



PECOS

Predictive Engineering and Computational Sciences

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



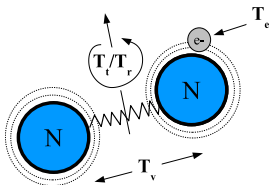
Acknowledgments

- 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

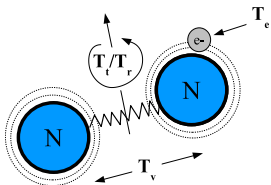
- When chemical kinetic timescales are approximately equal to flow timescales, the chemical composition of a flowfield must be determined as part of a simulation procedure. Such flows are in *chemical nonequilibrium*.

- 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.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \boldsymbol{\tau}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) = -\nabla \cdot \dot{\mathbf{q}} + \nabla \cdot (\boldsymbol{\tau} \mathbf{u})$$

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.

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) = \nabla \cdot (\rho \mathcal{D}_s \nabla c_s) + \dot{\omega}_s$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \boldsymbol{\tau}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) = -\nabla \cdot \dot{\mathbf{q}} + \nabla \cdot (\boldsymbol{\tau} \mathbf{u}) + \nabla \cdot \left(\rho \sum_{s=1}^{ns} h_s \mathcal{D}_s \nabla c_s \right)$$

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.

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}) = \nabla \cdot (\rho \mathcal{D}_s \nabla c_s) + \dot{\omega}_s$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \boldsymbol{\tau}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) = -\nabla \cdot \dot{\mathbf{q}} + \nabla \cdot (\boldsymbol{\tau} \mathbf{u}) + \nabla \cdot \left(\rho \sum_{s=1}^{ns} h_s \mathcal{D}_s \nabla c_s \right)$$

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

$$\frac{\partial \rho e_V}{\partial t} + \nabla \cdot (\rho e_V \mathbf{u}) = -\nabla \cdot \dot{\mathbf{q}}_V + \nabla \cdot \left(\rho \sum_{s=1}^{ns} e_{V_s} \mathcal{D}_s \nabla c_s \right) + \dot{\omega}_V$$

Thermodynamics & Transport Properties

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

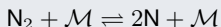
$$\begin{aligned}
 e^{\text{int}} &= e^{\text{trans}} + e^{\text{rot}} + e^{\text{vib}} + e^{\text{elec}} + h^0 \\
 &= \sum_{s=1}^{ns} c_s e_s^{\text{trans}}(T) + \sum_{s=\text{mol}} c_s e_s^{\text{rot}}(T) + \\
 &\quad \sum_{s=\text{mol}} c_s e_s^{\text{vib}}(T_V) + \sum_{s=1}^{ns} c_s e_s^{\text{elec}}(T_V) + \sum_{s=1}^{ns} c_s h_s^0
 \end{aligned}$$

Here we have assumed that $T^{\text{trans}} = T^{\text{rot}} = T$ and $T^{\text{vib}} = T^{\text{elec}} = T_V$

- 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



...



...

- The reactions are of the form

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

where α_{sr} and β_{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}

$$k_{fr}(\bar{T}) = C_{fr} \bar{T}^{\eta_r} \exp(-E_{ar}/R\bar{T})$$

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

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

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

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

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

$$\dot{Q}_{vs} = \dot{\omega}_s (e_s^{\text{vib}} + e_s^{\text{elec}})$$

so the net vibrational energy production rate is

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

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

$$\dot{Q}_{vs} = \dot{\omega}_s (e_s^{\text{vib}} + e_s^{\text{elec}})$$

so the net vibrational energy production rate is

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

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

$$\dot{\omega}_V = \sum_{s=1}^{ns} \dot{Q}_s^{\text{tr-vib}} + \sum_{s=1}^{ns} \dot{\omega}_s (e_s^{\text{vib}} + e_s^{\text{elec}})$$

$$\frac{\partial U}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial G_i}{\partial x_i} + \dot{S}$$

$$\frac{\partial U}{\partial t} + (\mathbf{A}_i^c + \mathbf{A}_i^P) \frac{\partial U}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\mathbf{K}_{ij} \frac{\partial U}{\partial x_j} \right) + \dot{\mathbf{S}}$$

$$\frac{\partial U}{\partial t} + (\mathbf{A}_i^c + \mathbf{A}_i^P) \frac{\partial U}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\mathbf{K}_{ij} \frac{\partial U}{\partial x_j} \right) + \dot{\mathbf{S}}$$

Find U satisfying the essential boundary and initial conditions such that

$$\begin{aligned} & \int_{\Omega} \left[\mathbf{W} \cdot \left(\frac{\partial U}{\partial t} + \mathbf{A}_i^P \frac{\partial U}{\partial x_i} - \dot{\mathbf{S}} \right) + \frac{\partial \mathbf{W}}{\partial x_i} \cdot \left(\mathbf{K}_{ij} \frac{\partial U}{\partial x_j} - \mathbf{A}_i^c U \right) \right] d\Omega \\ & + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \tau_{\text{SUPG}} \frac{\partial \mathbf{W}}{\partial x_k} \cdot \mathbf{A}_k \left[\frac{\partial U}{\partial t} + \mathbf{A}_i \frac{\partial U}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\mathbf{K}_{ij} \frac{\partial U}{\partial x_j} \right) - \dot{\mathbf{S}} \right] d\Omega \\ & + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \nu \left(\frac{\partial \mathbf{W}}{\partial x_i} \cdot g^{ij} \frac{\partial U}{\partial x_j} \right) d\Omega - \oint_{\Gamma} \mathbf{W} \cdot (\mathbf{g} - \mathbf{f}) d\Gamma = 0 \end{aligned}$$

for all \mathbf{W} in an appropriate function space.

Stabilization Parameters

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

$$\boldsymbol{\tau}_{\text{SUPG}} = \text{diag} (\tau_{c,s}, \tau_{m,j}, \tau_E, \tau_{ev})$$

where $\tau_{c,s}$, $\tau_{m,j}$, τ_E , and τ_{ev} are given by

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

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

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

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

Inviscid Cylinder

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

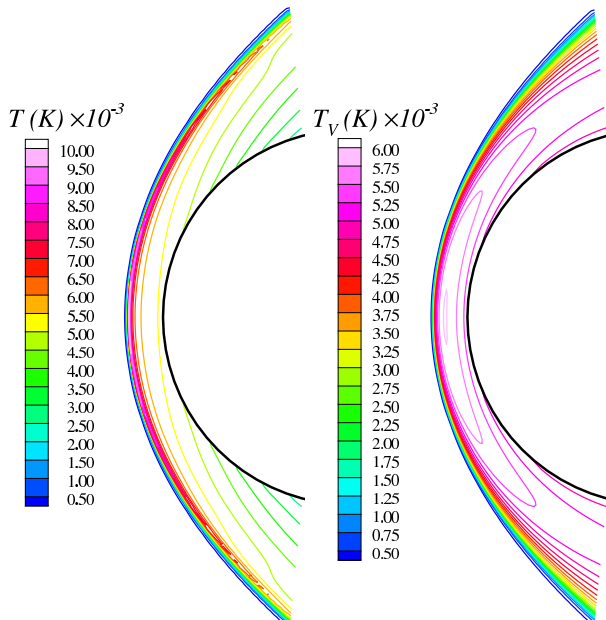
$$cN_{2,\infty} = 0.78, cO_{2,\infty} = 0.22$$

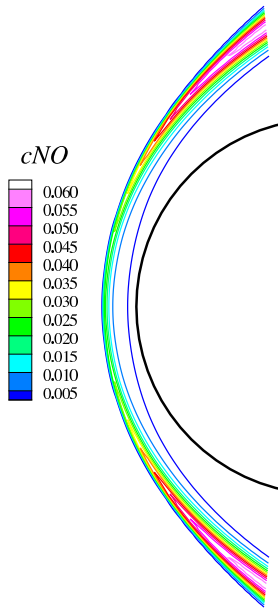
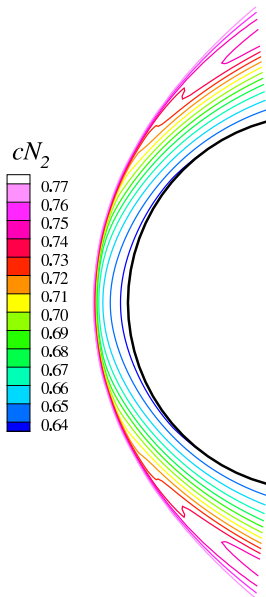
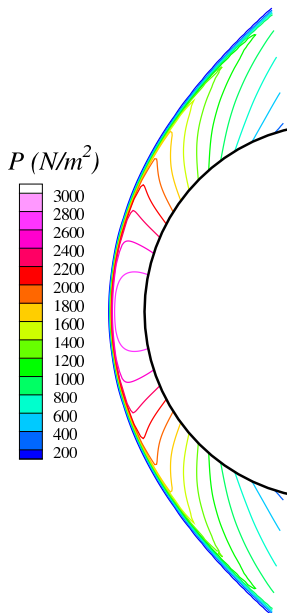
$$U_\infty = 5,500 \text{ m/sec}$$

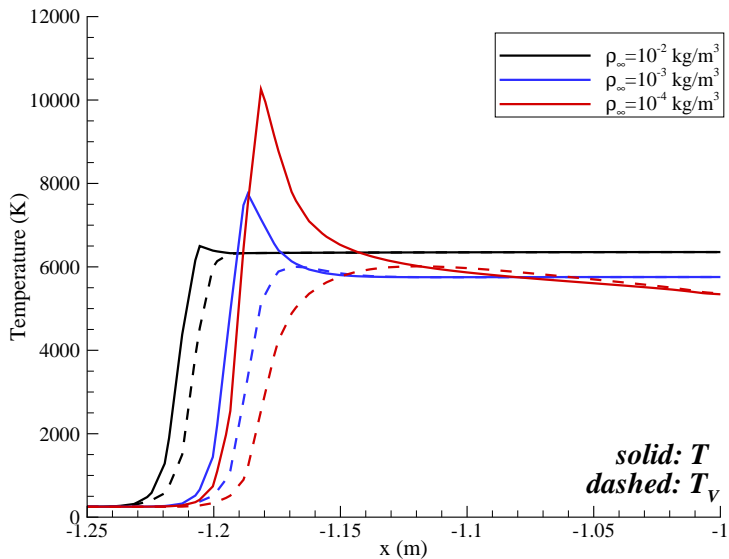
$$\rho_\infty = 10^{-2} - 10^{-4} \text{ kg/m}^3$$

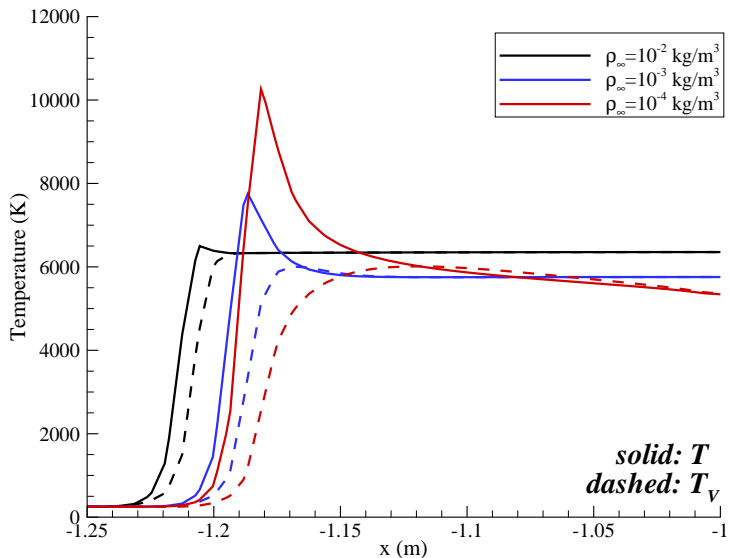
$$T_\infty = 250 \text{ K} = T_{V,\infty}$$

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









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

2D Extended Cylinder

- Laminar flow in thermal equilibrium
- No-slip, adiabatic, noncatalytic wall
- Chemical nonequilibrium, 5 species air (N_2 , O_2 , NO , N , O)
- 5 reaction model with Park 1990 rates

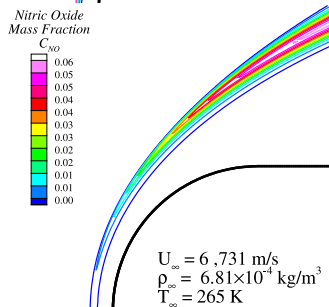
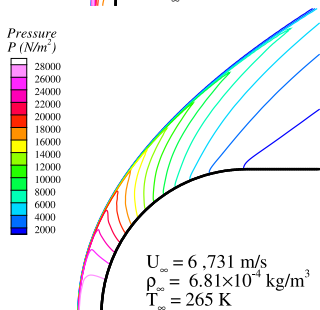
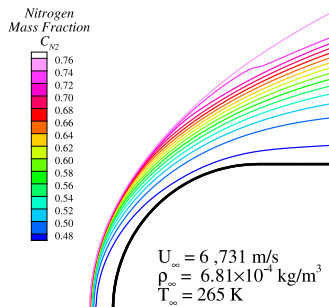
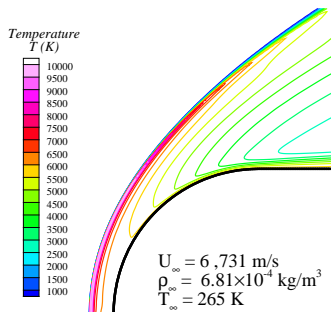
$$cN_{2,\infty} = 0.78, cO_{2,\infty} = 0.22$$

$$U_{\infty} = 6,731 \text{ m/sec}$$

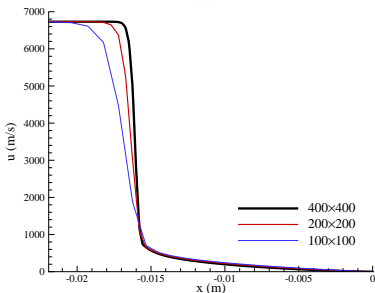
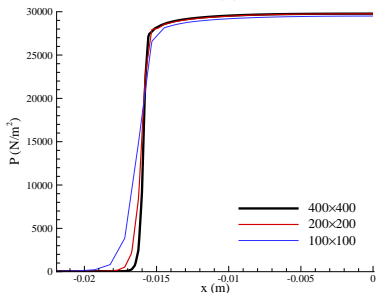
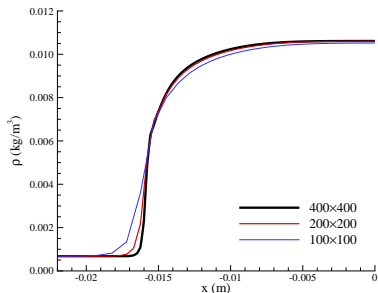
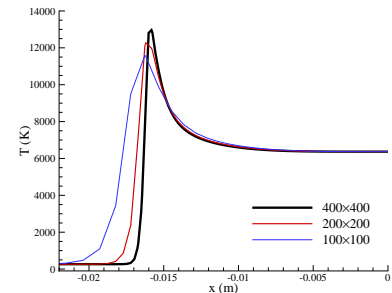
$$\rho_{\infty} = 6.81 \times 10^{-4} \text{ kg/m}^3$$

$$T_{\infty} = 265 \text{ K}$$

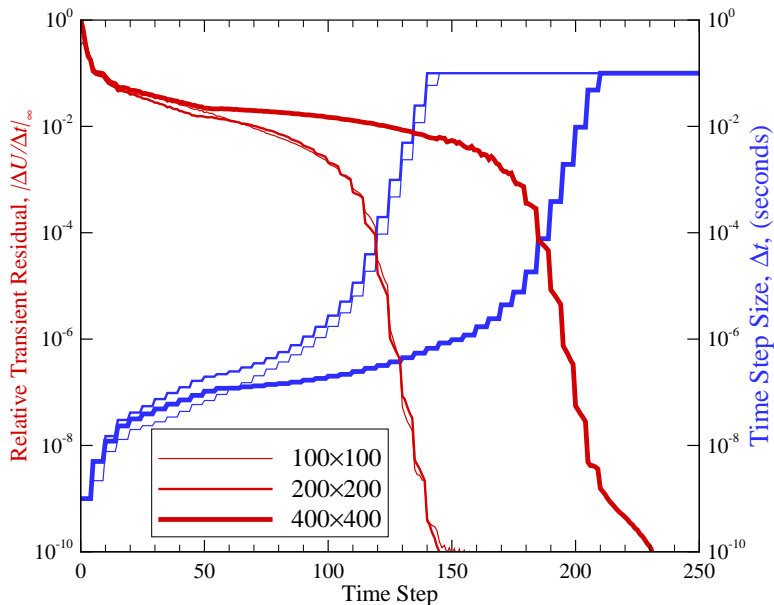
- Blottner/Wilke/Eucken with constant Lewis number $Le = 1.4$ for transport properties
- Mesh, iterative convergence
- FIN-S/DPLR comparison
- Weak & Strong Scaling



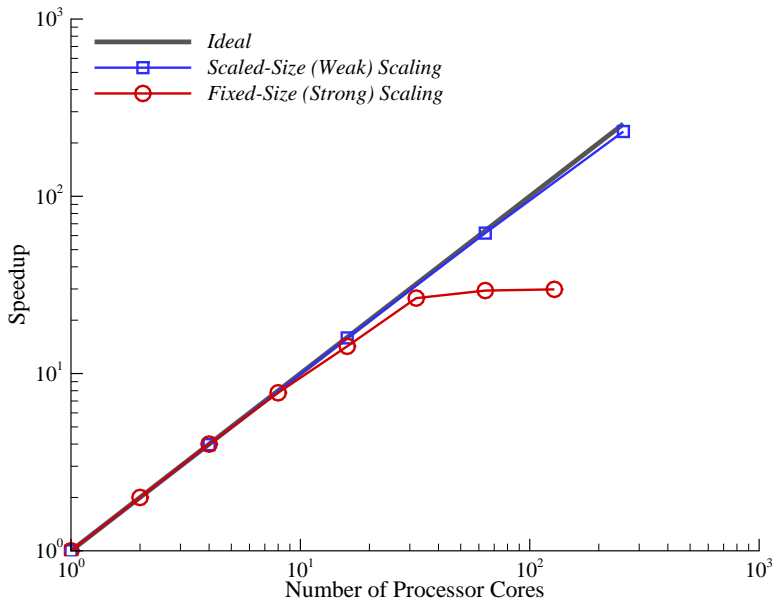
Mesh Convergence



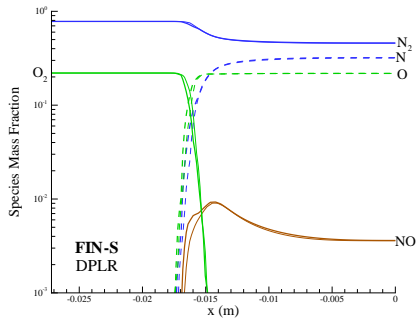
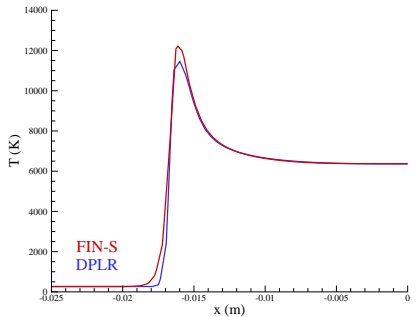
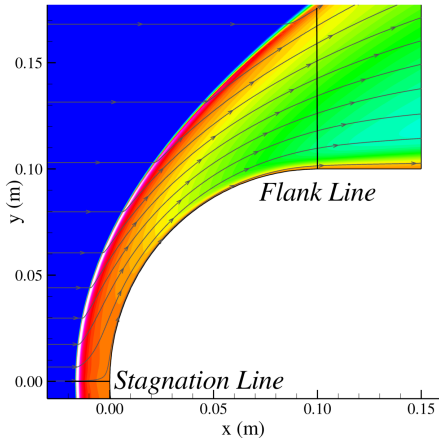
Iterative Convergence



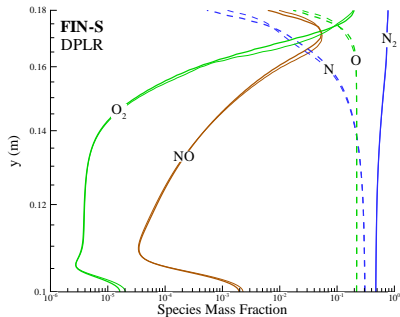
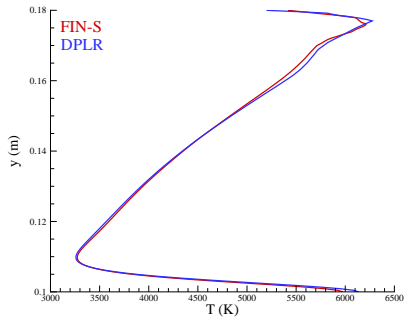
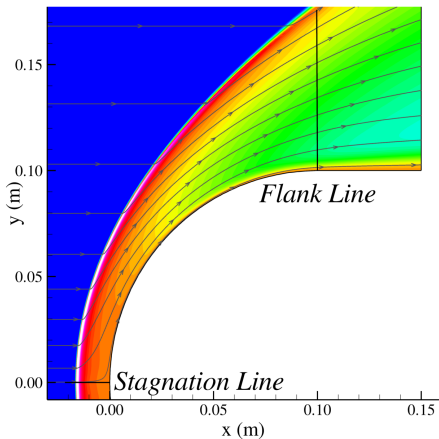
Speedup



Code-to-Code Comparison – Stagnation Line

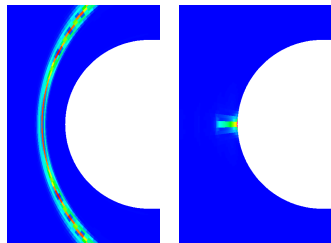


Code-to-Code Comparison – Flank Line

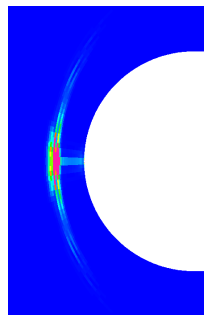


Additional Focus Areas

- 1 Physics Modeling
 - ▶ Weakly Ionized Flows
 - ▶ Surface Catalycity
 - ▶ Additional Boundary Conditions
- 2 Ablation coupling
- 3 Adjoints
 - ▶ Sensitivity analysis
 - ▶ Adaptivity



Primal & Dual Error



Combined QoI Error

Thank you!

Questions?