Parameter Sensitivity Analysis for Hypersonic Viscous Flow using a Discrete Adjoint Approach

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Outline

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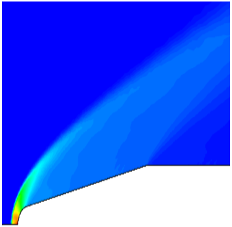
- Introduction
- Overview of Flow Solver and Physical Models
- Solution Scheme Details
- Sensitivity Formulation
- Flow and Sensitivity Results for Perfect Gas Model
- Flow and Sensitivity Results for Real Gas Model
- Conclusion

Introduction

- Simulation of complex problems rely heavily on empirical relations
- Relations can require hundreds of parameters to define
- Sensitivity and uncertainty can enhance analysis and design capability
- Sampling currently used due to nonlinear nature of flows
  - Thousands of flow solutions required
  - Computationally expensive

Introduction

- Localized sensitivity calculated using flow adjoint
- Sensitivity to large number of inputs with cost approximately equal to flow solve
- Possibilities for uncertainty quantification, adaptation and simulation optimization.
- Should be possible to augment weaknesses of sampling with an adjoint based approach



Flow Solver Details

- Navier Stokes Equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \vec{F}(\mathbf{U}) = \nabla \cdot \vec{F}_v(\mathbf{U}) + \mathbf{S}(\mathbf{U}) \quad (1)$$

- Two dimensional, cell-centered finite volume solver using unstructured triangles and/or quadrilaterals
- Solver uses a fully implicit, pseudo-time stepping method
- Perfect gas and Real gas models examined

Physical Model

- Perfect gas variables

$$\mathbf{U} = \left\{ \begin{array}{c} \rho \\ \rho\vec{u} \\ \rho e_t \end{array} \right\} \quad \vec{F} = \left\{ \begin{array}{c} \rho\vec{u} \\ \rho\vec{u}\otimes\vec{u} + P \\ \rho\vec{u}h_t \end{array} \right\} \quad \vec{F_v} = \left\{ \begin{array}{c} 0 \\ \underline{\tau} \\ \underline{\tau}\cdot\vec{u} - \vec{q} \end{array} \right\}$$

- Sutherland's Law used for viscosity
- 5 Parameters required to define model:
  - Ratio of Specific Heats γ
  - Reynolds Number
  - Prandtl Number
  - Two constants within Sutherland's Law

Physical Model

- 5 species, Two Temperature Real Gas Model

$$\mathbf{U} = \left\{ \begin{array}{c} \rho_s \\ \rho\vec{u} \\ \rho e_t \\ \rho e_v \end{array} \right\} \quad \vec{F} = \left\{ \begin{array}{c} \rho_s\vec{u} \\ \rho\vec{u}\otimes\vec{u}+P \\ \rho\vec{u}h_t \\ \rho\vec{u}h_v \end{array} \right\} \quad \mathbf{S} = \left\{ \begin{array}{c} \omega_s \\ 0 \\ 0 \\ \sum_s \omega_s \hat{D}_{v,s} + Q_{T-V} \end{array} \right\}$$

$$\vec{F}_v = \left\{ \begin{array}{c} -\rho_s\tilde{V}_s \\ \underline{\mathcal{T}} \\ \underline{\mathcal{T}}\cdot\vec{u} - \vec{q} - \vec{q}_v - \sum_s h_{t,s}\rho_s\tilde{V}_s \\ -\sum_s h_{v,s}\rho_s\tilde{V}_s - \vec{q}_v \end{array} \right\}$$

- Dunn-Kang chemical kinetics model used
- Transport quantities calculated using curve fits from Blottner *et al*
- Approximately 250 constants required to define physical model

Solver Description

- Solution marched to steady state using implicit pseudo-time stepping
- Method of Lines:

$$\frac{d\mathbf{U}}{dt} + \mathbf{R}(\mathbf{U}) = 0 \tag{2}$$

- BDF1 discretization used for pseudo-time derivative
- Unsteady residual given by:

$$\mathbf{J}(\mathbf{U}^n, \mathbf{U}^{n-1}) = \frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t} + \mathbf{R}(\mathbf{U}^n) \tag{3}$$

- Nonlinear equation $\mathbf{J}(\mathbf{U}^n, \mathbf{U}^{n-1}) = 0$ solved approximately at each time step

Solution Scheme

- Fixed number of inexact Newton iterations performed per time step (~ 10)

$$\delta \mathbf{U}^k = -[P]^{-1}\,\mathbf{J}(\mathbf{U}^k, \mathbf{U}^{n-1}) \qquad (4)$$

$$\mathbf{U}^{k+1} = \mathbf{U}^k + \lambda \delta \mathbf{U}^k \qquad (5)$$

- $[P]$ chosen to approximate $\frac{\partial \mathbf{J}}{\partial \mathbf{U}^k}$, 1st order Van-Leer-Hänel
- Preconditioner matrix and transport quantities calculated once per time step and frozen.
- Global time stepping used for start-up, local time stepping for full convergence
- λ used to keep updates sensible

Spatial Discretization

- Gradient reconstruction of primitives
- Green-Gauss contour integration used to calculate gradients
- Smooth Van Albada Limiter with Pressure Switch used:

$$\Psi_k = max(0, 1 - K\nu_k)\frac{1}{\Delta^-}\frac{({\Delta^+}^2 + \varepsilon^2)\Delta^- + 2{\Delta^-}^2\Delta^+}{{\Delta^+}^2 + 2\Delta^- + \Delta^-\Delta^+ + \varepsilon^2} \quad (6)$$

$$\nu_i = \frac{\sum_k |P_R - P_L|}{\sum_k P_R + P_L} \quad (7)$$

- Face based Gradients calculated using averaging and correction term:

$$\nabla \mathbf{V}_k = \tilde{\nabla \mathbf{V}} + \frac{\mathbf{V}_R - \mathbf{V}_L - \tilde{\nabla \mathbf{V}} \cdot \Delta \vec{T}}{|\Delta \vec{T}|}\frac{\Delta \vec{T}}{|\Delta \vec{T}|} \quad (8)$$

- Inviscid Flux Calculated Using AUSM+UP flux function with Frozen Speed of Sound

Sensitivity Derivation

- Let the objective and constraint have following functional dependence

$$L = L(D, \mathbf{U}(D)) \tag{9}$$
$$\mathbf{R} = \mathbf{R}(D, \mathbf{U}(D)) = 0 \tag{10}$$

- Objective and Constraint may be differentiated using the Chain rule

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial \mathbf{U}} \frac{\partial \mathbf{U}}{\partial D} \tag{11}$$
$$\frac{d\mathbf{R}}{dD} = \frac{\partial \mathbf{R}}{\partial D} + \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \frac{\partial \mathbf{U}}{\partial D} = 0 \tag{12}$$

- Solve Constraint Equation for $\frac{\partial \mathbf{U}}{\partial D}$

Sensitivity Derivation

- Forward Sensitivity Equation Given by:

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} - \frac{\partial L}{\partial \mathbf{U}} \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-1} \frac{\partial \mathbf{R}}{\partial D} \tag{13}$$

- Transpose Equation

$$\frac{dL}{dD}^{T} = \frac{\partial L}{\partial D}^{T} - \frac{\partial \mathbf{R}}{\partial D}^{T} \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-T} \frac{\partial L}{\partial \mathbf{U}}^{T} \tag{14}$$

- Define Flow Adjoint with Equation:

$$\frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{T} \boldsymbol{\Lambda} = -\frac{\partial \mathbf{L}}{\partial \mathbf{U}}^{\mathbf{T}} \tag{15}$$

- Sensitivity Calculated by:

$$\frac{dL}{dD}^{T} = \frac{\partial L}{\partial D}^{T} + \frac{\partial \mathbf{R}}{\partial D}^{T} \boldsymbol{\Lambda} \tag{16}$$

Parameter Sensitivity

- For Model Parameters, D dependence enters through field variables $\boldsymbol{\mu}$

$$L = L(\mathbf{U}(D), \boldsymbol{\mu}(D, \mathbf{U}(D))) \quad (17)$$

$$\mathbf{R} = \mathbf{R}(\mathbf{U}(D), \boldsymbol{\mu}(D, \mathbf{U}(D))) \quad (18)$$

- Sutherland's Law Example

$$\frac{\mu}{\mu_{ref}} = \frac{C_1 T^{3/2}}{T + S} \quad (19)$$

- Forward Sensitivity Equation for Model Parameters

$$\frac{dL}{dD} = \frac{\partial L}{\partial \boldsymbol{\mu}} \frac{\partial \boldsymbol{\mu}}{\partial D} + \left(\frac{\partial L}{\partial \mathbf{U}} + \frac{\partial L}{\partial \boldsymbol{\mu}} \frac{\partial \boldsymbol{\mu}}{\partial \mathbf{U}} \right) \frac{\partial \mathbf{U}}{\partial D} \quad (20)$$

Parameter Sensitivity

- Adjoint Sensitivity Equation for Model Parameters

$$\frac{\partial L}{\partial D}^T = \frac{\partial \boldsymbol{\mu}}{\partial D}^T \left(\frac{\partial L}{\partial \boldsymbol{\mu}}^T + \frac{\partial \mathbf{R}}{\partial \boldsymbol{\mu}}^T \boldsymbol{\Lambda} \right) \tag{21}$$

- Flow Adjoint Found by Solving Equation:

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{U}} + \frac{\partial \mathbf{R}}{\partial \boldsymbol{\mu}} \frac{\partial \boldsymbol{\mu}}{\partial \mathbf{U}} \right]^T \boldsymbol{\Lambda} = - \left(\frac{\partial L}{\partial \mathbf{U}}^T + \frac{\partial \boldsymbol{\mu}}{\partial \mathbf{U}}^T \frac{\partial L}{\partial \boldsymbol{\mu}}^T \right) \tag{22}$$

- Adjoint Equation solved with Defect Correction:

$$[P]^T \delta \boldsymbol{\Lambda}^k = -\frac{\partial L}{\partial \mathbf{U}}^T - \left[\frac{\partial \boldsymbol{\mu}}{\partial \mathbf{U}}^T \frac{\partial \mathbf{R}}{\partial \boldsymbol{\mu}}^T + \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^T \right] \boldsymbol{\Lambda}^k \tag{23}$$

$$\boldsymbol{\Lambda}^{k+1} = \boldsymbol{\Lambda}^k + \delta \boldsymbol{\Lambda}^k \tag{24}$$

Field Variable Sensitivity

- Set $\frac{\partial \boldsymbol{\mu}}{\partial D} = 1$ and $\frac{\partial \boldsymbol{\mu}}{\partial \mathbf{U}} = 0$:

$$\frac{\partial L}{\partial \boldsymbol{\mu}}^T = \frac{\partial L}{\partial \boldsymbol{\mu}}^T + \frac{\partial R}{\partial \boldsymbol{\mu}}^T \boldsymbol{\Lambda}_\mu \tag{25}$$

- Formally, Adjoint Solution with Frozen $\boldsymbol{\mu}$ required:

$$\left[\left.\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)_\mu \right]^T \boldsymbol{\Lambda}_\mu = -\left.\frac{\partial L}{\partial \mathbf{U}}\right)_\mu^T \tag{26}$$

- Field Variables defined throughout domain (at cell centers or face centers)
- May be used for Uncertainty Propagation or Model Adaptation

$$\delta L^2 = \sum_i \frac{\partial L}{\partial \mu_i}^2 \delta \mu_i^2(\mathbf{U}_i) \tag{27}$$

Perfect Gas Results

- 5 km/s cylinder test case
- Fixed Wall temperature
- Results compared against LAURA and FUN2D

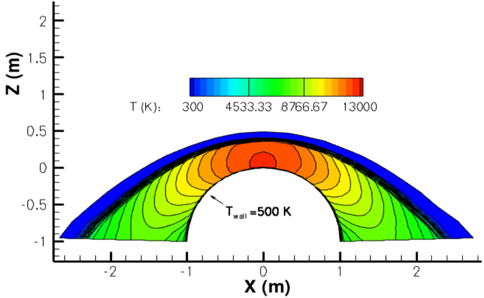
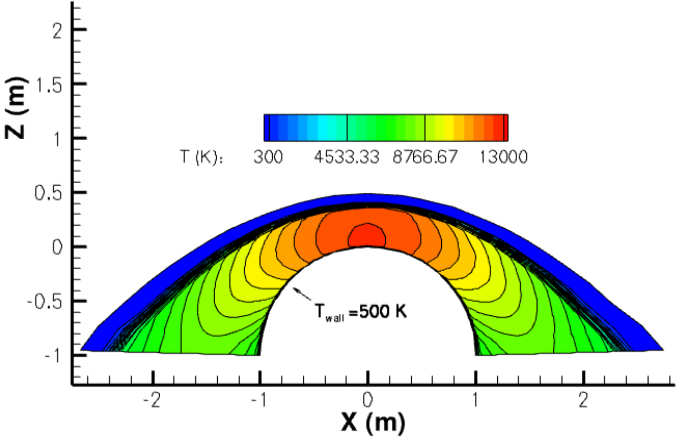


Table: Benchmark Flow Conditions

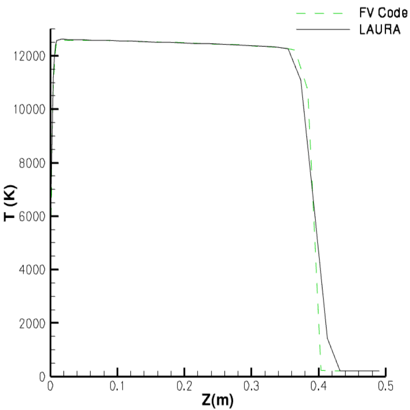
$V_\infty =$	5 km/s
$\rho_\infty =$	0.001 kg/m^3
$T_\infty =$	200 K
$T_{wall} =$	500 K
$M_\infty =$	17.605
$Re_\infty =$	753,860
$Pr_\infty =$	0.72

Perfect Gas Results

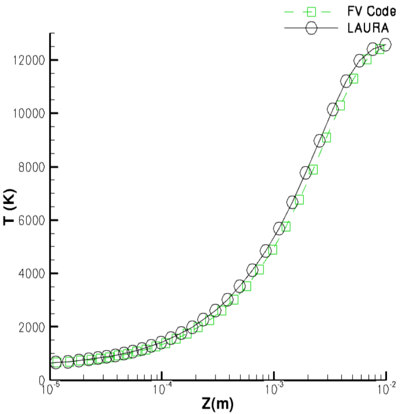


Temperature Contour for 5 km/s case

Perfect Gas Results

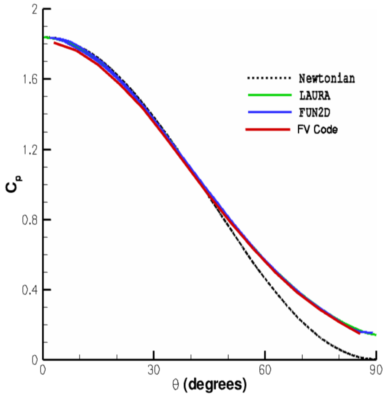


Temperature along Stagnation Streamline

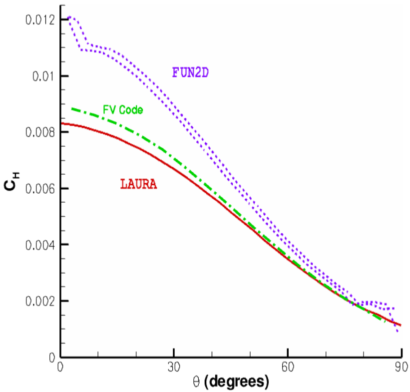


Temperature along Stagnation Streamline(Boundary Layer)

Perfect Gas Results



Surface Pressure Distribution



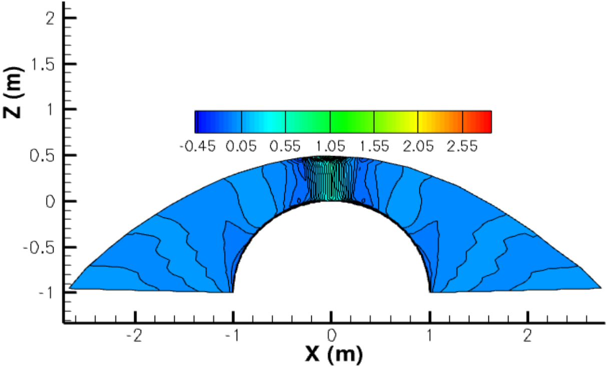
Surface Heating Distribution

Perfect Gas Sensitivity

- Geometric and Parameter Sensitivities for 5 km/s Benchmark Case
- Sensitivities computed for Integrated Surface heating Objective:

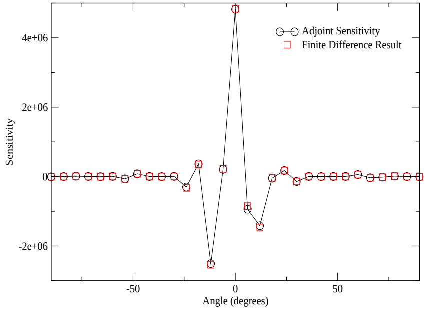
$$L = \int_A -k \nabla T \cdot \vec{n} dA \qquad (28)$$

- Sensitivities Validated using Finite Difference
- Adjoint Solution for Velocity



Geometric Sensitivity

- Sensitivity of Surface Heating to surface geometry calculated
- Normal displacement of surface grid points used as design variable
- 31 total design variables



Heat Flux Sensitivity to Surface Point Displacements

Parameter Sensitivity

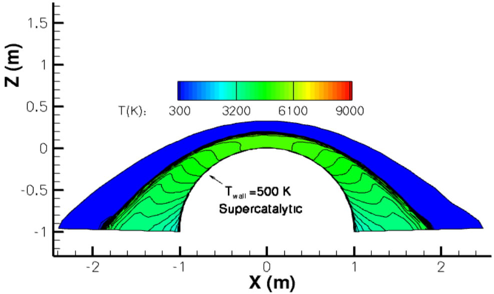
- Sensitivity to Perfect Gas Parameter γ
- Fixed Freestream Velocity and Fixed Freestream Mach Number Considered

Table: Sensitivity of Surface Heating to γ

	Fixed Velocity	Fixed Mach Number
Objective Value	1.628×10^{-2}	1.628×10^{-2}
Finite Difference	-3.111×10^{-2}	-1.198×10^{-2}
Adjoint	-3.109×10^{-2}	-1.206×10^{-2}
Relative Error	7.279×10^{-4}	7.186×10^{-4}

Real Gas Results

- 5 km/s cylinder test case
- Fixed Wall temperature
- Super-catalytic Wall
- Results compared with LAURA



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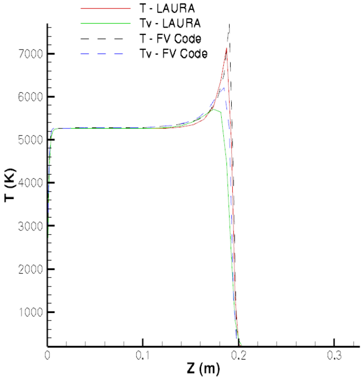
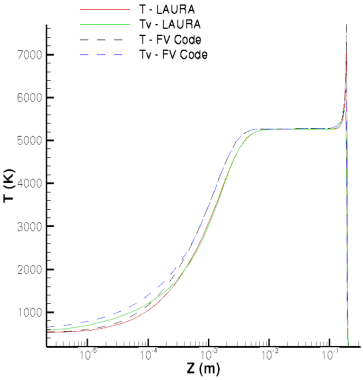
Real Gas Results

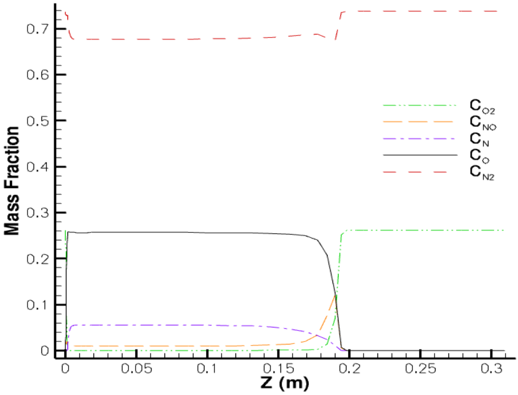


Temperature along Stagnation Streamline



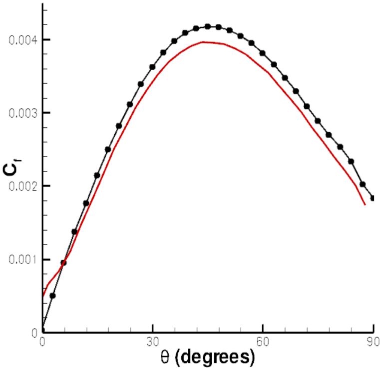
Temperature along Stagnation Streamline (Log Scale)

Real Gas Results

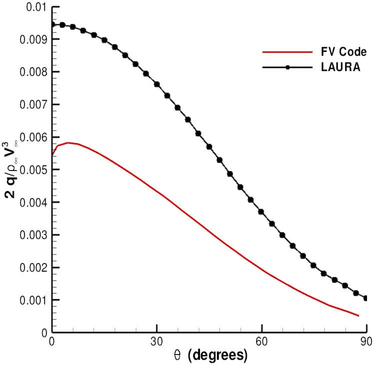


Mass Fraction along Stagnation Streamline for 5 km/s case

Real Gas Results



Skin Friction Distribution



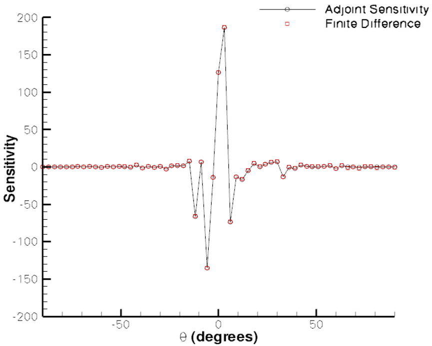
Surface Heating Distribution

Real Gas Sensitivity

- Sensitivities computed for Integrated Surface heating Objective:

$$L = -\int_A k\nabla T \cdot \vec{n} + k_v \nabla T_v \cdot \vec{n} dA \qquad (29)$$

- Sensitivities Validated using Finite Difference
- Geometric Sensitivity, 61 Design Variables



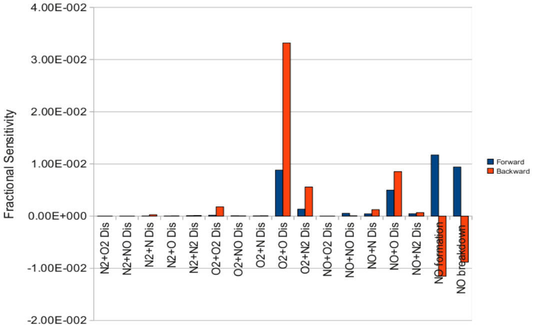
Real Gas Sensitivity

- Sensitivity of Surface Heating to Arrhenius Coefficients:

$$K_f = C_f T_a^{\eta_f} e^{-\frac{E_{a,f}}{kT_a}} \quad (30)$$

$$K_b = C_b T_a^{\eta_b} e^{-\frac{E_{a,b}}{kT_a}} \quad (31)$$

- Sensitivities Expressed as fractional changes (i.e. $\frac{dL/L}{dD/D}$)

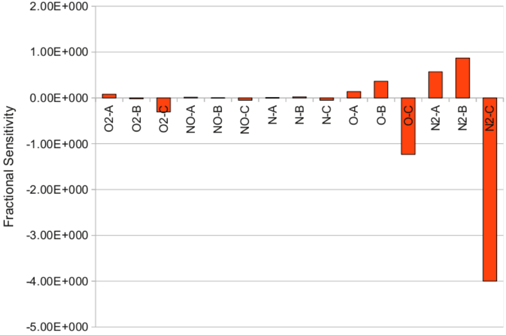


Real Gas Sensitivity

- Sensitivity of Surface Heating to Species Viscosity Curve Fit Parameters:

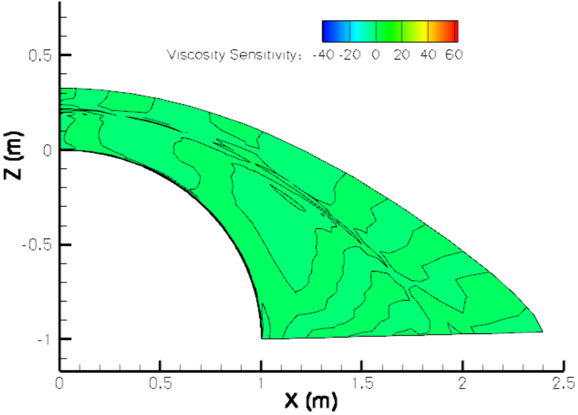
$$\mu_s = 0.1 e^{(A_s ln(T)+B_s) ln(T)+C_s} \tag{32}$$

- Significantly Higher Sensitivity than Reaction Parameters

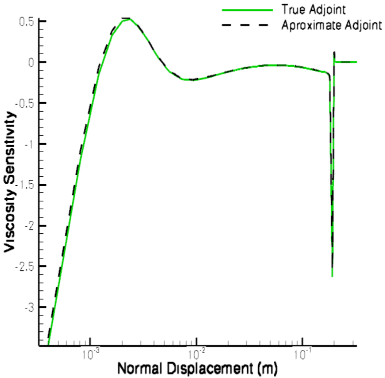


Real Gas Sensitivity

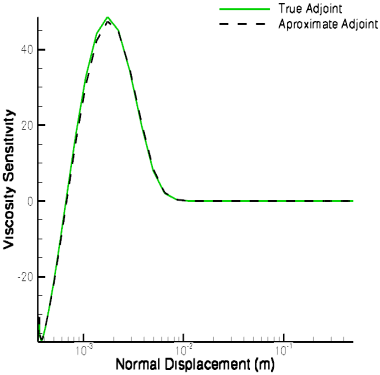
- Sensitivity of Surface Heating to Face-centered Viscosity throughout Domain
- 7800 Faces within Computational Grid
- Exact and Approximate Adjoints used to Compute Sensitivity



Real Gas Sensitivity



Viscosity Sensitivity along Stagnation Streamline



Viscosity Sensitivity at 45 degrees

Conclusions

Conclusions:

- Sensitivity to large number of parameters with minimal effort possible with adjoint
- Parameter sensitivity can be used to determine most important model components
- Field variable sensitivity possible; identifying regions/ranges of greatest importance

Future Work:

- Extend valid range of sensitivities by including higher order terms
- Investigate simulation adaptation using adjoint
- Explore hybrid sensitivity/sampling approaches to uncertainty quantification