

Discretely entropy stable weight-adjusted discontinuous Galerkin methods: curvilinear meshes and GPU acceleration

Jesse Chan, Lucas Wilcox

Abstract

Things to include: entropy conservation and stability on curvilinear meshes, choosing geometric factors to ensure constant state preservation, high order accuracy. Computational considerations for curvilinear meshes.

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1 Introduction

Introducing WADG [1, 2].

Matrix WADG: GPU efficiency of WADG vs storing weighted inverses [3].

2 Systems of nonlinear conservation laws

This work addresses is high order schemes for the following system of n nonlinear conservation laws in d dimensions

$$\frac{\partial \mathbf{u}}{\partial t} + \sum_{j=1}^d \frac{\partial \mathbf{f}_j(\mathbf{u})}{\partial x_j} = 0, \quad \mathbf{u} \in \mathbb{R}^n, \quad \mathbf{f}_j : \mathbb{R}^n \rightarrow \mathbb{R}^n, \quad (1)$$

where $\mathbf{u}(\mathbf{x}, t)$ denote the *conservative variables* for this system. We will specify boundary conditions in a later section.

We are interested in nonlinear conservation laws for which an entropy function $U(\mathbf{u})$ exists, where $U(\mathbf{u})$ is convex with respect to the conservative variables \mathbf{u} . If this function exists, then it is possible to define *entropy variables* $\mathbf{v}(\mathbf{u}) = \frac{\partial U}{\partial \mathbf{u}}$. These functions symmetrize the system of nonlinear conservation laws (1) [4].

It can be shown (see, for example, [5]) that symmetrization is equivalent to the existence of an entropy flux function $F(\mathbf{u})$ and entropy potential ψ such that

$$\mathbf{v}^T \frac{\partial \mathbf{f}_j}{\partial \mathbf{u}} = \frac{\partial F_j(\mathbf{u})}{\partial \mathbf{u}}^T, \quad \psi_j(\mathbf{v}) = \mathbf{v}^T \mathbf{f}_j(\mathbf{u}(\mathbf{v})) - F_j(\mathbf{u}(\mathbf{v})), \quad \psi'_j(\mathbf{v}) = \mathbf{f}_j(\mathbf{u}(\mathbf{v})).$$

Smooth solutions of (1) can be shown to satisfy a conservation of entropy by multiplying (1) by $\mathbf{v}(\mathbf{u})$. Using the definition of the entropy variables, entropy flux, and the chain rule yields

$$\mathbf{v}^T \frac{\partial \mathbf{f}_j(\mathbf{u})}{\partial x_j} = \frac{\partial U(\mathbf{u})}{\partial \mathbf{u}}^T \frac{\partial \mathbf{f}_j(\mathbf{u})}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial x_j} = \frac{\partial F_j(\mathbf{u})}{\partial x_j}, \quad (2)$$

and that

$$\frac{\partial U(\mathbf{u})}{\partial t} + \sum_{j=1}^d \frac{\partial F_j(\mathbf{u})}{\partial x_j} = 0.$$

Let $\Omega \subset \mathbb{R}^d$ now be a closed domain with boundary $\partial\Omega$. Integrating over Ω and using Gauss' theorem on the spatial derivative yields

$$\int_{\Omega} \frac{\partial U(\mathbf{u})}{\partial t} \, dx + \int_{\partial\Omega} \sum_{j=1}^d (\mathbf{v}(\mathbf{u})^T \mathbf{f}_j(\mathbf{u}) - \psi_j(\mathbf{v}(\mathbf{u}))) n_j \, dx = 0, \quad (3)$$

where $\mathbf{n} = (n_1, \dots, n_d)^T$ denotes the unit outward normal vector on $\partial\Omega$.

General solutions (including non-smooth solutions such as shocks) satisfy an entropy *inequality*

$$\int_{\Omega} \frac{\partial U(\mathbf{u})}{\partial t} \, dx + \int_{\partial\Omega} \sum_{j=1}^d (\mathbf{v}(\mathbf{u})^T \mathbf{f}_j(\mathbf{u}) - \psi_j(\mathbf{v}(\mathbf{u}))) n_j \, dx \leq 0, \quad (4)$$

which results from considering solutions of an appropriate viscous form of the equations (1) and taking the limit as viscosity vanishes. In this work, schemes which satisfy a discrete form of (4) will be constructed by first enforcing a discrete version of entropy conservation (3), then adding an appropriate numerical dissipation which will enforce the entropy inequality (4).

2.1 Standard DG formulations for nonlinear conservation laws

We begin by reviewing the construction of standard high order DG formulations for (1).

2.1.1 Mathematical notation

Let the domain $\Omega \subset \mathbb{R}^d$ be decomposed into elements (subdomains) D^k , and let \hat{D} denote a d -dimensional reference element with boundary $\partial\hat{D}$. Let $\hat{\mathbf{x}}$ denote coordinates on \hat{D} , and let \hat{n}_i denote the i th component of the unit normal vector on $\partial\hat{D}$. We assume that \hat{n}_i is constant; i.e., that the faces of the reference element are planar (this assumption holds for all commonly used reference elements [6]).

We will assume that each physical element D^k is the image of \hat{D} under some smoothly differentiable mapping $\Phi_k(\hat{\mathbf{x}})$ such that

$$\mathbf{x} = \Phi_k(\hat{\mathbf{x}}), \quad \mathbf{x} \in D^k.$$

This also implies that integrals over physical elements can be mapped back to the reference element as follows

$$\int_{D^k} u \, d\mathbf{x} = \int_{\hat{D}} u J^k \, d\hat{\mathbf{x}},$$

where J^k denotes the determinant of the Jacobian of Φ_k . Integrals over physical faces of D^k can similarly be mapped back to reference faces.

We define an approximation space using degree N polynomials on the reference element. For example, on a d -dimensional reference simplex, the natural polynomial space are total degree N polynomials

$$P^N(\hat{D}) = \left\{ \hat{x}_1^{i_1} \dots \hat{x}_d^{i_d}, \quad \hat{\mathbf{x}} \in \hat{D}, \quad 0 \leq \sum_{k=1}^d i_k \leq N \right\}.$$

Other element types possess different natural polynomial spaces [6], but typically contain the space of total degree N polynomials. This work is directly applicable to other elements and spaces as well. We denote the dimension of the approximation space P^N as $N_p = \dim(P^N(\hat{D}))$.

Finally, we define the L^2 norm and inner products over the reference element \hat{D} and the surface of the reference element $\partial\hat{D}$

$$(\mathbf{u}, \mathbf{v})_{\hat{D}} = \int_{\hat{D}} \mathbf{u} \cdot \mathbf{v} \, d\mathbf{x} = \int_{\hat{D}} \mathbf{u} \cdot \mathbf{v} J^k \, d\hat{\mathbf{x}}, \quad \|\mathbf{u}\|_{\hat{D}}^2 = (\mathbf{u}, \mathbf{u})_{\hat{D}}, \quad \langle \mathbf{u}, \mathbf{v} \rangle_{\partial\hat{D}} = \int_{\partial\hat{D}} \mathbf{u} \cdot \mathbf{v} \, d\mathbf{x},$$

Finally, we introduce the continuous L^2 projection operator Π_N and lifting operator L . For $u \in L^2(\hat{D})$, the L^2 projection $\Pi_N u$ is defined through

$$\int_{\hat{D}} \Pi_N u v \, d\hat{\mathbf{x}} = \int_{\hat{D}} u v \, d\hat{\mathbf{x}}, \quad \forall v \in P^N(\hat{D}). \quad (5)$$

Likewise, for a boundary function $u \in L^2(\partial\hat{D})$, the lifting operator L [7, 8] is defined through

$$(Lu, v)_{\hat{D}} = \langle u, v \rangle_{\partial\hat{D}}, \quad \forall v \in P^N(\hat{D}). \quad (6)$$

2.1.2 Discontinuous Galerkin formulations and the L^2 projection

Discontinuous Galerkin methods have been very widely applied to systems of nonlinear conservation laws (1) [9, 10, 11, 12]. The development of new discontinuous Galerkin methods for nonlinear conservation laws have focused heavily on the choice of numerical flux [13] or the development of slope limiters [14, 15, 16] and artificial viscosity strategies [17, 18, 19]. However, the treatment of the underlying volume discretization remains relatively unchanged between each of these approaches.

Ignoring terms involving filters, limiters, or artificial viscosity, a semi-discrete “weak” DG formulation for (1) can be given locally over an element D^k : find $\mathbf{u} \in (P^N(D^k))^n$ such that

$$\int_{D^k} \left(\frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{v} - \sum_{j=1}^d \mathbf{f}_j(\mathbf{u}) \cdot \frac{\partial \mathbf{v}}{\partial x_j} \right) d\mathbf{x} + \sum_{j=1}^d \int_{\partial D^k} (\mathbf{f}_j^*(\mathbf{u}^+, \mathbf{u})) \cdot \mathbf{v} n_j \, d\mathbf{x} = 0, \quad \forall \mathbf{v} \in (P^N(D^k))^n, \quad (7)$$

where the numerical flux \mathbf{f}^* is a function of the solution \mathbf{u} on both D^k and neighboring elements.

Unfortunately, solutions to (7) do not (in general) obey a discrete version of the entropy inequality (4). Since (4) is a generalized statement of energy stability, the lack of a discrete entropy inequality implies that the discrete solution can blow up in finite time. The reason for this is due the fact that, in practice, the integrals in (7) are not computed exactly and are instead approximated using polynomially exact quadratures. This is compounded by the fact that the nonlinear flux function $\mathbf{f}_j(\mathbf{u})$ is often rational and impossible to integrate exactly using polynomial quadratures. To account for the inexactness of quadrature, we rewrite (7) in strong form using a discrete quadrature-based L^2 projection.

For polynomial approximation spaces, $\frac{\partial \mathbf{v}}{\partial x_i}$ is polynomial. Then, mapping (7) back to the reference element \hat{D} and using the L^2 projection and (5), we have that

$$\int_{D^k} \mathbf{f}_j(\mathbf{u}) \cdot \frac{\partial \mathbf{v}}{\partial x_i} d\mathbf{x} = \int_{\hat{D}} \Pi_N \mathbf{f}_j(\mathbf{u}) \cdot \frac{\partial \mathbf{v}}{\partial x_i} J^k d\mathbf{x}.$$

Thus, integrating by parts (7) recovers a “strong” DG formulation involving the projection operator

$$\begin{aligned} & \int_{D^k} \left(\frac{\partial \mathbf{u}}{\partial t} - \sum_{j=1}^d \frac{\partial \Pi_N \mathbf{f}_j(\mathbf{u})}{\partial x_j} \right) \cdot \mathbf{v} d\mathbf{x} \\ & + \sum_{j=1}^d \int_{\partial D^k} (\mathbf{f}_j^*(\mathbf{u}^+, \mathbf{u}) - \Pi_N \mathbf{f}_j(\mathbf{u})) \cdot \mathbf{v} n_j d\mathbf{x} = 0, \quad \forall \mathbf{v} \in (P^N(D^k))^n. \end{aligned} \quad (8)$$

From this, we see that our discrete scheme does not differentiate the nonlinear flux function $\mathbf{f}_j(\mathbf{u})$ exactly, but instead differentiates the projection of $\Pi_N \mathbf{f}_j(\mathbf{u})$ onto polynomials of degree N . Because the L^2 projection operator is introduced, the chain rule no longer holds at the discrete level and step (2) of the proof of entropy conservation is no longer valid. Thus, ensuring discrete entropy stability will require a discrete formulation of the system of nonlinear conservation laws (1) from which we can prove a discrete entropy inequality without relying on the chain rule.

3 Discretely entropy stable DG methods on curved meshes

We will first show how to construct discretely entropy stable high order DG methods on curvilinear meshes, but will present this using a matrix formulation as opposed to a continuous formulation. This is to ensure that the effects of discretization, nonlinear, and quadrature are accounted for in the proof of semi-discrete entropy stability. We first introduce quadrature-based matrices, which we will then use to construct discretely entropy stable DG formulations.

3.1 Basis and quadrature rules

We now introduce quadrature-based matrices for the d -dimensional reference element \hat{D} , which we will use to construct matrix-vector formulations of DG methods. Assuming $u(\mathbf{x}) \in P^N(\hat{D})$, it can be represented in terms of the vector of coefficients \mathbf{u} using some polynomial basis ϕ_i of degree N and dimension N_p

$$u(\mathbf{x}) = \sum_{j=1}^{N_p} \mathbf{u}_j \phi_j(\hat{\mathbf{x}}), \quad P^N(\hat{D}) = \text{span} \{ \phi_i(\hat{\mathbf{x}}) \}_{i=1}^{N_p}.$$

We construct quadrature-based based on ϕ_i and appropriate volume and surface quadrature rules. The volume and surface quadrature rules are given by points and positive weights $\{(\mathbf{x}_i, w_i)\}_{i=1}^{N_q}$ and $\{(\mathbf{x}_i^f, w_i^f)\}_{i=1}^{N_q^f}$, respectively. We make the following assumptions on the strength of these quadratures:

Assumption 1. The volume quadrature rule $\{(\mathbf{x}_i, w_i)\}_{i=1}^{N_q}$ is exact for polynomials of degree $2N - 1$. Additionally, for any $u, v \in P^N(\hat{D})$, integration by parts

$$\left(\frac{\partial u}{\partial x_i}, v\right)_{\hat{D}} = \langle u, v n_i \rangle_{\partial \hat{D}} - \left(u, \frac{\partial v}{\partial x_i}\right)_{\hat{D}}$$

holds when volume and surface integrals are approximated using quadrature.

Assumption (1) holds, for example, for any surface quadrature rule which is exact for degree $2N$ polynomials on the boundary of the reference element $\partial \hat{D}$.

3.2 Reference element matrices

Let \mathbf{W}, \mathbf{W}_f denote diagonal matrices whose entries are volume and surface quadrature weights, respectively. The surface quadrature weights are given by quadrature weights on reference faces, which are mapped to faces of the reference element. We define the volume and surface quadrature interpolation matrices \mathbf{V}_q and \mathbf{V}_f

$$\begin{aligned} (\mathbf{V}_q)_{ij} &= \phi_j(\hat{\mathbf{x}}_i), & 1 \leq j \leq N_p, & \quad 1 \leq i \leq N_q, \\ (\mathbf{V}_f)_{ij} &= \phi_j(\hat{\mathbf{x}}_i^f), & 1 \leq j \leq N_p, & \quad 1 \leq i \leq N_q^f, \end{aligned} \quad (9)$$

which map coefficients \mathbf{u} to evaluations of u at volume and surface quadrature points.

Next, let \mathbf{D}_i denote the differentiation matrix with respect to the i th coordinate, defined implicitly through the relation

$$u(\hat{\mathbf{x}}) = \sum_{j=1}^{N_p} \mathbf{u}_j \phi_j(\hat{\mathbf{x}}), \quad \frac{\partial u}{\partial \hat{x}_i} = \sum_{j=1}^{N_p} (\mathbf{D}_i \mathbf{u})_j \phi_j(\hat{\mathbf{x}}).$$

The matrix \mathbf{D}_i maps basis coefficients of some polynomial $u \in P^N$ to coefficients of its i th derivative with respect to the reference coordinate $\hat{\mathbf{x}}$, and is sometimes referred to as a “modal” differentiation matrix (with respect to a general non-nodal “modal” basis [20]).

Using the volume quadrature interpolation matrix \mathbf{V}_q , we can compute a quadrature-based mass matrix \mathbf{M} by evaluating L^2 inner products of different basis functions using quadrature

$$\mathbf{M} = \mathbf{V}_q^T \mathbf{W} \mathbf{V}_q, \quad \mathbf{M}_{ij} = \sum_{k=1}^{N_q} w_k \phi_j(\mathbf{x}_k) \phi_i(\mathbf{x}_k) \approx \int_{\hat{D}} \phi_j \phi_i d\hat{\mathbf{x}} = (\phi_j, \phi_i)_{\hat{D}}.$$

The approximation in the formula for the mass matrix becomes an equality if the volume quadrature rule is exact for polynomials of degree $2N$. The mass matrix is symmetric and positive definite under Assumption 1; however, we do not make any distinctions between diagonal and dense (lumped) mass matrices in this work.

The mass matrix appears in the discretization of L^2 projection (5) and lift operators (6) using quadrature. The result are quadrature-based L^2 projection and lift operators $\mathbf{P}_q, \mathbf{L}_q$,

$$\mathbf{P}_q = \mathbf{M}^{-1} \mathbf{V}_q^T \mathbf{W}, \quad \mathbf{L}_q = \mathbf{M}^{-1} \mathbf{V}_f^T \mathbf{W}_f, \quad (10)$$

which are discretizations of the continuous L^2 projection operator Π_N and continuous lift operator L . The matrix \mathbf{P}_q maps a function (in terms of its evaluation at quadrature points) to coefficients of the L^2 projection in the basis $\phi_j(x)$, while the matrix \mathbf{L}_q “lifts” a function (evaluated at surface quadrature points) from the boundary of an element to coefficients of a basis defined in the interior of the element.

Finally, we introduce quadrature-based operators \mathbf{D}_N^i which will be used to construct discretizations of our nonlinear conservation laws. This operator was introduced in [21] as a “decoupled summation by parts” operator

$$\mathbf{D}_N^i = \begin{bmatrix} \mathbf{V}_q \mathbf{D}_i \mathbf{P}_q - \frac{1}{2} \mathbf{V}_q \mathbf{L}_q \text{diag}(\hat{\mathbf{n}}_i \hat{\mathbf{J}}_f) \mathbf{V}_f \mathbf{P}_q & \frac{1}{2} \mathbf{V}_q \mathbf{L}_q \text{diag}(\hat{\mathbf{n}}_i \hat{\mathbf{J}}_f) \\ -\frac{1}{2} \text{diag}(\hat{\mathbf{n}}_i \hat{\mathbf{J}}_f) \mathbf{V}_f \mathbf{P}_q & \frac{1}{2} \text{diag}(\hat{\mathbf{n}}_i \hat{\mathbf{J}}_f) \end{bmatrix} \quad (11)$$

where $\hat{\mathbf{n}}_i$ is the vector containing values of the i th component of the unit normal on the surface of the reference element \hat{D} , and $\hat{\mathbf{J}}_f$ contains values of the face Jacobian factor \hat{J}_f which result from mapping a face of \hat{D} to a reference face. When combined with projection and lifting matrices, \mathbf{D}_N^i produces a high order approximation of non-conservative products. Let \mathbf{f}, \mathbf{g} denote vectors containing the evaluation of functions $f(\mathbf{x}), g(\mathbf{x})$ at both volume and surface quadrature points

$$\begin{bmatrix} \mathbf{P}_q & \mathbf{L}_q \end{bmatrix} \text{diag}(\mathbf{f}) \mathbf{D}_N^i \mathbf{g} \approx f \frac{\partial g}{\partial \hat{x}_i}.$$

It can be observed that the matrix \mathbf{D}_N^i satisfies several key properties. First, it can be observed that $\mathbf{D}_N^i \mathbf{1} = 0$, where $\mathbf{1}$ is the vector of all ones. Second, \mathbf{D}_N^i satisfies a summation-by-parts property. Let \mathbf{Q}_N^i be the scaling of \mathbf{D}_N^i by the diagonal matrix of volume and surface quadrature weights

$$\mathbf{Q}_N^i = \mathbf{W}_N \mathbf{D}_N^i, \quad \mathbf{W}_N = \begin{pmatrix} \mathbf{W} & \\ & \mathbf{W}_f \end{pmatrix}.$$

Then, \mathbf{Q}_N^i satisfies the following discrete analogue of integration by parts

$$\mathbf{Q}_N^i + (\mathbf{Q}_N^i)^T = \mathbf{B}_N^i, \quad \mathbf{B}_N = \begin{pmatrix} 0 & \\ & \mathbf{W}_f \text{diag}(\hat{\mathbf{n}}_i \hat{\mathbf{J}}_f) \end{pmatrix}. \quad (12)$$

3.3 Curvilinear differentiation and projection matrices

The key difference between curvilinear and affine meshes is that geometric terms now vary spatially over each element. In practice, derivatives are computed over the reference element and mapped to the physical element D^k through a change of variables formula

$$\frac{\partial u}{\partial x_i} = \sum_{j=1}^d \mathbf{G}_{ij}^k \frac{\partial u}{\partial \hat{x}_j}, \quad \mathbf{G}_{ij}^k = \frac{\partial \hat{x}_j}{\partial x_i}.$$

where we have defined the elements of the matrix \mathbf{G}^k as the derivatives of the reference coordinates \hat{x}_j with respect to the physical coordinates x_i on D^k . We refer to the determinant of \mathbf{G}^k as J^k .

We assume in this work that the mesh is stationary. It can be shown at the continuous level that, for any differentiable and invertible mapping, the quantity $J^k \mathbf{G}^k$ satisfies a geometric conservation law (GCL) [22, 23]

$$\sum_{j=1}^d \frac{\partial}{\partial \hat{x}_j} J^k \mathbf{G}_{ij}^k = 0, \quad (13)$$

or that $\hat{\nabla} \cdot (J^k \mathbf{G}^k)^T = 0$. Using (13), the scaled physical derivative $J^k \frac{\partial u}{\partial x_i}$ can be computed via

$$J^k \frac{\partial u}{\partial x_i} = \frac{1}{2} \sum_{j=1}^d \left(J^k \mathbf{G}_{ij}^k \frac{\partial u}{\partial \hat{x}_j} + \frac{\partial (J^k \mathbf{G}_{ij}^k u)}{\partial \hat{x}_j} \right). \quad (14)$$

We define physical differentiation matrices based on the approximation of (14). Define \mathbf{D}_k^i as

$$\mathbf{D}_k^i = \sum_{j=1}^d \text{diag}(\mathbf{J} \mathbf{G}_{ij}^k) \mathbf{D}_N^j + \mathbf{D}_N^j \text{diag}(\mathbf{J} \mathbf{G}_{ij}^k)$$

where $\mathbf{J} \mathbf{G}_{ij}^k$ refers to the vector containing evaluations of $J^k \mathbf{G}_{ij}^k$ at both volume and surface quadrature points. Using properties of the Hadamard product [24], we can rewrite \mathbf{D}_k^i as

$$\mathbf{D}_k^i = \sum_{j=1}^d \left(\mathbf{D}_N^j \circ \{\{\mathbf{J} \mathbf{G}_{ij}^k\}\} \right), \quad \{\{\mathbf{J} \mathbf{G}_{ij}^k\}\}_{mn} = \frac{1}{2} \left((\mathbf{J} \mathbf{G}_{ij}^k)_m + (\mathbf{J} \mathbf{G}_{ij}^k)_n \right), \quad (15)$$

where $\{\{JG_{ij}^k\}\}$ denotes the matrix of averages between each of the entries of JG_{ij}^k . From (15), it is straightforward to show that $Q_k^i = W_N D_k^i$ also satisfies a summation by parts property

$$Q_k^i + (Q_k^i)^T = B_k^i, \quad B_k^i = \begin{pmatrix} 0 & \\ & W_f \text{diag}(\mathbf{n}_i J_f^k) \end{pmatrix}, \quad (16)$$

where \mathbf{n}_i and J_f^k are vectors containing evaluations of the physical unit normals and face Jacobian factors for D^k at surface quadrature points, respectively. Here, we have used that the scaled matrix of geometric factors transforms scaled reference normal vectors to scaled physical normals [25], such that

$$\sum_{j=1}^d JG_{ij} \hat{n}_j \hat{J}_f = n_i J_f^k, \quad \left(\sum_{j=1}^d (JG_{ij}^k) \circ (\hat{n}_j \hat{J}_f) \right) = (n_i J_f^k).$$

Curvilinear mappings also imply that integrals over each physical element D^k are no longer simple scalings of integrals over \hat{D} . The L^2 projection of $u \in L^2(D^k)$ over a curvilinear element D^k is defined through

$$(\Pi_N u, v)_{D^k} = (u, v)_{D^k}. \quad (17)$$

Mapping integrals to the reference element \hat{D} yields

$$(\Pi_N u, vJ)_{\hat{D}} = (u, vJ)_{\hat{D}}. \quad (18)$$

For affine elements, J is constant and can be cancelled. Thus, the L^2 projection over affine elements is equivalent to simply taking the L^2 projection of a function over the reference element. However, for curved elements, J acts as a spatially varying weight within the L^2 inner product.

Discretizing (18) requires a weighted mass matrix. We define a curved mass matrix over an element D^k by weighting the discrete L^2 norm with values of J at quadrature points

$$M_k = V_q^T W_J V_q, \quad (W_J)_{ij} = \delta_{ij} w_i J(\mathbf{x}_i), \quad i = 1, \dots, N_q. \quad (19)$$

Then, a curvilinear L^2 projection and lift matrices can be defined in a manner analogous to (10)

$$P_q^k = (M^k)^{-1} V_q^T W \text{diag}(J^k), \quad L_q^k = (M^k)^{-1} V_f^T W_f \text{diag}(J_f^k). \quad (20)$$

These matrices are distinct from element to element, reflecting the fact that problem (18) is distinct from element to element.

3.4 A discretely entropy stable DG formulation on curved meshes

Given the matrices in Section 3.3, we can now define a local entropy stable DG formulation on an element D^k . Here, we seek an approximation solution $\mathbf{u}_N(\mathbf{x}, t)$ to (1), which is represented using vector-valued coefficients $\mathbf{u}_h(t)$ such that

$$\mathbf{u}_N(\mathbf{x}, t) = \sum_{j=1}^{N_p} (\mathbf{u}_h(t))_j \phi_j(\mathbf{x}), \quad (\mathbf{u}_h(t))_j \in \mathbb{R}^n.$$

Since the coefficients are vector valued, we assume that all matrices act component-wise on \mathbf{u}_h in the Kronecker product sense.

We first define the numerical fluxes $\mathbf{f}_{i,S}(\mathbf{u}_L, \mathbf{u}_R)$ as the bivariate function of “left” and “right” conservative variable states $\mathbf{u}_L, \mathbf{u}_R$. Such a numerical flux is referred to as entropy conservative (or entropy stable) if it satisfies the following conditions:

Definition 1. The numerical flux $\mathbf{f}_{i,S}(\mathbf{u}_L, \mathbf{u}_R)$ is entropy conservative (or entropy stable) if it satisfies the following conditions

1. $\mathbf{f}_{i,S}(\mathbf{u}_L, \mathbf{u}_R) = \mathbf{f}_{i,S}(\mathbf{u}_R, \mathbf{u}_L)$ (symmetry),
2. $\mathbf{f}_{i,S}(\mathbf{u}, \mathbf{u}) = \mathbf{f}_i(\mathbf{u})$ (consistency),
3. $\mathbf{f}_{i,S}$ is referred to as entropy conservative if it satisfies conditions 1, 2, and

$$(\mathbf{v}_L - \mathbf{v}_R)^T \mathbf{f}_{i,S}(\mathbf{u}_L, \mathbf{u}_R) = \psi_i(\mathbf{u}_L) - \psi_i(\mathbf{u}_R).$$

4. $\mathbf{f}_{i,S}$ is referred to as entropy stable if it satisfies conditions 1, 2, and

$$(\mathbf{v}_L - \mathbf{v}_R)^T \mathbf{f}_{i,S}(\mathbf{u}_L, \mathbf{u}_R) \leq \psi_i(\mathbf{u}_L) - \psi_i(\mathbf{u}_R).$$

We now introduce the L^2 projection of the entropy variables \mathbf{v}_h and the entropy-projected conservative variables $\tilde{\mathbf{u}}$

$$\mathbf{u}_q = \mathbf{V}_q \mathbf{u}_h, \quad \mathbf{v}_h = \mathbf{P}_q \mathbf{v}(\mathbf{u}_q), \quad \tilde{\mathbf{v}} = \begin{bmatrix} \mathbf{V}_q \\ \mathbf{V}_f \end{bmatrix} \mathbf{v}_h, \quad \tilde{\mathbf{u}} = \begin{bmatrix} \tilde{\mathbf{u}}_q \\ \tilde{\mathbf{u}}_f \end{bmatrix} = \mathbf{u}(\tilde{\mathbf{v}}). \quad (21)$$

Here, the entropy-projected conservative variables $\tilde{\mathbf{u}}$ denote the evaluation of the conservative variables in terms of the projected entropy variables at volume and face quadrature points. We note that, under an appropriate choice of quadrature on quadrilaterals and hexahedra, this approach is equivalent to the approach taken in [26], where the entropy variables are evaluated at Gauss nodes, then interpolated to a different set of nodes and used to compute the nonlinear fluxes.

We now introduce a semi-discrete DG formulation for \mathbf{u}_h

$$\begin{aligned} \frac{d\mathbf{u}_h}{dt} + \begin{bmatrix} \mathbf{P}_q^k & \mathbf{L}_q^k \end{bmatrix} \sum_{j=1}^d \left(\mathbf{D}_k^j \circ \mathbf{F}_S \right) \mathbf{1} + \sum_{j=1}^d \mathbf{L}_q^k \text{diag}(\mathbf{n}_i) (\mathbf{f}^* - \mathbf{f}(\tilde{\mathbf{u}}_f)) &= 0, \\ (\mathbf{F}_S)_{ij} = \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j), \quad 1 \leq i, j \leq N_q + N_q^f, \\ \mathbf{f}^* = \mathbf{f}_S(\tilde{\mathbf{u}}_f^+, \tilde{\mathbf{u}}_f) \text{ on interior faces,} \end{aligned} \quad (22)$$

where $\tilde{\mathbf{u}}^+$ denotes the values of the entropy-projected conservative variables on the neighboring element across each face of D^k , and \mathbf{f}^* on the boundary denotes some numerical flux through which boundary conditions are imposed.

Define the boundary quadrature matrix $\mathbf{W}_{\partial\Omega}$ such that

$$(\mathbf{W}_{\partial\Omega})_{ii} = \begin{cases} \mathbf{W}_f \text{diag}(\mathbf{J}_f^k), & \text{if } \mathbf{x}_i^f \text{ is on the } \partial\Omega \\ 0, & \text{otherwise.} \end{cases}$$

We have the following semi-discrete statement of entropy conservation:

Theorem 1. Assume that $\mathbf{Q}_k^j \mathbf{1} = 0$ for $j = 1, \dots, d$ over each element D^k . Then, (22) is entropy conservative in the sense that

$$\sum_k \mathbf{1}^T \mathbf{J}^k \mathbf{W} \frac{d\mathbf{u}}{dt} = \sum_k \sum_{j=1}^d \mathbf{1}^T \mathbf{W}_{\partial\Omega} (\psi_j(\tilde{\mathbf{u}}_f) - \tilde{\mathbf{v}}_f^T \mathbf{f}^*).$$

Proof. Using that $\mathbf{Q}_k^j \mathbf{1} = 0$ for $i = 1, \dots, d$ over each element and (16), the proof of entropy conservation is identical to that of [21]. \square

3.5 A discrete geometric conservation law

An important aspect of Theorem 1 is the assumption that $\mathbf{Q}_k^j \mathbf{1} = 0$ for $j = 1, \dots, d$. However, this is not always guaranteed to hold for \mathbf{Q}_k^j as defined through (15). In this section, we discuss methods of constructing the geometric terms $J\mathbf{G}_{ij}$ for curvilinear meshes in a way that ensures $\mathbf{Q}_k^j \mathbf{1} = 0$.

From (15), the condition $\mathbf{Q}_k^j \mathbf{1} = 0$ is equivalent to

$$\begin{aligned} \mathbf{W}_N \sum_{j=1}^d \mathbf{D}_N^j \{ \{ J\mathbf{G}_{ij}^k \} \} \mathbf{1} &= \frac{1}{2} \mathbf{W}_N \sum_{j=1}^d \left(\text{diag} (J\mathbf{G}_{ij}^k) \mathbf{D}_N^j \mathbf{1} + \mathbf{D}_N^j \text{diag} (J\mathbf{G}_{ij}^k) \mathbf{1} \right) \\ &= \frac{1}{2} \mathbf{W}_N \sum_{j=1}^d \mathbf{D}_N^j (J\mathbf{G}_{ij}^k) = 0, \end{aligned}$$

where we have used that $\mathbf{D}_N^j \mathbf{1} = 0$ to eliminate the first term. Since \mathbf{W}_N is a diagonal matrix with positive entries, $\mathbf{Q}_k^j \mathbf{1} = 0$ is equivalent to ensuring that

$$\sum_{j=1}^d \mathbf{D}_N^j (J\mathbf{G}_{ij}^k) = 0, \quad (23)$$

a discrete version of the GCL (13). This condition is also related to free-stream preservation, which ensures (at the discrete level) that for \mathbf{u} constant,

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u} = \frac{\partial \mathbf{u}}{\partial t} = 0.$$

For isoparametric mappings in two dimensions, free stream preservation is naturally enforced by noting that the scaled metric terms $J\mathbf{G}_{ij}$ are exactly polynomials of degree N . As a result, computing the metric terms exactly naturally enforces that both the continuous GCL (13) and the discrete GCL (23) are satisfied. However, the discrete GCL is not always maintained at the discrete level in 3D due to the fact that geometric factors for a degree N geometric mapping are polynomials of degree $2N - 2$. Because the degree of $J\mathbf{G}_{ij}$ is higher than the degree of the underlying polynomial space, these metric terms are not represented exactly through their values at nodal or quadrature points, resulting in aliasing errors and the loss of the discrete GCL (23) [23, 27].

This can be remedied by using an interpolation of the curl-conservative form of the geometric factors, which ensures that $\widehat{\nabla} \cdot (J\mathbf{G}^T) = 0$ locally [28, 23]. However, because the geometric factors are computed by applying the curl, the geometric factors are approximated as degree $(N - 1)$ polynomials rather than degree N polynomials, which can reduce accuracy. We take a different approach, based on a strategy described in [29, 30]. Integrating by parts the DG formulation yields, for any constant \mathbf{u}

$$\begin{aligned} (\nabla_h \cdot \mathbf{u}, v)_\Omega &= \sum_k \left(\widehat{\nabla} \cdot (J\mathbf{G}^T \mathbf{u}), v \right)_{\widehat{D}} + \langle J\mathbf{G}^T \mathbf{u} - \Pi_N (J\mathbf{G}^T \mathbf{u}), v \widehat{\mathbf{n}} \rangle_{\partial \widehat{D}} \\ &= \sum_k \left(-J\mathbf{G}^T \mathbf{u}, \widehat{\nabla} v \right)_{\widehat{D}} + \langle (J\mathbf{G} \widehat{\mathbf{n}})^T \mathbf{u}, v \rangle_{\partial \widehat{D}} \\ &= \sum_k \left(-J\mathbf{G}^T \mathbf{u}, \widehat{\nabla} v \right)_{\widehat{D}} + \langle \mathbf{n} \cdot \mathbf{u}, v \rangle_{\partial \widehat{D}}. \end{aligned}$$

for any $v \in V_h$. Thus, to ensure that this sums to zero, we modify the geometric factors by seeking $J\mathbf{G}$ which minimizes the L^2 error for a degree N polynomial approximation to the true geometric factors, subject to a weakly divergence-free constraint

$$\begin{aligned} \min_{J\tilde{\mathbf{G}}_i \in P^N} \frac{1}{2} \left\| J\tilde{\mathbf{G}}_i - J\mathbf{G}_i \right\|_{L^2(\widehat{D})}^2, \\ \text{s.t. } \langle \mathbf{n}_i, v \rangle_{\partial \widehat{D}} - \left(J\tilde{\mathbf{G}}_i, \nabla v \right)_{\widehat{D}} = 0, \quad \forall v \in P^N. \end{aligned}$$

We note that the constraint corresponding to $v = 1$ yields that $\langle \mathbf{n}_i, v \rangle_{\partial \hat{D}} = 0$. Thus, in order to guarantee a solution to this problem, we require that $\langle \mathbf{n}_i, v \rangle_{\partial \hat{D}} = 0$ for consistency of the right hand side. [Clarify when this is satisfied!!](#).

This strategy was first introduced in the context of SBP-SAT terms in [29]. We approach its implementation slightly differently, and use the fact that the quadratic program can be solved explicitly using the null space method, which is computationally feasible since the null space of the constraint matrix is computed only once on the reference element. This null space corresponds to a discretely divergence-free basis, which we extract using the SVD.

The resulting free-stream preserving geometric factors result in separate approximations of the volume and surface geometric factors. The surface geometric factors are constructed at surface quadrature points, which guarantees that neighboring surface normal terms cancel for watertight meshes. The volume geometric factors are constructed at quadrature points and projected onto a polynomial basis of degree N with weakly divergence-free constraints involving the surface normals.

4 Discretely stable and low storage DG methods on curved meshes

A disadvantage of the formulation (22) is high storage costs, especially at high orders of approximation. While the matrices \mathbf{Q}_k^i can be applied to a vector without needing to explicitly store the matrix, the projection and lifting matrices (20) differ from element to element, necessitating either explicit pre-computation and storage or the assembly and inversion of a weighted mass matrix for each right hand side evaluation. The latter option is computationally expensive, while the former option increases storage costs. This increase in storage can result in suboptimal performance on modern computational architectures [3], due to the increasing cost of memory operations and data movement compared to arithmetic operations.

In this section, we present a discretely entropy stable scheme which avoids this high storage cost through the use of a weight-adjusted approximation to the inverse of a weighted mass matrix.

4.1 A weight-adjusted approximation to the curvilinear mass matrix

Recall that the L^2 projection on a curvilinear domain Π_N^k is defined as

$$(\Pi_N^k u, v)_{D^k} = (J \Pi_N^k u, v)_{\hat{D}} = (uJ, v)_{\hat{D}} = (u, v)_{D^k}, \quad \forall v \in V_h.$$

To define a weight-adjusted approximation to the curvilinear L^2 inner product, we first define the operator T_w^{-1} as follows

$$(w T_w^{-1} u, v)_{\hat{D}} = (u, v)_{\hat{D}}, \quad \forall v \in V_h.$$

Taking $w = 1/J$ then provides an approximation of the curvilinear L^2 inner product

$$(Ju, v)_{\hat{D}} \approx (T_{1/J}^{-1} u, v)_{\hat{D}}, \quad \forall u, v \in V_h.$$

This forms the basis of the weight-adjusted approximation of weighted L^2 inner products.

[Add matrix stuff](#)

4.2 Weight-adjusted projection

We now define the weight-adjusted projection operator P_N as

$$P_N u = \Pi_N \left(\frac{1}{J} \Pi_N (uJ) \right).$$

Note that P_N is self-adjoint with respect to the J -weighted L^2 inner product

$$(JP_N u, v) = \left(\Pi_N \left(\frac{1}{J} \Pi_N (uJ) \right), vJ \right) = \left(uJ, \Pi_N \left(\frac{1}{J} \Pi_N (vJ) \right) \right) = (uJ, P_N v). \quad (24)$$

Furthermore, using that $T_{1/J}^{-1}$ is self-adjoint for $v \in V_h$ with respect to the L^2 inner product [1], we have that a projection-like property holds for the weight-adjusted L^2 inner product

$$\left(T_{1/J}^{-1} P_N u, v \right) = \left(\frac{1}{J} \Pi_N(uJ), T_{1/J}^{-1} v \right) = (\Pi_N(uJ), v) = (uJ, v), \quad \forall v \in V_h. \quad (25)$$

Let $\Pi_N^k u$ be the L^2 projection of u with respect to the weighted (curvilinear) L^2 inner product. We observe in numerical experiments that for a fixed geometric mapping, $\|\Pi_N^k u - P_N u\|_{L^2(\Omega)} = O(h^{N+2})$. Because the difference between the L^2 and WADG projection is superconvergent, the results are indistinguishable for a fixed geometric mapping.

We can prove this bound using results from [1, 2]. The first theorem we need shows that $T_{1/J}^{-1}$ can be used to approximate weighted curvilinear L^2 inner products with order $(2N+2)$ accuracy.

Theorem 2. *Let $u \in W^{N+1,2}(D^k)$ and $v \in V_h(D^k)$. Then,*

$$\left| (u, vJ)_{\hat{D}} - \left(T_{1/J}^{-1} u, v \right)_{\hat{D}} \right| \leq Ch^{2N+2} \|J\|_{L^\infty(D^k)} \left\| \frac{1}{J} \right\|_{L^\infty(D^k)}^2 \|J\|_{W^{N+1,\infty}(D^k)}^2 \|u\|_{W^{N+1,2}(D^k)} \|v\|_{W^{N+1,2}(D^k)}.$$

Proof. The proof involves straightforward adaptations of Theorem 4, Theorem 5, and Theorem 6 in [1] to the reference element \hat{D} . \square

The next result we need is a generalized inverse inequality.

Lemma 1. *Let $v \in P^N(D^k)$, and let $h = \text{diam}(D^k)$. Then,*

$$\|v\|_{W^{N+1,2}(D^k)} \leq C_N h^{-N} \|v\|_{L^2(D^k)}.$$

where C_N is independent of h .

Proof. The result is the consequence of a scaling argument and a Rayleigh quotient bound involving the largest eigenvalue of the generalized eigenvalue problem

$$\mathbf{K}_N \mathbf{u} = \lambda \mathbf{M} \mathbf{u},$$

where \mathbf{M} is the L^2 mass matrix over D^k and \mathbf{K}_N is the Gram matrix corresponding to the Sobolev inner product for $W^{N+1,2}(D^k)$. We note that the constant C_N depends on the largest eigenvalue, which in turn depends on the order N and dimension d . \square

We can now prove that $P_N u$ is superconvergent to the curvilinear L^2 projection $\Pi_N^k u$

Theorem 3. *Let $u \in W^{N+1,2}(D^k)$. The difference between the L^2 projection $\Pi_N^k u$ and the weight-adjusted projection $P_N u$ is*

$$\|\Pi_N^k u - P_N u\|_{L^2(D^k)} \leq C \|J\|_{L^\infty(D^k)} \left\| \frac{1}{J} \right\|_{L^\infty(D^k)}^2 \|J\|_{W^{N+1,\infty}(D^k)}^2 h^{N+2} \|u\|_{W^{N+1,2}(D^k)}.$$

where C is a mesh-independent constant.

Proof. Let $\Pi_N^k u$ be the L^2 projection over the curved element D^k , such that

$$(J \Pi_N^k u, v) = (uJ, v), \quad \forall v \in V_h.$$

Using the fact that $P_N u$ satisfies an analogous property (25), we can rewrite the norm of the difference between the weight-adjusted and L^2 projections

$$\|\Pi_N^k u - P_N u\|_{L^2(D^k)}^2 = (\Pi_N^k u - P_N u, vJ)_{\widehat{D}}, \quad v = \Pi_N^k u - P_N u.$$

Because $v \in P^N(D^k)$, we can also evaluate the squared error as

$$\begin{aligned} \|\Pi_N^k u - P_N u\|_{L^2(D^k)}^2 &= |(\Pi_N^k u, vJ)_{\widehat{D}} - (P_N u, vJ)_{\widehat{D}}| \\ &= |(u, vJ)_{\widehat{D}} - (P_N u, vJ)_{\widehat{D}}| = \left| \left(T_{1/J}^{-1} P_N u, v \right)_{\widehat{D}} - (JP_N u, v)_{\widehat{D}} \right|. \end{aligned}$$

Applying Theorem 2 and Lemma 1 then yields that

$$\begin{aligned} \|\Pi_N^k u - P_N u\|_{L^2(D^k)}^2 &\leq Ch^{2N+2} C_J \|u\|_{W^{N+1,2}(D^k)} \|v\|_{W^{N+1,2}(\widehat{D})} \\ &\leq Ch^{N+2} C_J \|u\|_{W^{N+1,2}(D^k)} \|v\|_{L^2(D^k)}, \end{aligned}$$

where C_J is a mesh-independent constant depending on J . Dividing through by

$$\|v\|_{L^2(D^k)} = \|\Pi_N^k u - P_N u\|_{L^2(D^k)}$$

gives the desired result. \square

5 Limiting

The evaluation of $\mathbf{u}_v = \mathbf{u}(\Pi_N v)$ can increase entropy pointwise, such that $S(\mathbf{u}_v) \geq S(\mathbf{u})$. This can manifest as spikes in \mathbf{u}_v . We wish to mollify the effect of such spikes.

The first approach is to limit the conservative variable \mathbf{u}

$$\tilde{\mathbf{u}} = \bar{\mathbf{u}} + \Theta(\mathbf{u} - \bar{\mathbf{u}})$$

where Θ is some diagonal matrix with entries in $[0, 1]$. We want to ensure that $\rho, E - \frac{\rho u^2}{2} > 0$.

The entropy for the compressible Euler equations is

$$U(\mathbf{u}) = -\frac{\rho s}{\gamma - 1},$$

where $s = \log\left(\frac{p}{\rho^\gamma}\right)$ is the physical specific entropy. The entropy variables under this choice of entropy are then

$$v_1 = \frac{\gamma - s}{\gamma - 1} - \frac{\rho u^2}{2p}, \quad v_2 = \frac{\rho u}{\rho e}, \quad v_3 = -\frac{\rho}{\rho e}.$$

where the internal energy $\rho e = E - u^2/2$.

The inverse mapping is given by

$$\rho = -(\rho e)v_3, \quad m = (\rho e)v_2, \quad E = (\rho e) \left(1 - \frac{v_2^2}{2v_3} \right),$$

where ρe and s in terms of the entropy variables are

$$\rho e = \left(\frac{(\gamma - 1)}{(-v_3)^\gamma} \right)^{1/(\gamma-1)} e^{\frac{-s}{\gamma-1}}, \quad s = \gamma - v_1 + \frac{v_2^2}{2v_3}.$$

The mapping is invertible so long as $\rho, E - \frac{\rho u^2}{2} > 0$, which can be ensured using standard limiters. However, we have to ensure also that $\rho(\Pi_N \mathbf{v}) > 0$ (similarly for internal energy). This boils down to ensuring that $\Pi_N v_3(x) < 0$, which guarantees that $(\rho e) > 0$ as well.

It can be helpful to ensure a stronger condition, that $\Pi_N v_3(x) \leq \max_x v_3(x)$. This guarantees a bound constraint on the conservative variables evaluated using the projected entropy variables.

Another approach is to change the time-step size based on the difference between \mathbf{u} and \mathbf{u}_v . This would be similar to local time-stepping (high order interpolation of the numerical fluxes and multiple evaluations of)

- Adaptively choose time-step size?
- Expensive option: bisection or Newton algorithm for finding theta.

6 Numerical experiments

6.1 Super-convergence of the weight-adjusted projection

6.2 Compressible Euler equations

6.2.1 Two dimensional experiments

[Shock propagation on a curved mesh: testing entropy conservation](#)

[Isentropic vortex on curved and non-curved meshes](#)

6.2.2 Three dimensional experiments

[Isentropic vortex on curved and non-curved meshes](#)

7 Computational results

The semi-discrete evolution equation is as follows

$$\frac{\partial \mathbf{u}}{\partial t} = \begin{bmatrix} \mathbf{P}_q & \mathbf{L}_q \end{bmatrix} \left(\begin{bmatrix} 2\mathbf{D}_q & \mathbf{V}_q \mathbf{L}_q \\ \mathbf{V}_f \mathbf{P}_q & \mathbf{I} \end{bmatrix} \circ \begin{bmatrix} \mathbf{f}_S(\mathbf{u}, \mathbf{u}_f) & \mathbf{f}_S(\mathbf{u}, \mathbf{u}_f) \\ \mathbf{f}_S(\mathbf{u}, \mathbf{u}_f) & \mathbf{f}_S(\mathbf{u}_f^+, \mathbf{u}_f) \end{bmatrix} \mathbf{1} \right).$$

where \mathbf{u}, \mathbf{u}_f are evaluations at volume and surface quadrature points.

The method is outlined as follows: we store the conservation variables \mathbf{u} at quadrature points, and compute projected entropy variables $\mathbf{v}_u = \Pi_N(\mathbf{v}(\mathbf{u}))$

1. Apply volume flux differencing (\mathbf{D}_q and $\mathbf{V}_q \mathbf{L}_q$) and projection ($\mathbf{V}_q \mathbf{P}_q$) (volume kernel)
2. Apply surface flux differencing ($\mathbf{V}_f \mathbf{P}_q$) and lifting ($\mathbf{V}_q \mathbf{L}_q$) (volume kernel)
3. Apply WADG (scale by $1/J$ and apply $\mathbf{V}_q \mathbf{P}_q$ and update \mathbf{u} at volume quad points. Compute curvilinear projected entropy variables $\mathbf{v}_u = P_N \mathbf{v}(\mathbf{u}) = \Pi_N(\frac{1}{J} \Pi_N(\mathbf{v}(\mathbf{u})J))$, interpolate to volume quad points, and compute conservative variable volume values (update)
4. Interpolate entropy variables at surface quadrature points and write out conservative variable surface values (face).

8 Conclusions

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