Aerothermodynamic Design Sensitivities for a Reacting Gas Flow Solver on an Unstructured Mesh Using a Discrete Adjoint Formulation

Kyle B. Thompson

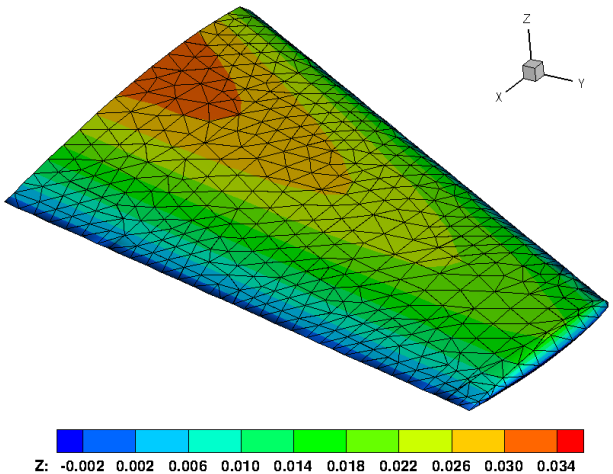
Mechanical and Aerospace Engineering Department
North Carolina State University

Aerothermodynamics Branch
NASA Langley Research Center

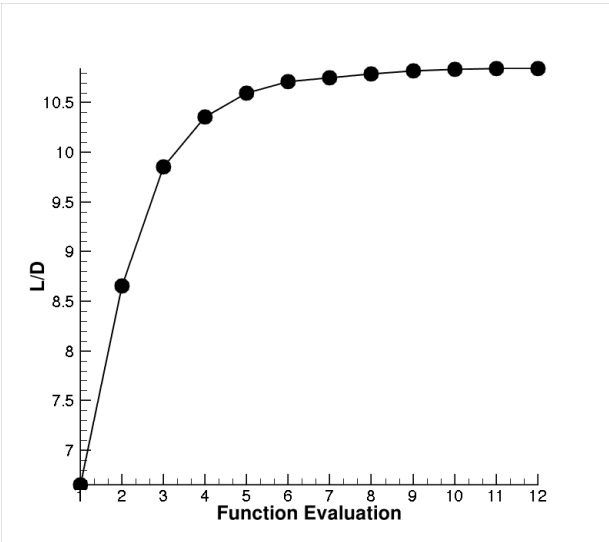
April 20, 2016

Outline

Introduction - Design



Shape Design Mesh Movement[1]



Lift/Drag Objective Function[1]

- Exploring design space using high-fidelity CFD is challenging
- zero-order methods (sampling) are prohibitively expensive
- Need to be intelligent about techniques for evaluating sensitivity to design parameters
- Gradient-based optimization much more efficient than sampling, but requires calculating sensitivity derivatives

[1] **Credit: FUN3D Tutorial Examples**.

Introduction - Design

- $>$ **100 design variables** in OM6 wing shape optimization

Introduction - Design

- $>$ **100 design variables** in OM6 wing shape optimization
- How do you to compute sensitivity of that many DVs?

Introduction - Design

- $>$ **100 design variables** in OM6 wing shape optimization
- How do you to compute sensitivity of that many DVs?

Direct differentiation approach - Expensive

- Navier-Stokes equations can be directly differentiated to yield sensitivity derivatives necessary for gradient-based optimization
- Finite difference requires a minimum of **one flow solution for each design variable sensitivity**
- Prohibitively expensive for large number of design parameters

Introduction - Design

- $>$ **100 design variables** in OM6 wing shape optimization
- How do you to compute sensitivity of that many DVs?

Adjoint approach - More efficient

- Solve adjoint equations in addition to Navier Stokes flow equations to obtain sensitivity derivatives
- **One flow and adjoint solution needed for each cost function**, regardless of number of design variables
- Considerably more efficient than direct differentiation approach for large number of design parameters

Introduction - Design

- Adjoint-based design optimization has recieved considerable attention in compressible, perfect gas CFD solvers[2,3], but very little in reacting flow solvers
- Difficulty of adjoint approach lies in implementating exact linearizations for 2nd-order flux construction scheme
- Particularly difficult for reacting flows, due to
  - Complexity of linearizing the additional equations for multi-species chemical kinetics
  - Resorting to Automatic Differentiation tools incurs performance overhead that is implementation-specific[4]
  - Serious memory and computational cost concerns when simulating a large number of species

[2] E. J. Nielsen et al. *Computers & Fluids* 33.9 (2004), pp. 1131–1155.

[3] J. E. Peter and R. P. Dwight. *Computers & Fluids* 39.3 (2010), pp. 373–391.

[4] J.-D. Müller and P. Cusdin. *International Journal for Numerical Methods in Fluids* 47.8-9 (2005), pp. 939–945.

Introduction - Improvement to State of the Art

- Current state of the art
  - Attempts made at both continuous[5] and discrete[6] adjoint formulations for a compressible reacting flow solver
  - These attempts suffer from quadratic scaling in memory and computational cost with number of species
  - Recent scheme at Barcelona Supercomputing Center[7] is promising, but only for incompressible reacting flows
- Proposed improvement to the state of the art
  - New decoupled scheme for both hypersonic flow solver and adjoint solver that is robust for high-speed flows in chemical non-equilibrium
  - New scheme significantly improves scaling in computational cost and memory with number of species

[5] S. R. Copeland, F. Palacios, and J. J. Alonso. *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, 2014.

[6] B. Lockwood et al. *49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition*. American Institute of Aeronautics and Astronautics, 2011.

[7] M. K. Esfahani and G. Houzeaux. *57th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*. American Institute of Aeronautics and Astronautics, 2016.

Introduction - Decoupled Approach

- Reacting gas simulations require solving a large number of conservation equations
- Memory concerns
  - Size of Jacobians scales quadratically with number species in gas mixture
  - Solving system of equations in a tightly-coupled fashion can be limited by memory constraints
- Cost concerns
  - Cost of solving the linear system scales quadratically with number of species in gas mixture
- Efficiently solving adjoint problem is a primary motivator
  - Solving adjoint system particularly costly if linear solver is slow
  - Can be necessary to store jacobian twice $\rightarrow$ large memory overhead

Introduction - Decoupled Approach

- Loosely-coupled solvers have become popular in the combustion community[8]
  - Decouple species conservation equations from meanflow equations, and solve two smaller systems

$$\underbrace{\begin{pmatrix} \square & \square & \cdots & \square \\ \square & \square & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \square & \cdots & \cdots & \square \end{pmatrix}}_{(4+ns)\times(4+ns)} \rightarrow \underbrace{\begin{pmatrix} \square & \cdots & \square \\ \vdots & \ddots & \vdots \\ \square & \cdots & \square \end{pmatrix}}_{5\times 5} \text{ and } \underbrace{\begin{pmatrix} \square & \boxslash & \cdots & \boxslash \\ \boxslash & \square & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \boxslash & \cdots & \cdots & \square \end{pmatrix}}_{ns\times ns}$$

- Candler, et al.[9] originally derived this for Steger-Warming scheme, this work extends to Roe FDS scheme

[8] V. Sankaran and M. Olsen. *16th AIAA Computational Fluid Dynamics Conference*. 2003.

[9] G. V. Candler, P. K. Subbareddy, and I. Nompelis. *AIAA Journal* 51.5 (2013), pp. 1245–1254.

Introduction - Choice of Code and Implementation

- FUN3D chosen as code to facilitate all research presented, because
  - Excellent infrastructure for adjoint-based design analysis and optimization
  - Robust hypersonic flow solver
  - NASA Langley Research Center supporting me through the Pathways program
- Decision to pursue discrete adjoint, rather than continuous adjoint, due to current FUN3D implementation

Outline

Fully-Coupled Point Implicit Method

- All work presented is for inviscid flows in chemical non-equilibrium, using a one-temperature model, but is extendable to viscous flows.
- Beginning with the semi-discrete form

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{1}{V}\sum_f (\mathbf{F}\cdot\mathbf{S})^f = \mathbf{W}$$

$$\mathbf{U} = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix}, \quad \mathbf{F}\cdot\mathbf{S} = \begin{pmatrix} \rho_1 \overline{U} \\ \vdots \\ \rho_{ns} \overline{U} \\ \rho u \overline{U} + p s_x \\ \rho u \overline{U} + p s_y \\ \rho u \overline{U} + p s_z \\ (\rho E + p)\overline{U} \end{pmatrix} S, \quad \mathbf{W} = \begin{pmatrix} \dot{\rho}_1 \\ \vdots \\ \dot{\rho}_{ns} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Fully-Coupled Point Implicit Method

- Using the Roe FDS scheme to compute the inviscid flux at the face, $\mathbf{F}^f$, and linearizing the system results in

$$\frac{\delta \mathbf{U}^n}{\Delta t} + \frac{1}{V}\sum_f \left(\frac{\partial \mathbf{F}^f}{\partial \mathbf{U^L}}\delta \mathbf{U}^L + \frac{\partial \mathbf{F}^f}{\partial \mathbf{U^R}}\delta \mathbf{U}^R\right)^n \mathbf{S}^f - \frac{\partial \mathbf{W}}{\partial \mathbf{U}}\delta \mathbf{U}^n = -\frac{1}{V}\sum_f (\mathbf{F}^f \cdot \mathbf{S}^f)^n + \mathbf{W}^n$$

- Which can be thought of more simply as

$$\mathbf{Au} = \mathbf{b}$$

$$\mathbf{A} \rightarrow \begin{array}{c}(4+ns)\times(4+ns)\\ \text{Jacobian Block}\end{array}$$

$$\mathbf{b} \rightarrow \begin{array}{c}(4+ns)\times 1\\ \text{Residual}\end{array}$$

Fully-Coupled Point Implicit Method

- Constructing the Jacobian in a fully-coupled fashion results in large, dense block matricies
- Using a stationary iterative method (i.e., Gauss-Seidel, SSOR, etc.), work is dominated by matrix-vector products

$$\text{Cost} \rightarrow O((4 + ns)^2)$$

- Leads to onerous quadratic scaling with respect to number of species

Decoupled Point Implicit Method

- The main idea is to separate the meanflow and species composition equations, adding a new equation for the total mixture density
- Leads to two sets of conserved variables

$$\mathbf{U}' = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix} \qquad \hat{\mathbf{U}} = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \end{pmatrix}$$

Meanflow Species Composition

Decoupled Point Implicit Method

- The fluxes are solved in two sequential steps
  - The mixture fluxes are first solved as

$$\frac{\partial \mathbf{U}'}{\partial t} + \frac{1}{V}\sum_f (\mathbf{F}' \cdot \mathbf{S})^f = 0$$

  - Followed by the species fluxes

$$\frac{\partial \hat{\mathbf{U}}}{\partial t} + \frac{1}{V}\sum_f (\hat{\mathbf{F}} \cdot \mathbf{S})^f = \hat{\mathbf{W}}$$

- Since the mixture density was determined in the first step, step two actually solves for the species mass fractions

$$\delta\hat{\mathbf{U}}^n = \rho^{n+1}\hat{\mathbf{V}}^{n+1} - \rho^n\hat{\mathbf{V}}^n = \rho^{n+1}\delta\hat{\mathbf{V}}^n + \hat{\mathbf{V}}^n\delta\rho^n$$

$$\hat{\mathbf{V}} = (c_1, \ldots, c_{ns})^T, c_s = \rho_s/\rho$$

Decoupled Point Implicit Method

- The Roe FDS scheme species mass fluxes can be rewritten as

$$\hat{\mathbf{F}}_{\rho_s} = c_s \mathbf{F}'_{\rho} + (c_s^L - \tilde{c}_s)\rho^L \lambda^+ + (c_s^R - \tilde{c}_s)\rho^R \lambda^-$$

$$\frac{\partial \hat{\mathbf{F}}_{\rho_s}}{\partial c_s^L} = w\mathbf{F}_{\rho} + (1-w)\rho^L \lambda^+ - w\rho^R \lambda^-$$

$$\frac{\partial \hat{\mathbf{F}}_{\rho_s}}{\partial c_s^R} = (1-w)\mathbf{F}_{\rho} + (w-1)\rho^L \lambda^+ + w\rho^R \lambda^-$$

- Jacobian Approximations

$$\text{Step 1:} \quad \left.\frac{\partial \mathbf{F}}{\partial \mathbf{U}'}\right|_{\hat{\mathbf{V}}} = 5 \times 5 \underset{c_s=\text{Constant}}{\text{Roe FDS Jacobian}}$$

$$\text{Step 2:} \quad \left.\frac{\partial \mathbf{F}}{\partial \hat{\mathbf{V}}}\right|_{\hat{\mathbf{U}}'} = \begin{pmatrix} \frac{\partial F_{\rho_1}}{\partial c_1} & & 0 \\ & \ddots & \\ 0 & & \frac{\partial F_{\rho_{ns}}}{\partial c_{ns}} \end{pmatrix}$$

Decoupled Point Implicit Method

- Chemical source term linearized via

$$\hat{\mathbf{W}}^{n+1} = \hat{\mathbf{W}}^{n} + \left.\frac{\partial \hat{\mathbf{W}}}{\partial \mathbf{U}}\right|_{\mathbf{U}'} \frac{\partial \mathbf{U}}{\partial \hat{\mathbf{V}}}$$

$$\mathbf{C} = \left.\frac{\partial \hat{\mathbf{W}}}{\partial \mathbf{U}}\right|_{\mathbf{U}'} \frac{\partial \mathbf{U}}{\partial \hat{\mathbf{V}}}$$

- Full system to be solved in step two

$$\rho^{n+1}\frac{\delta \hat{\mathbf{V}}^{n}}{\Delta t} + \frac{1}{V}\sum_{f}\left(\frac{\partial \hat{\mathbf{F}}^{f}}{\partial \mathbf{V}^{L}}\delta \mathbf{V}^{L} + \frac{\partial \hat{\mathbf{F}}^{f}}{\partial \hat{\mathbf{V}}^{R}}\delta \hat{\mathbf{V}}^{R}\right)^{n,n+1}\mathbf{S}^{f} - \mathbf{C}^{n,n+1}\delta \mathbf{V}^{n}$$

$$= -\frac{1}{V}\sum_{f}(\hat{\mathbf{F}}^{n,n+1}\cdot\mathbf{S})^{f} + \mathbf{W}^{n,n+1} - \hat{\mathbf{V}}^{n}\left(\frac{\delta \rho^{n}}{\Delta t} - R_{\rho}\right)$$

$$R_{\rho} = -\frac{1}{V}\sum_{f}\sum_{s}(\hat{F}^{n,n+1}_{\rho_s}\cdot\mathbf{S})$$

- R_{ρ} is included to preserve $\sum_{s} c_s = 1$, $\sum_{s} \delta c_s = 0$.

Outline

Cost and Memory Savings of the Decoupled Flow Solver

- Most significant savings comes from the source term linearization being purely node-based
  - Convective contributions to block Jacobians are diagonal
  - Source term jacobian is dense block Jacobian
  - In the global system (w/chemistry), all off-diagonal block jacobians are diagonal

$$\begin{pmatrix} \square & & & & \\ & \ddots & & & \\ & & \square & & \\ & & & \ddots & \\ & & & & \square \end{pmatrix} \begin{pmatrix} \delta\hat{\mathbf{V}}_1 \\ \vdots \\ \delta\hat{\mathbf{V}}_i \\ \vdots \\ \delta\hat{\mathbf{V}}_{nodes} \end{pmatrix} = \begin{pmatrix} \hat{b}_1 \\ \vdots \\ \hat{b}_i \\ \vdots \\ \hat{b}_{nodes} \end{pmatrix} - \begin{pmatrix} (\sum_{j=1}^{N_{nb}} [\diagdown] \delta\hat{\mathbf{V}}_j)_1 \\ \vdots \\ (\sum_{j=1}^{N_{nb}} [\diagdown] \delta\hat{\mathbf{V}}_j)_i \\ \vdots \\ (\sum_{j=1}^{N_{nb}} [\diagdown] \delta\hat{\mathbf{V}}_j)_{nodes} \end{pmatrix}$$

- Matrix-vector products $\rightarrow$ inner products: $O(ns^2) \rightarrow O(ns)$

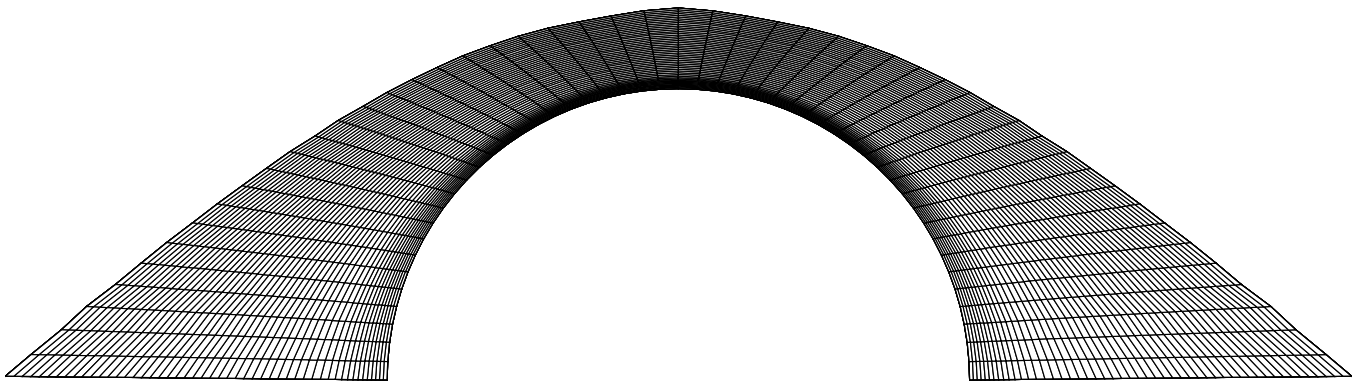
Cost and Memory Savings of the Decoupled Flow Solver

- Comparing size of Jacobian systems, using Compressed Row Storage

$$\mathbf{A}_d = \text{Decoupled system Jacobians}$$
$$\mathbf{A} = \text{Fully-coupled system Jacobians}$$

$$\begin{aligned} \textit{Relative Memory Cost} &= \frac{size(\mathbf{A}_d)}{size(\mathbf{A})} \\ &= \lim_{ns\to\infty} \frac{(ns^2+5^2)(N_{nodes})+(ns+5^2)(N_{nbrs})}{(ns+4)^2(N_{nodes}+N_{nbrs})} \\ &= \frac{N_{nodes}}{N_{nodes}+N_{nbrs}} \end{aligned}$$

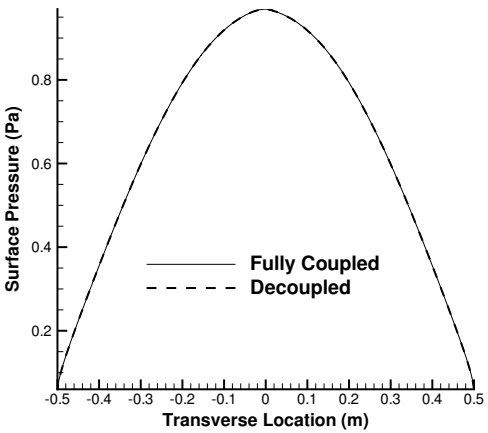
Numerical Results: 2D Cylinder

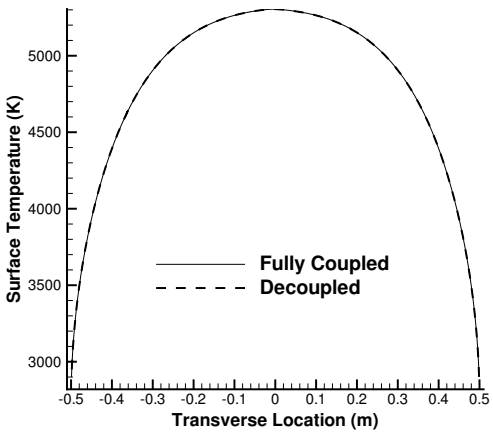


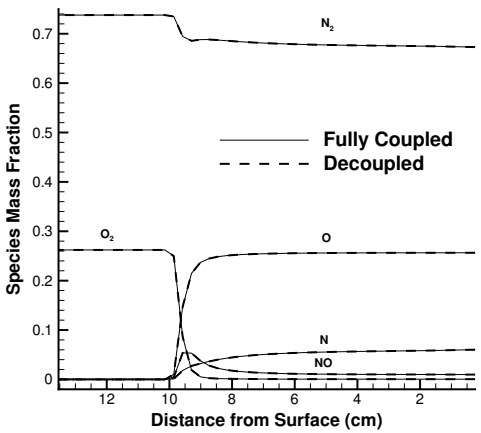
- Fully-coupled and decoupled methods both implemented in the Generic Gas Path of FUN3D
- Tested on 2D cylinder case
  - $V_\infty = 5000\ m/s$, $\rho_\infty = 0.001\ kg/m^3$, and $T_\infty = 200\ K$
- Inviscid flow, with 1-Temperature model

Numerical Results: 2D Cylinder

- Verification of implementation
  - 5-species air model: N, N_2, O, O_2, and NO with five reactions

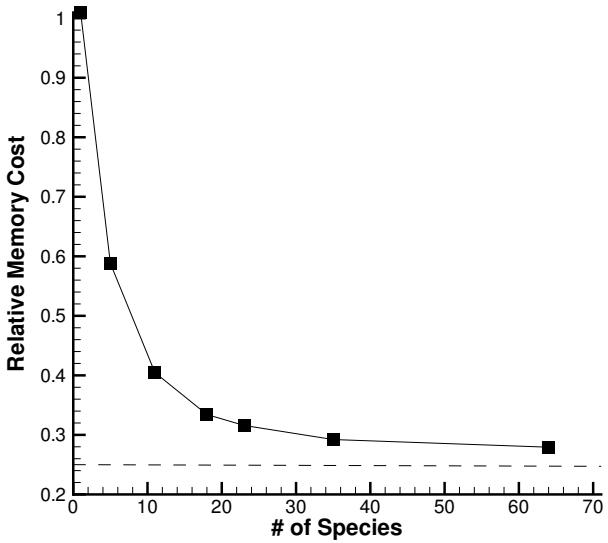


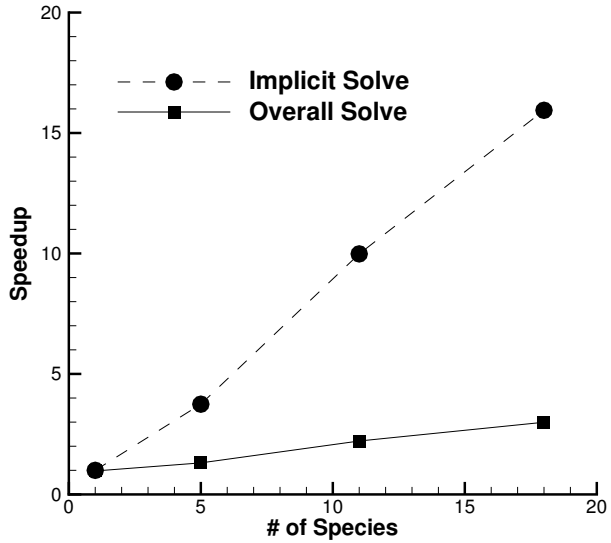




  - Surface pressure, surface temperature, and mass fractions on stagnation line agree between decoupled and fully coupled implementations

Numerical Results: 2D Cylinder



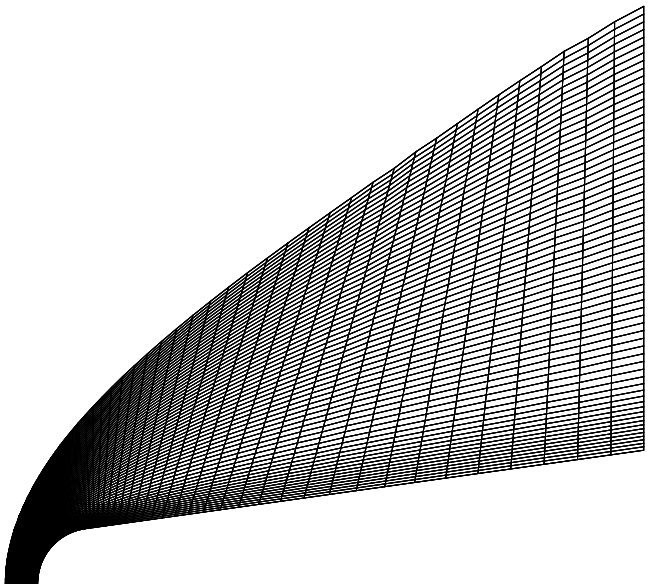


- On structured grids $N_{nbrs} \approx 6N_{nodes}$
  - Half precision off-diagonal $N_{nbrs} = \frac{6N_{nodes}}{2}$

$$Memory\ \ Cost \approx \frac{N_{nodes}}{N_{nodes} + N_{nbrs}} = \frac{N_{nodes}}{N_{nodes} + 6N_{nodes}/2} = \frac{1}{4}$$

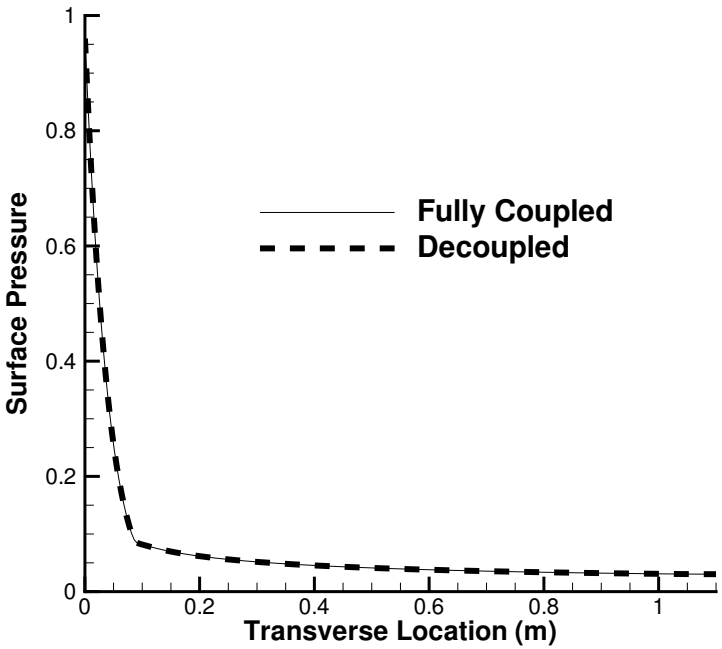
  - Linear speedup in solver: $\frac{O(ns^2)}{O(ns)} = O(ns)$

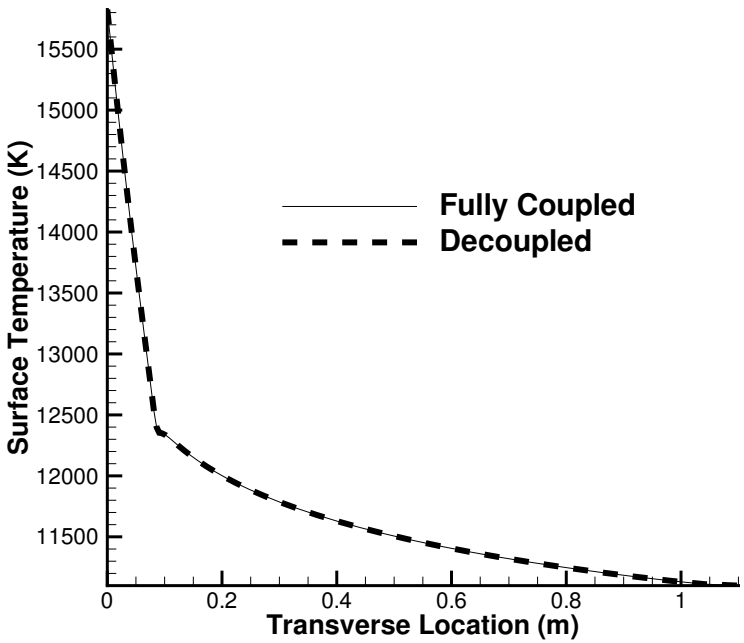
Numerical Results: Axisymmetric Spherically Capped Cone



- Verify that the decoupled scheme is robust at high velocities
  - $V_\infty = 15000\ m/s$, $\rho_\infty = 0.001\ kg/m^3$, $T_\infty = 200\ K$.
  - 11-species air model N, N_2, O, O_2, NO, N^+, N_2^+, O^+, O_2^+, NO^+, and electrons, with 22 possible reactions.
  - Inviscid flow, with 1-Temperature model

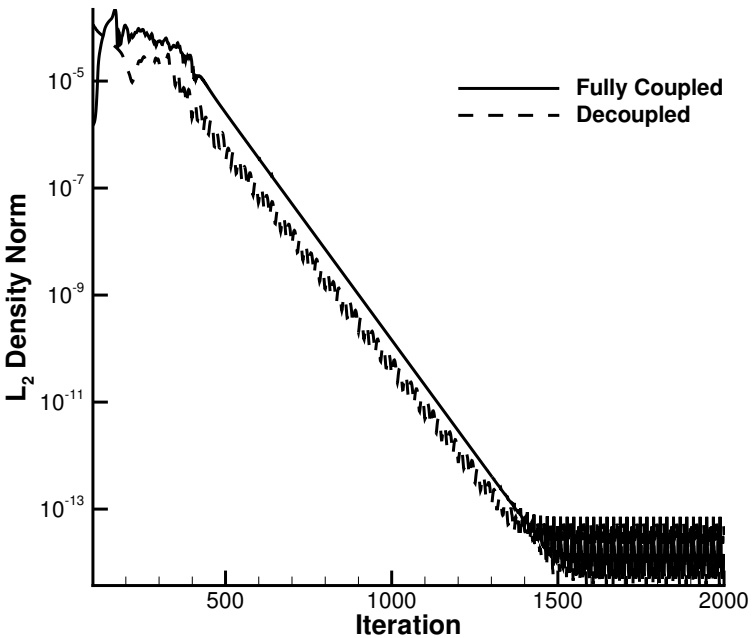
Numerical Results: Axisymmetric Spherically Capped Cone

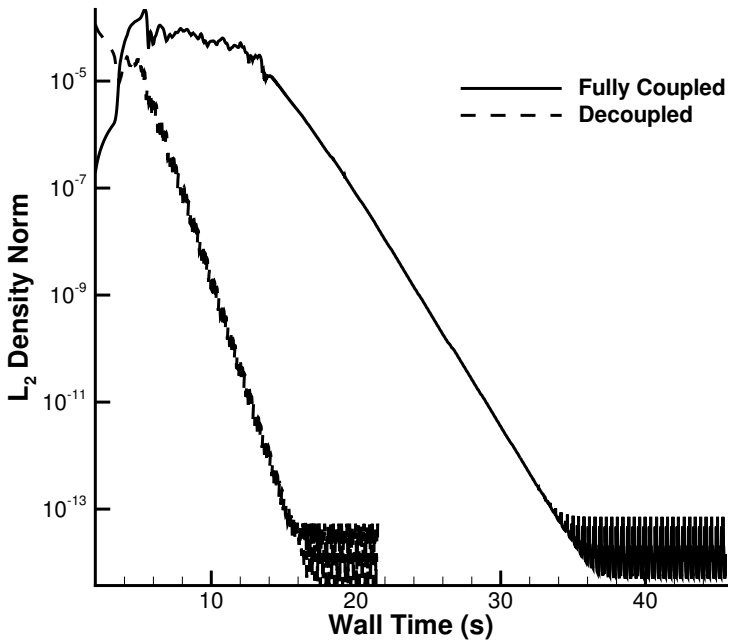




- Surface pressure and surface temperature agree between decoupled and fully coupled implementations

Numerical Results: Axisymmetric Spherically Capped Cone





- Necessary to scale source term magnitude by $0.001 \leq w \leq 1$ for the first 500 iterations, due to extreme reaction rates
- Both schemes converge in a similar number of iterations
- Decoupled scheme $\approx$ 2x faster

Outline

Derivation of Discrete Adjoint Formulation

- The derivation of the adjoint approach to compute design sensitivities begins with forming the Lagrangian and differentiating with respect to the design variables

$$L(\mathbf{D}, \mathbf{Q}, \mathbf{X}, \mathbf{\Lambda}) = f(\mathbf{D}, \mathbf{Q}, \mathbf{X}) + \mathbf{\Lambda}^T \mathbf{R}(\mathbf{D}, \mathbf{Q}, \mathbf{X})$$

$\mathbf{D}$ = design variables

$\mathbf{Q}$ = flow variables

$\mathbf{X}$ = computational grid

f = cost function

$\mathbf{R}$ = flow residual

$\mathbf{\Lambda}$ = costate variables

Derivation of Discrete Adjoint Formulation

- The derivation of the adjoint approach to compute design sensitivities begins with forming the Lagrangian and differentiating with respect to the design variables

$$L(\mathbf{D}, \mathbf{Q}, \mathbf{X}, \mathbf{\Lambda}) = f(\mathbf{D}, \mathbf{Q}, \mathbf{X}) + \mathbf{\Lambda}^T \mathbf{R}(\mathbf{D}, \mathbf{Q}, \mathbf{X})$$

$$\frac{\partial L}{\partial \mathbf{D}} = \left\{ \frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \frac{\partial f}{\partial \mathbf{X}} \right\} + \left[\frac{\partial \mathbf{Q}}{\partial \mathbf{D}}\right]^T \left\{ \frac{\partial f}{\partial \mathbf{Q}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T \mathbf{\Lambda} \right\}$$

$$+ \left\{ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \right\} \mathbf{\Lambda}$$

$\mathbf{D}$ = design variables $\quad f$ = cost function

$\mathbf{Q}$ = flow variables $\quad \mathbf{R}$ = flow residual

$\mathbf{X}$ = computational grid $\quad \mathbf{\Lambda}$ = costate variables

Derivation of Discrete Adjoint Formulation

- The derivation of the adjoint approach to compute design sensitivities begins with forming the Lagrangian and differentiating with respect to the design variables

$$L(\mathbf{D}, \mathbf{Q}, \mathbf{X}, \mathbf{\Lambda}) = f(\mathbf{D}, \mathbf{Q}, \mathbf{X}) + \mathbf{\Lambda}^T \mathbf{R}(\mathbf{D}, \mathbf{Q}, \mathbf{X})$$

$$\frac{\partial L}{\partial \mathbf{D}} = \left\{ \frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \frac{\partial f}{\partial \mathbf{X}} \right\} + \left[\frac{\partial \mathbf{Q}}{\partial \mathbf{D}}\right]^T \left\{ \frac{\partial f}{\partial \mathbf{Q}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T \mathbf{\Lambda} \right\}$$

$$+ \left\{ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \right\} \mathbf{\Lambda}$$

$\mathbf{D}$ = design variables $\quad f$ = cost function

$\mathbf{Q}$ = flow variables $\quad \mathbf{R}$ = flow residual

$\mathbf{X}$ = computational grid $\quad \mathbf{\Lambda}$ = costate variables

Derivation of Discrete Adjoint Formulation

- Need to eliminate flow variable dependence on design variables, $\frac{\partial \mathbf{Q}}{\partial \mathbf{D}}$
- Adjoint equation

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T \mathbf{\Lambda} = -\frac{\partial f}{\partial \mathbf{Q}}$$

- Solve for $\mathbf{\Lambda}$ and compute sensitivity derivatives

$$\frac{\partial L}{\partial \mathbf{D}} = \left\{\frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \frac{\partial f}{\partial \mathbf{X}}\right\} + \left\{\left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T\right\} \mathbf{\Lambda}$$

Fully Coupled Iterative Method

- Adjoint problem is a linear system

$$\begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_i}}{\partial \rho_j}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho_j}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_j}^T \\ \frac{\partial \mathbf{R}_{\rho_i}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}^T \\ \frac{\partial \mathbf{R}_{\rho_i}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T \end{pmatrix} \begin{pmatrix} \Lambda_{\rho_i} \\ \Lambda_{\rho\mathbf{u}} \\ \Lambda_{\rho E} \end{pmatrix} = - \begin{pmatrix} \frac{\partial f}{\partial \rho_i} \\ \frac{\partial f}{\partial \rho\mathbf{u}} \\ \frac{\partial f}{\partial \rho E} \end{pmatrix}$$

- Can be solved with Krylov method (i.e. GMRES), but time marching similar to flow solver shown to be more robust

$$\left(\frac{V}{\Delta t}\mathbf{I} + \frac{\partial \mathbf{R}_1}{\partial \mathbf{Q}}^T \right) \Delta\Lambda = -\frac{\partial f}{\partial \mathbf{Q}} - \frac{\partial \mathbf{R}_2}{\partial \mathbf{Q}}^T \Lambda$$

- Straightforward to formulate, but cost and memory requirements scale quadratically with number of species

Decoupled Iterative Method

- Rewrite conserved variables similar to decoupled flow solver

$$\begin{pmatrix} \frac{\partial \mathbf{R}_\rho}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho s}}{\partial \rho}^T \\ \frac{\partial \mathbf{R}_\rho}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho s}}{\partial \rho\mathbf{u}}^T \\ \frac{\partial \mathbf{R}_\rho}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho s}}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_\rho}{\partial c_s}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial c_s}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}^T & \frac{\partial \mathbf{R}_{\rho s}}{\partial c_s}^T \end{pmatrix} \begin{pmatrix} \Lambda_\rho \\ \Lambda_{\rho\mathbf{u}} \\ \Lambda_{\rho E} \\ \Lambda_{c_s} \end{pmatrix} = - \begin{pmatrix} \frac{\partial f}{\partial \rho} \\ \frac{\partial f}{\partial \rho\mathbf{u}} \\ \frac{\partial f}{\partial \rho E} \\ \frac{\partial f}{\partial c_s} \end{pmatrix}$$

Decoupled Iterative Method

- Rewrite conserved variables similar to decoupled flow solver

$$\begin{pmatrix} \frac{\partial \mathbf{R}_\rho}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho}^T \\ \frac{\partial \mathbf{R}_\rho}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho\mathbf{u}}^T \\ \frac{\partial \mathbf{R}_\rho}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_\rho}{\partial c_s}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial c_s}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}^T & \frac{\partial \mathbf{R}_{\rho_s}}{\partial c_s}^T \end{pmatrix} \begin{pmatrix} \Lambda_\rho \\ \Lambda_{\rho\mathbf{u}} \\ \Lambda_{\rho E} \\ \Lambda_{c_s} \end{pmatrix} = - \begin{pmatrix} \frac{\partial f}{\partial \rho} \\ \frac{\partial f}{\partial \rho\mathbf{u}} \\ \frac{\partial f}{\partial \rho E} \\ \frac{\partial f}{\partial c_s} \end{pmatrix}$$

- Recognize that there is an analogue to the species mass equation decoupling used in the flow solver
- Linear system can be decomposed as block jacobi scheme

Decoupled Iterative Method

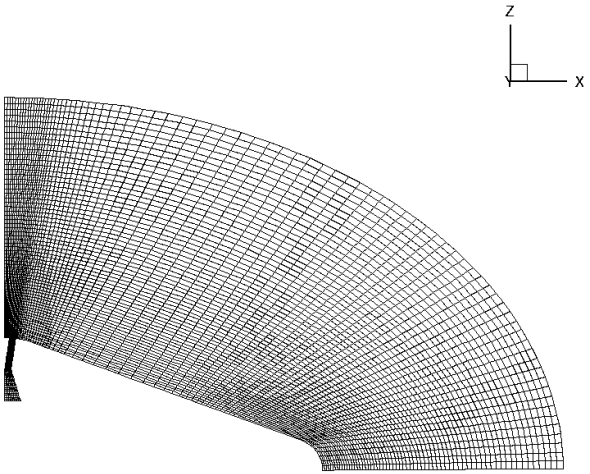
- Separate into two systems and solve as block jacobi scheme

$$\left(\frac{V}{\Delta t}\mathbf{I}+\frac{\partial \mathbf{R}_{\rho_s}}{\partial c_s}^T\right)\Delta\Lambda_{c_s}=-\frac{\partial f}{\partial c_s}-\frac{\partial \mathbf{R}_{\rho_s}}{\partial c_s}^T\Lambda_{c_s}-\frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho}^T\Lambda_{\rho}-\frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho\mathbf{u}}^T\Lambda_{\rho\mathbf{u}}-\frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho E}^T\Lambda_{\rho E}$$

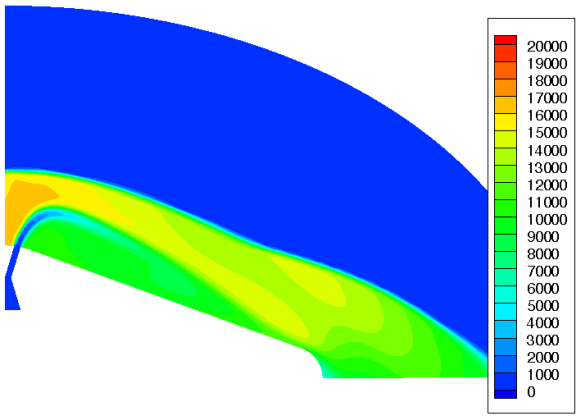
$$\begin{aligned}\left[\frac{V}{\Delta t}\mathbf{I}+\begin{pmatrix}\frac{\partial \mathbf{R}_{\rho}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho E}^T\\ \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}^T\\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T\end{pmatrix}\right]\begin{pmatrix}\Delta\Lambda_{\rho}\\ \Delta\Lambda_{\rho\mathbf{u}}\\ \Delta\Lambda_{\rho E}\end{pmatrix}=\\ -\begin{pmatrix}\frac{\partial f}{\partial \rho}\\ \frac{\partial f}{\partial \rho\mathbf{u}}\\ \frac{\partial f}{\partial \rho E}\end{pmatrix}-\begin{pmatrix}\frac{\partial \mathbf{R}_{\rho}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho E}^T\\ \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}^T\\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T\end{pmatrix}\begin{pmatrix}\Lambda_{\rho}\\ \Lambda_{\rho\mathbf{u}}\\ \Lambda_{\rho E}\end{pmatrix}-\begin{pmatrix}\frac{\partial \mathbf{R}_{\rho}}{\partial c_s}^T\\ \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial c_s}^T\\ \frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}^T\end{pmatrix}\Lambda_{c_s}\end{aligned}$$

Outline

Design Problem: Hypersonic Retro Propulsion Vehicle



Annular nozzle mesh



Temperature Contour

- Apply adjoint to design Reaction Control System (RCS) jet system to shape shock interaction to maintain maximum drag at minimum surface temperature
- This annular nozzle configuration has been shown to have a steady solution for inviscid flow

Design Problem: Parameterization

- Design sensitivities given by

$$\frac{\partial L}{\partial \mathbf{D}} = \left\{ \frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \frac{\partial f}{\partial \mathbf{X}} \right\} + \left\{ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \right\} \mathbf{\Lambda}$$

- Define cost functions $=> f$
  - Total vehicle drag (with and without jet thrust contribution)
  - Total vehicle surface temperature (in lieu of heating, since these are inviscid simulations)
- Define design parameters $=> \mathbf{D}$
  - Plenum pressure
  - Plenum temperature
  - Jet placement and geometry
- Define mesh parameters $=> \mathbf{X}$
  - Custom grid generation utility
  - Faciliate all grid dependencies by wrapping in complex variables

Design Problem: Grid Generation and Governing Equations

- Grid generation tool provides straightforward way to get mesh sensitivities
  - All parameters can be perturbed by a complex source term, and jacobian calculated via frechet derivatives
  - Structured mesh generation is fast and robust
  - Easy to convert to unstructured grid accepted by FUN3D
- Propose to limit research to inviscid flow, due to large jump in complexity going to full Navier-Stokes
  - Decoupled approach changes very little with addition of viscous terms
  - Viscous terms considerably more exhausting to implement
  - Grid generation process significantly more complicated
  - Scope of research is to demonstrate the new decoupled formulation for flow and adjoint solvers

Outline

Concluding Remarks - Summary of work

- Completed work
  - Derivation of decoupled method for Roe FDS in adjoint and flow solver
  - Implementation/verification of decoupled scheme in flow solver
  - Exact linearization of 2nd-order Roe FDS scheme and chemical source term for both fully coupled and decoupled methods
  - Implementation of fully coupled adjoint scheme for inviscid flow
- Proposed work
  - Implementation of decoupled adjoint scheme
  - Optimization of Hypersonic Retro Propulsion configuration using fully coupled and decoupled schemes for inviscid flow and adjoint solvers

Concluding Remarks

- Design problem provides good testbed for a truly unique hypersonic application
  - Parameterization is well defined
  - Non-linearity of design space is a concern
  - Optimal steady solution exists?
- Decoupling the species equations yield impressive benefits at minimal cost in robustness
  - 2 times faster and 1/3 required memory for both 2D Cylinder and Sphere-Cone 11-species cases
  - Convergence issues at very high velocities can be offset by scaling source term as solution progresses
- Decoupled adjoint approach is a significant improvement to the state of the art
  - Preliminary testing has shown that memory overhead in adjoint is significantly reduced with decoupled scheme
  - Can expect speedup in adjoint solve similar to flow solve

Acknowledgements

- Thanks to the FUN3D team at NASA Langley Research Center, for their support in integrating aspects of the compressible gas path into the reacting gas path of FUN3D.
- Thanks to the Entry Systems Modeling Project within the NASA Game Changing Development Program for their funding and support of this research.

References I

References II

References III


Candler, G. V., Subbareddy, P. K., and Nompelis, I. "Decoupled Implicit Method for Aerothermodynamics and Reacting Flows". In: *AIAA Journal* 51.5 (2013), pp. 1245–1254.


Copeland, S. R., Palacios, F., and Alonso, J. J. "Adjoint-Based Aerothermodynamic Shape Design of Hypersonic Vehicles in Non-Equilibrium Flows". In: *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, 2014.


Esfahani, M. K. and Houzeaux, G. "Implementation of discrete adjoint method for parameter sensitivity analysis in chemically reacting flows". In: *57th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*. American Institute of Aeronautics and Astronautics, 2016.

References IV


Lockwood, B. et al. "Uncertainty Quantification in Viscous Hypersonic Flows using Gradient Information and Surrogate Modeling". In: *49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition*. American Institute of Aeronautics and Astronautics, 2011.


Müller, J.-D. and Cusdin, P. "On the performance of discrete adjoint CFD codes using automatic differentiation". In: *International Journal for Numerical Methods in Fluids* 47.8-9 (2005), pp. 939–945.

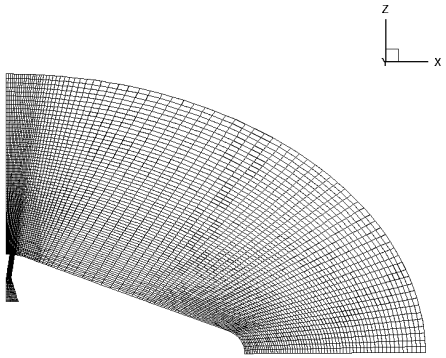

Nielsen, E. J. et al. "An implicit, exact dual adjoint solution method for turbulent flows on unstructured grids". In: *Computers & Fluids* 33.9 (2004), pp. 1131–1155.


Peter, J. E. and Dwight, R. P. "Numerical sensitivity analysis for aerodynamic optimization: A survey of approaches". In: *Computers & Fluids* 39.3 (2010), pp. 373–391.

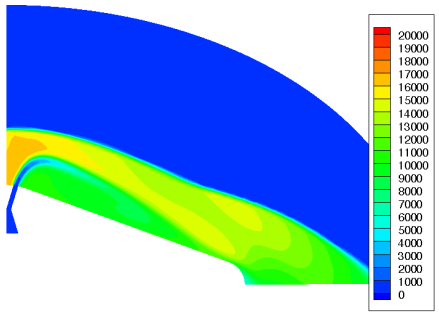
References V

Sankaran, V. and Olsen, M. "Stability Analysis of Fully-Coupled and Loosely-Coupled Schemes for Combustion CFD". In: *16th AIAA Computational Fluid Dynamics Conference*. 2003.

Design Problem: Hypersonic Retro Propulsion Vehicle



Annular nozzle mesh



Temperature Contour

- Benefits of using RCS jet shape shock interaction to maintain maximum drag at minimum surface temperature
  - **Lower total mass**: Jet propellent mass is less than equivalent TPS material required
  - **Lower surface temperature**: Jet stream "shrouds" surface in cooler pocket
  - **Higher total drag**: Jet could propel combustable gas (i.e. methane) to ignite in shock layer and increase drag

Backup: Derivation

- For the Roe flux difference splitting scheme, the species mass fluxes are given by

$$F_{\rho_s} = \frac{\rho_s^L \mathbf{U}^L + \rho_s^R \mathbf{U}^R}{2} - \frac{\tilde{c}_s(\lambda_1 dv_1 + \lambda_2 dv_2) + \lambda_3 dv_{3_s}}{2}$$

$$dv_1 = \frac{p^R - p^L + \tilde{\rho}\tilde{a}(\mathbf{U}^R - \mathbf{U}^L)}{\tilde{a}^2}$$

$$dv_2 = \frac{p^R - p^L - \tilde{\rho}\tilde{a}(\mathbf{U}^R - \mathbf{U}^L)}{\tilde{a}^2}$$

$$dv_{3_s} = \frac{\tilde{a}^2(\rho_s^R - \rho_s^L) - \tilde{c}_s(p^R - p^L)}{\tilde{a}^2}$$

$$\lambda_1 = \mid \tilde{\mathbf{U}} + \tilde{a} \mid, \quad \lambda_2 = \mid \tilde{\mathbf{U}} - \tilde{a} \mid, \quad \lambda_3 = \mid \tilde{\mathbf{U}} \mid$$

Backup: Derivation

- The $\tilde{}$ notation signifies a Roe-averaged quantity

$$\tilde{\mathbf{U}} = wU^L + (1-w)\mathbf{U}^R$$

$$w = \frac{\tilde{\rho}}{\tilde{\rho} + \rho^R}$$

$$\tilde{\rho} = \sqrt{\rho^R \rho^L}$$

- The species mass fluxes must sum to the total mass flux

$$F_\rho = \sum_s F_{\rho_s} = \frac{\rho^L \mathbf{U}^L + \rho^R \mathbf{U}^R}{2} - \frac{\tilde{c}_s(\lambda_1 dv_1 + \lambda_2 dv_2) + \lambda_3 dv_3}{2}$$

$$dv_3 = \frac{\tilde{a}^2(\rho^R - \rho^L) - (p^R - p^L)}{\tilde{a}^2}$$

Backup: Derivation

- Substituting back into species mass flux equation

$$F_{\rho_s} = \tilde{c}_s F_\rho + \frac{(c_s^L - \tilde{c}_s)\rho^L(\mathbf{U}^L + \mid \tilde{\mathbf{U}} \mid)}{2} + \frac{(c_s^R - \tilde{c}_s)\rho^R(\mathbf{U}^R - \mid \tilde{\mathbf{U}} \mid)}{2}$$

- This can be simplified to yield a form similar to that derived by Candler, et. al for the Steger-Warming scheme

$$F_{\rho_s} = \tilde{c}_s F_\rho + (c_s^L - \tilde{c}_s)\rho^L \lambda^+ + (c_s^R - \tilde{c}_s)\rho^R \lambda^-$$

$$\lambda^+ = \frac{\mathbf{U}^L + \mid \tilde{\mathbf{U}} \mid}{2}, \quad \lambda^- = \frac{\mathbf{U}^R - \mid \tilde{\mathbf{U}} \mid}{2}$$

Backup: Derivation

- Differentiating with respect to the mass fraction, c_s, the left and right state contributions are

$$\frac{\partial F_{\rho_s}}{\partial c_s^L} = wF_\rho + (1-w)\rho^L\lambda^+ - w\rho^R\lambda^-$$
$$\frac{\partial F_{\rho_s}}{\partial c_s^R} = (1-w)F_\rho + (w-1)\rho^L\lambda^+ + w\rho^R\lambda^-$$

- Again, where w is the Roe-averaged density weighting

$$w = \frac{\tilde{\rho}}{\tilde{\rho}+\rho^R}, \quad \tilde{\rho} = \sqrt{\rho^R\rho^L}$$