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A FAST AND PORTABLE HIGH-ORDER IN TEMPORAL METHOD FOR COMPUTATIONAL FLUID DYNAMICS

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Abstract

A Fast and Portable High-Order in Temporal Method for Computational Fluid Dynamics

by

Youngjun Lee

A clear, concise abstract explaining the why, what, and how of your work.

A loving dedication.

Acknowledgments

The text of this dissertation includes reprints of the following previously published material:

- Youngjun Lee and Dongwook Lee. A single-step third-order temporal discretization with jacobian-free and hessian-free formulations for finite difference methods. *Journal of Computational Physics*, 427:110063, 2021.

- Youngjun Lee, Dongwook Lee, and Adam Reyes. A recursive system-free single-step temporal discretization method for finite difference methods. *Journal of Computational Physics: X*, 12:100098, 2021.

The primary co-author Dongwook Lee listed in these publications directed and supervised the research which forms the basis for this dissertation.

Chapter 1

Introduction

In past decades, the rapid evolution of the high-performance computing (HPC) systems offers growing computational capacity for the numerical simulations of various scientific fields, where conducting a direct experiment is extremely expensive or notoriously complicated. As the computing power of HPC systems gradually increases, scientists can compute more complex and computationally intensive physical models such as visualizing black holes [26, 1], simulating nuclear fusions [24, 19], studying laser-plasma interactions [32, 40], to name a few.

In order to simulate these physical phenomena, it demands meticulously designed numerical algorithms for solving nonlinear, multidimensional, and multiphysics equations judiciously. Generally speaking, numerical algorithms require more computational power for better solution accuracy, *i.e.*, using high-resolution grid configuration.

However, the recent hardware development trend – the progression of the memory capacity per compute core has become gradually saturated [2] – is compelling the HPC community to find more efficient ways that can best exercise computing resources in pursuing computer simulations. As reported in 2014 [15], decreasing memory density per compute core will be the primary limiting factor to the

scalability of scientific simulation codes.

To meet this end, modern practitioners have relentlessly delved into advancing high-arithmetic-intensity models that can increase numerical accuracy per degree of freedom while operating with reduced memory requirements and data transfers in HPC architectures. For example, in the computational fluid dynamics (CFD) community, one such computing paradigm is to promote high-order methods in which high arithmetic intensity is achieved by using an increasing number of higher-order terms. Due to its high availability in increasing the quality of numerical solutions with fewer grid points, high-order discrete methods for hyperbolic conservation laws have become primary themes in the CFD community.

Under the dual computational need for accuracy and stability, the CFD community has developed high-order reconstruction and interpolation strategies that can achieve spatially high-order approximation. [41, 12, 30, 27, 7, 9, 33, 3] However, efforts to achieve a high-order accuracy in the temporal axis have seen a renewed effort. For decades, multi-stage time integrators [22, 23, 21] have been considered as the standard temporal integration strategy for an extensive range of high-order numerical schemes for partial differential equation (PDE) solvers.

This dissertation develops a single-stage, high-order time integration scheme for hyperbolic PDEs. The core design concept is to achieve high-order accuracy within a single step to reduce computational costs for the overall numerical schemes. Another important objective for designing a high-order time integrator in this dissertation is to increase its portability. By designing a time integrator independent of the system of equations, one can provide increased flexibility and ease of code implementation.

Consequently, a newly developed time integrator showed more than two times faster performance gain than the conventional multi-stage methods. Also, it can

readily replace only the temporal part of any existing simulation code.

Chapter 2

Discretization Methods

This dissertation interests in solving the general conservation laws of hyperbolic PDEs, predicting numerical solutions with high-order accuracy. This chapter introduces two general ways to discretize the Euler equations, which will be of particular interest in this dissertation.

2.1 Euler Equations

In three dimensions, the conservation laws may be written as,

$$\partial_t \mathbf{U} + \nabla \cdot \mathcal{F}(\mathbf{U}) = \partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) + \partial_y \mathbf{G}(\mathbf{U}) + \partial_z \mathbf{H}(\mathbf{U}) = 0, \tag{2.1}$$

where $\mathbf{U}$ is a vector of conserved variables and $\mathcal{F} = (\mathbf{F}(\mathbf{U}), \mathbf{G}(\mathbf{U}), \mathbf{H}(\mathbf{U}))^T$ is the flux function in the x, y, and z directions. The conservation law is considered hyperbolic if the flux Jacobian has only real eigenvalues and is diagonalizable. Thus,

$$\mathbf{A} = \partial_{\mathbf{U}} \mathbf{F} = \mathbf{R}\mathbf{\Lambda}\mathbf{L}, \tag{2.2}$$

where $\mathbf{A}$ is the flux Jacobian in x-direction, $\mathbf{\Lambda}$ is a diagonal matrix with real eigenvalues, and $\mathbf{L}$ and $\mathbf{R}$ are corresponding left and right eigenvectors.

This dissertation focuses on solving Euler equations, which govern compressible, adiabatic inviscid flow. In the Euler equations, the conserved variables and the flux functions are defined as,

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{bmatrix}, \quad \mathbf{F}(\mathbf{U}) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u\,(E+p) \end{bmatrix}, \quad \mathbf{G}(\mathbf{U}) = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ v\,(E+p) \end{bmatrix}, \quad \mathbf{H}(\mathbf{U}) = \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w\,(E+p) \end{bmatrix}. \tag{2.3}$$

In the above equations, ρ is the density, $\mathbf{u} = (u, v, w)^T$ is the velocity, E is the total energy, and p is the pressure of the fluid. E, the total energy of the fluid represents the sum of internal and kinetic energy,

$$E = \epsilon + \frac{1}{2}\rho \mathbf{u}^2, \tag{2.4}$$

where the internal energy of the fluid, ϵ, obeys the equation of state. (EOS) This dissertation uses the ideal gas law:

$$\epsilon = \frac{p}{\gamma - 1}, \tag{2.5}$$

where γ is the specific heat ratio.

In the following, this dissertation uses the Euler equation as an example of the conserved hyperbolic system. However, numerical methods presented in this dissertation are valid for any system of the form of Eq. (2.1). Magnetohydrodynamics (MHD) equations, for example, the general numerical strategies will

be nearly identical to the Euler equations except for the solenoidal constraint of the magnetic field. ($\nabla \cdot \mathbf{B} = 0$) Thus, the high-order methods presented in this dissertation can be applied to the MHD simulation code easily.

2.2 Finite Volume Method

The popular way to consider discretized variables for the conserved system is to cast volume integrals to the governing equations, called the finite volume method. (FVM) Consider Eq. (2.1) discretized on a uniform grid containing cells with equal spacing $(\Delta x, \Delta y, \Delta z)$ in the three spatial dimensions. Then, each cell's center can be indexed by (i, j, k) at (x_i, y_j, z_k) and the cell's face centers at each interface by $(i \pm \frac{1}{2}, j, k), (i, j \pm \frac{1}{2}, k), (i, j, k \pm \frac{1}{2})$. Taking the volume average of each computational cell ($\frac{1}{\mathcal{V}_{ijk}} \int_{\mathcal{V}_{ijk}} \cdot \, d\mathcal{V}$) to Eq. (2.1) and applying the divergence theorem, we have,

$$\frac{1}{\mathcal{V}_{ijk}} \int_{\mathcal{V}_{ijk}} \partial_t \mathbf{U} \, d\mathcal{V} + \frac{1}{\mathcal{V}_{ijk}} \oint_{\mathcal{S}_{ijk}} \mathcal{F}(\mathbf{U}) \cdot \mathbf{n} \, d\mathcal{S} = 0, \tag{2.6}$$

where $\mathcal{V}_{ijk}$ is the volume of the cell at i, j, k, and $\mathcal{S}_{ijk}$ is the surrounding surfaces of the cell at i, j, k.

The semi-discretized form of FVM representation of the conserved system is obtained by substituting the dimensionally split flux functions $(\mathbf{F}(\mathbf{U}), \mathbf{G}(\mathbf{U}), \mathbf{H}(\mathbf{U}))$:

$$\begin{aligned} \partial_t \overline{\mathbf{U}}_{i,j,k} = &- \frac{1}{\Delta x} \left(\widetilde{\mathbf{F}}_{i+\frac{1}{2},j,k} - \widetilde{\mathbf{F}}_{i-\frac{1}{2},j,k} \right) \\ &- \frac{1}{\Delta y} \left(\widetilde{\mathbf{G}}_{i,j+\frac{1}{2},k} - \widetilde{\mathbf{G}}_{i,j-\frac{1}{2},k} \right) \\ &- \frac{1}{\Delta z} \left(\widetilde{\mathbf{H}}_{i,j,k+\frac{1}{2}} - \widetilde{\mathbf{H}}_{i,j,k-\frac{1}{2}} \right). \end{aligned} \tag{2.7}$$

In the above equation, the overline indicates a volume-averaged quantity, while

the tilde indicates a surface average at half-indexed cell face. Note that the above semi-discretized form of FVM scheme is a purely analytical result without any numerical approximation. The numerical methods are used to estimate surface-averaged fluxes at each cell's interfaces and update the volume-averaged conserved variables to the next time step.

The most common way to approximate interfacial fluxes for FVM solver for Euler equations is to solve the Riemann problem at cell interfaces following the Godunov method [20]. The Riemann problem is composed of a conservation equation with a single discontinuity in its initial condition. As firstly introduced by Godunov in [20], the Riemann solver ($\mathcal{RS}$) gives a numerical flux across the discontinuity in the Riemann problem. For example, the numerical flux across the discontinuity at $x_{i+\frac{1}{2},j,k}$ can be calculated as,

$$\hat{\mathbf{f}}_{i+\frac{1}{2},j,k} = \mathcal{RS}(\mathbf{U}^{\mathrm{L}}_{i+\frac{1}{2},j,k},\ \mathbf{U}^{\mathrm{R}}_{i+\frac{1}{2},j,k}). \tag{2.8}$$

The precedent task for solving the Riemann problem is to determining Riemann states at interfaces. Note that the inputs of the Riemann solver are regarded as *pointwise* values, ($\mathbf{U}^{\mathrm{L}}_{i+\frac{1}{2},j,k},\ \mathbf{U}^{\mathrm{R}}_{i+\frac{1}{2},j,k}$) while the fundamental data type of FVM is the *volume-averaged* values. ($\overline{\mathbf{U}}_{i,j,k}$) To specify the pointwise Riemann states at interfaces with given volume-averaged conserved variables, they must be reconstructed from the neighboring volume-averaged quantities. For example, a one-dimensional stencil with radius=r, the left Riemann states at $i+\frac{1}{2}$ can be reconstructed from cell-centered volume-averaged conserved variables ($\overline{\mathbf{U}}_{i-r,j,k},\ldots,\overline{\mathbf{U}}_{i,j,k},\ldots,\overline{\mathbf{U}}_{i+r,j,k}$), using p-th order accurate reconstruction operator $\mathcal{R}(\cdot)$:

$$\mathbf{U}^{\mathrm{L}}_{i+\frac{1}{2},j,k} = \mathcal{R}(\overline{\mathbf{U}}_{i-r,j,k},\ldots,\overline{\mathbf{U}}_{i+r,j,k}) + \mathcal{O}(\Delta x^p). \tag{2.9}$$

The spatial order of accuracy, p, of the FVM solver is thereby determined by choice of the reconstruction operator, $\mathcal{R}(\cdot)$ which will be discussed in **find my ref!**.

It is important to note that the numerical flux resulting from the Riemann solver is also a pointwise representation, while the surface-averaged fluxes ($\widetilde{\mathbf{F}}_{i\pm\frac{1}{2},j,k}, \widetilde{\mathbf{G}}_{i,j\pm\frac{1}{2},k}, \widetilde{\mathbf{H}}_{i,j,k\pm\frac{1}{2}}$) are needed for FVM formulation as presented in Eq. (2.7). This should be addressed thoroughly, as a naive approximation of the pointwise flux to the surface-averaged flux is bounded by second-order accuracy no matter the accuracy of the Riemann states:

$$\begin{aligned}\widetilde{\mathbf{F}}_{i+\frac{1}{2},j,k} &= \frac{1}{\Delta y \Delta z}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}}\int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \mathbf{F}(x_{i+\frac{1}{2}}, y, z)\, dz\, dy \\ &= \mathbf{F}_{i+\frac{1}{2},j,k} + \mathcal{O}(\Delta y^2, \Delta z^2).\end{aligned} \tag{2.10}$$

The conventional way to achieve higher than second-order accuracy in FVM solver is to solve the Riemann problem at multiple quadrature points on each face. [39, 31, 42] More recent studies proposed ways to avoid multiple calls of Riemann solver, reconstructing surface-averaged fluxes from pointwise Riemann fluxes, [8, 18] using linear combinations of Riemann fluxes, [17, 16] to name a few.

2.3 Finite Difference method

As it firstly proposed in [38], the finite difference method (FDM) seeks a discretization of the spatial derivatives of the fluxes in *pointwise* representation.

Assuming that there exist numerical fluxes satisfy the conservative form as,

$$\begin{aligned}\partial_t \overline{\mathbf{U}}_{i,j,k} = &- \frac{1}{\Delta x}\left(\hat{\mathbf{f}}_{i+\frac{1}{2},j,k} - \hat{\mathbf{f}}_{i-\frac{1}{2},j,k}\right) \\ &- \frac{1}{\Delta y}\left(\hat{\mathbf{g}}_{i,j+\frac{1}{2},k} - \hat{\mathbf{g}}_{i,j-\frac{1}{2},k}\right) \\ &- \frac{1}{\Delta z}\left(\hat{\mathbf{h}}_{i,j,k+\frac{1}{2}} - \hat{\mathbf{h}}_{i,j,k-\frac{1}{2}}\right),\end{aligned} \tag{2.11}$$

where $\hat{\mathbf{f}}_{i\pm\frac{1}{2},j,k}, \hat{\mathbf{g}}_{i,j\pm\frac{1}{2},k}, \hat{\mathbf{h}}_{i,j,k\pm\frac{1}{2}}$ are the *pointwise* numerical fluxes in each direction at half-indexed cell-face centers. The remaining task is to identify the numerical fluxes in desired order of accuracy, p, which satisfy,

$$\partial_x \mathbf{F}|_{\mathbf{x}=\mathbf{x}_{ijk}} = \frac{1}{\Delta x}\left(\hat{\mathbf{f}}_{i+\frac{1}{2},j,k} - \hat{\mathbf{f}}_{i-\frac{1}{2},j,k}\right) + \mathcal{O}(\Delta x^p), \quad \mathbf{x}_{ijk} = (x_i, y_j, z_k), \tag{2.12}$$

and similarly in y and z fluxes.

In order to specify the numerical fluxes for FDM, consider the pointwise x-flux $\mathbf{F}(x, y_j, z_k)$ as a one-dimensional cell average of an auxiliary function $\hat{\mathbf{F}}$,

$$\mathbf{F}(x, y_j, z_k) = \frac{1}{\Delta x}\int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} \hat{\mathbf{F}}(\xi, y_j, z_k)\, d\xi\,. \tag{2.13}$$

Then the analytic derivative of Eq. (2.13) at $x = x_i$ in x-direction becomes

$$\partial_x \mathbf{F}|_{x=x_i} = \frac{1}{\Delta x}\left(\hat{\mathbf{F}}(x_{i+\frac{1}{2}}, y_j, z_k) - \hat{\mathbf{F}}(x_{i-\frac{1}{2}}, y_j, z_k)\right). \tag{2.14}$$

Comparing Eq. (2.12) and Eq. (2.14), the numerical fluxes in FDM are obtained with desired order of accuracy, p, if they can be defined with the following relationship with $\hat{\mathbf{F}}$,

$$\hat{\mathbf{f}}_{i+\frac{1}{2},j,k} = \hat{\mathbf{F}}(x_{i+\frac{1}{2}}, y_j, z_k) + \mathcal{O}(\Delta x^p). \tag{2.15}$$

Mathematically speaking, the inverse problem of Eq. (2.15) is exactly the same

as the conventional 1D reconstruction problem in FVM, the operation of which is specifically designed to find the primitive function value $\hat{\mathbf{F}}$ at a certain location (mostly, $x_{i\pm\frac{1}{2}}$) in the i-th cell, given the integral-averaged (or volume-averaged) values $\mathbf{F}$ at nearby stencil points as input. Namely, this can be written as

$$\hat{\mathbf{F}}(\xi, y_j, z_k) = \mathcal{R}\left(\mathbf{F}_{i-r,j,k}, \ldots, \mathbf{F}_{i+r,j,k}\right) + \mathcal{O}(\Delta x^p), \quad \xi \in [x_{i-\frac{1}{2}}, x_{i-\frac{1}{2}}], \tag{2.16}$$

where $\mathcal{R}(\cdot)$ is a p-th order accurate reconstruction operator that used for FVM formulation in Section 2.2, and will be discussed in **find my ref!**.

Contrary to FVM, the conservative FDM uses only the pointwise values for constructing numerical strategies, not requiring the data conversion between pointwise and volume-averaged quantities. In addition, the high-order reconstruction schemes used for constructing Riemann states in FVM can be used for constructing numerical fluxes in FDM without intense changes in the simulation code – only a simple change in the input variables for the reconstruction operator. This simplicity in numerical strategy attracts researchers in the CFD community, leading various adoptions in high-order solvers. [27, 37, 33, 11, 35]

Compared to FVM, the major difference of FDM is obtaining high-order numerical fluxes directly from the reconstruction operator. Although it simplifies the numerical schemes, the direct formulation of the numerical fluxes hinders its further modifications while keeping a high-order convergence rate.

For example, the adaptive mesh refinement (AMR) grid configuration [5, 6] requires numerical fluxes splitting between the coarse grid to the fine grid in a conservative manner. Conventionally, this is ensured by an additional flux correction step in FVM formulation. [6] However, in FDM, a different approach should be taken because modifying the high-order numerical fluxes may spoil the order of accuracy. One possible way to maintain conservation across coarse to the fine

grid points is to apply nonlinear interpolation on the conserved variables, imply them as boundary conditions, and distribute the calculated errors among coarse grid points. [36]

Another limitation on the direct formulation of numerical fluxes in FDM is the lack of the option to include substructure in the wave model, which Riemann solver typically does in FVM to resolve certain features better. Del Zanna proposed one alternative way of FDM [13, 14], which views numerical fluxes as the Riemann fluxes with the series of high-order correction terms. This approach can achieve a high-order convergence rate with Riemann fluxes like in FVM, without the additional data type conversions required of conventional FVM. [34]

2.4 Conclusion

Two major discretization strategies for conservative systems have been presented. Both the finite difference and finite volume methods are able to achieve high-order spatial accuracy by reconstructing volume-averaged quantities to the pointwise values.

The finite difference method

- evolves the pointwise conserved variables,
- provides a straightforward framework without data type conversions,
- requires high-order numerical fluxes constructed from the pointwise, cell-centered physical fluxes directly from the high-order reconstruction methods and
- may be delicate with the additional modifications on the numerical fluxes.

The finite volume method

- evolves the volume-averaged conserved variables,
- requires rigorous data type conversions to maintain high-order accuracy,
- requires high-order reconstruction of the Riemann states from the cell-centered conserved variables and
- guarantees the conservation laws over the whole spatiotemporal domain by design.

Chapter 3

High-Order Methods for FDM

3.1 High-Order Reconstruction Schemes

3.1.1 Weighted Essentially Non-Oscillatory Methods

3.1.2 Nested Multi-Resolution WENO Method

3.1.3 Gaussian Process Reconstruction

3.2 High-Order Time Integration Schemes

3.2.1 Strong Stability Preserving Runge-Kutta Methods

3.2.2 Lax–Wendroff Type Method.

Chapter 4

System-Free Picard Integral Formulation

4.1 Picard Integral Formulation

4.2 System-Free Approach

4.3 Recursive System-Free Approach

Chapter 5

Results

Chapter 6

Conclusion

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