Adjoints for Scientists and Engineers
Spring 2018
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Assignment #2 **Due Date: Mar 6, 2018**

For this assignment you will apply the discrete adjoint method to the quasi-1D Euler equations and use the adjoint to evaluate the gradient of a functional. If you need a refresher, Anderson's aerodynamics textbook [1] provides a good introduction to quasi-1D nozzle flows.

1 Boundary Value Problem and Functional

1.1 The Quasi-1D Euler Equations

The quasi-1D Euler equations are a system of coupled nonlinear PDEs given by

$$R(q, A) \equiv \frac{d}{dx}\left[F(q, A)\right] - G(q, A) = 0, \qquad \forall\, x \in [0, 1], \tag{1}$$

where the flux and source are

$$F(q, A) = \begin{pmatrix}\rho u A, & (\rho u^2 + p)A, & u(e + p)A\end{pmatrix}^T \qquad \text{and} \qquad G(q, A) = \begin{pmatrix}0, & p\frac{dA}{dx}, & 0\end{pmatrix}^T,$$

respectively. The unknown state vector is $q = [\rho, \rho u, e]^T$, where $q_1 = \rho$ is the density, $q_2 = \rho u$ is the momentum per unit volume, and $q_3 = e$ is the energy per unit volume. Pressure is determined using the ideal-gas equation of state: $p(q) = (\gamma-1)(e-\frac{1}{2}\rho u^2)$, where $\gamma = 1.4$ here. In the implementation, the equations and variables have been nondimensionalized using the density and sound speed at the inlet, $x = 0$.

The function $A = A(x)$ is the spatially varying nozzle area. We will use a cubic area that defines a converging-diverging nozzle. In particular, the four coefficients in the cubic area are found using the following conditions:

$$\begin{aligned} A(0) &= 2.0, & A(1) &= 1.5, \\ A(0.5) &= 1.0, & \frac{dA}{dx}(0.5) &= 0.0. \end{aligned}$$

The function $A(x)$ is nondimensionalized using the area at the midpoint (i.e. the throat) of the nozzle.

The PDE (1) has an exact solution that can be found using the Mach relations; see, for example, [1]. The source code provides a function — `getFlowExact` — that computes this exact solution for a given area, stagnation temperature, and stagnation pressure. For the present study, the exact solution is based on a stagnation temperature of 300 K and stagnation pressure of 100 kPa. The critical nozzle area is $A^* = 0.8$ and the gas constant is 287 J/(kg K).

1.2 Boundary Conditions

The quasi-1D Euler equations require boundary conditions at the inlet and outlet, but the number and type of boundary conditions depend on whether the flow is subsonic or supersonic. For this assignment, we will assume that the flow is subsonic everywhere.

At a subsonic one-dimensional inlet, there are two waves entering the domain and one wave exiting the domain. There needs to be a boundary condition for each of the incoming waves. The inlet boundary conditions in the provided code are applied to the incoming characteristic variables, which are evaluated based on the exact solution at $x = 0$.

At a subsonic outlet, there are two waves exiting the domain and one wave entering the domain. Therefore, we need only one boundary condition, which is again applied to the one left-travelling characteristic.

1.3 Functionals

We will consider two functionals in this assignment. The first is the integrated momentum source,

$$J_1(q) = \int_{x=0}^{1} p \frac{dA}{dx}\, dx.$$

The second functional is the outlet pressure computed using the numerical solution:

$$J_2(q) = p(q)\big|_{x=1}.$$

Note that J_2 is a boundary functional, while J_1 is a volume functional.

2 Discretization

The quasi-1D Euler equations are discretized using a nodal discontinuous Galerkin method [2], which is a collocation finite-element method in which the discrete solution is stored at the Lobatto-Gauss-Legendre quadrature points. On node i of element κ the discrete residual takes the form

$$R_{\kappa,i}(q_h, A_h) = -\sum_{j=1}^{N} \mathsf{Q}_{j,i} F_{\kappa,j} + \delta_{iN} \hat{F}_{\kappa,N} - \delta_{i1} \hat{F}_{\kappa,1} - G_{\kappa,i} = 0,$$

where δ_{ij} is the Kronecker delta, and the flux and source are evaluated as follows:

$$F_{\kappa,j} \equiv F(q_{\kappa,j}, A_{\kappa,j}), \qquad G_{\kappa,i} \equiv \begin{pmatrix} 0 \\ p(q_{\kappa,i}) \sum_{j=1}^{N} \mathsf{Q}_{i,j} A_{\kappa,j} \\ 0 \end{pmatrix}.$$

In the above expressions, $\mathsf{Q}_{i,j}$ denotes the (i,j)th entry in the stiffness matrix $\int_\kappa L_i \frac{\partial L_j}{\partial \xi} d\xi$, where L_i is the ith Legendre polynomial evaluated on the $[-1, 1]$ reference element.

2.1 Continuity and Boundary Condition Imposition

The numerical fluxes at the end nodes, $\hat{F}_{\kappa,1}$ and $\hat{F}_{\kappa,N}$, change depending on whether the element boundary is adjacent to another element or adjacent to the domain boundary. For element boundaries at interfaces, we use the Roe numerical flux and supply the states on either side of the interface. For element boundaries at domain boundaries, we use the Roe numerical flux and supply the discrete solution and the relevant boundary state; this has the effect of applying the characteristic boundary conditions described earlier.

3 Provided Code

The supplementary zip file contains source code that implements the baseline discretization and solves for the steady-state solution. The code is written in Julia, which you can find more information about at `www.julialang.org`.

You will need to follow the steps below to get the code working.

1. Install the current release of Julia, version v0.6.2. Go to `https://julialang.org/downloads/` then choose the appropriate link for your operating system.

2. Once Julia is installed you need to add a few packages. To do so, start Julia and type the following:
```
julia> Pkg.add("Roots")
julia> Pkg.add("PyPlot")
julia> Pkg.clone("https://github.com/OptimalDesignLab/SummationByParts.jl.git")
```

3. Finally, to run the provided code, you will have to start Julia from the same directory in which you saved the assignment files. Then, at the Julia prompt type
```
julia> include("assign2_example.jl")
```

4 Questions

1. Adapt the provided source code to perform grid convergence studies of the two discrete functionals, $J_{1,h}(q_h)$ and $J_{2,h}(q_h)$. The studies should include discretizations of degree $p = 1$, $p = 2$, $p = 3$, and $p = 4$. The degree is set using the `degree` keyword in the `EulerSolver` constructor; see the provided example code. The number of elements, `numelem`, should be sufficient to infer the asymptotic rate of convergence of the functional. Also, **make sure that the there are a sufficient number of time-step iterations to reach the desired convergence tolerance.** If your solution is not sufficiently converged, your functional values will be incorrect.

   You can assume that the "exact" value of the integrated-source functional is

   $$J_1(q) \approx -0.35194635479522557,$$

   and that the "exact" value of the outlet-pressure functional is

   $$J_2(q) \approx 0.6896586332699256$$

What do these studies suggest about the corresponding adjoint problems?

2. Compute and plot the adjoints of $J_{1,h}(q_h)$ and $J_{2,h}(q_h)$ using the discrete adjoint method. This will require several steps:

   (a) Write some code to compute the Jacobian of the discrete residual R_h with respect to q_h. You can use any method you want to evaluate the Jacobian.

   (b) Write code to evaluate the right-hand-side of the adjoint, $-\partial J_{i,h}/\partial q_h$ where $i = 1, 2$. Again, you can use any method you want.

   (c) Use the first two steps to solve for the discrete adjoints of the two functionals. Watch out for sign errors.

   (d) For each functional, plot the three adjoint variables versus x. That is, plot ψ_ρ, $\psi_{\rho u}$, and ψ_e. Consider several different values of `degree` and `numelem` to ensure your solution is grid independent.

   Comment on the qualitative behavior of the adjoints for $J_{1,h}$ and $J_{2,h}$.

3. Use the discrete adjoint to evaluate the (total) gradient of the integrated-source functional with respect to the area, $DJ_{1,h}/DA_h$, where A_h is the vector of nozzle areas at each mesh node. Recall

$$\frac{DJ_{1,h}}{DA_h} = \frac{\partial J_{1,h}}{\partial A_h} + \psi_h^T \frac{\partial R_h}{\partial A_h},$$

   so you will need to evaluate the partial derivatives of $J_{1,h}$ and $\psi_h^T R_h$ with respect to A_h. You can do this with any method you want.

   Plot the gradient $DJ_{1,h}/DA_h$ versus x. What do you notice? Explain the behavior by rewriting the volume functional as a surface functional.

   Hint: Keep in mind that $A_{i,N} = A_{i+1,1}$, that is, the area is continuous at the element interfaces. This relationship is important to respect when you evaluate the gradient, otherwise you will see odd behavior at the interfaces.

5 Report and Code Expectations

Your report should be typeset in LaTeX. As before, the report should be fewer than 10 pages if you use a 12 point font. This is a "soft" page limit, but please do not be overly verbose.

The following should be included in the report.

- An abstract that summarizes your results.
- Provide a separate section or subsection in which you answer each question in the above list of questions.

You do not need to include an introduction, since your audience (me!) knows the background. You can include the results of additional studies that you performed out of interest.

The report will include several figures as requested in the questions. Please use an adequate font size on the figures! It should be legible if printed.

Please provide the modified code for your project as a separate zip file. You do not need to include in the report itself. All code should have adequate commenting.

Collaboration

You are permitted and encouraged to discuss the assignment with each other, provided each of you writes your own code and report. A good policy to follow in order to avoid academic misconduct is to not take notes or exchange files with one another; i.e. exchange information verbally and you should be fine.

References

[1] Anderson, J. D., *Fundamentals of Aerodynamics: second edition*, McGraw-Hill, Inc., New York, NY, 1991.

[2] Hesthaven, J. S. and Warburton, T., *Nodal discontinuous Galerkin methods: algorithms, analysis, and applications*, Springer-Verlag, New York, 2008.