Scalable Laplacian Eigenfluids (Supplementary Material)

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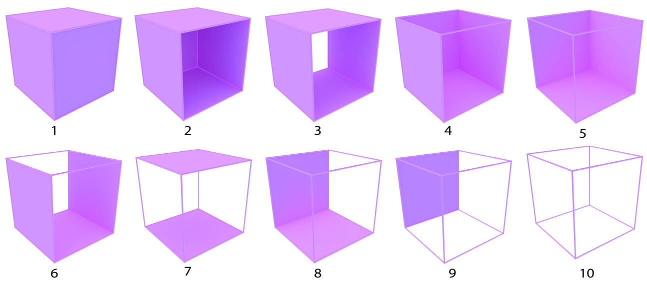

Fig. 1. Visualization of all 10 possible boundary conditions, with associated indices.

1 3D NEUMANN BASIS

For a box domain with six boundary walls, there are 10 possible combinations of Dirichlet and Neumann boundary conditions (up to symmetry). Figure 1 is a visualization of all 10 combinations. We list all the basis functions we derived for these combinations.

1. Six Dirichlet walls:

$$\begin{cases}\Phi_x = a(\sin(k_x x)\cos(k_y y)\cos(k_z z))\\ \Phi_y = b(\cos(k_x x)\sin(k_y y)\cos(k_z z))\\ \Phi_z = c(\cos(k_x x)\cos(k_y y)\sin(k_z z))\end{cases} \tag{1}$$

$k_x, k_y, k_z \in \mathbb{Z}^+ \cup 0$. The constants a, b, c need to satisfy the divergence free condition: $ak_x + bk_y + ck_z = 0$.

2. One Neumann wall, Φ_x at $x = \pi$:

$$\begin{cases}\Phi_x = a(\sin(k_x x)\cos(k_y y)\cos(k_z z))\\ \Phi_y = b(\cos(k_x x)\sin(k_y y)\cos(k_z z))\\ \Phi_z = c(\cos(k_x x)\cos(k_y y)\sin(k_z z))\end{cases} \tag{2}$$

$k_x \in \left(\mathbb{Z}^+ - \frac{1}{2}\right) \cup 0$, $k_y, k_z \in \mathbb{Z}^+ \cup 0$. Divergence free condition: $ak_x + bk_y + ck_z = 0$.

3. Two Neumann walls, Φ_x at $x = 0, x = \pi$:

$$\begin{cases}\Phi_x = a(\cos(k_x x)\cos(k_y y)\cos(k_z z))\\ \Phi_y = b(\sin(k_x x)\sin(k_y y)\cos(k_z z))\\ \Phi_z = c(\sin(k_x x)\cos(k_y y)\sin(k_z z))\end{cases} \tag{3}$$

$k_x, k_y, k_z \in \mathbb{Z}^+ \cup 0$. Divergence free condition: $-ak_x + bk_y + ck_z = 0$.

4. Two Neumann walls for Φ_x at $x = \pi$ and Φ_y at $y = \pi$:

$$\begin{cases}\Phi_x = a(\sin(k_x x)\cos(k_y y)\cos(k_z z))\\ \Phi_y = b(\cos(k_x x)\sin(k_y y)\cos(k_z z))\\ \Phi_z = c(\cos(k_x x)\cos(k_y y)\sin(k_z z))\end{cases} \tag{4}$$

$k_x, k_y \in \left(\mathbb{Z}^+ - \frac{1}{2}\right) \cup 0$, $k_z \in \mathbb{Z}^+ \cup 0$. Divergence free condition: $ak_x + bk_y + ck_z = 0$.

5. Three Neumann walls, Φ_x at $x = \pi$, Φ_y at $y = \pi$ and Φ_z at $z = \pi$:

$$\begin{cases}\Phi_x = a(\sin(k_x x)\cos(k_y y)\cos(k_z z))\\ \Phi_y = b(\cos(k_x x)\sin(k_y y)\cos(k_z z))\\ \Phi_z = c(\cos(k_x x)\cos(k_y y)\sin(k_z z))\end{cases} \tag{5}$$

$k_x, k_y, k_z \in \left(\mathbb{Z}^+ - \frac{1}{2}\right) \cup 0$. Divergence free condition: $ak_x + bk_y + ck_z = 0$.

6. Three Neumann walls, Φ_x at $x = \pi, x = 0$ and Φ_y at $y = \pi$:

$$\begin{cases}\Phi_x = a(\cos(k_x x)\cos(k_y y)\cos(k_z z))\\ \Phi_y = b(\sin(k_x x)\sin(k_y y)\cos(k_z z))\\ \Phi_z = c(\sin(k_x x)\cos(k_y y)\sin(k_z z))\end{cases} \tag{6}$$

$k_y \in \left(\mathbb{Z}^+ - \frac{1}{2}\right) \cup 0$, $k_x, k_z \in \mathbb{Z}^+ \cup 0$, Divergence free condition: $-ak_x + bk_y + ck_z = 0$.

7. Four Neumann walls, Φ_x at $x = 0, x = \pi$ and Φ_z at $z = 0, z = \pi$:

$$\begin{cases}\Phi_x = a(\cos(k_x x)\cos(k_y y)\sin(k_z z))\\ \Phi_y = b(\sin(k_x x)\sin(k_y y)\sin(k_z z))\\ \Phi_z = c(\sin(k_x x)\cos(k_y y)\cos(k_z z))\end{cases} \tag{7}$$

$k_x, k_y, k_z \in \mathbb{Z}^+ \cup 0$. Divergence free condition: $-ak_x + bk_y - ck_z = 0$.

8. Four Neumann walls, Φ_x at $x = \pi$, Φ_y at $y = \pi$ and Φ_z at $z = 0, z = \pi$.

$$\begin{cases}\Phi_x = a(\sin(k_x x)\cos(k_y y)\sin(k_z z))\\ \Phi_y = b(\cos(k_x x)\sin(k_y y)\sin(k_z z))\\ \Phi_z = c(\cos(k_x x)\cos(k_y y)\cos(k_z z))\end{cases} \tag{8}$$

$k_x, k_y \in \left(\mathbb{Z}^+ - \frac{1}{2}\right) \cup 0$, $k_z \in \mathbb{Z}^+ \cup 0$. Divergence free condition: $ak_x + bk_y - ck_z = 0$

9. Five Neumann walls, Φ_x at $x = \pi$, Φ_y at $y = 0, y = \pi$ and Φ_z at $z = 0, z = \pi$:

$$\begin{cases}\Phi_x = a(\sin(k_x x)\sin(k_y y)\sin(k_z z))\\ \Phi_y = b(\cos(k_x x)\cos(k_y y)\sin(k_z z))\\ \Phi_z = c(\cos(k_x x)\sin(k_y y)\cos(k_z z))\end{cases} \tag{9}$$

$k_x \in \left(\mathbb{Z}^+ - \frac{1}{2}\right) \cup 0$, $k_y, k_z \in \mathbb{Z}^+ \cup 0$. Divergence free condition: $ak_x - bk_y - ck_z = 0$

10. Six Neumann walls for all three axes.

$$\begin{cases}\Phi_x = a(\cos(k_x x)\sin(k_y y)\sin(k_z z))\\ \Phi_y = b(\sin(k_x x)\cos(k_y y)\sin(k_z z))\\ \Phi_z = c(\sin(k_x x)\sin(k_y y)\cos(k_z z))\end{cases} \tag{10}$$

$k_x, k_y, k_z \in \mathbb{Z}^+ \cup 0$. Divergence free condition: $ak_x + bk_y + ck_z = 0$.

All the above basis functions need to be normalized, which places another constraint on the three constants. Assuming we are given a fixed wave number k_x, k_y, k_z, we need to solve for a, b and c. There are currently only two constraints, the normalization and

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divergence-free constraint. Another constraint needs to be added in order to determine a, b and c. Functions of the same form as ours are used to describe the electric field in a box cavity resonator, see e.g. Cheng [1989]. In this case, a "direction of propagation" is chosen, and then the functions to describe the electric field are derived. For example, if the basis in equation 10 and the x axis is chosen as the "direction of propagation", then the constants become : $a = -(k_y^2 + k_z^2), b = k_x k_y, c = k_x k_z$. The constants are then normalized. We found that choosing the constants this way maximizes a under both the divergence-free and normalization constraint. Thus, the velocity along the direction x is maximized. One can also derive the same formula by solving the constrained maximization problem where a is maximized under the divergence-free and normalization constraints.

When we determine the constants a, b, c, we take the scene into consideration. For example, for a scene where the fluid flows predominantly along y direction (e.g. due to buoyancy), we choose the constant by maximizing the velocity along the y direction. If there is no prior knowledge about the direction of the fluid, we then choose the constant by maximize a, b and c individually, and then use the average value for each constant.

2 ENERGY CONSERVATION OF CHEBYSHEV COLLOCATION METHODS

In spectral collocation (pseudospectral) methods, differentiation matrices are used to compute the derivative of a given function on a grid. For example, given a discretized function $v(x_i),\ \ i = 0, 1, ..., N-1$, the discretized derivative of v can be written as $\mathbf{v}' = \mathbf{D}\mathbf{v}$, where $\mathbf{D}$ is an $N \times N$ matrix, and $\mathbf{v}', \mathbf{v} \in \mathbb{R}^N$. Generally, $\mathbf{D}$ is a dense matrix. However, the matrix is usually never constructed explicitly, and a transformation method is used to compute the derivative $\mathbf{v}'$ given $\mathbf{v}$. For Fourier series and Chebyshev polynomials, the derivative can be evaluated in $N \log(N)$ time complexity using the FFT.

When the N-S equation is discretized in space, it is desirable for the spatially-discretized, time-continuous equation to conserve some important properties of the N-S equations. It is advised in [Canuto et al. 1988] that the convection form of N-S equation will lead to instabilities at various Reynolds numbers, bcause the discretized convection form may not conserve momentum and energy. Thus, the rotation form of the N-S equations should be used instead. We can show that Chebyshev collocation does not conserve energy under rotation form when the viscosity is zero. In contrast to the Chebyshev differential matrix, the Fourier differential matrix is skew-symmetric, thus its semi-discretized equation conserves energy [Canuto et al. 2007]. However, the Fourier basis assumes periodic boundary conditions.

The rotation form of the N-S equations is:

$$\begin{aligned} &\frac{\partial \mathbf{u}}{\partial t} + \mathbf{w} \times \mathbf{u} = -\nabla q + \nu \nabla^2 \mathbf{u} \\ &\nabla \cdot \mathbf{u} = 0 \end{aligned} \tag{11}$$

where $\mathbf{w} = \nabla \times \mathbf{u}$ and $q = p + 0.5|\mathbf{u}|^2$. This form is equivalent to the common convection form of the N-S equations.

First, let us denote spatially-discretized velocity as $\mathbf{u}^N$. Define the discrete gradient operator $\mathbb{G}_N q^N = \begin{bmatrix} \mathbf{D}_N^x q^N & \mathbf{D}_N^y q^N & \mathbf{D}_N^z q^N \end{bmatrix}^T$ where $\mathbf{D}$ is the Chebyshev differentiation matrix with size N along desired direction. And define the discrete divergence operator $\mathbb{D}_N \mathbf{u}^N = \mathbf{D}_N^x \mathbf{u}_x^N + \mathbf{D}_N^y \mathbf{u}_y^N + \mathbf{D}_N^z \mathbf{u}_z^N$. Omitting the viscosity, the space discretized inviscid N-S equation can be written as:

$$\begin{aligned} &\frac{d\mathbf{u}^N}{dt} + \mathbf{w}^N \times \mathbf{u}^N + \mathbb{G}_N q^N = 0 \\ &\mathbb{D}_N \mathbf{u}^N = 0 \end{aligned} \tag{12}$$

Taking the first equation of above and performing a dot product on both sides using $\mathbf{u}^N$ yields:

$$\frac{d|\mathbf{u}|^2}{dt} + (\mathbf{w}^N \times \mathbf{u}^N, \mathbf{u}^N) + (\mathbb{G}_N q^N, \mathbf{u}^N) = 0. \tag{13}$$

The product $(\mathbf{w}^N \times \mathbf{u}^N, \mathbf{u}^N)$ is zero since the cross product is orthogonal to $\mathbf{u}^N$. Thus, in order for energy to be conserved, $(\mathbb{G}_N q^N, \mathbf{u}^N)$ must be equal to zero. In addition to this, since $\mathbb{D}_N \mathbf{u}^N = 0$, we can construct the equation $(q^N, \mathbb{D}_N \mathbf{u}^N) = 0$. Thus, assuming that energy is conserved, the below two equations must hold:

$$\begin{aligned} (\mathbb{G}_N q^N, \mathbf{u}^N) &= (\mathbf{D}_N^x q^N, \mathbf{u}_x^N) + (\mathbf{D}_N^y q^N, \mathbf{u}_y^N) + (\mathbf{D}_N^z q^N, \mathbf{u}_z^N) = 0 \\ (q^N, \mathbb{D}_N \mathbf{u}^N) &= (q^N, \mathbf{D}_N^x \mathbf{u}_x^N) + (q^N, \mathbf{D}_N^y \mathbf{u}_y^N) + (q^N, \mathbf{D}_N^z \mathbf{u}_z^N) = 0 \end{aligned} \tag{14}$$

Writing the above two equations as matrix products yields:

$$\begin{aligned} &(\mathbf{u}_x^N)^T \mathbf{D}_N^x q^N + (\mathbf{u}_y^N)^T \mathbf{D}_N^y q^N + (\mathbf{u}_z^N)^T \mathbf{D}_N^z q^N = 0 \\ &(q^N)^T \mathbf{D}_N^x \mathbf{u}_x^N + (q^N)^T \mathbf{D}_N^y \mathbf{u}_y^N + (q^N)^T \mathbf{D}_N^z \mathbf{u}_z^N = 0. \end{aligned} \tag{15}$$

Taking the transpose of the first equation, and then adding the second one, we get:

$$\begin{aligned} (q^N)^T (\mathbf{D}_N^x + (\mathbf{D}_N^x)^T) \mathbf{u}_x^N + (q^N)^T (\mathbf{D}_N^y + (\mathbf{D}_N^y)^T) \mathbf{u}_y^N + \\ (q^N)^T (\mathbf{D}_N^z + (\mathbf{D}_N^z)^T) \mathbf{u}_z^N = 0. \end{aligned} \tag{16}$$

For arbitrary $\mathbf{u}$ and q, the above equation only holds when $\mathbf{D}_N + (\mathbf{D}_N)^T = 0$ (skew-symmetric), or when $\mathbf{D}_N = (\mathbf{D}_N)^T$ (symmetric). As shown in page 53 of [Trefethen 2000], the Chebyshev differentiation matrix is:

$$\mathbf{D}_N = \begin{bmatrix} \frac{2(N-1)^2+1}{6} & \cdots & 2\frac{(-1)^j}{1-x_j} & \cdots & \frac{1}{2}(-1)^{(N-1)} \\ \vdots & \ddots & & \frac{(-1)^{i+j}}{x_i - x_j} & \vdots \\ -\frac{1}{2}\frac{(-1)^i}{1-x_i} & & \frac{-x_j}{2(1-x_j^2)} & & \frac{1}{2}\frac{(-1)^{N-1+i}}{1+x_i} \\ \vdots & \frac{(-1)^{i+j}}{x_i - x_j} & & \ddots & \vdots \\ -\frac{1}{2}(-1)^{(N-1)} & \cdots & -2\frac{(-1)^{N-1+j}}{1+x_j} & \cdots & -\frac{2(N-1)^2+1}{6} \end{bmatrix} \tag{17}$$

where i, j is integer index from 0 to $N-1$, and $x_j = \cos(\frac{j\pi}{N-1})$. It is clear that this Chebyshev differentiation matrix is neither skew-symmetric, nor symmetric. So the equation 16 does not hold. Thus, $(\mathbb{G}_N q^N, \mathbf{u}^N) = 0$ does not hold since $\mathbb{D}_N \mathbf{u}^N = 0$, and Chebyshev collocation methods are not energy-conserving.

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