Comparison Between Finite Difference and Spectral Methods in Computational Fluid Dynamics.

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Introduction

The study of fluid dynamics encompasses a wide range of phenomena, from the flow of air over an aircraft wing to the circulation of blood in the human body. Central to this field are the Navier-Stokes equations, which describe the motion of fluid substances. These equations, derived from the principles of conservation of mass, momentum, and energy, form the foundation for understanding both laminar and turbulent flows. In many practical applications, such as environmental engineering, aerodynamics, and meteorology, fluid flows can often be approximated as incompressible. This simplification assumes that the fluid density remains constant, which is valid for many liquids and low-speed gas flows.

So, the incompressible Navier-Stokes equations describe the motion of fluid substances under the assumption that the fluid density is constant. These equations can be written as follows:

1. **Momentum Equations:**

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}$$

2. **Continuity Equation (Incompressibility Condition):**

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

where:

- $\mathbf{u} = (u, v, w)$ is the velocity vector field.

- p is the pressure field.

- ρ is the fluid density (constant for incompressible flow).

- ν is the kinematic viscosity of the fluid.

- $\mathbf{f}$ represents body forces (e.g., gravity) acting on the fluid.

To solve these partial differential equations (PDEs) numerically, one of the most widely used approaches is the finite difference method (FDM).

Another widely used approach, applied only in the periodic problems, is the spectral method.

The purpose of this work is to compare and demonstrate the consistency between these two approaches: the finite difference method and the spectral method.

Formulation of the 2D Finite Difference Method for the Incompressible Navier-Stokes Equations

The finite difference method approximates the derivatives in the Navier-Stokes equations by differences between function values at discrete grid points. This method is particularly advantageous for its simplicity and straightforward implementation, making it accessible for various applications and educational purposes.

The incompressible Navier-Stokes equations in two dimensions (2D) are given by:

1. **Momentum Equations:**

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

2. **Continuity Equation (Incompressibility Condition):**

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

where u and v are the velocity components in the x and y directions, respectively, p is the pressure, ρ is the fluid density, and ν is the kinematic viscosity.

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The firs step is to set the spatial and time discretization grid.

In the simplest case we discretize the computational domain into a uniform grid with N_x points in the x direction and N_y points in the y direction. Grid spacings are $\Delta x = \frac{L_x}{N_x - 1}$ and $\Delta y = \frac{L_y}{N_y - 1}$, where L_x and L_y are the lengths of the domain in the x and y directions. Time is discretized into steps of size Δt.

The second step is the finite difference approximations for spatial derivatives. The simplest scheme is the central difference approach.

- Central difference approximations for spatial derivatives:

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} \approx \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} \tag{1}$$

$$\left(\frac{\partial u}{\partial y}\right)_{i,j} \approx \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y} \tag{2}$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \tag{3}$$

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} \tag{4}$$

- Similar approximations are used for v and p.

The next step is the time integration. Explicit time integration schemes like Forward Euler or Runge-Kutta methods can be used for the time-stepping of velocity components.

Enforcing Incompressibility

To ensure the incompressibility condition $\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$, a pressure correction step is introduced through the Pressure Poisson Equation (PPE). The intermediate velocity fields u^* and v^* are computed without considering the pressure gradient. These intermediate fields do not necessarily satisfy the incompressibility condition. To correct this, the pressure p^{n+1} at the next time step is computed by solving the following Pressure Poisson Equation:

$$\nabla^2 p^{n+1} = \frac{\rho}{\Delta t} \left(\frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial y} \right) \tag{5}$$

The finite difference form of this equation is:

$$\frac{p_{i+1,j}^{n+1} - 2p_{i,j}^{n+1} + p_{i-1,j}^{n+1}}{\Delta x^2} + \frac{p_{i,j+1}^{n+1} - 2p_{i,j}^{n+1} + p_{i,j-1}^{n+1}}{\Delta y^2} = \frac{\rho}{\Delta t} \left(\frac{u_{i+1,j}^* - u_{i-1,j}^*}{2\Delta x} + \frac{v_{i,j+1}^* - v_{i,j-1}^*}{2\Delta y} \right) \tag{6}$$

This equation is solved iteratively using methods like Gauss-Seidel or Successive Over-Relaxation (SOR).

Corrector Step

After solving for the pressure p^{n+1}, the velocity fields are corrected to enforce incompressibility:

$$u^{n+1} = u^* - \frac{\Delta t}{\rho} \frac{\partial p^{n+1}}{\partial x} \tag{7}$$

$$v^{n+1} = v^* - \frac{\Delta t}{\rho} \frac{\partial p^{n+1}}{\partial y} \tag{8}$$

The finite difference approximations for the corrected velocities are:

$$u_{i,j}^{n+1} = u_{i,j}^* - \frac{\Delta t}{\rho} \frac{p_{i+1,j}^{n+1} - p_{i-1,j}^{n+1}}{2\Delta x} \tag{9}$$

$$v_{i,j}^{n+1} = v_{i,j}^* - \frac{\Delta t}{\rho} \frac{p_{i,j+1}^{n+1} - p_{i,j-1}^{n+1}}{2\Delta y} \tag{10}$$

Entire Algorithm

1. **Initialize** the velocity fields u and v, and the pressure field p.

2. **Time-stepping loop**:

   - For each time step $n \to n + 1$:
     - **Predictor Step** (explicit time integration for the intermediate velocity field):

$$u^* = u^n + \Delta t \left(-\left(u^n \frac{\partial u^n}{\partial x} + v^n \frac{\partial u^n}{\partial y} \right) + \nu \left(\frac{\partial^2 u^n}{\partial x^2} + \frac{\partial^2 u^n}{\partial y^2} \right) \right) \tag{11}$$

$$v^* = v^n + \Delta t \left(-\left(u^n \frac{\partial v^n}{\partial x} + v^n \frac{\partial v^n}{\partial y} \right) + \nu \left(\frac{\partial^2 v^n}{\partial x^2} + \frac{\partial^2 v^n}{\partial y^2} \right) \right) \tag{12}$$

   - **Apply boundary conditions** to u, v, and p.

– **Pressure Poisson Equation** (to enforce incompressibility):

$$\nabla^2 p^{n+1} = \frac{\rho}{\Delta t} \left(\frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial y} \right) \tag{13}$$

This equation can be solved using iterative solvers like Gauss-Seidel or Successive Over-Relaxation (SOR).

– **Corrector Step** (update velocities with the pressure gradient):

$$u^{n+1} = u^* - \frac{\Delta t}{\rho} \frac{\partial p^{n+1}}{\partial x} \tag{14}$$

$$v^{n+1} = v^* - \frac{\Delta t}{\rho} \frac{\partial p^{n+1}}{\partial y} \tag{15}$$

– **Again enforce boundary conditions** to u, v, and p.
– **Repeat** the time-stepping loop until the desired simulation time is reached.

Spectral Method Formulation

For a periodic domain, we expand the velocity and pressure fields using Fourier series:

$$u(x, y, t) = \sum_{k_x, k_y} \hat{u}_{k_x, k_y}(t) e^{i(k_x x + k_y y)} \tag{16}$$

$$v(x, y, t) = \sum_{k_x, k_y} \hat{v}_{k_x, k_y}(t) e^{i(k_x x + k_y y)} \tag{17}$$

$$p(x, y, t) = \sum_{k_x, k_y} \hat{p}_{k_x, k_y}(t) e^{i(k_x x + k_y y)} \tag{18}$$

Substitute the Fourier expansions into the governing equations and use the orthogonality of the exponential functions to derive equations for the Fourier coefficients $\hat{u}_{k_x, k_y}$, $\hat{v}_{k_x, k_y}$, and $\hat{p}_{k_x, k_y}$.

Momentum Equations

For the u-momentum equation:

$$\frac{d\hat{u}_{k_x, k_y}}{dt} + \sum_{k'_x, k'_y} \left(\hat{u}_{k'_x, k'_y} i(k_x - k'_x) \hat{u}_{k_x - k'_x, k_y - k'_y} + \hat{v}_{k'_x, k'_y} i(k_y - k'_y) \hat{u}_{k_x - k'_x, k_y - k'_y} \right) = -ik_x \hat{p}_{k_x, k_y} + \nu \left(-k_x^2 - k_y^2 \right) \hat{u}_{k_x, k_y} \tag{19}$$

For the v-momentum equation:

$$\frac{d\hat{v}_{k_x, k_y}}{dt} + \sum_{k'_x, k'_y} \left(\hat{u}_{k'_x, k'_y} i(k_x - k'_x) \hat{v}_{k_x - k'_x, k_y - k'_y} + \hat{v}_{k'_x, k'_y} i(k_y - k'_y) \hat{v}_{k_x - k'_x, k_y - k'_y} \right) = -ik_y \hat{p}_{k_x, k_y} + \nu \left(-k_x^2 - k_y^2 \right) \hat{v}_{k_x, k_y} \tag{20}$$

The second term in momentum equations presents the sum of different three wave interactions. Due to its complexity, this term is typically handled in the physical space before being transformed into the Fourier domain.

$$\frac{\hat{u}_{k_x, k_y}^{n+1} - \hat{u}_{k_x, k_y}^n}{\Delta t} = -(\widehat{u \cdot \nabla u})_{k_x, k_y}^n - ik_x \hat{p}_{k_x, k_y}^n + \nu \left(-k_x^2 - k_y^2 \right) \hat{u}_{k_x, k_y}^n$$

$$\frac{\hat{v}_{k_x, k_y}^{n+1} - \hat{v}_{k_x, k_y}^n}{\Delta t} = -(\widehat{v \cdot \nabla v})_{k_x, k_y}^n - ik_y \hat{p}_{k_x, k_y}^n + \nu \left(-k_x^2 - k_y^2 \right) \hat{v}_{k_x, k_y}^n$$

Solving for Pressure: Enforcing incompressibility in Fourier space gives:

$$k_x \hat{u}_{k_x,k_y} + k_y \hat{v}_{k_x,k_y} = 0$$

Taking the divergence of the momentum equations and using the incompressibility condition leads to the pressure Poisson equation in Fourier space:

$$(k_x^2 + k_y^2)\hat{p}_{k_x,k_y} = ik_x(\widehat{u \cdot \nabla u})^n_{k_x,k_y} + ik_y(\widehat{v \cdot \nabla v})^n_{k_x,k_y}$$

This is similar to the analogous situation in the previous finite difference approach. Now we have to solve for $\hat{p}_{k_x,k_y}$ using the above relation.

Updating Velocity: Solve for the velocity components in Fourier space:

$$\hat{u}^{n+1}_{k_x,k_y} = \hat{u}^n_{k_x,k_y} - \Delta t \left((\widehat{u \cdot \nabla u})^n_{k_x,k_y} + ik_x \hat{p}^n_{k_x,k_y} \right) + \nu \Delta t \left(-k_x^2 - k_y^2 \right) \hat{u}^n_{k_x,k_y}$$

$$\hat{v}^{n+1}_{k_x,k_y} = \hat{v}^n_{k_x,k_y} - \Delta t \left((\widehat{v \cdot \nabla v})^n_{k_x,k_y} + ik_y \hat{p}^n_{k_x,k_y} \right) + \nu \Delta t \left(-k_x^2 - k_y^2 \right) \hat{v}^n_{k_x,k_y}$$
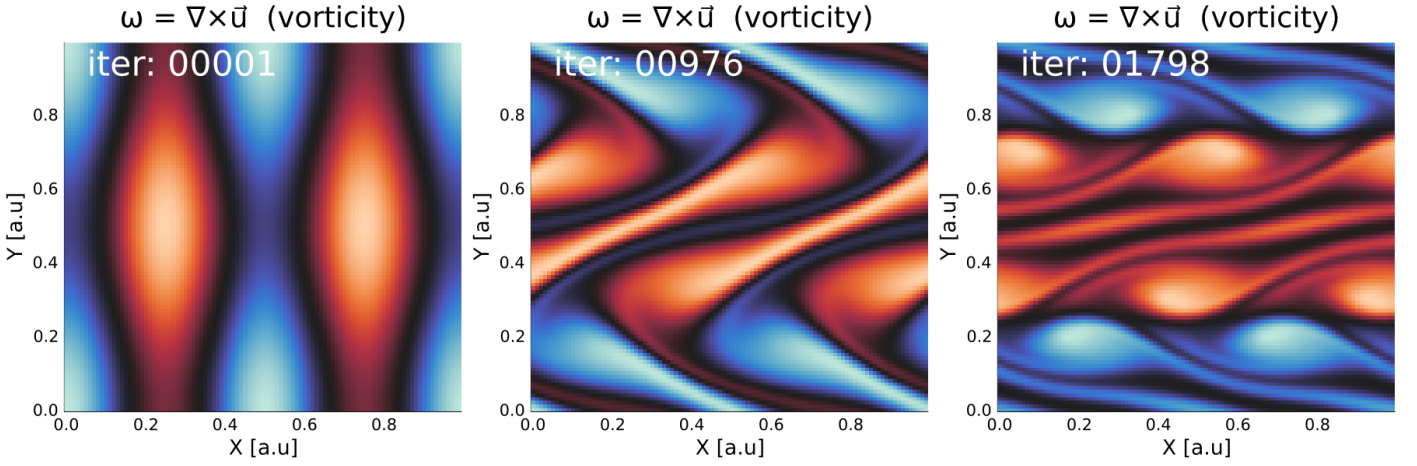

Figure 1: The development of the periodic vorticity structure. **The simulation has been done with the finite difference method.** The Figures (i),(ii) and (iii) show the development of the initial perturbation in three different moments: at initial moment, in the middle of the simulation and in the end of the simulation.

Comparison between two approaches

The goal of this work is to compare these two computational methods and show that they are generally equivalent to each other. We will conduct the comparison using the example of the development of a periodic vorticity perturbation. Let us recall that the Fourier decomposition method is periodic by nature and is applicable only for solving exclusively periodic problems. The finite element method is more general and does not have periodicity constraints. Nevertheless, for the purpose of comparing these two methods, we will implement the finite difference scheme so that it is adapted specifically for solving periodic problems.

The Figure 1 shows a periodic vorticity perturbation and its development over time. These calculations were performed using the finite element method. It is evident that a fairly simple perturbation develops into regular turbulent structures over time.

In the Figure 2, similar calculations were performed using the Spectral method. It can be seen that both methods produce very similar results and are essentially equivalent.
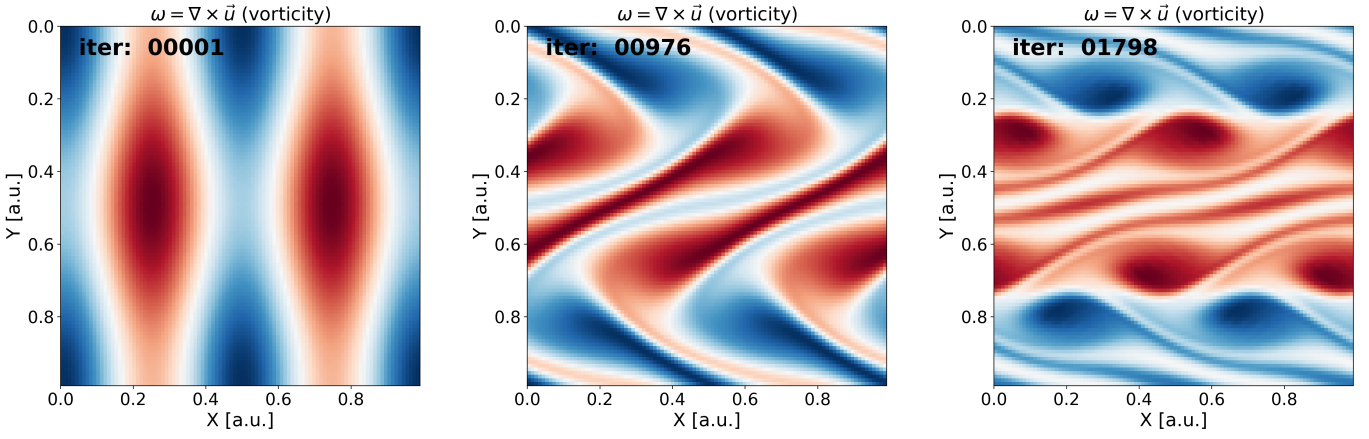
Figure 2: The development of the periodic vorticity structure. **The simulation has been done with the spectral approach.** The three Figures (i),(ii) and (iii) show the development of the initial perturbation in three different moments: at initial moment, in the middle of the simulation and in the end of the simulation.

Summary

The Finite Difference Method (FDM) and the Spectral Method offer different approaches to solving the Navier-Stokes equations, each with its advantages and limitations.

FDM approximates derivatives using finite differences, dividing the spatial domain into a grid and approximating derivatives using neighboring grid points. It typically has lower accuracy compared to spectral methods and requires finer grids to achieve higher accuracy, especially in regions with high gradients. The computational cost of FDM is linear with respect to the number of grid points, making it efficient for large, sparse systems and easy to parallelize due to the local nature of operations. FDM is also flexible in handling complex geometries and various types of boundary conditions, although special treatment is required at boundaries to maintain accuracy. Stability considerations for FDM involve careful time-stepping methods to adhere to conditions like the Courant-Friedrichs-Lewy (CFL) condition, with implicit methods available to alleviate stability constraints but at increased computational complexity.

In contrast, the Spectral Method expands the solution in terms of global basis functions, such as Fourier series for periodic domains, and transforms the problem into spectral space where derivatives become algebraic operations. Spectral methods are known for their high accuracy and rapid convergence for smooth problems, often requiring fewer grid points than FDM for a given accuracy. The computational cost involves global operations, such as the Fast Fourier Transform (FFT), with a complexity of $O(N \log N)$. FFTs can be parallelized, but the global nature of operations can be a bottleneck. Spectral methods are naturally suited for periodic boundary conditions, though handling non-periodic boundaries is more complex and requires additional techniques. The implementation of spectral methods is more challenging due to the global nature of basis functions and the handling of boundary conditions. Explicit time-stepping in spectral methods can be constrained by stability considerations similar to FDM, and nonlinear terms need careful treatment to avoid aliasing errors.

In summary, spectral methods provide high efficiency and accuracy for smooth solutions and periodic boundary conditions, while FDM offers greater flexibility and simplicity, particularly for complex geometries and boundary conditions. The choice between the two depends on the specific problem requirements and the nature of the solution.