

ABSTRACT

THOMPSON, KYLE B. A North Carolina State University Sample L^AT_EX Thesis with a Title
So Long it Needs a Line Break. (Under the direction of Hassan Hassan and Peter Gnoffo.)

This is my abstract.

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A North Carolina State University Sample L^AT_EX Thesis
with a Title So Long it Needs a Line Break

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DEDICATION

To my parents and friends.

BIOGRAPHY

The author was born in a small town ...

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I would like to thank my advisor for his help.

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Chapter 1

Introduction

1.1 Flow Solver Decoupled Approach

1.1.1 Introduction

The usability of hypersonic solvers on complex geometries is often limited by the extreme problem size associated with high energy physics. The additional equations required in reacting gas simulations lead to large Jacobians that scale quadratically in size to the number of governing equations. This leads to a significant increase in the memory required to store the flux linearizations and the computational cost of the point solver. As reacting gas CFD solvers are used to solve increasingly more complex problems, this onerous quadratic scaling of computational cost and Jacobian size will ultimately surpass the current limits of hardware and time constraints on achieving a flow solution[2].

The proposed method is based heavily upon the work of Candler et al.[1]. In that work, it was shown that quadratic scaling between the cost of solving the implicit system and adding species mass equations can be reduced from quadratic to linear scaling by decoupling the species mass equations from the mixture mass, momentum, and energy equations and solving the two systems sequentially. In the aforementioned work, the scheme was derived for a modified form of the Steger-Warming flux vector splitting method[6], whereas the work presented here is derived for the Roe flux difference splitting (FDS) scheme[9].

A primary motivator for the presented work is to prepare for the implementation of an adjoint capability in a reacting gas solver that employs the Roe scheme. Developing an adjoint implementation for non-equilibrium flows is an extremely challenging problem, because deriving exact Jacobians for a reacting gas system is particularly difficult. Decoupling the system also simplifies the derivation of exact Jacobians. If the species mass equations are decoupled, the mixture mass, momentum, and energy flux Jacobians can be easily derived[7], and a weighting

scheme can be used to correct the non-uniqueness of the pressure linearization[11]. For the decoupled species fluxes, we derive an exact linearization in the presented work. Future work will include an adjoint-based error estimation capability that leverages these exact linearizations.

1.1.2 Background: Fully-Coupled Point Implicit Method

All work presented here is for the inviscid conservation equations, but it can be extended to include viscous terms. For an inviscid, multi-species mixture, the governing equations in vector form are:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{W} \quad (1.1)$$

or, in semi-discrete form,

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{1}{V} \sum_f (\mathbf{F} \cdot \mathbf{S})^f = \mathbf{W} \quad (1.2)$$

summing over all faces, f , in the domain, where V is the cell volume, \mathbf{W} is the chemical source term vector, and \mathbf{S} is the face outward normal vector. The vectors of conserved variables and fluxes are:

$$\mathbf{U} = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho_1 \bar{U} \\ \vdots \\ \rho_{ns} \bar{U} \\ \rho u \bar{U} + p s_x \\ \rho u \bar{U} + p s_y \\ \rho u \bar{U} + p s_z \\ (\rho E + p) \bar{U} \end{pmatrix} \quad (1.3)$$

where \bar{U} is the outward pointing normal velocity, and E is the total energy of the mixture per unit mass, defined as:

$$E = \sum c_s e_s + \frac{u^2 + v^2 + w^2}{2} \quad (1.4)$$

where e_s is the internal energy of species s . By using the Roe FDS scheme,

$$\mathbf{F}^{n+1} \approx \mathbf{F}^n + \frac{\partial \mathbf{F}}{\partial \mathbf{U}} \delta \mathbf{U}^n \quad (1.5)$$

$$\mathbf{W}^{n+1} \approx \mathbf{W}^n + \frac{\partial \mathbf{W}}{\partial \mathbf{U}} \delta \mathbf{U}^n$$

where $\delta \mathbf{U}^n = \mathbf{U}^{n+1} - \mathbf{U}^n$. By using an implicit time integration, the implicit scheme becomes:

$$\frac{\delta \mathbf{U}^n}{\Delta t} + \frac{1}{V} \sum_f \left(\frac{\partial \mathbf{F}^f}{\partial \mathbf{U}^L} \delta \mathbf{U}^L + \frac{\partial \mathbf{F}^f}{\partial \mathbf{U}^R} \delta \mathbf{U}^R \right)^n \mathbf{S}^f - \frac{\partial \mathbf{W}}{\partial \mathbf{U}} \delta \mathbf{U}^n = -\frac{1}{V} \sum_f (\mathbf{F}^f \cdot \mathbf{S}^f)^n + \mathbf{W}^n \quad (1.6)$$

or, put more simply:

$$A\delta\mathbf{U}^n = \mathbf{b} \quad (1.7)$$

where A is the Jacobian matrix of the fully coupled system, and \mathbf{b} is the residual vector. For a point implicit relaxation scheme, the Jacobian matrix can be split into its diagonal and off-diagonal elements, with the latter moved to the RHS:

$$A = O + D \quad (1.8)$$

Each matrix element is a square $(ns+4) \times (ns+4)$ matrix. One method of solving this system is a Red-Black Gauss-Seidel scheme[10], where matrix coefficients with even indices are updated first and, subsequently, the coefficients with odd indices are updated. This red-black ordering enables better vectorization in solving the linear system. The computational work for the Gauss-Seidel scheme is dominated by matrix-vector multiplications of elements of O with $\delta\mathbf{U}$, which are $O(N^2)$ operations, where $N = ns + 4$. In the next section, it is shown that decoupling the system reduces these matrix-vector multiplications to $O(N^2 + M)$ operations, where $N = ns$ and $M = ns$.

1.1.3 Background: Decoupled Point Implicit Method

If the species mass equations are replaced by a single mixture mass equation, the mixture equations can be separated from the species mass equations and the conserved variables become

$$\mathbf{U}' = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix} \quad \hat{\mathbf{U}} = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \end{pmatrix} \quad (1.9)$$

Solving the flux vector is performed in two sequential steps. The mixture fluxes are first solved as

$$\frac{\partial \mathbf{U}'}{\partial t} + \frac{1}{V} \sum_f (\mathbf{F}' \cdot \mathbf{S})^f = 0 \quad (1.10)$$

followed by the species fluxes as

$$\frac{\partial \hat{\mathbf{U}}}{\partial t} + \frac{1}{V} \sum_f (\hat{\mathbf{F}} \cdot \mathbf{S})^f = \hat{\mathbf{W}} \quad (1.11)$$

Point relaxation uses Red-Black Gauss-Seidel to update the conserved variables in \mathbf{U}' and all associated auxiliary variables, such as temperature, pressure, speed of sound, etc. This is done

by holding the thermo-chemical state constant, and will always result in the relaxation of a five-equation system. This does trade an implicit relationship between the mixture and species equations for an explicit one; thus, this decoupling can have an impact on the stability of the scheme, especially due to the non-linearity of the chemical source term[8].

The solution of the species mass equations takes a different form. Based on the work of Candler et al.[1], the decoupled variables can be rewritten in terms of mass fraction, as follows:

$$\delta \hat{\mathbf{U}}^n = \rho^{n+1} \hat{\mathbf{V}}^{n+1} - \rho^n \hat{\mathbf{V}}^n = \rho^{n+1} \delta \hat{\mathbf{V}}^n + \hat{\mathbf{V}}^n \delta \rho^n \quad (1.12)$$

where $\hat{\mathbf{V}} = (c_1, \dots, c_{ns})^T$, and $c_s = \rho_s / \rho$ the mass fraction of species s . While the derivation of the species mass equations is different for the Roe FVS scheme from that of Steger-Warming proposed by Candler et al.[1], the final result takes a similar form:

$$\hat{F}_{\rho_s} = c_s F'_\rho + (c_s^L - \tilde{c}_s) \rho^L \lambda^+ + (c_s^R - \tilde{c}_s) \rho^R \lambda^- \quad (1.13)$$

where F'_ρ is the total mass flux computed previously using all \mathbf{U}' variables, and $\tilde{\cdot}$ denotes a Roe-averaged quantity. Likewise, linearizing the species mass fluxes with respect to the $\hat{\mathbf{V}}$ variables yields

$$\hat{\mathbf{F}}^{n+1} = \hat{\mathbf{F}}^n + \frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{V}}^L} \delta \hat{\mathbf{V}}^L + \frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{V}}^R} \delta \hat{\mathbf{V}}^R \quad (1.14)$$

$$\frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{V}}^L} = w F_\rho + (1 - w) \rho^L \lambda^+ - w \rho^R \lambda^- \quad (1.15)$$

$$\frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{V}}^R} = (1 - w) F_\rho + (w - 1) \rho^L \lambda^+ + w \rho^R \lambda^- \quad (1.16)$$

A full derivation of Eqs. (1.13-1.16), along with the definition of w , is included in Appendix A. The chemical source term is linearized in the same manner as the fully coupled scheme; however, the updated \mathbf{U}' variables are used to evaluate the Jacobian, and the chain rule is applied to linearize $\hat{\mathbf{W}}$ with respect to the species mass fractions:

$$\hat{\mathbf{W}}^{n+1} = \hat{\mathbf{W}}^n + \frac{\partial \hat{\mathbf{W}}}{\partial \mathbf{U}} \bigg|_{\mathbf{U}'} \frac{\partial \mathbf{U}}{\partial \hat{\mathbf{V}}} \quad (1.17)$$

For simplicity of notation, we define

$$C = \frac{\partial \hat{\mathbf{W}}}{\partial \mathbf{U}} \bigg|_{\mathbf{U}'} \frac{\partial \mathbf{U}}{\partial \hat{\mathbf{V}}} \quad (1.18)$$

The decoupled system to be solved becomes:

$$\rho^{n+1} \frac{\delta \hat{\mathbf{V}}^n}{\Delta t} + \frac{1}{V} \sum_f \left(\frac{\partial \hat{\mathbf{F}}^f}{\partial \hat{\mathbf{V}}^L} \delta \hat{\mathbf{V}}^L + \frac{\partial \hat{\mathbf{F}}^f}{\partial \hat{\mathbf{V}}^R} \delta \hat{\mathbf{V}}^R \right)^{n,n+1} \mathbf{S}^f - C^{n,n+1} \delta \mathbf{V}^n \quad (1.19)$$

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

$$R_\rho = -\frac{1}{V} \sum_f \sum_s (\hat{F}_{\rho_s}^{n,n+1} \cdot \mathbf{S}) \quad (1.20)$$

where R_ρ is included to preserve the constraint that the mass fractions sum to unity, i.e., $\sum_s c_s = 1$, $\sum_s \delta c_s = 0$.

1.1.4 Cost and Memory Savings of the Decoupled Implicit Problem

In decoupling the species equations, the most significant savings comes from the source term linearization being purely node-based[4]. Solving the mean flow equations is conducted in the same manner as the fully coupled system. All entries in the Jacobian A_m are linearizations of the mixture equation fluxes, which results in 5×5 matrices. All entries in the Jacobian A_d are linearizations of the species mass fluxes, which results in $ns \times ns$ matrices. Because there is no interdependence of species, except through the chemical source term, all contributions due to linearizing the convective flux are purely diagonal $ns \times ns$ matrices. Via Eq. (1.8), we decompose A_d into its diagonal and off-diagonal elements, resulting in the following linear system:

$$\begin{pmatrix} \square & & & \\ & \ddots & & \\ & & \square & \\ & & & \ddots \\ & & & & \square \end{pmatrix} \begin{pmatrix} \delta \hat{\mathbf{V}}_1 \\ \vdots \\ \delta \hat{\mathbf{V}}_i \\ \vdots \\ \delta \hat{\mathbf{V}}_{nodes} \end{pmatrix} = \begin{pmatrix} \hat{b}_1 \\ \vdots \\ \hat{b}_i \\ \vdots \\ \hat{b}_{nodes} \end{pmatrix} - \begin{pmatrix} (\sum_{j=1}^{N_{nb}} [\mathcal{N}] \delta \hat{\mathbf{V}}_j)_1 \\ \vdots \\ (\sum_{j=1}^{N_{nb}} [\mathcal{N}] \delta \hat{\mathbf{V}}_j)_i \\ \vdots \\ (\sum_{j=1}^{N_{nb}} [\mathcal{N}] \delta \hat{\mathbf{V}}_j)_{nodes} \end{pmatrix} \quad (1.21)$$

where \square represents a dense $ns \times ns$ matrix, $[\mathcal{N}]$ represents a diagonal matrix, and $\delta \hat{\mathbf{V}}_j$ is the decoupled variable update on the node j that neighbors node i , where N_{nb} is the number of nodes neighboring node i . Thus, the non-zero entries in the off-diagonal matrix can be reduced from diagonal matrices to vectors. This results in significant savings in both computational cost and memory, as the only quadratic operation left in solving the implicit system is dealing with the diagonal entries in the Jacobian. Because the off-diagonal entries significantly outnumber the diagonal entries, we can expect nearly linear scaling in cost with the number of species. If compressed row storage[3] is used to only store non-zero off-diagonal entries, the relative

memory savings in the limit of a large number of species for the Jacobian is given by

$$\begin{aligned}
\text{Relative Memory Cost} &= \frac{\text{size}(A_d)}{\text{size}(A)} \\
&= \lim_{ns \rightarrow \infty} \frac{(ns^2 + 5^2)(N_{nodes}) + (ns + 5^2)(N_{nz})}{(ns + 4)^2(N_{nodes} + N_{nz})} \\
&= \frac{N_{nodes}}{N_{nodes} + N_{nz}}
\end{aligned} \tag{1.22}$$

where N_{nodes} is the number of nodes, and N_{nz} is the number of non-zero off-diagonal entries stored using compressed row storage. For a structured grid, each node has six neighbors in 3D, i.e., $N_{nz} = 6N_{nodes}$; therefore, we can expect the Jacobian memory required to decrease by a factor of seven using this decoupled scheme. Interestingly, for a grid that is not purely hexahedral, $N_{nz} > 6N_{nodes}$; thus, this decoupled scheme provides higher relative memory savings on unstructured grids than structured grids when using compressed row storage.

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APPENDIX

Appendix A

Derivations

A.1 Decoupled Flux Derivation

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

$$F_{\rho_s} = \frac{\rho_s^L \bar{U}^L + \rho_s^R \bar{U}^R}{2} - \frac{\tilde{c}_s(\lambda_1 dv_1 + \lambda_2 dv_2) + \lambda_3 dv_{3_s}}{2} \quad (\text{A.1})$$

$$dv_1 = \frac{p^R - p^L + \tilde{\rho} \tilde{a}(\bar{U}^R - \bar{U}^L)}{\tilde{a}^2} \quad (\text{A.2})$$

$$dv_2 = \frac{p^R - p^L - \tilde{\rho} \tilde{a}(\bar{U}^R - \bar{U}^L)}{\tilde{a}^2} \quad (\text{A.3})$$

$$dv_{3_s} = \frac{\tilde{a}^2(\rho_s^R - \rho_s^L) - \tilde{c}_s(p^R - p^L)}{\tilde{a}^2} \quad (\text{A.4})$$

$$\lambda_1 = |\bar{\mathbf{U}} + \tilde{\mathbf{a}}|, \quad \lambda_2 = |\bar{\mathbf{U}} - \tilde{\mathbf{a}}|, \quad \lambda_3 = |\bar{\mathbf{U}}| \quad (\text{A.5})$$

where the $\tilde{}$ notation signifies a Roe-averaged quantity, given by:

$$\tilde{\mathbf{U}} = w \tilde{\mathbf{U}}^L + (1 - w) \tilde{\mathbf{U}}^R \quad (\text{A.6})$$

$$w = \frac{\tilde{\rho}}{\tilde{\rho} + \rho^R} \quad (\text{A.7})$$

$$\tilde{\rho} = \sqrt{\rho^R \rho^L} \quad (\text{A.8})$$

The species mass fluxes must sum to the total mass flux; thus, the total mixture mass flux is given as

$$F_\rho = \sum_s F_{\rho_s} = \frac{\rho^L \bar{U}^L + \rho^R \bar{U}^R}{2} - \frac{\tilde{c}_s(\lambda_1 dv_1 + \lambda_2 dv_2) + \lambda_3 dv_3}{2} \quad (\text{A.9})$$

$$dv_3 = \frac{\tilde{a}^2(\rho^R - \rho^L) - (p^R - p^L)}{\tilde{a}^2} \quad (\text{A.10})$$

Multiplying Eq. (A.9) by the Roe-averaged mass fraction and substituting it into Eq. (A.1) results in:

$$F_{\rho_s} = \tilde{c}_s F_\rho + \frac{(c_s^L - \tilde{c}_s)\rho^L(\bar{U}^L + |\tilde{U}|)}{2} + \frac{(c_s^R - \tilde{c}_s)\rho^R(\bar{U}^R - |\tilde{U}|)}{2} \quad (\text{A.11})$$

It should be noted here that the Roe-averaged normal velocity, \tilde{U} , requires an entropy correction in the presence of strong shocks[5]. This correction has no dependence on the species mass fractions; therefore, it does not change the form of the Jacobian for this decoupled scheme. The notation can be further simplified by defining the normal velocities as follows:

$$\lambda^+ = \frac{\bar{U}^L + |\tilde{U}|}{2}, \quad \lambda^- = \frac{\bar{U}^R - |\tilde{U}|}{2} \quad (\text{A.12})$$

Finally, substituting Eq. (A.12) into Eq. (A.11) yields the final result for calculating the species flux in the decoupled system:

$$F_{\rho_s} = \tilde{c}_s F_\rho + (c_s^L - \tilde{c}_s)\rho^L \lambda^+ + (c_s^R - \tilde{c}_s)\rho^R \lambda^- \quad (\text{A.13})$$

Forming the convective contributions to the Jacobians is straightforward. Because the \mathbf{U}' level variables are constant, only the left, right, and Roe-averaged state mass fractions vary. Differentiating Eq. (A.13) with respect to the mass fraction, c_s , the left and right state contributions are

$$\frac{\partial F_{\rho_s}}{\partial c_s^L} = w F_\rho + (1 - w)\rho^L \lambda^+ - w\rho^R \lambda^- \quad (\text{A.14})$$

$$\frac{\partial F_{\rho_s}}{\partial c_s^R} = (1 - w)F_\rho + (w - 1)\rho^L \lambda^+ + w\rho^R \lambda^- \quad (\text{A.15})$$

Because there is no dependence between species in decoupled convective formulation, the Jacobian block elements are purely diagonal for the convective contributions, of the form

$$\begin{pmatrix} \frac{\partial F_{\rho_1}}{\partial c_1} & & 0 \\ & \ddots & \\ 0 & & \frac{\partial F_{\rho_{ns}}}{\partial c_{ns}} \end{pmatrix} \quad (\text{A.16})$$