CODE-VERIFICATION TECHNIQUES FOR HYPERSONIC REACTING FLOWS IN THERMOCHEMICAL NONEQUILIBRIUM

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Outline

• Introduction

• Governing Equations

• Verification Techniques for Spatial Accuracy

• Spatial-Discretization Verification Results

• Verification Techniques for Thermochemical Source Term

• Thermochemical-Source-Term Verification Results

• Summary
• Introduction
  – Hypersonic Flow
  – Sandia Parallel Aerodynamics and Reentry Code (SPARC)
  – Verification and Validation

• Governing Equations

• Verification Techniques for Spatial Accuracy

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• Summary
Hypersonic flows and underlying aerothermochemical phenomena

- Important in design & analysis of vehicles exiting/reentering atmosphere

- High flow velocities and stagnation enthalpies
  - Induce chemical reactions
  - Excite thermal energy modes

- Aerodynamic and thermochemical models require full coupling
Sandia Parallel Aerodynamics and Reentry Code (SPARC)

- Under development at Sandia National Laboratories

- Compressible computational fluids dynamics code

- Models transonic and hypersonic reacting turbulent flows

- Solves transient heat equation and equations associated with decomposing and non-decomposing ablators

- One- and two-way couplings between fluid-dynamics and ablation solvers
Credibility of computational physics codes requires verification and validation

- **Validation** assesses how well models represent physical phenomena
  - Computational results are compared with experimental results
  - Assess suitability of models, model error, and bounds of validity

- **Verification** assesses accuracy of numerical solutions against expectations
  - *Solution verification* estimates numerical error for particular solution
  - *Code verification* verifies correctness of numerical-method implementation
Code verification is focus of this work

- Governing equations are numerically discretized
  - Discretization error is introduced in solution

- Seek to verify discretization error decreases with refinement of discretization
  - Should decrease at an expected rate

- Use manufactured and exact solutions to compute error
Code verification demonstrated in many computational physics disciplines

- Fluid dynamics
- Solid mechanics
- Heat transfer
- Multiphase flows
- Electrodynamics
- Electromagnetism
- Fluid–structure interaction
- Radiation hydrodynamics

Code-verification techniques for hypersonic flows have been presented

- Single-species perfect gas
- Multi-species gas in thermal equilibrium

We present code-verification techniques for hypersonic reacting flows in thermochemical nonequilibrium and demonstrate effectiveness

- Spatial discretization
- Thermochemical source term
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• Governing Equations
  – Conserved Quantities
  – Vibrational Energy
  – Translational–Vibrational Energy Exchange
  – Chemical Kinetics
  – Scope of Code Verification

• Verification Techniques for Spatial Accuracy

• Spatial-Discretization Verification Results

• Verification Techniques for Thermochemical Source Term

• Thermochemical-Source-Term Verification Results

• Summary
Governing Equations: $n_s$ Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

$$
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_c (\mathbf{U}) = -\nabla \cdot \mathbf{F}_p (\mathbf{U}) + \nabla \cdot \mathbf{F}_d (\mathbf{U}) + \mathbf{S} (\mathbf{U}),
$$

where

$$
\mathbf{U} = \begin{bmatrix} \rho \\ \rho v \\ \rho E \\ \rho e_v \end{bmatrix}, \quad \mathbf{F}_c (\mathbf{U}) = \begin{bmatrix} \rho v^T \\ \rho v v^T \\ \rho E v^T \\ \rho e_v v^T \end{bmatrix}, \quad \mathbf{F}_p (\mathbf{U}) = \begin{bmatrix} 0 \\ pv^T \\ pI \end{bmatrix}, \quad \mathbf{F}_d (\mathbf{U}) = \begin{bmatrix} -\mathbf{J} \\ \tau (\mathbf{v} - \mathbf{q} - \mathbf{q}_v - \mathbf{J}^T \mathbf{h})^T \\ (-\mathbf{q}_v - \mathbf{J}^T \mathbf{e}_v)^T \end{bmatrix},
$$

$$
\mathbf{S} (\mathbf{U}) = \begin{bmatrix} \dot{\mathbf{w}} \\ 0 \\ 0 \end{bmatrix}, \quad \rho = \begin{bmatrix} \rho_1, \ldots, \rho_{n_s} \end{bmatrix}^T, \quad \dot{\mathbf{w}} = \begin{bmatrix} \dot{w}_1, \ldots, \dot{w}_{n_s} \end{bmatrix}^T: \text{mass production rates per volume},
$$

$$
e_v = \begin{bmatrix} e_{v_1}, \ldots, e_{v_{n_s}} \end{bmatrix}^T: \text{mixture vibrational energy per mass},
$$

$$
p = \sum_{s=1}^{n_s} \frac{\rho_s}{M_s} \bar{R} T, \quad e_v = \begin{bmatrix} e_{v_1}, \ldots, e_{v_{n_s}} \end{bmatrix}^T: \text{vibrational energies per mass},
$$

$$
Q_{t-v} : \text{translational–vibrational energy exchange},
$$

$$
E = \frac{|v|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} (c_{v_s} T + e_{v_s} + h^0_s)
$$
Governing Equations: \( n_s \) Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

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\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_c (\mathbf{U}) = -\nabla \cdot \mathbf{F}_p (\mathbf{U}) + \nabla \cdot \mathbf{F}_d (\mathbf{U}) + \mathbf{S} (\mathbf{U}),
\]

where

\[
\mathbf{U} = \begin{cases} 
\rho, \\
\rho v, \\
\rho E, \\
\rho e_v
\end{cases}, \quad \mathbf{F}_c (\mathbf{U}) = \begin{bmatrix} \rho v^T \\ \rho vv^T \\ \rho E v^T \\ \rho e_v v^T \end{bmatrix}, \quad \mathbf{F}_p (\mathbf{U}) = \begin{bmatrix} 0 \\ p I \\ p v^T \\ 0 \end{bmatrix}, \quad \mathbf{F}_d (\mathbf{U}) = \begin{bmatrix} -J \\ \tau \\ (\tau v - q - q_v - J^T h)^T \\ (-q_v - J^T e_v)^T \end{bmatrix},
\]

Multiple species

\[
\mathbf{S} (\mathbf{U}) = \begin{cases} 
\mathbf{\dot{w}}, \\
0, \\
0, \quad Q_{t-v} + \mathbf{e}_v^T \mathbf{\dot{w}}
\end{cases},
\]

\[
\mathbf{\dot{w}} = \begin{bmatrix} \dot{w}_1, \ldots, \dot{w}_{n_s} \end{bmatrix}^T: \text{mass production rates per volume},
\]

\[
e_v = \begin{bmatrix} e_{v_1}, \ldots, e_{v_{n_s}} \end{bmatrix}^T: \text{mixture vibrational energy per mass},
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Q_{t-v} : \text{translational–vibrational energy exchange},
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E = \frac{|v|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} \left( c_{v_s} T + e_{v_s} + h_s^0 \right)
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\]

where

\[
\mathbf{U} = \begin{\{ \begin{array}{c}
\rho \\
\rho v \\
\rho E \\
\rho e_v 
\end{array} \end{\{}, \quad \mathbf{F}_c (\mathbf{U}) = \begin{bmatrix}
\rho v^T \\
\rho vv^T \\
\rho E v^T \\
\rho e_v v^T
\end{bmatrix}, \quad \mathbf{F}_p (\mathbf{U}) = \begin{bmatrix}
0 \\
\rho I \\
pv^T \\
0
\end{bmatrix}, \quad \mathbf{F}_d (\mathbf{U}) = \begin{bmatrix}
-J \\
\tau \\
(\tau v - q - q_v - J^T h)^T \\
(-q_v - J^T e_v)^T
\end{bmatrix}, \quad \mathbf{S} (\mathbf{U}) = \begin{\{ \begin{array}{c}
\dot{\mathbf{w}} \\
0 \\
0 \\
Q_{t-v} + e_v^T \dot{\mathbf{w}}
\end{array} \end{\{},
\]

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\rho = \{\rho_1, \ldots, \rho_{n_s}\}^T, \quad \dot{\mathbf{w}} = \{\dot{w}_1, \ldots, \dot{w}_{n_s}\}^T : \text{mass production rates per volume},
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e_v = \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} e_{v_s} : \text{mixture vibrational energy per mass},
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Governing Equations: $n_s$ Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

\[
\frac{\partial U}{\partial t} + \nabla \cdot F_c (U) = -\nabla \cdot F_p (U) + \nabla \cdot F_d (U) + S (U),
\]

where

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U = \begin{cases}
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\rho e_v
\end{cases}, \quad F_c (U) = \begin{bmatrix}
\rho v^T \\
\rho vv^T \\
\rho E v^T \\
\rho e_v v^T
\end{bmatrix}, \quad F_p (U) = \begin{bmatrix}
0 \\
pI \\
pv^T \\
0
\end{bmatrix}, \quad F_d (U) = \begin{bmatrix}
-J \\
\tau \\
(\tau v - q - q_v - J^T h)^T \\
(-q_v - J^T e_v)^T
\end{bmatrix},
\]

\[
S (U) = \begin{cases}
\dot{w} \\
0 \\
0 \\
Q_{t-v} + e_v^T \dot{w}
\end{cases},
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\rho = \{\rho_1, \ldots, \rho_{n_s}\}^T, \quad \dot{w} = \{\dot{w}_1, \ldots, \dot{w}_{n_s}\}^T : \text{mass production rates per volume},
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\rho = \sum_{s=1}^{n_s} \rho_s, \quad e_v = \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} e_{v_s} : \text{mixture vibrational energy per mass},
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p = \sum_{s=1}^{n_s} \frac{\rho_s}{M_s} \bar{R}T, \quad e_v = \{e_{v_1}, \ldots, e_{v_{n_s}}\}^T : \text{vibrational energies per mass},
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\rho E v^T \\
\rho e_v v^T 
\end{bmatrix}, \quad \mathbf{F}_p (\mathbf{U}) = \begin{bmatrix} 0 \\
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p v^T \\
0 
\end{bmatrix}, \quad \mathbf{F}_d (\mathbf{U}) = \begin{bmatrix} -J \\
\tau \\
(\tau v - q - q_v - J^T h)^T \\
(-q_v - J^T e_v)^T 
\end{bmatrix},
\]

\[
\mathbf{S} (\mathbf{U}) = \begin{cases} 
\dot{\mathbf{w}} \\
0 \\
0 \\
Q_{t-v} + e_v^T \dot{\mathbf{w}} 
\end{cases},
\]

\[
\rho = \{\rho_1, \ldots, \rho_{n_s}\}^T, \quad \mathbf{w} = \{\dot{w}_1, \ldots, \dot{w}_{n_s}\}^T: \text{mass production rates per volume,}
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\mathbf{S} (\mathbf{U}) = \begin{cases} 
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Q_{t-v} + \mathbf{e}_v^T \dot{\mathbf{w}} 
\end{cases},
$$

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0 \\
\dot{Q}_{t-v} + \mathbf{e}_v^T \dot{\mathbf{w}} 
\end{bmatrix}^T: \text{mass production rates per volume},
$$

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\rho = \begin{bmatrix} 
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\end{bmatrix}^T, \quad 
\dot{\mathbf{w}} = \begin{bmatrix} 
\dot{w}_1, \ldots, \dot{w}_{n_s} 
\end{bmatrix}^T: \text{mass production rates per volume},
$$

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$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_c (\mathbf{U}) = -\nabla \cdot \mathbf{F}_p (\mathbf{U}) + \nabla \cdot \mathbf{F}_d (\mathbf{U}) + \mathbf{S} (\mathbf{U}),$$

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$$\mathbf{S} (\mathbf{U}) = \left\{ \begin{array}{c} \dot{\mathbf{w}} \\ 0 \\ 0 \\ Q_{t-v} + e_v^T \dot{\mathbf{w}} \end{array} \right\}.$$

$$\rho = \{\rho_1, \ldots, \rho_{n_s}\}^T, \quad \dot{\mathbf{w}} = \{\dot{w}_1, \ldots, \dot{w}_{n_s}\}^T: \text{mass production rates per volume},$$

$$\rho = \sum_{s=1}^{n_s} \rho_s, \quad e_v = \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} e_{v_s}: \text{mixture vibrational energy per mass},$$

$$\dot{\mathbf{w}} = \{\dot{w}_1, \ldots, \dot{w}_{n_s}\}^T: \text{vibrational energies per mass},$$

$$Q_{t-v}: \text{translational–vibrational energy exchange},$$

$$E = \frac{|v|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} (c_{v_s} T + e_{v_s} + h_s^0)$$
Vibrational Energy

Mixture vibrational energy per mass:

\[ e_v = \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} e_{v_s}, \]

where

\[ e_{v_s} = \begin{cases} \sum_{m=1}^{n_{v_s}} e_{v_s,m}(T_v) & \text{for molecules,} \\ 0 & \text{for atoms,} \end{cases} \]

and

\[ e_{v_s,m}(T') = \frac{\bar{R}}{M_s} \frac{\theta_{v_s,m}}{\exp(\theta_{v_s,m}/T') - 1} \]

- \( n_{v_s} \): number of vibrational modes of species \( s \) (\( n_{v_s} = 0 \) for atoms)
- \( \theta_{v_s,m} \): characteristic vibrational temperature of mode \( m \) of species \( s \)
Translational–Vibrational Energy Exchange

Landau–Teller model:

\[ Q_{t-v} = \sum_{s=1}^{n_s} \rho_s \sum_{m=1}^{n_{vs}} \frac{e_{v_s,m}(T) - e_{v_s,m}(T_v)}{\langle \tau_{s,m} \rangle} \]

Translational–vibrational energy relaxation time for mode \( m \) of species \( s \):

\[ \langle \tau_{s,m} \rangle = \left( \sum_{s'=1}^{n_s} \frac{y_{s'}}{\tau_{s,m,s'}} \right)^{-1} + \left[ \left( N_A \sum_{s'=1}^{n_s} \frac{\rho_{s'}}{M_{s'}} \right) \sigma_{v_s} \sqrt{\frac{8}{\pi}} \frac{\bar{R}T}{M_s} \right]^{-1} \]

where

\[ y_s = \frac{\rho_s / M_s}{\sum_{s'=1}^{n_s} \rho_{s'/M_{s'}}}, \quad \tau_{s,m,s'} = \frac{\exp \left[ a_{s,m,s'} \left( T^{-1/3} - b_{s,m,s'} \right) - 18.42 \right]}{p'} \]

\[ \sigma_{v_s} = \sigma'_{v_s} \left( \frac{50,000 \text{ K}}{T} \right)^2 \]

\( p' \): pressure in atmospheres.

\( a_{s,m,s'} \) and \( b_{s,m,s'} \): vibrational constants for mode \( m \) of species \( s \) with colliding species \( s' \)

\( N_A \): Avogadro constant

\( \sigma_{v_s} \): collision-limiting vibrational cross section

\( \sigma'_{v_s} \): collision-limiting vibrational cross section at 50,000 K.
Chemical Kinetics

Mass production rate per volume for species \( s \): \[ \dot{w}_s = M_s \sum_{r=1}^{n_r} (\beta_{s,r} - \alpha_{s,r}) (R_{f,r} - R_{b,r}) \]

Forward and backward reaction rates for reaction \( r \):
\[ R_{f,r} = \gamma k_{f,r} \prod_{s=1}^{n_s} \left( \frac{1}{\gamma M_s} \right)^{\alpha_{s,r}} \]
\[ R_{b,r} = \gamma k_{b,r} \prod_{s=1}^{n_s} \left( \frac{1}{\gamma M_s} \right)^{\beta_{s,r}} \]

Forward and backward reaction rate coefficients:
\[ k_{f,r}(T_c) = C_{f,r} T_c^{\eta_r} \exp \left( -\theta_r / T_c \right) \]
\[ k_{b,r}(T) = \frac{k_{f,r}(T)}{K_{e,r}(T)} \]

Equilibrium constant for reaction \( r \):
\[ K_{e,r}(T) = \exp \left[ A_{1,r} \left( \frac{T}{10000} \right) + A_{2,r} + A_{3,r} \ln \left( \frac{10000}{T} \right) + A_{4,r} \frac{10000}{T} + A_{5,r} \left( \frac{10000}{T} \right)^2 \right] \]

\( \alpha_{s,r} \) and \( \beta_{s,r} \): stoichiometric coefficients for species \( s \) in reaction \( r \)

\( \gamma \): unit conversion factor

\( C_{f,r}, \eta_r, A_{i,r} \): empirical parameters

\( \theta_r \): activation energy of reaction \( r \), divided by Boltzmann constant

\( T_c \): rate-controlling temperature (\( T_c = \sqrt{TT_v} \) for dissociation, \( T_c = T \) for exchange)
Scope of Code Verification

Conservation of mass, momentum, and energy:

\[
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_c (\mathbf{U}) = -\nabla \cdot \mathbf{F}_p (\mathbf{U}) + \nabla \cdot \mathbf{F}_d (\mathbf{U}) + \mathbf{S} (\mathbf{U}),
\]

where

\[
\mathbf{U} = \left\{ \begin{array}{c} \rho \\ \rho \mathbf{v} \\ \rho E \\ \rho e_v \end{array} \right\}, \quad \mathbf{F}_c (\mathbf{U}) = \left[ \begin{array}{c} \rho \mathbf{v}^T \\ \rho \mathbf{v} \mathbf{v}^T \\ \rho E \mathbf{v}^T \\ \rho e_v \mathbf{v}^T \end{array} \right], \quad \mathbf{F}_p (\mathbf{U}) = \left[ \begin{array}{c} 0 \\ \rho \mathbf{I} \\ \rho \mathbf{v} \mathbf{v}^T \\ 0 \end{array} \right], \quad \mathbf{F}_d (\mathbf{U}) = \left[ \begin{array}{c} -\mathbf{J} \\ \mathbf{J} \mathbf{v} - \mathbf{q} - \mathbf{q} v - \mathbf{q} v - \mathbf{J} \mathbf{T} \mathbf{h} \\ \mathbf{J} \mathbf{T} \mathbf{e}_v \\ \mathbf{J} \mathbf{T} \mathbf{e}_v \end{array} \right],
\]

\[
\mathbf{S} (\mathbf{U}) = \left\{ \begin{array}{c} \dot{\mathbf{w}} \\ 0 \\ 0 \end{array} \right\}, \quad \rho = \left\{ \rho_1, \ldots, \rho_{n_s} \right\}^T, \quad \dot{\mathbf{w}} = \left\{ \dot{\mathbf{w}}_1, \ldots, \dot{\mathbf{w}}_{n_s} \right\}^T: \text{mass production rates per volume},
\]

\[
\rho = \sum_{s=1}^{n_s} \rho_s, \quad e_v = \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} e_{v_s}: \text{mixture vibrational energy per mass},
\]

\[
p = \sum_{s=1}^{n_s} \frac{\rho_s}{M_s} \bar{R} T, \quad e_v = \left\{ e_{v_1}, \ldots, e_{v_{n_s}} \right\}^T: \text{vibrational energies per mass},
\]

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Q_{t-v} : \text{translational–vibrational energy exchange},
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E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} (c_{v_s} T + e_{v_s} + h_s^0)
\]
Conservation of mass, momentum, and energy:

\[ \frac{\partial U}{\partial t} + \nabla \cdot F_c(U) = -\nabla \cdot F_p(U) + \nabla \cdot F_d(U) + S(U), \]

where

\[ U = \begin{bmatrix} \rho \\ \rho v \\ \rho E \\ \rho e_v \end{bmatrix}, \quad F_c(U) = \begin{bmatrix} \rho v^T \\ \rho vv^T \\ \rho E v^T \\ \rho e_v v^T \end{bmatrix}, \quad F_p(U) = \begin{bmatrix} 0 \\ p I \\ p v^T \end{bmatrix}, \quad F_d(U) = \begin{bmatrix} -J^T \\ \tau (\tau v - q - q_v - J^T h)^T \\ (-q_v - J^T e_v)^T \end{bmatrix}, \]

\[ S(U) = \begin{bmatrix} \dot{w} \\ 0 \\ 0 \end{bmatrix}, \quad \dot{w} = \{\dot{w}_1, \ldots, \dot{w}_{n_s}\}^T: \text{mass production rates per volume,} \]

\[ \rho = \{\rho_1, \ldots, \rho_{n_s}\}^T, \quad e_v = \{e_{v_1}, \ldots, e_{v_{n_s}}\}^T: \text{mixture vibrational energy per mass,} \]

\[ e_v = \frac{\rho_s e_{v_s}}{\rho}: \text{mixture vibrational energy per mass,} \]

\[ p = \sum_{s=1}^{n_s} \frac{\rho_s}{M_s} \bar{R} T, \quad e_v = \{e_{v_1}, \ldots, e_{v_{n_s}}\}^T: \text{vibrational energies per mass,} \]

\[ Q_{t-v} : \text{translational–vibrational energy exchange,} \]

\[ E = \frac{|v|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} (\rho v_s T + e_{v_s} + h_s^o) \]
Scope of Code Verification

Conservation of mass, momentum, and energy:

\[ \frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_c (\mathbf{U}) = -\nabla \cdot \mathbf{F}_p (\mathbf{U}) + \nabla \cdot \mathbf{F}_d (\mathbf{U}) + \mathbf{S} (\mathbf{U}), \]

where

\[ \mathbf{U} = \left\{ \frac{\rho}{\rho v}, \frac{\rho v}{\rho v_T}, \frac{\rho E}{\rho E v_T}, \rho_e v_T \right\}, \quad \mathbf{F}_c (\mathbf{U}) = \begin{bmatrix} \rho v^T \\ \rho v v_T \\ \rho E v_T \\ \rho e v_T \end{bmatrix}, \quad \mathbf{F}_p (\mathbf{U}) = \begin{bmatrix} 0 \\ p I \\ p v_T \end{bmatrix}, \quad \mathbf{F}_d (\mathbf{U}) = \begin{bmatrix} -J \\ \tau (\tau v - q - q_v - J^T h) \\ (-q_v - J^T e_v) \end{bmatrix}, \]

\[ \mathbf{S} (\mathbf{U}) = \left\{ \begin{array}{c} \dot{\mathbf{w}} \\ 0 \\ 0 \\ Q_{t-v} + e^T_v \dot{\mathbf{w}} \end{array} \right\}, \quad \rho = \left\{ \rho_1, \ldots, \rho_{n_s} \right\}^T, \quad \dot{\mathbf{w}} = \left\{ \dot{\mathbf{w}}_1, \ldots, \dot{\mathbf{w}}_{n_s} \right\}^T : \text{mass production rates per volume}, \]

\[ e_v = \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} e_{v_s} : \text{mixture vibrational energy per mass}, \]

\[ e_v = \left\{ e_{v_1}, \ldots, e_{v_{n_s}} \right\}^T : \text{vibrational energies per mass}, \quad Q_{t-v} : \text{translational–vibrational energy exchange}, \]

\[ E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} (c_{v_s} T + e_{v_s} + h_s^0) \]
Scope of Code Verification

Conservation of mass, momentum, and energy:

\[
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_c (\mathbf{U}) = -\nabla \cdot \mathbf{F}_p (\mathbf{U}) + \nabla \cdot \mathbf{F}_d (\mathbf{U}) + \mathbf{S} (\mathbf{U}),
\]

where

\[
\mathbf{U} = \begin{cases} 
\rho \\
\rho v \\
\rho E \\
\rho e_v 
\end{cases}, \quad \mathbf{F}_c (\mathbf{U}) = \begin{bmatrix} 
\rho v^T \\
\rho vv^T \\
\rho E v^T \\
\rho e_v v^T 
\end{bmatrix}, \quad \mathbf{F}_p (\mathbf{U}) = \begin{bmatrix} 
0 \\
pI \\
pv^T \\
0
\end{bmatrix}, \quad \mathbf{F}_d (\mathbf{U}) = \begin{bmatrix} 
-J \\
\tau v - q - q_v - J^T h \\
-q_v - J^T e_v
\end{bmatrix},
\]

\[
\mathbf{S} (\mathbf{U}) = \begin{cases} 
\dot{\mathbf{w}} \\
0 \\
0 \\
Q_{t-v} + e_v^T \dot{\mathbf{w}}
\end{cases}, \quad \rho = \begin{cases} 
\rho_1, \ldots, \rho_{n_s} \end{cases}^T, \quad \dot{\mathbf{w}} = \begin{cases} 
\dot{\mathbf{w}}_1, \ldots, \dot{\mathbf{w}}_{n_s} \end{cases}^T : \text{mass production rates per volume},
\]

\[
\rho = \sum_{s=1}^{n_s} \rho_s, \quad e_v = \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} e_{v_s} : \text{mixture vibrational energy per mass},
\]

\[
e_v = \begin{cases} 
e_{v_1}, \ldots, e_{v_{n_s}} \end{cases}^T : \text{vibrational energies per mass}, \quad Q_{t-v} : \text{translational–vibrational energy exchange},
\]

\[
E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} (c_{v_s} T + e_{v_s} + h_{s}^0)
\]
Outline

• Introduction

• Governing Equations

• Verification Techniques for Spatial Accuracy
  – Spatial Accuracy
  – Solutions
  – Error Norms

• Spatial-Discretization Verification Results

• Verification Techniques for Thermochemical Source Term

• Thermochemical-Source-Term Verification Results

• Summary
Spatial Accuracy (Steady State)

Governing equations

\[ r(U; \mu) = 0 \]

Discretized equations

\[ \tilde{r}(\tilde{U}; \mu) = 0 \]

For \( \hat{p}^{th} \)-order-accurate discretization, error is

\[ e(x) = \tilde{U}(x) - U(x) = C(x) h^{\hat{p}(x)} + O(h^{\hat{p}(x)+1}) \]

\( h \): relative characterization of cell sizes

- Between meshes, with respect to one dimension
- Individual cell sizes may be non-uniform functions of \( h \)
- Sufficiently fine meshes \( \rightarrow \) asymptotic region \( (h^{\hat{p}(x)+1} \ll h^{\hat{p}(x)}) \)

\[ e(x) \approx C(x) h^{\hat{p}(x)} \]

\( C(x) \): function of derivative(s) of the state vector \( U \) at \( x \)

- Approximately constant between meshes in asymptotic region
Order of Accuracy

Observed accuracy $\tilde{p}(x)$ computed using 2 meshes:
Order of Accuracy

Observed accuracy $\tilde{\rho}(x)$ computed using 2 meshes:

Coarser mesh ($h$)

$$e_1(x) = C(x) h \tilde{\rho}(x)$$
Order of Accuracy

Observed accuracy $\tilde{\rho}(\mathbf{x})$ computed using 2 meshes:

- Coarser mesh $(h)$
  
  $$e_1(\mathbf{x}) = C(\mathbf{x}) h \tilde{\rho}(\mathbf{x})$$

- Finer mesh $(h/q)$
  
  $$(q\text{-times as fine in each dimension})$$
  
  $$e_2(\mathbf{x}) = C(\mathbf{x}) (h/q) \tilde{\rho}(\mathbf{x})$$
Order of Accuracy

Observed accuracy $\tilde{p}(\mathbf{x})$ computed using 2 meshes:

Coarser mesh ($h$)

$$e_1(\mathbf{x}) = C(\mathbf{x}) h^{\tilde{p}(\mathbf{x})}$$

Finer mesh ($h/q$) (q-times as fine in each dimension)

$$e_2(\mathbf{x}) = C(\mathbf{x})(h/q)^{\tilde{p}(\mathbf{x})}$$

$\tilde{p}(\mathbf{x})$ is computed by

$$\tilde{p}(\mathbf{x}) = \frac{\log |e_1(\mathbf{x})/e_2(\mathbf{x})|}{\log q} = \log_q |e_1(\mathbf{x})/e_2(\mathbf{x})|$$
Solutions

Need solution to compute error
Solutions

Exact Solutions
Exact Solutions

- **Negligible implementation effort:** \( r(U_{\text{Exact}}; \mu) = 0 \)
Exact Solutions

- **Negligible implementation effort**: \( r(U_{\text{Exact}}; \mu) = 0 \)
- **Limited cases**
Solutions

Exact Solutions

- **Negligible implementation effort**: $r(U_{\text{Exact}}; \mu) = 0$
- **Limited cases**
- **Span small subset of application space**
Solutions

Exact Solutions

- Negligible implementation effort: \( r(U_{\text{Exact}}; \mu) = 0 \)
- Limited cases
- Span small subset of application space

Manufactured Solutions
Solutions

Exact Solutions

- **Negligible implementation effort**: \( r(U_{\text{Exact}}; \mu) = 0 \)
- **Limited cases**
- **Span small subset of application space**

Manufactured Solutions

- **Do not satisfy original equations**: \( r(U_{\text{MS}}; \mu) \neq 0 \)
Solutions

Exact Solutions

- **Negligible** implementation effort: \( r(U_{\text{Exact}}; \mu) = 0 \)
- **Limited** cases
- **Span small subset** of application space

Manufactured Solutions

- **Do not** satisfy original equations: \( r(U_{\text{MS}}; \mu) \neq 0 \)
- **Require source term**: \( \tilde{r}(\tilde{U}; \mu) = r(U_{\text{MS}}; \mu) \)
Solutions

Exact Solutions

- **Negligible implementation effort:** \( r(U_{\text{Exact}}; \mu) = 0 \)
- **Limited cases**
- **Span small subset of application space**

Manufactured Solutions

- **Do not satisfy original equations:** \( r(U_{MS}; \mu) \neq 0 \)
- **Require source term:** \( \tilde{r}(\tilde{U}; \mu) = r(U_{MS}; \mu) \)
- **Manufactured to exercise features of interest**
Solutions

Exact Solutions

- **Negligible implementation effort:** $r(U_{\text{Exact}}; \mu) = 0$
- **Limited cases**
- **Span small subset** of application space

Manufactured Solutions

- **Do not** satisfy original equations: $r(U_{\text{MS}}; \mu) \neq 0$
- **Require source term:** $\tilde{r}(\tilde{U}; \mu) = r(U_{\text{MS}}; \mu)$
- Manufactured to exercise features of interest
- Should be **smooth, continuously differentiable functions with generally nonzero derivatives and moderate variations**
Solutions

Exact Solutions

- **Negligible implementation effort**: \( r(U_{\text{Exact}}; \mu) = 0 \)
- **Limited cases**
- **Span small subset of application space**

Manufactured Solutions

- **Do not** satisfy original equations: \( r(U_{\text{MS}}; \mu) \neq 0 \)
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Solutions

Exact Solutions

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• Do not satisfy original equations: \( r(U_{\text{MS}}; \mu) \neq 0 \)
• Require source term: \( \tilde{r}(\tilde{U}; \mu) = r(U_{\text{MS}}; \mu) \)
• Manufactured to exercise features of interest
• Should be smooth, continuously differentiable functions with generally nonzero derivatives and moderate variations
Error Norms

Computing $p = f(\tilde{p}(x))$ (e.g., $p = \min_{x \in \Omega} \tilde{p}(x)$) has two shortcomings:

• For cell-centered schemes, cell centers vary with mesh refinement
• In regions where error vanishes, computed $\tilde{p}(x)$ is meaningless

Error norms to quantify spatial accuracy:

- $L_1$-norm: $\epsilon_{1} = \| \alpha(x) - \tilde{\alpha}(x) \|_1 = \int_{\Omega} | \alpha(x) - \tilde{\alpha}(x) | d\Omega$
  - Average error
  - Not significantly contaminated by localized deviations (e.g., discontinuities, lower-order boundary conditions)

- $L_\infty$-norm: $\epsilon_{\infty} = \| \alpha(x) - \tilde{\alpha}(x) \|_\infty = \max_{x \in \Omega} | \alpha(x) - \tilde{\alpha}(x) |$
  - Maximum error
  - Catches localized deviations (expected and unexpected)

• Without discontinuities, both norms should yield same
Error Norms

Computing \( p = f(\tilde{p}(\mathbf{x})) \) (e.g., \( p = \min_{\mathbf{x} \in \Omega} \tilde{p}(\mathbf{x}) \)) has two shortcomings:

- For cell-centered schemes, cell centers vary with mesh refinement

\[ \epsilon_1(\alpha) = \| \alpha(x) - \tilde{\alpha}(x) \|_1 = \int_{\Omega} | \alpha(x) - \tilde{\alpha}(x) | \, d\Omega \]

- Average error
- Not significantly contaminated by localized deviations (e.g., discontinuities, lower-order boundary conditions)

\[ \epsilon_\infty(\alpha) = \| \alpha(x) - \tilde{\alpha}(x) \|_\infty = \max_{x \in \Omega} | \alpha(x) - \tilde{\alpha}(x) | \]

- Maximum error
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Error norms to quantify spatial accuracy: $p = \log_q \left( \varepsilon_{\alpha_1} / \varepsilon_{\alpha_2} \right)$
Error Norms

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Error norms to quantify spatial accuracy: \( p = \log_q (\varepsilon_{\alpha_1}/\varepsilon_{\alpha_2}) \)

- \( L^1 \)-norm: \( \varepsilon^1_{\alpha} = \| \alpha(x) - \tilde{\alpha}(x) \|_1 = \int_{\Omega} |\alpha(x) - \tilde{\alpha}(x)| d\Omega \)
Error Norms

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Error norms to quantify spatial accuracy: \( p = \log_q (\varepsilon_{\alpha_1}/\varepsilon_{\alpha_2}) \)

- **\( L^1 \)-norm:** \( \varepsilon^1_{\alpha} = \|\alpha(x) - \tilde{\alpha}(x)\|_1 = \int_{\Omega} |\alpha(x) - \tilde{\alpha}(x)| \, d\Omega \)
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Error Norms

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Error Norms

Computing \( p = f(\tilde{p}(\mathbf{x})) \) (e.g., \( p = \min_{\mathbf{x} \in \Omega} \tilde{p}(\mathbf{x}) \)) has two shortcomings:

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Error norms to quantify spatial accuracy: \( p = \log_q \left( \varepsilon_{\alpha_1} / \varepsilon_{\alpha_2} \right) \)

- \( L^1 \)-norm: \( \varepsilon_{\alpha}^1 = \| \alpha(\mathbf{x}) - \tilde{\alpha}(\mathbf{x}) \|_1 = \int_{\Omega} |\alpha(\mathbf{x}) - \tilde{\alpha}(\mathbf{x})| d\Omega \)
  - Average error
  - Not significantly contaminated by localized deviations (e.g., discontinuities, lower-order boundary conditions)

- \( L^\infty \)-norm: \( \varepsilon_{\alpha}^\infty = \| \alpha(\mathbf{x}) - \tilde{\alpha}(\mathbf{x}) \|_\infty = \max_{\mathbf{x} \in \Omega} |\alpha(\mathbf{x}) - \tilde{\alpha}(\mathbf{x})| \)
  - Maximum error
  - Catches localized deviations (expected and unexpected)
Error Norms

Computing \( p = f(\tilde{p}(x)) \) (e.g., \( p = \min_{x \in \Omega} \tilde{p}(x) \)) has two shortcomings:

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- \( L^1 \)-norm: \( \varepsilon^1_{\alpha} = \|\alpha(x) - \tilde{\alpha}(x)\|_1 = \int_{\Omega} |\alpha(x) - \tilde{\alpha}(x)| \, d\Omega \)
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- \( L^\infty \)-norm: \( \varepsilon^\infty_{\alpha} = \|\alpha(x) - \tilde{\alpha}(x)\|_\infty = \max_{x \in \Omega} |\alpha(x) - \tilde{\alpha}(x)| \)
  - Maximum error
  - Catches localized deviations (expected and \textit{unexpected})

- Without discontinuities, both norms should yield same \( p \)
Outline

• Introduction

• Governing Equations

• Verification Techniques for Spatial Accuracy

• Spatial-Discretization Verification Results
  – Single-Species Inviscid Flow in Thermochemical Equilibrium
  – Five-Species Inviscid Flow in Chemical Nonequilibrium

• Verification Techniques for Thermochemical Source Term

• Thermochemical-Source-Term Verification Results

• Summary
1D Supersonic Flow using a Manufactured Solution

- One-dimensional domain: $x \in [0, 1]$ m

- Boundary conditions:
  - Supersonic inflow ($x = 0$ m)
  - Supersonic outflow ($x = 1$ m)

- 5 uniform meshes: 50, 100, 200, 400, 800 elements

- Solution consists of small, smooth perturbations to uniform flow:
  \begin{align*}
  \rho(x) &= \bar{\rho} \left[1 - \epsilon \sin(\pi x) \right], \\
  u(x) &= \bar{u} \left[1 - \epsilon \sin(\pi x) \right], \\
  T(x) &= \bar{T} \left[1 + \epsilon \sin(\pi x) \right],
  \end{align*}

  $\bar{\rho} = 1$ kg/m$^3$, $\bar{T} = 300$ K, $\bar{M} = 2.5$, $\epsilon = 0.05$
1D Supersonic Flow using a Manufactured Solution

First-order accurate

| Mesh | $\rho$ | $u$ | $T$ |
|------|--------|-----|-----|
| 1–2  | 1.0008 | 1.0008 | 1.0008 |
| 2–3  | 1.0002 | 1.0002 | 1.0002 |
| 3–4  | 1.0001 | 1.0001 | 1.0000 |
| 4–5  | 1.0000 | 1.0000 | 1.0000 |

Second-order accurate

| Mesh | $\rho$ | $u$ | $T$ |
|------|--------|-----|-----|
|      | 2.0313 | 2.0362 | 2.0351 |
| 2–3  | 2.0157 | 2.0184 | 2.0178 |
| 3–4  | 2.0079 | 2.0093 | 2.0090 |
| 4–5  | 2.0040 | 2.0047 | 2.0045 |

Observed accuracy $p$ using $L^\infty$-norms of the error

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2D Supersonic Flow using a Manufactured Solution

- Two-dimensional domain: \((x, y) \in [0, 1] \text{ m} \times [0, 1] \text{ m}\)

- Boundary conditions:
  - Supersonic inflow \((x = 0 \text{ m})\)
  - Supersonic outflow \((x = 1 \text{ m})\)
  - Slip wall (tangent flow) \((y = 0 \text{ m} \& y = 1 \text{ m})\)

- 5 nonuniform meshes: \(25 \times 25 \rightarrow 400 \times 400\)

- Solution consists of small, smooth perturbations to uniform flow:
  \[
  \begin{align*}
  \rho (x, y) &= \bar{\rho} \left[ 1 - \epsilon \sin \left( \frac{5}{4} \pi x \right) \left( \sin \left( \pi y \right) + \cos \left( \pi y \right) \right) \right], \\
  u (x, y) &= \bar{u} \left[ 1 + \epsilon \sin \left( \frac{1}{4} \pi x \right) \left( \sin \left( \pi y \right) + \cos \left( \pi y \right) \right) \right], \\
  v (x, y) &= \bar{v} \left[ -\epsilon \sin \left( \frac{5}{4} \pi x \right) \left( \sin \left( \pi y \right) \right) \right], \\
  T(x, y) &= \bar{T} \left[ 1 + \epsilon \sin \left( \frac{5}{4} \pi x \right) \left( \sin \left( \pi y \right) + \cos \left( \pi y \right) \right) \right], \\
  \bar{\rho} &= 1 \text{ kg/m}^3, \bar{T} = 300 \text{ K}, \bar{M} = 2.5, \epsilon = 0.05
  \end{align*}
\]
2D Supersonic Flow using a Manufactured Solution
2D Supersonic Flow using a Manufactured Solution

First-order accurate

| Mesh | $\rho$ | $u$ | $v$ | $T$ |
|------|-------|-----|-----|-----|
| 1–2  | 0.9420| 0.9409| 0.9721| 0.9628|
| 2–3  | 0.9850| 0.9902| 0.9910| 0.9874|
| 3–4  | 0.9960| 1.0002| 0.9924| 0.9952|
| 4–5  | 0.9989| 1.0009| 0.9959| 0.9984|

Second-order accurate

| Mesh | $\rho$ | $u$ | $v$ | $T$ |
|------|-------|-----|-----|-----|
| 1–2  | 2.0623| 1.9188| 1.8174| 1.8598|
| 2–3  | 2.1304| 1.9450| 1.9221| 1.9280|
| 3–4  | 2.0902| 1.9603| 1.9671| 1.9586|
| 4–5  | 2.0128| 1.9823| 1.9860| 1.9809|

Observed accuracy $p$ using $L^\infty$-norms of the error
2D Supersonic Flow using an Exact Solution

- Two-dimensional domain: \((r, \theta) \in [1, 1.384] \times [0, 90]^\circ\)

- Boundary conditions:
  - Supersonic inflow \((\theta = 90^\circ)\)
  - Supersonic outflow \((\theta = 0^\circ)\)
  - Slip wall (tangent flow) \((r = 1 \& r = 1.384)\)

- 6 meshes: \(32 \times 8 \rightarrow 1024 \times 256\)

- Solution is steady isentropic vortex:
  \[
  \rho(r) = \rho_i \left[ 1 + \frac{\gamma - 1}{2} M_i^2 \left( 1 - \left( \frac{r_i}{r} \right)^2 \right) \right]^{\frac{1}{\gamma - 1}},
  \]
  
  \[
  u_r(r) = 0,
  \]
  
  \[
  u_\theta(r) = -a_i M_i \frac{r_i}{r},
  \]
  
  \[
  T(r) = T_i \left[ 1 + \frac{\gamma - 1}{2} M_i^2 \left( 1 - \left( \frac{r_i}{r} \right)^2 \right) \right],
  \]
  
  \(\rho_i = 1, \ a_i = 1, \ M_i = 2.25, \ T_i = 1/(\gamma R)\)
2D Supersonic Flow using an Exact Solution
2D Supersonic Flow using an Exact Solution

| Mesh | $\rho$  | $u$  | $v$  | $T$  |
|------|--------|------|------|------|
| 1–2  | 1.9896 | 1.9119 | 1.9943 | 1.9699 |
| 2–3  | 1.9735 | 1.9589 | 2.0070 | 1.9979 |
| 3–4  | 1.9954 | 1.9760 | 2.0099 | 2.0076 |
| 4–5  | 1.9972 | 1.9879 | 2.0054 | 2.0044 |
| 5–6  | 1.9986 | 1.9940 | 2.0029 | 2.0025 |

Observed accuracy $p$ using $L^\infty$-norms of the error
3D Supersonic Flow using a Manufactured Solution

- Three-dimensional domain: \((x, y, z) \in [0, 1] \text{ m} \times [0, 1] \text{ m} \times [0, 1] \text{ m}\)

- Boundary conditions:
  - Supersonic inflow \((x = 0 \text{ m})\)
  - Supersonic outflow \((x = 1 \text{ m})\)
  - Slip wall (tangent flow)
    \((y = 0 \text{ m}, y = 1 \text{ m}, z = 0 \text{ m}, z = 1 \text{ m})\)

- 5 nonuniform meshes:
  \(25 \times 25 \times 25 \rightarrow 400 \times 400 \times 400\)

- Solution consists of small, smooth perturbations to uniform flow:
  \[
  \begin{align*}
  \rho(x, y, z) &= \bar{\rho}\left[1 - \epsilon \sin\left(\frac{5}{4}\pi x\right) (\sin(\pi y) + \cos(\pi y))(\sin(\pi z) + \cos(\pi z))\right], \\
  u(x, y, z) &= \bar{u}\left[1 + \epsilon \sin\left(\frac{1}{4}\pi x\right) (\sin(\pi y) + \cos(\pi y))(\sin(\pi z) + \cos(\pi z))\right], \\
  v(x, y, z) &= \bar{v}\left[-\epsilon \sin\left(\frac{5}{4}\pi x\right) (\sin(\pi y)) (\sin(\pi z) + \cos(\pi z))\right], \\
  w(x, y, z) &= \bar{w}\left[-\epsilon \sin\left(\frac{5}{4}\pi x\right) (\sin(\pi y) + \cos(\pi y))(\sin(\pi z))\right], \\
  T(x, y, z) &= \bar{T}\left[1 + \epsilon \sin\left(\frac{5}{4}\pi x\right) (\sin(\pi y) + \cos(\pi y))(\sin(\pi z) + \cos(\pi z))\right], \\
  \bar{\rho} &= 1 \text{ kg/m}^3, \bar{T} = 300 \text{ K}, \bar{M} = 2.5, \epsilon = 0.05
  \end{align*}
  \]
3D Supersonic Flow using a Manufactured Solution

![Graph showing spatial accuracy results](image)

| Mesh | $\rho$  | $u$  | $v$  | $w$  | $T$  |
|------|--------|------|------|------|------|
| 1–2  | 2.0849 | 1.8731 | 1.9841 | 1.7039 | 1.9404 |
| 2–3  | 2.1406 | 1.9923 | 1.9295 | 1.8621 | 1.9774 |
| 3–4  | 2.0990 | 2.0115 | 1.9623 | 1.9349 | 1.9922 |
| 4–5  | 2.0585 | 2.0100 | 1.9820 | 1.9571 | 1.9964 |

Observed accuracy $p$ using $L^\infty$-norms of the error

$$\log_{10}(\varepsilon_\alpha^\infty/\bar{\alpha}), \alpha=\{\rho, u, v, w, T\} \approx O(h^2)$$
Five-Species Air Model

5 species: N₂, O₂, NO, N, and O

17 reactions:

| r | Reaction                     | Type of Reaction |
|---|------------------------------|------------------|
| 1–5 | N₂ + \( M \) ⇌ N + N + \( M \), \( M = \{N₂, O₂, NO, N, O\} \) | Dissociation     |
| 6–10 | O₂ + \( M \) ⇌ O + O + \( M \), \( M = \{N₂, O₂, NO, N, O\} \) | Dissociation     |
| 11–15 | NO + \( M \) ⇌ N + O + \( M \), \( M = \{N₂, O₂, NO, N, O\} \) | Dissociation     |
| 16 | N₂ + O ⇌ N + NO              | Exchange         |
| 17 | NO + O ⇌ N + O₂              | Exchange         |
Five-Species Inviscid Flow in Chemical Nonequilibrium

- Two-dimensional domain: \((x, y) \in [0, 1] \text{ m} \times [0, 1] \text{ m}\)
- Same boundary conditions
- 7 nonuniform meshes: \(25 \times 25 \rightarrow 1600 \times 1600\)
- Solution consists of small, smooth perturbations to uniform flow

\[
\begin{align*}
\rho_{N_2}(x, y) &= \bar{\rho}_{N_2} \left[1 - \epsilon \sin\left(\frac{5}{4} \pi x\right) \left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right], \\
\rho_{O_2}(x, y) &= \bar{\rho}_{O_2} \left[1 + \epsilon \sin\left(\frac{3}{4} \pi x\right) \left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right], \\
\rho_{NO}(x, y) &= \bar{\rho}_{NO} \left[1 + \epsilon \sin\left(\pi x\right) \left(\sin\left(\pi y\right)\right)\right], \\
\rho_{N}(x, y) &= \bar{\rho}_{N} \left[1 + \epsilon \sin\left(\pi x\right) \left(\cos\left(\frac{1}{4} \pi y\right)\right)\right], \\
\rho_{O}(x, y) &= \bar{\rho}_{O} \left[1 + \epsilon \sin\left(\pi x\right) \left(\sin\left(\pi y\right) + \cos\left(\frac{1}{4} \pi y\right)\right)\right], \\
u(x, y) &= \bar{u} \left[1 + \epsilon \sin\left(\frac{1}{4} \pi x\right) \left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right], \\
v(x, y) &= \bar{v} \left[-\epsilon \sin\left(\frac{5}{4} \pi x\right) \left(\sin\left(\pi y\right)\right)\right], \\
T(x, y) &= \bar{T} \left[1 + \epsilon \sin\left(\frac{5}{4} \pi x\right) \left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right], \\
T_v(x, y) &= \bar{T_v} \left[1 + \epsilon \sin\left(\frac{3}{4} \pi x\right) \left(\sin\left(\frac{5}{4} \pi y\right) + \cos\left(\frac{3}{4} \pi y\right)\right)\right]
\end{align*}
\]
Five-Species Inviscid Flow in Chemical Nonequilibrium

Spatial Results

Source Results

Summary

Equations

Spatial Accuracy

Source Term

Introduction

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Sandia National Laboratories
2D Supersonic Flow in Thermal Equilibrium using a Manufactured Solution

| Variable | Value   | Units   |
|----------|---------|---------|
| \(\bar{\rho}_{N_2}\) | 0.77    | kg/m³   |
| \(\bar{\rho}_{O_2}\) | 0.20    | kg/m³   |
| \(\bar{\rho}_{NO}\) | 0.01    | kg/m³   |
| \(\bar{\rho}_N\) | 0.01    | kg/m³   |
| \(\bar{\rho}_O\) | 0.01    | kg/m³   |
| \(\bar{T}\) | 3500    | K       |
| \(\bar{M}\) | 2.5     |         |
| \(\epsilon\) | 0.05    |         |

![Graph showing \(\log_{10}(\sqrt{n})\) vs. \(\log_{10}(\epsilon_{\infty}(\alpha)/\bar{\alpha})\) for different variables and \(O(h^2)\)](image)

Mesh | \(\rho_{N_2}\) | \(\rho_{O_2}\) | \(\rho_{NO}\) | \(\rho_N\) | \(\rho_O\) | \(u\)  | \(v\)  | \(T\)     |
---   |-------|-------|-------|-------|-------|------|------|-------|
1–2   | 2.0608| 2.1382| 2.0698| 2.0644| 2.1885| 1.8425| 1.8289| 1.7351   
2–3   | 2.1161| 2.1219| 2.1127| 2.1072| 2.1697| 1.8875| 1.9220| 1.7923   
3–4   | 2.0798| 2.0813| 1.8555| 2.0754| 2.0971| 1.9200| 1.9686| 1.8525   
4–5   | 2.0456| 2.0458| 1.8917| 2.0428| 2.0806| 1.9522| 1.9871| 1.9079   
5–6   | 2.0243| 2.0243| 1.9427| 2.0228| 2.0529| 1.9735| 1.9939| 1.9485   
6–7   | 2.0125| 2.0125| 1.9790| 2.0118| 2.0318| 1.9865| 1.9969| 1.9737   

2D MMS, \(n_s = 5\), \(T_v = T\), \(\dot{w} \neq 0\): Observed accuracy \(p\) using \(L^\infty\)-norms of the error
### 2D Hypersonic Flow in Thermal Nonequilibrium using a Manufactured Solution

| Variable | Value | Units |
|----------|-------|-------|
| $\bar{\rho}_{N_2}$ | 0.0077 | kg/m$^3$ |
| $\bar{\rho}_{O_2}$ | 0.0020 | kg/m$^3$ |
| $\bar{\rho}_{NO}$ | 0.0001 | kg/m$^3$ |
| $\bar{\rho}_N$ | 0.0001 | kg/m$^3$ |
| $\bar{\rho}_O$ | 0.0001 | kg/m$^3$ |
| $\bar{T}$ | 5000 | K |
| $\bar{T}_v$ | 1000 | K |
| $\bar{M}$ | 8 | |
| $\epsilon$ | 0.05 | |

**Mesh**

| Mesh | $\rho_{N_2}$ | $\rho_{O_2}$ | $\rho_{NO}$ | $\rho_N$ | $\rho_O$ | $u$ | $v$ | $T$ | $T_v$ |
|------|--------------|--------------|--------------|----------|----------|-----|-----|-----|-----|
| 1–2  | 1.5659       | 1.6370       | 1.6555       | 1.6046   | 1.5869   | 1.7742| 1.7337| 1.7814| 1.5545|
| 2–3  | 1.9067       | 1.6944       | 1.6986       | 1.7598   | 1.8819   | 1.8916| 1.8701| 1.8768| 1.9150|
| 3–4  | 1.9868       | 2.0475       | 2.0698       | 2.0477   | 2.0110   | 1.9488| 1.9357| 1.9349| 2.0082|
| 4–5  | 2.0074       | 1.9941       | 2.0138       | 1.9936   | 2.0089   | 1.9752| 1.9684| 1.9672| 2.0168|
| 5–6  | 2.0062       | 1.9939       | 2.0004       | 1.9935   | 2.0061   | 1.9879| 1.9843| 1.9836| 2.0111|
| 6–7  | 2.0037       | 1.9965       | 1.9994       | 1.9962   | 1.9955   | 1.9940| 1.9922| 1.9918| 2.0063|

2D MMS, $n_s = 5$, $T_v \neq T$, $\dot{w} \neq 0$: Observed accuracy $p$ using $L^\infty$-norms of the error
## Outline

- Introduction
- Governing Equations
- Verification Techniques for Spatial Accuracy
- Spatial-Discretization Verification Results
- Verification Techniques for Thermochemical Source Term
  - Techniques
  - Distinctive Features
- Thermochemical-Source-Term Verification Results
- Summary
Verification Techniques for Thermochemical Source Term

• $S(U) = [\dot{w}; 0; 0; Q_{t-v} + e_v^T \dot{w}]$ is algebraic
Verification Techniques for Thermochemical Source Term

\[ S(\mathbf{U}) = \begin{bmatrix} \dot{\mathbf{w}}; 0; 0; Q_{t-v} + \mathbf{e}_v^T \dot{\mathbf{w}} \end{bmatrix} \text{ is algebraic} \]

- \[ S(\mathbf{U}) \text{ computed by same code for both sides of } \mathbf{\tilde{r}}(\mathbf{\tilde{U}}; \mu) = \mathbf{r}(\mathbf{U}_{MS}; \mu) \]
Verification Techniques for Thermochemical Source Term

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- \( S(U) \) computed by same code for both sides of \( \tilde{r}(\tilde{U}; \mu) = r(U_{MS}; \mu) \)
- Manufactured solutions will **not** detect implementation errors
Verification Techniques for Thermochemical Source Term

- $\mathbf{S}(\mathbf{U}) = [\dot{\mathbf{w}}; 0; 0; \dot{Q}_{t-v} + \mathbf{e}^T_v \dot{\mathbf{w}}]$ is algebraic
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- Compute $\dot{Q}_{t-v}(\rho, T, T_v)$, $\mathbf{e}_v(\rho, T, T_v)$, and $\dot{\mathbf{w}}(\rho, T, T_v)$
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- Compute \( Q_{t-v}(\rho, T, T_v), e_v(\rho, T, T_v), \) and \( \dot{w}(\rho, T, T_v) \)
  - For single-cell mesh when initialized to \( \{\rho, T, T_v\} \) with no velocity
Verification Techniques for Thermochemical Source Term

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  - For many values of \( \{\rho, T, T_v\} \)
  - Compare with independently developed code
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  - For single-cell mesh when initialized to \( \{\rho, T, T_v\} \) with no velocity
  - For many values of \( \{\rho, T, T_v\} \)
  - Compare with independently developed code

- For each query, compute symmetric relative difference

\[
\delta_\beta = 2 \left| \frac{\beta_{\text{SPARC}} - \beta'}{\beta_{\text{SPARC}} + \beta'} \right|
\]

\[\beta = \{Q_{t-v}, e_{vN_2}, e_{vO_2}, e_{vNO}, \dot{w}_{N_2}, \dot{w}_{O_2}, \dot{w}_{NO}, \dot{w}_N, \dot{w}_O\}\]
Distinctive Features

This is **not** typical low-rigor code-to-code comparison
Distinctive Features

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Distinctive and rigorous features:
Distinctive Features

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Distinctive and rigorous features:

- Code is independently developed internally
Distinctive Features

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Distinctive and rigorous features:

- Code is independently developed **internally**
  - Uses **same** models and material properties expected from **SPARC**
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  - Comparison is queried for 1000s of conditions, spans extreme ranges
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  - Models and material properties are the same
  - Typically code-to-code comparison accepts a few percent

- **Wide** condition coverage
  - Comparison is queried for 1000s of conditions, spans extreme ranges
  - Code-to-code comparison typically considers single or few conditions
• Introduction

• Governing Equations

• Verification Techniques for Spatial Accuracy

• Spatial-Discretization Verification Results

• Verification Techniques for Thermochemical Source Term

• Thermochemical-Source-Term Verification Results
  – Samples of $Q_{t-v}(\rho, T, T_v)$, $e_v(\rho, T, T_v)$, and $\dot{w}(\rho, T, T_v)$
  – Nonzero Relative Differences in $Q_{t-v}$ and $e_v$
  – Nonzero Relative Differences in $\dot{w}$

• Summary
Samples of $Q_{t-v}(\rho, T, T_v)$, $e_v(\rho, T, T_v)$, and $\dot{w}(\rho, T, T_v)$

| Variable | Minimum | Maximum | Units     | Spacing   |
|----------|---------|---------|-----------|-----------|
| $\rho_{N_2}$ | $10^{-6}$ | $10^1$  | kg/m$^3$  | Logarithmic |
| $\rho_{O_2}$ | $10^{-6}$ | $10^1$  | kg/m$^3$  | Logarithmic |
| $\rho_{NO}$  | $10^{-6}$ | $10^1$  | kg/m$^3$  | Logarithmic |
| $\rho_N$    | $10^{-6}$ | $10^1$  | kg/m$^3$  | Logarithmic |
| $\rho_O$    | $10^{-6}$ | $10^1$  | kg/m$^3$  | Logarithmic |
| $T$         | 100     | 15,000  | K         | Linear    |
| $T_v$       | 100     | 15,000  | K         | Linear    |

Ranges and spacings for 100,000 Latin hypercube samples of $\rho$, $T$, and $T_v$
Original Nonzero Relative Differences in $Q_{t-v}$ and $e_v$
• Relative differences are not near machine precision
• Relative differences are **not** near machine precision

• $\delta_{Q_{t-v}} > 10\%$ in 8.8% of simulations
• Relative differences are not near machine precision
• $\delta_{Q_{t-v}} > 10\%$ in 8.8% of simulations
• $\delta_{Q_{t-v}} > 1\%$ in 29% of simulations
Relative differences are not near machine precision.

- $\delta_{Q_{t-v}} > 10\%$ in 8.8% of simulations.
- $\delta_{Q_{t-v}} > 1\%$ in 29% of simulations.
- $\delta_{e_v} > 100\%$ for some simulations.
Causes of Large Relative Differences in $Q_{t-v}$ and $e_v$

Two causes:

• Incorrect lookup table values for vibrational constants
  – For $N_2$ and $O_2$ when the colliding species is NO
  – Introduced error in $Q_{t-v}$ for all simulations
  – For high-enthalpy (20 MJ/kg), hypersonic, laminar double-cone flow, 1.4% change in pressure and 2.7% change in heat flux

• Loose convergence criteria for computing $T_v$ from $\rho e_v$
  – Unsuitable for low values of $T_v$
  – Introduced errors in $Q_{t-v}$ and $e_v$ for a few simulations
  – For converged, steady problem, original criteria are acceptable
Causes of Large Relative Differences in $Q_{t-v}$ and $e_v$

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Corrected Nonzero Relative Differences in $Q_{t-v}$ and $e_v$

Original lookup table and convergence criteria

![Graph showing corrected nonzero relative differences in $Q_{t-v}$ and $e_v$]
Corrected Nonzero Relative Differences in $Q_{t-v}$ and $e_v$

Original lookup table and convergence criteria

![Graph 1](#)

Corrected lookup table and tighter convergence criteria

![Graph 2](#)
Corrected Nonzero Relative Differences in $Q_{t-v}$ and $e_v$

- Relative differences are consistent with our expectations

![Histogram of $\log_{10} \delta_{Q_{t-v}}$](image1)

![Histogram of $\log_{10} \delta_{e_v}$](image2)
• Relative differences are consistent with our expectations

• $\delta_{Q_{t-v}} < 10^{-10}$ and $\delta_{e_v} < 10^{-14}$ in all simulations
Corrected Nonzero Relative Differences in $Q_{t-v}$ and $e_v$

- Relative differences are consistent with our expectations
- $\delta_{Q_{t-v}} < 10^{-10}$ and $\delta_{e_v} < 10^{-14}$ in all simulations
- $\delta_{Q_{t-v}} > 10^{-12}$ in 28/100,000 simulations
Corrected Nonzero Relative Differences in $Q_{t-v}$ and $e_v$

- Relative differences are consistent with our expectations
- $\delta_{Q_{t-v}} < 10^{-10}$ and $\delta_{e_v} < 10^{-14}$ in all simulations
- $\delta_{Q_{t-v}} > 10^{-12}$ in 28/100,000 simulations
  - $T$ and $T_v$ have relative difference less than 0.2%
Corrected Nonzero Relative Differences in $Q_{t-v}$ and $e_v$

- Relative differences are consistent with our expectations
- $\delta_{Q_{t-v}} < 10^{-10}$ and $\delta_{e_v} < 10^{-14}$ in all simulations
- $\delta_{Q_{t-v}} > 10^{-12}$ in 28/100,000 simulations
  - $T$ and $T_v$ have relative difference less than 0.2%
  - In numerator of $\frac{e_{v_s,m}(T) - e_{v_s,m}(T_v)}{\langle \tau_{s,m} \rangle}$, $e_{v_s,m}(T)$ and $e_{v_s,m}(T_v)$ share many leading digits
Corrected Nonzero Relative Differences in $Q_{t-v}$ and $e_v$

- Relative differences are consistent with our expectations
- $\delta_{Q_{t-v}} < 10^{-10}$ and $\delta_{e_v} < 10^{-14}$ in all simulations
- $\delta_{Q_{t-v}} > 10^{-12}$ in 28/100,000 simulations
  - $T$ and $T_v$ have relative difference less than 0.2%
  - In numerator of $\frac{e_{v_{s,m}}(T) - e_{v_{s,m}}(T_v)}{\langle \tau_{s,m} \rangle}$, $e_{v_{s,m}}(T)$ and $e_{v_{s,m}}(T_v)$ share many leading digits
  - Precision lost when computing difference
Nonzero Relative Differences in $\dot{w}$

![Graph showing the distribution of nonzero relative differences in $\dot{w}$.]
Nonzero Relative Differences in $\dot{w}$

- Relative differences are consistent with our expectations

![Bar chart showing nonzero relative differences in $\dot{w}$]
Nonzero Relative Differences in $\dot{w}$

- Relative differences are consistent with our expectations
- $\dot{w} < 10^{-9}$ in all simulations
Nonzero Relative Differences in $\dot{w}$

- Relative differences are consistent with our expectations
- $\dot{w} < 10^{-9}$ in all simulations
- $\dot{w} > 10^{-12}$ for 87/500,000 computed values (5 species, 100,000 simulations)
Nonzero Relative Differences in $\dot{w}$

- Relative differences are consistent with our expectations
- $\dot{w} < 10^{-9}$ in all simulations
- $\dot{w} > 10^{-12}$ for 87/500,000 computed values (5 species, 100,000 simulations)
  - Due to precision loss that can occur from subtraction in
    \[
    \dot{w}_s = M_s \sum_{r=1}^{n_r} (\beta_{s,r} - \alpha_{s,r}) (R_{f_r} - R_{b_r})
    \]
Outline

- Introduction
- Governing Equations
- Verification Techniques for Spatial Accuracy
- Spatial-Discretization Verification Results
- Verification Techniques for Thermochemical Source Term
- Thermochemical-Source-Term Verification Results
- Summary
  - Code-Verification Techniques
Code-Verification Techniques

• Manufactured and exact solutions
  – Effective approaches for verifying spatial accuracy – detected multiple issues
  – Rigorous norms improve effectiveness – $L^\infty$-norm of error more useful
  – Insufficient for algebraic source terms – both evaluations the same

• Thermochemical-source-term approach
  – Effective approach for verifying implementation – detected multiple issues
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