

Accurate Calculation of Detonation with an Adaptive Wavelet Method

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PROJECT SUMMARY

- An adaptive method is applied to problems in hypersonic propulsion.
- Compressible, reactive Navier-Stokes model includes detailed chemical kinetics, multi-species transport, momentum and energy diffusion.
- These problems are typically multidimensional and contain a wide range of spatial and temporal scales.
- Our adaptive wavelet method allows this range of scales to be resolved while greatly reducing the required computer time and automatically produces verified solutions.

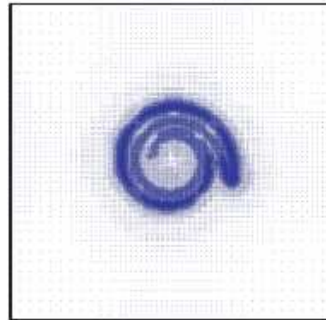
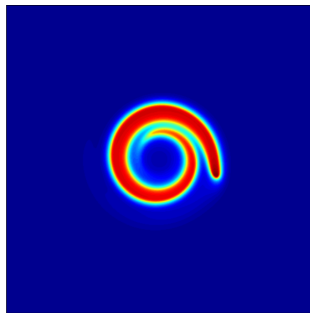


Figure: Flameball-vortex interaction—
computed temperature field and
adaptive grid.

WAVELET APPROXIMATION IN DOMAIN $[0, 1]^d$

Approximation of $u(\mathbf{x})$ by the interpolating wavelet, a multiscale basis, on $\mathbf{x} \in [0, 1]^d$ is given by

$$u(\mathbf{x}) \approx u^J(\mathbf{x}) = \sum_{\mathbf{k}} u_{j_0, \mathbf{k}} \Phi_{J_0, \mathbf{k}}(\mathbf{x}) + \sum_{j=J_0}^{J-1} \sum_{\lambda} d_{j, \lambda} \Psi_{j, \lambda}(\mathbf{x}),$$

where $\mathbf{x} \in \mathbb{R}^d$, $\lambda = (\mathbf{e}, \mathbf{k})$ and $\Psi_{j, \lambda}(\mathbf{x}) \equiv \Psi_{j, \mathbf{k}}^{\mathbf{e}}(\mathbf{x})$.

- Scaling function:

$$\Phi_{j, \mathbf{k}}(\mathbf{x}) = \prod_{i=1}^d \phi_{j, \mathbf{k}}(x_i), \quad k_i \in \kappa_j^0$$

- Wavelet function:

$$\Psi_{j, \mathbf{k}}^{\mathbf{e}}(\mathbf{x}) = \prod_{i=1}^d \psi_{j, \mathbf{k}}^{\mathbf{e}_i}(x_i), \quad k_i \in \kappa_j^{\mathbf{e}_i}$$

where $\mathbf{e} \in \{0, 1\}^d \setminus \mathbf{0}$, $\psi_{j, \mathbf{k}}^0(x) \equiv \phi_{j, \mathbf{k}}(x)$ and $\psi_{j, \mathbf{k}}^1(x) \equiv \psi_{j, \mathbf{k}}(x)$, and $\kappa_j^0 = \{0, \dots, 2^j\}$ and $\kappa_j^1 = \{0, \dots, 2^j - 1\}$.

1-D INTERPOLATING SCALING FUNCTION AND WAVELET

Some properties of $\phi_{j,k}$ and $\psi_{j,k}$ of order p ($p \in \mathbb{N}$, even):

- $\phi_{j,k}$ is defined through $\phi(2^j x - k)$ where $\phi(x) = \int \varphi_p(y)\varphi_p(y-x)dy$, the auto-correlation of the Daubechies wavelet $\varphi_p(x)$.
- The support of $\phi_{j,k}$ is compact, *i.e.* $\text{supp}\{\phi_{j,k}\} \sim |O(2^{-j})|$.
- $\phi_{j,k}(x_{j,n} = n2^{-j}) = \delta_{k,n}$, *i.e.* satisfies the *interpolation property*.
- $\psi_{j,k} = \phi_{j+1,2k+1}$.
- $\text{span}\{\phi_{j,k}\} = \text{span}\{\{\phi_{j-1,k}\}, \{\psi_{j-1,k}\}\}$.
- $\{1, x, \dots, x^{p-1}\}$, for $x \in [0, 1]$, can be written as a linear combination of $\{\phi_{j,k}, k = 0, \dots, 2^j\}$.
- $\{\{\phi_{J_0,k}\}, \{\psi_{j,k}\}_{j=J_0}^\infty\}$ forms a basis of a continuous 1-D function on the unit interval $[0, 1]$.

SPARSE WAVELET REPRESENTATION (SWR) AND IRREGULAR SPARSE GRID

- For a given threshold parameter ε , the multiscale approximation of a function $u(\mathbf{x})$ can be written as

$$\begin{aligned}
 u^J(\mathbf{x}) &= \sum_{\mathbf{k}} u_{J_0, \mathbf{k}} \Phi_{j_0, \mathbf{k}}(\mathbf{x}) + \sum_{j=j_0}^{J-1} \sum_{\{\lambda : |d_{j, \lambda}| \geq \varepsilon\}} d_{j, \lambda} \Psi_{j, \lambda}(\mathbf{x}) \\
 &\quad + \underbrace{\sum_{j=j_0}^{J-1} \sum_{\{\lambda : |d_{j, \lambda}| < \varepsilon\}} d_{j, \lambda} \Psi_{j, \lambda}(\mathbf{x})}_{R_\varepsilon^J},
 \end{aligned}$$

and the SWR is obtained by discarding the term R_ε^J .

- For interpolating wavelets, each basis function is associated with one dyadic grid point, *i.e.*

$$\Phi_{j, \mathbf{k}}(\mathbf{x}) \quad \text{with} \quad \mathbf{x}_{j, \mathbf{k}} = (k_1 2^{-j}, \dots, k_d 2^{-j})$$

$$\Psi_{j, \lambda}(\mathbf{x}) \quad \text{with} \quad \mathbf{x}_{j, \lambda} = \mathbf{x}_{j+1, 2\mathbf{k} + \mathbf{e}}$$

SWR AND IRREGULAR SPARSE GRID (CONTINUED)

- For a given SWR, one has an associated grid composed of *essential* points, whose wavelet amplitudes are greater than the threshold parameter ε

$$\mathcal{V}_e = \{\mathbf{x}_{j_0, \mathbf{k}}, \bigcup_{j \geq j_0} \mathbf{x}_{j, \boldsymbol{\lambda}} : \boldsymbol{\lambda} \in \Lambda_j\}, \quad \Lambda_j = \{\boldsymbol{\lambda} : |d_{j, \boldsymbol{\lambda}}| \geq \varepsilon\}.$$

- To accommodate the possible advection and sharpening of solution features, we determine the *neighboring* grid points:

$$\mathcal{V}_b = \bigcup_{\{j, \boldsymbol{\lambda} \in \Lambda\}} \mathcal{N}_{j, \boldsymbol{\lambda}},$$

where $\mathcal{N}_{j, \boldsymbol{\lambda}}$ is the set of neighboring points to $x_{j, \boldsymbol{\lambda}}$.

- The new sparse grid, \mathcal{V} , is then given by

$$\mathcal{V} = \mathbf{x}_{j_0, \mathbf{k}} \cup \mathcal{V}_e \cup \mathcal{V}_b.$$

SWR AND IRREGULAR SPARSE GRID (CONTINUED)

- There exists an adaptive fast wavelet transform (*AFWT*), with $O(N)$, $N = \dim\{\mathcal{V}\}$ operations, mapping the function values on the irregular grid \mathcal{V} to the associated wavelet coefficients and *vice-versa*:

$$AFWT(\{u(\mathbf{x}) : \mathbf{x} \in \mathcal{V}\}) \rightarrow \mathcal{D} = \{\{u_{j_0, \mathbf{k}}\}, \{d_{j, \boldsymbol{\lambda}}, \boldsymbol{\lambda} \in \Lambda_j\}_{j > j_0}\}.$$

- Provided that the function $u(\mathbf{x})$ is continuous, the error in the SWR $u_\varepsilon^J(\mathbf{x})$ is bounded by

$$\|u - u_\varepsilon^J\|_\infty \leq C_1 \varepsilon.$$

- Furthermore, for the function that is smooth enough, the number of basis functions $N = \dim\{u_\varepsilon^J\}$ required for a given ε satisfies

$$N \leq C_2 \varepsilon^{-d/p}, \quad \text{and} \quad \|u - u_\varepsilon^J\|_\infty \leq C_2 N^{-p/d}.$$

DERIVATIVE APPROXIMATION OF SWR

- Direct differentiation of wavelets is costly (with $O(p(J - j_0)N)$ operations) because of different support sizes of wavelet basis on different levels.
- Alternatively, we use finite differences to approximate the derivative on a grid of irregular points. The procedure can be summarized as follows:
 - ❶ For a given SWR of a function, perform the inverse interpolating wavelet transform to obtain the function values at the associated irregular points.
 - ❷ Apply locally a finite difference scheme of order n to approximate the derivative at each grid point.
- Estimate shows that the pointwise error of the derivative approximation has the following bound:

$$\|\partial^i u / \partial x^i - D_x^{(i)} u_\varepsilon^J\|_{\mathbf{V}, \infty} \leq CN^{-\min((p-i), n)/2}, \quad \|f\|_{\mathcal{G}, \infty} = \max_{x \in \mathcal{V}} |f(x)|.$$

DYNAMICALLY ADAPTIVE ALGORITHM FOR SOLVING TIME-DEPENDENT PDES

Given the set of PDEs

$$\frac{\partial u}{\partial t} = F(t, u, u_x, u_{xx}, \dots),$$

with initial conditions

$$u(x, 0) = u^0.$$

- ❶ Obtain sparse grid, \mathcal{V}^m , based on thresholding of magnitudes of wavelet amplitudes of the approximate solution u^m .
- ❷ Integrate in time using an explicit time integrator with error control to obtain the new solution u^{m+1} .
- ❸ Assign $u^{m+1} \rightarrow u^m$ and return to step ❶.

COMPRESSIBLE REACTIVE FLOW

Code solves the n -D compressible reactive Navier-Stokes equations:

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= -\frac{\partial}{\partial x_i} (\rho u_i) \\ \frac{\partial \rho u_i}{\partial t} &= -\frac{\partial}{\partial x_j} (\rho u_j u_i) - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \\ \frac{\partial \rho E}{\partial t} &= -\frac{\partial}{\partial x_j} (u_j (\rho E + p)) + \frac{\partial u_j \tau_{ji}}{\partial x_i} - \frac{\partial q_i}{\partial x_i} \\ \frac{\partial \rho Y_k}{\partial t} &= -\frac{\partial}{\partial x_i} (u_i \rho Y_k) + M_k \dot{\omega}_k - \frac{\partial j_{k,i}}{\partial x_i}, \quad k = 1, \dots, K\end{aligned}$$

Where ρ -density, u_i -velocity vector, E -specific total energy, Y_k -mass fraction of species k , τ_{ij} -viscous stress tensor, q_i -heat flux, $j_{k,i}$ -species mass flux, M_k - molecular weight of species k , and $\dot{\omega}_k$ -reaction rate of species k .

COMPRESSIBLE REACTIVE FLOW (CONT.)

Where,

$$E = e + \frac{1}{2}u_i u_i$$

$$\tau_{ij} = -\frac{2}{3}\mu \frac{\partial u_l}{\partial x_l} \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

$$q_i = -k \frac{\partial T}{\partial x_i} + \sum_{k=1}^K \left(h_k j_{k,i} - \frac{RT}{m_k X_k} D_k^T d_{k,i} \right)$$

$$j_{k,i} = \frac{\rho Y_k}{X_k \bar{M}} \sum_{j=1, j \neq k}^K M_j D_{kj} d_{j,i} - \frac{D_k^T}{T} \frac{\partial T}{\partial x_i}$$

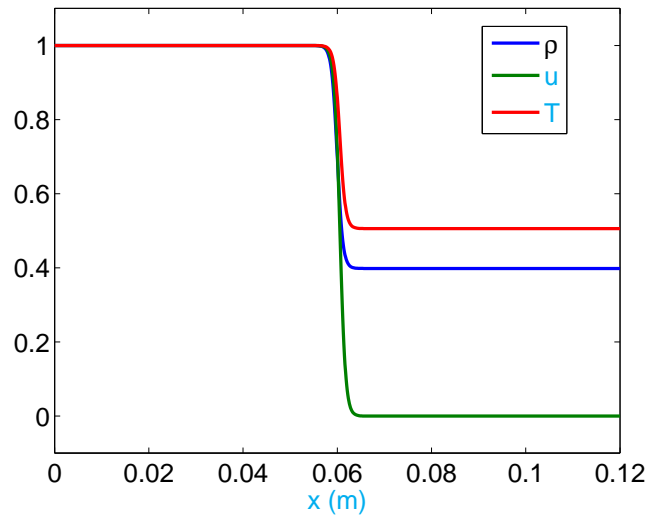
$$d_{k,i} = \frac{\partial X_k}{\partial x_i} + (X_k - Y_k) \frac{1}{p} \frac{\partial p}{\partial x_i}$$

1-D VISCOUS DETONATION

Initial conditions:

$2H_2 : 1O_2 : 7Ar$ mixture

9 species, 37 reactions



State 1: $0 \text{ m} \leq x < 0.06 \text{ m}$

$$\rho_1 = 0.18075 \text{ kg m}^{-3}$$

$$P_1 = 35594 \text{ Pa}$$

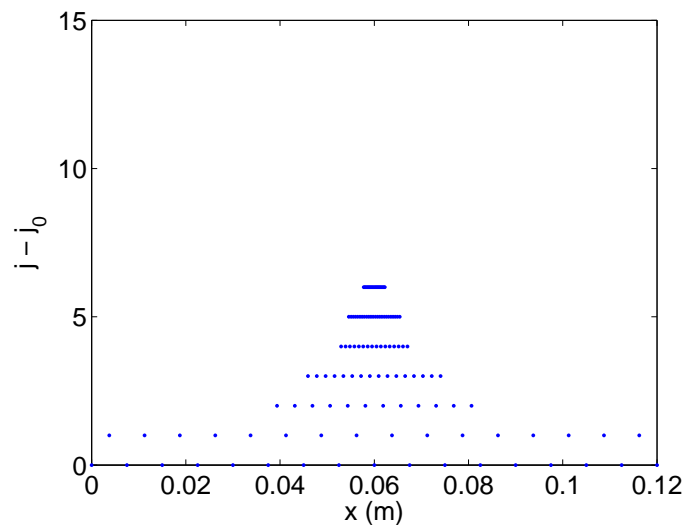
$$u_1 = 487.34 \text{ m s}^{-1}$$

State 2: $0.06 \text{ m} \leq x \leq 0.12 \text{ m}$

$$\rho_2 = 0.072 \text{ kg m}^{-3}$$

$$P_2 = 7173 \text{ Pa}$$

$$u_2 = 0 \text{ m s}^{-1}$$



Wavelet parameters:

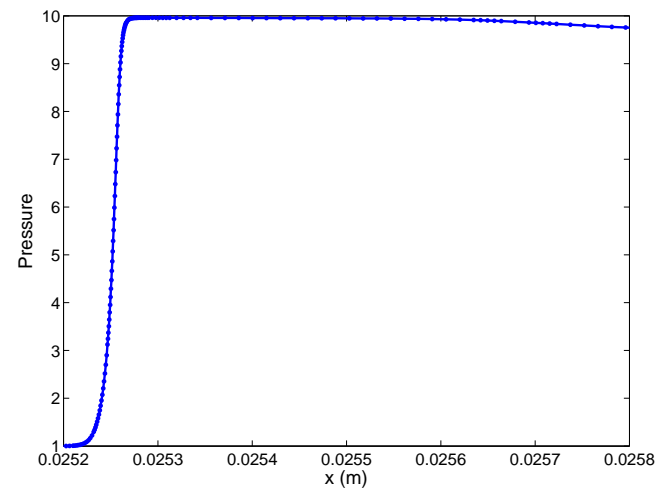
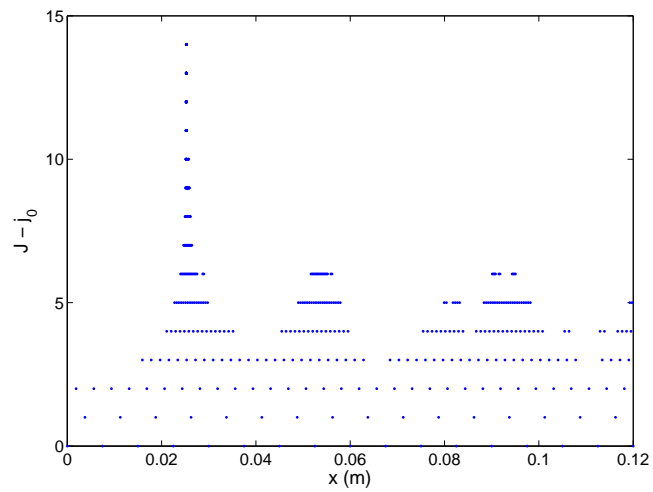
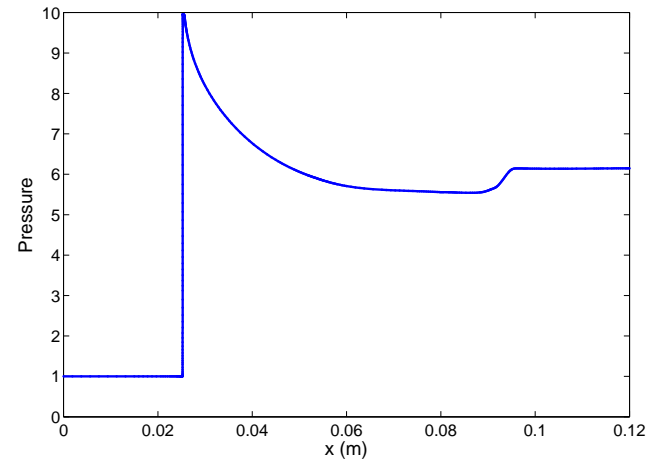
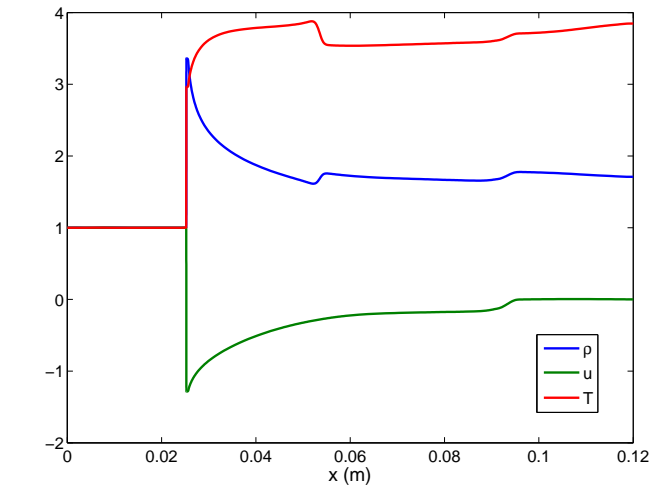
$$\epsilon = 1 \times 10^{-4}$$

$$p = 6, \quad n = 4$$

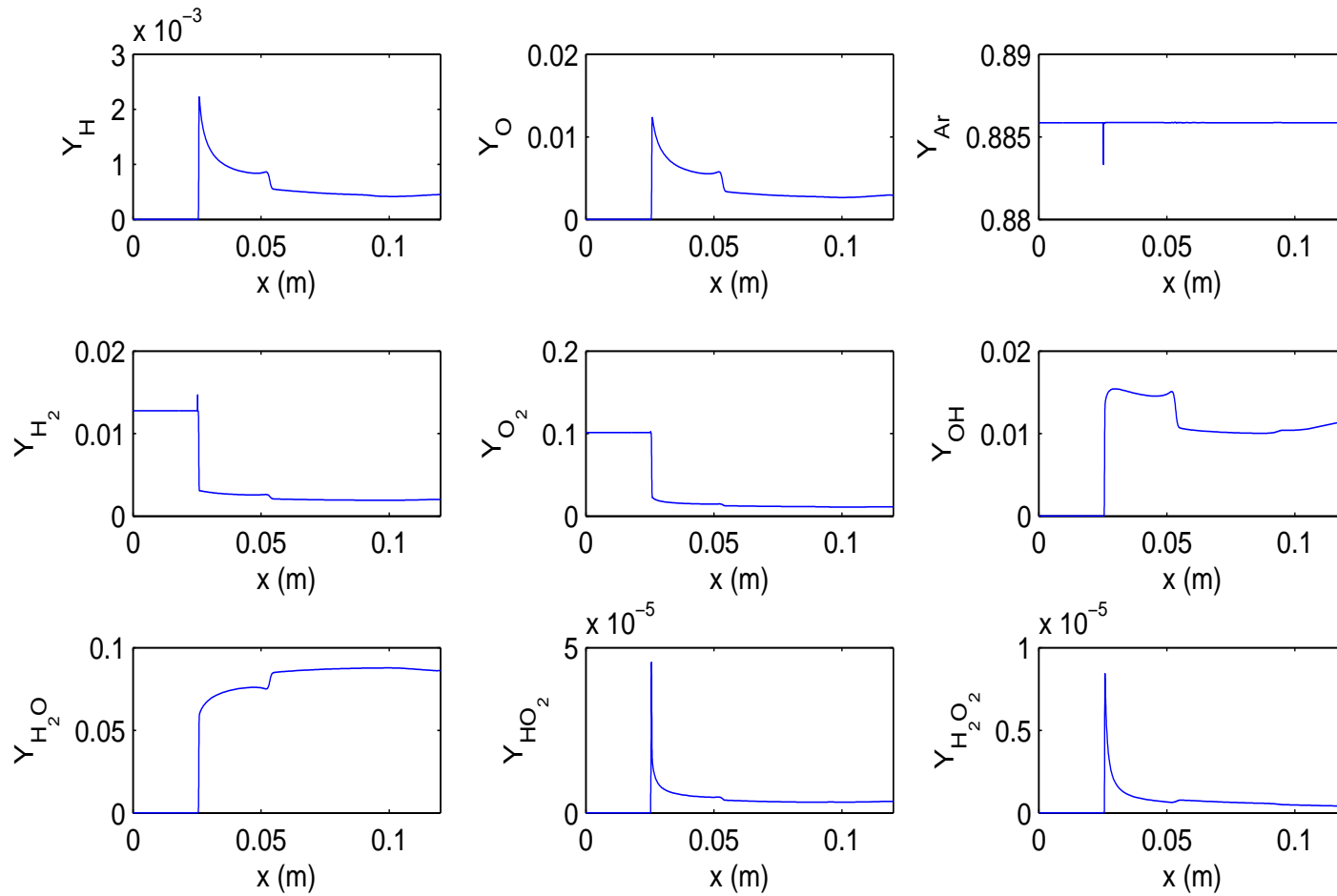
$$j_0 = 4, \quad J - j_0 = 15$$

1-D VISCOUS DETONATION (CONT.)

$t = 230 \mu s$

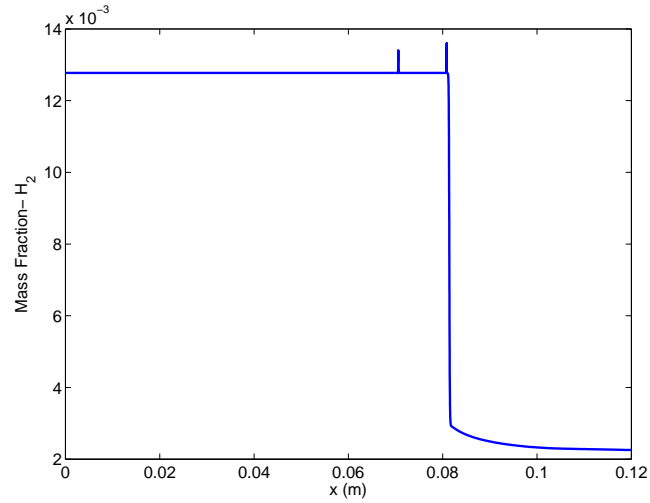


SPECIES MASS FRACTIONS AT $t = 230 \mu s$

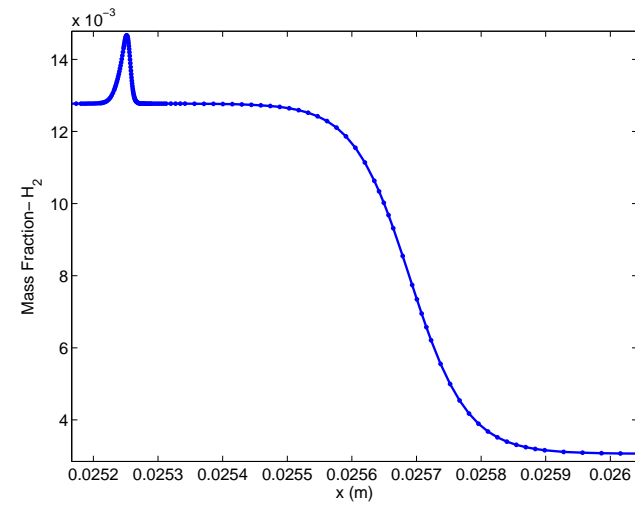
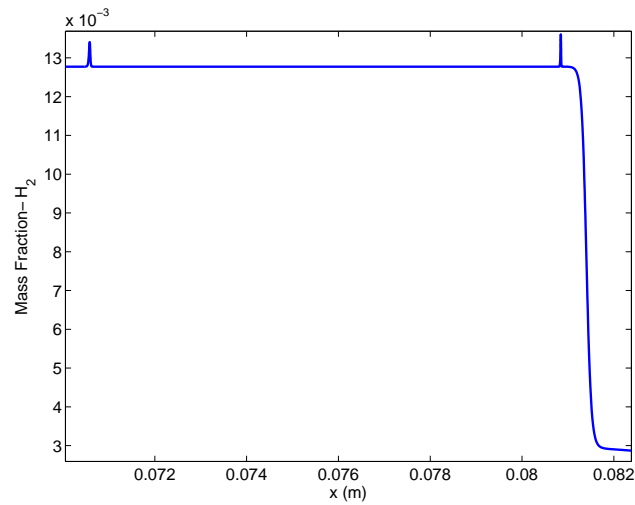
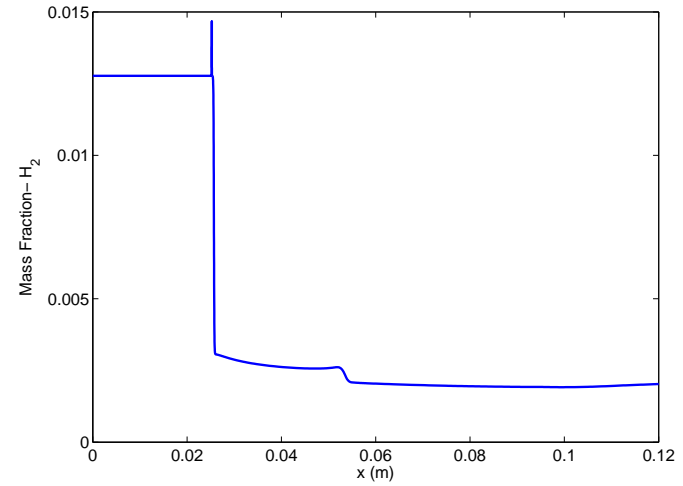


EFFECT OF MULTI-COMPONENT MASS DIFFUSION

$t = 180 \mu s$



$t = 230 \mu s$



SUMMARY

- An adaptive wavelet method is used to simulate a 1-d viscous detonation in a $H_2 - O_2 - Ar$ mixture.
- Detailed chemical kinetics, state-dependent thermodynamic and transport properties, and mass and thermal diffusions are included.
- The method distributes collocation points satisfying a given error tolerance.
- For the detonation problem considered, micron-scale resolution is needed:

Domain length:	12 cm
Induction zone:	$\approx 0.5 \text{ mm}$
Shock thickness:	$\approx 10 \text{ }\mu\text{m}$
Mean-free path:	$\approx 0.5 \text{ }\mu\text{m}$
Minimum Δx :	$\approx 0.5 \text{ }\mu\text{m}$
Average DOF:	275
Compression ratio (N_{full}/N_{adap}):	950