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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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- At hypersonic conditions these modes may not be in equilibrium, resulting in \textit{thermal nonequilibrium}.
• 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.

• 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.

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \, u) = 0 \]
\[ \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu) = -\nabla P + \nabla \cdot \tau \]
\[ \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H u) = -\nabla \cdot \dot{q} + \nabla \cdot (\tau u) \]
Governing Equations

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

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

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

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

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

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

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

$$N_2 + M \rightleftharpoons 2N + M$$

$$\ldots$$

$$N_2 + O \rightleftharpoons NO + N$$

$$\ldots$$

- 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 $\bar{T}$

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

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 $\bar{T} = T$. We are currently using CANtera in this regime.

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

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

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We adopt the Landau-Teller vibrational energy exchange model

\[ \dot{Q}_s^{\text{tr-vib}} = \rho_s \frac{\hat{e}_s^{\text{vib}} - e_s^{\text{vib}}}{\tau_s^{\text{vib}}} \] (1)

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

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

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

\[ \dot{\omega}_V = \dot{Q}_v + \dot{Q}_{\text{transfer}} \]

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

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

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

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

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

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

\[
\int_{\Omega} \left[ W \cdot \left( \frac{\partial U}{\partial t} + A_i^p \frac{\partial U}{\partial x_i} - \dot{S} \right) + \frac{\partial W}{\partial x_i} \cdot \left( K_{ij} \frac{\partial U}{\partial x_j} - A_i^c U \right) \right] \, d\Omega \\
+ \sum_{e=1}^{n_{el}} \int_{\Omega_e} \tau_{\text{SUPG}} \frac{\partial W}{\partial x_k} \cdot A_k \left[ \frac{\partial U}{\partial t} + A_i \frac{\partial U}{\partial x_i} - \frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial U}{\partial x_j} \right) - \dot{S} \right] \, d\Omega \\
+ \sum_{e=1}^{n_{el}} \int_{\Omega_e} \nu \left( \frac{\partial W}{\partial x_i} \cdot g^{ij} \frac{\partial U}{\partial x_j} \right) \, d\Omega - \int_{\Gamma} W \cdot (g - f) \, d\Gamma = 0
\]

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

\[ \nu = \left[ \frac{\left\| \frac{\partial U}{\partial t} + A_i \frac{\partial U}{\partial x_i} - \frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial U}{\partial x_j} \right) \right\|^2}{A_0^{-1}} \right]^{1/2} \]

\[ (\Delta U_h)^T A_0^{-1} \Delta U_h + g^{ij} \left( \frac{\partial U_h}{\partial x_i} \right)^T A_0^{-1} \frac{\partial U_h}{\partial x_j} \]

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

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

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

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

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

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

$T(K) \times 10^{-3}$

$T_v(K) \times 10^{-3}$
\[ \tau_{sr}^{\text{vib}} = \frac{1}{P} \exp \left[ A_{sr} \left( T^{-1/3} - 0.015 \mu_{sr}^{1/4} \right) - 18.42 \right] \]
2D Extended Cylinder

- Laminar flow in thermal equilibrium
- No-slip, adiabatic, noncatalytic wall
- Chemical nonequilibrium, 5 species air (N\textsubscript{2}, O\textsubscript{2}, NO, N, O)
- 5 reaction model with Park 1990 rates

\[
\begin{align*}
    c_{N_2,\infty} &= 0.78, \\
    c_{O_2,\infty} &= 0.22, \\
    U_\infty &= 6,731 \text{ m/sec}, \\
    \rho_\infty &= 6.81 \times 10^{-4} \text{ kg/m}^3, \\
    T_\infty &= 265 \text{ K}
\end{align*}
\]

- 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

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

![Graph showing iterative convergence of relative transient residual and time step size for different mesh sizes (100x100, 200x200, 400x400).]
Results
Viscous Thermal Equilibrium Chemical Reacting Flow

### Speedup

*Ideal*

*Scaled-Size (Weak) Scaling*

*Fixed-Size (Strong) Scaling*

Number of Processor Cores

- 10
- 1
- 2
- 3

The graph illustrates the speedup for different scenarios of scaling with varying numbers of processor cores.
Code-to-Code Comparison – Stagnation Line

Flank Line

Stagnation Line

Species Mass Fraction

$O_2$

$N_2$

$N$

$O$

$NO$

$\text{FIN-S}$

$\text{DPLR}$

T (K)

Species Mass Fraction

$10^6$

$10^3$

$10^1$

$10^{-1}$

$10^{-2}$

$10^{-3}$

$10^{-6}$
Results

Viscous Thermal Equilibrium Chemical Reacting Flow

Code-to-Code Comparison – Flank Line

Flank Line

Stagnation Line

Species Mass Fraction

FIN-S
DPLR

O$_2$
NO
N
N$_2$

Species Mass Fraction

T (K)

y (m)

10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}

0.1
0.12
0.14
0.16
0.18

FIN-S
DPLR

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SUPG FEM for Thermochem. Noneq. Flows

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Near-term Effort

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?