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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

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- Introduction
  - Hypersonic Flow
  - Sandia Parallel Aerodynamics and Reentry Code (SPARC)
  - Verification and Validation
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Hypersonic Flow

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)

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

Verification and Validation

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

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

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

Outline

- Introduction
- 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
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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

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

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

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

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

$p = \sum_{s=1}^{n_s} \frac{\rho_s}{M_s} \bar{R} T$, $\mathbf{e}_v = \left\{e_{v_1}, \ldots, e_{v_{n_s}}\right\}^T$: vibrational energies per mass,

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

$$E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho}\left(c_{\mathcal{V}_s} T + e_{v_s} + h_s^o\right)$$

Governing Equations: n_s Species in Vibrational Nonequilibrium

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Multiple species

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

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

$p = \sum_{s=1}^{n_s} \frac{\rho_s}{M_s} \bar{R}T$, $\quad \mathbf{e}_v = \{e_{v_1}, \dots, e_{v_{n_s}}\}^T$: vibrational energies per mass,

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

$$E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho}\left(c_{\mathcal{V}_s}T + e_{v_s} + h_s^o\right)$$

Governing Equations: n_s Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

Local time derivative

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

where

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

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

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

$$E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho}\left(c_{\mathcal{V}_s} T + e_{v_s} + h_s^o\right)$$

Governing Equations: n_s Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

Convective flux gradient

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

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

$$E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho} \left(c_{\mathcal{V}_s} T + e_{v_s} + h_s^o\right)$$

Governing Equations: n_s Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

Pressure flux gradient

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

where

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Governing Equations: n_s Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

Diffusive flux gradient

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Governing Equations: n_s Species in Vibrational Nonequilibrium

Conservation of mass, momentum, and energy:

Thermochemical source term

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

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

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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

$$e_{v_{s,m}}(T') = \frac{\bar{R}}{M_s} \frac{\theta_{v_{s,m}}}{\exp\left(\theta_{v_{s,m}}/T'\right) - 1}$$

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:

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

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

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

where

$$y_s = \frac{\rho_s / M_s}{\sum_{s'=1}^{n_s} \rho_{s'}/M_{s'}}, \quad \tau_{s,m,s'} = \frac{\exp\left[a_{s,m,s'} \left(T^{-1/3} - b_{s,m,s'} \right) - 18.42 \right]}{p'}, \quad \sigma_{v_s} = \sigma'_{v_s} \left(\frac{50{,}000 \text{ K}}{T} \right)^2$$

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

σ_{v_s}: collision-limiting vibrational cross section

σ'_{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:

$$R_{f_r} = \gamma k_{f_r} \prod_{s=1}^{n_s} \left(\frac{1}{\gamma}\frac{\rho_s}{M_s}\right)^{\alpha_{s,r}} \quad \text{and} \quad R_{b_r} = \gamma k_{b_r} \prod_{s=1}^{n_s} \left(\frac{1}{\gamma}\frac{\rho_s}{M_s}\right)^{\beta_{s,r}}$$

Forward and backward reaction rate coefficients:

$$k_{f_r}(T_c) = C_{f_r} T_c^{\eta_r} \exp\left(-\theta_r/T_c\right) \quad \text{and} \quad k_{b_r}(T) = \frac{k_{f_r}(T)}{K_{e_r}(T)}$$

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

γ: unit conversion factor

C_{f_r}, η_r, A_{i_r}: empirical parameters

θ_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:

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Scope of Code Verification

Conservation of mass, momentum, and energy:

Non-diffusive flux gradients

Thermochemical source term

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

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

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$p = \sum_{s=1}^{n_s} \frac{\rho_s}{M_s} \bar{R} T$, $\quad \mathbf{e}_v = \{e_{v_1}, \dots, e_{v_{n_s}}\}^T$: vibrational energies per mass,

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

$$E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho}(c_{\mathcal{V}_s} T + e_{v_s} + h_s^o)$$

Scope of Code Verification

Conservation of mass, momentum, and energy:

Non-diffusive flux gradients

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

where

Spatial discretization

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

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

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

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

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

$$E = \frac{|\mathbf{v}|^2}{2} + \sum_{s=1}^{n_s} \frac{\rho_s}{\rho}\left(c_{\mathcal{V}_s} T + e_{v_s} + h_s^o\right)$$

Scope of Code Verification

Conservation of mass, momentum, and energy:

Thermochemical source term

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

where

Implementation

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

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Outline

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- Governing Equations
- Verification Techniques for Spatial Accuracy
  - Spatial Accuracy
  - Solutions
  - Error Norms
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Spatial Accuracy (Steady State)

Governing equations
$\mathbf{r}(\mathbf{U};\boldsymbol{\mu}) = \mathbf{0}$

Discretized equations
$\tilde{\mathbf{r}}(\tilde{\mathbf{U}};\boldsymbol{\mu}) = \mathbf{0}$

For $\tilde{p}^{\text{th}}$-order-accurate discretization, error is

$$\mathbf{e}(\mathbf{x}) = \tilde{\mathbf{U}}(\mathbf{x}) - \mathbf{U}(\mathbf{x}) = \mathbf{C}(\mathbf{x})h^{\tilde{p}(\mathbf{x})} + \mathcal{O}(h^{\tilde{p}(\mathbf{x})+1})$$

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 → asymptotic region ($h^{\tilde{p}(\mathbf{x})+1} \ll h^{\tilde{p}(\mathbf{x})}$)

$$\mathbf{e}(\mathbf{x}) \approx \mathbf{C}(\mathbf{x})h^{\tilde{p}(\mathbf{x})}$$

$\mathbf{C}(\mathbf{x})$: function of derivative(s) of the state vector $\mathbf{U}$ at $\mathbf{x}$

- Approximately constant between meshes in asymptotic region

Order of Accuracy

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

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Finer mesh (h/q)

(q-times as fine in each dimension)

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

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

$\tilde{p}(\mathbf{x})$ 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

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- Do not satisfy original equations: $\mathbf{r}(\mathbf{U}_{\text{MS}}; \boldsymbol{\mu}) \neq \mathbf{0}$

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  - Catches localized deviations (expected and **unexpected**)
- Without discontinuities, both norms should yield same p

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  - Single-Species Inviscid Flow in Thermochemical Equilibrium
  - Five-Species Inviscid Flow in Chemical Nonequilibrium
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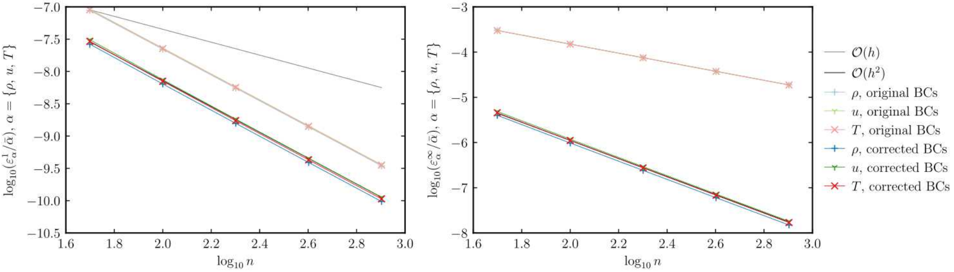
1D Supersonic Flow using a Manufactured Solution

- 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:

$$\begin{aligned} \rho(x) &= \bar{\rho}\left[1 - \epsilon \sin(\pi x)\right], \\ u(x) &= \bar{u}\left[1 - \epsilon \sin(\pi x)\right], \\ T(x) &= \bar{T}\left[1 + \epsilon \sin(\pi x)\right], \end{aligned}$$

$\bar{\rho} = 1$ kg/m^3, $\bar{T} = 300$ K, $\bar{M} = 2.5$, $\epsilon = 0.05$

1D Supersonic Flow using a Manufactured Solution



	First-order accurate			Second-order accurate		
	Original boundary conditions			Corrected boundary conditions		
Mesh	ρ	u	T	ρ	u	T
1–2	1.0008	1.0008	1.0008	2.0313	2.0362	2.0351
2–3	1.0002	1.0002	1.0002	2.0157	2.0184	2.0178
3–4	1.0001	1.0001	1.0000	2.0079	2.0093	2.0090
4–5	1.0000	1.0000	1.0000	2.0040	2.0047	2.0045

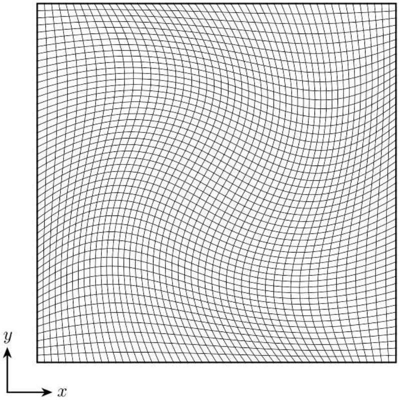
Observed accuracy p using L^∞-norms of the error

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 ($x = 0$ m)
  - Supersonic outflow ($x = 1$ m)
  - Slip wall (tangent flow) ($y = 0$ m & $y = 1$ m)
- 5 nonuniform meshes: $25 \times 25 \rightarrow 400 \times 400$
- Solution consists of small, smooth perturbations to uniform flow:

$$\rho\,(x, y) = \bar{\rho}\left[1 - \epsilon \sin\left(\tfrac{5}{4}\pi x\right)\left(\sin\left(\quad \pi y\right) + \cos\left(\quad \pi y\right)\right)\right],$$
$$u\,(x, y) = \bar{u}\left[1 + \epsilon \sin\left(\tfrac{1}{4}\pi x\right)\left(\sin\left(\quad \pi y\right) + \cos\left(\quad \pi y\right)\right)\right],$$
$$v\,(x, y) = \bar{v}\left[\quad - \epsilon \sin\left(\tfrac{5}{4}\pi x\right)\left(\sin\left(\quad \pi y\right) \qquad\qquad\qquad \right)\right],$$
$$T(x, y) = \bar{T}\left[1 + \epsilon \sin\left(\tfrac{5}{4}\pi x\right)\left(\sin\left(\quad \pi y\right) + \cos\left(\quad \pi y\right)\right)\right],$$

$\bar{\rho} = 1\ \text{kg/m}^3$, $\bar{T} = 300$ K, $\bar{M} = 2.5$, $\epsilon = 0.05$



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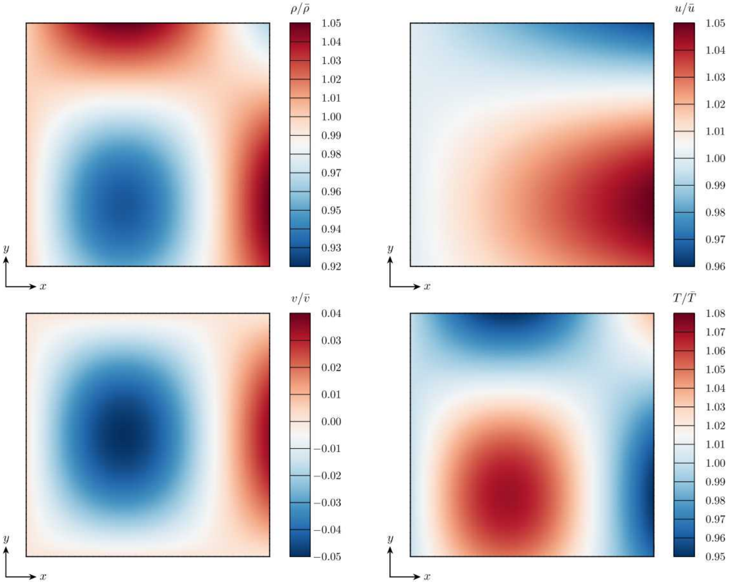

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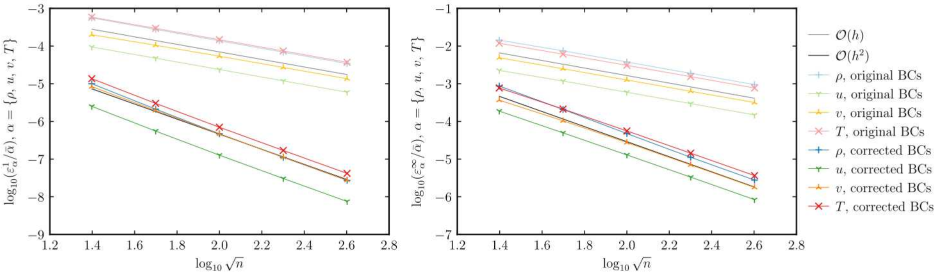
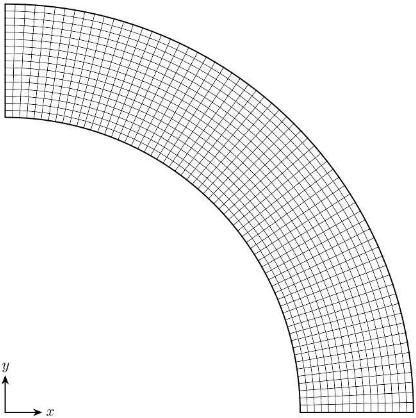


	First-order accurate				Second-order accurate			
	Original boundary conditions				Corrected boundary conditions			
Mesh	ρ	u	v	T	ρ	u	v	T
1–2	0.9420	0.9409	0.9721	0.9628	2.0623	1.9188	1.8174	1.8598
2–3	0.9850	0.9902	0.9910	0.9874	2.1304	1.9450	1.9221	1.9280
3–4	0.9960	1.0002	0.9924	0.9952	2.0902	1.9603	1.9671	1.9586
4–5	0.9989	1.0009	0.9959	0.9984	2.0128	1.9823	1.9860	1.9809

Observed accuracy p using L^∞-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:



$$\rho(r) = \rho_i \left[1 + \frac{\gamma - 1}{2} M_i^2 \left(1 - \left(\frac{r_i}{r}\right)^2\right)\right]^{\frac{1}{\gamma-1}},$$

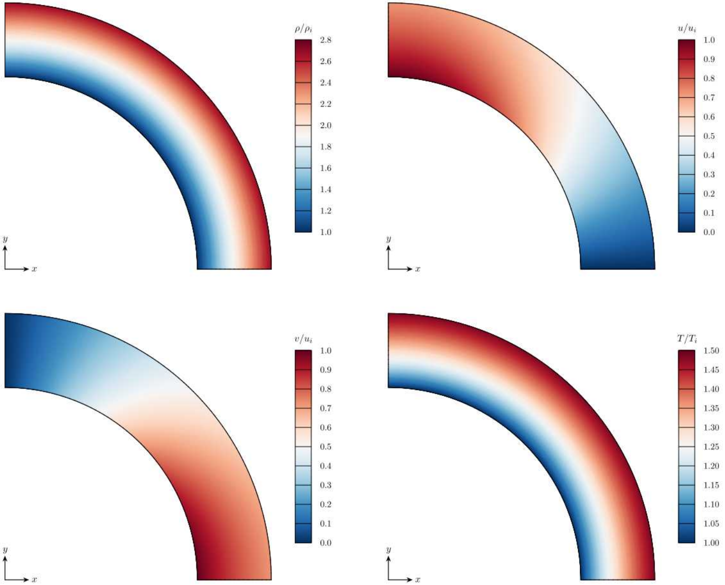
$$u_r(r) = 0,$$

$$u_\theta(r) = -a_i M_i \frac{r_i}{r},$$

$$T(r) = T_i \left[1 + \frac{\gamma - 1}{2} M_i^2 \left(1 - \left(\frac{r_i}{r}\right)^2\right)\right],$$

$\rho_i = 1,\ a_i = 1,\ M_i = 2.25,\ T_i = 1/(\gamma R)$

2D Supersonic Flow using an Exact Solution



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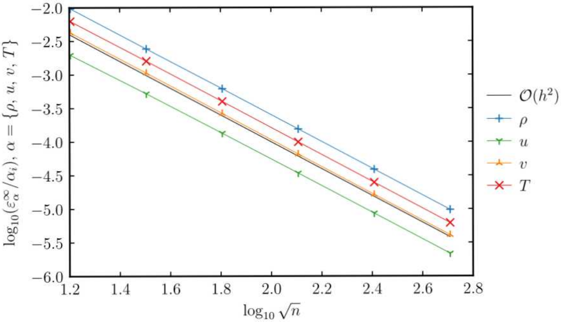


Mesh	ρ	u	v	T
1–2	1.9896	1.9119	1.9943	1.9699
2–3	1.9735	1.9589	2.0070	1.9979
3–4	1.9954	1.9760	2.0099	2.0076
4–5	1.9972	1.9879	2.0054	2.0044
5–6	1.9986	1.9940	2.0029	2.0025

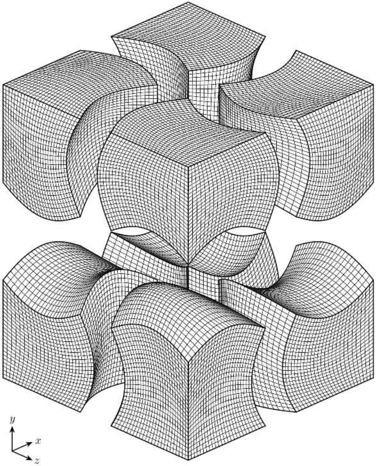
Observed accuracy p using L^∞-norms of the error

3D Supersonic Flow using a Manufactured Solution

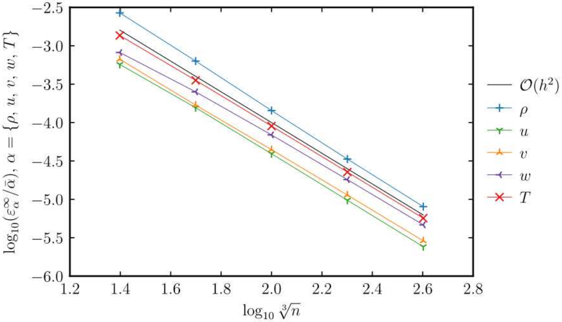
- Three-dimensional domain: $(x, y, z) \in [0,\ 1]\ \text{m} \times [0,\ 1]\ \text{m} \times [0,\ 1]\ \text{m}$
- Boundary conditions:
  - Supersonic inflow ($x = 0$ m)
  - Supersonic outflow ($x = 1$ m)
  - Slip wall (tangent flow)
    ($y = 0$ m, $y = 1$ m, $z = 0$ m, $z = 1$ m)
- 5 nonuniform meshes:
  $25 \times 25 \times 25 \rightarrow 400 \times 400 \times 400$
- Solution consists of small, smooth perturbations to uniform flow:

$$\begin{aligned}
\rho(x,y,z) &= \bar{\rho}\big[1 - \epsilon \sin\left(\tfrac{5}{4}\pi x\right)(\sin(\pi y) + \cos(\pi y))(\sin(\pi z) + \cos(\pi z))\big],\\
u(x,y,z) &= \bar{u}\big[1 + \epsilon \sin\left(\tfrac{1}{4}\pi x\right)(\sin(\pi y) + \cos(\pi y))(\sin(\pi z) + \cos(\pi z))\big],\\
v(x,y,z) &= \bar{v}\big[\ \ - \epsilon \sin\left(\tfrac{5}{4}\pi x\right)(\sin(\pi y) \qquad\qquad)(\sin(\pi z) + \cos(\pi z))\big],\\
w(x,y,z) &= \bar{w}\big[\ \ - \epsilon \sin\left(\tfrac{5}{4}\pi x\right)(\sin(\pi y) + \cos(\pi y))(\sin(\pi z) \qquad\qquad)\big],\\
T(x,y,z) &= \bar{T}\big[1 + \epsilon \sin\left(\tfrac{5}{4}\pi x\right)(\sin(\pi y) + \cos(\pi y))(\sin(\pi z) + \cos(\pi z))\big],
\end{aligned}$$

$\bar{\rho} = 1\ \text{kg/m}^3$, $\bar{T} = 300$ K, $\bar{M} = 2.5$, $\epsilon = 0.05$



3D Supersonic Flow using a Manufactured Solution



Mesh	ρ	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^∞-norms of the error

Five-Species Air Model

5 species: N_2, O_2, NO, N, and O

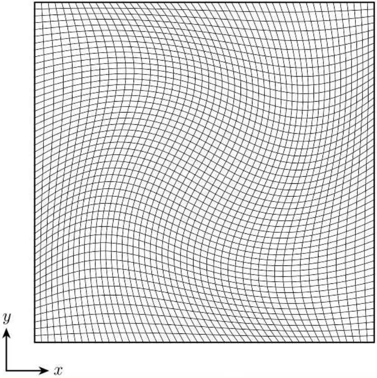
17 reactions:

r	Reaction	Type of Reaction
1–5	$N_2 + \mathcal{M} \leftrightharpoons N + N + \mathcal{M}, \quad \mathcal{M} = \{N_2, O_2, NO, N, O\}$	Dissociation
6–10	$O_2 + \mathcal{M} \leftrightharpoons O + O + \mathcal{M}, \quad \mathcal{M} = \{N_2, O_2, NO, N, O\}$	Dissociation
11–15	$NO + \mathcal{M} \leftrightharpoons N + O + \mathcal{M}, \quad \mathcal{M} = \{N_2, O_2, NO, N, O\}$	Dissociation
16	$N_2 + O \leftrightharpoons N + NO$	Exchange
17	$NO + O \leftrightharpoons N + O_2$	Exchange

Five-Species Inviscid Flow in Chemical Nonequilibrium

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

$$
\begin{aligned}
\rho_{\mathrm{N}_2}(x, y) &= \bar{\rho}_{\mathrm{N}_2}\left[1 - \epsilon \sin\left(\tfrac{5}{4}\pi x\right)\left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right],\\
\rho_{\mathrm{O}_2}(x, y) &= \bar{\rho}_{\mathrm{O}_2}\left[1 + \epsilon \sin\left(\tfrac{3}{4}\pi x\right)\left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right],\\
\rho_{\mathrm{NO}}(x, y) &= \bar{\rho}_{\mathrm{NO}}\left[1 + \epsilon \sin\left(\pi x\right)\left(\sin\left(\pi y\right)\right)\right],\\
\rho_{\mathrm{N}}(x, y) &= \bar{\rho}_{\mathrm{N}}\left[1 + \epsilon \sin\left(\pi x\right)\left(\cos\left(\tfrac{1}{4}\pi y\right)\right)\right],\\
\rho_{\mathrm{O}}(x, y) &= \bar{\rho}_{\mathrm{O}}\left[1 + \epsilon \sin\left(\pi x\right)\left(\sin\left(\pi y\right) + \cos\left(\tfrac{1}{4}\pi y\right)\right)\right],\\
u(x, y) &= \bar{u}\left[1 + \epsilon \sin\left(\tfrac{1}{4}\pi x\right)\left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right],\\
v(x, y) &= \bar{v}\left[\ - \epsilon \sin\left(\tfrac{5}{4}\pi x\right)\left(\sin\left(\pi y\right)\right)\right],\\
T(x, y) &= \bar{T}\left[1 + \epsilon \sin\left(\tfrac{5}{4}\pi x\right)\left(\sin\left(\pi y\right) + \cos\left(\pi y\right)\right)\right],\\
T_v(x, y) &= \bar{T}_v\left[1 + \epsilon \sin\left(\tfrac{3}{4}\pi x\right)\left(\sin\left(\tfrac{5}{4}\pi y\right) + \cos\left(\tfrac{3}{4}\pi y\right)\right)\right]
\end{aligned}
$$



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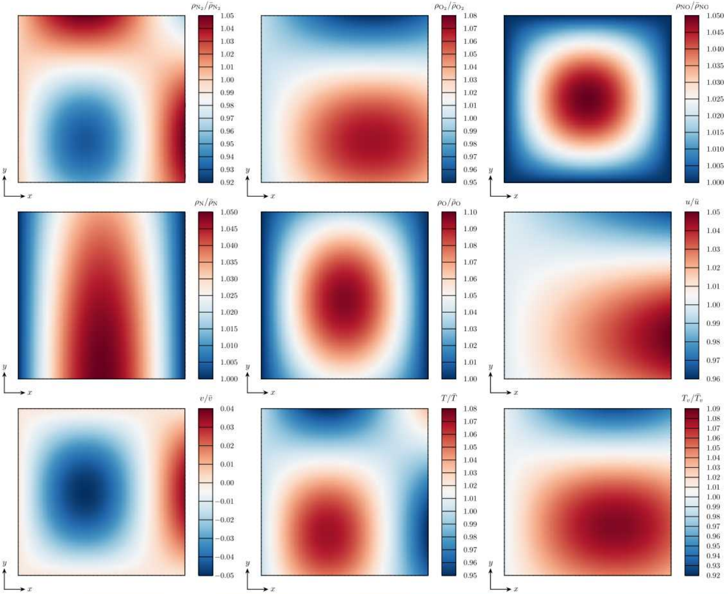
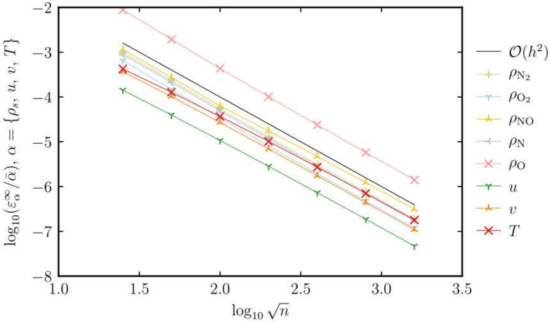


2D Supersonic Flow in Thermal Equilibrium using a Manufactured Solution

Variable	Value	Units
$\bar{\rho}_{N_2}$	0.77	kg/m^3
$\bar{\rho}_{O_2}$	0.20	kg/m^3
$\bar{\rho}_{NO}$	0.01	kg/m^3
$\bar{\rho}_{N}$	0.01	kg/m^3
$\bar{\rho}_{O}$	0.01	kg/m^3
$\bar{T}$	3500	K
$\bar{M}$	2.5	
ϵ	0.05	

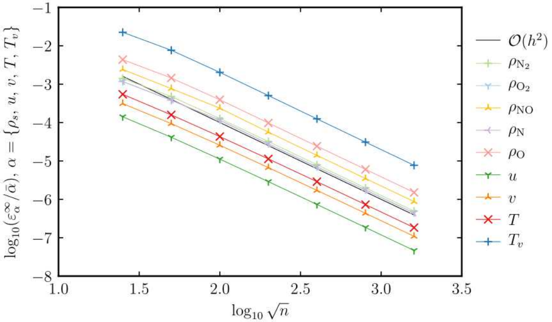


Mesh	ρ_{N_2}	ρ_{O_2}	ρ_{NO}	ρ_N	ρ_O	u	v	T
1–2	2.0608	2.1382	2.0698	2.0644	2.1885	1.8425	1.8289	1.7351
2–3	2.1161	2.1219	2.1127	2.1072	2.1697	1.8875	1.9220	1.7923
3–4	2.0798	2.0813	1.8555	2.0754	2.0971	1.9200	1.9686	1.8525
4–5	2.0456	2.0458	1.8917	2.0428	2.0806	1.9522	1.9871	1.9079
5–6	2.0243	2.0243	1.9427	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, $n_s = 5$, $T_v = T$, $\dot{\mathbf{w}} \neq \mathbf{0}$: Observed accuracy p using L^∞-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	
ϵ	0.05	



Mesh	ρ_{N_2}	ρ_{O_2}	ρ_{NO}	ρ_N	ρ_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, $n_s = 5$, $T_v \neq T$, $\dot{\mathbf{w}} \neq \mathbf{0}$: Observed accuracy p using L^∞-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
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Verification Techniques for Thermochemical Source Term

- $\mathbf{S}(\mathbf{U}) = \left[\dot{\mathbf{w}};\, \mathbf{0};\, 0;\, Q_{t-v} + \mathbf{e}_v^T \dot{\mathbf{w}}\right]$ is algebraic

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  - For single-cell mesh when initialized to $\{\boldsymbol{\rho},\, T,\, T_v\}$ with no velocity
  - For many values of $\{\boldsymbol{\rho},\, T,\, T_v\}$
  - Compare with independently developed code
- For each query, compute symmetric relative difference

$$\delta_\beta = 2\left|\frac{\beta_{\texttt{SPARC}} - \beta'}{\beta_{\texttt{SPARC}} + \beta'}\right|$$

$$\beta = \left\{Q_{t-v},\, e_{v_{\mathrm{N}_2}},\, e_{v_{\mathrm{O}_2}},\, e_{v_{\mathrm{NO}}},\, \dot{w}_{\mathrm{N}_2},\, \dot{w}_{\mathrm{O}_2},\, \dot{w}_{\mathrm{NO}},\, \dot{w}_{\mathrm{N}},\, \dot{w}_{\mathrm{O}}\right\}$$

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- **Wide** condition coverage
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  - Nonzero Relative Differences in Q_{t-v} and $\mathbf{e}_v$
  - Nonzero Relative Differences in $\dot{\mathbf{w}}$
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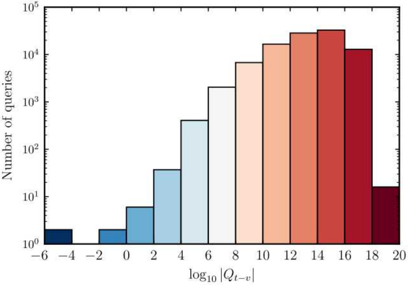
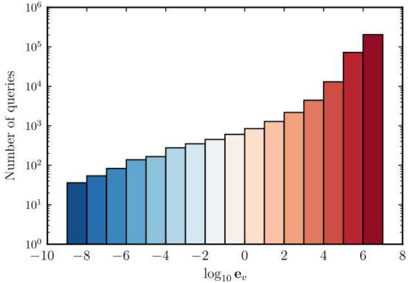
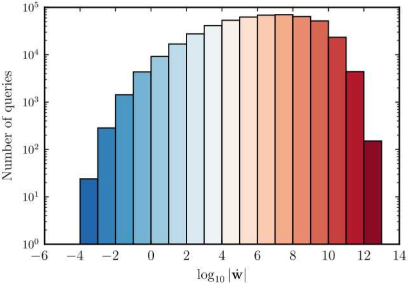
Samples of $Q_{t-v}(\boldsymbol{\rho}, T, T_v)$, $\mathbf{e}_v(\boldsymbol{\rho}, T, T_v)$, and $\dot{\mathbf{w}}(\boldsymbol{\rho}, T, T_v)$

Variable	Minimum	Maximum	Units	Spacing
ρ_{N_2}	10^{-6}	10^{1}	kg/m^3	Logarithmic
ρ_{O_2}	10^{-6}	10^{1}	kg/m^3	Logarithmic
ρ_{NO}	10^{-6}	10^{1}	kg/m^3	Logarithmic
ρ_{N}	10^{-6}	10^{1}	kg/m^3	Logarithmic
ρ_{O}	10^{-6}	10^{1}	kg/m^3	Logarithmic
T	100	15,000	K	Linear
T_v	100	15,000	K	Linear

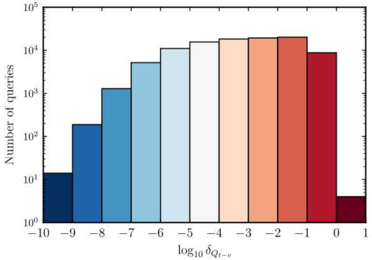
Ranges and spacings for 100,000 Latin hypercube samples of $\boldsymbol{\rho}$, T, and T_v

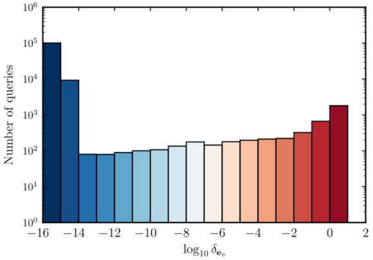






Original Nonzero Relative Differences in Q_{t-v} and $\mathbf{e}_v$





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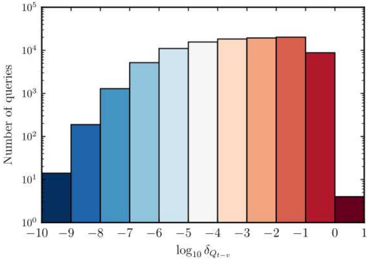

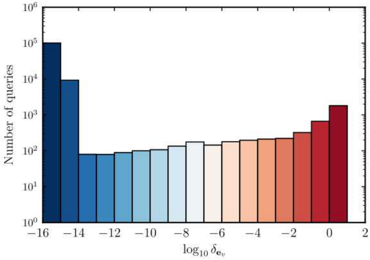

- Relative differences are not near machine precision

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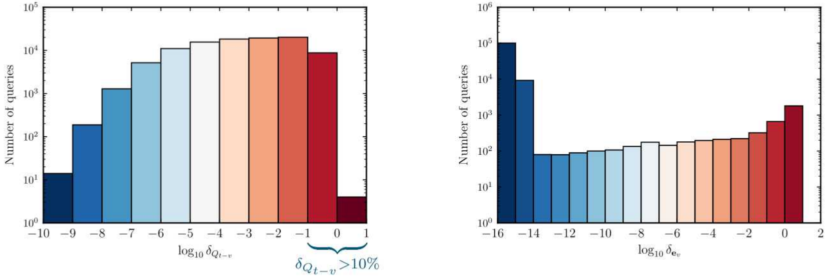
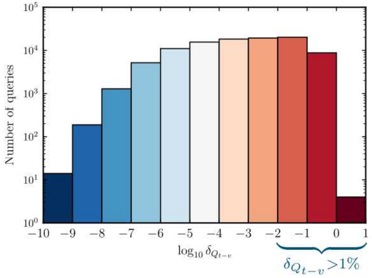
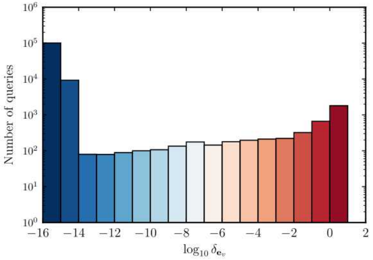


- Relative differences are not near machine precision
- $\delta_{Q_{t-v}} > 10\%$ in 8.8% of simulations

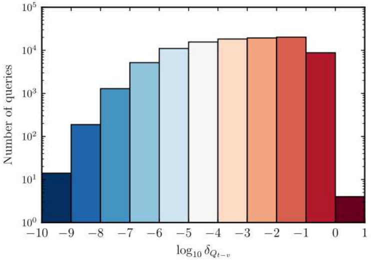
Original Nonzero Relative Differences in Q_{t-v} and $\mathbf{e}_v$

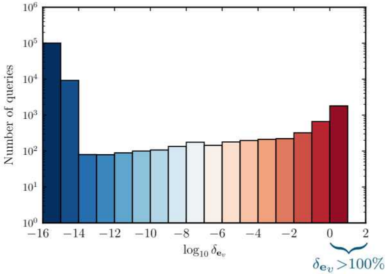




- Relative differences are not near machine precision
- $\delta_{Q_{t-v}} > 10\%$ in 8.8% of simulations
- $\delta_{Q_{t-v}} > 1\%$ in 29% of simulations

Original Nonzero Relative Differences in Q_{t-v} and $\mathbf{e}_v$





- 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
- $\delta_{\mathbf{e}_v} > 100\%$ for some simulations

Causes of Large Relative Differences in Q_{t-v} and $\mathbf{e}_v$

Two causes:

Causes of Large Relative Differences in Q_{t-v} and $\mathbf{e}_v$

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- **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

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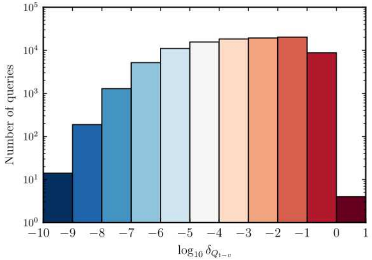
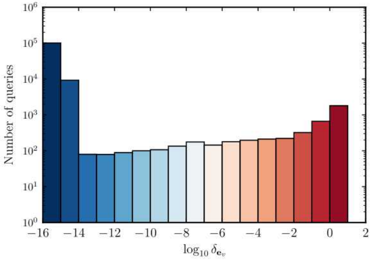
- **Loose convergence criteria** for computing T_v from ρe_v
  - Unsuitable for low values of T_v
  - Introduced errors in Q_{t-v} and $\mathbf{e}_v$ for a few simulations
  - For converged, steady problem, original criteria are acceptable

Corrected Nonzero Relative Differences in Q_{t-v} and $\mathbf{e}_v$

Original lookup table and convergence criteria





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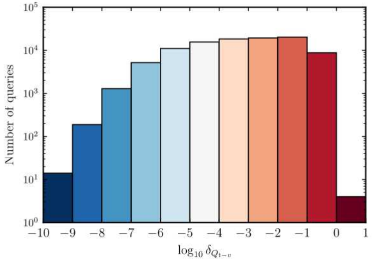
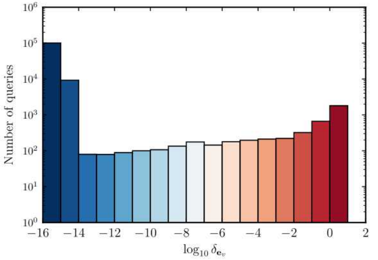
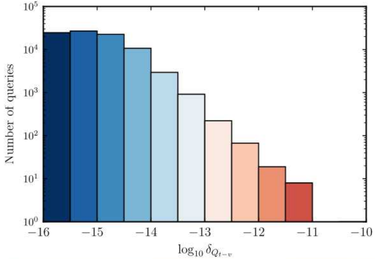
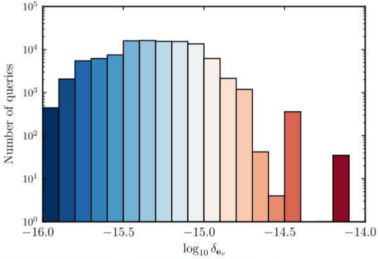




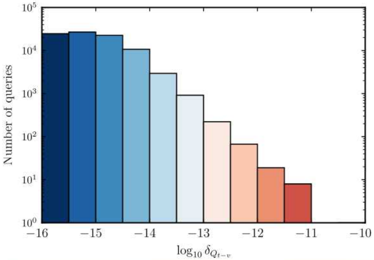
Corrected lookup table and tighter convergence criteria

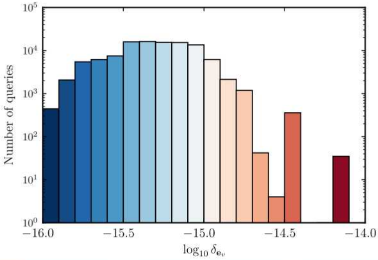




Corrected Nonzero Relative Differences in Q_{t-v} and $\mathbf{e}_v$

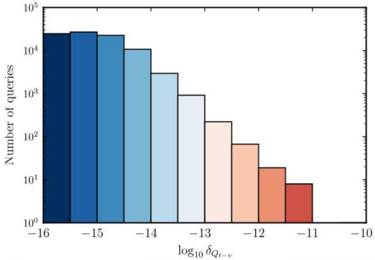
- Relative differences are consistent with our expectations

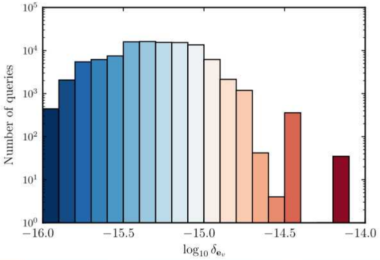




Corrected Nonzero Relative Differences in Q_{t-v} and $\mathbf{e}_v$

- Relative differences are consistent with our expectations
- $\delta_{Q_{t-v}} < 10^{-10}$ and $\delta_{\mathbf{e}_v} < 10^{-14}$ in all simulations





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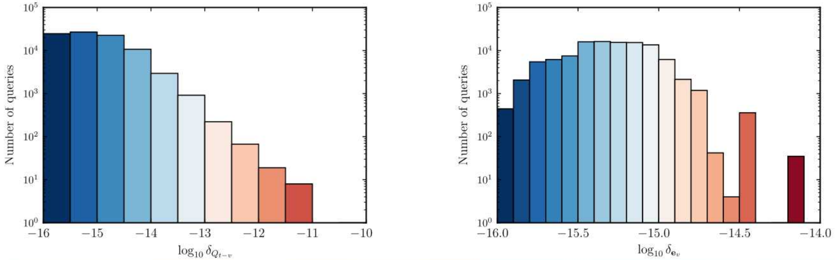
- $\delta_{Q_{t-v}} < 10^{-10}$ and $\delta_{\mathbf{e}_v} < 10^{-14}$ in all simulations
- $\delta_{Q_{t-v}} > 10^{-12}$ in 28/100,000 simulations



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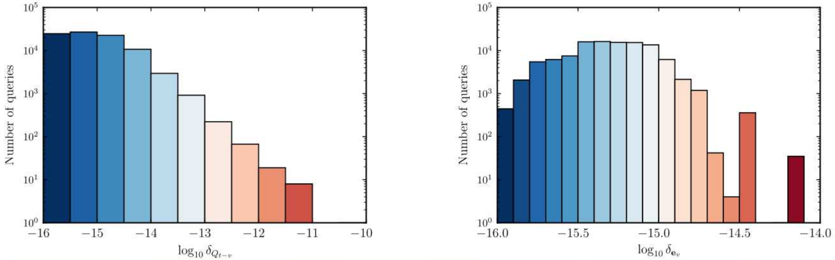

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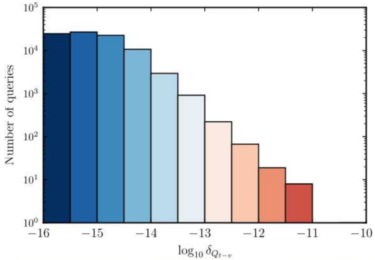

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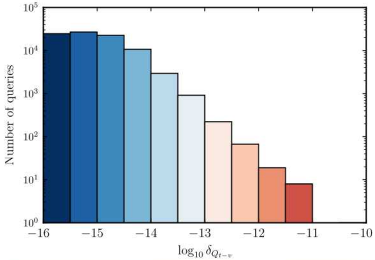
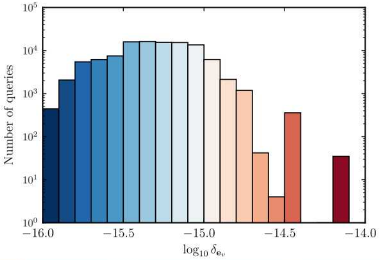
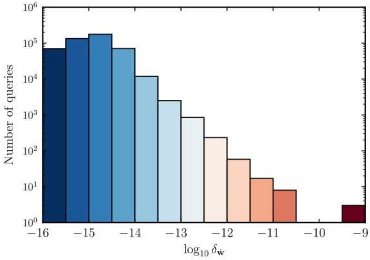
  - Precision lost when computing difference





Nonzero Relative Differences in $\dot{\mathbf{w}}$



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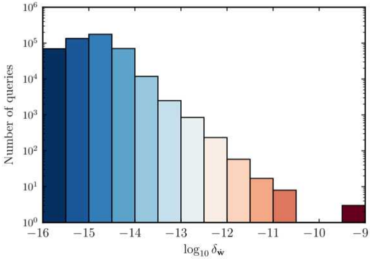

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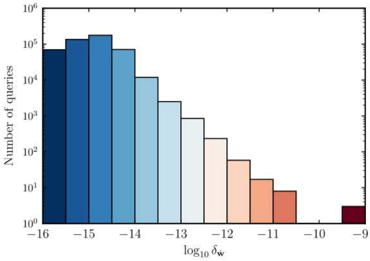
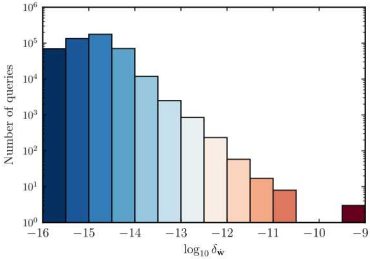


- Relative differences are consistent with our expectations
- $\dot{\mathbf{w}} < 10^{-9}$ in all simulations

Nonzero Relative Differences in $\dot{\mathbf{w}}$



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

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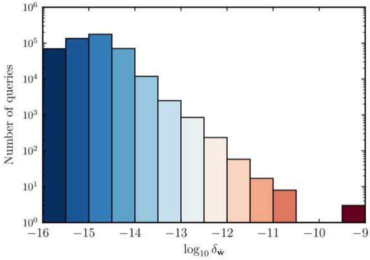

- Relative differences are consistent with our expectations
- $\dot{\mathbf{w}} < 10^{-9}$ in all simulations
- $\dot{\mathbf{w}} > 10^{-12}$ for 87/500,000 computed values (5 species, 100,000 simulations)
  - Due to precision loss that can occur from subtraction in $\dot{w}_s = M_s \sum_{r=1}^{n_r}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

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^∞-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

Questions?

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