

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

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Introduction and Motivation

- 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

Introduction and Motivation

- How to compute sensitivity of design variables?
- Direct differentiation approach
 - Navier-Stokes equations can be directly differentiated to yield sensitivity derivatives necessary for gradient-based optimization
 - Requires a minimum of one flow solution for each design variable sensitivity
 - Prohibitively expensive for large number of design parameters
- Adjoint approach
 - 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 and Motivation

- Adjoint-based design optimization has recieved considerable attention in compressible, perfect gas CFD solvers, but very little in reacting flow solvers
- Difficulty of adjoint approach lies in implementing 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
 - Serious memory and computational cost concerns

Introduction and Motivation

- 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 → large memory overhead

Introduction and Motivation

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

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

- Beneficial for adjoint formulation
 - Two smaller systems are considerably easier to linearize
 - Storing jacobian for adjoint solve becomes practical
- Candler, et al. originally derived this for Steger-Warming scheme, this work extends to Roe FDS scheme
 - Candler, G. V., Subbareddy, P. K., and Nompelis, I. "Decoupled Implicit Method for Aerothermodynamics and Reacting Flows." *AIAA Journal*, Vol. 51, no. 5, pp. 1-11, 2013.

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

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

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

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

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

- Which can be thought of more simply as

$$\mathbf{A} \mathbf{u} = \mathbf{b}$$

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

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

Fully-Coupled Point Implicit Method

- Constructing the Jacobian in a fully-coupled fashion results in large, dense block matrices
- 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

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

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

$$\begin{aligned} \delta \hat{\mathbf{U}}^n &= \rho^{n+1} \hat{\mathbf{V}}^{n+1} - \rho^n \hat{\mathbf{V}}^n = \rho^{n+1} \delta \hat{\mathbf{V}}^n + \hat{\mathbf{V}}^n \delta \rho^n \\ \hat{\mathbf{V}} &= (c_1, \dots, c_{ns})^T, c_s = \rho_s / \rho \end{aligned}$$

Decoupled Point Implicit Method

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

$$\begin{aligned}\hat{\mathbf{F}}_{\rho_s} &= c_s \mathbf{F}'_{\rho} + (c_s^L - \tilde{c}_s) \rho^L \lambda^+ + (c_s^R - \tilde{c}_s) \rho^R \lambda^- \\ \frac{\partial \hat{\mathbf{F}}_{\rho_s}}{\partial c_s^L} &= w \mathbf{F}_{\rho} + (1 - w) \rho^L \lambda^+ - w \rho^R \lambda^- \\ \frac{\partial \hat{\mathbf{F}}_{\rho_s}}{\partial c_s^R} &= (1 - w) \mathbf{F}_{\rho} + (w - 1) \rho^L \lambda^+ + w \rho^R \lambda^-\end{aligned}$$

- Jacobian Approximations

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

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

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

$$\begin{aligned} \rho^{n+1} \frac{\delta \hat{\mathbf{V}}^n}{\Delta t} + \frac{1}{V} \sum_f \left(\frac{\partial \hat{\mathbf{F}}^f}{\partial \mathbf{V}^L} \delta \mathbf{V}^L + \frac{\partial \hat{\mathbf{F}}^f}{\partial \hat{\mathbf{V}}^R} \delta \hat{\mathbf{V}}^R \right)^{n,n+1} \mathbf{S}^f - \mathbf{C}^{n,n+1} \delta \mathbf{V}^n \\ = -\frac{1}{V} \sum_f (\hat{\mathbf{F}}^{n,n+1} \cdot \mathbf{S})^f + \mathbf{W}^{n,n+1} - \hat{\mathbf{V}}^n \frac{\delta \rho^n}{\Delta t} - R_\rho \end{aligned}$$

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

- R_ρ is included to preserve $\sum_s c_s = 1$, $\sum_s \delta c_s = 0$.

Derivation

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

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

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

\mathbf{D} = design variables

f = cost function

\mathbf{Q} = flow variables

\mathbf{R} = flow residual

\mathbf{X} = computational grid

$\boldsymbol{\Lambda}$ = costate variables

Derivation

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

\mathbf{D} = design variables

f = cost function

\mathbf{Q} = flow variables

\mathbf{R} = flow residual

\mathbf{X} = computational grid

$\boldsymbol{\Lambda}$ = costate variables

Derivation

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

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

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

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

Fully Coupled Iterative Method

- Adjoint problem is a linear system

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

- 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

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

- Decoupled Iterative Method

- Rewrite conserved variables similar to decoupled flow solver

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

- 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

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

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

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

Cost and Memory Savings of the Decoupled Implicit Problem

- 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

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

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

Cost and Memory Savings of the Decoupled Implicit Problem

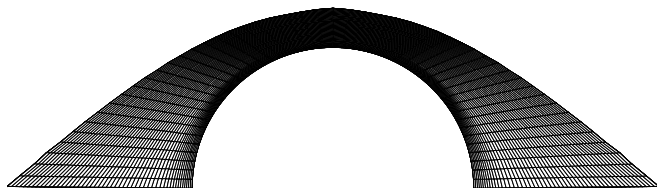
- Comparing size of Jacobian systems, using Compressed Row Storage

\mathbf{A}_d = Decoupled system Jacobians

\mathbf{A} = Fully-coupled system Jacobians

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

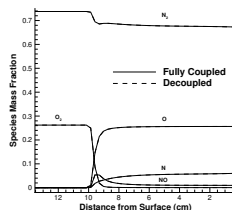
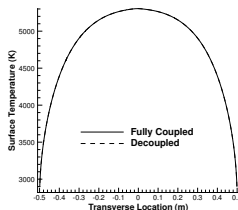
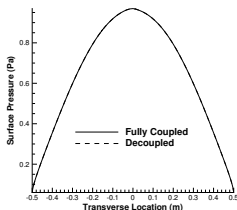
Numerical Results: 2D Cylinder



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

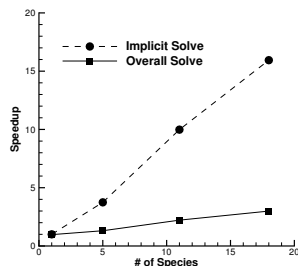
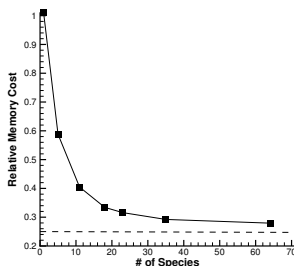
Numerical Results: 2D Cylinder

- Verification of implementation
 - 5-species air model: N, N₂, O, O₂, and NO with five reactions



- Surface pressure and surface temperature agree discretely to 8 significant figures
- Mass fractions on stagnation line agree to 4 significant figures

Numerical Results: 2D Cylinder

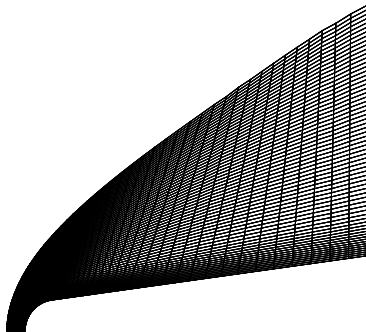


- On structured grids $N_{nbrs} \approx 6N_{nodes}$
 - Half precision off-diagonal $N_{nbrs} = \frac{6N_{nodes}}{2}$

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

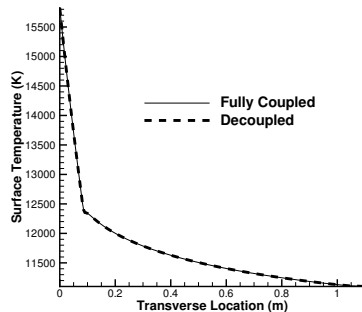
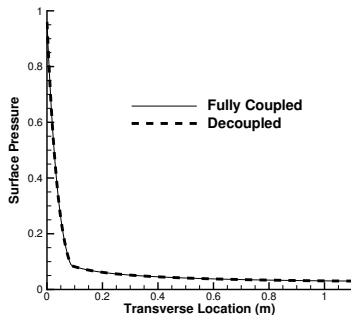
- Linear speedup in solver: $\frac{O(N^2)}{O(N)} = O(N)$

Numerical Results: Axisymmetric Spherically Capped Cone



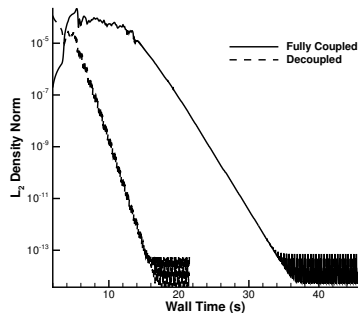
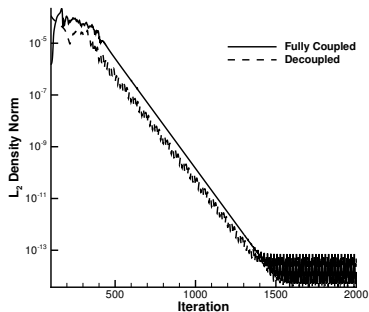
- Verify that the decoupled scheme is robust at high velocities
 - $V_\infty = 15000 \text{ m/s}$, $\rho_\infty = 0.001 \text{ kg/m}^3$, $T_\infty = 200 \text{ K}$.
 - 11-species air model N, N₂, O, O₂, NO, N⁺, N₂⁺, O⁺, O₂⁺, NO⁺, and electrons, with 22 possible reactions.

Numerical Results: Axisymmetric Spherically Capped Cone



- Surface pressure and surface temperature agree discretely to 8 significant figures

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 $\approx 2\times$ faster

Design Problem: Hypersonic SRP Vehicle

Conclusions

- 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
- Improvements valuable for adjoint work
 - Preliminary testing has shown that memory overhead in adjoint is significantly reduced with decoupled scheme
 - Can expect similar speedup in adjoint solve
 - Differences between fully-coupled and decoupled method results may impact adjoint and require further study

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Backup: Derivation

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

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

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

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

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

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

Backup: Derivation

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

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

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

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

- 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

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

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

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

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

Backup: Derivation

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

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

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

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

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