

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

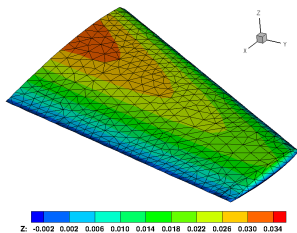
Aerothermodynamics Branch
NASA Langley Research Center

April 20, 2016

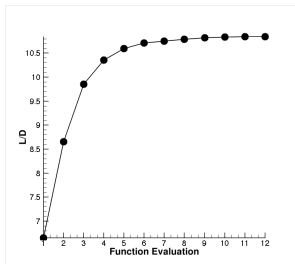
Outline

- 1 Introduction
- 2 Flow Solver
 - Fully-Coupled Method
 - Decoupled Method
- 3 Cost and Memory Savings
 - Cost and Memory Savings of the Decoupled Flow Solver
 - Numerical Results: 2D Cylinder
 - Numerical Results: Axisymmetric Spherically Capped Cone
- 4 Adjoint Solver
 - Derivation of Discrete Adjoint Formulation
 - Fully Coupled Iterative Method
 - Decoupled Iterative Method
- 5 Design Problem
- 6 Concluding Remarks

Introduction - Design



Shape Design Mesh Movement¹



Lift/Drag Objective Function¹

- 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

¹Credit: 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 received considerable attention in compressible, perfect gas CFD solvers^{2,3}, 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
 - Resorting to Automatic Differentiation tools incurs performance overhead that is implementation-specific⁴
 - Serious memory and computational cost concerns when simulating a large number of species

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

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

⁴J.-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 continuous⁵ and discrete⁶ 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 Center⁷ 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

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

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

⁷M. 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 → large memory overhead

Introduction - Decoupled Approach

- Loosely-coupled solvers have become popular in the combustion community⁸
 - Decouple species conservation equations from meanflow equations, and solve two smaller systems

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

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

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

⁹G. 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

- 1 Introduction
- 2 Flow Solver
 - Fully-Coupled Method
 - Decoupled Method
- 3 Cost and Memory Savings
 - Cost and Memory Savings of the Decoupled Flow Solver
 - Numerical Results: 2D Cylinder
 - Numerical Results: Axisymmetric Spherically Capped Cone
- 4 Adjoint Solver
 - Derivation of Discrete Adjoint Formulation
 - Fully Coupled Iterative Method
 - Decoupled Iterative Method
- 5 Design Problem
- 6 Concluding Remarks

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

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

$$= -\frac{1}{V} \sum_f (\mathbf{F}^f \cdot \mathbf{S}^f)^n + \mathbf{W}^n$$

- Which can be thought of more simply as

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

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

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

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

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

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

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

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

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

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

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

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

Outline

- 1 Introduction
- 2 Flow Solver
 - Fully-Coupled Method
 - Decoupled Method
- 3 Cost and Memory Savings
 - Cost and Memory Savings of the Decoupled Flow Solver
 - Numerical Results: 2D Cylinder
 - Numerical Results: Axisymmetric Spherically Capped Cone
- 4 Adjoint Solver
 - Derivation of Discrete Adjoint Formulation
 - Fully Coupled Iterative Method
 - Decoupled Iterative Method
- 5 Design Problem
- 6 Concluding Remarks

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

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

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

Cost and Memory Savings of the Decoupled Flow Solver

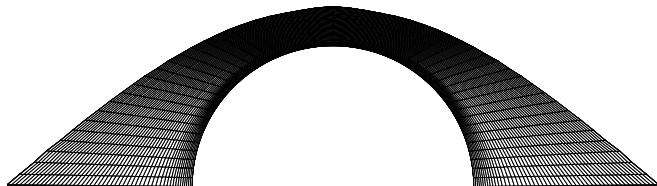
- Comparing size of Jacobian systems, using Compressed Row Storage

\mathbf{A}_d = Decoupled system Jacobians

\mathbf{A} = Fully-coupled system Jacobians

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

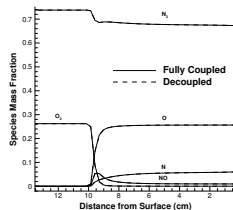
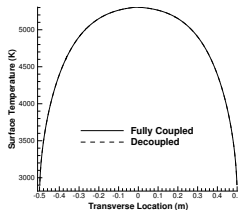
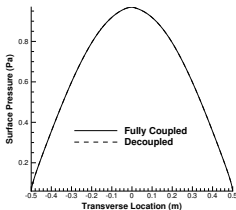
Numerical Results: 2D Cylinder



- 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 $T_{\infty} = 200 \text{ K}$
- Inviscid flow, with 1-Temperature model

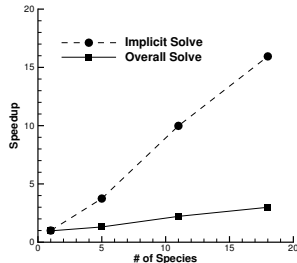
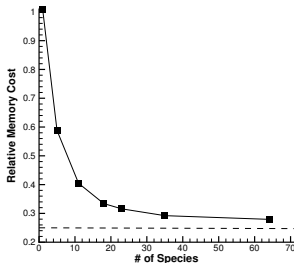
Numerical Results: 2D Cylinder

- Verification of implementation
 - 5-species air model: N, N₂, O, O₂, 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

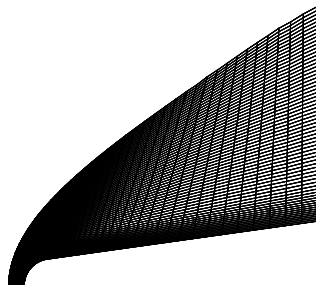


- On structured grids $N_{nbrs} \approx 6N_{nodes}$
 - Half precision off-diagonal $N_{nbrs} = \frac{6N_{nodes}}{2}$

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

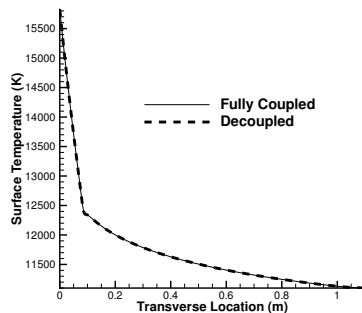
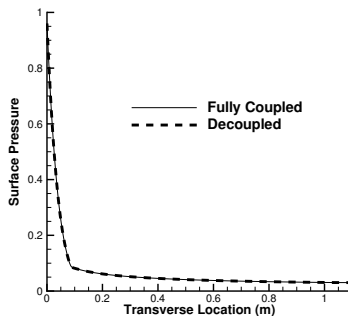
- Linear speedup in solver: $\frac{O(ns^2)}{O(ns)} = O(ns)$

Numerical Results: Axisymmetric Spherically Capped Cone



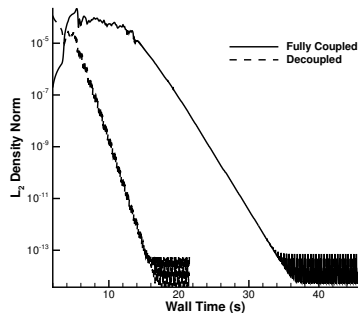
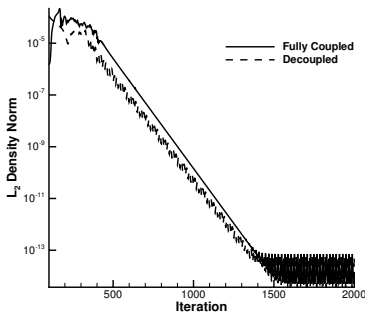
- Verify that the decoupled scheme is robust at high velocities
 - $V_{\infty} = 15000 \text{ m/s}$, $\rho_{\infty} = 0.001 \text{ kg/m}^3$, $T_{\infty} = 200 \text{ K}$.
 - 11-species air model N, N₂, O, O₂, NO, N⁺, N₂⁺, O⁺, O₂⁺, NO⁺, and electrons, with 22 possible reactions.
 - Inviscid flow, with 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 $\approx 2\times$ faster

Outline

- 1 Introduction
- 2 Flow Solver
 - Fully-Coupled Method
 - Decoupled Method
- 3 Cost and Memory Savings
 - Cost and Memory Savings of the Decoupled Flow Solver
 - Numerical Results: 2D Cylinder
 - Numerical Results: Axisymmetric Spherically Capped Cone
- 4 Adjoint Solver
 - Derivation of Discrete Adjoint Formulation
 - Fully Coupled Iterative Method
 - Decoupled Iterative Method
- 5 Design Problem
- 6 Concluding Remarks

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

f = cost function

\mathbf{Q} = flow variables

\mathbf{R} = flow residual

\mathbf{X} = computational grid

$\mathbf{\Lambda}$ = 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

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

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

\mathbf{D} = design variables

f = cost function

\mathbf{Q} = flow variables

\mathbf{R} = flow residual

\mathbf{X} = computational grid

$\boldsymbol{\Lambda}$ = costate variables

Derivation 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

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

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

\mathbf{D} = design variables

f = cost function

\mathbf{Q} = flow variables

\mathbf{R} = flow residual

\mathbf{X} = computational grid

$\boldsymbol{\Lambda}$ = costate variables

Derivation of Discrete Adjoint Formulation

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

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

- 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

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

- 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

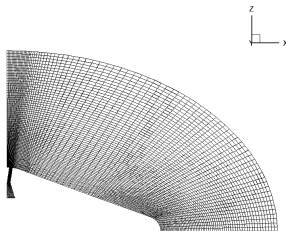
$$\left(\frac{V}{\Delta t} \mathbf{I} + \frac{\partial \mathbf{R}_{\rho s}}{\partial c_s}^T \right) \Delta \Lambda_{c_s} = -\frac{\partial f}{\partial c_s} - \frac{\partial \mathbf{R}_{\rho s}}{\partial c_s}^T \Lambda_{c_s} - \frac{\partial \mathbf{R}_{\rho s}}{\partial \rho}^T \Lambda_{\rho} - \frac{\partial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

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

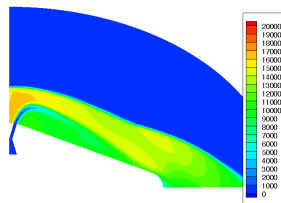
Outline

- 1 Introduction
- 2 Flow Solver
 - Fully-Coupled Method
 - Decoupled Method
- 3 Cost and Memory Savings
 - Cost and Memory Savings of the Decoupled Flow Solver
 - Numerical Results: 2D Cylinder
 - Numerical Results: Axisymmetric Spherically Capped Cone
- 4 Adjoint Solver
 - Derivation of Discrete Adjoint Formulation
 - Fully Coupled Iterative Method
 - Decoupled Iterative Method
- 5 Design Problem
- 6 Concluding Remarks

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

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

- Define cost functions $\Rightarrow f$
 - 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 $\Rightarrow \mathbf{D}$
 - Plenum pressure
 - Plenum temperature
 - Jet placement and geometry
- Define mesh parameters $\Rightarrow \mathbf{X}$
 - Custom grid generation utility
 - Facilitate 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

- 1 Introduction
- 2 Flow Solver
 - Fully-Coupled Method
 - Decoupled Method
- 3 Cost and Memory Savings
 - Cost and Memory Savings of the Decoupled Flow Solver
 - Numerical Results: 2D Cylinder
 - Numerical Results: Axisymmetric Spherically Capped Cone
- 4 Adjoint Solver
 - Derivation of Discrete Adjoint Formulation
 - Fully Coupled Iterative Method
 - Decoupled Iterative Method
- 5 Design Problem
- 6 Concluding Remarks

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

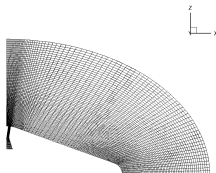
-  Lockwood, B. et al. “Uncertainty Quantification in Viscous Hypersonic Flows using Gradient Information and Surrogate Modeling”. In: *49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition*. American Institute of Aeronautics and Astronautics, 2011.
-  Müller,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

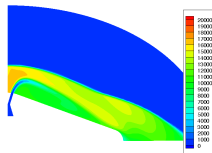


Sankaran, V. and Olsen, M. "Stability Analysis of Fully-Coupled and Loosely-Coupled Schemes for Combustion CFD". In: *16th AIAA Computational Fluid Dynamics Conference*. 2003.

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 propellant mass is less than equivalent TPS material required
 - **Lower surface temperature:** Jet stream “shrouds” surface in cooler pocket
 - **Higher total drag:** Jet could propel combustible 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

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

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

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

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

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

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

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