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

Benjamin S. Kirk, Steven W. Bova, and Ryan B. Bond

NASA Lyndon B. Johnson Space Center

March 23, 2011
Acknowledgments

1. This work was supported in part by the Entry, Descent and Landing Project in the NASA/ESMD Enabling Technology Development and Demonstration Program.

2. This work was supported in part by a cooperative agreement with the Predictive Engineering and Computational Sciences (PECOS) Center at The University of Texas at Austin.
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.
• 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.
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.

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \, u) = 0
\]

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

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H u) = -\nabla \cdot \dot{q} + \nabla \cdot (\tau u)
\]
Governed 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.

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

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s u) = \nabla \cdot (\rho D_s \nabla c_s) + \dot{\omega}_s
\]

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

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

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

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

\[
\begin{align*}
N_2 + M & \rightleftharpoons 2N + M \\
\cdots \\
N_2 + O & \rightleftharpoons NO + N \\
\cdots
\end{align*}
\]

- The reactions are of the form

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

where \( \alpha_{sr} \) and \( \beta_{sr} \) are the stoichiometric coefficients for reactants and products

- The source terms are then

\[
\dot{\omega}_s = M_s \sum_{r=1}^{nr} \left( \alpha_{sr} - \beta_{sr} \right) \left( R_{br} - R_{fr} \right)
\]

Kirk, Bova, Bond
SUPG FEM for Thermochem. Noneq. Flows
March 23, 2011 7 / 25
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

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

We adopt the Landau-Teller vibrational energy exchange model

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

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

\[ \tau_s^\text{vib} = \frac{\sum_{r=1}^{n_s} \chi_r}{\sum_{r=1}^{n_s} \chi_r / \tau_{sr}^\text{vib}} \]

\[ \chi_r = c_r \frac{M}{M_r} \]

\[ M = \left( \sum_{s=1}^{n_s} \frac{c_s}{M_s} \right)^{-1} \]

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

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

so the net vibrational energy production rate is

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

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

so the net vibrational energy production rate is

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

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

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

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.
Finite Element Formulation

Stabilization Parameters

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

\[ \tau_{\text{SUPG}} = \text{diag} (\tau_c, \tau_m, \tau_E, \tau_{\text{ev}}) \]

where \( \tau_c, \tau_m, \tau_E, \) and \( \tau_{\text{ev}} \) are given by

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

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

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

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

- Inviscid flow in thermochemical nonequilibrium
- 5 species air (N₂, O₂, 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

Temperature (K)

\[ \text{solid: } T \]
\[ \text{dashed: } T_v \]

\( \rho_\infty = 10^{-2} \text{ kg/m}^3 \)
\( \rho_\infty = 10^{-3} \text{ kg/m}^3 \)
\( \rho_\infty = 10^{-4} \text{ kg/m}^3 \)
\[
\tau_{sR}^{\text{vib}} = \frac{1}{P} \exp \left[ A_{sR} \left( T^{-1/3} - 0.015 \mu_{sR}^{1/4} \right) - 18.42 \right]
\]
2D Extended Cylinder

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

\[
c_{N_2,\infty} = 0.78, \quad c_{O_2,\infty} = 0.22 \\
U_\infty = 6,731 \text{ m/seg} \\
\rho_\infty = 6.81 \times 10^{-4} \text{ kg/m}^3 \\
T_\infty = 265 \text{ K}
\]

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

- **Nitrogen Mass Fraction** $C_{\text{N}_2}$
  - $U_\infty = 6,731$ m/s
  - $\rho_\infty = 6.81 \times 10^{-4}$ kg/m$^3$
  - $T_\infty = 265$ K

- **Nitric Oxide Mass Fraction** $C_{\text{NO}}$
  - $U_\infty = 6,731$ m/s
  - $\rho_\infty = 6.81 \times 10^{-4}$ kg/m$^3$
  - $T_\infty = 265$ K
Mesh Convergence
Iterative Convergence
Results

Viscous Thermal Equilibrium Chemical Reacting Flow

Speedup

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

Number of Processor Cores

Speedup

10

0

10

1

10

2

10

3

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

Kirk, Bova, Bond

SUPG FEM for Thermochem. Noneq. Flows

March 23, 2011

21 / 25
Code-to-Code Comparison – Stagnation Line

Flank Line

Stagnation Line

FIN-S

DPLR

Species Mass Fraction

$O_2$

$N_2$

$N$

$O$

$NO$
Code-to-Code Comparison –
Flank Line
Additional Focus Areas

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

2. Ablation coupling

3. Adjoint
   - Sensitivity analysis
   - Adaptivity

Primal & Dual Error

Combined QoI Error
Thank you!

Questions?