Computer Simulation（2022）: FINAL Report due 2023 Feb. 16

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Answer Problem 1 through Problem 3.

Problem 1: Briefly explain each of the following terms.

(1) Conserved Quantities

Conserved quantities are physical quantities that remain constant in physical processes. They are unchanged (or conserved) in total, regardless of the physical process that occurs within the system. Examples include momentum conservation described by the Navier-Stokes equation and mass conservation stated by the continuity equation.

(2) Finite Difference Method

Finite Difference Method (FDM) is one of the numerical simulation methods. Specifically, FDM discretizes the physical quantities in a uniform, finite number of grids to approximate solutions to ordinary/partial differential equations and their derivatives with finite difference (Newton quotient).

Advantages include:

1) Ease of implementation: Many of differential operators are approximated via Taylor expansion.
2) High accuracy: It is relatively easy to obtain high-order approximations.
3) High scalability: Suitable to parallel computing thanks to efficient memory access.

On the other hand, it involves several disadvantages such as:

1) Numerical viscosity: It is prone to numerical viscosity if the system includes advection.
2) Enforcement of conservation laws: It is difficult to impose conservation laws unless special care is provided.

(3) CFL Conditions

CFL conditions state the maximum possible timestep in explicit Euler scheme. It is defined as ratio of physical and numerical propagation speed of physical quantities, derived by considering the characteristic length and speed of the system (the smallest grid size and the fastest possible wave speed). This corresponds to the numerical simulation being able to capture the fastest wave in the system, and without satisfying the CFL condition, explicit scheme fluctuates and diverges during the computation.

(4) Truncation Errors

Truncation errors are numerical errors that appear when approximating quantities. For example, Taylor's theorem states any C^∞-continuous real-valued functions are represented by infinite number of polynomials. Yet, one often drops the summation at 2nd or 3rd-order polynomials, resulting in finite approximation to have remainders, which are called truncation errors. They are distinguished from round-off errors, which are categorized into another class of numerical errors.

Problem 2: Answer the following questions.

(1) Show that the following finite difference approximation has the fourth-order spatial accuracy. *Tips: You can use Taylor-series expansion both for function q and its derivative q'.*

$$q'_{j+1} + 4q'_j + q'_{j-1} = 3\frac{q_{j+1} - q_{j-1}}{\Delta x}$$

Taylor expansion of q_{j+1} and $q'_{j\pm1}$ gives:

$$q_{j\pm1} = q_j \pm \Delta x q'_j + \frac{(\Delta x)^2}{2!}q''_j \pm \frac{(\Delta x)^3}{3!}q'''_j + \frac{(\Delta x)^4}{4!}q''''_j + \mathcal{O}((\Delta x)^5) \tag{1}$$

$$q'_{j\pm1} = q'_j \pm \Delta x q''_j + \frac{(\Delta x)^2}{2!}q'''_j \pm \frac{(\Delta x)^3}{3!}q''''_j + \frac{(\Delta x)^4}{4!}q'''''_j + \mathcal{O}((\Delta x)^5) \tag{2}$$

From equation (1), we have the following:

$$q_{j+1} - q_{j-1} = 2\Delta x q'_j + \frac{(\Delta x)^3}{3}q'''_j + \mathcal{O}((\Delta x)^5) \tag{3}$$

$$3\frac{q_{j+1} - q_{j-1}}{\Delta x} = 6q'_j + (\Delta x)^2 q'''_j + \mathcal{O}((\Delta x)^4) \tag{4}$$

Similarly, equation (2) yields:

$$q'_{j+1} + q'_{j-1} = 2q'_j + (\Delta x)^2 q'''_j + \frac{(\Delta x)^4}{12}q'''''_j + \mathcal{O}((\Delta x)^5) \tag{5}$$

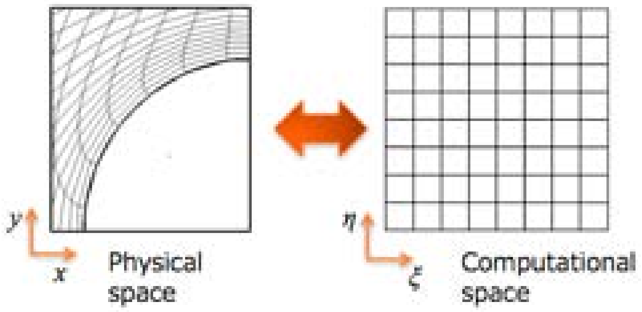
$$(\Delta x)^2 q'''_j = q'_{j+1} + q'_{j-1} - 2q'_j - \frac{(\Delta x)^4}{12}q'''''_j + \mathcal{O}((\Delta x)^5) \tag{6}$$

Substituting equation (6) for equation (4), we obtain:

$$\begin{aligned} 3\frac{q_{j+1} - q_{j-1}}{\Delta x} &= 6q'_j + (\Delta x)^2 q'''_j + \mathcal{O}((\Delta x)^4) \\ &= 6q'_j + q'_{j+1} + q'_{j-1} - 2q'_j - \frac{(\Delta x)^4}{12}q'''''_j + \mathcal{O}((\Delta x)^4) \\ &= q'_{j+1} + 4q'_j + q'_{j-1} - \frac{(\Delta x)^4}{12}q'''''_j + \mathcal{O}((\Delta x)^4) \\ &= q'_{j+1} + 4q'_j + q'_{j-1} + \mathcal{O}((\Delta x)^4) \end{aligned} \tag{7}$$

In equation (7), the leading error term is the fourth power of discretization length, Δx. Hence, the above expression has the fourth-order spatial accuracy.

Problem 3: In calculations using a general curvilinear coordinate grid system, the basic equations are solved by transforming them from the curvilinear coordinate system in the physical space to the orthogonal coordinate system in the computational space as shown below.



Three-dimensional coordinate transformation assumes the local relationship described by equation [1] between the physical space (x, y, z) and the computational space (ξ, η, ζ).

$$x = x(\xi,\eta,\zeta), y = y(\xi,\eta,\zeta), z = z(\xi,\eta,\zeta),$$
$$\xi = \xi(x,y,z), \eta = \eta(x,y,z), \zeta = \zeta(x,y,z) \qquad [1]$$

The Jacobian of the coordinate transformation, $\boldsymbol{J}$, is defined by equation [2] and the metrics have relations [3],

$$\boldsymbol{J} \equiv \frac{\partial(x,y,z)}{\partial(\xi,\eta,\zeta)} = \begin{vmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{vmatrix} = x_\xi(y_\eta z_\zeta - y_\zeta z_\eta) + y_\xi(z_\eta x_\zeta - z_\zeta x_\eta) + z_\xi(x_\eta y_\zeta - x_\zeta y_\eta) \quad [2]$$

$$\begin{pmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{pmatrix}\begin{pmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \; or \; \begin{pmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{pmatrix}^{-1} \quad [3]$$

where, for example, x_ξ denotes $\partial x/\partial\xi$. Answer the following questions.

(1) Convert the first-order differential operators $\partial/\partial x$, $\partial/\partial y$ and, $\partial/\partial z$ in the physical space to the operators in the computational space by using the chain rule of differential operators. *Tips: consider the relationship between physical and computational spaces through equation [1].*

Consider a physical quantity $\phi = \phi(x, y, z)$. Applying the chain rule, its derivative in x-direction can be computed as:

$$\frac{\partial\phi}{\partial x} = \frac{\partial\phi}{\partial\xi}\frac{\partial\xi}{\partial x} + \frac{\partial\phi}{\partial\eta}\frac{\partial\eta}{\partial x} + \frac{\partial\phi}{\partial\zeta}\frac{\partial\zeta}{\partial x} \tag{8}$$

$$\therefore \frac{\partial}{\partial x}\phi = \left(\frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial x}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial x}\frac{\partial}{\partial\zeta}\right)\phi \tag{9}$$

With index notation, equation (9) is re-written as:

$$\frac{\partial}{\partial x_i}\phi = \frac{\partial\xi_l}{\partial x_i}\frac{\partial}{\partial\xi_l}\phi \quad (i = 1, 2, 3) \tag{10}$$

Thus, 3 differential operators $\partial/\partial x$, $\partial/\partial y$ and, $\partial/\partial z$ in the physical space are converted into:

$$\frac{\partial}{\partial x} = \frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial x}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial x}\frac{\partial}{\partial\zeta} \tag{11}$$

$$\frac{\partial}{\partial y} = \frac{\partial\xi}{\partial y}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial y}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial y}\frac{\partial}{\partial\zeta} \tag{12}$$

$$\frac{\partial}{\partial z} = \frac{\partial\xi}{\partial z}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial z}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial z}\frac{\partial}{\partial\zeta} \tag{13}$$

(2) Transform the continuity equation of the incompressible fluid flow [4] to the computational space. u, v, and w are the velocity components represented in the orthogonal coordinate system.

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial v}{\partial z} = 0 \quad [4]$$

Reflecting question (1), derivative terms on the left-hand side are transformed.

$$\frac{\partial u}{\partial x} = \left(\frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial x}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial x}\frac{\partial}{\partial\zeta}\right)u \tag{14}$$

$$\frac{\partial v}{\partial y} = \left(\frac{\partial\xi}{\partial y}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial y}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial y}\frac{\partial}{\partial\zeta}\right)v \tag{15}$$

$$\frac{\partial w}{\partial z} = \left(\frac{\partial\xi}{\partial z}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial z}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial z}\frac{\partial}{\partial\zeta}\right)w \tag{16}$$

Therefore, the continuity equation of the incompressible fluid flow is:

$$\begin{aligned} 0 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} &= \left(\frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial x}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial x}\frac{\partial}{\partial\zeta}\right)u \\ &+ \left(\frac{\partial\xi}{\partial y}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial y}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial y}\frac{\partial}{\partial\zeta}\right)v \\ &+ \left(\frac{\partial\xi}{\partial z}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial z}\frac{\partial}{\partial\eta} + \frac{\partial\zeta}{\partial z}\frac{\partial}{\partial\zeta}\right)w \end{aligned} \tag{17}$$

Or, with index notation, we have the following:

$$\frac{\partial}{\partial x_i}u_i = \frac{\partial\xi_l}{\partial x_i}\frac{\partial}{\partial\xi_l}u_i = 0 \tag{18}$$

(3) Describe the physical meaning of the Jacobian, $\boldsymbol{J}$.

Jacobi matrix, $\boldsymbol{J} = [J_{il}] = [\partial x_i/\partial\xi_l]$, describes the change ratio between 2 coordinate systems. Indeed, $\partial x_i/\partial\xi_l$ means sensitivity in x_i when infinitesimal change occurs in ξ_l. As $\partial x_i/\partial\xi_l$ only explains the length change between x_i and ξ_l, we consider its determinant $|J_{il}|$, which describe area change ratio in 2D and volume change ratio in 3D.

Appendix A: 2D Lid-Driven Cavity Flow

(A) Problem setup

We consider 2D lid-driven cavity flow, which is well-known problem to model the flow of an incompressible fluid in a closed square cavity. Cavity is consisted of 3 fixed walls and 1 driving wall which moves along x-axis at a constant velocity. As for pressure boundary condition, we impose homogeneous Neumann condition at each wall, and enforce homogeneous Dirichlet condition at $(x, y) = (0.5, 0)$; see Figure A1.

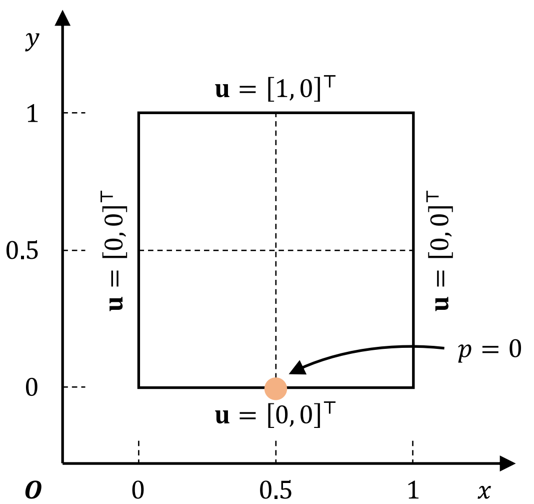


Figure A1: Problem setup and boundary conditions

(B) Governing equation and discretization

Fluid motion is generally governed by the continuity equation and a set of the Navier-Stokes equations.

$$\nabla \cdot \mathbf{u} = 0 \tag{A1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u} \tag{A2}$$

where $\mathbf{u}$ is fluid velocity, p is pressure, Re is Reynolds number. We apply the fractional step method as time integration scheme. The fractional step method splits the single timestep in the momentum equation (the Navier-Stokes equation, equation (A2)) into 2 parts: one with convection and viscosity (intermediate velocity field, $\mathbf{u}^{(*)}$), another with pressure gradient (next velocity field, $\mathbf{u}^{(n+1)}$).

$$\begin{gathered} \frac{\mathbf{u}^{(*)} - \mathbf{u}^{(n)}}{\Delta t} + \left(\mathbf{u}^{(n)} \cdot \nabla\right)\mathbf{u}^{(n)} = \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}^{(n)} \\ \therefore \mathbf{u}^{(*)} = \mathbf{u}^{(n)} + \Delta t \left(-\left(\mathbf{u}^{(n)} \cdot \nabla\right)\mathbf{u}^{(n)} + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}^{(n)}\right) \end{gathered} \tag{A3}$$

$$\begin{gathered} \frac{\mathbf{u}^{(n+1)} - \mathbf{u}^{(*)}}{\Delta t} = -\nabla p^{(n+1)} \\ \therefore \mathbf{u}^{(n+1)} = \mathbf{u}^{(*)} - \Delta t \nabla p^{(n+1)} \end{gathered} \tag{A4}$$

Considering the mass conservation at $(n+1)^{\text{th}}$ step, we apply equation (A4) to equation (A1) to obtain the following PPE.

$$\begin{gathered} \nabla \cdot \mathbf{u}^{(n+1)} = \nabla \cdot \left(\mathbf{u}^{(*)} - \Delta t \nabla p^{(n+1)}\right) = 0 \\ \therefore \nabla^2 p^{(n+1)} = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^{(*)} \end{gathered} \tag{A5}$$

As for spatial discretization, we employ regular uniform grid ($\Delta x = \Delta y = 5 \times 10^{-3}$), where all independent variables ($\mathbf{u} = [u, v]^\top$ and p) are allocated at the same vertices. In particular, we adopt Kawamura-Kuwahara scheme (KK scheme) for convection term (see Appendix B for details), and 2^{nd}-order central difference scheme for pressure gradient and viscosity terms. In addition, we apply Jacobi's iterative method to solve the PPE in equation (A5).

(C) Numerical results

Cavity flow is a steady problem. We assume the field has reached to a steady state when the following is satisfied.

$$\max\left(\frac{\left\|u^{(n+1)} - u^{(n)}\right\|_2}{\left\|u^{(n)}\right\|_2}, \frac{\left\|v^{(n+1)} - v^{(n)}\right\|_2}{\left\|v^{(n)}\right\|_2}\right) < \delta \tag{A6}$$

where $\|\cdot\|_2$ is ℓ^2-norm over the spatial dimension, δ is the convergence tolerance, set to $\delta = 1 \times 10^{-6}$ in this study. Figure A2 shows the results and the velocity distribution at the geometric center, compared to the reference presented in [1].

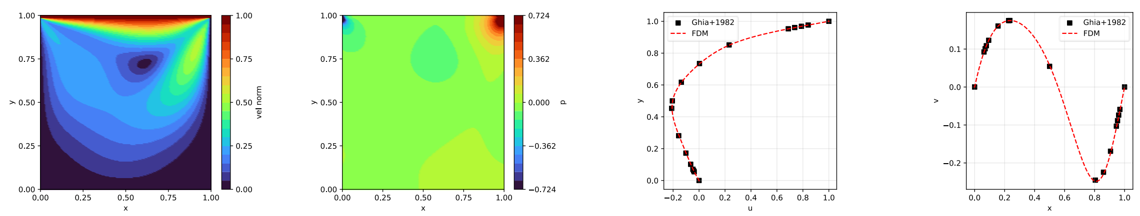
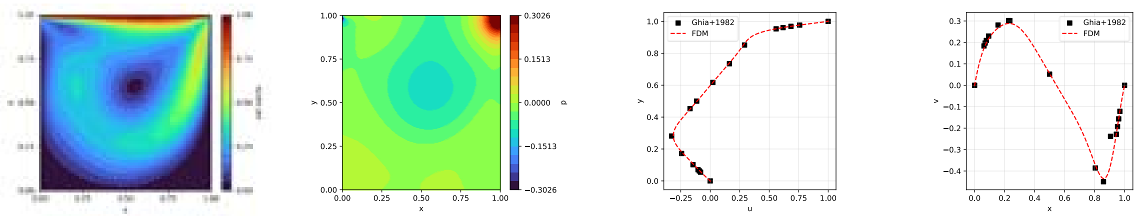
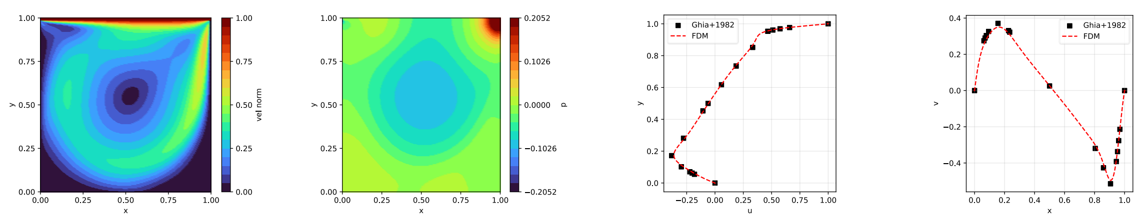
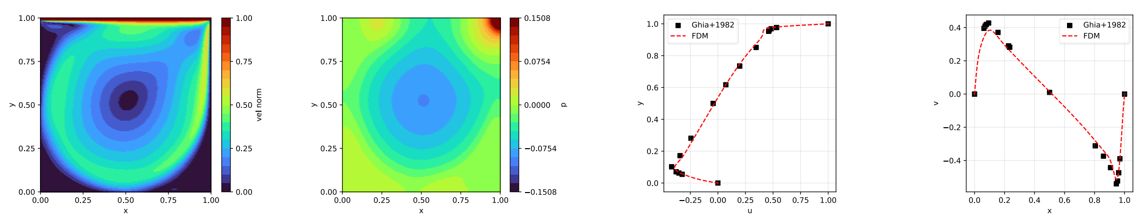
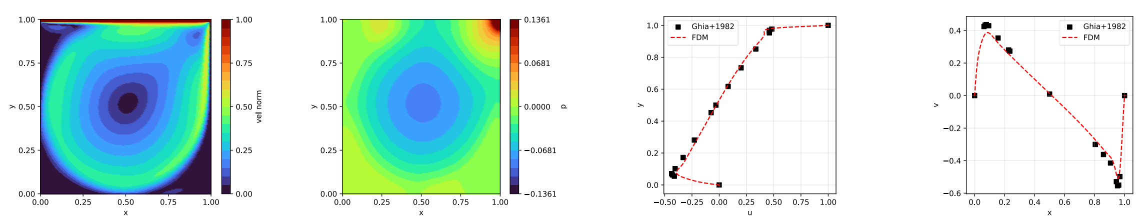
Re	Velocity norm	Pressure	u at $x = 0.5$	v at $y = 0.5$
100 (15.4s)				
400 (26.8s)				
1,000 (36.4s)				
3,200 (87.5s)				
5,000 (148.5s)				

Figure A2: FDM results with different Reynolds numbers, Re

(D) Discussion

We were able to perform 2D cavity flow simulation using the finite difference method. We obtained a smooth distribution for both velocity and pressure fields for various Reynolds numbers. For relatively low Reynolds numbers ($\mathrm{Re} = 100$ and 400), the results show a good agreement with the reference solution [1], however, as the Reynolds number increases, the obtained velocity fields are found to be slower than that of [1]. The following points are considered as factors of the difference:

(i) Governing equation: We used the continuity and the Navier-Stokes equations, while the stream function-vorticity formulation is applied in [1]. The stream function-vorticity formulation has a strong advantage as in exact mass conservation, although its applicability is limited to 2D problems. On the other hand, it is well known that the exact mass conservation in the formulation given in equation (A1) and (A2) is challenging, especially when the discretization is performed on a simple regular grid. In fact, we find that the velocity divergence has many non-zero values violating the mass conservation near the singularity points at the upper left and right corners as the Reynolds number increases (see Figure A3), which may have affected the evaluation of pressure, and pressure gradient-driven velocity fields. Improvement may be achieved by introducing staggered or collocated grids to better satisfy the continuity equation.

(ii) Boundary condition: [2] presents the Finite Element Method (FEM) results using the continuity and the Navier-Stokes equations formulation, similar to the present approach, having a good agreement with [1] even for high Reynolds numbers. In [2], the Dirichlet condition for the pressure is given at the bottom left corner of the cavity. As mentioned above, an accurate evaluation of the pressure field is essential since its gradient drives the velocity. Imposing the homogeneous Dirichlet condition at the bottom left corner may improve the accuracy, although it requires a diagonal stencil to compute the pressure gradient, which is not implemented in the presented study.

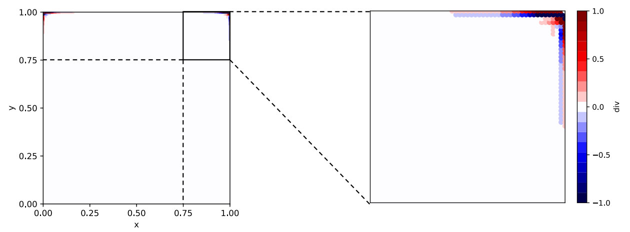
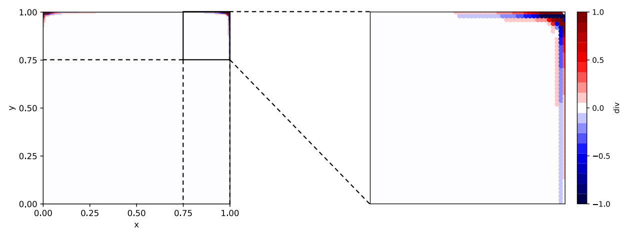
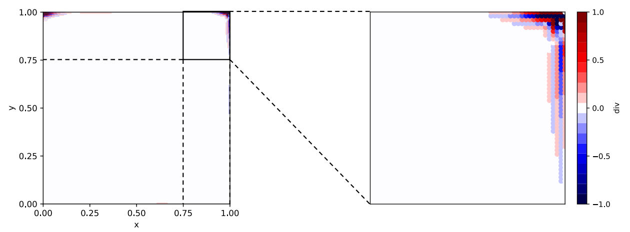
Re	Velocity divergence
100	
1,000	
5,000	

Figure A3: Velocity divergence at $\mathrm{Re} = 100,\ 1{,}000$ and $5{,}000$

Appendix B: Kawamura-Kuwahara Scheme

Convection term is discretized with Kawamura-Kuwahara (KK) scheme. We first discretize the convection term as follows:

$$u\frac{\partial \phi}{\partial x} = \begin{cases} u\dfrac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6\Delta x} \\ u\dfrac{-\phi_{i+2} + 6\phi_{i+1} - 3\phi_i - 2\phi_{i-1}}{6\Delta x} \end{cases} \tag{B1}$$

Considering the sign of convection speed u, we have the following expression.

$$\begin{aligned} u\frac{\partial \phi}{\partial x} &= \frac{u+|u|}{2}\frac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6\Delta x} \\ &+ \frac{u-|u|}{2}\frac{-\phi_{i+2} + 6\phi_{i+1} - 3\phi_i - 2\phi_{i-1}}{6\Delta x} \\ &= u\frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\Delta x} \\ &+ |u|(\Delta x)^3\frac{\phi_{i+2} - 4\phi_{i+1} + 6\phi_i - 4\phi_{i-1} + \phi_{i-2}}{12(\Delta x)^4} \end{aligned} \tag{B2}$$

By Taylor expansion, we find that the 1st term in equation (B2) is the 4th-order central difference, and the 2nd term is the 4th-order numerical viscosity. Here, KK scheme introduces a constant $\beta = 1/4$ to the numerical viscosity term, resulting in:

$$\begin{aligned} u\frac{\partial \phi}{\partial x} &\approx u\frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\Delta x} \\ &+ \beta|u|(\Delta x)^3\frac{\phi_{i+2} - 4\phi_{i+1} + 6\phi_i - 4\phi_{i-1} + \phi_{i-2}}{(\Delta x)^4} \end{aligned} \tag{B3}$$

Reference:

[1] U. Ghia, K.N. Ghia, C.T. Shin: High-Re solutions for incompressible flow using the Navier-Stokes equations and a multigrid method, *Journal of Computational Physics*, Vol. 48, No. 3, pp. 387-411, 1982.

[2] O.C. Zienkiewicz, R.L. Taylor, P. Nithiarasu: The Finite Element Method for Fluid Dynamics, pp. 97-102, Oxford, 2014.