High Order Structure-Preserving Numerical Methods for Evolution PDEs

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The research group of Prof. Chi-Wang Shu focuses on algorithm development, analysis, implementation and application of high order structure-preserving numerical methods for evolutionary PDEs. Entropy condition, positivity-preserving and other structure stability considerations are addressed in our research.

(1) High Order Explicit-Implicit-Null (EIN) Time Discretizations:

- ***Motivation:*** Temporal methods cannot perform to the needs of MHD equations, nor the extreme anisotropy of their anisotropic thermal diffusion. In nonlinear cases, standard Explicit-Implicit (IMEX) methods must solve large algebraic systems that are computationally costly.
- ***Proposal:*** We extend existing EIN methods to the anisotropic diffusion equation with extreme anisotropy, *linearly* handling equations with *nonlinear* stiff terms.

Methodology.

Via method of lines, consider $du/dt = F(t,u)$, where $F(t,u)$ is any terms apart from time derivatives.

1. Identify which terms in $F(t,u)$ contribute severe stiffness.
2. Add & subtract a simple approximation to such terms, called $G(t,u)$:

$$du/dt = \underbrace{F(t,u) - G(t,u)}_{T_1} + \underbrace{G(t,u).}_{T_2}$$

3. Apply standard IMEX of explicit treatment on T_1 and implicit on T_2.

- **Goal:** $G(t,u)$ is well-chosen to remove the stiffness in $F(t,u)$ and preferably linear.

In two-dimensions, we propose $G(t,u) = a_0(a_1 u_{xx} + a_2 u_{yy})$, where constant a_0 guarantees stability and constants a_1, a_2 represent anisotropy present.

(2) Proof of Entropy Condition for Runge-Kutta Discontinuous Galerkin Methods:

- ***Motivation:*** The entropy solution of the 1D nonlinear scalar conservation law is uniquely characterized by the *entropy inequality*. Harten's 1976 *discrete entropy inequality* result holds only for numerical solutions of the first-order monotone scheme.
- ***Method:*** We extended this to explicit fully-discrete high-order Runge-Kutta discontinuous Galerkin (RKDG) methods and nonlinear conservation laws:
  - Proved L^2-stability of an explicit second order RKDG method with P^1 elements and Heun's method. The result holds for the general strictly convex conservation laws, achieved via cyclic inequality **Theorem 1**. [2]
  - Presented a counterexample to L^2-stability for a class of explicit 3-stage, third-order Runge-Kutta methods (including SSP-RK3) when in the RKDG method with P^2 elements and consistent locally Lipschitz numerical flux for Burgers' equation, via **Theorem 2.** [3]
  - Proved the fully-discrete cell square entropy inequality of explicit RKDG methods with P^1, P^2, P^3 elements and general non-uniform meshes while using a class of explicit third-order Runge-Kutta methods not considered in [3]. For P^1, we proved the results for the general strictly convex conservation laws, while for P^2 and P^3 we only proved for Burgers' equation. [4]

Theorem 1. For any real $b_1, b_2, \dots, b_{2N}$ satisfying

$$b_{2i-1} - 2b_{2i} + b_{2i+1} \geq 0, \qquad \forall i = 1, 2, \dots, N$$

with $b_{2N+1} = b_1$ and $b_{2N+2} = b_2$, we have

$$\sum_{i=1}^{N} (b_{2i-1} - 2b_{2i} + b_{2i+1})^3 \leq 1024 \max_{1\leq i\leq 2N} |b_i| \sum_{i=1}^{N} (b_{2i} - 2b_{2i+1} + b_{2i+2})^2 .$$

Theorem 2.

$$\sup \frac{\int_0^{2\pi} v(x)^2 v'(x)^4 \, dx}{\int_0^{2\pi} v(x)^4 v''(x)^2 \, dx} = 1,$$

taken over all 2π-periodic smooth functions $v(x)$ on the interval $[0,2\pi]$.

(3) Efficient Riemann invariant-based local characteristic decompositions for compressible Euler equations:

- ***Motivation:*** Standard Local Characteristic Decomposition (LCD) is necessary for combined shocks but computationally expensive, often dominating the runtime of high-order WENO schemes.

$$\begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & 0 & x & 0 \\ x & x & x & x \end{pmatrix}$$

Figure (1a): Original left eigenmatrix

$$\begin{pmatrix} 1 & a & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -a & 0 & 1 \end{pmatrix}$$

Figure (1b): New left eigenmatrix

- ***Method:*** We proposed using Riemann invariants as transform variables for WENO interpolation, which yields nearly diagonal eigenmatrices for the compressible Euler equations. [5]
- ***Efficiency:*** This sparsity reduces the floating-point multiplications for left eigenmatrix-vector multiplication from 16 to 1 in 2D, cutting LCD computational time by 60%–90%.
- ***Accuracy & Robustness:*** The method satisfies the "E-property" so that oscillation near contact waves are eliminated. Both high order in smooth region and ENO property are maintained. PP limiters are applied to avoid undesirable breakdowns.

(4) Positivity-preserving Sweeping for Euler equations:

- ***Motivation:*** High-order numerical methods often crash during simulations of extreme flows, such as high-Mach astrophysical jets (Figure (2)), due to unphysical negative density or pressure errors near strong shocks.
- ***Method:*** We developed a novel conservative sweeping procedure that redistributes mass, momentum, and energy to strictly enforce physical constraints without destroying high-order accuracy. [1]

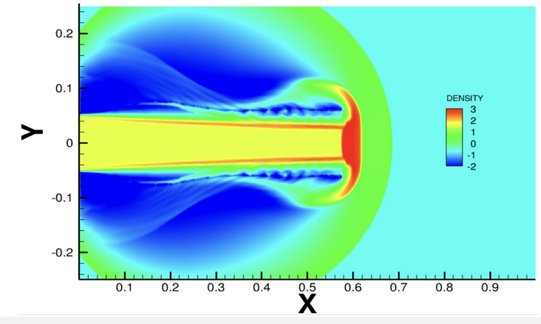


Figure (2): Density (log scale) of a Mach 2000 astrophysical jet using the sweeping framework [1]. The method stably captures turbulent structures.

- ***Wide Applicability:*** Acts as a standalone post-processor for finite difference, finite volume, and discontinuous Galerkin methods without modifying underlying spatial discretization.
- ***Impact:*** Enables robust simulations of astrophysical explosions (supernovae), hypersonic shock waves (aerospace), and combustion engines (detonations).

[1] D.C. Griffin and C.-W. Shu, A sweeping positivity-preserving high order finite difference WENO scheme for Euler equations, *Research in the Mathematical Sciences*, accepted upon minor revision.
[2] Y. Wei and C.-W. Shu, L^2-stability of explicit second order Runge-Kutta discontinuous Galerkin method for nonlinear conservation laws, *Journal of Scientific Computing*, v105 (2025), 12.
[3] Y. Wei and C.-W. Shu, Counterexample to the one-step strong L^2-stability of a class of third order Runge-Kutta discontinuous Galerkin methods for Burgers equation, *Pure and Applied Functional Analysis*, to appear.
[4] Y. Wei and C.-W. Shu, Fully-discrete cell entropy inequality of third-order explicit Runge-Kutta discontinuous Galerkin method for nonlinear conservation laws, submitted to *Mathematics of Computation*.
[5] Y. Wu and C.-W. Shu, Finite difference alternative WENO schemes with Riemann invariant-based local characteristic decompositions for compressible Euler equations, *Journal of Computational Physics*, v537 (2025), 114104.