MÉTHODES ITÉRATIVES POUR LE TRANSPORT MULTIESPÈCE

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TRANSPORT-PROPERTY COMPUTATIONAL METHODS

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Transport Coefficients in Weak Magnetic Fields (0)

- **Monatomic/Polyatomic/Reactive**

  Chapman and Cowling (1939), Hischfelder, Curtiss, and Bird (1954)

  Waldmann (1958), Devoto (1966), Ferziger and Kaper (1972)

  Wang-Chang Uhlenbeck (1964), De Boer (1951)

  Waldmann and Trubenbacher (1962), Monchick, Yun, and Mason (1963)

  Ludwig and Heil (1960), Nagnibeda and Kustova (1983), Grunfeld (1993), Alexeev, Chikhaoui, and Grushin (1994)

  Zhdanov (2002), Magin and Degrez (2004)

  Giovangigli (1991), Ern and Giovangigli (1994), García Muñoz (2007)

  Nagnibeda and Kustova (2009),

Transport Coefficients in Weak Magnetic Fields (1)

- **Kinetic theory**

  Mixtures

  Ionized gases

  Polyatomic gases

  Reactive gases

- **Semiclassical Boltzmann equations**

$$\partial_t f_k + \boldsymbol{c}_k \cdot \boldsymbol{\nabla} f_k + \boldsymbol{b}_k \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_k} f_k = \frac{1}{\epsilon} \mathcal{J}_k + \epsilon^\alpha \mathcal{R}_k, \qquad k \in \mathcal{S},$$

$$\boldsymbol{b}_k = \boldsymbol{g} + z_k (\boldsymbol{E} + \boldsymbol{c}_k \wedge \boldsymbol{B}) \qquad \mathcal{S} = \{1, \dots, n\}$$

- **Chapman-Enskog expansion**

Transport Coefficients in Weak Magnetic Fields (2)

- **Transport fluxes**

$$\boldsymbol{\Pi} = -\kappa(\boldsymbol{\nabla}\cdot\boldsymbol{v})\mathbb{I} - \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t - \tfrac{2}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{v})\mathbb{I}\big),$$

$$\boldsymbol{\mathcal{V}}_k = -\sum_{l\in\mathcal{S}} D_{kl}\boldsymbol{d}_l - \theta_k\boldsymbol{\nabla}\log T, \qquad k\in\mathcal{S},$$

$$\boldsymbol{Q} = \sum_{k\in\mathcal{S}}\rho h_k Y_k \boldsymbol{\mathcal{V}}_k - \widehat{\lambda}\boldsymbol{\nabla}T - p\sum_{k\in\mathcal{S}}\theta_k\boldsymbol{d}_k,$$

- **Diffusion driving forces**

$$\boldsymbol{d}_k = \frac{\boldsymbol{\nabla}p_k}{p} - \frac{\rho_k z_k}{p}(\boldsymbol{E} + \boldsymbol{v}\wedge\boldsymbol{B}),$$

Transport Coefficients in Weak Magnetic Fields (3)

- **Alternative formulation**

$$\mathcal{V}_k = -\sum_{l \in \mathcal{S}} D_{kl} (\boldsymbol{d}_l + \chi_l \boldsymbol{\nabla} \log T), \qquad l \in \mathcal{S},$$

$$\boldsymbol{Q} = \sum_{k \in \mathcal{S}} \rho h_k Y_k \mathcal{V}_k - \lambda \boldsymbol{\nabla} T + p \sum_{k \in \mathcal{S}} \chi_k \mathcal{V}_k,$$

- **Transport linear systems**

  Integral equations with constraints (linearized Boltzmann)

  Galerkin variational procedure (Standard and Reduced spaces)

  Linear systems with constraints

  Natural symmetric singular formalism

Isotropic Transport Linear Systems (1)

- **Form of the linear systems**

  Regular case $G\alpha = \beta,$

  Singular case $\begin{cases} G\alpha = & \beta, \\ \langle \alpha, \mathcal{G} \rangle = & 0, \end{cases}$

  Transport coefficient $\mu = \langle \alpha, \beta' \rangle$

- **Symmetric formalism**

  Calculation of the symmetric systems/ Comparison with Monchick, Yun and Mason

  $G^{\mathrm{MYM}} = G - \mathcal{C} \otimes \mathcal{G}$ (up to scaling factors)

  Reduced basis coefficients

  Variational framework for λ and χ

  Mathematical structure of the linear systems and Iterative algorithms

Isotropic Transport Linear Systems (2)

- **System to be solved**

$$\begin{cases} G\alpha &= \beta, & G \in \mathbb{R}^{\omega,\omega}, \\ \langle \alpha, \mathcal{G} \rangle &= 0, & \alpha, \beta, \mathcal{G} \in \mathbb{R}^{\omega}, \end{cases}$$

$$\mu = \langle \alpha, \beta' \rangle$$

- **Mathematical structure**

$$\begin{cases} G \ \text{ is symmetric positive semi-definite,} \qquad N(G) = \mathbb{R}\mathcal{N}, \\ N(G) \oplus \mathcal{G}^{\perp} = \mathbb{R}^{\omega}, \\ \beta \in R(G), \end{cases}$$

- **The sparse transport matrix $db(G)$**

  $db(G)$ is composed of diagonal of blocs of G and is easily invertible

  $2db(G) - G$ and $db(G)$ are symmetric positive definite for $n \geq 3$,

Isotropic Transport Linear Systems (3)

- **Direct method with a symmetric formulation**

$$\widetilde{G}\alpha = \beta, \qquad \widetilde{G} = G + \mathcal{G} \otimes \mathcal{G},$$

- **Generalized conjugate gradient**

  Conjugate gradient algorithm for singular matrices,

- **Stationary iterative methods**

  $G = M - W, \quad M = db(G) + \text{diag}(\sigma_1, \ldots, \sigma_\omega),$

  $T = M^{-1}W, \quad P = \text{Proj}\big(\mathcal{G}^\perp, N(G)\big) = I - \mathcal{N}\otimes\mathcal{G}/\langle\mathcal{N}, \mathcal{G}\rangle,$

  T is convergent, $\varrho(T) = 1$, $\varrho(PT) < 1$, and

$$\alpha = \sum_{0\leq j<\infty} (PT)^j PM^{-1}P^t\beta \qquad \mu = \langle \sum_{0\leq j<\infty} (PT)^j PM^{-1}P^t\beta, \beta' \rangle.$$

  Important point $M + W = 2db(G) - G \; + \; 2\text{diag}(\sigma_1, \ldots, \sigma_n)$ is positive definite,

First Order Diffusion Coefficients

- **First order transport linear systems**

$$\begin{cases} \Delta D &= Q, \\ D\mathsf{y} &= 0, \end{cases} \qquad Q = \mathbb{I} - \mathsf{y}\otimes\mathsf{u}, \qquad P = Q^t = \mathbb{I} - \mathsf{u}\otimes\mathsf{y}, \qquad \mathsf{y} = (Y_1, \ldots, Y_n)^t, \quad \mathsf{u} = (1, \ldots, 1)^t \in \mathbb{R}^n$$

$$\Delta_{kk} = \sum_{\substack{l\in\mathcal{S} \\ l\neq k}} \frac{X_k X_l}{\mathcal{D}_{kl}}, \quad k \in \mathcal{S}, \qquad \Delta_{kl} = -\frac{X_k X_l}{\mathcal{D}_{kl}}, \quad k, l \in \mathcal{S}, \quad k \neq l,$$

- **Asymptotic expansion**

$$\Delta = M - W, \qquad M = \mathrm{diag}\Big(\frac{\Delta_{11}}{1-Y_1}, \ldots, \frac{\Delta_{nn}}{1-Y_n}\Big), \qquad T = M^{-1}W,$$

$$D = \sum_{0\leq j<\infty} (PT)^j P M^{-1} P^t,$$

Transport Coefficients in Strong Magnetic Fields (0)

- **Monatomic/Polyatomic/Reactive**

  Chapman and Cowling (1939),

  Braginsky (1958)(1965),

  Kanenko (1960),

  Ferziger and Kaper (1972),

  Kanenko and Yamao (1980),

  Bruno, Capitelli and Dangola (2003),

  Giovangigli and Graille (2003),

  Bruno, Catalfamo, Laricchiuta, Giordano, and Capitelli (2006)

  Bruno, Laricchiuta, Capitelli, and Catalfamo (2007)

  Giovangigli and Graille (2009)

Transport Coefficients in Strong Magnetic Fields (1)

- **Kinetic theory**

  Mixtures

  Ionized gases

  Polyatomic gases

  Reactive gases

- **Semiclassical Boltzmann equations**

$$\partial_t f_k + \boldsymbol{c}_k \cdot \boldsymbol{\nabla} f_k + \widetilde{\boldsymbol{b}}_k \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_k} f_k + \frac{1}{\epsilon}(\boldsymbol{c}_k - \boldsymbol{v}) \wedge \boldsymbol{B} \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_k} f_k = \frac{1}{\epsilon} \mathcal{J}_k + \epsilon^{\alpha} \mathcal{R}_k, \qquad k \in \mathcal{S},$$

$$\widetilde{\boldsymbol{b}}_k = \boldsymbol{g} + z_k(\boldsymbol{E} + \boldsymbol{v} \wedge \boldsymbol{B})$$

- **Chapman-Enskog expansion**

Transport Coefficients in Strong Magnetic Fields (2)

- **Rotation matrix $R^{\mathcal{B}}$**

$$\boldsymbol{\mathcal{B}} = \boldsymbol{B}/\|\boldsymbol{B}\|, \qquad \boldsymbol{R}^{\mathcal{B}} = \begin{pmatrix} 0 & -\mathcal{B}_3 & \mathcal{B}_2 \\ \mathcal{B}_3 & 0 & -\mathcal{B}_1 \\ -\mathcal{B}_2 & \mathcal{B}_1 & 0 \end{pmatrix}.$$

- **Viscous tensor**

$$\boldsymbol{\Pi} = -\kappa \nabla\cdot\boldsymbol{v}\,\mathbb{I} - \eta_1 \mathsf{S} - \eta_2\left(\boldsymbol{R}^{\mathcal{B}}\,\mathsf{S} - \mathsf{S}\,\boldsymbol{R}^{\mathcal{B}}\right) - \eta_3\left(-\boldsymbol{R}^{\mathcal{B}}\,\mathsf{S}\,\boldsymbol{R}^{\mathcal{B}} + \langle \mathsf{S}\boldsymbol{\mathcal{B}}, \boldsymbol{\mathcal{B}}\rangle\,\boldsymbol{\mathcal{B}}\otimes\boldsymbol{\mathcal{B}}\right)$$
$$- \eta_4\left(\mathsf{S}\,\boldsymbol{\mathcal{B}}\otimes\boldsymbol{\mathcal{B}} + \boldsymbol{\mathcal{B}}\otimes\boldsymbol{\mathcal{B}}\,\mathsf{S} - 2\langle \mathsf{S}\boldsymbol{\mathcal{B}}, \boldsymbol{\mathcal{B}}\rangle\,\boldsymbol{\mathcal{B}}\otimes\boldsymbol{\mathcal{B}}\right) - \eta_5\left(\boldsymbol{\mathcal{B}}\otimes\boldsymbol{\mathcal{B}}\,\mathsf{S}\,\boldsymbol{R}^{\mathcal{B}} - \boldsymbol{R}^{\mathcal{B}}\,\mathsf{S}\,\boldsymbol{\mathcal{B}}\otimes\boldsymbol{\mathcal{B}}\right),$$

$$\mathsf{S} = (\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^t) - \tfrac{2}{3}(\nabla\cdot\boldsymbol{v})\,\mathbb{I},$$

Transport Coefficients in Strong Magnetic Fields (3)

- **Orthogonal vectors associated with $\mathbf{X} \in \mathbb{R}^3$**

$$\mathbf{X}^{\parallel} = (\boldsymbol{\mathcal{B}} \cdot \mathbf{X})\boldsymbol{\mathcal{B}}, \qquad \mathbf{X}^{\perp} = \mathbf{X} - \mathbf{X}^{\parallel} \qquad \mathbf{X}^{\odot} = \boldsymbol{\mathcal{B}} \wedge \mathbf{X},$$

- **Diffusion velocities and heat flux**

$$\begin{aligned}\boldsymbol{\mathcal{V}}_i = & -\sum_{j\in\mathcal{S}} \left(D_{ij}^{\parallel} \boldsymbol{d}_j^{\parallel} + D_{ij}^{\perp} \boldsymbol{d}_j^{\perp} + D_{ij}^{\odot} \boldsymbol{d}_j^{\odot} \right) \\ & - \left(\theta_i^{\parallel} (\boldsymbol{\nabla} \log T)^{\parallel} + \theta_i^{\perp} (\boldsymbol{\nabla} \log T)^{\perp} + \theta_i^{\odot} (\boldsymbol{\nabla} \log T)^{\odot} \right),\end{aligned}$$

$$\begin{aligned}\boldsymbol{\mathcal{Q}} = & - \left(\widehat{\lambda}^{\parallel} (\boldsymbol{\nabla} T)^{\parallel} + \widehat{\lambda}^{\perp} (\boldsymbol{\nabla} T)^{\perp} + \widehat{\lambda}^{\odot} (\boldsymbol{\nabla} T)^{\odot} \right) \\ & - p \sum_{i\in\mathcal{S}} \left(\theta_i^{\parallel} \boldsymbol{d}^{\parallel} + \theta_i^{\perp} \boldsymbol{d}^{\perp} + \theta_i^{\odot} \boldsymbol{d}^{\odot} \right) + \sum_{i\in\mathcal{S}} h_i \rho Y_i \boldsymbol{\mathcal{V}}_i,\end{aligned}$$

Transport Coefficients in Strong Magnetic Fields (4)

- **Alternative formulation**

$$\begin{aligned}
\mathcal{V}_i &= -\sum_{j\in\mathcal{S}} D_{ij}^{\parallel}\big(\boldsymbol{d}_j^{\parallel} + \chi_j^{\parallel}(\boldsymbol{\nabla}\log T)^{\parallel}\big) \\
&\quad -\sum_{j\in\mathcal{S}} D_{ij}^{\perp}\big(\boldsymbol{d}_j^{\perp} + \chi_j^{\perp}(\boldsymbol{\nabla}\log T)^{\perp} + \chi_j^{\odot}(\boldsymbol{\nabla}\log T)^{\odot}\big) \\
&\quad -\sum_{j\in\mathcal{S}} D_{ij}^{\odot}\big(\boldsymbol{d}_j^{\odot} + \chi_j^{\perp}(\boldsymbol{\nabla}\log T)^{\odot} - \chi_j^{\odot}(\boldsymbol{\nabla}\log T)^{\perp}\big), \\
\boldsymbol{\mathcal{Q}} &= -\big(\lambda^{\parallel}(\boldsymbol{\nabla}T)^{\parallel} + \lambda^{\perp}(\boldsymbol{\nabla}T)^{\perp} + \lambda^{\odot}(\boldsymbol{\nabla}T)^{\odot}\big) \\
&\quad + p\sum_{i\in\mathcal{S}}(\chi_i^{\parallel}\boldsymbol{\mathcal{V}}_i^{\parallel} + \chi_i^{\perp}\boldsymbol{\mathcal{V}}_i^{\perp} + \chi_i^{\odot}\boldsymbol{\mathcal{V}}^{\odot}) + \sum_{i\in\mathcal{S}} h_i\rho Y_i\boldsymbol{\mathcal{V}}_i.
\end{aligned}$$

Anisotropic Transport Linear Systems (1)

- **Form of the complex linear systems (properly restructured)**

Regular case $$(G + \mathrm{i}G')\alpha = \beta,$$

Singular case $$\begin{cases} (G + \mathrm{i}G')\alpha = & \beta, \\ \langle \alpha, \mathcal{G} \rangle = & 0, \end{cases}$$

Transport coefficient $$\mu = \langle \alpha, \beta' \rangle$$

- **Polyatomic/Reactive**

New symmetry properties

New definition and variational framework for λ and χ

Reduced basis coefficients and simplified tensor expansion

Mathematical structure of the linear systems and Iterative algorithms

Anisotropic Transport Linear Systems (2)

- **System to be solved**

$$\begin{cases} (G + \mathsf{i}G')\alpha &= \beta, \qquad\qquad G, G' \in \mathbb{R}^{\omega,\omega}, \\ \langle \alpha, \mathcal{G} \rangle &= 0, \qquad\qquad \alpha \in \mathbb{C}^{\omega}, \quad \beta, \mathcal{G} \in \mathbb{R}^{\omega}, \end{cases}$$

$$\mu = \langle \alpha, \beta' \rangle$$

- **Mathematical structure**

$$\begin{cases} G \;\text{ as in the isotropic case,} \\ G' = Q\mathcal{D}'P \text{ where } \mathcal{D}' \text{ is diagonal,} \quad Q = \mathbb{I} - \mathcal{G}\otimes\mathcal{N}/\langle \mathcal{G}, \mathcal{N} \rangle \\ P = \mathbb{I} - \mathcal{N}\otimes\mathcal{G}/\langle \mathcal{G}, \mathcal{N} \rangle, \qquad N(G + \mathsf{i}G') = \mathbb{C}\mathcal{N} \\ N(G + \mathsf{i}G') \oplus \mathcal{G}^{\perp} = \mathbb{C}^{\omega}, \\ \beta \in R(G + \mathsf{i}G') \end{cases}$$

Anisotropic Transport Linear Systems (3)

- **Direct method with a symmetric formulation (complex Choleski)**

$$\widetilde{G}\alpha = \beta, \qquad \widetilde{G} = G + \mathcal{G} \otimes \mathcal{G} + \mathrm{i}G'$$

- **Generalized conjugate gradient**

  Orthogonal residuals algorithm for singular matrices

- **Stationary iterative methods**

  $G + \mathrm{i}G' = M - W, \quad M = db(G) + \mathrm{diag}(\sigma_1, \ldots, \sigma_\omega) + \mathrm{i}G',$

  $\mathcal{T} = M^{-1}W, \quad P = I - \mathcal{N} \otimes \mathcal{G} / \langle \mathcal{N}, \mathcal{G} \rangle,$

  $\mathcal{T}$ is convergent, $\varrho(\mathcal{T}) = 1$, $\varrho(P\mathcal{T}) \le \varrho(PT) < 1$, and

$$\alpha = \sum_{0 \le j < \infty} (P\mathcal{T})^j P M^{-1} P^t \beta \qquad \mu = \langle \sum_{0 \le j < \infty} (P\mathcal{T})^j P M^{-1} P^t \beta, \beta' \rangle.$$

  Easy inversion of $M = db(G) + \mathrm{diag}(\sigma_1, \ldots, \sigma_\omega) + \mathrm{i}G'$

First Order Magnetized Diffusion Coefficients

- **First order magnetized transport linear systems**

$$\begin{cases} (\Delta + \mathsf{i}\Delta')(D^{\perp} + \mathsf{i}D^{\odot}) &= Q, \\ (D^{\perp} + \mathsf{i}D^{\odot})\mathsf{y} &= 0, \end{cases} \qquad \begin{array}{ll} Q = \mathbb{I} - \mathsf{y}\otimes\mathsf{u}, & P = \mathbb{I} - \mathsf{u}\otimes\mathsf{y} \\ \mathsf{y} = (Y_1,\dots,Y_n)^t & \mathsf{u} = (1,\dots,1)^t \in \mathbb{R}^n, \end{array}$$

$$\Delta' = Q \ \mathrm{diag}(\mu_1,\dots,\mu_n)\ P, \qquad \mu_i = n_i q_i B/p, \quad i \in \mathcal{S},$$

- **Asymptotic expansion**

$$\Delta + \mathsf{i}\Delta' = M - W, \qquad M = \mathrm{diag}\Big(\frac{\Delta_{11}}{1-Y_1},\dots,\frac{\Delta_{nn}}{1-Y_n}\Big) + \mathsf{i}\Delta' \qquad \mathfrak{T} = M^{-1}W,$$

$$D^{\perp} + \mathsf{i}D^{\odot} = \sum_{0\le j<\infty} (P\mathfrak{T})^j P M^{-1} P^t,$$

- **Complex Stefan-Maxwell equations**

$$(\Delta + \mathsf{i}\Delta')(\boldsymbol{\mathcal{V}}^{\perp} - \mathsf{i}\,\boldsymbol{\mathcal{V}}^{\odot}) = \boldsymbol{d}^{\perp} - \mathsf{i}\boldsymbol{d}^{\odot} - \mathsf{y}\sum_{i\in\mathcal{S}}(\boldsymbol{d}_i^{\perp} - \mathsf{i}\boldsymbol{d}_i^{\odot}),$$

Transport Coefficients in a Two-Temperature Plasma (0)

- **Thermodynamic Nonequilibrium : State to State or Multi-Temperature Models**

  Bruno and Capitelli (1990–2009), Chikhaoui (1999),

  Kustova and Nagnibeda (1990–2009),

- **Two-Temperature Plasma : Monatomic/Strong electric or magnetic fields**

  Braginsky (1958), Ferziger and Kaper (1972),

  Braginsky (1965), Chemielsky and Ferziger (1966)

  Daybelge (1970), Kolesnikov (1974),

  Petit and Darrozes (1975), Mason and Daniel (1988),

  Zhdanov (2002), Graille, Magin, and Massot (2009)

Transport Coefficients in a Two-Temperature Plasma (1)

- **Kinetic theory**

  Mixtures $\quad \mathcal{S} = \mathcal{H} \cup \mathrm{e}$

  Ionized gases

  Strong magnetic field

  Nonequilibrium $\quad \epsilon \sim \mathrm{Kn} \sim \sqrt{m_\mathrm{e}/m_h}$

- **Multiscale Boltzmann equations**

$$\partial_t f_k + \boldsymbol{c}_k \cdot \boldsymbol{\nabla} f_k + \boldsymbol{b}_k \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_k} f_k = \frac{1}{\epsilon}\Big(\sum_{j \in \mathcal{H}} \mathcal{J}_{kj} + \frac{1}{\epsilon} \mathcal{J}_{\mathrm{e}k} \Big), \qquad k \in \mathcal{H},$$

$$\partial_t f_\mathrm{e} + \frac{1}{\epsilon} \boldsymbol{c}_\mathrm{e} \cdot \boldsymbol{\nabla} f_\mathrm{e} + \frac{1}{\epsilon} \widetilde{\boldsymbol{b}}_\mathrm{e} \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_\mathrm{e}} f_\mathrm{e} + \frac{1}{\epsilon^2} (\boldsymbol{c}_\mathrm{e} - \boldsymbol{v}_h) \wedge \boldsymbol{B} \cdot \boldsymbol{\nabla}_{\boldsymbol{c}_\mathrm{e}} f_\mathrm{e} = \frac{1}{\epsilon^2} \Big(\sum_{j \in \mathcal{H}} \mathcal{J}_{\mathrm{e}j} + \mathcal{J}_{\mathrm{ee}} \Big),$$

$$\boldsymbol{b}_k = \boldsymbol{g} + z_k (\boldsymbol{E} + \boldsymbol{c}_k \wedge \boldsymbol{B}) \qquad \widetilde{\boldsymbol{b}}_\mathrm{e} = \boldsymbol{g} + z_\mathrm{e} (\boldsymbol{E} + \boldsymbol{v}_h \wedge \boldsymbol{B})$$

Transport Coefficients in a Two-Temperature Plasma (2)

- **Multiscale Chapman-Enskog**

  Expansion of collision and streaming operators

  Expansion of collision invariants

  The reference velocity is $\boldsymbol{v}_h$

- **Multiscale steps**

Order	Heavy particles	Electrons
ϵ^{-2}	—	Thermalization at T_{e}
ϵ^{-1}	Thermalization at T_h	Zeroth order momentum
ϵ^{0}	Euler equations	$\mathcal{O}(\epsilon^0)$ Drift diffusion equations
ϵ^{1}	Navier-Stokes equations	$\mathcal{O}(\epsilon^1)$ Drift diffusion equations

Transport Coefficients in a Two-Temperature Plasma (3)

- **Heavy species transport fluxes**

$$\boldsymbol{\Pi}_h = -\kappa_h(\boldsymbol{\nabla}\cdot\boldsymbol{v}_h)\mathbb{I} - \eta_h\big(\boldsymbol{\nabla}\boldsymbol{v}_h + (\boldsymbol{\nabla}\boldsymbol{v}_h)^t - \tfrac{2}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{v}_h)\mathbb{I}\big),$$

$$\boldsymbol{\mathcal{V}}_k = -\sum_{l\in\mathcal{H}} D_{kl}\boldsymbol{d}_l - \theta_k\boldsymbol{\nabla}\log T_h, \qquad k\in\mathcal{H},$$

$$\boldsymbol{Q}_h = \sum_{k\in\mathcal{H}} \rho h_k Y_k \boldsymbol{\mathcal{V}}_k - \widehat{\lambda}_h\boldsymbol{\nabla}T_h - p\sum_{k\in\mathcal{H}}\theta_k\boldsymbol{d}_k,$$

- **Diffusion driving forces**

$$\boldsymbol{d}_k = \frac{\boldsymbol{\nabla}p_k}{p_h} - \frac{\rho_k z_k}{p_h}(\boldsymbol{E} + \boldsymbol{v}_h\wedge\boldsymbol{B}) - \frac{1}{p_h}\widetilde{\boldsymbol{F}}_{k\mathrm{e}}, \qquad k\in\mathcal{H},$$

$$\frac{\widetilde{\boldsymbol{F}}_{k\mathrm{e}}}{p_\mathrm{e}} = -\alpha_{k\mathrm{e}}^{\parallel}\boldsymbol{d}_\mathrm{e}^{\parallel} - \alpha_{k\mathrm{e}}^{\perp}\boldsymbol{d}_\mathrm{e}^{\perp} - \alpha_{k\mathrm{e}}^{\odot}\boldsymbol{d}_\mathrm{e}^{\odot} - \chi_{k\mathrm{e}}^{\parallel}\boldsymbol{\nabla}T_\mathrm{e}^{\parallel} - \chi_{k\mathrm{e}}^{\perp}\boldsymbol{\nabla}T_\mathrm{e}^{\perp} - \chi_{k\mathrm{e}}^{\odot}\boldsymbol{\nabla}T_\mathrm{e}^{\odot}, \qquad k\in\mathcal{H},$$

Transport Coefficients in a Two-Temperature Plasma (4)

- **Electron transport fluxes**

$$\begin{aligned}\mathcal{V}_{\mathrm{e}} =& - D_{ee}^{\|}\boldsymbol{d}_{\mathrm{e}}^{\|} - D_{ee}^{\perp}\boldsymbol{d}_{\mathrm{e}}^{\perp} - D_{ee}^{\odot}\boldsymbol{d}_{\mathrm{e}}^{\odot}\\ & - \theta_{\mathrm{e}}^{\|}(\boldsymbol{\nabla}\log T_{\mathrm{e}})^{\|} - \theta_{\mathrm{e}}^{\perp}(\boldsymbol{\nabla}\log T_{\mathrm{e}})^{\perp} - \theta_{\mathrm{e}}^{\odot}(\boldsymbol{\nabla}\log T_{\mathrm{e}})^{\odot}\\ & - \sum_{i\in\mathcal{H}}\left(\alpha_{ie}^{\|}\boldsymbol{d}_i^{2\|} + \alpha_{ie}^{\perp}\boldsymbol{d}_i^{2\perp} + \alpha_{ie}^{\odot}\boldsymbol{d}_i^{2\odot}\right),\end{aligned}$$

$$\begin{aligned}\boldsymbol{Q}_{\mathrm{e}} =& - \widehat{\lambda}_{\mathrm{e}}^{\|}(\boldsymbol{\nabla}T_{\mathrm{e}})^{\|} - \widehat{\lambda}_{\mathrm{e}}^{\perp}(\boldsymbol{\nabla}T_{\mathrm{e}})^{\perp} - \widehat{\lambda}_{\mathrm{e}}^{\odot}(\boldsymbol{\nabla}T_{\mathrm{e}})^{\odot}\\ & - p_{\mathrm{e}}\Big(\theta_{\mathrm{e}}^{\|}\boldsymbol{d}_{\mathrm{e}}^{\|} + \theta_{\mathrm{e}}^{\perp}\boldsymbol{d}_{\mathrm{e}}^{\perp} + \theta_{\mathrm{e}}^{\odot}\boldsymbol{d}_{\mathrm{e}}^{\odot}\Big)\\ & - p_{\mathrm{e}}\sum_{i\in\mathcal{H}}\left(\theta_{ie}^{\|}\boldsymbol{d}_{\mathrm{e}}^{2\|} + \theta_{ie}^{\perp}\boldsymbol{d}_{\mathrm{e}}^{2\perp} + \theta_{ie}^{\odot}\boldsymbol{d}_{\mathrm{e}}^{2\odot}\right) + \rho_{\mathrm{e}}h_{\mathrm{e}}\mathcal{V}_{\mathrm{e}},\end{aligned}$$

- **Diffusion driving forces**

$$\boldsymbol{d}_{\mathrm{e}} = \frac{\boldsymbol{\nabla}p_{\mathrm{e}}}{p_{\mathrm{e}}} - \frac{\rho_{\mathrm{e}}z_{\mathrm{e}}}{p_{\mathrm{e}}}(\boldsymbol{E} + v_h\wedge\boldsymbol{B}), \qquad \boldsymbol{d}_i^2 = -n_i\mathcal{V}_i, \quad i\in\mathcal{H},$$

Nonequilibrium Transport Linear Systems

- **Heavy species transport linear systems**

  Identical to the isotropic systems with $\mathcal{S}$ replaced by $\mathcal{H}$

  No polarisation effects

  Coupling with electrons through modified diffusion driving forces

- **Electrons transport linear systems**

  Small systems similar to the regular anisotropic case

  Second order expansion of the transport fluxes

- **Equilibrium $T_h = T_\mathrm{e}$**

  The fluxes can be recovered from the equilibrium theory

High Temperature Air (0)

- **High temperature air**

  Eleven species N_2 O_2 NO N O N_2^+ O_2^+ NO^+ N^+ O^+ E

  Thermodynamics from Gupta, Yos, Thomson and Lee (NASA 1990)

  Collision integrals from Wright, Bose, Palmer, and Levin (AIAA 2005)

$$X_{\mathrm{N_2}} = X_{\mathrm{O_2}} = X_{\mathrm{NO}} = X_{\mathrm{N}} = X_{\mathrm{O}} = 0.2(1 - 10x)$$

$$X_{\mathrm{N_2^+}} = X_{\mathrm{O_2^+}} = X_{\mathrm{NO^+}} = X_{\mathrm{N^+}} = X_{\mathrm{O^+}} = x, \qquad X_{\mathrm{e}} = 5x,$$

  Variable $0 \leq x \leq 0.1$ and variable B

  Pressure $p = 0.1$ atm and Temperature $T = T_h = 10000$K

- **Numerical tests**

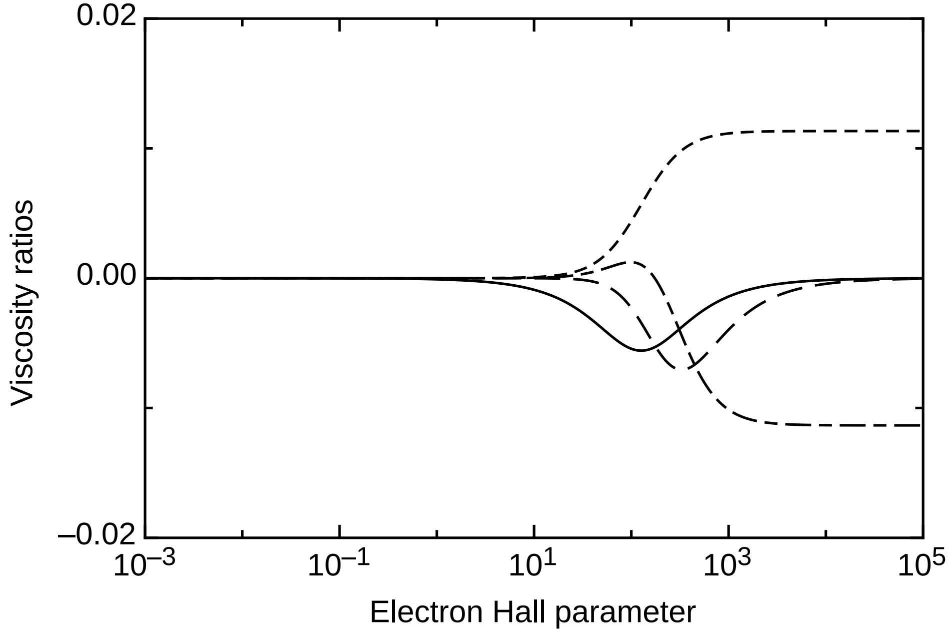
  Diffusion velocities, Viscosities, Thermal conductivities

  Diffusion matrices, Electrical Conductivities

High Temperature Air (1)

- **Viscosity ratios as function of the Electron Hall parameter**

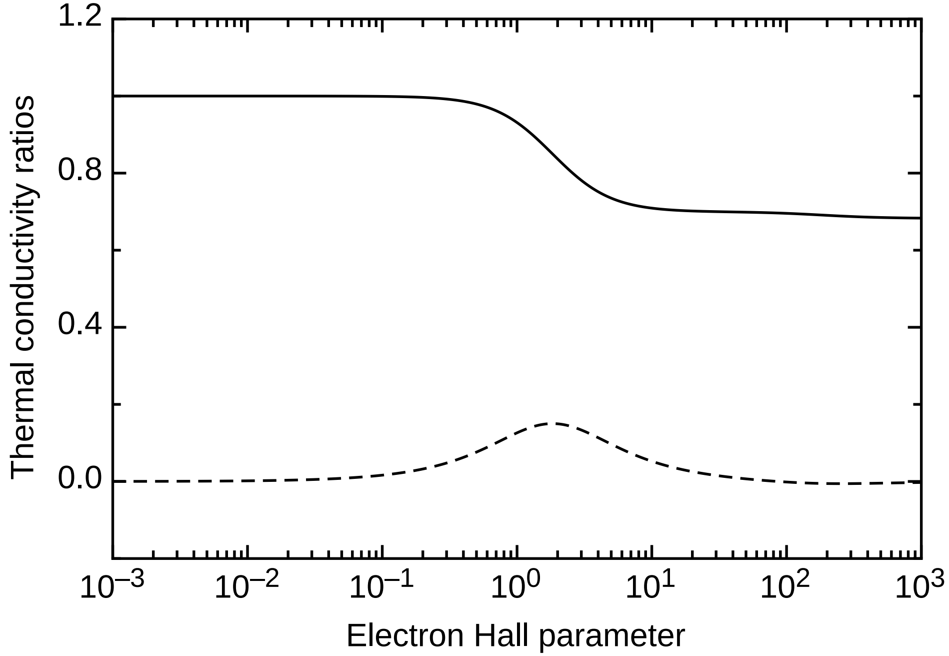
$$x = 10^{-2} \quad \beta_e = 3eB/16\rho_e\Omega_{e,h}^{(1,1)} \quad \eta_1 \simeq 2.31\ 10^{-4}\ \mathrm{Kg\ m^{-1}s^{-1}}$$



High Temperature Air (2)

- **Thermal conductivity ratios as function of the Electron Hall parameter**

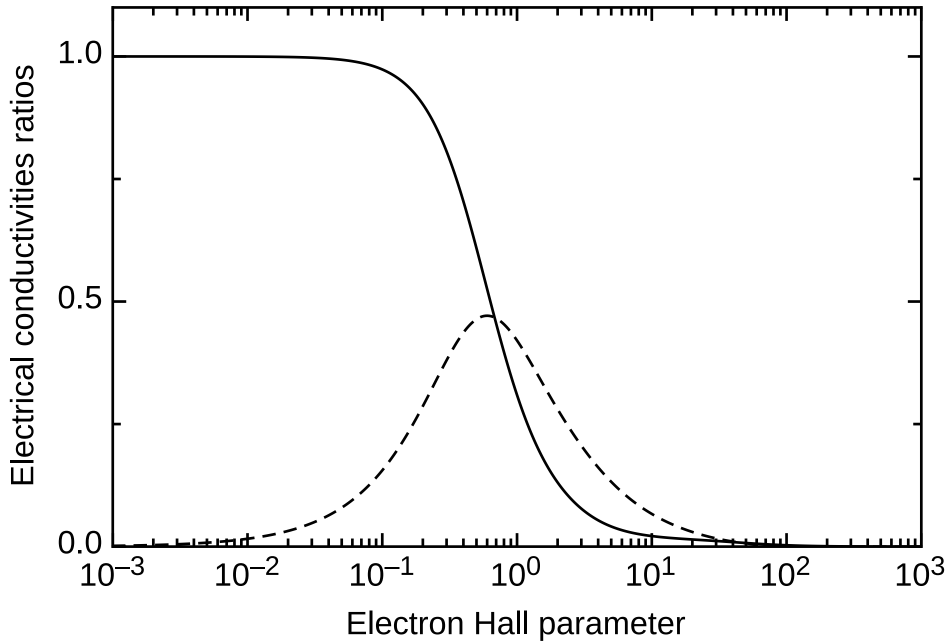
$$x = 10^{-2} \qquad \beta_{\mathrm{e}} = 3eB/16\rho_{\mathrm{e}}\Omega_{\mathrm{e},h}^{(1,1)} \qquad \lambda^{\parallel} = 0.646\ \mathrm{W\ m^{-1}K^{-1}}$$



High Temperature Air (3)

- **Electrical conductivity ratios as function of the Electron Hall parameter**

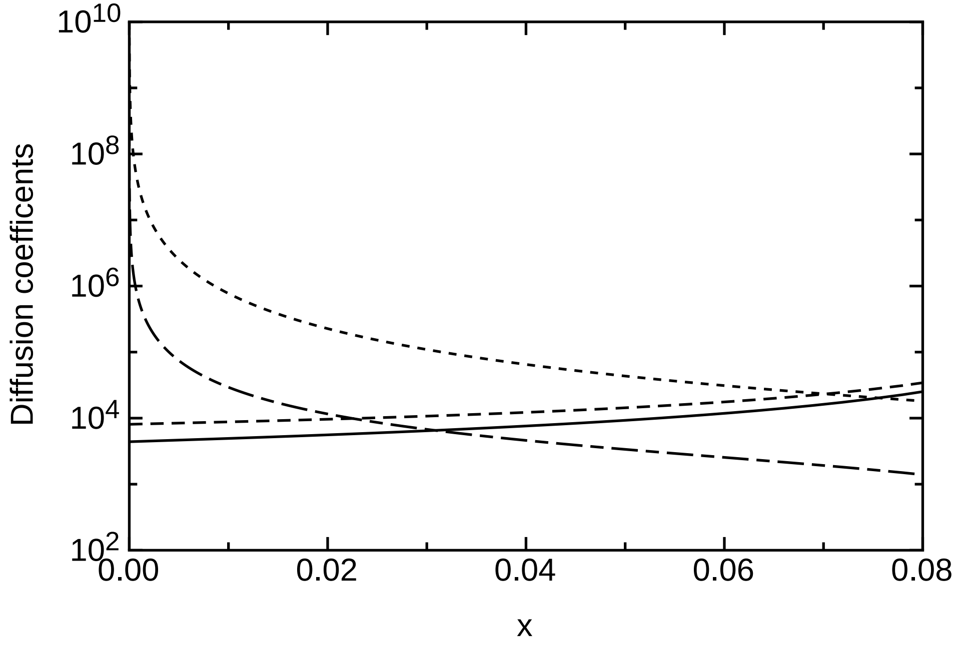
$$x = 10^{-2} \quad \beta_e = 3eB/16\rho_e\Omega^{(1,1)}_{e,h} \quad \sigma^{\parallel} = 2601\ \mathrm{A\,V^{-1}m^{-1}}$$



High Temperature Air (4)

- **Nitrogen/Electron diffusion coefficients as function of x**

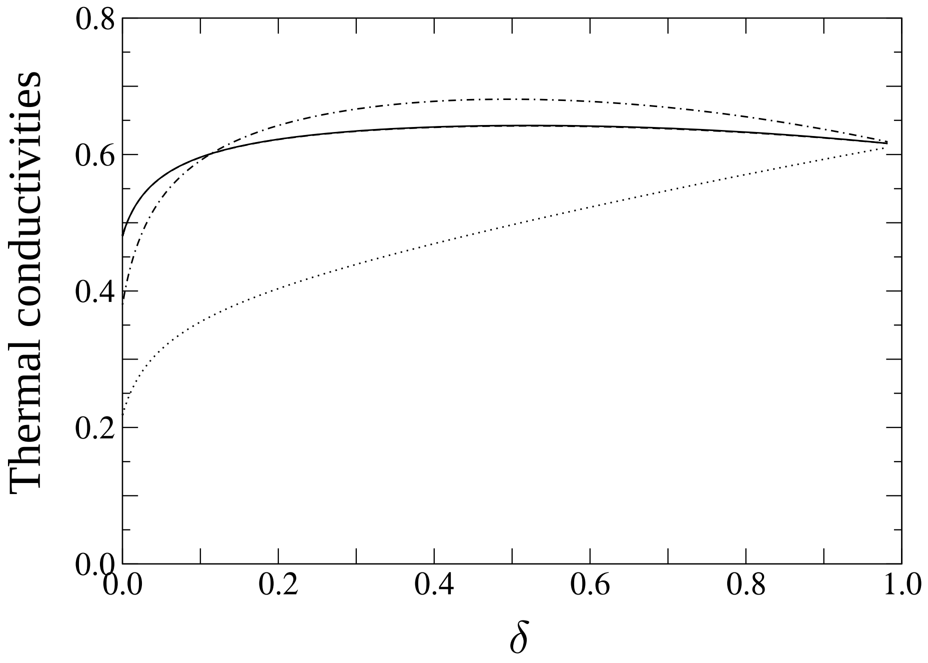
  $0 \leq x \leq 0.1 \quad B = 0 \quad D_{\mathrm{N_2N_2}} \quad D_{\mathrm{NN}} \quad D_{\mathrm{N^+N^+}} \quad D_{\mathrm{ee}}$



High Temperature Air (5)

- **Thermal conductivities λ, λ^{mon}, λ^{euk}, and $\lambda^{[\mathrm{e}]}$ as functions of δ**

$$0 \le \delta \le 1 \qquad B = 0 \qquad X_k = (1-\delta)X_k^{\mathrm{fr}} + \delta X_k^{\mathrm{eq}}, \quad k \in \mathcal{S}$$



Numerical Tests (0)

- **Approximated collision integrals**

  Physical constants are transformed into numerical parameters

  Mathematical structure still holds for approximated systems

- **Computational costs**

  Size of the systems $\omega \simeq rn, \quad r = 1, 2, 3, 4, 5$

  Systems evaluation $O(\omega^2) = O(n^2)$

  Direct method Gauss LU $\omega^3/3$ Choleski LL^t $\omega^3/6$

  Iterative methods $O(\omega^2)$

  Empirical methods $O(\omega)$ but no rigorous approximations at $O(\omega)$ cost

- **Truncation of convergent series**

  Truncation of iterative methods at 10^{-3} accuracy

Numerical Tests (1)

- **Mixtures**

  Gas mixtures associated with H_2 and CH_4 combustion chemistry

  H_2 chemistry, $n = 9$ CH_4 chemistry, $n = 16$

- **Number of nodes**

  $m = 2500$ nodes for a 50*50 grid

- **Mixtures**

  Mixture 1 H_2 mixture, equimolar

  Mixture 2 H_2 mixture, $X_k = \epsilon$ for $k \notin \{\mathrm{H}_2, \mathrm{O}_2, \mathrm{N}_2\}$, $X_k = 1/3 - 2\epsilon$ for $k \in \{\mathrm{H}_2, \mathrm{O}_2, \mathrm{N}_2\}$

  Mixture 3 CH_4 mixture, equimolar

Numerical Tests (2)

- **Shear viscosity (Conjugate gradient methods)**

	Mixture 1	Mixture 2	Mixture 3
1	4.00E-4	6.50E-5	1.71E-3
2	1.18E-7	8.63E-8	3.97E-8
3	3.66E-12	1.23E-12	8.46E-13
4	1.27E-16	3.17E-17	—

Numerical Tests (3)

- **Diffusion matrix (Standard iterative methods)**

	Mixture 1	Mixture 2	Mixture 3
1	2.92E-2	9.92E-6	7.87E-3
2	1.88E-3	1.39E-6	1.91E-4
3	1.01E-4	8.52E-8	6.22E-6
4	6.67E-6	9.06E-9	2.04E-7
ϱ	6.44E-2	8.17E-2	3.33E-2

Numerical Tests (4)

- **Thermal diffusion vector (Conjugate gradient methods)**

	Mixture 1	Mixture 2	Mixture 3
1	4.82E-2	1.65E-1	3.62E-2
2	6.14E-3	1.31E-2	1.07E-3
3	5.67E-4	2.76E-3	3.82E-5
4	1.99E-5	1.09E-3	6.66E-7

Numerical Tests (5)

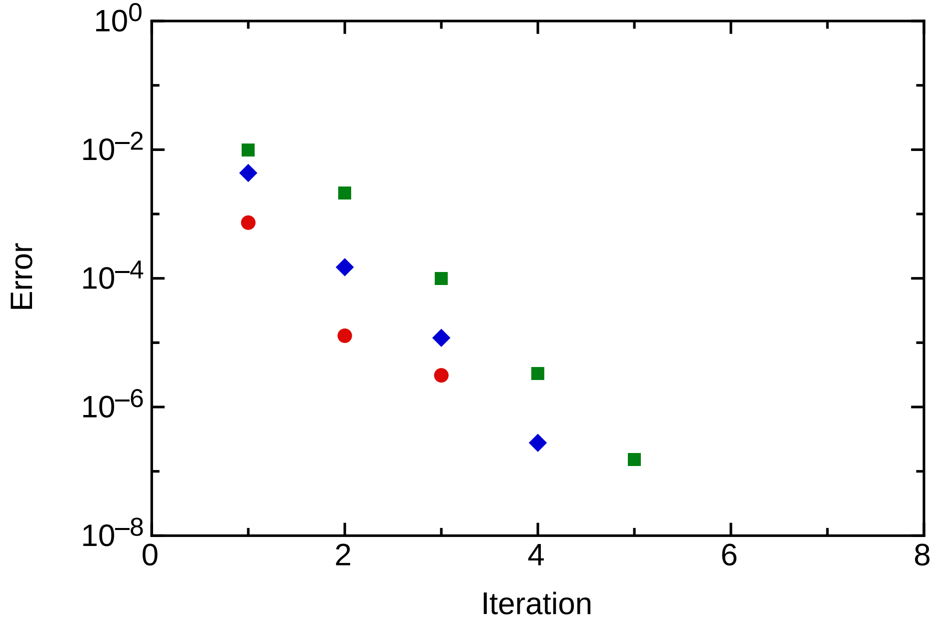
- **Performance with respect to existing transport software**

Coefficient	η		$\widehat{\lambda}, \theta, D_{[00]}$		$D_{[00]}$		$\Delta_{[00]}$
Method	IT	DS	IT	DS	IT	DS	IT
C98 scal	3.5	2.5	9.9	3.7	11.0	4.2	2.1
C98 vect	15.0	11.0	81.1	23.7	82.3	34.3	22.3
Convex C3	4.2	2.8	31.8	11.8	4.1	1.3	6.7
IBM RS6000	5.9	4.4	16.6	6.9	11.4	5.0	2.1
HP750	2.3	1.5	10.6	2.0	7.3	1.9	1.8

Numerical Experiments (1)

- **Evaluation of diffusion velocities $\mathcal{V}$ by solving Stefan-Maxwell equations**

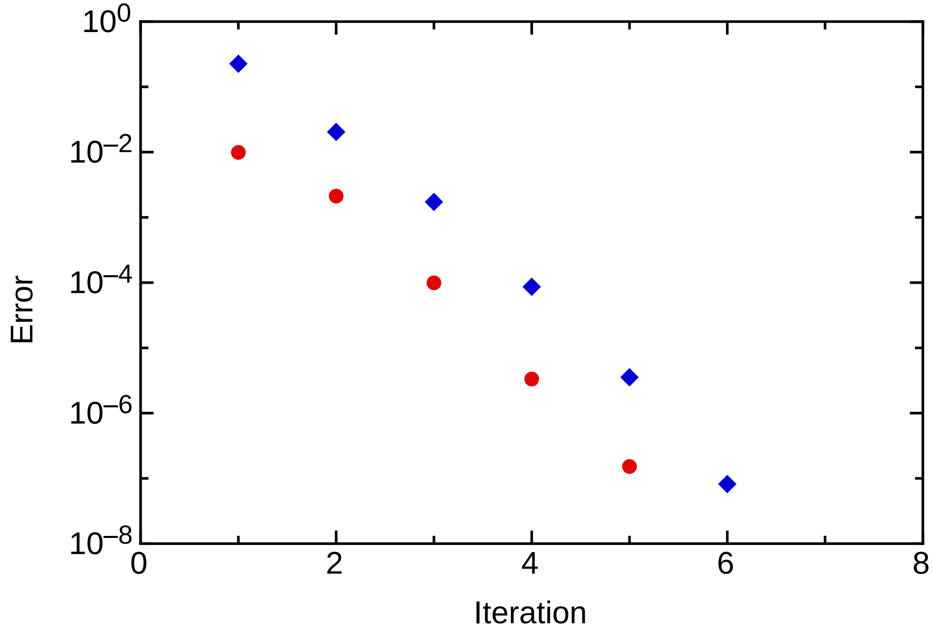
  $x = 10^{-4}$ $\quad x = 10^{-3}$ $\quad x = 10^{-2}$ $\quad B = 0$



Numerical Experiments (2)

- **Evaluation of diffusion velocities $\mathcal{V}^{\parallel}$ and $\mathcal{V}^{\perp}$ by solving Stefan-Maxwell equations**

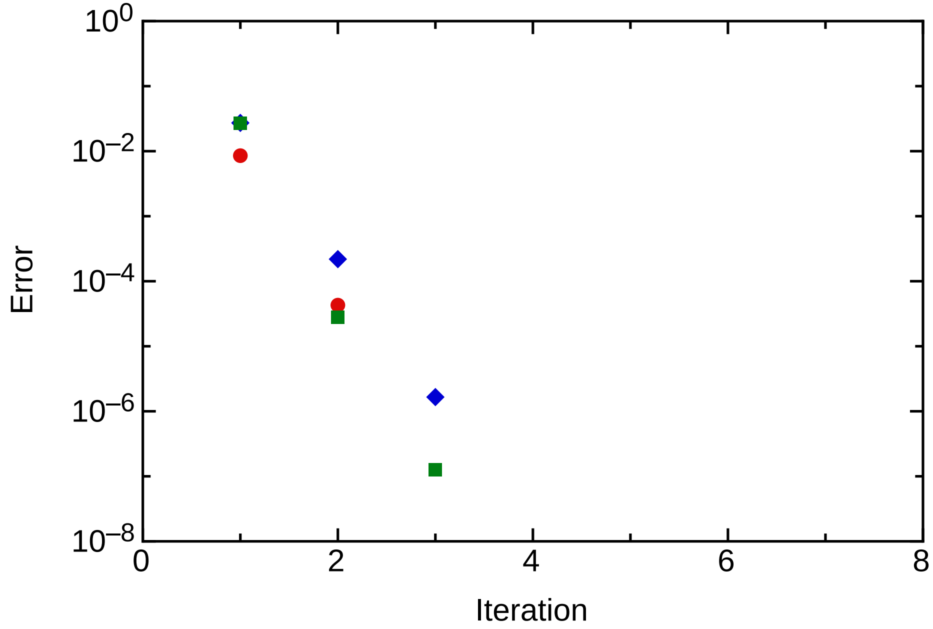
  $x = 10^{-2} \qquad B = 10^{3}$



Numerical Experiments (3)

- **Evaluation of the thermal conductivity λ**

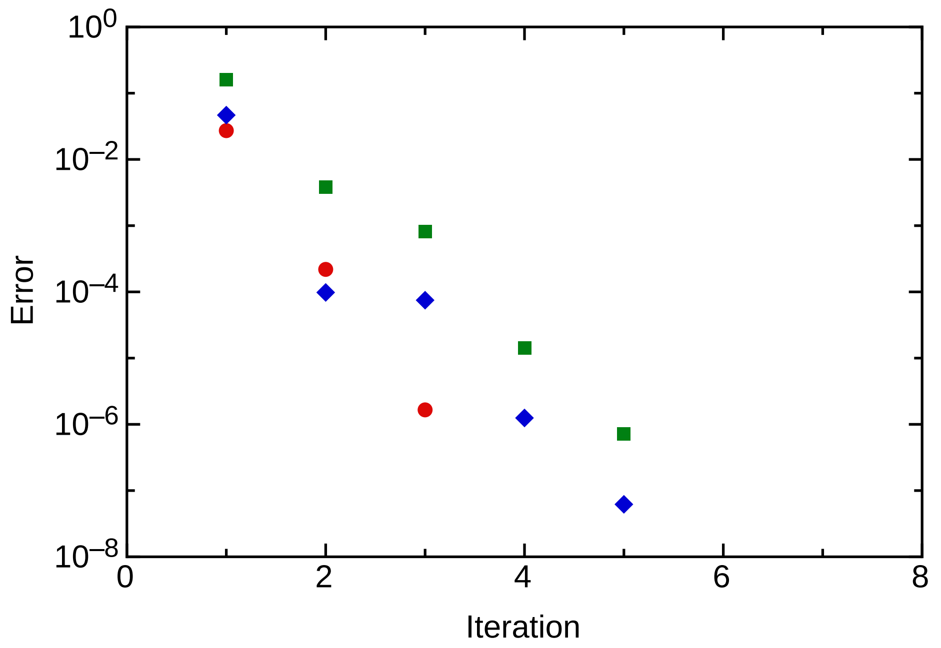
$x = 10^{-4}$ $\quad$ $x = 10^{-3}$ $\quad$ $x = 10^{-2}$ $\quad$ $B = 0$



Numerical Experiments (4)

- **Evaluation of thermal conductivities $\boldsymbol{\lambda}^{\parallel}, \boldsymbol{\lambda}^{\perp}, \boldsymbol{\lambda}^{\odot}$**

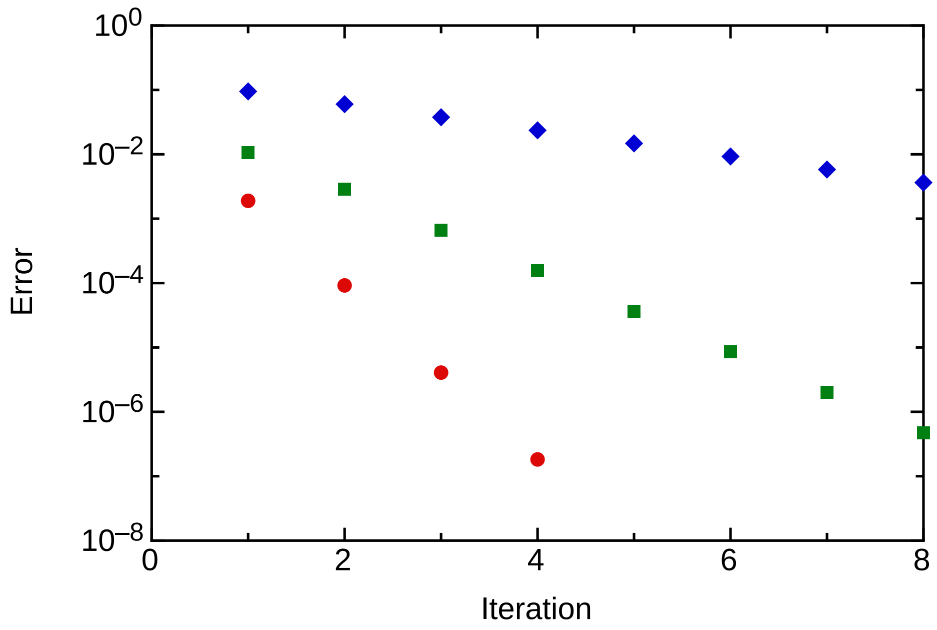
  $x = 10^{-2} \qquad B = 10^{3}$



Numerical Experiments (5)

- **Evaluation of diffusion matrices (similar results with $\mathcal{H}$)**

  $x = 10^{-4}$ $x = 10^{-3}$ $x = 10^{-2}$ $B = 0$



New Stationary Algorithms (1)

- **Reformulation of the transport linear system**

$$\mathsf{u}_2 \neq 0 \text{ with } \langle \mathsf{u}_2, \mathsf{y} \rangle = 0, \qquad \mathsf{y}_2 = \Delta \mathsf{u}_2 \qquad \mathsf{u}_2 = D \mathsf{y}_2$$

$$\Delta_2 = \Delta - \frac{\mathsf{y}_2 \otimes \mathsf{y}_2}{\langle \mathsf{y}_2, \mathsf{u}_2 \rangle}, \qquad D_2 = D - \frac{\mathsf{u}_2 \otimes \mathsf{u}_2}{\langle \mathsf{y}_2, \mathsf{u}_2 \rangle},$$

$$\begin{cases} \Delta_2 D_2 = Q_2, \\ D_2 \mathsf{y} = D_2 \mathsf{y}_2 = 0, \end{cases} \qquad Q_2 = P_2^t = \mathbb{I} - \frac{\mathsf{y} \otimes \mathsf{u}}{\langle \mathsf{y}, \mathsf{u} \rangle} - \frac{\mathsf{y}_2 \otimes \mathsf{u}_2}{\langle \mathsf{y}_2, \mathsf{u}_2 \rangle},$$

- **Asymptotic expansion**

$$\Delta_2 = M_2 - W_2, \qquad T_2 = M_2^{-1} W_2, \qquad D_2 = \sum_{0 \le j < \infty} (P_2 T_2)^j P_2 M_2^{-1} P_2^t,$$

$$D = \frac{\mathsf{u}_2 \otimes \mathsf{u}_2}{\langle \mathsf{y}_2, \mathsf{u}_2 \rangle} + \sum_{0 \le j < \infty} (P_2 T_2)^j P_2 M_2^{-1} P_2^t,$$

New Stationary Algorithms (2)

- **Spectra of iteration matrices**

  $\Delta = M - W \quad M = M^t \quad M + W$ positive definite $\quad T = M^{-1}W$

  T is symmetric for $\langle\langle x, y\rangle\rangle = \langle Mx, y\rangle$ and its powers are convergent

$$\sigma(T) \subset (-\alpha, \alpha) \cup \{1-\epsilon\} \cup \{1\}, \qquad \sigma(PT) \subset (-\alpha, \alpha) \cup \{1-\epsilon\},$$

$$0 < \alpha < 1 - \epsilon, \qquad Tv_2 = (1-\epsilon)v_2,$$

- **Vector $\mathbf{u_2}$**

  $u_2 \in \text{span}\{\mathsf{u}, v_2\}, \quad v_2 \in N(\Delta_2) = \text{span}\{\mathsf{u}, \mathsf{u}_2\}$

  $\Delta_2 = M_2 - W_2 \quad M_2 = M \quad M_2 + W_2$ positive definite $\quad T_2 = M_2^{-1}W_2$

$$\sigma(T_2) \subset (-\alpha, \alpha) \cup \{1\}, \qquad \sigma(P_2T_2) \subset (-\alpha, \alpha),$$

New Stationary Algorithms (3)

- **Approximate vector u_2**

$$(\mathsf{u}_2^*)_k = \begin{cases} 1, & \text{if } k \in \mathcal{I}, \\ 0, & \text{if } k \notin \mathcal{I}, \end{cases} \qquad \mathcal{I} = \text{Ionized species}, \qquad \mathsf{u}_2 \in \text{span}\{\mathsf{u}, \mathsf{u}_2^*\},$$

- **Rayleigh quotients**

$$\rho(PT) = \sup\Big\{ \frac{|\langle Wx, x\rangle|}{\langle Mx, x\rangle};\ x \in \mathbb{R}^n,\ x \neq 0,\ \langle M\mathsf{u}, x\rangle = 0 \Big\},$$

$$\rho(P_2T_2) = \sup\Big\{ \frac{|\langle W_2x, x\rangle|}{\langle M_2x, x\rangle};\ x \in \mathbb{R}^n,\ x \neq 0,\ \langle M_2\mathsf{u}, x\rangle = \langle M_2\mathsf{u}_2, x\rangle = 0 \Big\}.$$

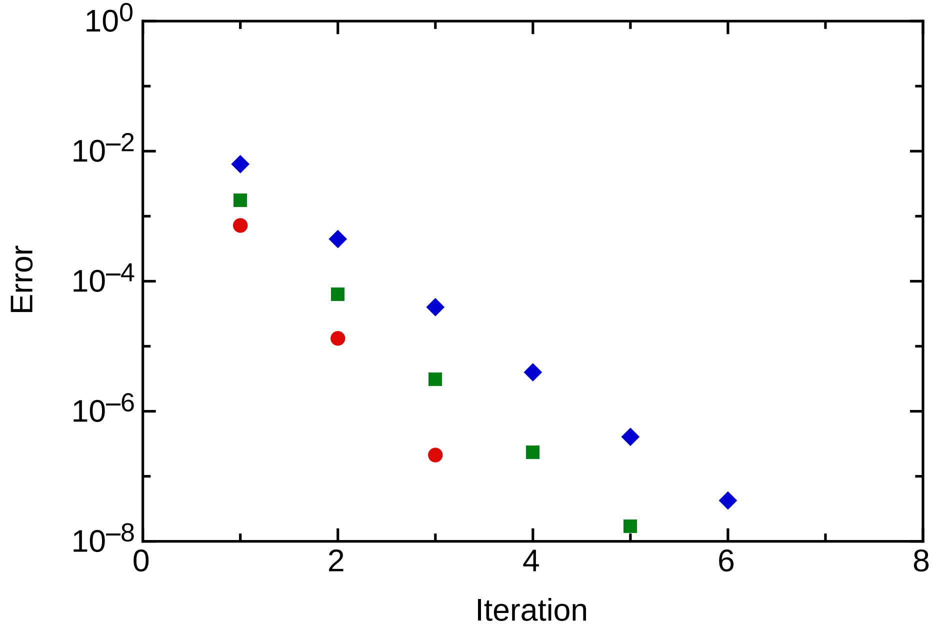
- **Origin of the problem**

Binary diffusion coefficients for positive ions pairs are very small

Numerical Experiments (6)

- **Evaluation of diffusion matrices**

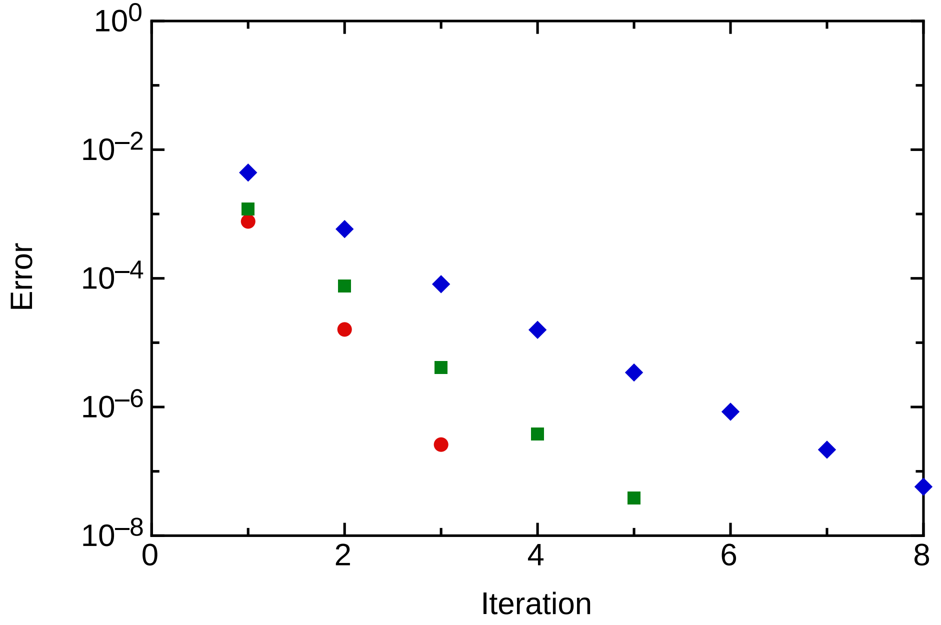
  $x = 10^{-4}$ $\quad x = 10^{-2}$ $\quad x = 10^{-2}$ $\quad B = 0$



Numerical Experiments (7)

- **Evaluation of higher order diffusion matrices**

  $x = 10^{-4} \quad x = 10^{-2} \quad x = 10^{-2} \quad B = 0$



A Bunsen Laminar Flame (1)

- **Flow configuration**

  Cylindrical geometry

  Computational domain $[0, 1.5] \times [0, 25]$ cm

  Mixture of 20% Hydrogen and 80 % Air , $v^{\mathrm{inj}} = 300$ cm/s

  Coflow of Air

- **Governing equations**

  Multicomponent reactive flow equations, Soret effect included

  Reaction mechanism : 9 species and 19 reactions

- **Numerical techniques**

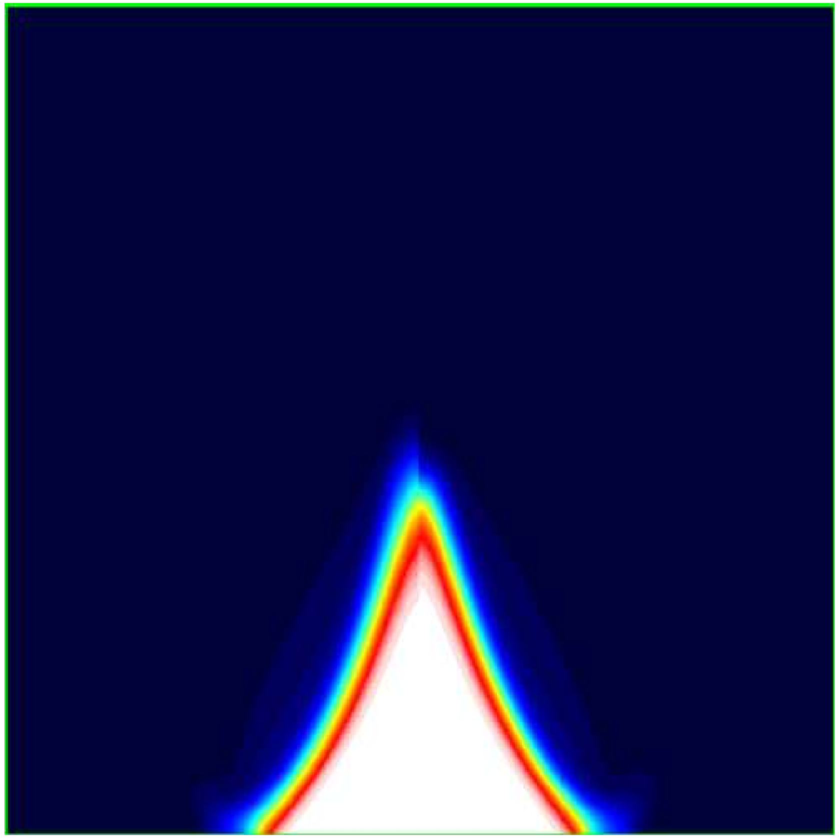
  Finite differences/Finite elements

  Newton iterations, unsteady/steady, Fully coupled algorithms

  Preconditioned BiCGStab or GMRes

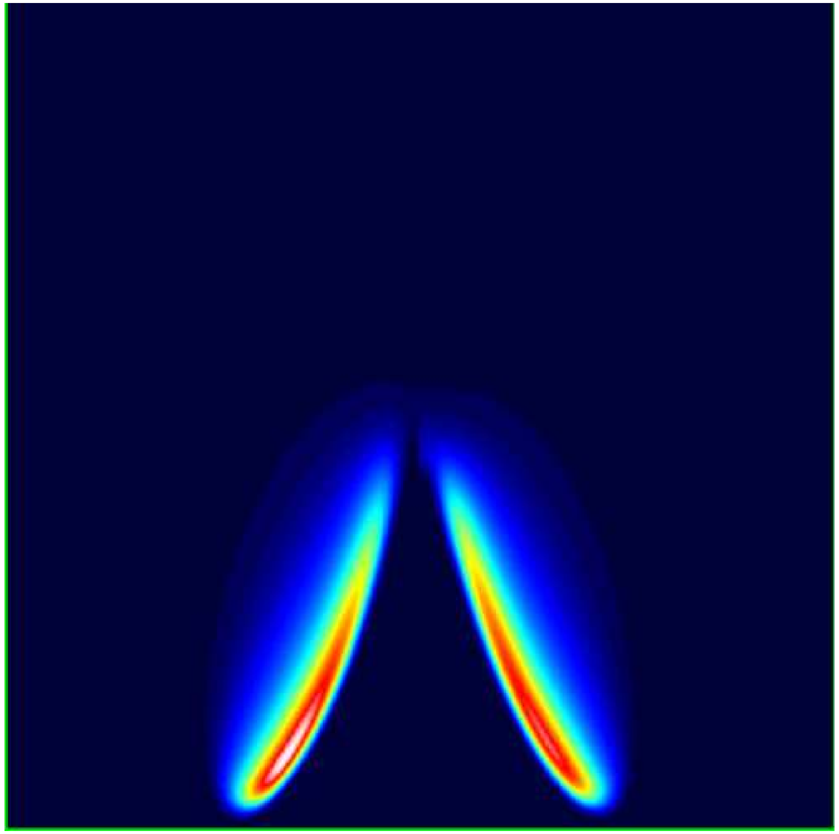
A Bunsen Laminar Flame (2)

- **Mole fraction of H_2**



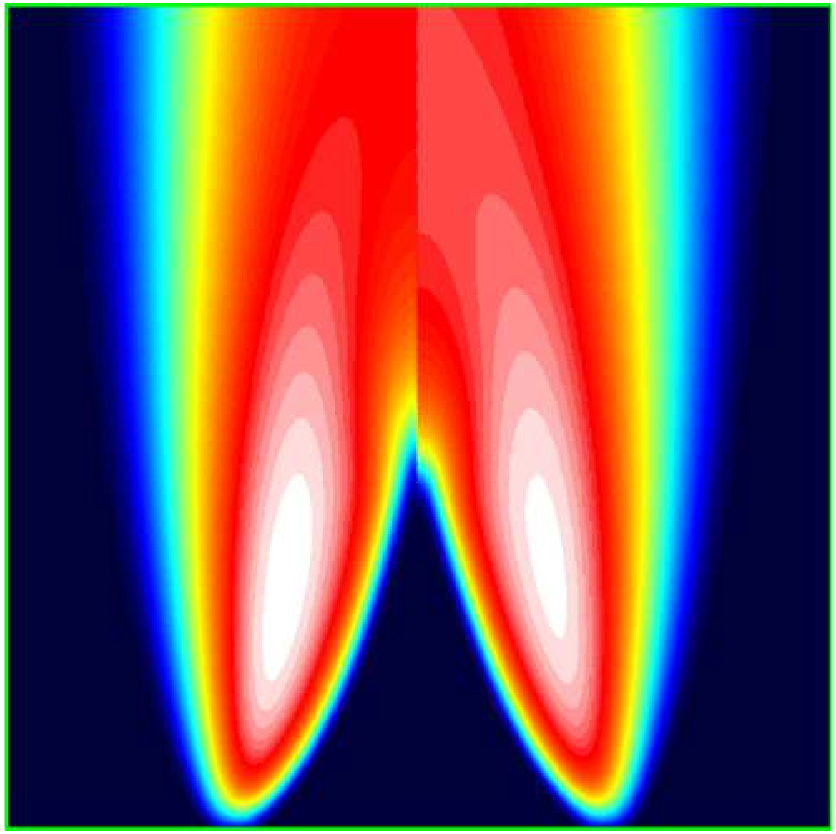
A Bunsen Laminar Flame (3)

- **Mole fraction of H**



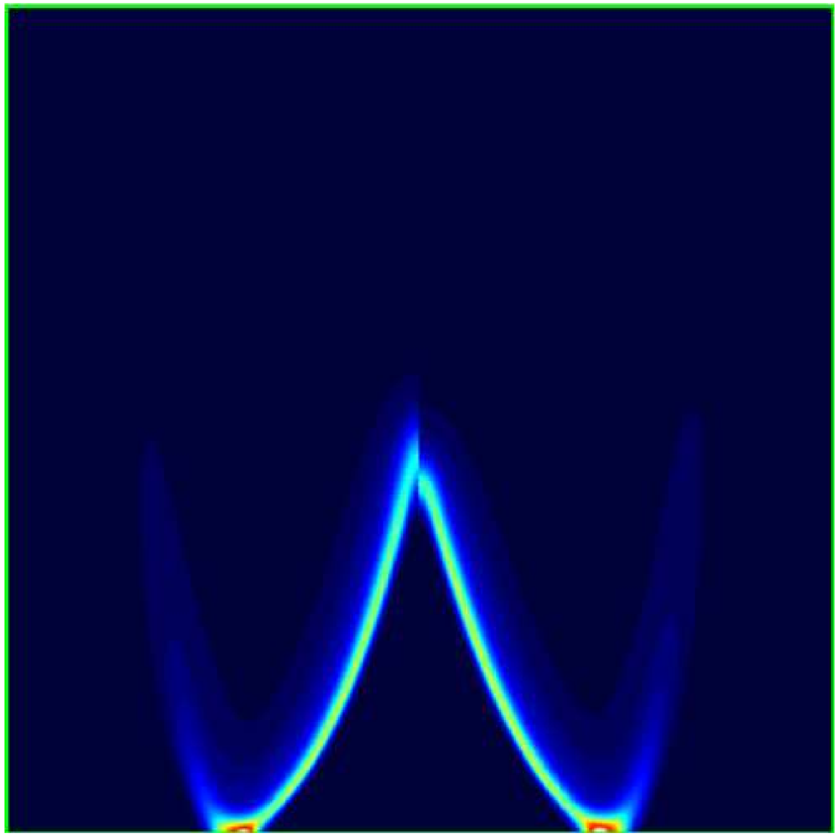
A Bunsen Laminar Flame (4)

- **Temperature**



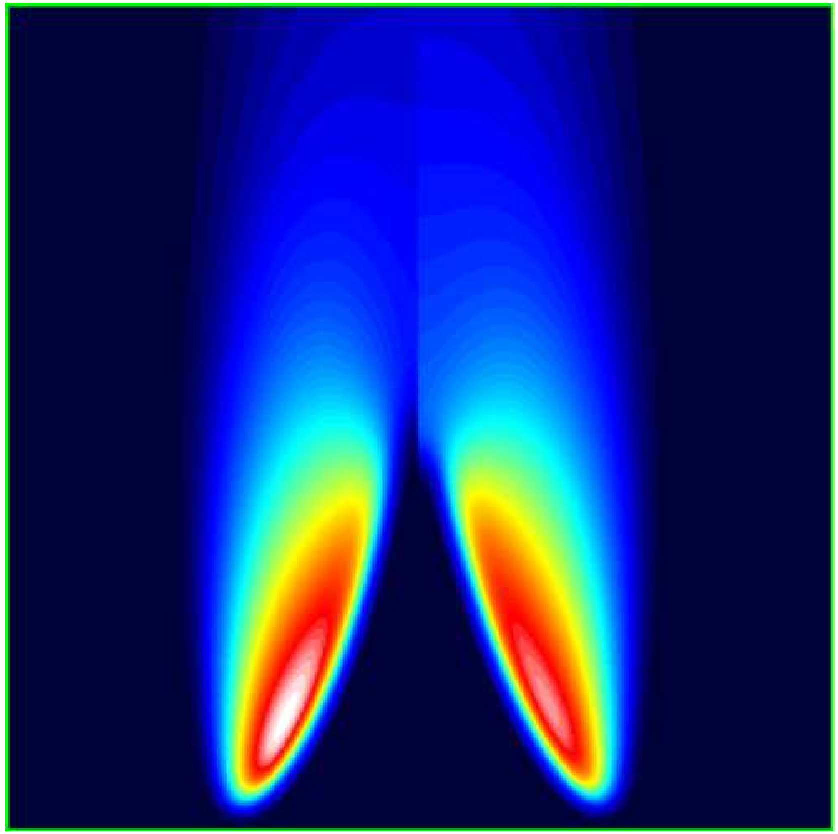
A Bunsen Laminar Flame (5)

- **Mole fraction of H_2O_2**



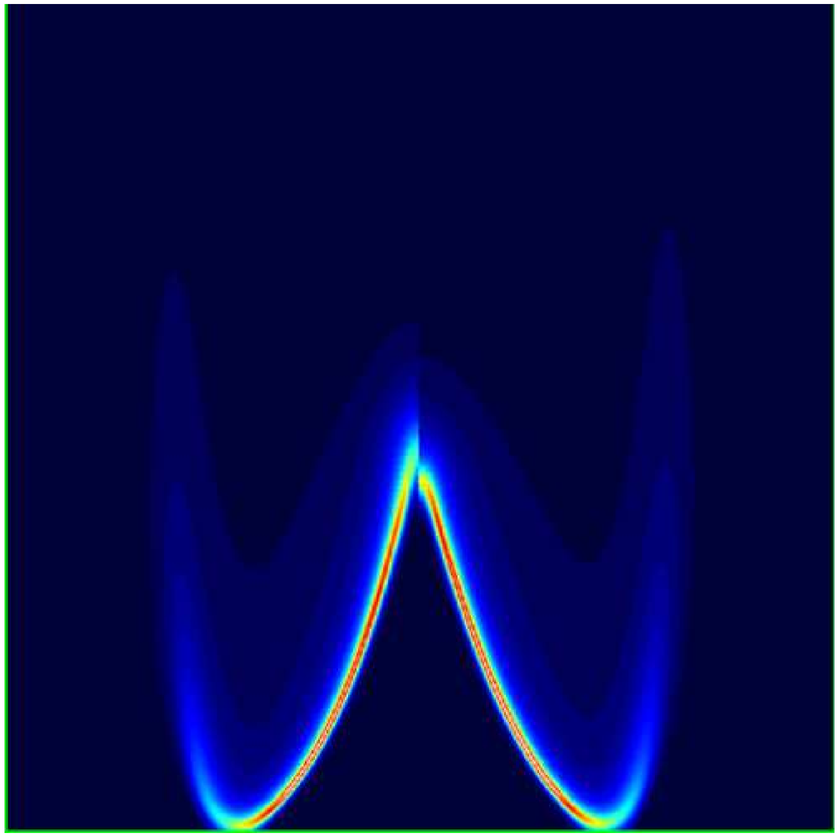
A Bunsen Laminar Flame (6)

- **Mole fraction of OH**



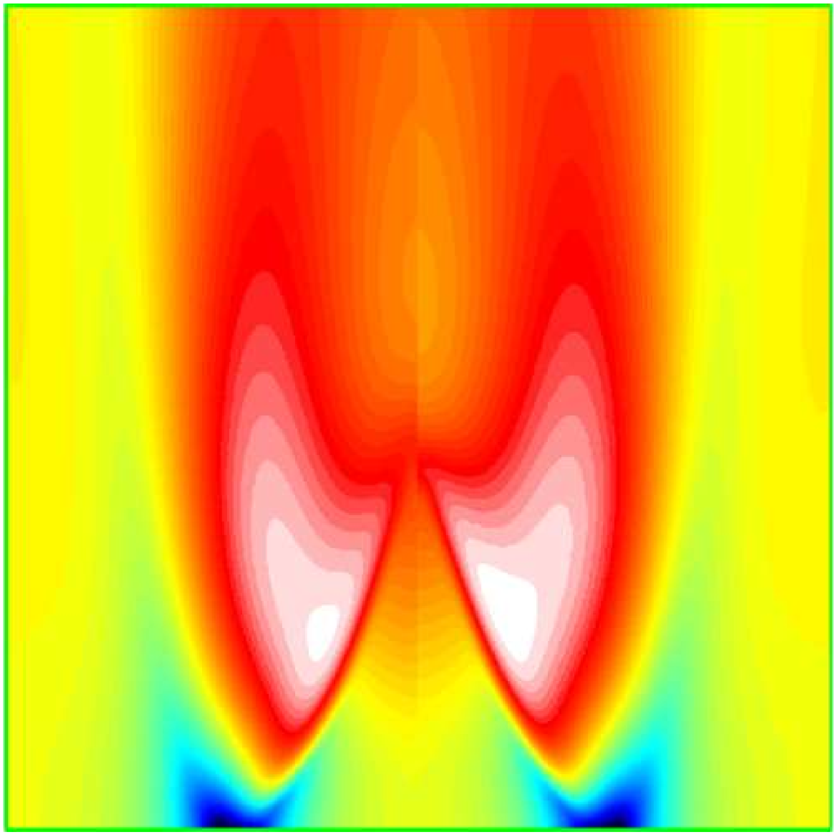
A Bunsen Laminar Flame (7)

- **Mole fraction of HO_2**



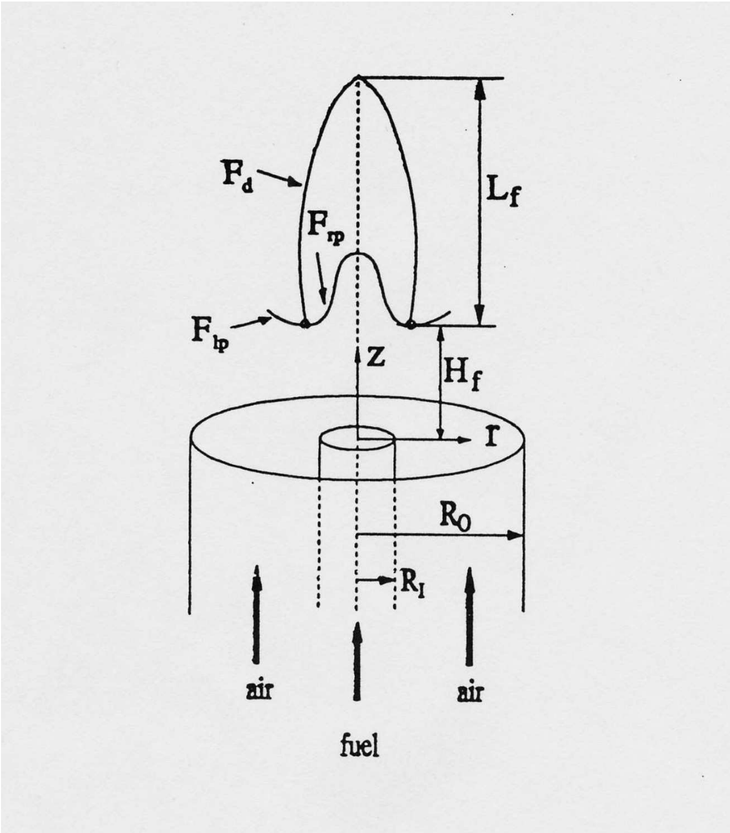
A Bunsen Laminar Flame (8)

- **Velocity**



Diffusion Laminar Flames (1)

- **Flow configuration**



Diffusion Laminar Flames (2)

- **Flow parameters**

  Cylindrical geometry, $R_I = 0.2$ cm, $\delta_B = 0.038$ cm, $R_O = 2.5$ cm,

  Computational domain $[0, 7.5] \times [0, 25]$ cm

  Fuel mixture of 65% Methane and 35 % Nitrogen, Parabolic flow $v^{\mathrm{inj}} = 35$ cm/s

  Plug coflow of Air $v^{\mathrm{inj}} = 35$ cm/s

- **Governing equations**

  Multicomponent reactive flow equations, Soret effect included

  Reaction mechanism : 31 species and 173 reactions

- **Numerical techniques**

  Finite differences/Finite elements

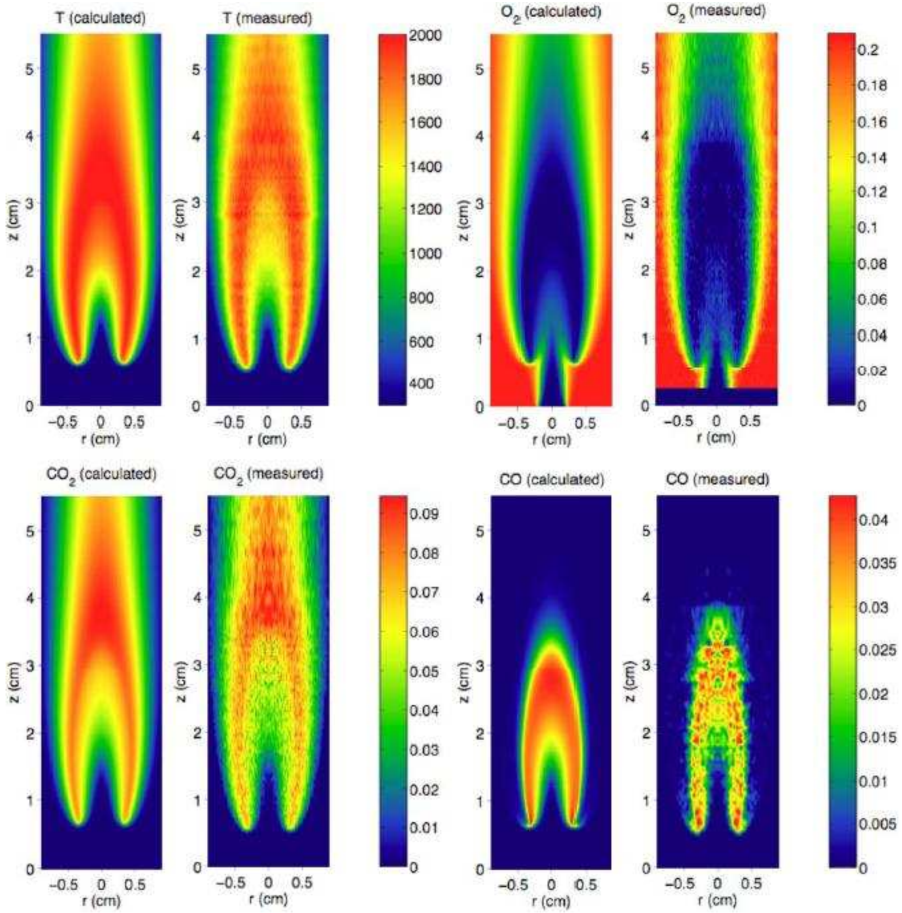
  Newton iterations, unsteady/steady

  Fully coupled algorithms

  Preconditioned BiCGStab or GMRes

Diffusion Laminar Flames (3)

- **Flame structure (Mitchell Smooke and Seth Dworkin YALE University)**



Diffusion Laminar Flames (4)

- **Flow parameters**

  Cylindrical geometry, $R_I = 0.2$ cm, $\delta_B = 0.038$ cm, $R_O = 2.5$ cm,

  Computational domain $[0, 7.5] \times [0, 25]$ cm

  Fuel mixture of 32% Ethylene and 68 % Nitrogen, Parabolic flow $v^{\mathrm{inj}} = 35$ cm/s

  Plug coflow of Air $v^{\mathrm{inj}} = 35$ cm/s

- **Governing equations**

  Multicomponent reactive flow equations, Soret effect included

  Soot section equations, Inception/Growth/Aging/Coalescence/Thermophoresis

  Reaction mechanism : 45 species and 233 reactions

- **Numerical techniques**

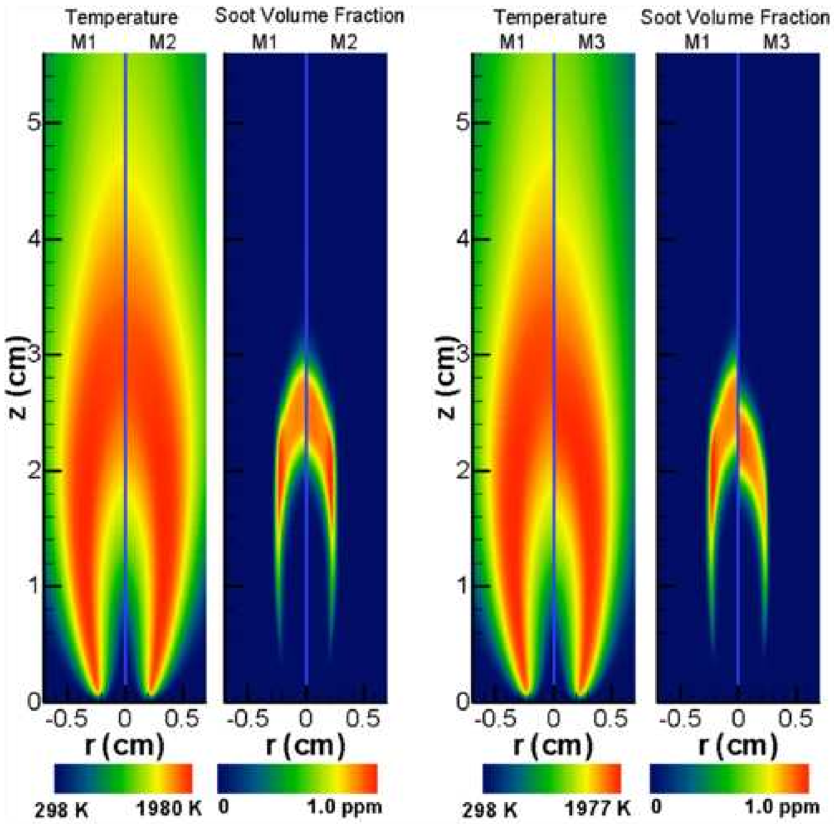
  Finite differences/Finite elements

  Newton iterations, unsteady/steady, Fully coupled algorithms

  Preconditioned BiCGStab or GMRes

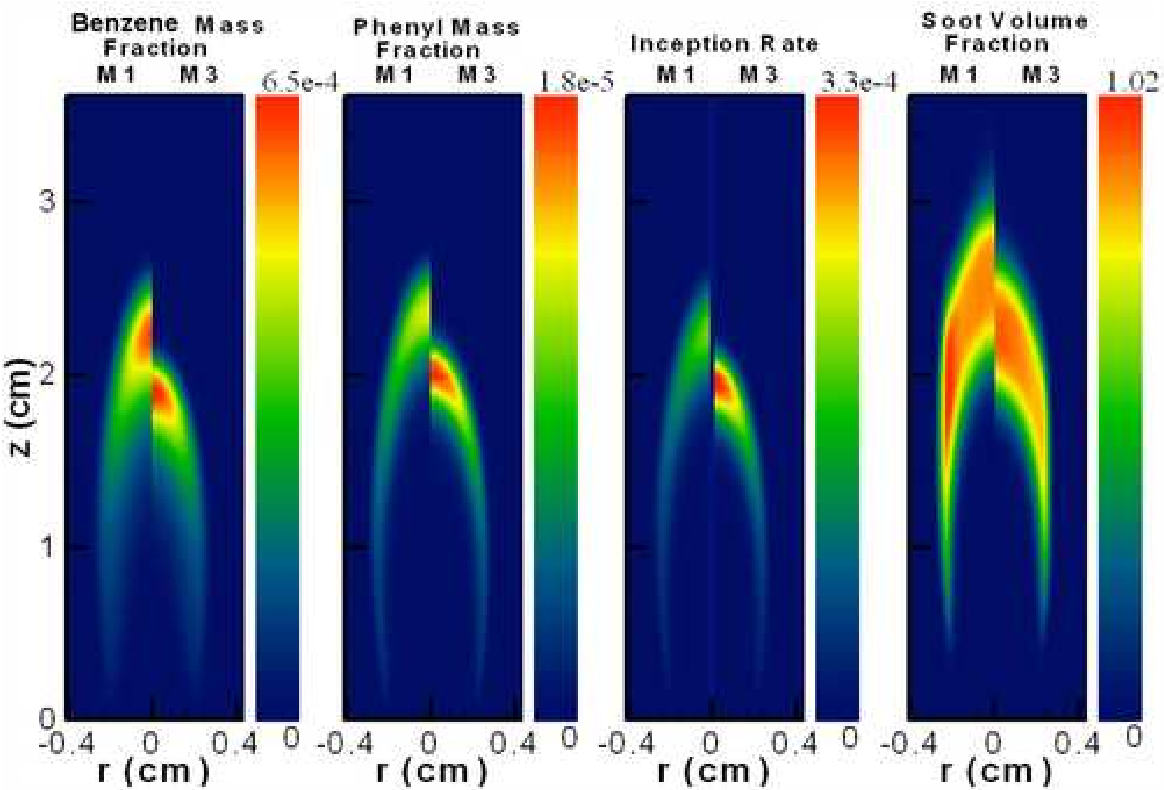
Diffusion Laminar Flames (5)

- **Soot formation (with Mitchell Smooke and Seth Dworkin YALE University)**



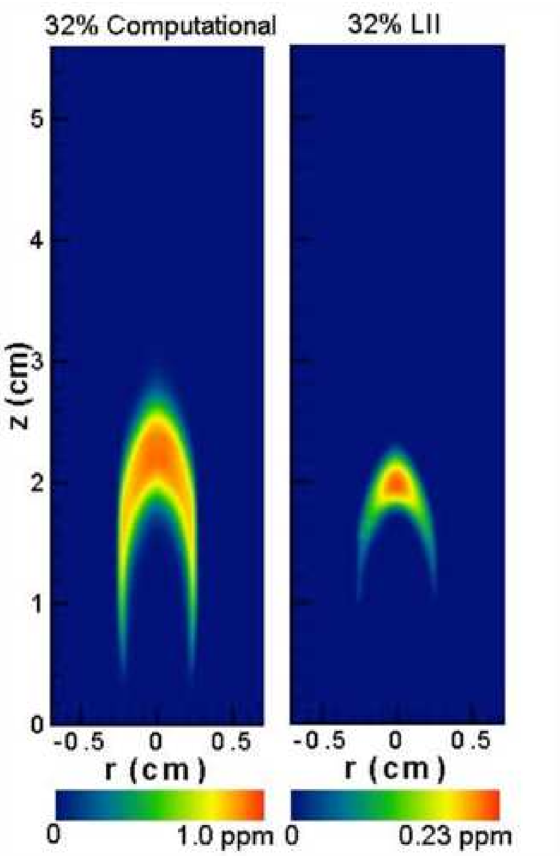
Diffusion Laminar Flames (6)

- **Soot formation**



Diffusion Laminar Flames (7)

- **Soot formation**



Volume viscosity (1)

- **Viscous tensor**

$$\boldsymbol{\Pi} = -\kappa(\boldsymbol{\nabla}\cdot\boldsymbol{v})\mathbb{I} - \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t - \tfrac{2}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{v})\mathbb{I}\big),$$

- **Stokes' hypothesis**

  $\kappa/\eta \simeq 0$ is basically wrong

- **Kinetic theory**

  $\kappa = 0$ only for dilute monatomic gases

  $\kappa/\eta = \mathcal{O}(1)$ for polyatomic gases

Volume viscosity (2)

- **Experimental measurements**

  Acoustic absorption of sound waves

$$\frac{\alpha}{\omega^2} = \frac{2\pi^2}{\rho c^3}\left(\tfrac{4}{3}\eta + \kappa + \frac{c_p - c_v}{c_p c_v}\lambda\right)$$

  α = sound absorption coefficient, c = sound velocity

  Typical values at room temperature of κ/η

Gas	N_2	H_2	D_2	CO	NH_3	CH_4	CD_4
κ/η	0.73	33.4	20.6	0.55	1.30	1.33	1.17

Volume viscosity (3)

- **Single polyatomic gas**

  T_{tr} = translational temperature

  T_{int} = internal temperature

  τ_{int} = internal energy relaxation time

- **Relaxation of internal energy**

$$\begin{cases} \partial_t T_{\mathrm{tr}} + \boldsymbol{v}.\boldsymbol{\nabla} T_{\mathrm{tr}} = -\dfrac{T_{\mathrm{tr}} - T}{\tau_{\mathrm{int}}}, \\ \partial_t T_{\mathrm{int}} + \boldsymbol{v}.\boldsymbol{\nabla} T_{\mathrm{int}} = -\dfrac{T_{\mathrm{int}} - T}{\tau_{\mathrm{int}}}, \end{cases} \qquad \kappa = p\,\frac{c_{\mathrm{int}} R}{c_v^2}\,\tau_{\mathrm{int}},$$

- **Independant internal modes and mixture of gases**

  Transport linear system

Volume viscosity (4)

- **Small Mach number limit**

  Pressure decomposition $p = p_{\rm u} + \widetilde{p}$ where $\widetilde{p}/p_{\rm u} = O({\rm Ma}^2)$

  Simplified state law $\rho = p_{\rm u} m/RT$ and simplified momentum equation

$$\partial_t(\rho \boldsymbol{v}) + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}\otimes\boldsymbol{v} + \widetilde{p}\,\mathbb{I}) - \boldsymbol{\nabla}\cdot\Big((\kappa - \tfrac{2}{3}\eta)\,\boldsymbol{\nabla}\cdot\boldsymbol{v}\,\mathbb{I} + \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t\big)\Big) = 0$$

  New perturbed pressure $\widehat{p} = \widetilde{p} - \kappa\,\boldsymbol{\nabla}\cdot\boldsymbol{v}$

$$\partial_t(\rho \boldsymbol{v}) + \boldsymbol{\nabla}\cdot(\rho \boldsymbol{v}\otimes\boldsymbol{v} + \widehat{p}\,\mathbb{I}) - \boldsymbol{\nabla}\cdot\Big(-\tfrac{2}{3}\eta\,\boldsymbol{\nabla}\cdot\boldsymbol{v}\,\mathbb{I} + \eta\big(\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t\big)\Big) = 0$$

  Volume viscosity only induces $O({\rm Ma}^2)$ effects with a full compressible model

- **Boundary layers**

  No volume viscosity terms in second order equations

- **Euler equations**

Volume viscosity (5)

- **Structure of weak compression waves**

  Upstream state $p_1, T_1, v_1 = v(-\infty)$, downstream state $p_2, T_2, v_2 = v(+\infty)$

  Taylor asymptotic analysis

$$p = \frac{p_2 + p_1}{2} + \frac{p_2 - p_1}{2} \tanh(\frac{x}{\delta})$$

$$\delta = \frac{4}{c_p/c_v + 1} \frac{1}{\rho(v_1 - v_2)} \left(\tfrac{4}{3}\eta + \kappa + \frac{c_p - c_v}{c_p c_v}\lambda \right),$$

  Volume viscosity thickens compression waves

- **Validity of Navier-Stokes equations in the Shock**

  Navier Stokes equations accurate up to $\mathrm{Ma} \leq 2$

  Navier Stokes are always a good approximation

Volume viscosity (6)

- **Vorticity equation** $\boldsymbol{\zeta} = \boldsymbol{\nabla} \wedge \boldsymbol{v}$

$$\partial_t \zeta + \boldsymbol{v}\cdot\boldsymbol{\nabla}\zeta = \zeta\cdot\boldsymbol{\nabla}\boldsymbol{v} - \zeta\boldsymbol{\nabla}\cdot\boldsymbol{v} + \frac{1}{\rho^2}\boldsymbol{\nabla}\rho \wedge \boldsymbol{\nabla}p - \frac{1}{\rho^2}\boldsymbol{\nabla}\rho \wedge \boldsymbol{\nabla}\big(\kappa\boldsymbol{\nabla}\cdot\boldsymbol{v}\big)$$
$$+ \boldsymbol{\nabla} \wedge \left(\frac{1}{\rho}\boldsymbol{\nabla}\cdot\big(\eta(\boldsymbol{\nabla}\boldsymbol{v} + (\boldsymbol{\nabla}\boldsymbol{v})^t - \tfrac{2}{3}\boldsymbol{\nabla}\cdot\boldsymbol{v}\mathbb{I})\big)\right).$$

- **Baroclinic term**

$$\frac{1}{\rho^2}\boldsymbol{\nabla}\rho \wedge \boldsymbol{\nabla}p$$

Volume viscosity (7)

- **Operator splitting**

  Finite differences

  $$\mathcal{L}_{H_x}(\delta t)\,\mathcal{L}_{H_y}(\delta t)\,\mathcal{L}_D(\delta t)\,\mathcal{L}_S(2\delta t)\,\mathcal{L}_D(\delta t)\,\mathcal{L}_{H_y}(\delta t)\,\mathcal{L}_{H_x}(\delta t)$$

- **Hyperbolic operators $\mathcal{L}_{H_x}$ or $\mathcal{L}_{H_y}$**

  Shock capturing

  Godunov/MUSCL with triad adaptive limiters

- **Dissipative operator $\mathcal{L}_D$**

  Centered differences

- **Numerical tests**

  Billet (JCP 2005), Billet and Abgrall (Comp. Fluids 2003),

  Billet and Louedin (JCP 2001)

- **Multicomponent transport**

  EGLIB library

Volume viscosity (8)

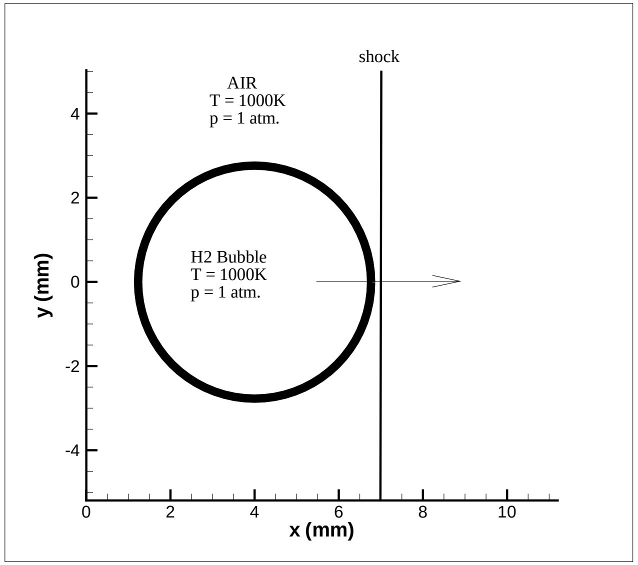
- **Reaction mechanism for Hydrogen/Air combustion**

1.	$H_2 + O_2 \rightleftharpoons 2OH$	1.70E+13	0.00	47780.
2.	$OH + H_2 \rightleftharpoons H_2O + H$	1.17E+09	1.30	3626.
3.	$H + O_2 \rightleftharpoons OH + O$	5.13E+16	-0.816	16507.
4.	$O + H_2 \rightleftharpoons OH + H$	1.80E+10	1.00	8826.
5.	$H + O_2 + M \rightleftharpoons HO_2 + M^a$	2.10E+18	-1.00	0.
6.	$H + O_2 + O_2 \rightleftharpoons HO_2 + O_2$	6.70E+19	-1.42	0.
7.	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$	6.70E+19	-1.42	0.
8.	$OH + HO_2 \rightleftharpoons H_2O + O_2$	5.00E+13	0.00	1000.
9.	$H + HO_2 \rightleftharpoons 2OH$	2.50E+14	0.00	1900.
10.	$O + HO_2 \rightleftharpoons O_2 + OH$	4.80E+13	0.00	1000.
11.	$2OH \rightleftharpoons O + H_2O$	6.00E+08	1.30	0.
12.	$H_2 + M \rightleftharpoons H + H + M^b$	2.23E+12	0.50	92600.
13.	$O_2 + M \rightleftharpoons O + O + M$	1.85E+11	0.50	95560.
14.	$H + OH + M \rightleftharpoons H_2O + M^c$	7.50E+23	-2.60	0.
15.	$H + HO_2 \rightleftharpoons H_2 + O_2$	2.50E+13	0.00	700.
16.	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	2.00E+12	0.00	0.
17.	$H_2O_2 + M \rightleftharpoons OH + OH + M$	1.30E+17	0.00	45500.
18.	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$	1.60E+12	0.00	3800.
19.	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	1.00E+13	0.00	1800.

Units are moles, centimeters, seconds, Kelvins, and calories.

Shock/hydrogen bubble interaction (1)

- **Initial configuration**



- **Initial state**

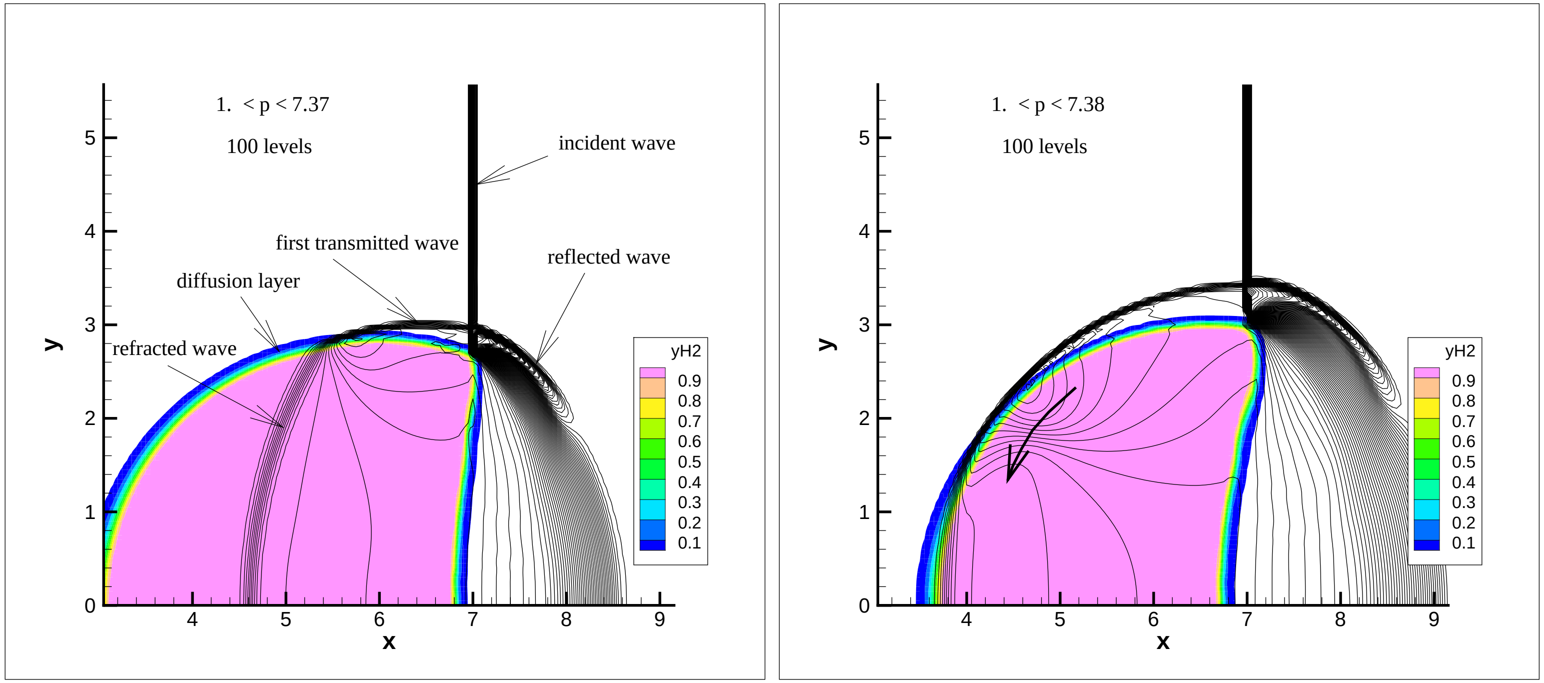
  Upstream : $T = 1000$ K, $p = 1$ atm, $v_x = 1240$ m/s, $M = 2$, $r = 2.8$ mm,

  Downstream : $T \simeq 1557$ K, $p \simeq 4.5$ atm, $v_x \simeq 450$ m/s

  $[0, 30]\times[0, 7.5]$ mm, $\Delta x = \Delta y = 0.025$ mm, 1201×301 uniform grid

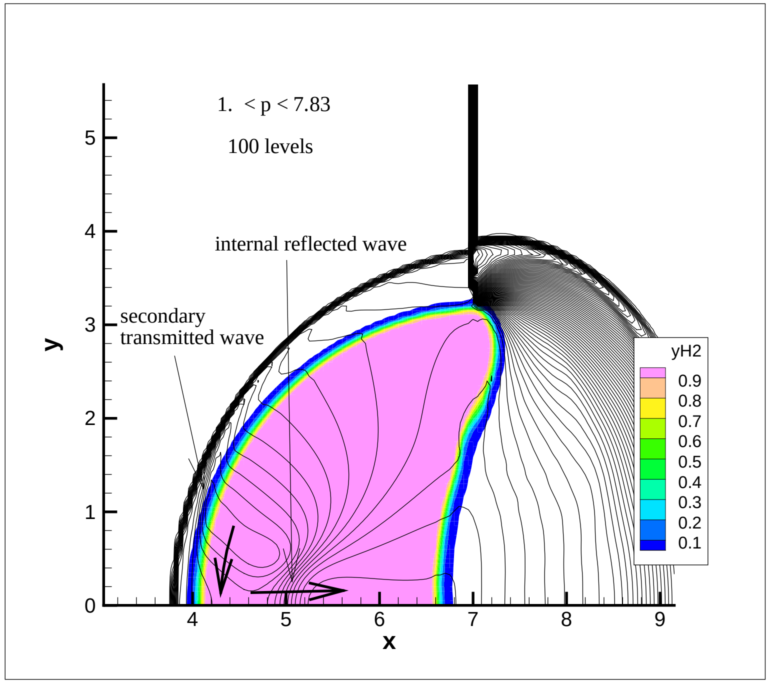
Shock/hydrogen bubble interaction (2)

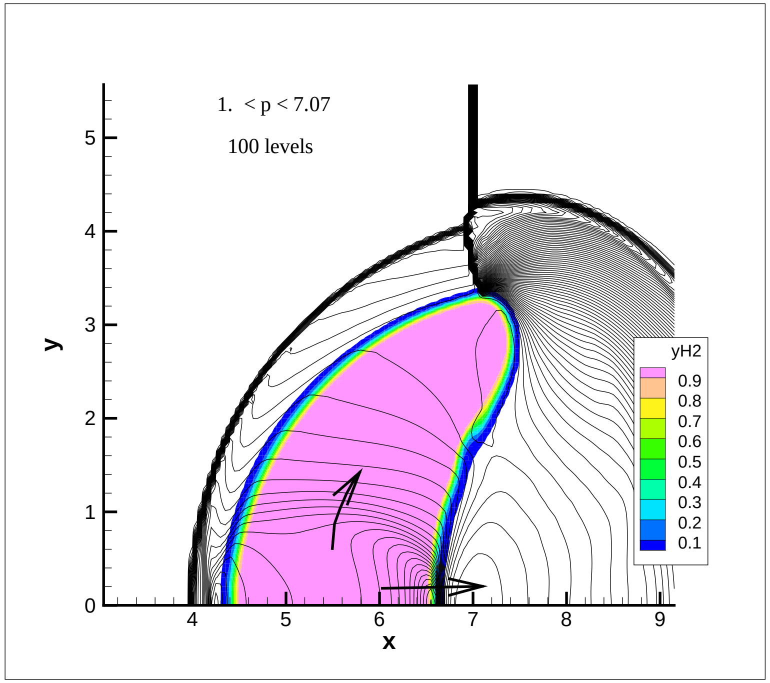
- **Pressure and hydrogen mass fraction at $t = 1.5,\ 2.0\ \mu s$**



Shock/hydrogen bubble interaction (3)

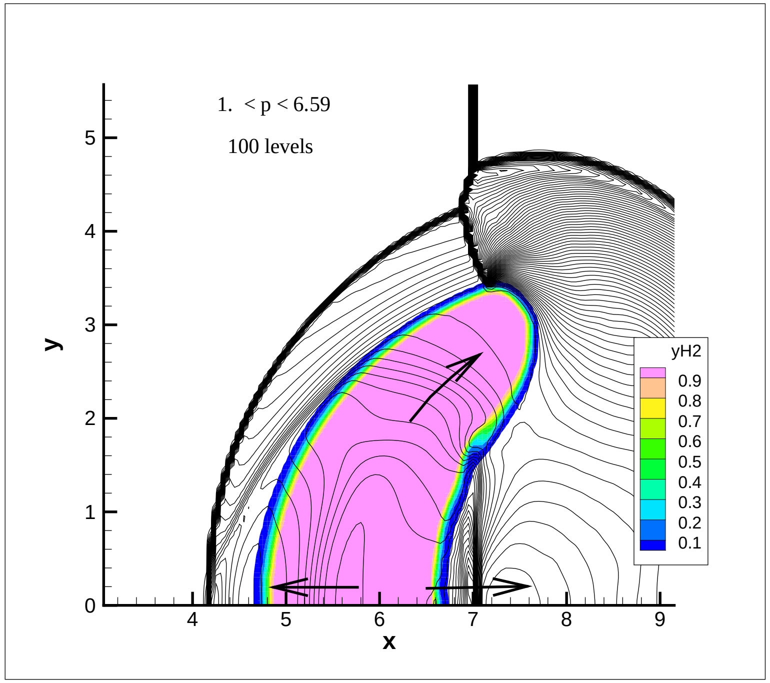
- **Pressure and hydrogen mass fraction at $t = 2.5,\ 3.0\ \mu s$**

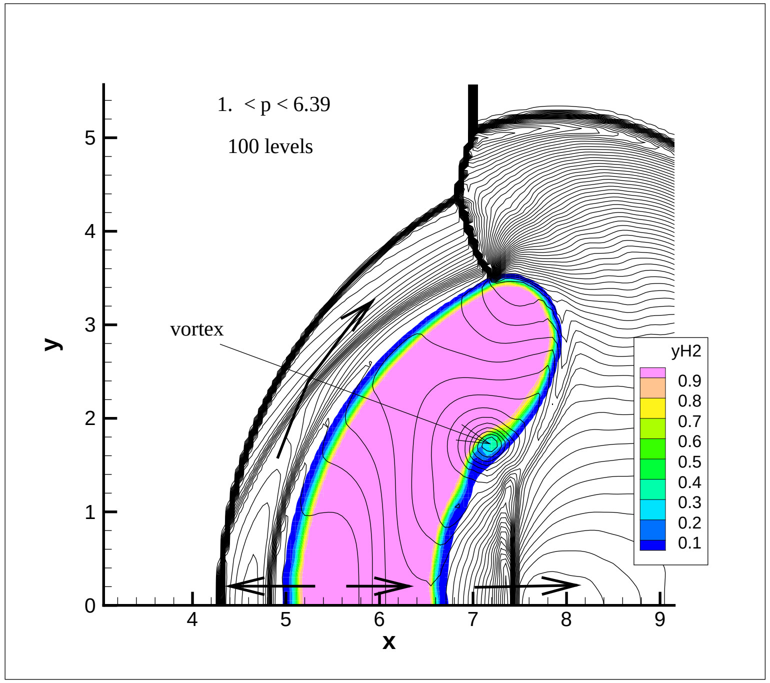




Shock/hydrogen bubble interaction (4)

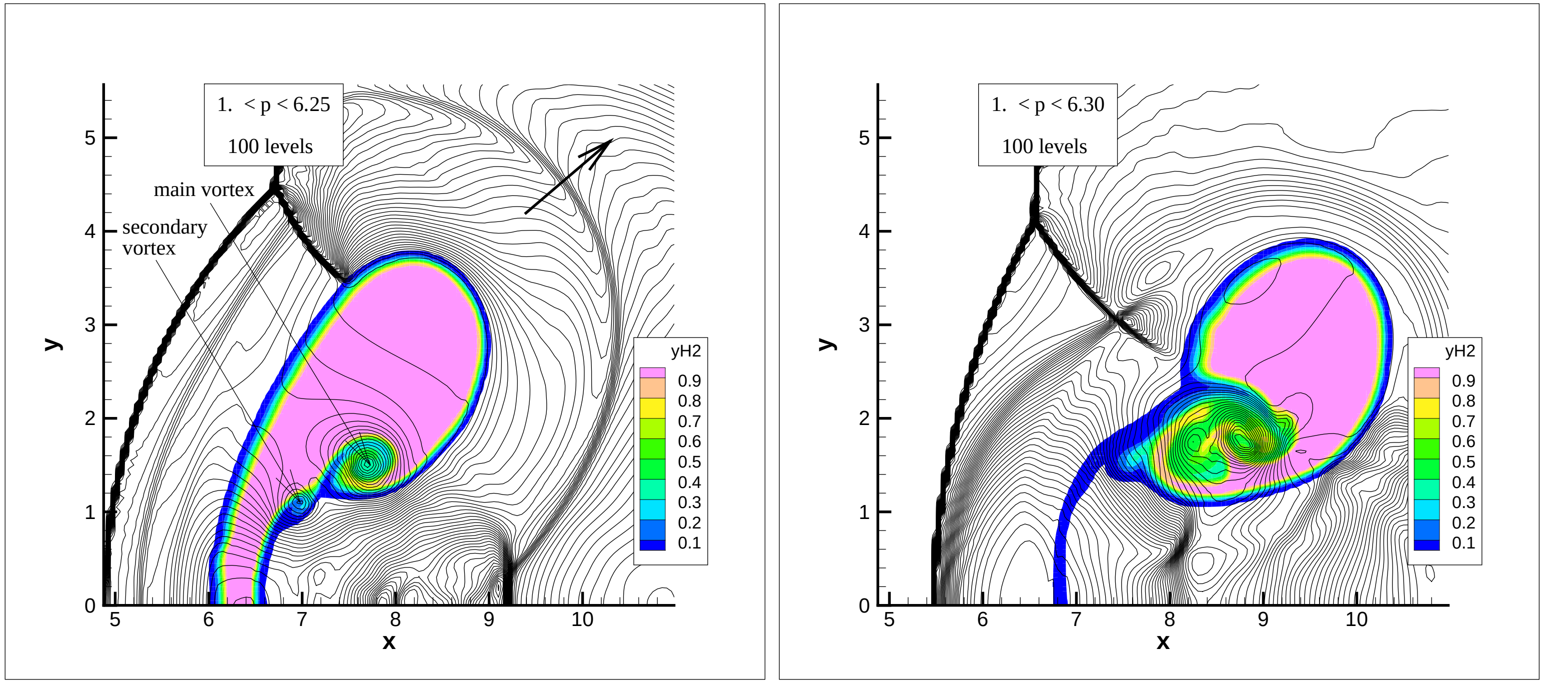
- **Pressure and hydrogen mass fraction at $t = 3.5,\ 4.0\ \mu s$**





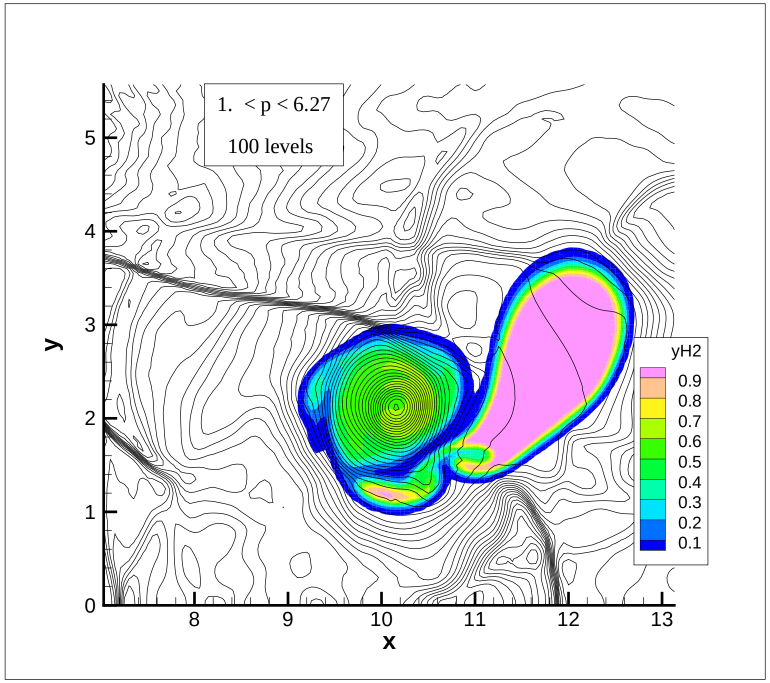
Shock/hydrogen bubble interaction (5)

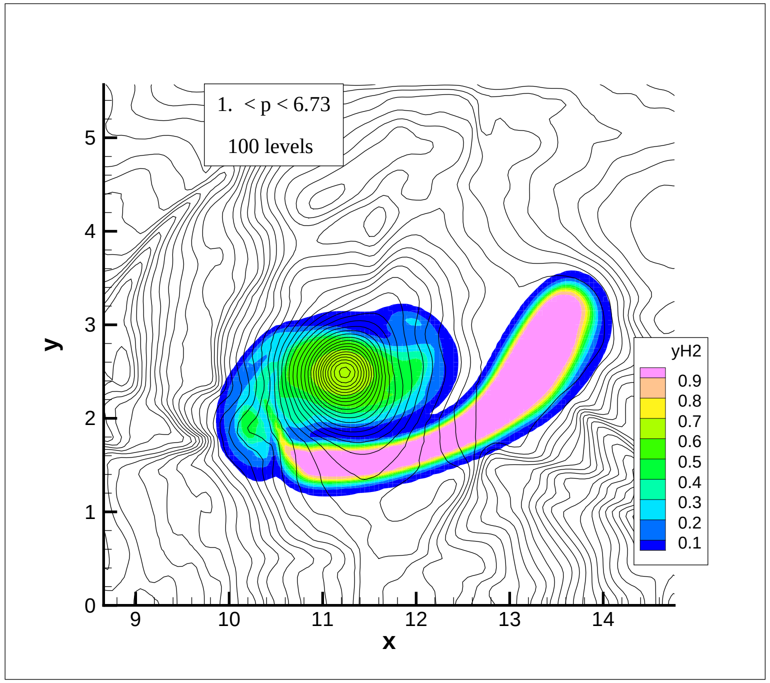
- **Pressure and hydrogen mass fraction at** $t = 6.0,\ 8.8\ \mu s$



Shock/hydrogen bubble interaction (6)

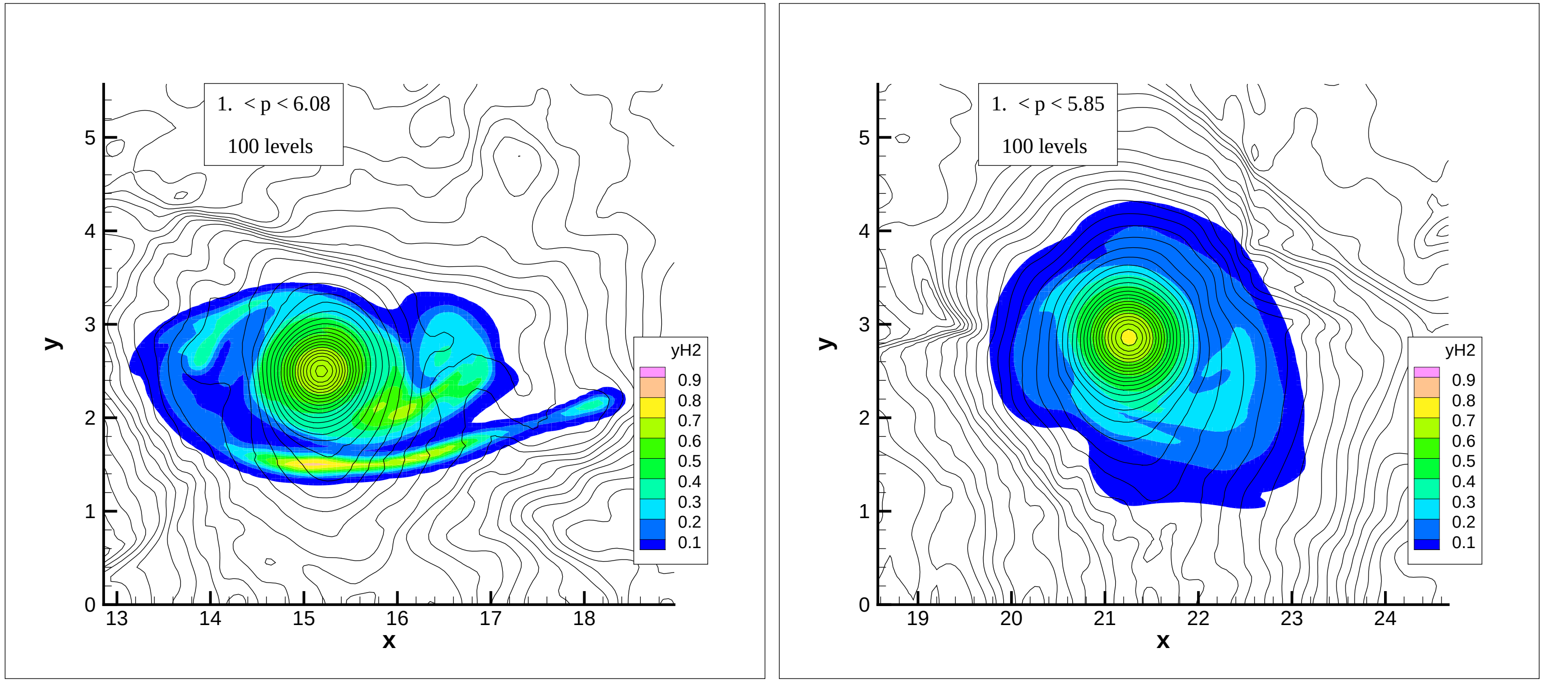
- **Pressure and hydrogen mass fraction at $t = 13.6,\ 16.6\ \mu s$**





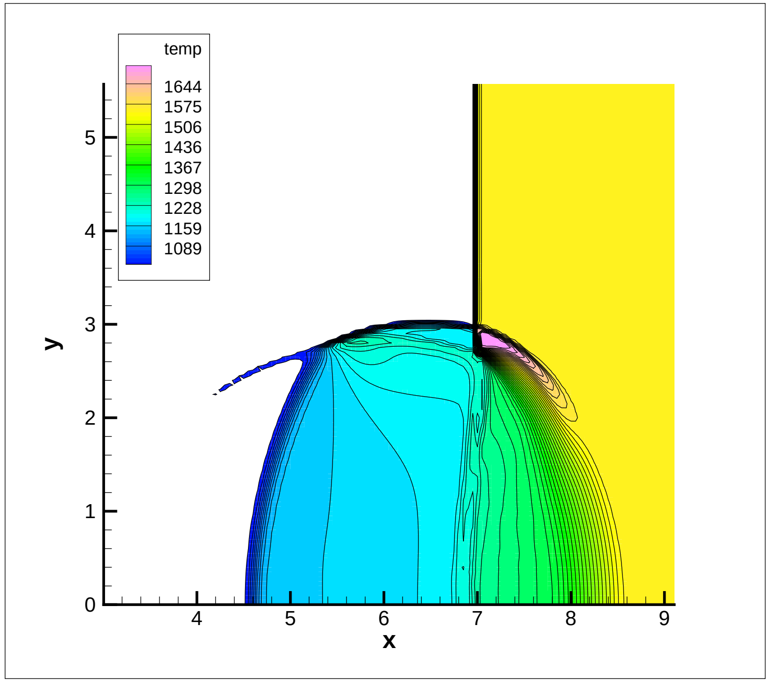
Shock/hydrogen bubble interaction (7)

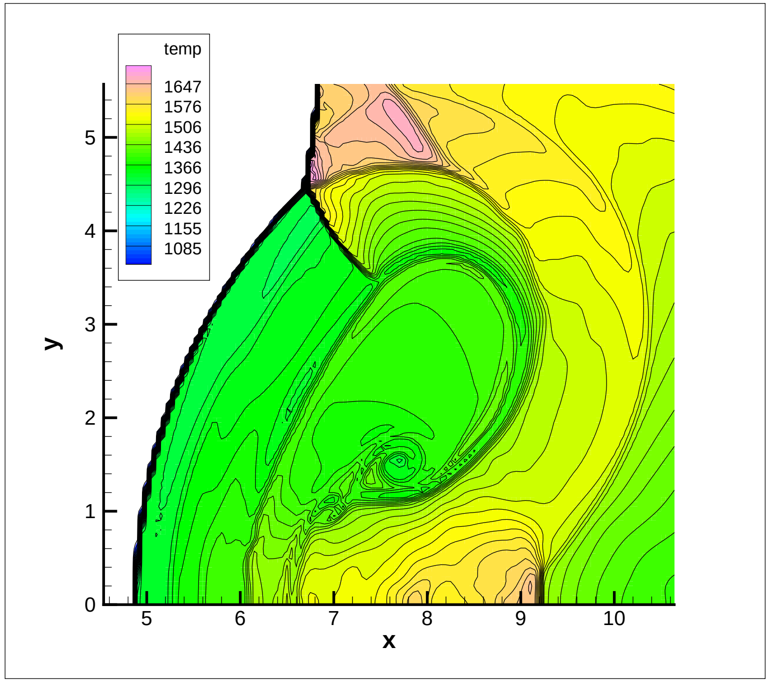
- **Pressure and hydrogen mass fraction at $t = 25.6,\ 41.6\ \mu s$**



Shock/hydrogen bubble interaction (8)

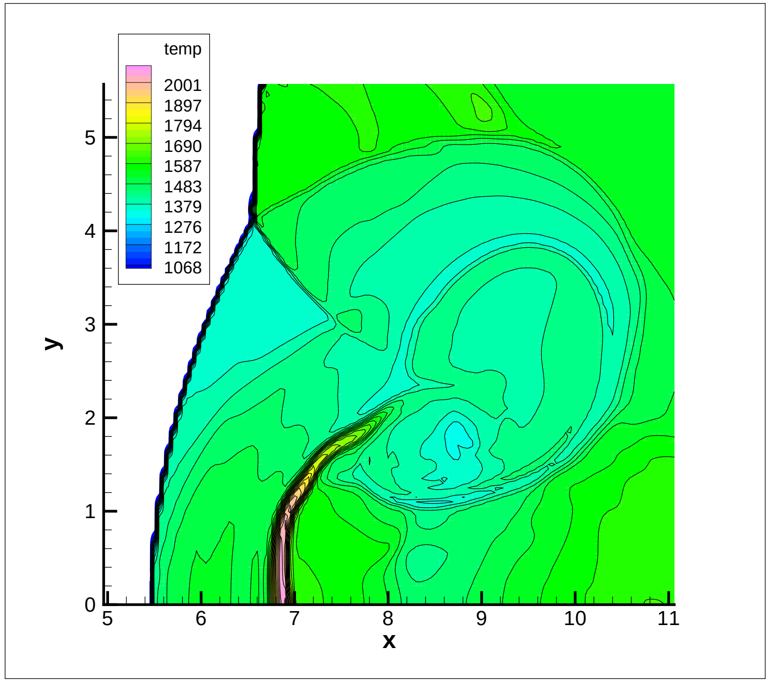
- **Temperature at** $t = 1.5, 6.0\ \mu s$

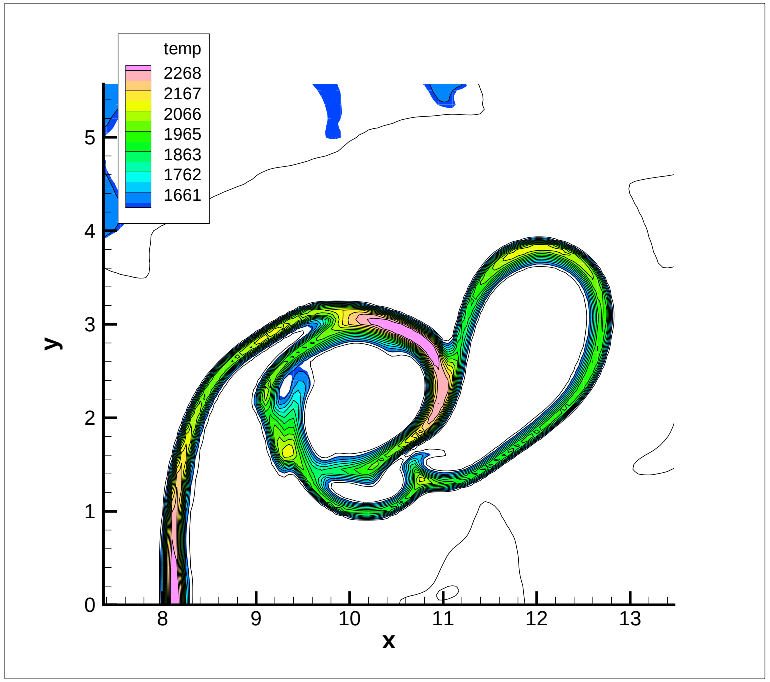




Shock/hydrogen bubble interaction (9)

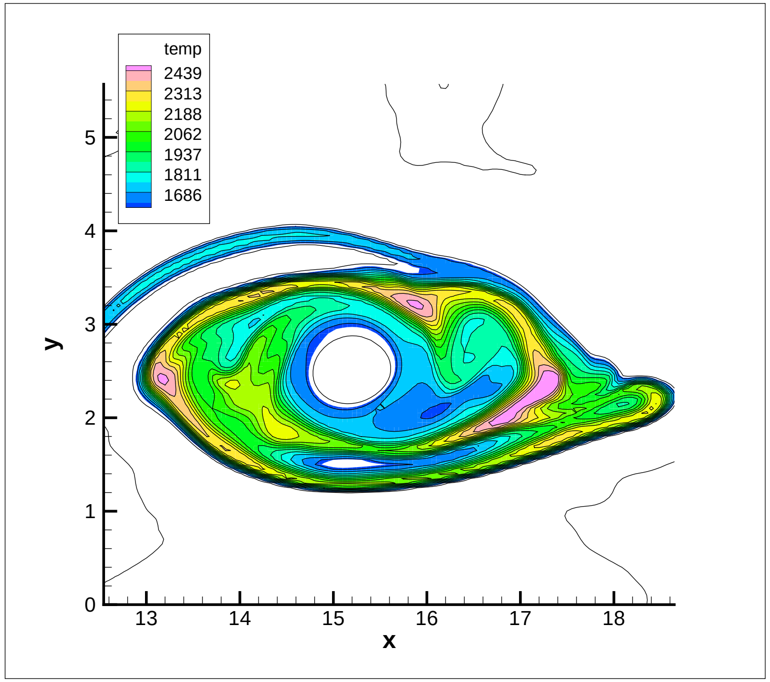
- **Temperature at $t = 8.8, 13.6\ \mu$s**

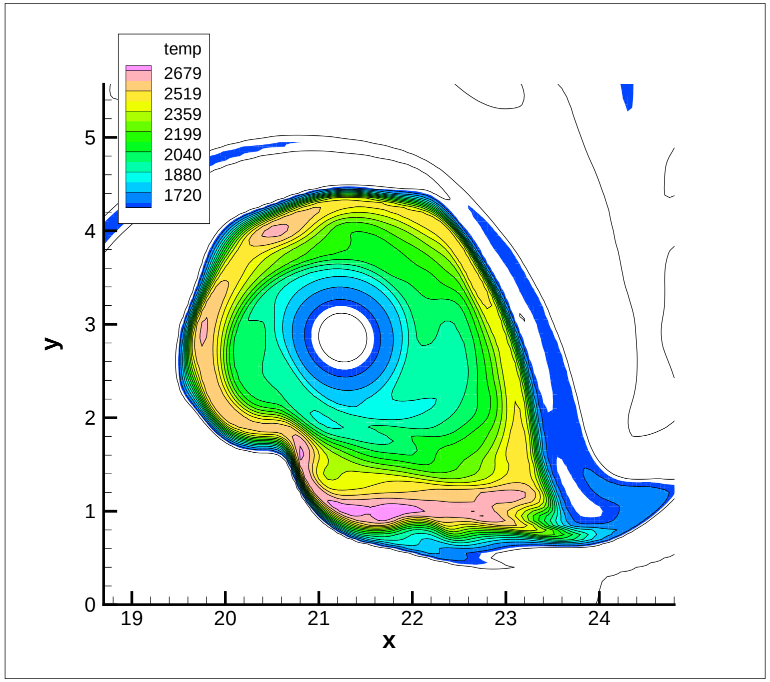




Shock/hydrogen bubble interaction (10)

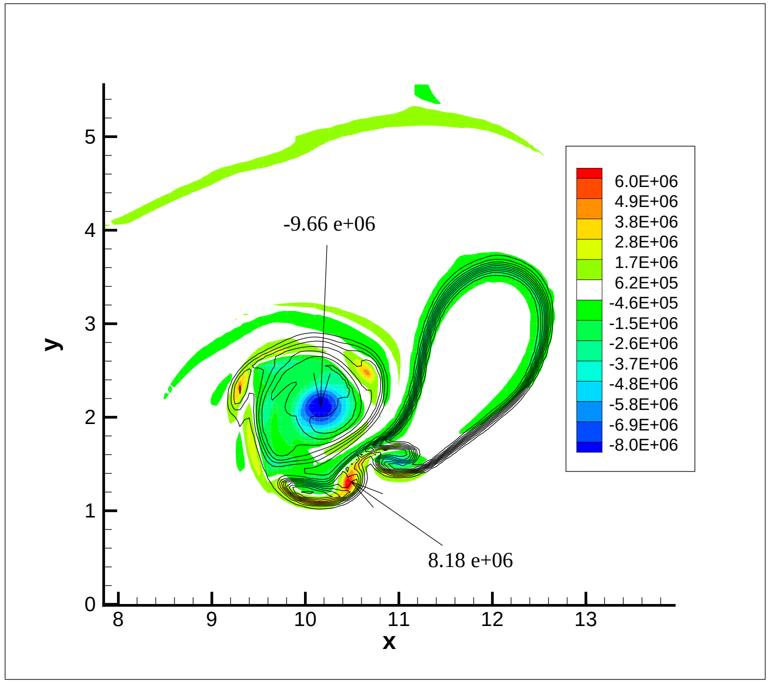
- **Temperature at** $t = 25.6, 41.6\ \mu s$

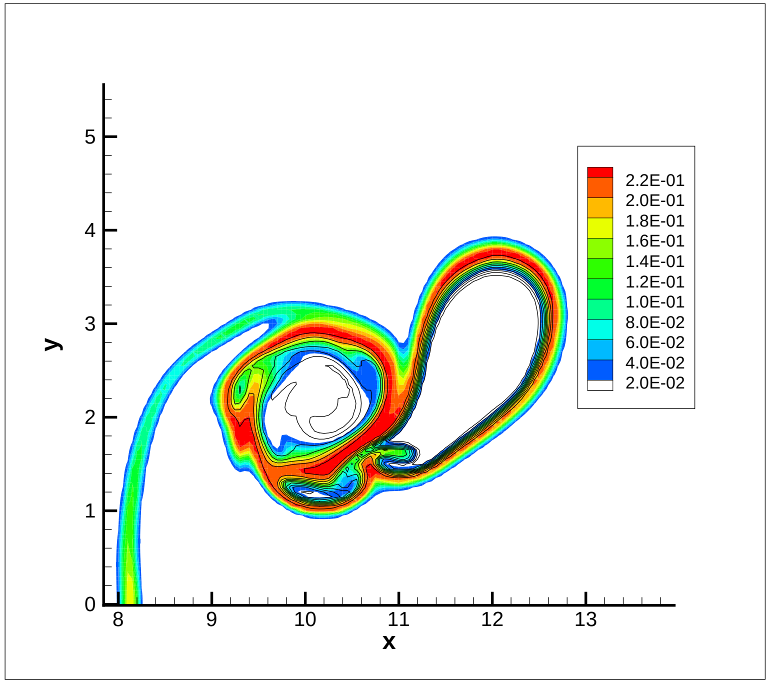




Shock/hydrogen bubble interaction (11)

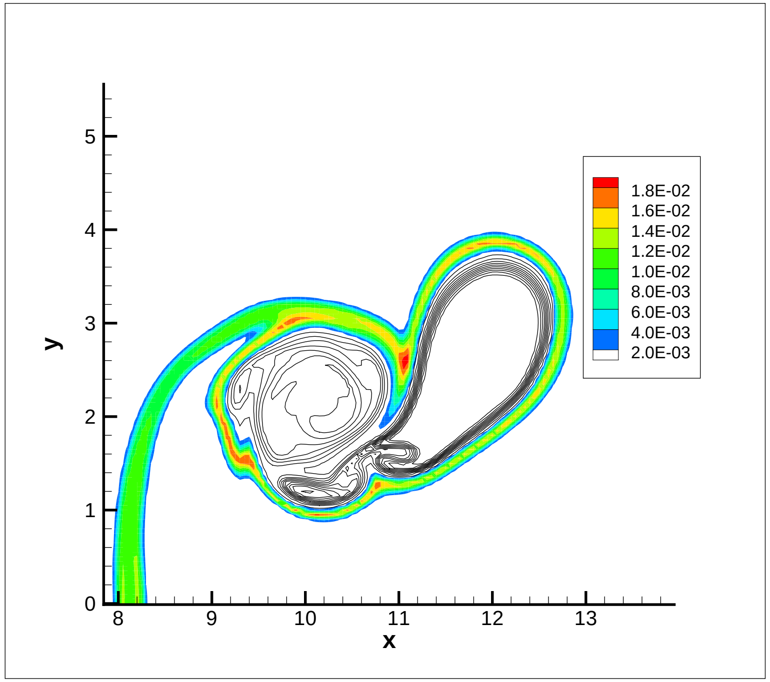
- **Vorticity and H_2O at $t = 13.6\ \mu s$**

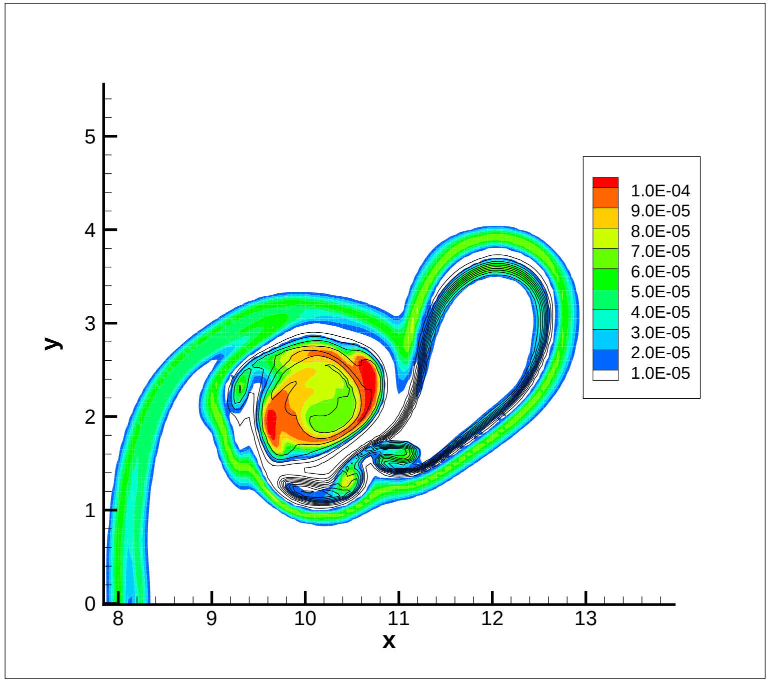




Shock/hydrogen bubble interaction (12)

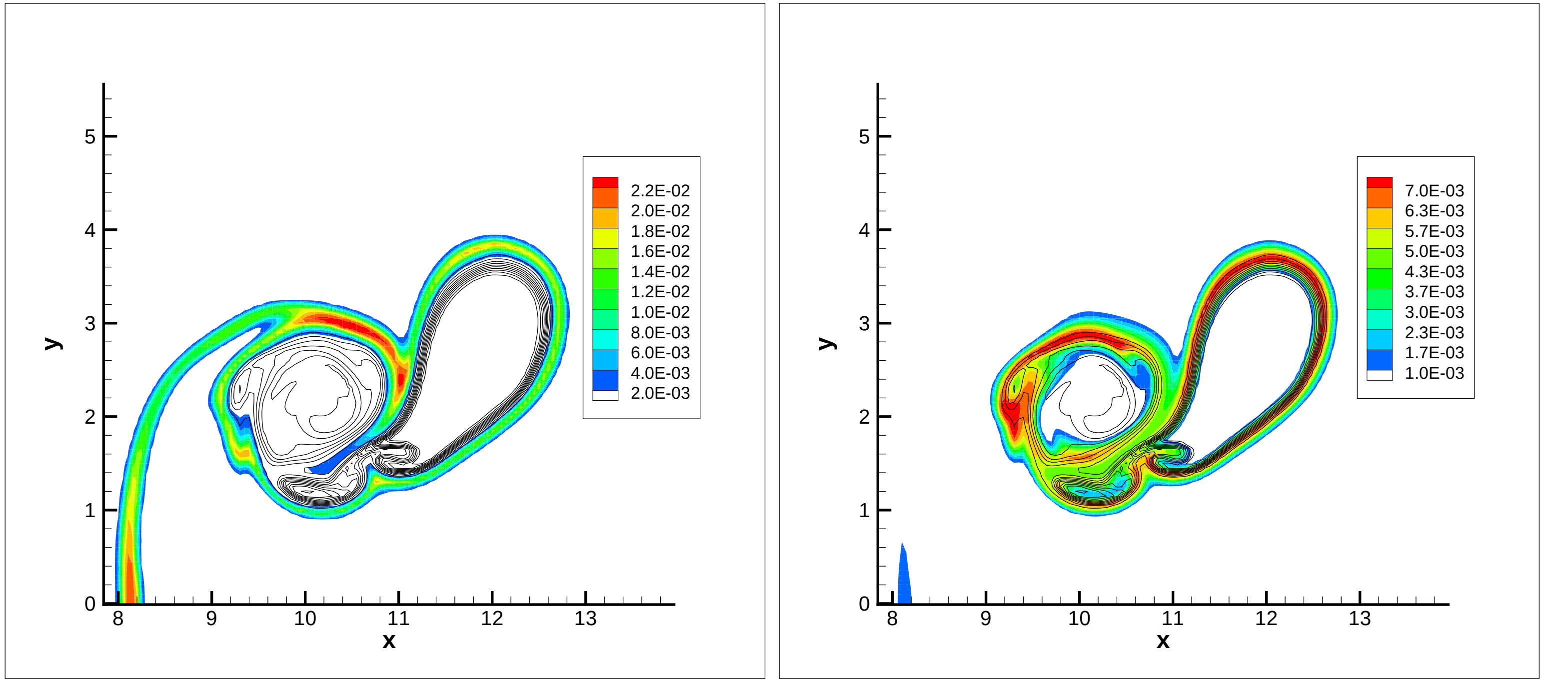
- **O and HO_2 at $t = 13.6\ \mu s$**





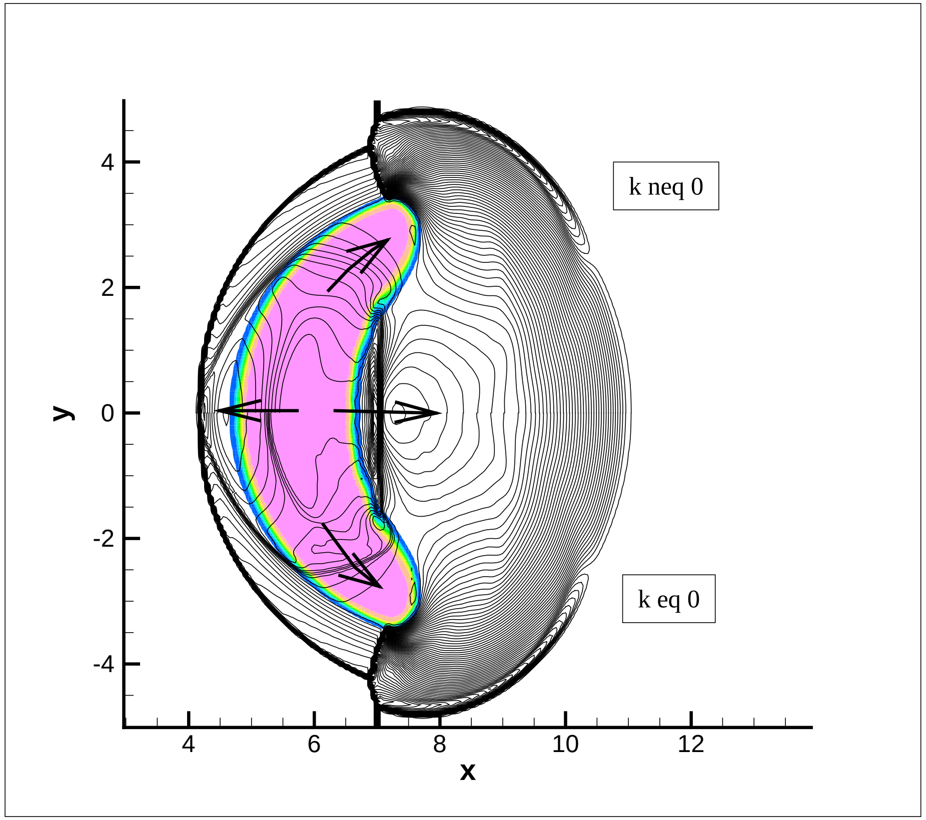
Shock/hydrogen bubble interaction (13)

- **OH and H at $t = 13.6\ \mu s$**



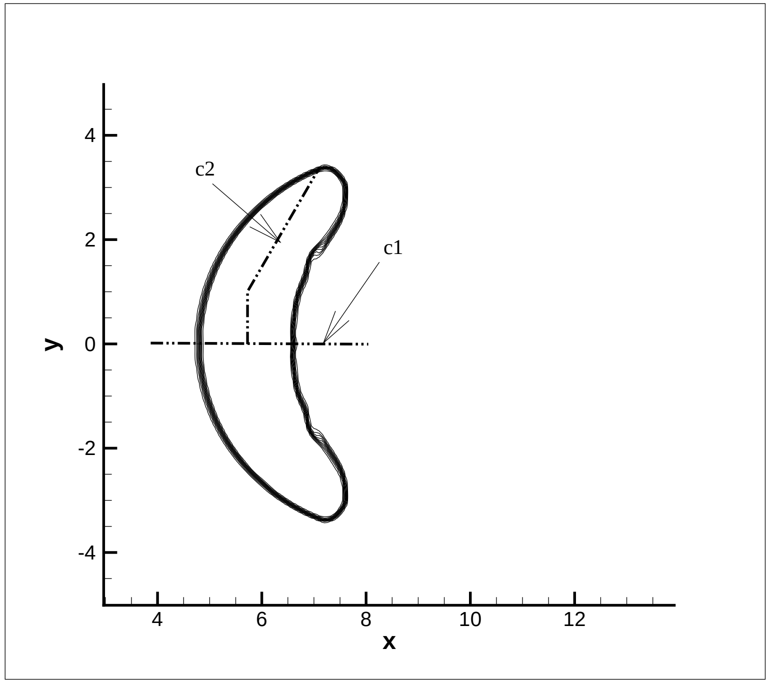
Shock/hydrogen bubble interaction (14)

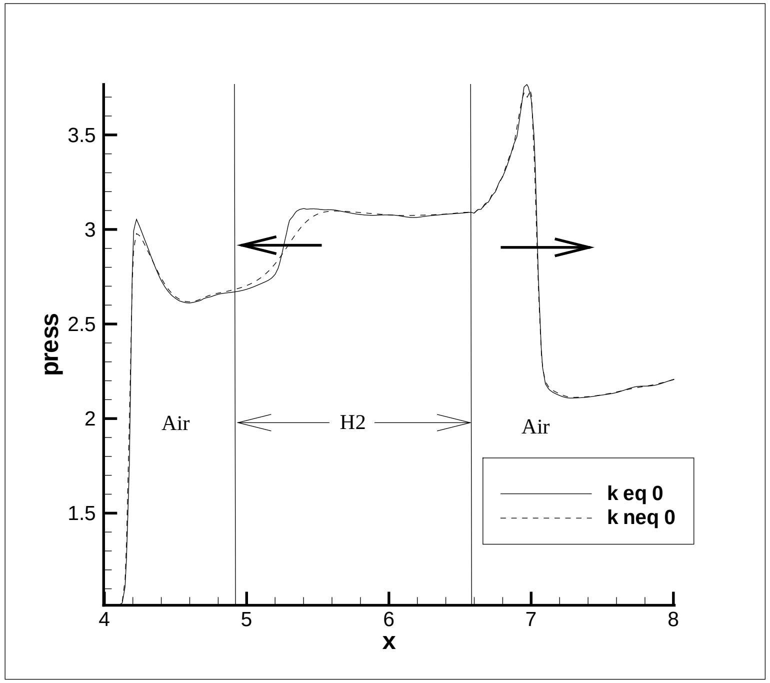
- **Pressure at $t = 3.5\ \mu s$**



Shock/hydrogen bubble interaction (15)

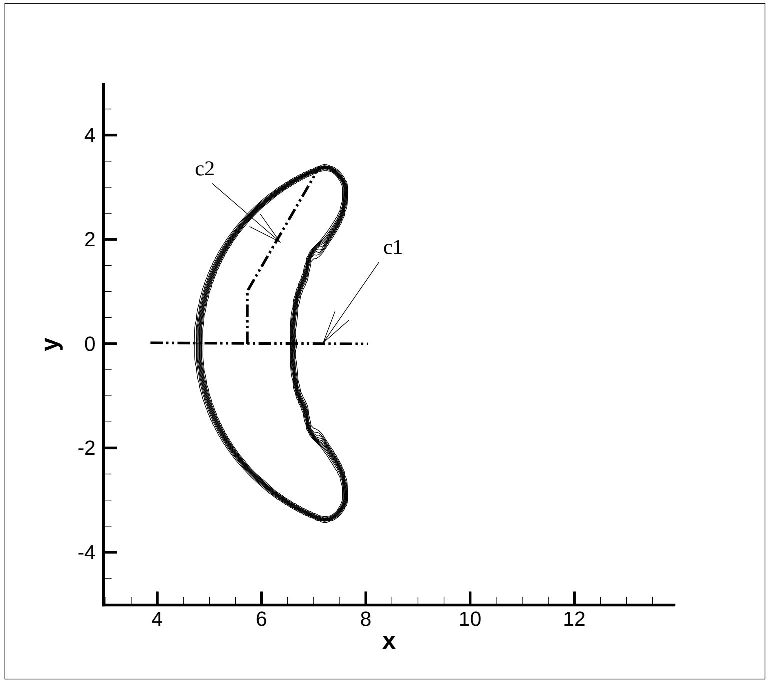
- **Pressure at $t = 3.5\ \mu s$**

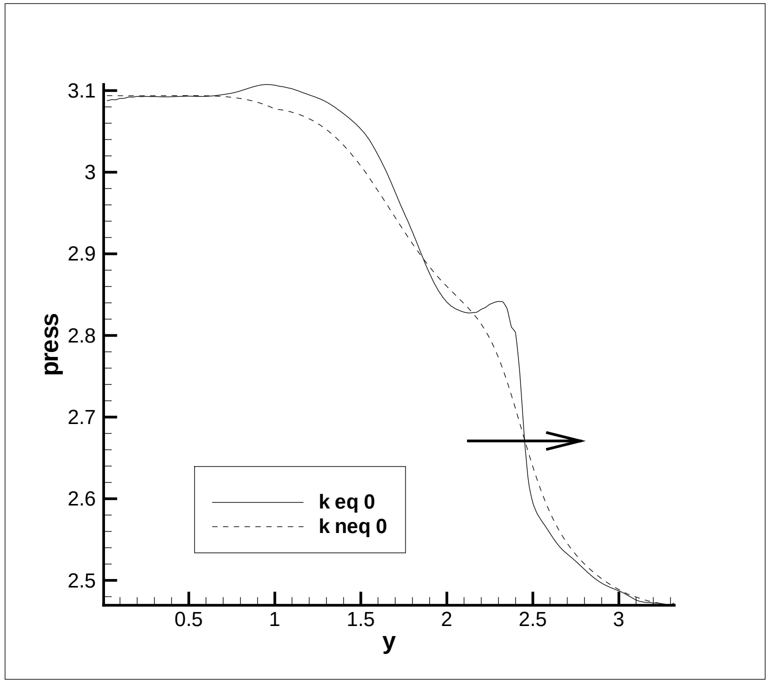




Shock/hydrogen bubble interaction (16)

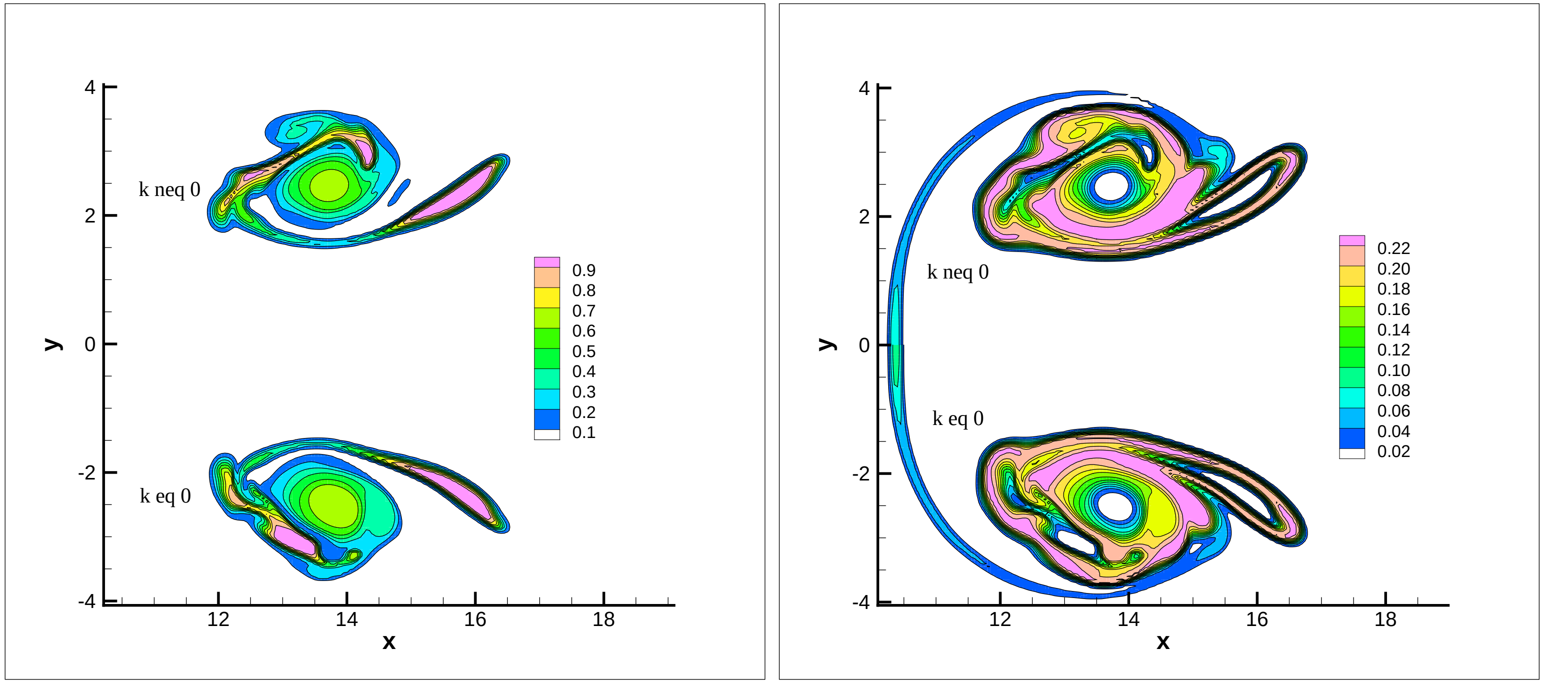
- **Pressure at $t = 3.5\ \mu s$**





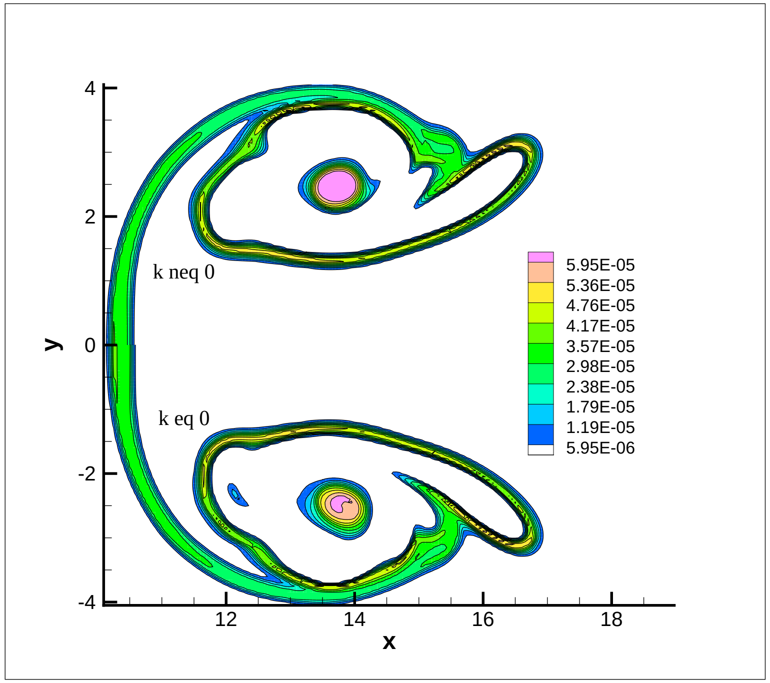
Shock/hydrogen bubble interaction (17)

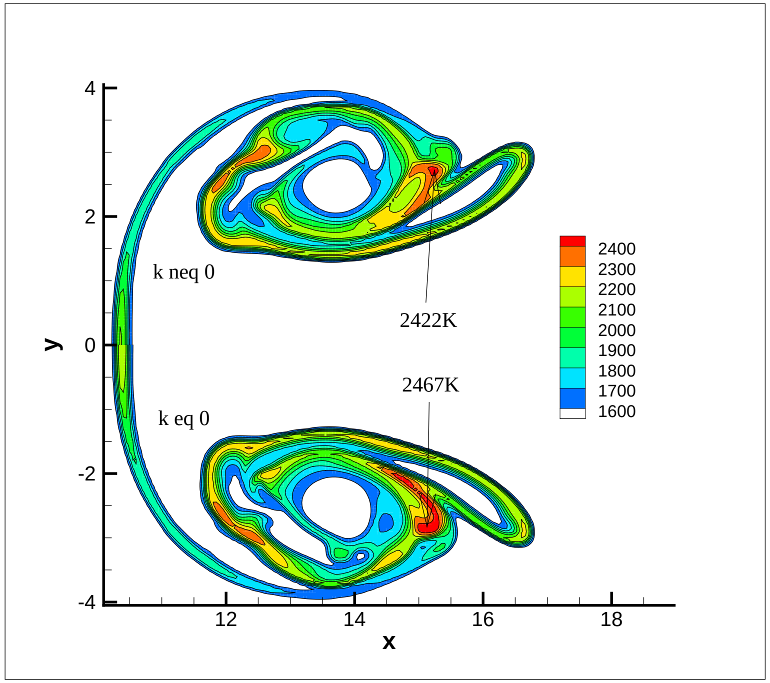
- **Impact of volume viscosity at $t = 21.6\ \mu s$**



Shock/hydrogen bubble interaction (18)

- **Impact of volume viscosity at $t = 21.6\ \mu s$**





Conclusion/Future work

- **Kinetic theory**

    Multi-Temperature theories for polyatomic molecules

    Electronic excited states

    Reactive mixtures

    Strong magnetic fields

- **Collision cross sections**

    Wide temperature range

    Polyatomic molecules

- **Numerics**

    Problem independent routines

    Open source environement