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A PREEMINENT
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Two accurate off-lattice pressure boundary algorithms in lattice Boltzmann method

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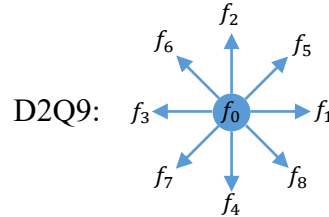
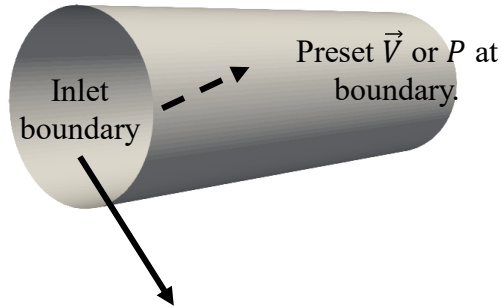
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Introduction:

- ❑ Interest in the lattice Boltzmann method (LBM) has been steadily increasing.
- ❑ Boundary condition (BC) is a necessity for numerical methods.
 - Uniquely determine the solution.
 - Affect stability and accuracy.
- ❑ Various choices for off-lattice velocity BC but rare choice for pressure BC.
 - Velocity BC: Bounce back^[1] (BB), Bouzidi^[2] (BFL), Zhao Yong^[3] (ZY), Yu^[4] (YLI) etc.
 - Pressure BC: Pressure anti-bounce back^[5] (PAB), pressure linear interpolation^[5] (PLI).
- ❑ Objective: develop an algorithm for off-lattice pressure BC.

Implementation of BC in LBM



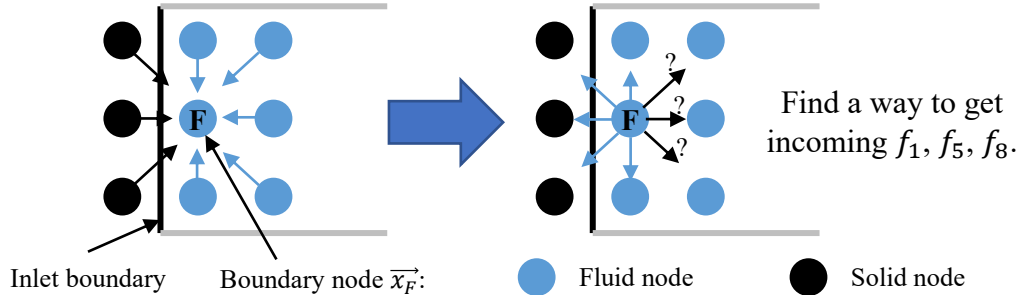
BGK collision operator

$$\Omega_i(\vec{x}, t) = -\frac{f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)}{\tau}$$

$$f_i^{eq}(\vec{x}, t) = \omega_i \rho \left(1 + \frac{\vec{u} \cdot \vec{c}_i}{c_s^2} + \frac{(\vec{u} \cdot \vec{c}_i)^2}{2c_s^4} - \frac{\vec{u} \cdot \vec{u}}{2c_s^2} \right)$$

Post collision $f_i^*(\vec{x}, t)$

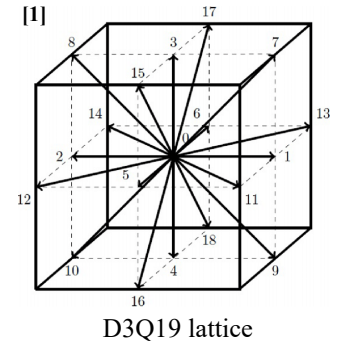
Post streaming $f_i(\vec{x} + \vec{c}_i, t + 1)$



Lattice Boltzmann equations:

$$\begin{aligned} f_i^*(\vec{x}, t) &= f_i(\vec{x}, t) + \Omega_i(\vec{x}, t) \\ f_i(\vec{x} + \vec{c}_i, t + 1) &= f_i^*(\vec{x}, t) \end{aligned}$$

$$\begin{aligned} \frac{P}{c_s^2} &= \rho = \sum_i f_i \\ \rho \vec{V} &= \sum_i f_i \vec{c}_i \end{aligned}$$



Common Dirichlet velocity boundary condition (link-wise algorithm)

BB^[1] (1994):
$$f_i(\vec{x}_F, t + 1) = f_i^*(\vec{x}_F, t) - 2\omega_i\rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2}$$

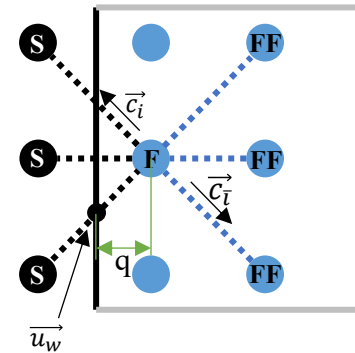
BFL^[2] (2001):
$$f_i(\vec{x}_F, t + 1) = 2qf_i^*(\vec{x}_F, t) + (1 - 2q)f_i^*(\vec{x}_{FF}, t) - 2\omega_i\rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2} \quad q < 0.5$$

$$f_i(\vec{x}_F, t + 1) = \frac{1}{2q}f_i^*(\vec{x}_F, t) + \frac{2q - 1}{2q}f_i^*(\vec{x}_F, t) - \frac{1}{q}\omega_i\rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2} \quad q \geq 0.5$$

YLI^[4] (2003):
$$f_i(\vec{x}_F, t + 1) = \frac{q}{1 + q}f_i^*(\vec{x}_F, t) + \frac{q}{1 + q}f_i^*(\vec{x}_F, t) + \frac{1 - q}{1 + q}f_i^*(\vec{x}_{FF}, t) - \frac{2}{1 + q}\omega_i\rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2}$$

CLI^[5] (2008):
$$f_i(\vec{x}_F, t + 1) = f_i^*(\vec{x}_F, t) + \frac{1 - 2q}{1 + 2q}f_i^*(\vec{x}_F, t) + \frac{1 - 2q}{1 + 2q}f_i^*(\vec{x}_{FF}, t) - \frac{4}{1 + 2q}\omega_i\rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2}$$

ZY^[3] (2017):
$$f_i(\vec{x}_F, t + 1) = \frac{1}{1 + 2q}f_i(\vec{x}_F, t) + \frac{2q}{1 + 2q}f_i^*(\vec{x}_F, t) - \frac{2}{1 + 2q}\omega_i\rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2}$$

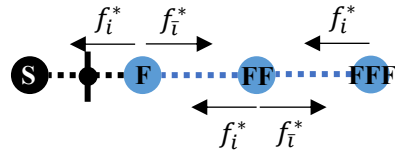


General equations

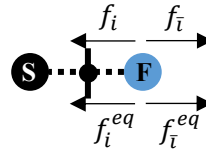
Ginzburg^[5] (2008): $f_i(\vec{x}_F, t + 1) = k_1 f_i^*(\vec{x}_F, t) + k_0 f_i^*(\vec{x}_{FF}, t) + k_{-1} f_i^*(\vec{x}_{FFF}, t) + \bar{k}_{-1} f_i^*(\vec{x}_F, t) + \bar{k}_{-2} f_i^*(\vec{x}_{FF}, t) + \varphi_i(\vec{x}_w, t) + f_i^{p.c.}(\vec{x}_F, t)$

Zhao, Yong^[3] (2017): $f_i(\vec{x}_F, t + 1) = a_1 f_i(\vec{x}_F, t) + a_2 f_i(\vec{x}_F, t) + a_3 f_i^{eq}(\vec{x}_F, t) + a_4 f_i^{eq}(\vec{x}_F, t) + a_5 \omega_i \rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2}$

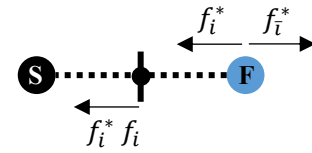
Marson^[7] (2021): $f_i(\vec{x}_F, t + 1) = a_1 f_i^*(\vec{x}_F, t) + a_2 f_i^*(\vec{x}_F, t) + a_3 f_i(\vec{x}_w, t + 1) + a_4 f_i^*(\vec{x}_w, t)$



Ginzburg



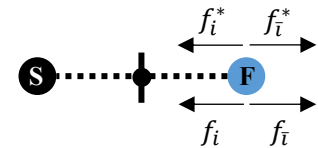
Zhao, Yong



Marson

Our goal: a single-node pressure BC, so our general equation is:

$$f_i(\vec{x}_F, t + 1) = A f_i^*(\vec{x}_F, t) + B f_i(\vec{x}_F, t) + C f_i^*(\vec{x}_F, t) + D f_i(\vec{x}_F, t) + E \omega_i \rho_F (1 + \frac{(\vec{c}_i \cdot \vec{u}_w)^2}{2c_s^4} - \frac{\vec{u}_w \cdot \vec{u}_w}{2c_s^2})$$



Our algorithm

Derivation of Single node (SN) algorithm

$$f_i(\vec{x}_F, t + 1) = Af_i^*(\vec{x}_F, t) + Bf_i(\vec{x}_F, t) + Cf_i^*(\vec{x}_F, t) + Df_i(\vec{x}_F, t)$$

Chapman-Enskog expansion

$$+ E\omega_i\rho_F\left(1 + \frac{(\vec{c}_i \cdot \vec{u}_w)^2}{2c_s^4} - \frac{\vec{u}_w \cdot \vec{u}_w}{2c_s^2}\right)$$

Taylor expansion

Make E = 2

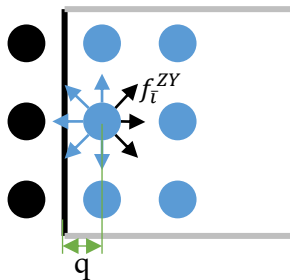
$$\begin{cases} A + B - C - D = -1 & \longrightarrow \text{Reach 1st order accuracy for velocity} \\ A + B + C + D + E = 1 & \longrightarrow \text{Reach 1st order accuracy for pressure} \\ A - C + qE = 0 & \longrightarrow \text{Reach 2nd order accuracy for pressure} \\ A + C + \tau E = 0 & \longrightarrow \text{Reach 2nd order accuracy for velocity} \end{cases}$$

$$\begin{cases} A = -q - \tau \\ B = q + \tau - 1 \\ C = q - \tau \\ D = \tau - q \\ E = 2 \end{cases}$$

$$\begin{aligned} f_i(\vec{x}_F, t + 1) &= (-q - \tau)f_i^*(\vec{x}_F, t) + (q + \tau - 1)f_i(\vec{x}_F, t) + (q - \tau)f_i^*(\vec{x}_F, t) + (\tau - q)f_i(\vec{x}_F, t) \\ &\quad + 2\omega_i\rho_F\left(1 + \frac{(\vec{c}_i \cdot \vec{u}_w)^2}{2c_s^4} - \frac{\vec{u}_w \cdot \vec{u}_w}{2c_s^2}\right) \end{aligned}$$

Density correction (DC) scheme

1. Apply ZY velocity:

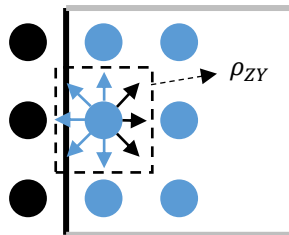


$$f_i^{ZY}(\vec{x}_F, t)$$

$$= \frac{1}{1+2q} f_i(\vec{x}_F, t) + \frac{2q}{1+2q} f_i^*(\vec{x}_F, t)$$

$$- \frac{2}{1+2q} \omega_i \rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2}$$

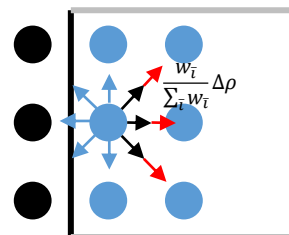
2. Find correction ($\Delta\rho$):



$$\rho_{ZY} = \sum_i f_i(\vec{x}_F, t)$$

$$\Delta\rho = \rho_F - \rho_{ZY}$$

3. Add correction:



$$f_{\bar{i}}(\vec{x}_F, t+1) = f_{\bar{i}}^{ZY}(\vec{x}_F, t) + \frac{w_{\bar{i}}}{\sum_i w_{\bar{i}}} \Delta\rho$$

\bar{i} : incoming direction

Macroscopic velocity and density in the algorithms

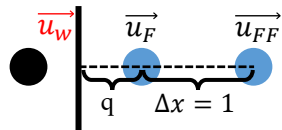
$$\text{SN: } f_i(x_F, t + 1) = (-q - \tau)f_i^*(x_F, t) + (q + \tau - 1)f_i(x_F, t) + (q - \tau)f_i^*(x_F, t) + (\tau - q)f_i(x_F, t) + 2\omega_i \rho_F (1 + \frac{(\vec{c}_i \cdot \vec{u}_w)^2}{2c_s^4} - \frac{\vec{u}_w \cdot \vec{u}_w}{2c_s^2})$$

$$\text{DC: } f_i(\vec{x}_F, t + 1) = \frac{1}{1+2q} f_i(\vec{x}_F, t) + \frac{2q}{1+2q} f_i^*(\vec{x}_F, t) - \frac{2}{1+2q} \omega_i \rho_0 \frac{\vec{c}_i \cdot \vec{u}_w}{c_s^2} + \frac{w_i}{\sum_i w_i} (\rho_F - \rho_{ZY})$$

Extrapolation of \vec{u}_w link-wise:

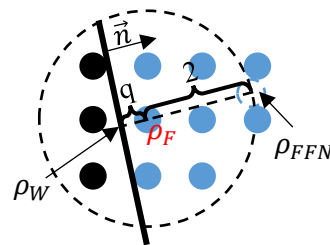
$$\vec{u}_w = q(\vec{u}_F - \vec{u}_{FF}) + \vec{u}_F$$

Has fluid neighbor:



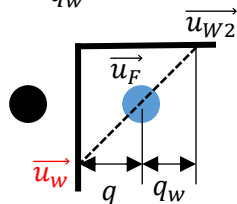
Interpolation of ρ_F in \vec{n} direction:

$$\rho_F = \frac{2}{2+q} (\rho_W - \rho_{FFN}) + \rho_{FFN}$$

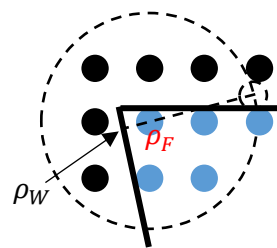


$$\vec{u}_w = \frac{q}{q_w} (\vec{u}_F - \vec{u}_{W2}) + \vec{u}_F$$

No fluid neighbor:



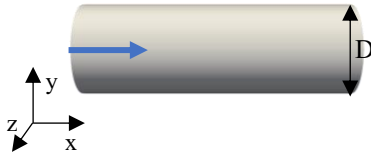
$$\rho_F = \rho_W$$



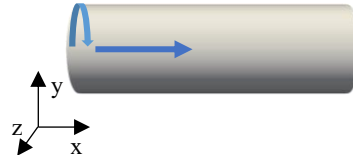
Simulation setup

Tested flow cases:

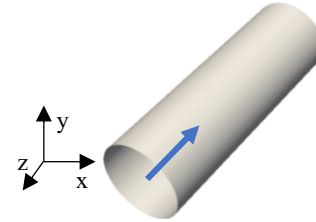
(1) Poiseuille flow;



(2) Taylor-Couette with axial flow;



(3) Poiseuille flow (arbitrary orientation);



Simulation setup:

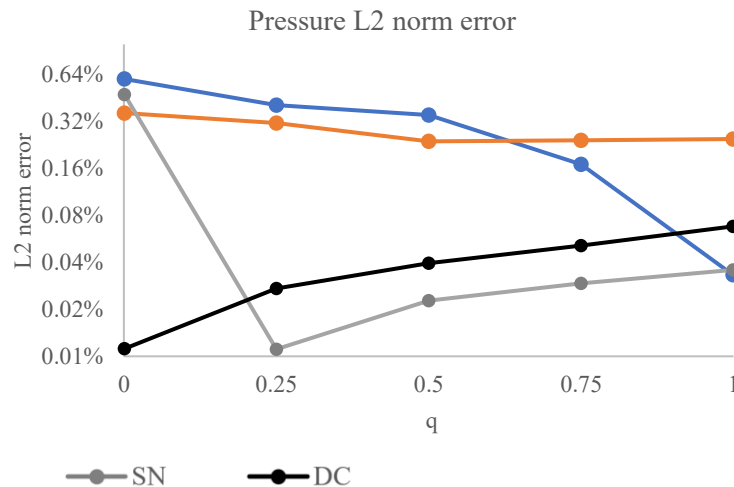
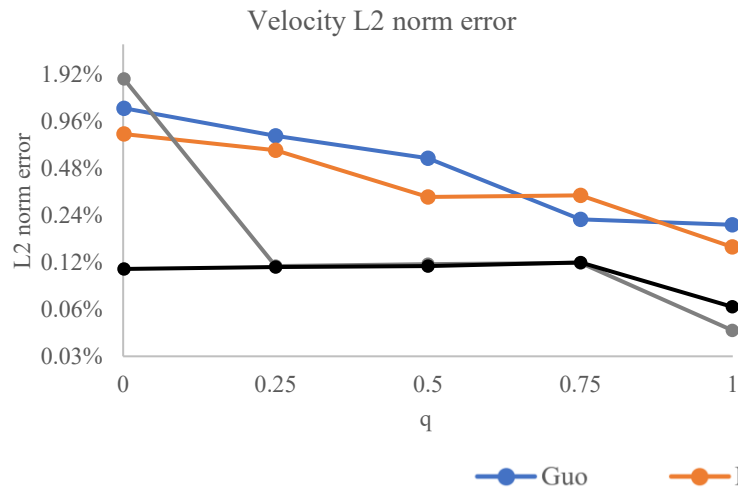
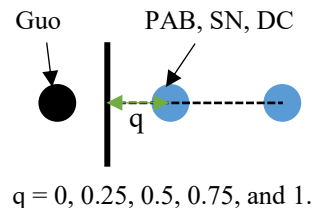
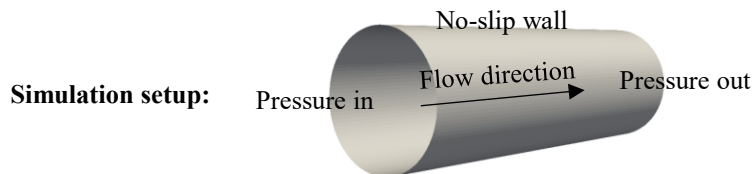
$$\frac{D}{dx} = 30; \tau = 1; \text{Incompressible BGK.}$$

Other comparison algorithms:

$$\text{PAB}^{[5]}: f_i(\vec{x}_F, t + 1) = -f_i^*(\vec{x}_F, t) + 2\omega_i\rho_w(1 + \frac{(\vec{c}_i \cdot \vec{u}_w)^2}{2c_s^4} - \frac{\vec{u}_w \cdot \vec{u}_w}{2c_s^2})$$

$$\text{Guo}^{[6,8]}: f_i(\vec{x}_S, t) = f_i^{eq}(\rho_w, \vec{u}_w) + f_i^{neq}(\vec{x}_F, t), \text{ where } \vec{u}_w = (\vec{u}_F \cdot \vec{n})\vec{n}$$

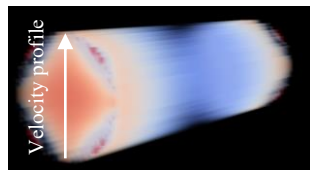
Accuracy with different q



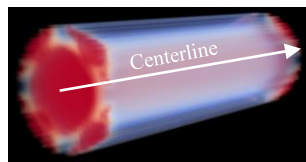
$$\text{L2 norm error} = \sqrt{\frac{\sum_{i=\text{node}} (\|\vec{v}_{\text{num}_i}\| - \|\vec{v}_{\text{theo}_i}\|)^2}{\sum_{i=\text{node}} (\|\vec{v}_{\text{theo}_i}\|)^2}}$$

Poiseuille flow in a cylinder

Velocity error field



Pressure error field



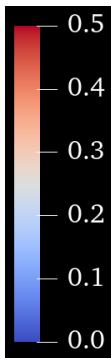
Guo

PAB

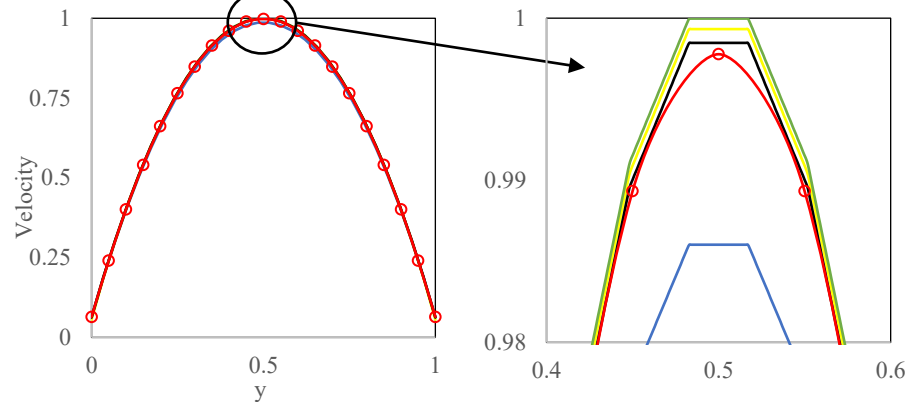
SN

DC

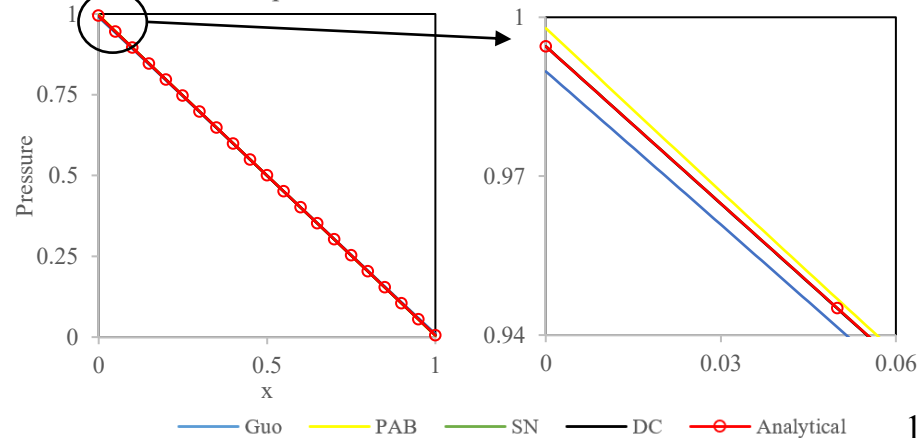
Unit: %



Velocity profile



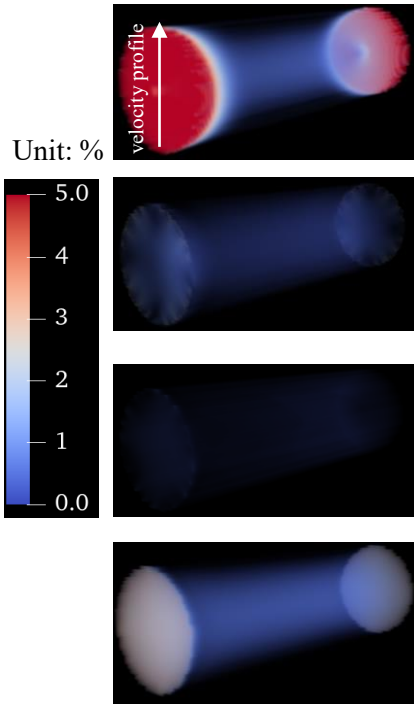
Centerline pressure



Taylor-Couette flow with axial velocity

Velocity error field

Pressure error field

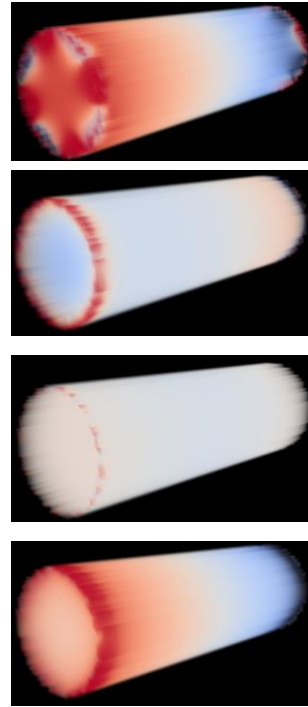


Guo

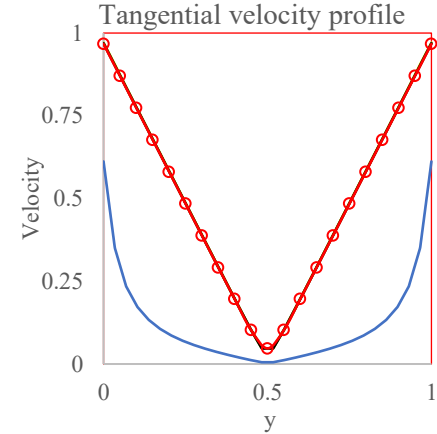
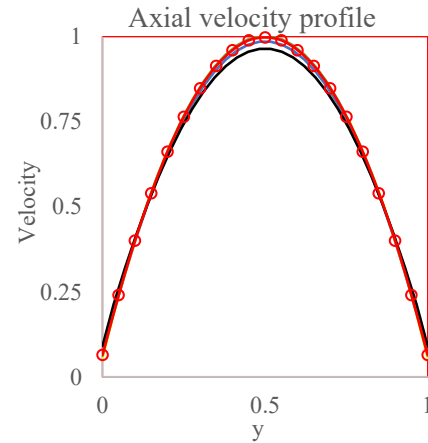
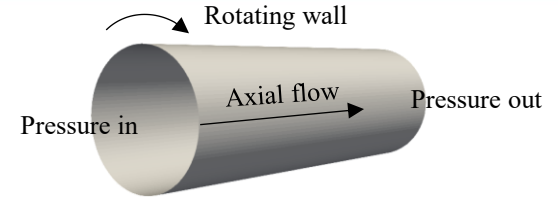
PAB

SN

DC

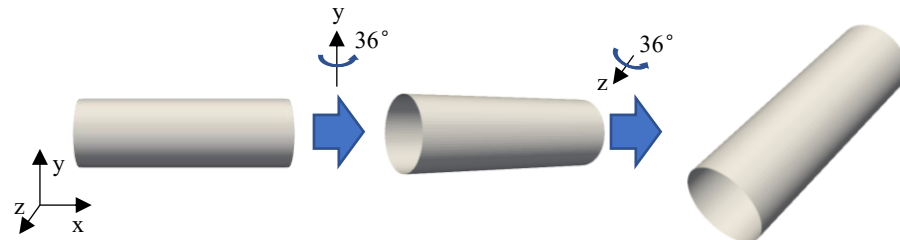
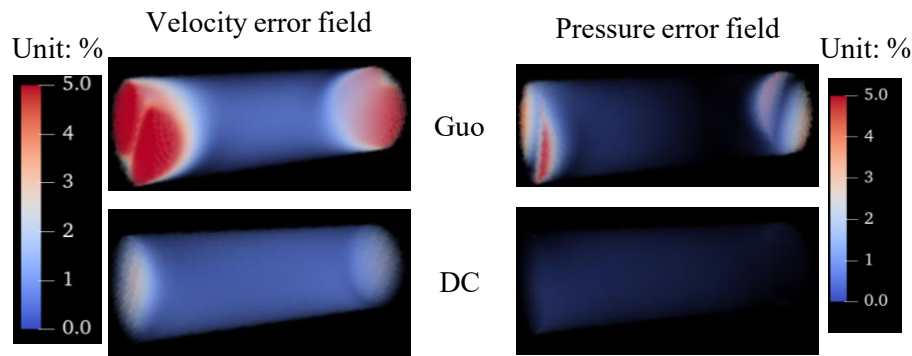


Simulation setup:



— Guo — PAB — SN — DC —○— Analytical

Poiseuille flow in a cylinder with arbitrary orientation



Usability

Algorithm	Normal flow	Tangential flow	Arbitrary orientation
Guo	√	×	√
PAB	√	√	×
SN	√	√	×
DC	√	√	√

Quantitative results

Poiseuille flow

Algorithm	V L2 norm error	P L2 norm error
Guo	0.56%	0.35%
PAB	0.31%	0.24%
SN	0.12%	0.02%
DC	0.11%	0.04%

Taylor-Couette flow with axial velocity

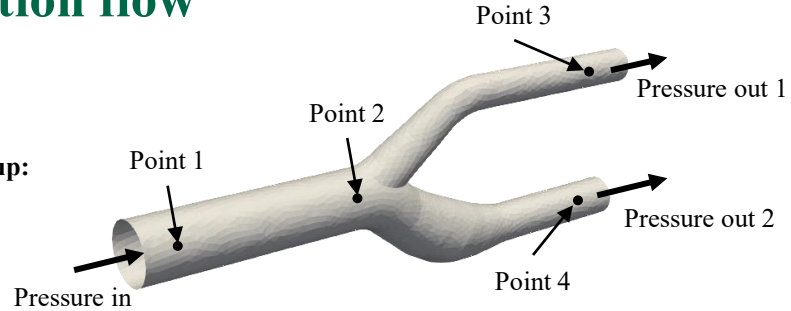
Algorithm	V L2 norm error	P L2 norm error
Guo	7.42%	1.06%
PAB	0.17%	0.90%
SN	0.05%	0.86%
DC	0.41%	0.96%

Poiseuille flow with arbitrary orientation

Algorithm	V L2 norm error	P L2 norm error
Guo	4.33%	1.32%
PAB	nan	nan
SN	nan	nan
DC	1.08%	0.36%

Bifurcation flow

Simulation setup:



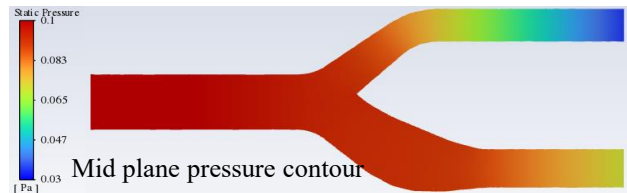
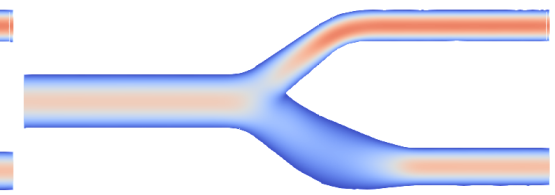
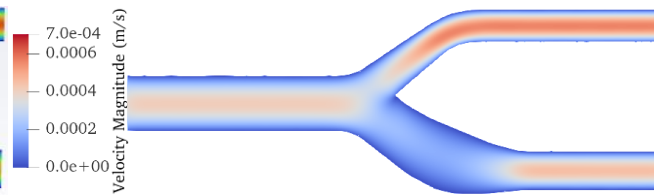
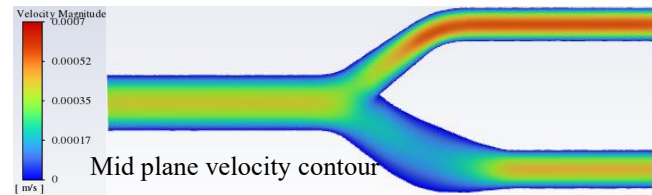
Algorithm	SN	DC	Benchmark	SN Difference	DC Difference
Inlet Q (m ³ /s)	1.01E-08	1.01E-08	1.01E-08	0.61%	0.45%
Outlet 1 Q (m ³ /s)	-4.80E-09	-4.80E-09	-4.82E-09	0.44%	0.37%
Outlet 2 Q (m ³ /s)	-5.32E-09	-5.32E-09	-5.33E-09	0.31%	0.13%
Point 1 V (m/s)	4.09E-04	4.09E-04	4.11E-04	0.43%	0.59%
Point 2 V (m/s)	2.37E-04	2.39E-04	2.38E-04	0.17%	0.41%
Point 3 V (m/s)	5.57E-04	5.56E-04	5.56E-04	0.13%	0.02%
Point 4 V (m/s)	4.48E-04	4.49E-04	4.47E-04	0.16%	0.43%
Point 2 P (Pa)	9.27E-02	9.27E-02	9.28E-02	0.13%	0.09%

$$\text{difference} = \left| \frac{\text{num}_{\text{LBM}} - \text{num}_{\text{Fluent}}}{\text{num}_{\text{Fluent}}} \right|$$

ANSYS Fluent benchmark

SN

DC





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Conclusion:

- Two off-lattice pressure boundary condition are developed and compared to existing algorithms.
- The proposed SN algorithm has smaller error in all presented flow cases.
- The proposed DC algorithm is applicable in arbitrary orientation with reasonable error.

Future work:

- Improve SN algorithm to support the boundary with arbitrary orientation.
- Analyze the stability and accuracy of the two proposed algorithms under various relaxation time (τ), Mach number, and resolution.



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Reference:

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Thank you!