Development of a hyperbolic solver for gyrokinetic equation using discontinuous Galerkin method

Gahyung Jo [1] Jae-Min Kwon [1] Janghoon Seo[1] Eisung Yoon[2]

[1]National Fusion Research Institute, Daejeon, Republic of Korea
[2]Ulsan National Institute of Science and Technology, Ulsan, Republic of Korea

December 15–16, 2022, 3rd Fusion HPC Workshop

한국핵융합에너지연구원
KOREA INSTITUTE OF FUSION ENERGY

Outline

Outline

Motivation

- We are developing a **whole device model** to simulate gyrokinetic equations with the **first walls** of fusion device as simulation boundaries.

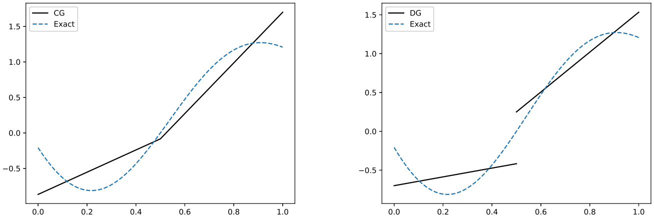
- The plasma fluctuation becomes strong as approaching **edge-SOL**(scrape-off layer) $(\delta n/n_0 \sim \mathcal{O}(1))$.
  - The conventional δf scheme is not applicable.
  - The **full-f** simulation and nonlinear collision operator are required.

- The magnetic field structure is complicated due to the separatrix and wall geometry.
  - A structured grid or ψ-θ grid is not appropriate.
  - An **unstructured** grid should be employed.

- The gradient of f is steep in space and velocity.
  - ρ_i/L_n can be $\sim \mathcal{O}(1)$ in H-mode pedestal and SOL region.
  - The open filed line in the SOL region.
  - The ion orbit loss hole, fast electron escape through the sheath potential barrier.
  - The **discontinuous Galerkin (DG)** approach can be a good candidate.
    N.R. Mandell, A. Hakim, G.W. Hammett, M. Francisquez, J. Plasma Phys. 86 (1) (2020) 905860109.

Discontinuous Galerkin method

- The DG method is a finite element (FE) method that uses a piecewise **discontinuous** basis.
  - A DG solution can be discontinuous at the interfaces of elements.

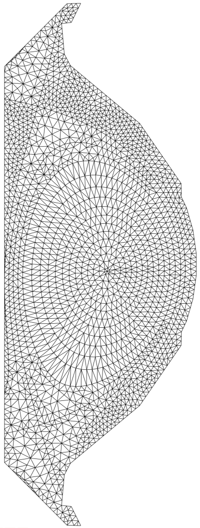


(a) FE method (b) DG method

- The DG method can be viewed as a combination of FE and finite volume (FV) methods.
  - The numerical flux is allowed. → The DG is more flexible and stable than the classic FE.
  - The DG has a higher order accuracy than the FV.
  - Information exchange is required only between the neighboring elements. → The DG is suitable for massive parallelization.

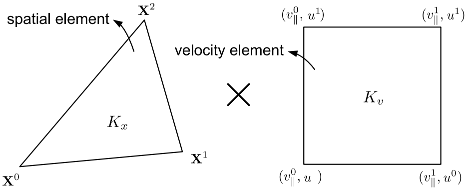
Outline

Computational Domain



- A toroidally axisymmetric domain is considered.
- No geometric constraint on the velocity space.
  $\rightarrow$ The **rectangular** elements are a good choice.
- **Triangular** elements are used to represent the complicated the wall structure.
- The finite element is constructed by the **Cartesian** product of the **triangle** and **rectangle**.

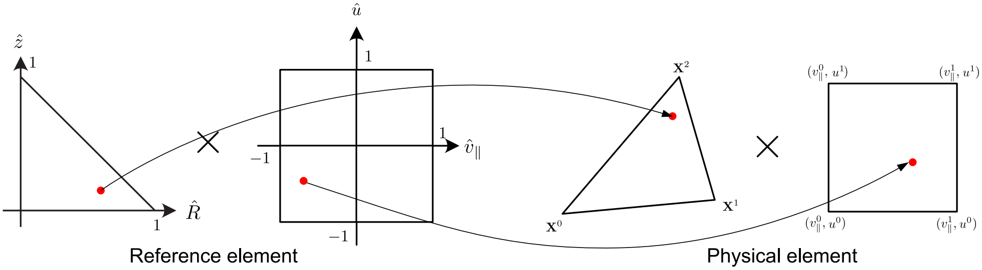
$$\mathcal{T}_h := \{K = K_x \times K_v : K_x \in \mathcal{T}_h^x, K_v \in \mathcal{T}_h^v\}.$$



- $\partial K = \partial(K_x \times K_v) = (\partial K_x \times K_v) \bigcup (K_x \times \partial K_v)$ where K_x and K_v are closed.

Affine transform

- The reference element technique improves the structure, efficiency, and re-usability of the finite element code.
- The basis functions are **once** constructed on the **reference** element and mapped to each **physical** element using the affine transforms.



- The basis function and local integration on a **physical** element can be evaluated on the **reference** element.

$$\mathcal{T} : \hat{K} \to K, \quad \zeta := \hat{\zeta} \circ \mathcal{T}^{-1}, \quad \int_K f(\mathbf{z}) d\mathbf{z} = |J\mathcal{T}| \int_{\hat{K}} (f \circ \mathcal{T})(\hat{\mathbf{z}}) d\hat{\mathbf{z}}.$$

Finite element spaces

- Two types of basis are employed to represent the numerical solution for the gyrokinetic equation.
  - Piecewise polynomial basis (Bubnov–Galerkin):

$$V_h := \{\xi = \xi_x \xi_v : \xi_x \in \mathbb{P}_m(K_x), \xi_v \in \mathbb{P}_m(K_v), K_x \times K_v \in \mathcal{T}_h\},$$

    - Linear basis $(m = 1)$

$$V_h = \{1, R, z\} \times \{1, v_\|, u\} \supset \mathbb{P}_1(K) = \{1, R, z, v_\|, u\}.$$

    - Quadratic basis $(m = 2)$

$$V_h = \{1, R, z, R^2, Rz, z^2\} \times \{1, v_\|, u, v_\|^2, v_\| u, u^2\} \supset \mathbb{P}_2(K).$$

  - Weighted polynomial basis (Petrov-Galerkin):

$$V_h' := \{\xi f_w : \xi \in V_h\},$$

    where f_w can be chosen as either the **local** or **canonical Maxwellian** functions.
    (E.L. Shi, G.W. Hammett, T. Stoltzfus-Dueck, A. Hakim, J. Plasma Phys. 83 (2017) 905830304.)

- The test function space is generated by the piecewise polynomial basis.

- The gyrokinetic equation in the **conservative** form is considered

$$\frac{\partial B_{\parallel}^{*} f}{\partial t} + \frac{\partial B_{\parallel}^{*} \dot{\mathbf{X}} f}{\partial \mathbf{X}} + \frac{\partial B_{\parallel}^{*} \dot{v}_{\parallel} f}{\partial v_{\parallel}} = 0,$$

where $f = f(\mathbf{z}; t)$, $\mathbf{z} = (\mathbf{X}, v_{\parallel}, u)$, $u = \sqrt{2\mu B_c / m_i}$, μ, B_c, and m_i are the magnetic moment, the equilibrium magnetic field at the magnetic axis, and the ion mass, respectively.

- The characteristic equations are given as follows:

$$\dot{\mathbf{X}} = v_{\parallel} \frac{\mathbf{B}^{*}}{B_{\parallel}^{*}} + \frac{\hat{b}}{B_{\parallel}^{*}} \times \frac{c}{q_s} \mu \nabla B,$$

$$\dot{v}_{\parallel} = -\frac{\mathbf{B}^{*}}{m_s B_{\parallel}^{*}} \cdot \mu \nabla B.$$

where $\mathbf{B}_{\parallel}^{*} = \hat{b} \cdot \mathbf{B}^{*}$, $\mathbf{B}^{*} = \mathbf{B} + \frac{m_s}{q_s} B v_{\parallel} \nabla \times \hat{b}$.

- Taking a **polynomial** test function $\zeta_\ell \in \mathbb{P}_m(K)$, $K \in \mathcal{T}_h$,

$$\int_K \zeta_\ell \frac{\partial B_\parallel^* f}{\partial t} d\mathbf{z} + \int_{\partial K} \zeta_\ell \underbrace{\mathcal{F}(\mathbf{n}, \mathbf{U})}_{\text{numerical flux}} dS_\sigma - \int_K \frac{\partial \zeta_\ell}{\partial \mathbf{z}} \cdot \mathbf{U} B_\parallel^* f d\mathbf{z} = 0.$$

  Here, an **upwind** numerical flux is applied.
- The solution can be approximated as

$$f(\mathbf{X}, v_\parallel, u; t) \approx \sum_\ell f_\ell(t) \zeta_\ell(\mathbf{X}, v_\parallel, u).$$

- Using the DG representation of f and summing over all $K \in \mathcal{T}_h$, we have that

$$\sum_{\ell'} \underbrace{\sum_{K \in \mathcal{T}_h} \langle \zeta_\ell, \xi_{\ell'} \rangle_K}_{\widehat{M}_{\ell\ell'} (= \widehat{M}_{\ell'\ell})} \frac{\partial f_{\ell'}}{\partial t} = - \underbrace{\sum_{K \in \mathcal{T}_h} \langle \zeta_\ell, \mathcal{F}(\mathbf{n}, \mathbf{U}_\Gamma) \rangle_{\partial K}}_{\widehat{S}_\ell} + \sum_{\ell'} \underbrace{\sum_{K \in \mathcal{T}_h} \left\langle \frac{\partial \zeta_\ell}{\partial \mathbf{z}} \cdot \mathbf{U}, \xi_{\ell'} \right\rangle_K}_{\widehat{E}_{\ell\ell'} (\neq \widehat{E}_{\ell'\ell})} f_{\ell'},$$

  where

$$\langle v, w \rangle_K = \int_K v w B_\parallel^* R du R dz dv_\parallel du, \quad \langle v, w \rangle_{\partial K} = \int_{\partial K} v w B_\parallel^* R du S_\sigma.$$

- A third-order SSP (Strong Stability Preserving) Runge–Kutta method.
  Sigal Gottlieb, Chi-Wang Shu and Eitan Tadmor, SIAM Review Vol. 43, No. 1 (2001), pp. 89-112

Implementation

- M is a **time-invariant** positive definite matrix.
  - Block diagonal matrix containing all elements of a parallel mesh part assigned to a single MPI process.
  - The PARDISO performs LDL^T-decomposition only **once** at the initial step.

- To reduce computation time, the code precomputes the time-invariant terms.

$$\int_\Gamma f_h R u B^* dS_\sigma \approx \sum_{ij} \underbrace{|JT| w_i R_i u_i B^*(\mathbf{z}_i) \hat{\varphi}_j(\hat{\mathbf{z}}_j)}_{C_{ij}} f_j(t),$$

where $w_i, \mathbf{z}_i$ are quadrature rule on Γ, JT is the Jacobian matrix of the affine transform.

	Process Time	Memory
w/o precomputation	4,175 secs	144.8 MB per PE
/o precomputation	1,395 secs	204.0 MB per PE
	-66.6%	+40.9%

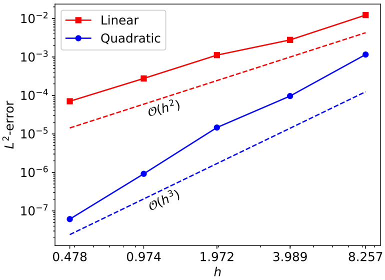
- Vectorization (AVX512 supported by MKL, Eigen3)

Outline

Convergence for interpolation

- A convergence test for interpolation with the following target function.

$$f(R, z, v_{\|}, u) = \sin \pi R \cos \pi z \times \sin 2\pi v_{\|} \cos 2\pi u.$$



- The convergence rates are good agreement with the analytic convergence rates.
- The L^2-errors are estimated using

$$\|e_h\|_{L^2}^2 = \int_\Omega |\mathcal{P} f_0 - f_0|^2 R u B_{\|}^* dR dz dv_{\|} du.$$

Conservation test

- For the conservation test, **mass** (ρ), **kinetic energy** (K), and **toroidal canonical angular momentum** (P_ϕ) are defined as follows.

$$\rho = \int_\Omega f_h B_\parallel^* d\mathbf{z},$$

$$K = \int_\Omega E_K f_h B_\parallel^* d\mathbf{z}, \quad E_K = v_\parallel^2 + u^2 B/B_c,$$

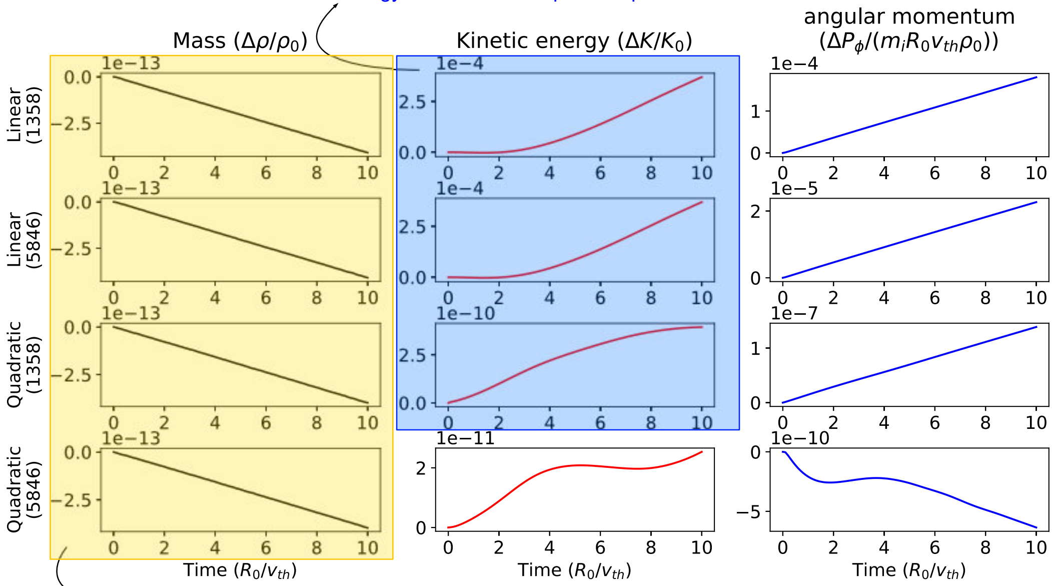
$$P_\phi = \int_\Omega p_\phi f_h B_\parallel^* d\mathbf{z}, \quad p_\phi = Z_i \psi - m_i R v_\parallel \frac{B_\phi}{B},$$

  where ψ, B_ϕ and Z_i are the poloidal magnetic flux, the toroidal component of magnetic field and the ion charge, respectively.

- In the **concentric circular domain**, an up-down symmetric boundary condition is assumed.

- The mesh for the velocity space is fixed.

Kinetic energy conservation requires a quadratic basis


Mass ($\Delta\rho/\rho_0$)
Kinetic energy ($\Delta K/K_0$)
Toroidal canonical angular momentum ($\Delta P_\phi/(m_i R_0 v_{th} \rho_0)$)
Linear (1358)
Linear (5846)
Quadratic (1358)
Quadratic (5846)
1e−13
1e−4
1e−10
1e−11
1e−5
1e−7
1e−10
Time (R_0/v_{th})

Mass is conserved nearly to a machine accuracy

- For a test function g, we have

$$\frac{dB_{\|}^{*} f_h}{dt} = 0 \Rightarrow \int_{\Omega} g \frac{dB_{\|}^{*} f_h}{dt} d\mathbf{z} = 0.$$

- The conservation properties can be expressed as

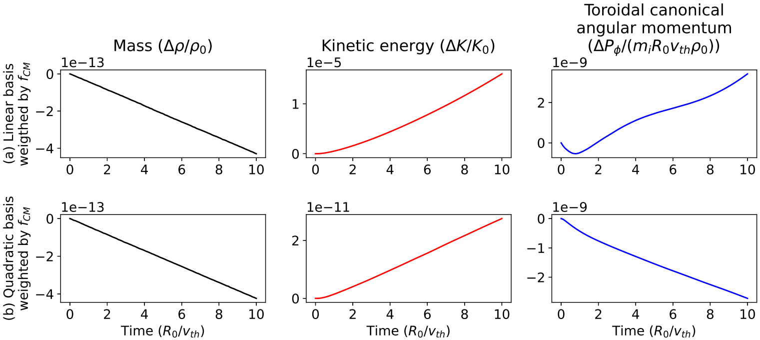
$$\begin{aligned}
\frac{d\rho}{dt} &= \frac{d}{dt} \int_{\Omega} 1 f_h B_{\|}^{*} d\mathbf{z} = \int_{\Omega} 1 \frac{dB_{\|}^{*} f_h}{dt} d\mathbf{z}, \\
\frac{dK}{dt} &= \int_{\Omega} E_K \frac{dB_{\|}^{*} f_h}{dt} d\mathbf{z}, \quad E_K = v_{\|}^2 + u^2 B/B_c, \\
\frac{dP_{\phi}}{dt} &= \int_{\Omega} p_{\phi} \frac{dB_{\|}^{*} f_h}{dt} d\mathbf{z}, \quad p_{\phi} = Z_i \psi - m_i R v_{\|} \frac{B_{\phi}}{B},
\end{aligned}$$

  - If $1 \in W_h$, then ρ is conserved. $\rightarrow$ Constant basis. (automatically satisfied)
  - If $E_K \in W_h$, then K is conserved. $\rightarrow$ Quadratic basis.

- The kinetic energy has quadratic terms in $v_{\|}$ and u along with spatially varying B.
- For the conservation of K, a **quadratic** basis is required.

Conservation property with weighted polynomial basis

- The weighed polynomial basis functions are used. For the weighting function, the **canonical Maxwellian** is considered.



- The canonical angular momentum shows good conservation even with the **linear weighted basis** function.
- The kinetic energy conservation still requires a quadratic basis.

Invariance test

- The **canonical Maxwellian** is a stationary solution of the gyrokinetic equation.
- As expected, the initial value f_{CM} shows little change.

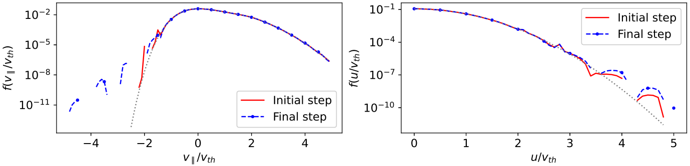


Figure: Quadratic polynomial basis

- The invariance is achieved even with the **linear weighted polynomial basis**.

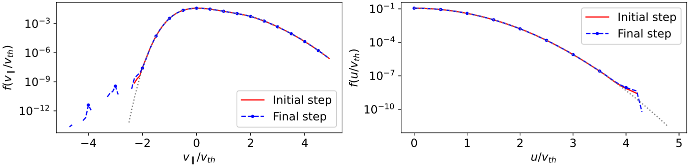
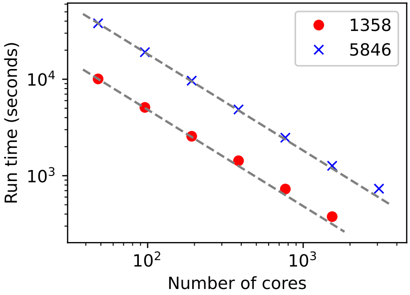
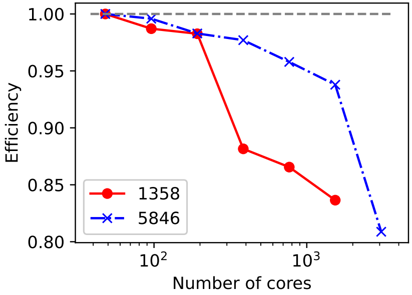


Figure: Linear weighted polynomial basis

Parallelization performance test



(a) Strong scaling: Measured run time



(b) Parallelization efficiency

- I_t is the ideal runtime, which is estimated as $I_t = M/N$ where M is the measured time when using smallest CPU cores.
- The efficiency is estimated by the ratio between I_t and the measured time.
  - **The efficiency remains fairly high up to a few thousand cores.**

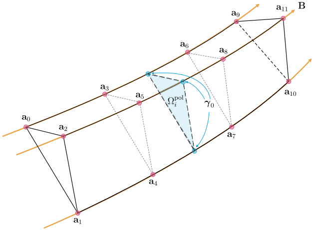
KFE 한국핵융합에너지연구원 KOREA INSTITUTE OF FUSION ENERGY

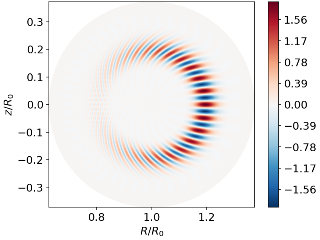
Outline

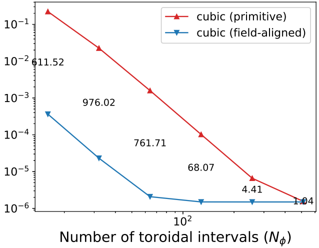
Summary

- A gyrokinetic hyperbolic solver for general tokamak geometry was developed.
  - The **discontinuous Galerkin method** with an **unstructured mesh** was employed.
- The impact of basis functions on the conservation properties.
  - The **conservation of the mass** was demonstrated up to the machine accuracy.
  - A **quadratic** basis for the **velocity** space is required for **kinetic energy**.
- Invariance in time with canonical Maxwellian initial value.
  - A **quadratic** basis shows the **invariance** up to machine accuracy.
  - A **linear** polynomial basis weighted by **canonical Maxwellian** can show the **invarinace** in a similar level.
- Parallelization performance.
  - The new code is parallelized by MPI library using domain decomposition method with ghost layers.
  - The solver has a good parallelization performance up to a few thousand ranks.

- Extending the solver to 5D by allowing toroidal variations.
  - In extending the spatial domain from 2D to 3D, it is critical to suppress the increase of overall **computing cost** within a manageable level.
  - The development of a new scheme discretizes the spatial domain into 3D elements, which are poloidally unstructured but **toroidally aligned** with equilibrium magnetic fields.







- Implementation of new numerical flux.
  - Lax-Fredrich numeric flux, etc.
- Collision operators and Maxwell equation solvers.
  - The nonlinear operator have been developed.
    (Dongkyu Kim, Janghoon Seo, Gahyung Jo, Jae-Min Kwon, Eisung Yoon*, Comput. Phys. Commun. (2022) 108459)