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

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Acknowledgments

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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*.

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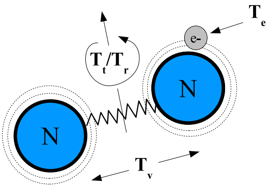

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- At hypersonic conditions these modes may not be in equilibrium, resulting in *thermal nonequilibrium*.

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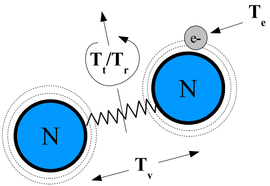

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- At hypersonic conditions these modes may not be in equilibrium, resulting in *thermal nonequilibrium*.

- 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.

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \ \boldsymbol{u}) &= 0 \\
\frac{\partial \rho \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u} \boldsymbol{u}) &= -\boldsymbol{\nabla} P + \boldsymbol{\nabla} \cdot \boldsymbol{\tau} \\
\frac{\partial \rho E}{\partial t} + \boldsymbol{\nabla} \cdot (\rho H \boldsymbol{u}) &= -\boldsymbol{\nabla} \cdot \dot{\boldsymbol{q}} + \boldsymbol{\nabla} \cdot (\boldsymbol{\tau} \boldsymbol{u})
\end{aligned}
$$

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

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

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

Thermodynamics & Transport Properties

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

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

  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

$$\mathsf{N}_2 + \mathcal{M} \rightleftharpoons 2\mathsf{N} + \mathcal{M}$$
$$\cdots$$
$$\mathsf{N}_2 + \mathsf{O} \rightleftharpoons \mathsf{NO} + \mathsf{N}$$
$$\cdots$$

- 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 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 $\bar{T}$

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

  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 $\bar{T} = \bar{T}\left(T, T_V\right)$ 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

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

where $\hat{e}_s^{\text{vib}}$ 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

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

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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

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

so the net vibrational energy production rate is

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

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

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

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}_i}{\partial x_i} = \frac{\partial \boldsymbol{G}_i}{\partial x_i} + \dot{\boldsymbol{\mathcal{S}}}$$

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

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

Find $\boldsymbol{U}$ satisfying the essential boundary and initial conditions such that

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

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

Stabilization Parameters

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

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

where τ_c, $\tau_{m,j}$, τ_E, and τ_{e_V} are given by

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

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

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

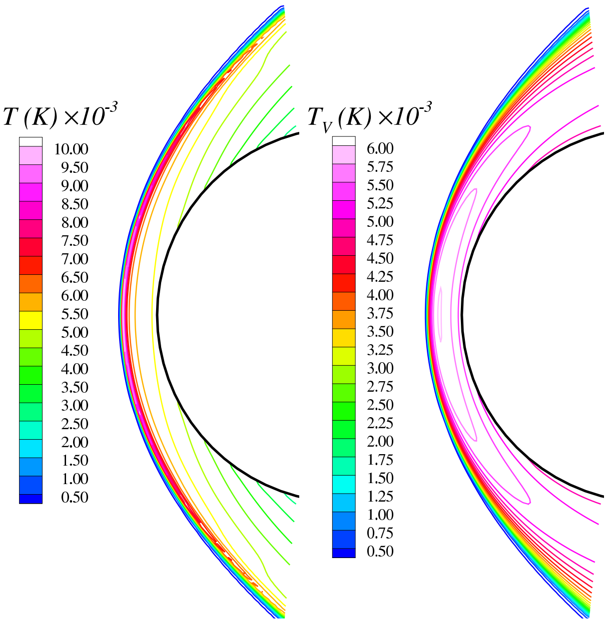
$$\tau_{ev} = \left[\left(\frac{2\left(\|\boldsymbol{u}\| + c\right)}{h_{\text{SUPG}}} \right)^2 + \left(\frac{4k_v}{\rho C_v^{\text{vib}} h^2_{\text{SUPG}}} \right)^2 + \nu^2 \right]^{-1/2}$$

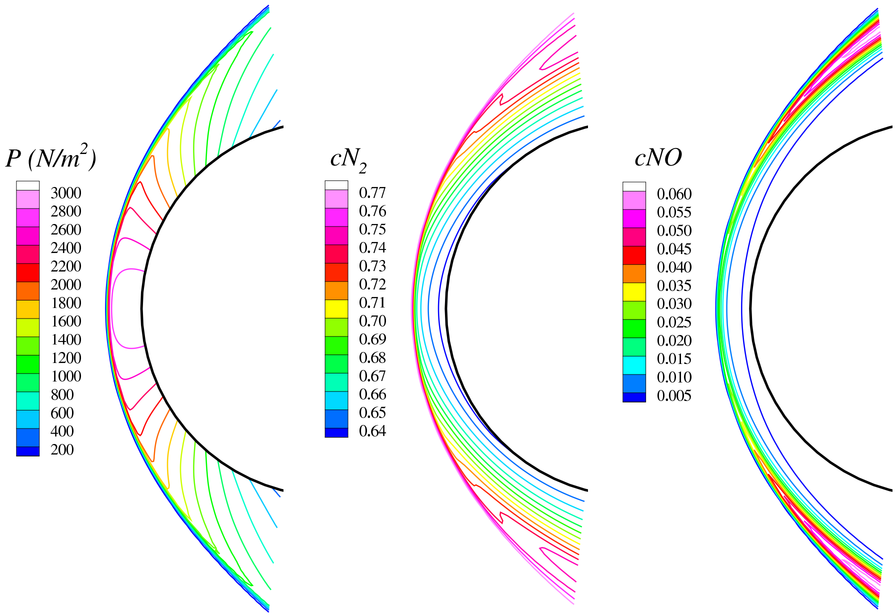
Inviscid Cylinder

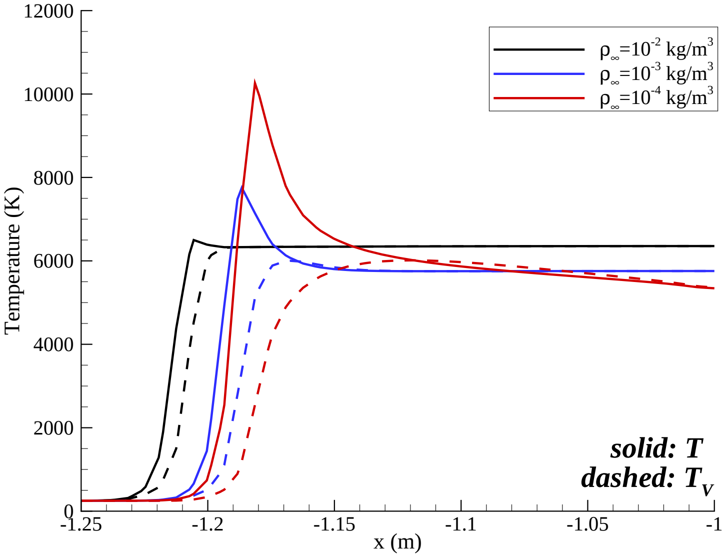
- Inviscid flow in thermochemical nonequilibrium
- 5 species air (N_2, O_2, NO, N, O)
- 5 reaction model with Park 1990 rates

$$
\begin{aligned}
c\mathsf{N}_{2,\infty} &= 0.78, c\mathsf{O}_{2,\infty} = 0.22 \\
U_\infty &= 5,500 \, {}^{\mathrm{m}}\!/\!_{\mathrm{sec}} \\
\rho_\infty &= 10^{-2} - 10^{-4} \, {}^{\mathrm{kg}}\!/\!_{\mathrm{m}^3} \\
T_\infty &= 250 \, \mathrm{K} = T_{V,\infty}
\end{aligned}
$$

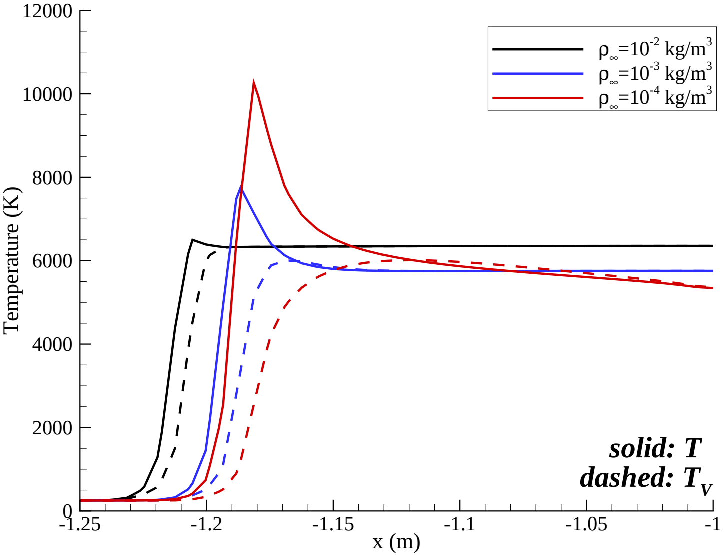
- Landau-Teller vibrational energy relaxation model, with Millikan and White vibrational relaxation time


$T\ (K) \times 10^{-3}$
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
$T_V\ (K) \times 10^{-3}$
6.00
5.75
5.50
5.25
5.00
4.75
4.50
4.25
4.00
3.75
3.50
3.25
3.00
2.75
2.50
2.25
2.00
1.75
1.50
1.25
1.00
0.75
0.50


P (N/m^2)
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
cN_2
0.77
0.76
0.75
0.74
0.73
0.72
0.71
0.70
0.69
0.68
0.67
0.66
0.65
0.64
cNO
0.060
0.055
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005



12000
10000
8000
6000
4000
2000
0
Temperature (K)
-1.25
-1.2
-1.15
-1.1
-1.05
-1
x (m)
$\rho_\infty = 10^{-2}$ kg/m^3
$\rho_\infty = 10^{-3}$ kg/m^3
$\rho_\infty = 10^{-4}$ kg/m^3
solid: T
dashed: T_V



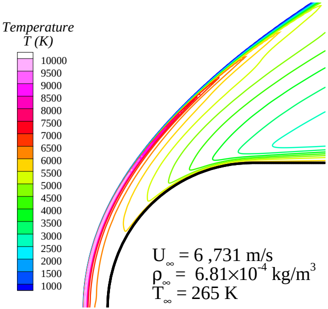
$$\tau_{sr}^{\text{vib}} = \frac{1}{P} \exp\left[A_{sr}\left(T^{-1/3} - 0.015\mu_{sr}^{1/4}\right) - 18.42\right]$$

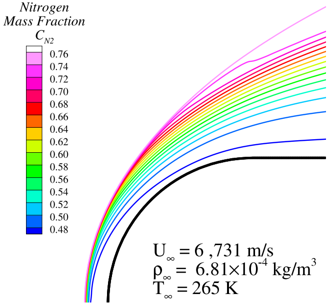
2D Extended Cylinder

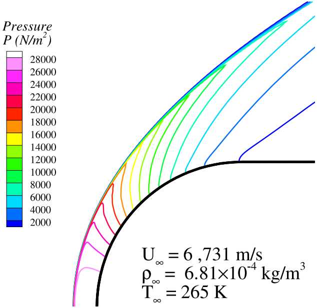
- Laminar flow in thermal equilibrium
- No-slip, adiabatic, noncatalytic wall
- Chemical nonequilibrium, 5 species air (N_2, O_2, NO, N, O)
- 5 reaction model with Park 1990 rates

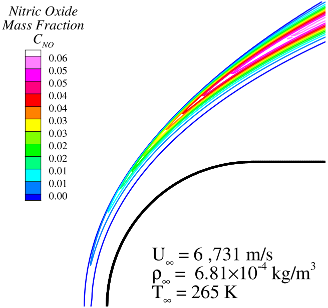
$$
\begin{aligned}
c\mathrm{N}_{2,\infty} &= 0.78, c\mathrm{O}_{2,\infty} = 0.22 \\
U_\infty &= 6,731\,\mathrm{m/sec} \\
\rho_\infty &= 6.81 \times 10^{-4}\,\mathrm{kg/m^3} \\
T_\infty &= 265\,\mathrm{K}
\end{aligned}
$$

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

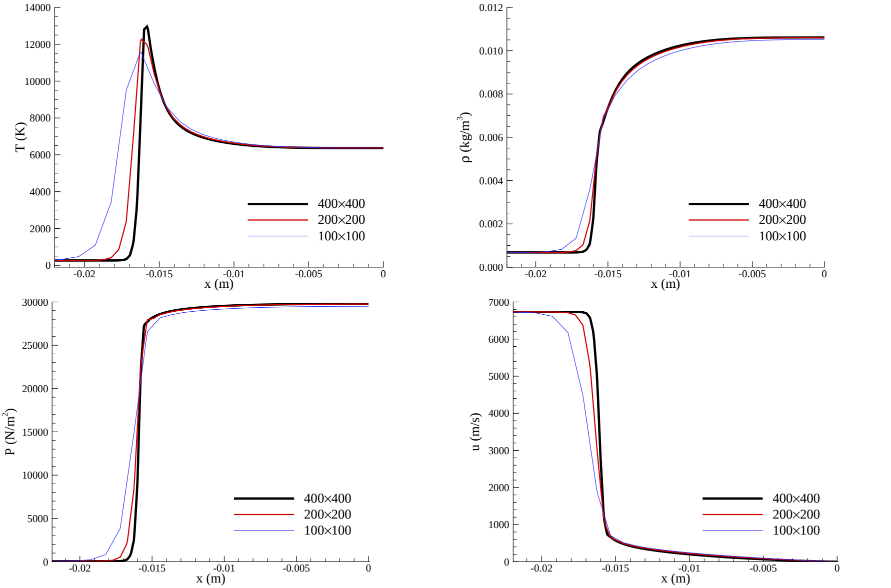

Temperature
T (K)
10000
9500
9000
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
U_∞ = 6 ,731 m/s
ρ_∞ = 6.81×10^{-4} kg/m^3
T_∞ = 265 K


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
U_∞ = 6 ,731 m/s
ρ_∞ = 6.81×10^{-4} kg/m^3
T_∞ = 265 K

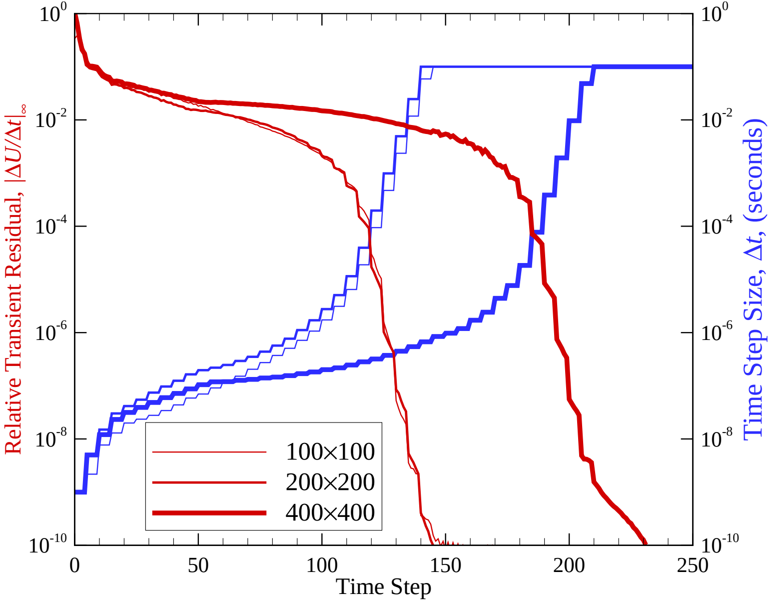

Pressure
P (N/m^2)
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
U_∞ = 6 ,731 m/s
ρ_∞ = 6.81×10^{-4} kg/m^3
T_∞ = 265 K


Nitric Oxide
Mass Fraction
C_{NO}
0.06
0.05
0.05
0.04
0.04
0.03
0.03
0.02
0.02
0.01
0.01
0.00
U_∞ = 6 ,731 m/s
ρ_∞ = 6.81×10^{-4} kg/m^3
T_∞ = 265 K

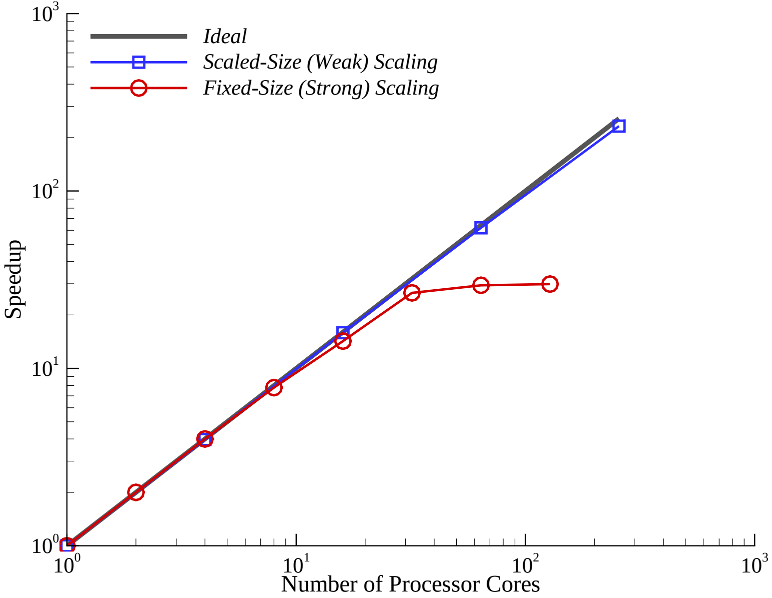
Mesh Convergence



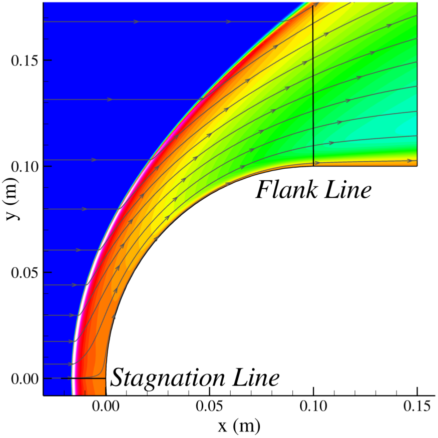
Iterative Convergence

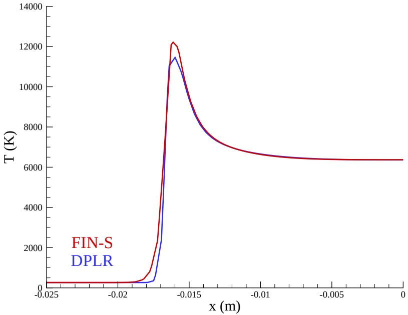


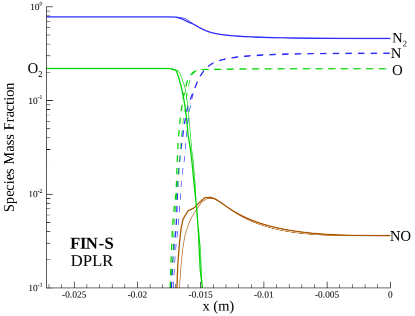
Speedup


Ideal
Scaled-Size (Weak) Scaling
Fixed-Size (Strong) Scaling
Speedup
Number of Processor Cores
10^0
10^1
10^2
10^3

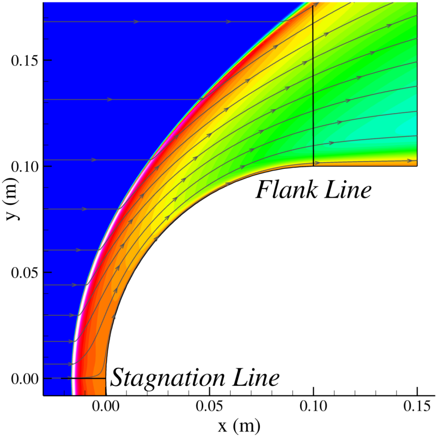
Code-to-Code Comparison –
Stagnation Line

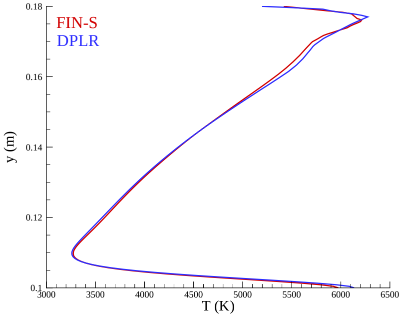


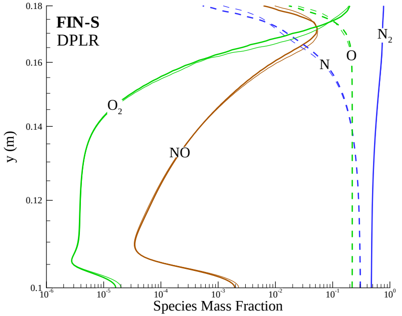




Code-to-Code Comparison –
Flank Line

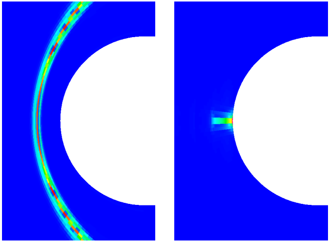




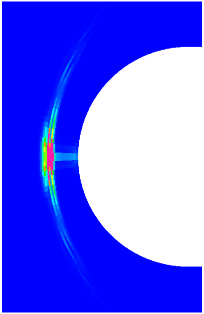


Additional Focus Areas

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?