#### CHOOSE AN APPROPRIATE TITLE

by

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### Dedication

This thesis is dedicated to those who have fuelled my interest in numerical analysis through their genious, creativity and passion. Include best graphic or logo

### Acknowledgments

### ToBeDone

Don't forget NSERC+McGill Funding

### Abstract

ToBeDone

### Abrégé

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# Chapter 1

# Introduction

 ${\bf To Be Modified}$ 

### Chapter 2

### Methodology

In this section, the governing equations of fluid mechanics and heat transfer, as well as the associated discretizations and boundary conditions employed are outlined. As this work is concerned with the solution of these equations through variants of the finite element method, we also outline the spaces used for the discretization.

Row-vector notation is assumed throughout with the following notation employed:

Object	Description	Example
Scalar variable	italic	a
Vector variable	italic boldface lowercase	a
Second-order tensor variable	italic boldface uppercase	$\boldsymbol{A}$
Vector	boldface lowercase	a
Matrix	boldface uppercase	A
Spaces	calligraphic uppercase	$\mathscr{A}$

#### Governing Equations

Following the notation of Pletcher et al. [1, Chapter 5], the continuity, Navier-Stokes and energy equations with source terms neglected are given by

$$\frac{\partial \boldsymbol{w}}{\partial t} + \nabla \cdot (\boldsymbol{F}^{i}(\boldsymbol{w}) - \boldsymbol{F}^{v}(\boldsymbol{w}, \boldsymbol{Q})) = 0, \tag{2.1}$$

where the vector of conservative variables and its gradients are defined as

$$\boldsymbol{w} := \begin{bmatrix} \rho & \rho \boldsymbol{v} & E \end{bmatrix} \in \mathbb{R}^{d+2}$$

$$\boldsymbol{Q} := \nabla^T \boldsymbol{w} \qquad \in \mathbb{R}^{d+2} \times \mathbb{R}^d, \tag{2.2}$$

where d is the problem dimension, and where the inviscid and viscous fluxes are defined as

$$\boldsymbol{F}^{i}(\boldsymbol{w}) := \begin{bmatrix} \rho \boldsymbol{v}^{T} & \rho \boldsymbol{v}^{T} \boldsymbol{v} + p \boldsymbol{I} & (E+p) \boldsymbol{v}^{T} \end{bmatrix} \in \mathbb{R}^{d+2} \times \mathbb{R}^{d}, \tag{2.3}$$

$$F^{v}(\boldsymbol{w}, \boldsymbol{Q}) := \begin{bmatrix} \boldsymbol{0}^{T} & \boldsymbol{\Pi} & \boldsymbol{\Pi} \boldsymbol{v}^{T} - \boldsymbol{q}^{T} \end{bmatrix} \in \mathbb{R}^{d+2} \times \mathbb{R}^{d}.$$
 (2.4)

The various symbols represent the density,  $\rho$ , the velocity,  $\boldsymbol{v}$ , the total energy per unit volume, E, the pressure, p, the stress tensor,  $\Pi$  and the energy flux,  $\boldsymbol{q}$ . The pressure is defined according to the equation of state for a calorically ideal gas,

$$p = (\gamma - 1) \left( E - \frac{1}{2} \rho \boldsymbol{v} \boldsymbol{v}^T \right) := (\gamma - 1) \rho e, \ \gamma = \frac{c_p}{c_v}, \ c_v = \frac{R_g}{\gamma - 1}, \ c_p = \frac{\gamma R_g}{\gamma - 1},$$

where e represents the specific internal energy,  $R_g$  is the gas constant and the specific heats at constant volume,  $c_v$ , and at constant pressure,  $c_p$ , are constant. The stress tensor is defined as

$$\mathbf{\Pi} = 2\mu \left( \mathbf{D} - \frac{1}{3} \nabla \cdot \mathbf{v} \mathbf{I} \right), \ \mathbf{D} \coloneqq \frac{1}{2} \left( \nabla^T \mathbf{v} + \left( \nabla^T \mathbf{v} \right)^T \right),$$

where  $\mu$  is the coefficient of shear viscosity (Add comment about how  $\mu$  is determined (Sutherland, p.259 pletcher(1997))) and where the coefficient of bulk viscosity was assumed to be zero. Finally, the energy flux is defined by

$$\mathbf{a} = \kappa \nabla T$$
.

where T represents the temperature and

$$\kappa = \frac{c_p \mu}{Pr},$$

with Pr representing the Prandtl number. In the case of the Euler equations, the contribution of the viscous flux is neglected.

#### **Discretizations**

#### **Preliminaries**

Let  $\Omega$  be a bounded simply connected open subset of  $\mathbb{R}^d$  with connected Lipschitz boundary  $\partial \Omega$  in  $\mathbb{R}^{d-1}$ . We let  $\Omega_h$  denote the disjoint partion of  $\Omega$  into "elements", V, and denote the element boundaries as  $\partial V$ . Elements and their boundaries are also referred to as volumes and faces respectively. We also define the following volume inner products,

$$(a,b)_D = \int_D ab; \quad a,b \in L^2(D),$$
$$(\mathbf{a},\mathbf{b})_D = \int_D \mathbf{a} \cdot \mathbf{b}; \quad \mathbf{a},\mathbf{b} \in L^2(D)^m,$$
$$(\mathbf{A},\mathbf{B})_D = \int_D \mathbf{A} : \mathbf{B}; \, \mathbf{A}, \mathbf{B} \in L^2(D)^{m \times d},$$

where D is a domain in  $\mathbb{R}^d$ , and where ':' denotes the inner product operator for two secondorder tensors. Analogous notation is used for face inner products,

$$\begin{split} \langle a,b\rangle_D &= \int_D ab; \qquad a,b \in L^2(D), \\ \langle \mathbf{a},\mathbf{b}\rangle_D &= \int_D \mathbf{a} \cdot \mathbf{b}; \quad \mathbf{a},\mathbf{b} \in L^2(D)^m, \\ \langle \mathbf{A},\mathbf{B}\rangle_D &= \int_D \mathbf{A} : \mathbf{B}; \ \mathbf{A},\mathbf{B} \in L^2(D)^{m \times d}, \end{split}$$

where D is a domain in  $\mathbb{R}^{d-1}$ . Denoting the polynomial space of order p on domain D as  $\mathscr{P}^p(D)$ , and letting n=d+2, we define the discontinuous discrete solution and gradient approximation spaces as

$$\mathcal{S}_h^v = \{ \boldsymbol{a} \in L^2(\Omega_h)^n : \boldsymbol{a}|_V \in \mathcal{P}^p(V)^n \ \forall V \in \Omega_h \}$$

$$\mathcal{S}_h^v = \{ \boldsymbol{A} \in L^2(\Omega_h)^{n \times d} : \boldsymbol{A}|_V \in \mathcal{P}^p(V)^{n \times d} \ \forall V \in \Omega_h \}.$$

We also define discontinuous test spaces

$$\mathcal{W}_{th}^{v} = \{ \mathbf{a_t} \in L^2(\Omega_h)^n : \mathbf{a_t}|_V \in \mathcal{P}^{p_t}(V)^n \ \forall V \in \Omega_h \}$$

$$\mathcal{Q}_{th}^{v} = \{ \mathbf{A_t} \in L^2(\Omega_h)^{n \times d} : \mathbf{A_t}|_V \in \mathcal{P}^{p_t}(V)^{n \times d} \ \forall V \in \Omega_h \},$$

where  $p_t \geq p$ . Will need additional spaces for DPG.

#### Discretized Equations

To obtain the discrete formulation, we first define a joint flux  $F(w, Q) := F^i(w) - F^v(w, Q)$ then integrate (2.2) and (2.1) with respect to test functions to obtain

$$\begin{split} &(\mathbf{Q_t}, \boldsymbol{Q})_V = \left(\mathbf{Q_t}, \nabla^T \boldsymbol{w}\right)_V, & \forall \mathbf{Q_t} \in \mathcal{Q}_t^v = \mathcal{Q}_h^v \\ &\left(\mathbf{w_t}, \frac{\partial \boldsymbol{w}}{\partial t}\right)_V + \left(\mathbf{w_t}, \nabla \cdot \boldsymbol{F}(\boldsymbol{w}, \boldsymbol{Q})\right)_V = \boldsymbol{0}, \, \forall \mathbf{w_t} \in \mathcal{W}_{th}^v = \mathcal{W}_h^v. \end{split}$$

Integrating by parts twice in the first equation and once in the second and choosing  $p_t = p$ , such that the approximation and test spaces are the same, results in the discontinuous Galerkin formulation,

$$egin{aligned} \left(\mathbf{Q_t}, oldsymbol{Q}
ight)_V &= \left(\mathbf{Q_t}, 
abla^T oldsymbol{w}
ight)_V + \left\langle \mathbf{Q_t}, \mathbf{n} \cdot (oldsymbol{w}^* - oldsymbol{w}) 
ight
angle_{\partial V}, & \forall \mathbf{Q_t} \in \mathcal{Q}_h^v \ \left(\mathbf{w_t}, rac{\partial oldsymbol{w}}{\partial t}
ight)_V - \left(\mathbf{w_t}, 
abla \cdot oldsymbol{F}(oldsymbol{w}, oldsymbol{Q})_V + \left\langle \mathbf{w_t}, \mathbf{n} \cdot oldsymbol{F}^* 
ight
angle_{\partial V}, & \forall \mathbf{w_t} \in \mathcal{W}_h^v. \end{aligned}$$

where  $\mathbf{n}$  denotes the outward pointing unit normal vector and where  $\mathbf{w}^*$  and  $\mathbf{F}^*$  represent the numerical solution and flux respectively.

### **Boundary Conditions**

Boundary conditions are imposed weakly through the specification of a 'ghost' state for elements in which  $V \cap \partial\Omega \neq \{0\}$ . The following boundary conditions are supported:

Boundary Condition	Reference(s)	Comments
Riemann Invariant	[2, section 2.2]	eq. (14) should read $c_b = \frac{\gamma - 1}{4} (R^+ - R^-)$
Slip-Wall	[3, eq. (10)]	
Back Pressure (Outflow)	[2, section 2.4]	
${\it Total\ Temperature/Pressure\ (Inflow)}$	[2, section 2.7]	
${\bf Supersonic\ Inflow/Outflow}$		imposes the exact/extrapolated solution
No-slip Overconstrained		imposes values for all primitive variables $^{\rm 1}$
No-slip Diabatic		imposes $\mathbf{v}$ and $(\mathbf{n}\cdot\mathbf{F}(\mathbf{W},\mathbf{Q}))_E=\text{constant}$

<sup>&</sup>lt;sup>1</sup>Add reference to Nordstrom explaining why this BC is overconstrained and add link to Taylor-Couette results where it is used.

### Chapter 3

### The DPG Methodology

In comparison to discontinuous Galerkin (DG) methods, the most noteworthy characteristic of the Discontinuous Petrov-Galerkin (DPG) methodology is that the optimal (to be defined below) test space is computed based on the minimization of the residual in a specified norm instead of simply being chosen to be the same as the trial space. Following Demkowicz et al. [4], note that DPG is generally referred to as a methodology, as opposed to a method, as different methods are obtained depending on the choice of inner product in the test space. Comment about requiring Hilbert based on use of term "inner product" here?

#### Linear DPG

In this section, we first outline the basic concepts of DPG methods in an abstract linear functional setting and then provide a concrete example through the application of the theory to the linear advection equation.

#### Abstract Functional Setting

Much of the theory outlined below is borrowed directly from the works of Demkowicz et al. [5, 4]. Of primary note, it is demonstrated that each DPG method can be interpreted as the *localization* of a method achieving optimal discrete stability through the choice of an optimal conforming test space.

#### A Petrov-Galerkin Variational Methodology with Optimal Stability

Consider the *linear* abstract variational problem

Find 
$$u \in \mathcal{U}$$
 such that  $b(v, u) = l(v) \ \forall v \in \mathcal{V}$ , (3.1)

where  $\mathscr{U}$  and  $\mathscr{V}$  denote the trial and test spaces, respectively, which are assumed to be Hilbert spaces, and where the bilinear form  $b(\cdot,\cdot)$  acting on  $\mathscr{V}\times\mathscr{U}$  and the linear form  $l(\cdot)$  acting on  $\mathscr{V}$  correspond to a particular variational formulation. It is assumed that the bilinear form satisfies a continuity condition with continuity constant M,

$$|b(v,u)| \le M||u||_{\mathscr{U}}||v||_{\mathscr{V}},\tag{3.2}$$

and an inf-sup condition with inf-sup constant  $\gamma$ ,

$$\exists \gamma > 0 : \inf_{u \in \mathcal{U}} \sup_{v \in \mathcal{V}} \frac{b(v, u)}{||v||_{\mathcal{V}}||u||_{\mathcal{U}}} \ge \gamma. \tag{3.3}$$

Further, it is assumed that the linear form is continuous and satisfies the following compatibility condition

$$l(v) = 0 \ \forall v \in \mathcal{V}_0, \text{ where } \mathcal{V}_0 := \{ v \in \mathcal{V} : b(v, u) = 0 \ \forall u \in \mathcal{U} \}.$$
 (3.4)

Then, by the Banach-Nečas-Babuška theorem (Add reference to Brener-Scott/Ciarlet), (3.1) has a unique solution, u, that depends continuously on the data,

$$||u||_{\mathscr{U}} \le \frac{M}{\gamma} ||l||_{\mathscr{V}'},\tag{3.5}$$

where  $\mathcal{V}'$  denotes the dual space of  $\mathcal{V}$ . Now let  $\mathcal{U}_h \subset \mathcal{U}$  and  $\mathcal{V}_h \subset \mathcal{V}$  be finite dimensional trial and test spaces and consider the finite dimensional variation problem

Find 
$$u_h \in \mathcal{U}_h$$
 such that  $b(v_h, u_h) = l(v_h) \ \forall v_h \in \mathcal{V}_h$ . (3.6)

If the form satisfies the discrete inf-sup condition with inf-sup constant  $\gamma_h$ ,

$$\exists \gamma_h > 0 : \inf_{u_h \in \mathcal{U}_h} \sup_{v_h \in \mathcal{V}_h} \frac{b(v_h, u_h)}{||v_h||_{\mathcal{V}_h}||u_h||_{\mathcal{U}_h}} \ge \gamma_h, \tag{3.7}$$

then Babuška's theorem [6, Theorem 2.2], demonstrates that the discrete problem, (3.6), is well-posed with the Galerkin error satisfying the error estimate,

$$||u_h - u||_{\mathcal{U}} \le \frac{M}{\gamma_h} \inf_{w_h \in \mathcal{U}_h} ||w_h - u||_{\mathcal{U}}. \tag{3.8}$$

where the original constant in the bound,  $\left(1+\frac{M}{\gamma_h}\right)$  [6, eq. (2.14)], has been sharpened to  $\frac{M}{\gamma_h}$  as demonstrated to be possible by Xu et al. [7, Theorem 2]. Generally, the well-posedness of the continuous problem does not imply the well-posedness of the discrete problem (i.e. (3.3)  $\Rightarrow$  (3.7)), and the fundamental motivation for the DPG methodology is then to choose the test space such that the supremum in the discrete inf-sup condition, (3.7), is obtained. (Potentially refer to where it is proven that DPG test functions are chosen in this way (following the demonstration in Demkowicz et al. [4, Section 4.1]))

A case of particular interest is then when the continuity and discrete inf-sup constants can be made equal,

$$M = \gamma_h, \tag{3.9}$$

so that the error incurred by the discrete approximation in (3.8) is smallest. As it is not immediately clear which norms should be selected for the trial and test spaces, the simplest strategy is to let the norm be selected as that which is naturally induced by the problem such that (3.9) is satisfied. Bui-Thanh et al. [8, Theorem 2.6] have proven that  $M = \gamma = 1$  if

$$\exists v_u \in \mathscr{V} \{0\} : b(v_u, u) = ||u||_{\mathscr{U}} ||v_u||_{\mathscr{V}} \ \forall u \in \mathscr{U} \setminus \{0\}, \tag{3.10}$$

where  $v_u$  is termed an optimal test function for the trial function u. Further, assuming that (3.10) holds, (3.9) is satisfied when the discrete test space is defined by

$$\mathscr{V} \supset \mathscr{V}_h = span\{v_{u_h} \in \mathscr{V} : u_h \in \mathscr{U}_h \subset \mathscr{U}, \ b(v_{u_h}, u_h) = ||u_h||_{\mathscr{U}} ||v_{u_h}||_{\mathscr{V}}\}; \tag{3.11}$$

see Bui-Thanh et al. [8, Lemma 2.8]. Defining the map from trial to test space,  $T: \mathcal{U} \ni u \to Tu := v_{Tu} \in \mathcal{V}$ , by

$$(v, Tu)_{\mathscr{V}} = b(v, u), \tag{3.12}$$

where  $(\cdot,\cdot)_{\mathscr{V}}$  represents the test space inner product, then

$$\mathcal{V}_h = span\{v_{Tu_h} \in \mathcal{V} : u_h \in \mathcal{U}_h\}; \tag{3.13}$$

see Bui-Thanh et al. [8, Theorem 2.9]. Defining the Riesz operator for the test inner product,

$$R_{\mathscr{V}}: \mathscr{V} \ni v \to (v, \cdot) \in \mathscr{V}',$$
 (3.14)

which is an isometric isomorphism by the Riesz Representation Theorem (Add reference), the test functions spanning  $\mathcal{V}_h$  in (3.13), which are henceforth referred to as *optimal* test functions, can be computed through the inversion of the Riesz operator by solving the auxiliary variational problem

Find 
$$v_{Tu_h} \in \mathcal{V}$$
 such that  $(w, v_{Tu_h})_{\mathcal{V}} = b(w, u_h), \ \forall w \in \mathcal{V}.$  (3.15)

#### DPG as a Localization of the Optimal Conforming PG Methodology

Note that no assumptions regarding the conformity of the trial and test spaces were imposed in §3.1.1. Specifically, the specification of the 'D' (discontinuous) in DPG, referring to a discontinuous test space, has not yet been made and the methodology described is thus of a general Petrov-Galerkin form. Denote the trial graph space over the domain  $\Omega$ ,  $\mathcal{H}_b(\Omega)$ , as that of the solution of (3.1),

$$\mathscr{H}_b(\Omega) := \{ u \in (L^2(\Omega))^n : b(v, u) \in (L^2(\Omega))^n \forall v \in \mathscr{V} \}, \tag{3.16}$$

where n denotes the number of scalar variables. Integration by parts of (3.1) leads to the

formal  $L^2$ -adjoint and a bilinear form representing the boundary terms

$$b(v, u) = b^*(v, u) + c(\operatorname{tr}_A^* v, \operatorname{tr}_A u)$$
(3.17)

where v is in the graph space for the adjoint

$$\mathcal{H}_b^*(\Omega) := \{ v \in (L^2(\Omega))^n : b^*(v, u) \in (L^2(\Omega))^n \forall u \in \mathcal{U} \}. \tag{3.18}$$

See Demkowicz et al. [5, eq. (4.18)] for a concrete example of these operators. When setting  $\mathcal{V} = \mathcal{H}_b^*(\Omega)$ , we say that the test space is  $\mathcal{H}_b$ -conforming.

As the eventual goal of the methodology is to solve (3.6) over a tesselation,  $T_h$ , of the discretized domain,  $\Omega_h$ , consisting of elements (referred to as volumes) V, we note that using a  $\mathcal{H}_b$ -conforming test space results in each of the optimal test functions computed by (3.15) having global support (i.e. potentially over all of  $\Omega_h$ ). To make the methodology practical, broken energy spaces are introduced such that the required inversion of the Riesz operator can be done elementwise, *localizing* (3.15),

Find 
$$v_{Tu_h} \in \mathcal{V}(V)$$
 such that  $(w, v_{Tu_h})_{\mathcal{V}(V)} = b(w, u_h), \ \forall w \in \mathcal{V}(V)$  (3.19)

where

$$\mathscr{V}(V) := \{ v \in L^2(\Omega) : v|_V \in \mathscr{H}_b^* \ \forall V \in T_h \}. \tag{3.20}$$

Noting that the test graph space is a subset of  $(L^2(\Omega))^n$ , it has been shown that the PG methodology of §3.1.1 is, in fact, a subset of this practical DPG methodology where  $L^2$ -conforming test spaces are used. Comment along the lines of: This comes at the cost of introducing trace unknowns over the interior volume boundaries? We now briefly reproduce the proof of Demkowicz et al. [5, Section 6].

Briefly reproduce the proof of [5], section 6 and make connections with DG.

### Bibliography

- [1] R. Pletcher, J. Tannehill, D. Anderson, Computational Fluid Mechanics and Heat Transfer, Second Edition, Series in Computational and Physical Processes in Mechanics and Thermal Sciences, Taylor & Francis, 1997.
  URL https://books.google.ca/books?id=ZJPbtHeilCgC
- J.-R. Carlson, Inflow/outflow boundary conditions with application to fun3d, Tech. Rep. NASA/TM-2011-217181, NASA Langley Research Center (2011).
   URL https://ntrs.nasa.gov/search.jsp?R=20110022658
- [3] L. Krivodonova, M. Berger, High-order accurate implementation of solid wall boundary conditions in curved geometries, J. Comput. Phys. 211 (2) (2006) 492-512. doi:10.1016/j.jcp.2005.05.029.
  URL http://dx.doi.org/10.1016/j.jcp.2005.05.029
- [4] L. Demkowicz, J. Gopalakrishnan, Discontinuous Petrov-Galerkin (DPG) Method, John Wiley & Sons, Ltd, 2017. doi:10.1002/9781119176817.ecm2105.
   URL http://dx.doi.org/10.1002/9781119176817.ecm2105
- [5] L. F. Demkowicz, J. Gopalakrishnan, An Overview of the Discontinuous Petrov Galerkin Method, Springer International Publishing, Cham, 2014, pp. 149–180. doi:10.1007/ 978-3-319-01818-8\_6.
   URL https://doi.org/10.1007/978-3-319-01818-8\_6
- I. Babuška, Error-bounds for finite element method, Numer. Math. 16 (4) (1971) 322–333. doi:10.1007/BF02165003.
   URL http://dx.doi.org/10.1007/BF02165003
- [7] J. Xu, L. Zikatanov, Some observations on babuAąka and brezzi theories 94 (2003) 195–202.
- [8] T. Bui-Thanh, L. Demkowicz, O. Ghattas, Constructively well-posed approximation methods with unity inf-sup and continuity constants for partial differential equations, Mathematics of Computation 82 (2013) 1923–1952.