A Streamline-Upwind Petrov-Galerkin Finite Element Scheme for Non-Ionized Hypersonic Flows in Thermochemical Nonequilibrium

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1 Background & Motivation

2 Physical Modeling
   - Governing Equations
   - Thermochemistry

3 Finite Element Formulation

4 Results
   - Inviscid Thermal Nonequilibrium Chemically Reacting Flow
   - Viscous Thermal Equilibrium Chemical Reacting Flow

5 Near-term Effort
When chemical kinetic timescales are approximately equal to flow timescales, the chemical composition of a flowfield must be determined as part of a simulation procedure. Such flows are in chemical nonequilibrium.
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• Molecules and atoms can store energy in various modes.
• At hypersonic conditions these modes may not be in equilibrium, resulting in thermal nonequilibrium.

• The physical models and governing equations for flows in thermochemical nonequilibrium have been simulated previously with finite difference and finite volume techniques.
• In this work we review the physical models and implement the first known SUPG finite element scheme for hypersonic flows in thermochemical nonequilibrium.
Governing Equations

- Extension from a single-species calorically perfect gas to a reacting mixture of thermally perfect gases requires species conservation equations and additional energy transport mechanisms.

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla P + \nabla \cdot \mathbf{\tau} \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) &= -\nabla \cdot \dot{q} + \nabla \cdot (\mathbf{\tau} \mathbf{u})
\end{align*}
\]
Governing Equations

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\[
\begin{align*}
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) &= \nabla \cdot (\rho D_s \nabla c_s) + \dot{\omega}_s \\
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \mathbf{u}) &= -\nabla P + \nabla \cdot \mathbf{\tau} \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) &= -\nabla \cdot \dot{\mathbf{q}} + \nabla \cdot (\mathbf{\tau u}) + \nabla \cdot \left( \rho \sum_{s=1}^{n_s} h_s D_s \nabla c_s \right)
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Governing Equations

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\]

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu) = -\nabla P + \nabla \cdot \tau
\]

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H u) = -\nabla \cdot \dot{q} + \nabla \cdot (\tau u) + \nabla \cdot \left( \rho \sum_{s=1}^{n_s} h_s D_s \nabla c_s \right)
\]

- Problem class may also require a multitemperature thermal nonequilibrium option.

\[
\frac{\partial \rho e_V}{\partial t} + \nabla \cdot (\rho e_V u) = -\nabla \cdot \dot{q}_V + \nabla \cdot \left( \rho \sum_{s=1}^{n_s} e_{Vs} D_s \nabla c_s \right) + \dot{\omega}_V
\]
Thermodynamics & Transport Properties

- Thermochemistry models must be extended for a mixture of vibrationally and electronically excited thermally perfect gases.

\[ e^{\text{int}} = e^{\text{trans}} + e^{\text{rot}} + e^{\text{vib}} + e^{\text{elec}} + h^0 \]

\[ = \sum_{s=1}^{ns} c_s e_s^{\text{trans}}(T) + \sum_{s=\text{mol}} c_s e_s^{\text{rot}}(T) + \sum_{s=\text{mol}} c_s e_s^{\text{vib}}(TV) + \sum_{s=1}^{ns} c_s h_s^0 \]

Here we have assumed that \( T^{\text{trans}} = T^{\text{rot}} = T \) and \( T^{\text{vib}} = T^{\text{elec}} = TV \)

- Additional transport property models are required. In this work we use
  - species viscosity given by Blottner curve fits,
  - species conductivities determined from an Eucken relation,
  - mixture transport properties computed via Wilke’s mixing rule, and
  - mass diffusion currently treated by assuming constant Lewis number.
Chemical Kinetics

- We consider $r$ general reactions of the form

\[ \text{N}_2 + \text{M} \rightleftharpoons 2\text{N} + \text{M} \]
\[ \ldots \]
\[ \text{N}_2 + \text{O} \rightleftharpoons \text{NO} + \text{N} \]
\[ \ldots \]

- The reactions are of the form

\[ \mathcal{R}_r = k_{br} \prod_{s=1}^{ns} \left( \frac{\rho_s}{M_s} \right)^{\beta_{sr}} - k_{fr} \prod_{s=1}^{ns} \left( \frac{\rho_s}{M_s} \right)^{\alpha_{sr}} \]

where $\alpha_{sr}$ and $\beta_{sr}$ are the stoichiometric coefficients for reactants and products.

- The source terms are then

\[ \dot{\omega}_s = M_s \sum_{r=1}^{nr} (\alpha_{sr} - \beta_{sr}) (\mathcal{R}_{br} - \mathcal{R}_{fr}) \]
Kinetic Rates

- The forward rate coefficients are defined with a modified Arrhenius law as a function of some temperature $\overline{T}$

$$k_{fr} (\overline{T}) = C_{fr} \overline{T}^{ηr} \exp \left( -\frac{E_{ar}}{R \overline{T}} \right)$$

where the rate constants are determined empirically.

- The corresponding backward rate coefficient can be found using the principle of detailed balance and the equilibrium constant $K_{eq}$

$$K_{eq} = \frac{k_{fr}}{k_{br}}$$

- In thermal equilibrium $\overline{T} = T$. We are currently using CANTERA in this regime.

- In thermal nonequilibrium $\overline{T} = \overline{T}(T, T_V)$ and typical hackery ensues.
Energy Exchange

\[ \dot{\omega}_V = \dot{Q}_v + \dot{Q}_{\text{transfer}} \]
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We adopt the Landau-Teller vibrational energy exchange model

\[ \dot{Q}_{s}^{\text{tr-vib}} = \rho_s \frac{\dot{\hat{e}}_{s}^{\text{vib}} - e_{s}^{\text{vib}}}{\tau_{s}^{\text{vib}}} \]  

(1)

where \( \dot{\hat{e}}_{s}^{\text{vib}} \) is the species equilibrium vibrational energy and the vibrational relaxation time \( \tau_{s}^{\text{vib}} \) is given by Millikan and White

\[ \tau_{s}^{\text{vib}} = \frac{\sum_{r=1}^{n_s} \chi_r}{\sum_{r=1}^{n_s} \chi_r / \tau_{sr}^{\text{vib}}} \quad \chi_r = c_r \frac{M}{M_r} \quad M = \left( \sum_{s=1}^{n_s} \frac{c_s}{M_s} \right)^{-1} \]

and

\[ \tau_{sr}^{\text{vib}} = \frac{1}{P} \exp \left[ A_{sr} \left( T^{-1/3} - 0.015 \mu_{sr}^{1/4} \right) - 18.42 \right] \]

\[ A_{sr} = 1.16 \times 10^{-3} \mu_{sr}^{1/2} \theta_{vs}^{4/3} \quad \mu_{sr} = \frac{M_s M_r}{M_s + M_r} \]
Vibrational Energy Production and Energy Exchange

\[ \dot{\omega}_V = \dot{Q}_v + \dot{Q}_{\text{transfer}} \]
Vibrational Energy Production and Energy Exchange

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When molecular species are created in the gas at rate \( \dot{\omega}_s \), they contribute vibrational/electronic energy at the rate

\[ \dot{Q}_{vs} = \dot{\omega}_s (e_{sv}^{\text{vib}} + e_{sv}^{\text{elec}}) \]

so the net vibrational energy production rate is

\[ \dot{Q}_v = \sum_{s=1}^{ns} \dot{\omega}_s (e_{sv}^{\text{vib}} + e_{sv}^{\text{elec}}) \]  \( \text{(2)} \)
Vibrational Energy Production and Energy Exchange

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\[ \dot{Q}_v = \sum_{s=1}^{ns} \dot{\omega}_s \left( e_{s}^{\text{vib}} + e_{s}^{\text{elec}} \right) \quad (2) \]

Combining (1) and (2) yields the desired net vibrational energy source term

\[ \dot{\omega}_V = \sum_{s=1}^{ns} \dot{Q}_{s}^{\text{tr-vib}} + \sum_{s=1}^{ns} \dot{\omega}_s \left( e_{s}^{\text{vib}} + e_{s}^{\text{elec}} \right) \]
\[ \frac{\partial U}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial G_i}{\partial x_i} + \dot{S} \]
\[
\frac{\partial U}{\partial t} + (A^c_i + A^P_i) \frac{\partial U}{\partial x_i} = \frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial U}{\partial x_j} \right) + \dot{S}
\]
\[
\frac{\partial U}{\partial t} + \left( A^c_i + A^P_i \right) \frac{\partial U}{\partial x_i} = \frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial U}{\partial x_j} \right) + \dot{S}
\]

Find \( U \) satisfying the essential boundary and initial conditions such that

\[
\int_{\Omega} \left[ W \cdot \left( \frac{\partial U}{\partial t} + A^P_i \frac{\partial U}{\partial x_i} - \dot{S} \right) + \frac{\partial W}{\partial x_i} \cdot \left( K_{ij} \frac{\partial U}{\partial x_j} - A^c_i U \right) \right] d\Omega + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \tau_{SUPG} \frac{\partial W}{\partial x_k} \cdot A_k \left[ \frac{\partial U}{\partial t} + A_i \frac{\partial U}{\partial x_i} - \frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial U}{\partial x_j} \right) - \dot{S} \right] d\Omega
\]

\[
+ \sum_{e=1}^{n_{el}} \int_{\Omega_e} \nu \left( \frac{\partial W}{\partial x_i} \cdot g^{ij} \frac{\partial U}{\partial x_j} \right) d\Omega - \oint_{\Gamma} W \cdot (g - f) d\Gamma = 0
\]

for all \( W \) in an appropriate function space.
Stabilization Parameters

\[
\nu = \left[ \frac{\left\| \frac{\partial \textbf{U}}{\partial t} + \textbf{A}_i \frac{\partial \textbf{U}}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \textbf{K}_{ij} \frac{\partial \textbf{U}}{\partial x_j} \right) \right\|^2_{\textbf{A}_0^{-1}}}{(\Delta \textbf{U}_h)^T \textbf{A}_0^{-1} \Delta \textbf{U}_h + g^{ij} \left( \frac{\partial \textbf{U}_h}{\partial x_i} \right)^T \textbf{A}_0^{-1} \frac{\partial \textbf{U}_h}{\partial x_j}} \right]^{1/2}
\]

\[\boldsymbol{\tau}_{\text{SUPG}} = \text{diag} \left( \tau_{c,s}, \tau_{m,j}, \tau_E, \tau_{eV} \right)\]

where \(\tau_{c}, \tau_{m,j}, \tau_E, \) and \(\tau_{eV}\) are given by

\[
\tau_{c,s} = \left[ \left( \frac{2 \left( \| \textbf{u} \| + c \right)}{h_{\text{SUPG}}} \right)^2 + \left( \frac{4D_s}{h_{\text{SUPG}}^2} \right)^2 + \nu^2 \right]^{-1/2}
\]

\[
\tau_{m,j} = \left[ \left( \frac{2 \left( \| \textbf{u} \| + c \right)}{h_{\text{SUPG}}} \right)^2 + \left( \frac{4\mu}{\rho h_{\text{SUPG}}^2} \right)^2 + \nu^2 \right]^{-1/2}
\]

\[
\tau_E = \left[ \left( \frac{2 \left( \| \textbf{u} \| + c \right)}{h_{\text{SUPG}}} \right)^2 + \left( \frac{4k}{\rho c_p h_{\text{SUPG}}^2} \right)^2 + \nu^2 \right]^{-1/2}
\]

\[
\tau_{eV} = \left[ \left( \frac{2 \left( \| \textbf{u} \| + c \right)}{h_{\text{SUPG}}} \right)^2 + \left( \frac{4k_v}{\rho C_{v}^{\text{vib}} h_{\text{SUPG}}^2} \right)^2 + \nu^2 \right]^{-1/2}
\]
Inviscid Cylinder

- Inviscid flow in thermochemical nonequilibrium
- 5 species air ($N_2$, $O_2$, NO, N, O)
- 5 reaction model with Park 1990 rates

\[
c_{N_2,\infty} = 0.78, \quad c_{O_2,\infty} = 0.22
\]
\[
U_\infty = 5,500 \text{ m/sec}
\]
\[
\rho_\infty = 10^{-2} - 10^{-4} \text{ kg/m}^3
\]
\[
T_\infty = 250 \text{ K} = T_{V,\infty}
\]

- Landau-Teller vibrational energy relaxation model, with Millikan and White vibrational relaxation time
Results

Inviscid Thermal Nonequilibrium Chemically Reacting Flow

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SUPG FEM for Thermochem. Noneq. Flows

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Results

Inviscid Thermal Nonequilibrium Chemically Reacting Flow

\[
\begin{align*}
\rho_\infty &= 10^{-2} \text{ kg/m}^3 \\
\rho_\infty &= 10^{-3} \text{ kg/m}^3 \\
\rho_\infty &= 10^{-4} \text{ kg/m}^3
\end{align*}
\]

\[
\tau_{\text{vib}} = 1
\]

\[
P_{\exp} \left[ A_{\text{sr}} (T - 1/3 - 0.015 \mu_{1/4}) - 18.42 \right]
\]

solid: \( T \)

dashed: \( T_V \)
\[ \tau_{sr}^{\text{vib}} = \frac{1}{P} \exp \left[ A_{sr} \left( T^{-1/3} - 0.015 \mu_{sr}^{1/4} \right) - 18.42 \right] \]
2D Extended Cylinder

- Laminar flow in thermal equilibrium
- No-slip, adiabatic, noncatalytic wall
- Chemical nonequilibrium, 5 species air (N₂, O₂, NO, N, O)
- 5 reaction model with Park 1990 rates

\[
\begin{align*}
c_{N_2,\infty} &= 0.78, \\
c_{O_2,\infty} &= 0.22 \\
U_{\infty} &= 6731 \text{ m/sec} \\
\rho_{\infty} &= 6.81 \times 10^{-4} \text{ kg/m}^3 \\
T_{\infty} &= 265 \text{ K}
\end{align*}
\]

- Blottner/Wilke/Eucken with constant Lewis number \( Le = 1.4 \) for transport properties
- Mesh, iterative convergence
- FIN-S/DPLR comparison
- Weak & Strong Scaling
Results

Viscous Thermal Equilibrium Chemical Reacting Flow

**Temperature**

$T (K)$

- $10000$
- $9500$
- $9000$
- $8500$
- $8000$
- $7500$
- $7000$
- $6500$
- $6000$
- $5500$
- $5000$
- $4500$
- $4000$
- $3500$
- $3000$
- $2500$
- $2000$
- $1500$
- $1000$

**Nitrogen Mass Fraction**

$C_{N2}$

- 0.76
- 0.74
- 0.72
- 0.70
- 0.68
- 0.66
- 0.64
- 0.62
- 0.60
- 0.58
- 0.56
- 0.54
- 0.52
- 0.50
- 0.48

**Pressure**

$P (N/m^2)$

- 28000
- 26000
- 24000
- 22000
- 20000
- 18000
- 16000
- 14000
- 12000
- 10000
- 8000
- 6000
- 4000
- 2000

**Nitric Oxide Mass Fraction**

$C_{NO}$

- 0.06
- 0.05
- 0.04
- 0.03
- 0.02
- 0.01
- 0.00

- $U_\infty = 6,731 \, m/s$
- $\rho_\infty = 6.81 \times 10^{-4} \, kg/m^3$
- $T_\infty = 265 \, K$

- $U_\infty = 6,731 \, m/s$
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Mesh Convergence
Iterative Convergence

![Graph showing iterative convergence with time step size and relative transient residual.](image-url)

- **Relative Transient Residual, $|\Delta U/\Delta t|_{\infty}$**
- **Time Step Size, $\Delta t$, (seconds)**

- Lines for different mesh sizes:
  - 100x100
  - 200x200
  - 400x400

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SUPG FEM for Thermochem. Noneq. Flows

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Results

Viscous Thermal Equilibrium Chemical Reacting Flow

Speedup

- Ideal
- Scaled-Size (Weak) Scaling
- Fixed-Size (Strong) Scaling

Number of Processor Cores

Speedup

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Code-to-Code Comparison – Stagnation Line

**Flank Line**

**Stagnation Line**
Code-to-Code Comparison –
Flank Line

Results
Viscous Thermal Equilibrium Chemical Reacting Flow
Additional Focus Areas

1. Physics Modeling
   - Weakly Ionized Flows
   - Surface Catalycity
   - Additional Boundary Conditions

2. Ablation coupling

3. Adjoint
   - Sensitivity analysis
   - Adaptivity
Thank you!

Questions?