A dual-weighted residual (DWR) error estimate for discontinuous solutions of hyperbolic problems

Hadi Minbashian

TECHNISCHE UNIVERSITÄT DARMSTADT

CEMRACS 19

Marseille, August 2nd, 2019

Outline

TECHNISCHE UNIVERSITÄT DARMSTADT

Motivation: Computing a quantity of interest

TECHNISCHE UNIVERSITÄT DARMSTADT

The reason for solving a PDE is alway to compute a physical quantity of interest. This quantity is given as a functional of the solution of the problem. For example, one physical quantity of interest in aerodynamics is the *total lift* over the airfoil surface S

$$L(p) = \oint p\mathbf{n} \cdot \mathbf{k}\, dS, \tag{1}$$

where pressure p is given by the solution of the Euler equations in 3-D

$$\begin{aligned} \rho_t + \operatorname{div}(\rho\mathbf{v}) &= 0 \\ (\rho\mathbf{v})_t + \operatorname{div}(\rho\mathbf{v} \otimes \mathbf{v} + p\mathbf{I}) &= 0 \\ E_t + \operatorname{div}((E + p)\mathbf{v}) &= 0 \end{aligned}$$

with the equation of state (for ideal gas)

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho|\mathbf{v}|^2.$$

Motivation: Computing a quantity of interest, cont'd

In practice we do discretize the equations through numerical methods. Therefore, one needs to control the error in computations. But, here, we are more interested in the error in quantity of interest rather than solution of the problem itself. For the above example we would like to control the following error.

$$e_L(\mathbf{u}_h) := \left| L(\mathbf{u}) - L(\mathbf{u}^h) \right| \leq ?\,,$$

where $\mathbf{u} = [\rho,\ \mathbf{v},\ E]^T$.

For the sake of simplicity, let us consider the following nonlinear scalar hyperbolic conservation law in 1-D:

$$\begin{aligned} \partial_t u + \partial_x f(u) &= 0, \quad \text{in } (0, T] \times \mathbb{R}, \\ u(x,0) &= u_0(x). \end{aligned} \tag{2}$$

where the flux function $f \in C^1$ is convex.
It is well-known that the solution u of (2) may develop shock discontinuities.
Therefore, the weak solution of (2) is defined as follows:

Definition (weak solution)

The function $u \in L^{\infty}((0, T] \times \Omega)$ is called a weak solution of (2) if

$$\int_0^T \int_{\mathbb{R}} u\,\partial_t \phi + f(u)\,\partial_x \phi\, dx\, dt + \int_0^T \int_{\mathbb{R}} u(x,0)\phi(x,0)\, dx\, dt = 0, \quad \forall \phi \in C_c^1((0, T] \times \mathbb{R}), \tag{3}$$

DWR for HCLs: Smooth solutions

- Assume u_h is the numerical solution of the scalar conservation law

$$\partial_t u + \partial_x f(u) = 0, \quad \text{in} \quad (0, T] \times \mathbb{R}, \tag{4}$$

  using a numerical method, in particular, Discontinuous Galerkin (DG).
- Let us consider a simple functional of interest (FoI) J, say

$$J(u) = \int_{\mathbb{R}} g(x)\, u(x, T)\, dx$$

- $J(u) - J(u^h) =?$

The formal approach to estimate the discretization error in J is based on the following Lagrangian.

$$L(u, p) = J(u) + (p, \partial_t u + \partial_x f(u))_{L^2((0,T]\times\mathbb{R})}.$$

DWR for HCLs: Smooth solutions, cont'd

TECHNISCHE UNIVERSITÄT DARMSTADT

Then the Lagrangian is given by

$$L(u;p) = \int_{\mathbb{R}} g(x)\, u(x,T)\, dx + \int_0^T \int_{\mathbb{R}} (p\,\partial_t u + p\,\partial_x f(u))\, dx\, dt.$$

Assuming all functions are smooth, then computing variation of the Lagrangian w. r. t. p leads to the primal problem

$$\partial_p L(u;\phi,p) = 0 \rightsquigarrow \int_0^T \int_{\mathbb{R}} \phi(\,\partial_t u + \,\partial_x f(u))\, dx\, dt = 0, \quad \forall \phi \in C_c^1((0,T] \times \mathbb{R},$$

and after integration by parts we get

$$A(u;\phi) := \int_0^T \int_{\mathbb{R}} u\,\partial_t \phi + f(u)\,\partial_x \phi\, dx\, dt + \int_0^T \int_{\mathbb{R}} u(x,0)\phi(x,0)\, dx\, dt = 0,$$

for all $\phi \in C_c^1((0,T] \times \mathbb{R})$.

DWR for HCLs: Smooth solutions, cont'd

TECHNISCHE UNIVERSITÄT DARMSTADT

In fact, after integration by parts for the second term of the Lagrangian, it would be of the following form.

$$L(u;p) = J(u) - A(u;p)$$

Now, one can compute the variation w. r. t. u, which results in the following dual problem

$$\begin{aligned} L'(u;\psi,p) &= J(\psi) - A'(u;\psi,p) \\ &= \int_0^T \int_{\mathbb{R}} \psi\,(\partial_t p + f'(u)\,\partial_x p)\,dx\,dt + \int_{\mathbb{R}} \psi(x,T)(p(x,T) - g(x))\,dx\,dt = 0, \end{aligned}$$

for all $\psi \in C_c^1((0,T] \times \mathbb{R})$. The above dual problem in differential form reads

$$\begin{aligned} \partial_t p + f'(u)\partial_x p &= 0, \\ p(x,T) &= g(x) \end{aligned}$$

DWR for HCLs: Smooth solutions, cont'd

Recall again the Lagrangian

$$L(u;p) = J(u) - A(u;p) \Rightarrow J(u) = L(u;p) + A(u;p)$$

and we assume that both dual and primal problem have been solved numerically using DG. Now for the error in FoI we have

$$\begin{aligned} J(u) - J(u^h) &= L(u;p) - L(u^h;p) + \underbrace{A(u;p)}_{=0} - A(u^h;p) \\ &= \int_0^1 L'(u_h + s\,(u-u^h); u-u^h, p)\, ds - A(u^h;p) \\ &= \frac{1}{2} L'(u^h; u-u^h, p) + \underbrace{\frac{1}{2} L'(u; u-u^h, p)}_{=0} + \mathcal{R}(u, u^h) - A(u^h;p) \end{aligned}$$

DWR for HCLs: Challenges in the presence of discontinuity

Finally we get the following estimate.

$$J(u) - J(u^h) \simeq \frac{1}{2} L'(u^h; u - u^h, p) - A(u^h; p)$$

DWR for HCLs: Challenges in the presence of discontinuity

TECHNISCHE UNIVERSITÄT DARMSTADT

Finally we get the following estimate.

$$J(u) - J(u^h) \simeq \frac{1}{2} L'(u^h; u - u^h, p) - A(u^h; p)$$

The above approach was based on smoothness assumptions which are not the case for hyperbolic conservation laws. In fact, there are two issues with the above approach.

- The residuals in the estimate may not be of optimal order.
- The discretization of the dual problem is challenging due to discontinuous coefficient.

Let's have a closer look at these issues.

Suboptimality of residuals

TECHNISCHE UNIVERSITÄT DARMSTADT

Let's consider the following simple ODE [1].

$$y'(t) = f(t), \;\; t \in [0, T]$$
$$y(0) = y_0$$

and we solve the above ODE using the Crank-Nicolson-Galerkin (CN-G) method.

- Let $0 = t_0 < t_1 < \cdots < t_N = T$, $I_n := (t_n, t_{n+1}]$ and $k_n := t_{n+1} - t_n$.
- $V_q := \{v \in C([0, T]) : v|_{I_n} \in \Pi_q(I_n)\}$.
- $V_q(I_n)$: The space consisting of the restrictions of the elements of V_q to I_n.

[1] C. Makridakis, ESAIM: Proc., 2007, Vol. 21, p. 31-44

Suboptimality of residuals

The CN-G method for the above ODE is defined with $q = 1$ as follows: We seek $Y \in V_1$ such that

$$(Y'(t), v)_{I_n} - (f(t), v)_{I_n} = 0, \ \ \forall v \in V_0(I_n),$$

for $n = 0, \cdots, N-1$. The above CN-G time discretization satisfies the following pointwise equation

$$Y'(t) - \mathcal{P}_0 f(t) = 0 \ \ \forall t \in I_n,$$

with $\mathcal{P}_0$ denoting the L^2 orthogonal projection operator onto $V_0(I_n)$. By plugging the approximate solution Y into the ODE, we obtain the following residual

$$R(t) = Y'(t) - f(t) = \mathcal{P}_0 f(t) - f(t) = \mathcal{O}(k_n) \ \forall t \in I_n,$$

while it is well-known that CN-G gives second order approximation to $y(t)$.

Dual problem with discontinuous coefficient

Let's recall again the dual problem.

$$\partial_t p + f'(u)\partial_x p = 0, \text{ in } [0, T] \times \mathbb{R},$$
$$p(x, T) = g(x)$$

In the presence of shock discontinuities, the above problem will be a linear backward transport problem with discontinuous coefficient $f'(u)$. Uniqueness for this kind of problems is ensured for some notion of solution called "*reversible solution*", but its discretization is still challenging.

Example:

$$\partial_t p + a(x)\partial_x p = 0, \text{ in } [0, T] \times \mathbb{R},$$
$$p(x, T) = p^T(x),$$

with $a(x) = -\text{sgn}(x)$.

Dual problem with discontinuous coefficient

Let's recall again the dual problem.

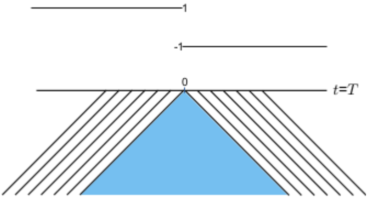
$$\partial_t p + f'(u)\partial_x p = 0, \quad \text{in } [0, T] \times \mathbb{R},$$
$$p(x, T) = g(x)$$

In the presence of shock discontinuities, the above problem will be a linear backward transport problem with discontinuous coefficient $f'(u)$. Uniqueness for this kind of problems is ensured for some notion of solution called "*reversible solution*", but its discretization is still challenging.

Example:

$$\partial_t p + a(x)\partial_x p = 0, \quad \text{in } [0, T] \times \mathbb{R},$$
$$p(x, T) = p^T(x),$$

with $a(x) = -\text{sgn}(x)$.



Reconstruction

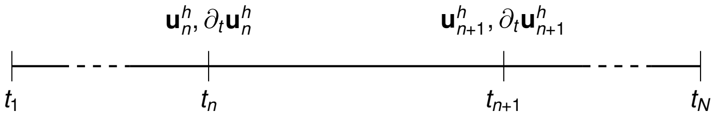
In order to get around of above difficulties, we rely on discrete setting based on some *space-time reconstruction*. Before going into detail let's see how this reconstruction looks like.

- Reconstruction in time

Let's assume that the DG semi-discrete form with N_x element of degree p is abstractly recast as the following system of ODEs.

$$\partial_t \mathbf{u}^h = F(\mathbf{u}^h), \quad \mathbf{u}^h(0) = \mathbf{u}_0^h \in \mathbb{R}^m, \tag{5}$$

where $m = N_x \times p$. The problem (5) is discretized to obtain approximate solutions $\mathbf{u}_1^h, \mathbf{u}_2^h, \cdots, \mathbf{u}_N^h$ at different time steps $t_1, t_2, \cdots, t_N$. Then we use Hermite interpolation on each subinterval $[t_n, t_{n+1}]$.



- Reconstruction in space

After reconstruction in time, we perform a local reconstruction in space over each spatial element [2]. It is illustrated as follows.

$$\partial_t u + b\,\partial_x u = 0, \quad \text{in } [0, T] \times \mathbb{R},$$
$$u(x,0) = u_0(x),$$

with $b > 0$. For the reconstruction we need to solve the following problem on each element $E_i = [x_i, x_{i+1}]$. Given $u^h \in V_q$ find $\hat{u} \in V_{q+1}$ s. t.

$$\left(\hat{u} - u^h, v\right)_{L^2(E_i)} = 0, \quad \forall v \in V_{q-1}$$

with $\hat{u}(x_i^+) = u^h(x_i^-), \hat{u}(x_{i+1}^-) = u^h(x_{i+1}^-)$.

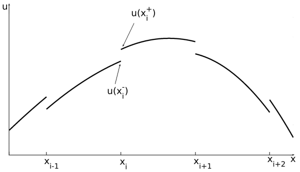
[2] J. Giesselmann et al., SIAM J. NUMER. ANAL., Vol. 53, No. 3, pp. 1280-1303.

Reconstruction cont'd

- Reconstruction in space

After reconstruction in time, we perform a local reconstruction in space over each spatial element [2]. It is illustrated as follows.

$$\partial_t u + b\,\partial_x u = 0, \quad \text{in } [0,T] \times \mathbb{R},$$
$$u(x,0) = u_0(x),$$



with $b > 0$. For the reconstruction we need to solve the following problem on each element $E_i = [x_i, x_{i+1}]$. Given $u^h \in V_q$ find $\hat{u} \in V_{q+1}$ s. t.

$$\left(\hat{u} - u^h, v\right)_{L^2(E_i)} = 0, \quad \forall v \in V_{q-1}$$

with $\hat{u}(x_i^+) = u^h(x_i^-)$, $\hat{u}(x_{i+1}^-) = u^h(x_{i+1}^-)$.

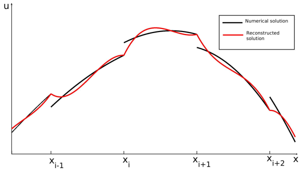
[2] J. Giesselmann et al., SIAM J. NUMER. ANAL., Vol. 53, No. 3, pp. 1280-1303.

Reconstruction cont'd

- Reconstruction in space

After reconstruction in time, we perform a local reconstruction in space over each spatial element [2]. It is illustrated as follows.

$$\partial_t u + b\,\partial_x u = 0, \quad \text{in } [0,T] \times \mathbb{R},$$
$$u(x,0) = u_0(x),$$



with $b > 0$. For the reconstruction we need to solve the following problem on each element $E_i = [x_i, x_{i+1}]$. Given $u^h \in V_q$ find $\hat{u} \in V_{q+1}$ s. t.

$$\left(\hat{u} - u^h, v\right)_{L^2(E_i)} = 0, \quad \forall v \in V_{q-1}$$

with $\hat{u}(x_i^+) = u^h(x_i^-), \hat{u}(x_{i+1}^-) = u^h(x_{i+1}^-)$.

[2] J. Giesselmann et al., SIAM J. NUMER. ANAL., Vol. 53, No. 3, pp. 1280-1303.

Dual problem: Revisited

TECHNISCHE UNIVERSITÄT DARMSTADT

Let's denote the reconstructed primal (res. dual) solution by $\hat{u}$ (res. $\hat{p}$). Now we define the following Lagrangian.

$$L_h(v; w) = J(v) - A_h(v; w)$$

for some functions v and w with the following dual residual when we plug in the reconstructed solutions:

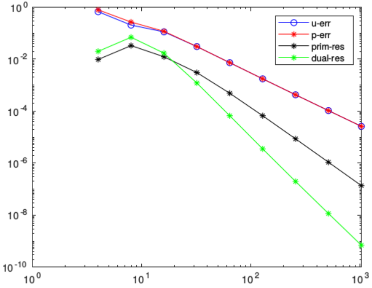
$$L_h'(\hat{u}; \psi, \hat{p}) = J(\psi) - A_h'(\hat{u}; \psi, \hat{p})$$

Now, following the same duality approach as before, we get an error representation as follows

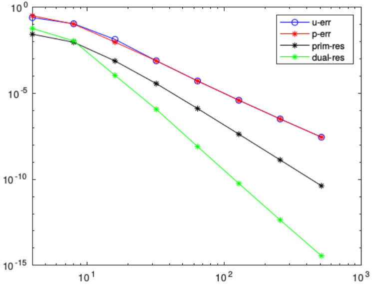
$$\begin{aligned} J(u) - J(\hat{u}) &= L_h(u; \hat{p}) + \underbrace{A_h(u; \hat{p})}_{=0} - L_h(\hat{u}; \hat{p}) - A_h(\hat{u}; \hat{p}) \\ &\simeq \frac{1}{2} L_h'(u; u - \hat{u}, \hat{p}) + \frac{1}{2} L_h'(\hat{u}; u - \hat{u}, \hat{p}) - A_h(\hat{u}; \hat{p}) \end{aligned}$$

Numerical results: Optimality of residuals

The following figures show the rate of residuals for the linear advection problem.



(a) Linear basis functions



(b) Quadratic basis functions

Concluding remarks

- A brief overview of DWR for hyperbolic problems with smooth solutions
- Encountering challenges in the presence of discontinuous solution
- Revisiting the DWR approach with space-time reconstruction
- Some numerical results to check the optimality of residuals

To-do list:

- We need to study the error propagation due to changing the dual problem.
- Looking at backward dual problem and its discretization using higher-order methods
- Extending the results to optimal control problems, in particular variational data assimilation.

Concluding remarks

- A brief overview of DWR for hyperbolic problems with smooth solutions
- Encountering challenges in the presence of discontinuous solution
- Revisiting the DWR approach with space-time reconstruction
- Some numerical results to check the optimality of residuals

To-do list:

- We need to study the error propagation due to changing the dual problem.
- Looking at backward dual problem and its discretization using higher-order methods
- Extending the results to optimal control problems, in particular variational data assimilation.

Thank you for your attention!