Efficient Kinetic Simulation of Two-Phase Flows: *Supplementary Material*

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CCS Concepts: • **Computing methodologies** → **Physical simulation**.

Additional Key Words and Phrases: Multiphase flow, turbulent flow simulation, lattice Boltzmann method

In this supplementary material, we discuss some of the details mentioned in the original ACM SIGGRAPH '22 technical paper entitled "*Efficient Kinetic Simulation of Two-Phase Flows*".

A VELOCITY-BASED LATTICE-BOLTZMANN EQUATIONS

After discretizing the mesoscopic velocities in Eq. (1) of the original paper, the evolution of the traditional density distribution function f_i satisfies the discrete Boltzmann equations:

$$\left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla\right) f_i = -\Omega_i(f_i - f_i^{\text{eq}}) + F_i, \tag{a}$$

where $\mathbf{c}_i$ denotes a D3Q27 lattice velocity (see Fig. 6 of the paper) and $\mathbf{F}_i$ is the projection in distribution space of the forcing terms. To obtain the pressure-velocity formulation (called the "velocity-based" formulation in [Fakhari et al. 2017]), we first transform the distribution component f_i into $\hat{f}_i$, with

$$\hat{f}_i = \frac{f_i}{\rho} + (p^* - 1) w_i^c, \tag{b}$$

where $p^* = p/\rho c^2$ is the LBM-normalized pressure and w_i^c the D3Q27 quadrature weight for link i. The corresponding $\hat{f}_i$'s evolution is:

$$\left(\frac{\partial}{\partial t} + \mathbf{c}_i \cdot \nabla\right) \hat{f}_i = -\Omega_i(\hat{f}_i - \hat{f}_i^{\text{eq}}) + \hat{F}_i, \tag{c}$$

where the equilibrium distributions $\hat{f}_i^{\text{eq}}$ and force terms are now:

$$\hat{f}_i^{\text{eq}} = \Gamma_i + (p^* - 1) w_i^c, \quad \text{and} \quad \hat{F}_i = F_i/\rho, \tag{d}$$

Γ being a dimensionless distribution function given in Eq. (5) of the original paper. Using a trapezoidal time integrator [Coreixas 2018] yields the update rule:

$$\hat{f}(\mathbf{x} + \Delta x, t + \Delta t) - \hat{f}(\mathbf{x}, t) = \frac{\Delta t}{2}\left[\hat{F}_i - \Omega_i(\hat{f} - \hat{f}_i^{\text{eq}})\right]_{(\mathbf{x}+\Delta x, t+\Delta t)} + \frac{\Delta t}{2}\left[\hat{F}_i - \Omega_i(\hat{f} - \hat{f}_i^{\text{eq}})\right]_{(\mathbf{x}, t)},$$

where $\delta x = c_i \delta t$. To turn this implicit update into an explicit one, we further use a change of variables from $\hat{f}$ to g through:

$$g_i = \hat{f}_i - \frac{\Delta t}{2}\left[\hat{F}_i - \Omega_i(\hat{f}_i - \hat{f}_i^{\text{eq}})\right], \tag{e}$$

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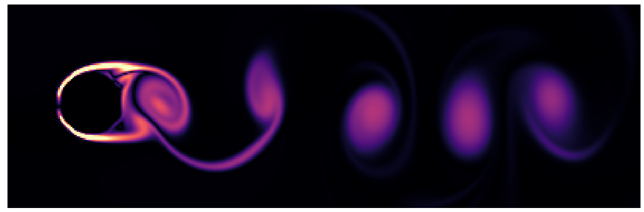

Fig. 1. **Von Kármán vortex street.** A vorticity plot of a simulation of a single-phase flow past a round obstacle in 2D shows the typical vortex shedding, even when a velocity-based (pressure-velocity) formulation based on distribution function g instead of f is used.

which does not affect mass, momentum or total energy preservation. We then obtain the final second-order accurate and explicit update rule of g_i with $\Delta x = \Delta t = 1$ given in Eq. (3) of the original paper, where the modified equilibrium distribution component $g_i{}^{\text{eq}}$ is:

$$g_i{}^{\text{eq}} = \hat{f}_i^{\text{eq}} - \frac{1}{2}\hat{F}_i. \tag{f}$$

This different formulation of LBM can still handle single-phase fluid simulation as it is just a rewriting of the original formulation; a vorticity visualization of a typical von Kármán vortex street, where a fluid flows past a disk-shaped obstacle, is shown in Fig. 1.

B EQUILIBRIUM DISTRIBUTION

From Eq. (5) of the original paper, the sixth-order Hermite expansion of Γ_i is written out as:

$$\begin{aligned}\Gamma_i \approx w_i^c \Bigg[& 1 + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c^2} + \frac{1}{2c^4}\mathbf{H}^{(2)}(\boldsymbol{c}_i) : \boldsymbol{u}\otimes\boldsymbol{u} \\ & + \frac{1}{2c^6}\Big(\mathbf{H}^{(3)}_{ixxy}\boldsymbol{u}_x^2\boldsymbol{u}_y + \mathbf{H}^{(3)}_{ixxz}\boldsymbol{u}_x^2\boldsymbol{u}_z + \mathbf{H}^{(3)}_{ixyy}\boldsymbol{u}_x\boldsymbol{u}_y^2 \\ & + \mathbf{H}^{(3)}_{ixzz}\boldsymbol{u}_x\boldsymbol{u}_z^2 + \mathbf{H}^{(3)}_{iyzz}\boldsymbol{u}_y\boldsymbol{u}_z^2 + \mathbf{H}^{(3)}_{iyzz}\boldsymbol{u}_y^2\boldsymbol{u}_z + \mathbf{H}^{(3)}_{ixyz}\boldsymbol{u}_x\boldsymbol{u}_y\boldsymbol{u}_z\Big) \\ & + \frac{1}{4c^8}\Big[\mathbf{H}^{(4)}_{ixxyy}\boldsymbol{u}_x^2\boldsymbol{u}_y^2 + \mathbf{H}^{(4)}_{ixxzz}\boldsymbol{u}_x^2\boldsymbol{u}_z^2 + \mathbf{H}^{(4)}_{iyyzz}\boldsymbol{u}_y^2\boldsymbol{u}_z^2 \\ & + 2\Big(\mathbf{H}^{(4)}_{ixyzz}\boldsymbol{u}_x\boldsymbol{u}_y\boldsymbol{u}_z^2 + \mathbf{H}^{(4)}_{ixyyz}\boldsymbol{u}_x\boldsymbol{u}_y^2\boldsymbol{u}_z + \mathbf{H}^{(4)}_{ixxyz}\boldsymbol{u}_x^2\boldsymbol{u}_y\boldsymbol{u}_z\Big)\Big] \\ & + \frac{1}{4c^{10}}\Big(\mathbf{H}^{(5)}_{ixxyzz}\boldsymbol{u}_x^2\boldsymbol{u}_y\boldsymbol{u}_z^2 + \mathbf{H}^{(5)}_{ixxyyz}\boldsymbol{u}_x^2\boldsymbol{u}_y^2\boldsymbol{u}_z \\ & + \mathbf{H}^{(5)}_{ixyyzz}\boldsymbol{u}_x\boldsymbol{u}_y^2\boldsymbol{u}_z^2\Big) + \frac{1}{8c^{12}}\mathbf{H}^{(6)}_{ixxyyzz}\boldsymbol{u}_x^2\boldsymbol{u}_y^2\boldsymbol{u}_z^2\Bigg],\end{aligned} \tag{g}$$

where $\mathbf{H}^{(n)}_{i\alpha_1\ldots\alpha_n}$ is a shorthand notation of the tensor element of the n-order Hermite polynomial basis $\mathbf{H}^{(n)}(\boldsymbol{c}_i)$ corresponding to the $\alpha_1 \ldots \alpha_n$ component.

C FORCE TERM

In 3D, the sixth-order Hermite expansion of the projection to the distribution space of a force $\mathbf{F}$ is:

$$\begin{aligned}
G_i &= \frac{\mathbf{F}}{\rho} \cdot \nabla_{\boldsymbol{c}_i} f_i \\
&= w_i^c \big(\frac{\boldsymbol{F} \cdot \boldsymbol{c}_i}{c^2} + \frac{1}{2c^4} [\mathbf{H}_{ixx}^{(2)} (2\boldsymbol{u}_x F_x) + \mathbf{H}_{iyy}^{(2)} (2\boldsymbol{u}_y F_y) + \mathbf{H}_{izz}^{(2)} (2\boldsymbol{u}_z F_z) \\
&+ 2\mathbf{H}_{ixy}^{(2)} (\boldsymbol{u}_x f_y + \boldsymbol{u}_y F_x) + 2\mathbf{H}_{ixz}^{(2)} (\boldsymbol{u}_x F_z + \boldsymbol{u}_z F_x) \\
&+ 2\mathbf{H}_{iyz}^{(2)} (\boldsymbol{u}_y f_z + \boldsymbol{u}_z F_y)] + \frac{1}{2c^6} [\mathbf{H}_{ixxy}^{(3)} (2\boldsymbol{u}_x \boldsymbol{u}_y F_x + \boldsymbol{u}_x^2 F_y) \\
&+ \mathbf{H}_{ixxz}^{(3)} (2\boldsymbol{u}_x \boldsymbol{u}_z F_x + \boldsymbol{u}_x^2 F_z) + \mathbf{H}_{ixyy}^{(3)} (2\boldsymbol{u}_x \boldsymbol{u}_y F_y + \boldsymbol{u}_y^2 F_x) \\
&+ \mathbf{H}_{ixzz}^{(3)} (2\boldsymbol{u}_x \boldsymbol{u}_z F_z + \boldsymbol{u}_z^2 F_x) + \mathbf{H}_{iyzz}^{(3)} (2\boldsymbol{u}_y \boldsymbol{u}_z F_z + \boldsymbol{u}_z^2 F_y) \\
&+ \mathbf{H}_{iyyz}^{(3)} (2\boldsymbol{u}_y \boldsymbol{u}_z F_y + \boldsymbol{u}_y^2 F_z) + 2\mathbf{H}_{ixyz}^{(3)} (\boldsymbol{u}_x \boldsymbol{u}_y F_z + \boldsymbol{u}_x F_y \boldsymbol{u}_z + F_x \boldsymbol{u}_y \boldsymbol{u}_z)] \\
&+ \frac{1}{4c^8} [\mathbf{H}_{ixxyy}^{(4)} (2\boldsymbol{u}_x^2 \boldsymbol{u}_y F_y + 2\boldsymbol{u}_x \boldsymbol{u}_y^2 F_x) + \mathbf{H}_{ixxzz}^{(4)} (2\boldsymbol{u}_x^2 \boldsymbol{u}_z F_z + \\
&2\boldsymbol{u}_x \boldsymbol{u}_z^2 F_x) + \mathbf{H}_{iyyzz}^{(4)} (2\boldsymbol{u}_y^2 \boldsymbol{u}_z F_z + 2\boldsymbol{u}_y \boldsymbol{u}_z^2 F_y) + 2\mathbf{H}_{ixyzz}^{(4)} (2\boldsymbol{u}_x \boldsymbol{u}_y \boldsymbol{u}_z F_z \\
&+ \boldsymbol{u}_x F_y \boldsymbol{u}_z^2 + F_x \boldsymbol{u}_y \boldsymbol{u}_z^2) + 2\mathbf{H}_{ixyyz}^{(4)} (2\boldsymbol{u}_x \boldsymbol{u}_y \boldsymbol{u}_z F_y + \boldsymbol{u}_x \boldsymbol{u}_y^2 F_z + F_x \boldsymbol{u}_y^2 \boldsymbol{u}_z) \\
&+ 2\mathbf{H}_{ixxyz}^{(4)} (2\boldsymbol{u}_x \boldsymbol{u}_y \boldsymbol{u}_z F_x + \boldsymbol{u}_y \boldsymbol{u}_x^2 F_z + \boldsymbol{u}_x^2 \boldsymbol{u}_z F_y)] \\
&+ \frac{1}{4c^{10}} [\mathbf{H}_{ixxyyz}^{(5)} (2\boldsymbol{u}_x \boldsymbol{u}_y^2 \boldsymbol{u}_z F_x + 2\boldsymbol{u}_x^2 \boldsymbol{u}_y \boldsymbol{u}_z F_y + \boldsymbol{u}_x^2 \boldsymbol{u}_y^2 F_z) \\
&+ \mathbf{H}_{ixxyzz}^{(5)} (2\boldsymbol{u}_x \boldsymbol{u}_y \boldsymbol{u}_z^2 F_x + \boldsymbol{u}_x^2 \boldsymbol{u}_z^2 F_y + 2\boldsymbol{u}_x^2 \boldsymbol{u}_y \boldsymbol{u}_z F_z) \\
&+ \mathbf{H}_{ixyyzz}^{(5)} (\boldsymbol{u}_y^2 \boldsymbol{u}_z^2 F_x + 2\boldsymbol{u}_x \boldsymbol{u}_y \boldsymbol{u}_z^2 F_y + 2\boldsymbol{u}_x \boldsymbol{u}_y^2 \boldsymbol{u}_z F_z)] \qquad \text{(h)} \\
&+ \frac{1}{8c^{12}} \mathbf{H}_{ixxyyzz}^{(6)} (2\boldsymbol{u}_x \boldsymbol{u}_y^2 \boldsymbol{u}_z^2 F_x + 2\boldsymbol{u}_x^2 \boldsymbol{u}_y \boldsymbol{u}_z^2 F_y + 2\boldsymbol{u}_x^2 \boldsymbol{u}_y^2 \boldsymbol{u}_z F_z) \big).
\end{aligned}$$

Fortunately, one can evaluate this expression far more efficiently through its expression in central moment space, see Sec. 3.2 in the original paper.

D D3Q7 LATTICE

The set of lattice velocities $\{\mathbf{d}_0, \mathbf{d}_1, ..., \mathbf{d}_6\}$ at a grid node in the D3Q27 model is defined as (see Fig. 6(right) of the original paper):

$$\mathbf{d}_0 = \begin{bmatrix}0\\0\\0\end{bmatrix}, \mathbf{d}_1 = \begin{bmatrix}1\\0\\0\end{bmatrix}, \mathbf{d}_2 = \begin{bmatrix}-1\\0\\0\end{bmatrix}, \mathbf{d}_3 = \begin{bmatrix}0\\1\\0\end{bmatrix}, \mathbf{d}_4 = \begin{bmatrix}0\\-1\\0\end{bmatrix}, \mathbf{d}_5 = \begin{bmatrix}0\\0\\1\end{bmatrix}, \mathbf{d}_6 = \begin{bmatrix}0\\0\\-1\end{bmatrix}.$$

The associated weights are:

$$w_0^d = \frac{1}{4},\ w_1^d = w_2^d = w_3^d = w_4^d = w_5^d = w_6^d = \frac{1}{8},$$

with a LBM speed of sound $d = 1/2$.

E CENTRAL MOMENT PROJECTION MATRIX

The projection matrix onto central moment space is expressed as:

$$\begin{gathered}
|M_0\rangle = \big|(1,1,1,1,1,1,1)\big\rangle, \quad |M_1\rangle = \big|\overline{d}_{xi}\big\rangle, \\
|M_2\rangle = \big|\overline{d}_{yi}\big\rangle, \quad |M_3\rangle = \big|\overline{d}_{zi}\big\rangle, \\
|M_4\rangle = \big|\overline{d}_{xi}^2 - \overline{d}_{yi}^2\big\rangle, \quad |M_5\rangle = \big|\overline{d}_{xi}^2 - \overline{d}_{zi}^2\big\rangle, \qquad \text{(i)} \\
|M_6\rangle = \big|\overline{d}_{xi}^2 + \overline{d}_{yi}^2 + \overline{d}_{zi}^2\big\rangle,
\end{gathered}$$

where we use the convention $\overline{\mathbf{d}}_{.} = \mathbf{d}_{.} - \mathbf{u} = (\overline{d}_{x.}, \overline{d}_{y.}, \overline{d}_{z.})$.

F HIGH-ORDER EQUILIBRIUM DISTRIBUTION $\mathbf{g}^{\mathrm{eq}}$

The expressions of $\hat{f}^{\,\mathrm{eq}}$ directly in central-moment space are:

$$\begin{gathered}
\hat{f}_0^{\mathrm{eq}} = p^*, \\
\hat{f}_1^{\mathrm{eq}} = -\mathbf{u}_x(p^*-1), \quad \hat{f}_2^{\mathrm{eq}} = -\mathbf{u}_y(p^*-1), \quad \hat{f}_3^{\mathrm{eq}} = -\mathbf{u}_z(p^*-1), \\
\hat{f}_4^{\mathrm{eq}} = \mathbf{u}_x\mathbf{u}_y(p^*-1), \quad \hat{f}_5^{\mathrm{eq}} = \mathbf{u}_x\mathbf{u}_z(p^*-1), \quad \hat{f}_6^{\mathrm{eq}} = \mathbf{u}_y\mathbf{u}_z(p^*-1), \\
\hat{f}_7^{\mathrm{eq}} = (\mathbf{u}_x\mathbf{u}_x - \mathbf{u}_y\mathbf{u}_y)(p^*-1), \quad \hat{f}_8^{\mathrm{eq}} = (\mathbf{u}_x\mathbf{u}_x - \mathbf{u}_z\mathbf{u}_z)(p^*-1), \\
\hat{f}_9^{\mathrm{eq}} = p^* + \mathbf{u}_x\mathbf{u}_x p^* + \mathbf{u}_y\mathbf{u}_y p^* + \mathbf{u}_z\mathbf{u}_z p^* - \mathbf{u}_x\mathbf{u}_x - \mathbf{u}_y\mathbf{u}_y - \mathbf{u}_z\mathbf{u}_z, \\
\hat{f}_{10}^{\mathrm{eq}} = -\frac{1}{3}\mathbf{u}_x(p^*-1)(3\mathbf{u}_y\mathbf{u}_y + 3\mathbf{u}_z\mathbf{u}_z + 2), \\
\hat{f}_{11}^{\mathrm{eq}} = -\frac{1}{3}\mathbf{u}_y(p^*-1)(3\mathbf{u}_x\mathbf{u}_x + 3\mathbf{u}_z\mathbf{u}_z + 2), \\
\hat{f}_{12}^{\mathrm{eq}} = -\frac{1}{3}\mathbf{u}_z(p^*-1)(3\mathbf{u}_x\mathbf{u}_x + 3\mathbf{u}_y\mathbf{u}_y + 2), \\
\hat{f}_{13}^{\mathrm{eq}} = -\mathbf{u}_x(\mathbf{u}_y\mathbf{u}_y - \mathbf{u}_z\mathbf{u}_z)(p^*-1), \quad \hat{f}_{14}^{\mathrm{eq}} = -\mathbf{u}_y(\mathbf{u}_x\mathbf{u}_x - \mathbf{u}_z\mathbf{u}_z)(p^*-1), \\
\hat{f}_{15}^{\mathrm{eq}} = -\mathbf{u}_z(\mathbf{u}_x\mathbf{u}_x - \mathbf{u}_y\mathbf{u}_y)(p^*-1), \quad \hat{f}_{16}^{\mathrm{eq}} = -\mathbf{u}_x\mathbf{u}_y\mathbf{u}_z(p^*-1) \\
\hat{f}_{17}^{\mathrm{eq}} = \frac{1}{3}p^* + \frac{2}{3}\mathbf{u}_x\mathbf{u}_x p^* + \frac{2}{3}\mathbf{u}_y\mathbf{u}_y p^* + \frac{2}{3}\mathbf{u}_z\mathbf{u}_z p^* - \frac{2}{3}\mathbf{u}_x\mathbf{u}_x \qquad \text{(j)} \\
-\frac{2}{3}\mathbf{u}_y\mathbf{u}_y - \frac{2}{3}\mathbf{u}_z\mathbf{u}_z - \mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y - \mathbf{u}_x\mathbf{u}_x\mathbf{u}_z\mathbf{u}_z \\
-\mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z + \mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y p^* + \mathbf{u}_x\mathbf{u}_x\mathbf{u}_z\mathbf{u}_z p^* + \mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z p^*, \\
\hat{f}_{18}^{\mathrm{eq}} = \frac{1}{9}p^* + \frac{2}{3}\mathbf{u}_x\mathbf{u}_x p^* - \frac{2}{3}\mathbf{u}_x\mathbf{u}_x - \mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y - \mathbf{u}_x\mathbf{u}_x\mathbf{u}_z\mathbf{u}_z \\
+\mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z + \mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y p^* + \mathbf{u}_x\mathbf{u}_x\mathbf{u}_z\mathbf{u}_z p^* - \mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z p^*, \\
\hat{f}_{19}^{\mathrm{eq}} = \frac{1}{3}(\mathbf{u}_y\mathbf{u}_y - \mathbf{u}_z\mathbf{u}_z)(3\mathbf{u}_x\mathbf{u}_x + 1)(p^*-1) \\
\hat{f}_{20}^{\mathrm{eq}} = \frac{1}{3}\mathbf{u}_y\mathbf{u}_z(3\mathbf{u}_x\mathbf{u}_x + 1)(p^*-1), \quad \hat{f}_{21}^{\mathrm{eq}} = \frac{1}{3}\mathbf{u}_x\mathbf{u}_z(3\mathbf{u}_y\mathbf{u}_y + 1)(p^*-1) \\
\hat{f}_{22}^{\mathrm{eq}} = \frac{1}{3}\mathbf{u}_x\mathbf{u}_y(3\mathbf{u}_z\mathbf{u}_z + 1)(p^*-1) \\
\hat{f}_{23}^{\mathrm{eq}} = -\frac{1}{9}\mathbf{u}_x(3\mathbf{u}_y\mathbf{u}_y + 1)(3\mathbf{u}_z\mathbf{u}_z + 1)(p^*-1) \\
\hat{f}_{24}^{\mathrm{eq}} = -\frac{1}{9}\mathbf{u}_y(3\mathbf{u}_x\mathbf{u}_x + 1)(3\mathbf{u}_z\mathbf{u}_z + 1)(p^*-1), \\
\hat{f}_{25}^{\mathrm{eq}} = -\frac{1}{9}\mathbf{u}_z(3\mathbf{u}_x\mathbf{u}_x + 1)(3\mathbf{u}_y\mathbf{u}_y + 1)(p^*-1) \\
\hat{f}_{26}^{\mathrm{eq}} = \frac{1}{27}p^* + \frac{1}{9}\mathbf{u}_x\mathbf{u}_x p^* + \frac{1}{9}\mathbf{u}_y\mathbf{u}_y p^* + \frac{1}{9}\mathbf{u}_z\mathbf{u}_z p^* - \frac{1}{9}\mathbf{u}_x\mathbf{u}_x \\
-\frac{1}{9}\mathbf{u}_y\mathbf{u}_y - \frac{1}{9}\mathbf{u}_z\mathbf{u}_z - \frac{1}{3}\mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y - \frac{1}{3}\mathbf{u}_x\mathbf{u}_x\mathbf{u}_z\mathbf{u}_z \\
-\frac{1}{3}\mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z + \frac{1}{3}\mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y p^* + \frac{1}{3}\mathbf{u}_x\mathbf{u}_x\mathbf{u}_z\mathbf{u}_z p^* \\
+\frac{1}{3}\mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z p^* - \mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z + \mathbf{u}_x\mathbf{u}_x\mathbf{u}_y\mathbf{u}_y\mathbf{u}_z\mathbf{u}_z p^*.
\end{gathered}$$

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