Dual-consistent treatment of functional output

James Lu, RICAM

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Dual-consistent treatment of functional output for compressible Navier-Stokes equations

James Lu (RICAM)

Overview

Dual-consistency for functional outputs
: definition, relation between discrete and continuous dual problems

Implications for DG treatment:
: inviscid Euler flow equation
: compressible Navier-Stokes equations

Numerical results
: discrete adjoint behavior, convergence rates for outputs

Dual problems

Application of duality-based techniques:

- error analysis
- design optimization, optimal control, ...

Introduce Lagrangian on appropraiate spaces, obtain either

- continuous dual problem
- discrete dual problem

For general discretizations, lack of correspondence between the two

Propose: dual-consistency property as a connection between the discrete and continuous dual problems.

Continuous Variational Setting

- Primal variation problem: $\mathbf{u} \in \mathscr{V}$ satisfy

$$\mathscr{F}(\mathbf{u}) = 0$$

where $\mathscr{F}$ is Frechét-differentiable, maps $\mathscr{V} \to \mathscr{W}'$.
- Functional of interest: $\mathscr{J}(\cdot) : \mathscr{V} \to \mathbb{R}$
- Introduce Lagrangian:

$$\mathscr{L}(\mathbf{u}, \boldsymbol{\psi}) \equiv \mathscr{J}(\mathbf{u}) - (\mathscr{F}(\mathbf{u}), \boldsymbol{\psi})_{\mathscr{W}', \mathscr{W}},$$

- Taking variations $\mathbf{u} \to \mathbf{u} + \delta\mathbf{v} \in \mathscr{V}$ in the permissible primal space, requiring the Lagrangian be stationary with respect to permissible $\delta\mathbf{v}$, obtain equation for the continuous dual variable $\boldsymbol{\psi}$:

$$\mathscr{F}'[\mathbf{u}]^* \boldsymbol{\psi} = \mathscr{J}'[\mathbf{u}]$$

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Discrete Setting for Finite Element Methods

- Finite dimensional test and trial spaces: $\mathscr{V}_h$ and $\mathscr{W}_h$, with bases $\{\phi_k\}$ and $\{\varphi_k\}$.
- FEM semilinear form: $R_h(\cdot,\cdot)$, functional $\mathscr{J}_h(\cdot)$.
- Define

$$\mathbf{u}_h = \mathbf{u}_h^D + \sum_{k=1}^{N} \mathbf{U}_k \phi_k, \mathbf{v}_h = \sum_{k=1}^{N} \mathbf{V}_k \varphi_k.$$

- The ith component of the nonlinear system of equations for the unknown coefficients $\mathbf{U} = \{\mathbf{U}_k\}$ is

$$R_h(\mathbf{u}_h, \varphi_i) = 0, \ i = 0, \dots, N.$$

- Then $\boldsymbol{\psi}_h = \sum_{k=1}^{N} \boldsymbol{\Psi}_k \varphi_k$ corresponding to the discrete adjoint solution satisfies

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Dual-consistency

Definition

The finite element formulation together with the discrete functional $\mathscr{J}_h(\cdot)$ is *dual-consistent* if given $\mathbf{u}$ and $\boldsymbol{\psi}$ solutions to the primal and adjoint PDE respectively, the following holds:

$$R'_h[\mathbf{u}](\mathbf{v}_h, \boldsymbol{\psi}) = \mathscr{J}'_h[\mathbf{u}](\mathbf{v}_h), \ \forall \mathbf{v}_h \in \mathscr{V}_h.$$

More generally, the formulation is said to be *asymptotically dual-consistent* if:

$$\lim_{h \to 0} \left(\sup_{\mathbf{v}_h \in \mathscr{V}_h} \frac{|R'_h[\mathbf{u}](\mathbf{v}_h, \boldsymbol{\psi}) - \mathscr{J}'_h[\mathbf{u}](\mathbf{v}_h)|}{\|\mathbf{v}_h\|_{\mathscr{V}_h}} \right) = 0.$$

Dual-consistency

- Factors to consider in showing dual-consistency of FE formulation:
  1. Treatment of interior terms
  2. Treatment of boundary condition and functional
- Lack of dual-consistency of NIP results in (Harriman, Houston and Süli):
  1. non-convergent discrete adjoint solution
  2. suboptimal functional output convergence
- Considerations at domain boundary demonstrate:
  1. necessary matching condition between boundary and functional treatment
  2. generalizes conservativity of functional treatment (Giles)

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First-order conservation laws

- Let $\mathbf{u} \in \mathscr{V}$ be a weak solution to the following system of conservation law,

$$\begin{cases} \nabla \cdot \mathscr{F}(\mathbf{u}) & = 0, \ \mathbf{x} \in \Omega, \\ \mathbf{D}(\mathbf{u}|_{\partial\Omega}, \mathrm{BC}) & = 0, \ \mathbf{x} \in \partial\Omega, \end{cases}$$

where Dirichlet conditions are imposed via the boundary operator $\mathbf{D}(\cdot, \mathrm{BC}) : \partial\mathscr{V} \to \partial\mathscr{V}$

- Adjoint state ψ associated with $\mathscr{J}(\cdot) \equiv \int_{\Gamma_{\text{output}}} J(\cdot) ds$, $\Gamma_{\text{output}} \subset \partial\Omega$ satisfies the PDE:

$$-\mathscr{F}'[\mathbf{u}]^T \cdot \nabla \psi = 0, \ \mathbf{x} \in \Omega,$$

subject to,

$$\int_{\partial\Omega} \psi^T \hat{\mathbf{n}} \cdot \mathscr{F}'[\mathbf{u}](\tilde{\mathbf{u}}) ds = \int_{\Gamma_{\text{output}}} J'[\mathbf{u}](\tilde{\mathbf{u}}) ds, \quad \forall \tilde{\mathbf{u}} \in \partial\mathscr{V}^0$$

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First-order conservation laws

- Trace space of $\mathscr{V}$ satisfying the linearized, homogeneous Dirichlet condition:

$$\partial\mathscr{V}^0 \equiv \left\{\tilde{\mathbf{u}} \in \partial\mathscr{V} : \mathbf{D}'[\mathbf{u}|_{\partial\Omega}](\tilde{\mathbf{u}}) = 0\right\}.$$

  $\therefore$ Components of variations $\tilde{\mathbf{u}}|_{\partial\Omega}$ allowed by the primal Dirichlet BC give rise to constraints on $\boldsymbol{\psi}|_{\partial\Omega}$.
- Existence of dual solutions for certain set of functionals, dependent on the boundary condition
- E.g., for inviscid Euler flow equations, on flow tangency boundaries only pressure based functionals are allowed

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DG for conservation laws

- Semilinear form:

$$R_h(\mathbf{u}_h,\mathbf{v}_h) \equiv \sum_{\kappa\in T_h}\Big\{-\int_\kappa \nabla\mathbf{v}_h^T\cdot\mathscr{F}(\mathbf{u}_h)d\mathbf{x}+\int_{\partial\kappa\setminus\partial\Omega}{\mathbf{v}_h^+}^T\mathscr{H}(\mathbf{u}_h^+,\mathbf{u}_h^-,\hat{\mathbf{n}})ds$$
$$+\int_{\partial\kappa\cap\partial\Omega}{\mathbf{v}_h^+}^T\mathscr{H}^b(\mathbf{u}_h^+,\mathbf{u}_h^b,\hat{\mathbf{n}})ds\Big\}$$

- Note:
  1. boundary conditions on $\partial\Omega$ weakly imposed via constructing a discrete boundary trace $\mathbf{u}_h^b(\mathbf{u}_h^+,\mathrm{BCData})$ being a function of the interior trace and BC data.
  2. boundary numerical flux $\mathscr{H}^b(\cdot,\cdot,\hat{\mathbf{n}})$ possibly different from $\mathscr{H}(\cdot,\cdot,\hat{\mathbf{n}})$

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$$+ \int_{\partial\kappa \cap \partial\Omega} \mathbf{v}_h^{+T} \mathscr{H}^b(\mathbf{u}_h^+, \mathbf{u}_h^b, \hat{\mathbf{n}}) ds \Big\}$$

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General prescription for dual-consistency

- Projective property of boundary trace map:
  $\mathbf{u}_h^b(\mathbf{u}_h^b(\cdot,\mathrm{BCData}),\mathrm{BCData}) = \mathbf{u}_h^b(\cdot,\mathrm{BCData})$
  $\therefore$ vector space decomposition:

$$\partial \mathscr{V}_h^p = \mathrm{range}\left(\left[\frac{\partial \mathbf{u}_h^b}{\partial \mathbf{u}_h^+}\right]\right) \oplus \mathrm{null}\left(\left[\frac{\partial \mathbf{u}_h^b}{\partial \mathbf{u}_h^+}\right]\right)$$

- Fixed point property:

$$\mathbf{D}(\mathbf{u}|_{\partial\Omega},\mathrm{BC}) = 0 \Rightarrow \mathbf{u}_h^b(\mathbf{u}|_{\partial\Omega},\mathrm{BCData}) = \mathbf{u}|_{\partial\Omega}.$$

- Following choice of boundary flux and functional constitute a dual-consistent treatment:

$$\begin{aligned} \mathscr{H}^b(\cdot) &= \hat{\mathbf{n}}\cdot\mathscr{F}(\mathbf{u}_h^b(\cdot,\mathrm{BCData})) \\ \mathscr{J}_h(\cdot) &= \int_{\Gamma_{\mathrm{output}}} J(\mathbf{u}_h^b(\cdot,\mathrm{BCData}))ds. \end{aligned}$$

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$$\mathbf{D}(\mathbf{u}|_{\partial\Omega},\mathrm{BC}) = 0 \Rightarrow \mathbf{u}_h^b(\mathbf{u}|_{\partial\Omega},\mathrm{BCData}) = \mathbf{u}|_{\partial\Omega}.$$

- Following choice of boundary flux and functional constitute a dual-consistent treatment:

$$\begin{aligned} \mathscr{H}^b(\cdot) &= \hat{\mathbf{n}}\cdot\mathscr{F}(\mathbf{u}_h^b(\cdot,\mathrm{BCData})) \\ \mathscr{J}_h(\cdot) &= \int_{\Gamma_{\mathrm{output}}} J(\mathbf{u}_h^b(\cdot,\mathrm{BCData}))ds. \end{aligned}$$

Test case: inviscid Euler equations

- Expression for the fluxes $\mathscr{F} = [\mathscr{F}^x, \mathscr{F}^y]$ are,

$$\mathscr{F}^x = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uH \end{pmatrix}, \quad \mathscr{F}^y = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vH \end{pmatrix}.$$

  H the total enthalpy, p the pressure given by
- Geometry: flow around Gaussian bump:
  $\Omega = \left\{ (x,y) \in (-6,6) \times (0,6) : y > \frac{1}{5} e^{-2x^2} \right\}$
- Output of interest

$$\mathscr{J}(\mathbf{u}) = \int_{x \in [-6,6],\, y = \frac{1}{5} e^{-2x^2}} n_y p(\mathbf{u}) e^{-\frac{1}{2}x^2} ds, \qquad (0.1)$$

Implications of different boundary treatments

(a) Dual-consistent (b) Dual-inconsistent

Figure: Comparison of $p = 3$ discrete adjoint solutions. $M_\infty = 0.5$.

Implications of different boundary treatments

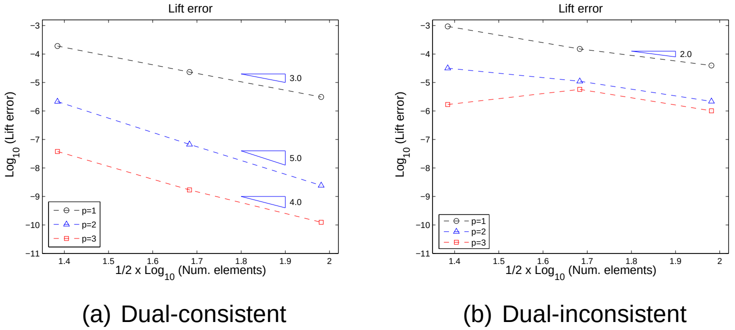


Figure: Comparison of functional output convergence. $M_\infty = 0.5$.

Discretization of elliptic operators

- Denote primal system: $\nabla \cdot (\mathscr{A}_v(\mathbf{u})\nabla \mathbf{u}) = 0, \mathbf{x} \in \Omega$,

$$\begin{cases} \mathbf{D}(\mathbf{u}|_{\partial\Omega}, \mathrm{BC}) & = 0, \ \mathbf{x} \in \partial\Omega, \\ \mathbf{N}(\hat{\mathbf{n}} \cdot \mathscr{A}_v(\mathbf{u})\nabla \mathbf{u}|_{\partial\Omega}, \mathrm{BC}) & = 0, \ \mathbf{x} \in \partial\Omega, \end{cases}$$

- Bassi-Rebay II DG discretization:

$$\begin{aligned} R_h(\mathbf{u}_h, \mathbf{v}_h) \ \equiv \ & \cdots - \int_{\partial\Omega} (\mathbf{u}_h^b - \mathbf{u}_h^+)^T (\hat{\mathbf{n}} \cdot \mathscr{A}_v(\mathbf{u}_h^b)^T \nabla \mathbf{v}_h^+) ds \\ + \ & \int_{\partial\Omega} {\mathbf{v}_h^+}^T \mathbf{F}_h^b \left(\hat{\mathbf{n}} \cdot \mathscr{A}_v(\mathbf{u}_h^b) \nabla \mathbf{u}_h^+ - \eta_f \hat{\mathbf{n}} \cdot \boldsymbol{\delta}_f^b \right) ds, \end{aligned}$$

where $\boldsymbol{\delta}_f^b \in [\mathscr{V}_h^p]^2$ such that

$$\int_\Omega \boldsymbol{\tau}_h^T \cdot \boldsymbol{\delta}_f^b d\mathbf{x} = \int_{\sigma_f} (\mathbf{u}_h^+ - \mathbf{u}_h^b)^T [\hat{\mathbf{n}} \cdot \mathscr{A}_v(\mathbf{u}_h^b)^T \boldsymbol{\tau}_h^+] ds,$$

- Consistent, dual-consistent on interior elements
- Stable for sufficiently large stabilization parameter η_f

General prescription for dual-consistency

- Projective property of boundary flux map:
  $\mathbf{F}_h^b(\mathbf{F}_h^b(\cdot, \mathrm{BCData}), \mathrm{BCData}) = \mathbf{F}_h^b(\cdot, \mathrm{BCData})$
- Fixed point property:

$$\begin{aligned} & \mathbf{N}(\hat{\mathbf{n}} \cdot \mathscr{A}_v \nabla \mathbf{u}|_{\partial\Omega}, \mathrm{BC}) = 0 \\ \Rightarrow \quad & \mathbf{F}_h^b(\hat{\mathbf{n}} \cdot \mathscr{A}_v \nabla \mathbf{u}|_{\partial\Omega}, \mathrm{BCData}) = \hat{\mathbf{n}} \cdot \mathscr{A}_v \nabla \mathbf{u}|_{\partial\Omega} \end{aligned}$$

- Form of functional for dual-consistent treatment:

$$\mathscr{J}_h(\nabla \mathbf{u}_h) = \int_{\Gamma_{\mathrm{output}}} J(\mathbf{F}_h^b(\hat{\mathbf{n}} \cdot \mathscr{A}_v \nabla \mathbf{u}_h^+ - \eta_f \hat{\mathbf{n}} \cdot \boldsymbol{\delta}_f^b))ds$$

Test case: compressible Navier-Stokes equations

- Viscous flux $\mathscr{A}_v(\mathbf{u})\nabla\mathbf{u}$, where components are:

$$x \;:\; \begin{pmatrix} 0 \\ \frac{2}{3}\mu(\mathbf{u})(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}) \\ \mu(\mathbf{u})(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) \\ \frac{2}{3}\mu(\mathbf{u})(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y})u + \mu(\mathbf{u})(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})v + \kappa(\mathbf{u})\frac{\partial T}{\partial x} \end{pmatrix}$$

$$y \;:\; \begin{pmatrix} 0 \\ \mu(\mathbf{u})(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) \\ \frac{2}{3}\mu(\mathbf{u})(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}) \\ \frac{2}{3}\mu(\mathbf{u})(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x})v + \mu(\mathbf{u})(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})u + \kappa(\mathbf{u})\frac{\partial T}{\partial y} \end{pmatrix}.$$

- Boundary condition on no-slip, adiabatic boundary: $u = v = 0$, $[\mathscr{A}_v(\mathbf{u})\nabla\mathbf{u}]_4 = 0$

Fine grid used for computation

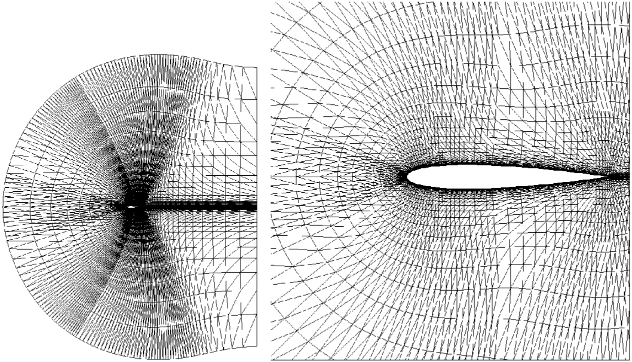
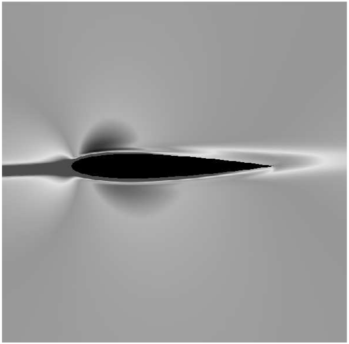
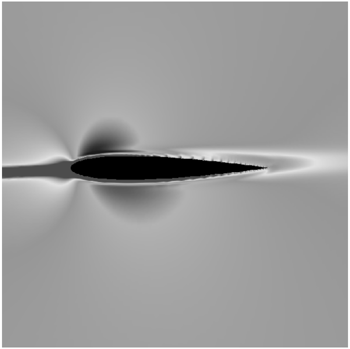


Figure: NACA 0012 grid, 10752 elements.

Implications of different boundary treatments



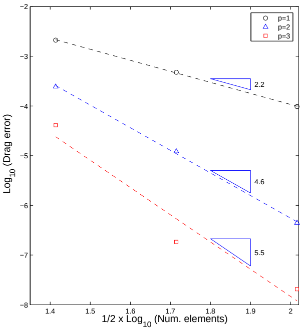
(a) Dual-consistent



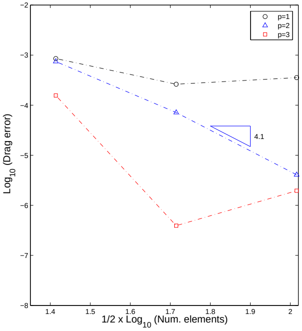
(b) A dual-inconsistent

Figure: Comparison of $p = 3$ discrete adjoint solutions.
$M_\infty = 0.5, Re = 5000$

Implications of different boundary treatments



(a) Dual-consistent



(b) Dual-inconsistent

Figure: Comparison of drag output convergence. $M_\infty = 0.5, Re = 5000$

Conclusions

- Proposed property of dual-consistency as a connection between duality in continuous and discrete settings
- Demonstrated the importance in the treatment of *boundary condition* and *functional output* important for dual-consistency
- Given a prescription for dual-consistent treatment of:
  1. DG discretization of first-order conservation laws
  2. Bassi-Rebay II DG discretization of elliptic operators
- Demonstrated implications in the context of flow equations:
  1. Regularity of discrete adjoint solution
  2. Rate of functional output convergence
  3. Effectivity of duality-based error estimates

Thank you for your attention!