independent moments of lowest possible order is captured in Table 7:

Table 7: Chosen moments for a cell with $(0, 1, -1)$ outer normal

Chosen moments	$\underline{m} = (m_{000}, m_{100}, m_{010}, m_{001}, m_{200}, m_{020}, m_{002}, m_{101}, m_{110}, m_{210}, m_{201}, m_{120}, m_{102}, m_{202}, m_{220})^T$

The chosen moments can be set to their Maxwell-Boltzman equilibrium [2] [1]. This is exact for raw moments up to first order. For higher order moments, using the equilibrium means that the non-equilibrium part is neglected. This approximation still recovers incompressible Navier-Stokes equations correctly [2].

Equilibrium moments can be expressed as

$$m_{abc}^{eq} = \sum_i f_i^{eq} c_{xi}^a c_{yi}^b c_{zi}^c \tag{2.2}$$

where f_i^{eq} is the Maxwell-Boltzman equilibrium:

$$f_i^{\mathrm{eq}} = w_i \rho \left[1 + 3\, \underline{c}_i \cdot \underline{u} + \frac{9}{2} \left(\underline{c}_i \cdot \underline{u} \right)^2 - \frac{3}{2}\, \underline{u} \cdot \underline{u} \right]. \tag{2.3}$$

Full set of Maxwell-Boltzman equilibrium moments is shown in Table 8.

Table 8: Maxwell-Boltzmann equilibrium for each moment

Moment	**Maxwell–Boltzmann equilibrium**
m_{000}	ρ
m_{100}	$\rho\, u_x$
m_{010}	$\rho\, u_y$
m_{001}	$\rho\, u_z$
m_{200}	$\frac{1}{3}\rho + \rho\, u_x^2$
m_{020}	$\frac{1}{3}\rho + \rho\, u_y^2$
m_{002}	$\frac{1}{3}\rho + \rho\, u_z^2$
m_{011}	$\rho\, u_y u_z$
m_{101}	$\rho\, u_x u_z$
m_{110}	$\rho\, u_x u_y$
m_{111}	0
m_{210}	$\frac{1}{3}\rho\, u_y + \rho\, u_x^2 u_y$
m_{201}	$\frac{1}{3}\rho\, u_z + \rho\, u_x^2 u_z$
m_{120}	$\frac{1}{3}\rho\, u_x + \rho\, u_x u_y^2$
m_{021}	$\frac{1}{3}\rho\, u_z + \rho\, u_y^2 u_z$
m_{102}	$\frac{1}{3}\rho\, u_x + \rho\, u_x u_z^2$
m_{012}	$\frac{1}{3}\rho\, u_y + \rho\, u_y u_z^2$
m_{022}	$\frac{1}{9}\rho + \frac{1}{3}\rho\, u_y^2 + \frac{1}{3}\rho\, u_z^2 + \rho\, u_y^2 u_z^2$
m_{202}	$\frac{1}{9}\rho + \frac{1}{3}\rho\, u_x^2 + \frac{1}{3}\rho\, u_z^2 + \rho\, u_x^2 u_z^2$
m_{220}	$\frac{1}{9}\rho + \frac{1}{3}\rho\, u_x^2 + \frac{1}{3}\rho\, u_y^2 + \rho\, u_x^2 u_y^2$
m_{211}	$\frac{1}{3}\rho\, u_y u_z$
m_{121}	$\frac{1}{3}\rho\, u_x u_z$
m_{112}	$\frac{1}{3}\rho\, u_x u_y$

All equilibrium moments are known. The equations can be expressed in a matrix form:

$$\underline{\underline{K}}\, \underline{f_k} + \underline{\underline{U}}\, \underline{f_u} = \underline{m} \tag{2.4}$$

where $\underline{\underline{U}}$ is the matrix of unknown distribution coefficients:

$$\underline{\underline{U}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & -1 & 1 & -1 & 0 & 1 & 0 & 0 & 1 & -1 & 1 & -1 & -1 & 1 \\ 0 & -1 & 0 & 0 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & -1 & 1 & -1 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & -1 & -1 & -1 & 1 & -1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & 1 & -1 & 1 & -1 & -1 & 1 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \tag{2.5}$$

$\underline{\underline{K}}$ is the matrix of known distribution coefficients:

$$\underline{\underline{K}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & -1 & 0 & -1 & -1 & 0 & -1 & 0 & -1 & -1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \end{bmatrix} \tag{2.6}$$

Equation 2.4 can be solved by inversion:

$$\underline{f_u} = \underline{\underline{U}}^{-1} \left(\underline{m} - \underline{\underline{K}} \underline{f_k} \right) \tag{2.7}$$

As $\underline{\underline{U}}$ is relatively small and nice, it can be inversed using a symbolic solver.

$$\underline{\underline{U^{-1}}} = \begin{bmatrix} 1 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & -1/2 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 & -1/2 \\ 0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & -1/2 & 0 & 0 & -1/2 \\ 0 & -1/2 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & -1/2 & 0 \\ -1 & 0 & -1/2 & 1/2 & 1 & 1/2 & 1/2 & 0 & 0 & 1/2 & -1/2 & 0 & 0 & -1/2 & -1/2 \\ 0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/2 & -1/2 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 & 0 & -1/2 & 0 & 0 & 0 & 0 & -1/2 \\ 0 & 0 & 0 & -1/2 & 0 & 0 & 1/2 & 0 & 0 & 0 & 1/2 & 0 & 0 & -1/2 & 0 \\ 0 & -1/2 & 0 & 0 & -1/2 & 0 & 0 & 1/4 & -1/4 & -1/4 & 1/4 & 1/4 & 1/4 & 1/4 & 1/4 \\ 0 & 1/2 & 0 & 0 & -1/2 & 0 & 0 & -1/4 & 1/4 & -1/4 & 1/4 & -1/4 & -1/4 & 1/4 & 1/4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/4 & 0 & 0 & -1/4 & 0 & 1/4 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/4 & 1/4 & 0 & -1/4 & 0 & 0 & 1/4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & -1/4 & 0 & -1/4 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 1/4 & 0 & 1/4 & 0 & 0 & 1/4 \end{bmatrix} \tag{2.8}$$

The code to calculate all this can be generated for all different cell types. Shortened C++ code is listed in Listing 1.

Listing 1: Generated C++ code for a face cell with $(0, 1, -1)$ outer normal

```
// Extracting known distributions
float f0 = f0ArrayView[shiftedIndex[0]];
float f1 = f1ArrayView[shiftedIndex[1]];
(...)
float f22 = f22ArrayView[shiftedIndex[22]];

// Multiply K fk
const float kf0 = + f0 + f1 + f2 + f3 + f6 + f7 + f10 + f12 + f13 + f15 + f19 +
    f22;
const float kf1 = + f1 - f2 + f7 - f10 + f12 - f15 - f19 + f22;
(...)
const float kf14 = + f12 + f15 + f19 + f22;

// Calculate equilibrium moments
const float m0 = rho;
const float m1 = rho * ux;
(...)
const float m14 = (1.f/9.f) * rho + (1.f/3.f) * rho * ux * ux + (1.f/3.f) * rho
    * uy * uy + rho * ux * ux * uy * uy;

// Subtract m - Kfk
const float s0 = m0 - kf0;
const float s1 = m1 - kf1;
(...)
const float s14 = m14 - kf14;

// Multiply U^-1 * (m - Kfk) to get unknown distributions
float f4 = + s0 - s4 - s5 + s14;
float f5 = + s0 - s4 - s6 + s13;
(...)
float f26 = + 0.25f * s8 + 0.25f * s9 + 0.25f * s11 + 0.25f * s14;
```

2.2 Consistency condition for face cells

For face cells that only miss neighbours in one direction, it is possible to find a relation between ρ, u_x, u_y, u_z and the known distributions $\underline{f_k}$. This can be used for example to determine ρ in a velocity inlet that has u_x, u_y, u_z given, or to determine the missing normal velocity component in a pressure outlet that has given ρ and two tangential velocity components. The derivation is explained in [3]. Let's now consider a cell with outer normal $(0, 0, -1)$ as example.

Table 9: Known and unknown distributions for a cell with $(0, 0, -1)$ outer normal

Known distributions	$\underline{f_k} = (f_0, f_1, f_2, f_3, f_5, f_6, f_7, f_{10}, f_{11}, f_{12}, f_{13}, f_{15}, f_{16}, f_{18}, f_{19}, f_{22}, f_{23}, f_{25})^T$
Unknown distributions	$\underline{f_u} = (f_4, f_8, f_9, f_{14}, f_{17}, f_{20}, f_{21}, f_{24}, f_{26})^T$

From m_{000} it yields that

$$\begin{aligned}\rho = \underline{f_k} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T \\ + \underline{f_u} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T\end{aligned} \tag{2.9}$$

Similarly, from m_{001} it yields that

$$\begin{aligned}\rho u_z = \underline{f_k} \cdot (\ 0,\ 0,\ 0, -1,\ 0,\ 0, -1, -1,\ 0,\ 0, -1,\ 0,\ 0, -1, -1, -1, -1, -1)^T \\ + \underline{f_u} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T\end{aligned} \tag{2.10}$$

Equation 2.10 can be multiplied by the only non-zero element of the outer normal and added to 2.9.

This removes dependency on $\underline{f_u}$ in all cases.

$$\begin{gathered}\rho + (-1)\rho u_z \\ = \\ \underline{f_k} \cdot (\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)^T \\ +(-1)\underline{f_k} \cdot (\ 0,\ 0,\ 0,-1,\ 0,\ 0,-1,-1,\ 0,\ 0,-1,\ 0,\ 0,-1,-1,-1,-1,-1)^T \\ = \\ \underline{f_k} \cdot (\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 2,\ 2,\ 1,\ 1,\ 2,\ 1,\ 1,\ 2,\ 2,\ 2,\ 2,\ 2)^T\end{gathered} \tag{2.11}$$

So

$$\rho = \frac{1}{(1+(-1)u_z)} \underline{f_k} \cdot (\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 2,\ 2,\ 1,\ 1,\ 2,\ 1,\ 1,\ 2,\ 2,\ 2,\ 2,\ 2)^T \tag{2.12}$$

Or

$$u_z = (-1)\left(-1 + \frac{1}{\rho}\underline{f_k} \cdot (\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 2,\ 2,\ 1,\ 1,\ 2,\ 1,\ 1,\ 2,\ 2,\ 2,\ 2,\ 2)^T\right) \tag{2.13}$$

depending on which variable is unknown.

2.3 Reconstructing tangential velocity components in a pressure outlet

A face cell pressure outlet has given ρ and the normal velocity component can be calculated from the consistency condition as shown previously. In order to use the moment based boundary condition scheme, the tangential velocity components are needed, too. These components could be set to values in the upstream cells to achieve zero gradient, but then the calculation is no longer local. To keep the pressure outlet boundary condition fully local, it is possible to reconstruct tangential velocity components from the known distributions.

Let's consider a pressure outlet with outer normal $(0, 0, 1)$. ρ is prescribed and u_z is known from the consistency condition. It remains to find u_x and u_y. Known and unknown distributions are captured in Table 10:

Table 10: Known and unknown distributions for a cell with $(0, 0, 1)$ outer normal

Known distributions	$\underline{f_k} = (f_0, f_1, f_2, f_4, f_5, f_6, f_8, f_9, f_{11}, f_{12}, f_{14}, f_{15}, f_{16}, f_{17}, f_{20}, f_{21}, f_{24}, f_{26})^T$
Unknown distributions	$\underline{f_u} = (f_3, f_7, f_{10}, f_{13}, f_{18}, f_{19}, f_{22}, f_{23}, f_{25})^T$

It turns out that some moments share the same unknown distribution groups. The idea is to pick the lowest order pair of moments which shares the same unknown distribution group and whose equilibrium expression contains u_x or u_y. Such moments are shown in Table 11:

Table 11: Selected moment pairs for a cell with $(0, 0, 1)$ outer normal

Unknown distribution group	**Moment pairs**
$\underline{f_u} \cdot (\ 0,\ 1,-1,\ 0,\ 0,-1,\ 1,\ 1,-1)^T$	m_{100}, m_{102}
$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 1,-1,\ 1,\ 1,-1,-1)^T$	m_{010}, m_{012}

The selected moments are expressed in Table 12:

Table 12: Selected moments for a cell with $(0, 0, 1)$ outer normal

Moment	**Known distributions**	**Unknown distributions**
m_{100}	$\underline{f_k} \cdot (\ 0,\ 1,-1,\ 0,\ 0,\ 0,-1,\ 1,-1,\ 1,\ 0,-1,\ 1,\ 0,\ 1,-1,-1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 1,-1,\ 0,\ 0,-1,\ 1,\ 1,-1)^T$
m_{010}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,-1,\ 1,\ 0,\ 0,-1,\ 1,-1,\ 1,-1,\ 1,-1,-1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 1,-1,\ 1,\ 1,-1,-1)^T$
m_{102}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,-1,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,-1,-1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 1,-1,\ 0,\ 0,-1,\ 1,\ 1,-1)^T$
m_{012}	$\underline{f_k} \cdot (\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,-1,\ 0,\ 0,\ 1,-1,-1,\ 1,\ 1)^T$	$\underline{f_u} \cdot (\ 0,\ 0,\ 0,\ 1,-1,\ 1,\ 1,-1,-1)^T$

From each pair of moments that share the same group, by subtracting the corresponding equations, unknown distributions get eliminated.

Using equilibrium of moments m_{100}, m_{102} gives

$$\begin{gathered} m_{100} = \rho\, u_x = \\ = \underline{f_k} \cdot (\ 0,\ \ 1,-1,\ \ 0,\ \ 0,\ \ 0,-1,\ \ 1,-1,\ \ 1,\ \ 0,-1,\ \ 1,\ \ 0,\ \ 1,-1,-1,\ \ 1)^T \\ +\underline{f_u} \cdot (\ 0,\ \ 1,-1,\ \ 0,\ \ 0,-1,\ \ 1,\ \ 1,-1)^T \end{gathered} \tag{2.14}$$

$$\begin{gathered} m_{102} = \frac{1}{3}\rho\, u_x + \rho\, u_x u_z^2 = \\ = \underline{f_k} \cdot (\ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,-1,\ \ 1,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 1,-1,-1,\ \ 1)^T \\ +\underline{f_u} \cdot (\ 0,\ \ 1,-1,\ \ 0,\ \ 0,-1,\ \ 1,\ \ 1,-1)^T \end{gathered} \tag{2.15}$$

Subtracting equation 2.15 from 2.14 gives

$$\begin{gathered} \rho\, u_x - \left(\frac{1}{3}\rho\, u_x + \rho\, u_x u_z^2\right) = \\ = \underline{f_k} \cdot (\ 0,\ \ 1,-1,\ \ 0,\ \ 0,\ \ 0,-1,\ \ 1,-1,\ \ 1,\ \ 0,-1,\ \ 1,\ \ 0,\ \ 1,-1,-1,\ \ 1)^T \\ -\underline{f_k} \cdot (\ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,-1,\ \ 1,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 1,-1,-1,\ \ 1)^T \end{gathered} \tag{2.16}$$

and so

$$u_x = \frac{1}{\left(\frac{2}{3}\rho - \rho\ u_z^2\right)} \underline{f_k} \cdot (\ 0,\ \ 1,-1,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0,-1,\ \ 1,\ \ 0,-1,\ \ 1,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0)^T \tag{2.17}$$

Similarly, using m_{010} and m_{012} gives

$$u_y = \frac{1}{\left(\frac{2}{3}\rho - \rho\ u_z^2\right)} \underline{f_k} \cdot (\ 0,\ \ 0,\ \ 0,\ \ 0,-1,\ \ 1,\ \ 0,\ \ 0,-1,\ \ 1,\ \ 0,\ \ 1,-1,\ \ 0,\ \ 0,\ \ 0,\ \ 0,\ \ 0)^T \tag{2.18}$$

3 Classification of cells

Cell types are sorted in Table 13:

Cell type	**Placement**	**Given**	**Local**	**Algorithm**
Ignore cell	Anywhere	None	Yes	None
Fluid	Interior	None	Yes	1. Read $\underline{f}$ 2. Calculate ρ, u_x, u_y, u_z from $\underline{f}$ 3. Apply collision + forcing 4. Write $\underline{f}$ 5. Write ρ 6. Write u_x, u_y, u_z
BC Bounceback	Anywhere	None	Yes	1. Read $\underline{f}$ 2. Apply bounceback 3. Write $\underline{f}$
BC Velocity inlet	Face	u_x, u_y, u_z explicitly, store in cell and prevent overwriting	Yes	1. Read $\underline{f_k}$ 2. Read u_x, u_y, u_z + calculate ρ from consistency condition 3. Apply MBBC 4. Apply collision + forcing 5. Write $\underline{f}$ 6. Write ρ
BC Pressure outlet	Face	ρ explicitly, store in cell and prevent overwriting	Yes	1. Read $\underline{f_k}$ 2. Read ρ + calculate normal u component from consistency condition + calculate tangential u components from moments 3. Apply MBBC 4. Apply collision + forcing 5. Write $\underline{f}$ 6. Write u_x, u_y, u_z

Table 13: Classification of cell types

4 References

[1] Alessandro De Rosis. Nonorthogonal central-moments-based lattice boltzmann scheme in three dimensions. *Phys. Rev. E*, 95:013310, Jan 2017.

[2] Pavel Eichler, Radek Fučík, and Pavel Strachota. Investigation of mesoscopic boundary conditions for lattice boltzmann method in laminar flow problems. *Computers & Mathematics with Applications*, 173:87–101, 2024.

[3] Ivars Krastins, Andrew Kao, Koulis Pericleous, and Tim Reis. Moment-based boundary conditions for straight on-grid boundaries in three dimensional lattice boltzmann simulations. *International Journal for Numerical Methods in Fluids*, 92:1948–1974, 05 2020.

[4] Adrian Kummerländer, Márcio Dorn, Martin Frank, and Mathias J. Krause. Implicit propagation of directly addressed grids in lattice boltzmann methods. *Concurrency and Computation: Practice and Experience*, 35(8):e7509, 2023.