Detonation Simulation Using the Parallel Wavelet Adaptive Multiresolution Representation

By

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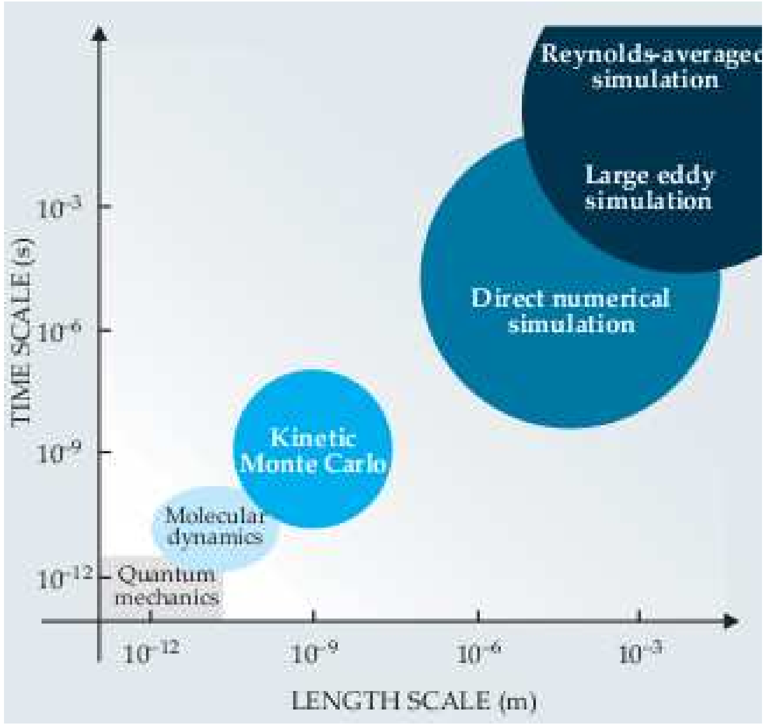
Project Summary

- An adaptive method is applied to the simulation of compressible reacting flow.
- Model includes detailed chemical kinetics, multi-species transport, momentum and energy diffusion.
- Problems are typically multi-dimensional and contain a wide range of spatial and temporal scales.
- Method resolves the range of scales present, while greatly reducing required computational effort and automatically produces verified solutions.



"Research needs for future internal combustion engines," *Physics Today*, Nov. 2008, pp 47-52.

Compressible Reactive Flow

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

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

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, $j_{i,k}$-species mass flux, M_k-molecular weight of species k, and $\dot{\omega}_k$-reaction rate of species k.

Compressible Reactive Flow (cont.)

Where,

$$
\begin{aligned}
\sum_{k=1}^{K} Y_k &= 1 \\
E &= e + \frac{1}{2} u_i u_i \\
\tau_{ij} &= -\frac{2}{3}\mu \frac{\partial u_l}{\partial x_l}\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \\
q_i &= -\mathsf{k}\frac{\partial T}{\partial x_i} + \sum_{k=1}^{K}\left(h_k j_{i,k} - \frac{RT}{m_k X_k} D_k^T d_{i,k}\right) \\
j_{i,k} &= \frac{\rho Y_k}{X_k \overline{M}} \sum_{j=1, j\neq k}^{K} M_j D_{jk} d_{i,j} - \frac{D_k^T}{T}\frac{\partial T}{\partial x_i} \\
d_{i,k} &= \frac{\partial X_k}{\partial x_i} + (X_k - Y_k)\frac{1}{p}\frac{\partial p}{\partial x_i}
\end{aligned}
$$

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 $\Psi_{j,\lambda}(\mathbf{x}) \equiv \Psi^{\mathbf{e}}_{j,\mathbf{k}}(\mathbf{x})$.

- Scaling function:

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

- Wavelet function:

$$\Psi^{\mathbf{e}}_{j,\mathbf{k}}(\mathbf{x}) = \prod_{i=1}^{d} \psi^{e_i}_{j,\mathbf{k}}(x_i), \; k_i \in \kappa_j^{e_i}$$

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

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

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

  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.*

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

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

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

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

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

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

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

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

SWR and Irregular Sparse grid (continued)

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

$$AFWT(\{u(\mathbf{x}) \,:\, \mathbf{x} \in \boldsymbol{\mathcal{V}}\}) \to \mathcal{D} = \{\{u_{j_0,\mathbf{k}}\}, \{d_{j,\boldsymbol{\lambda}},\ \boldsymbol{\lambda} \in \boldsymbol{\Lambda}_j\}_{j>j0}\}.$$

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

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

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

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

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 the connection with Lagrange interpolating polynomials to approximate the derivative on a grid of irregular points. The procedure can be summarized as follows:

  1. For a given SWR of a function, perform the inverse interpolating wavelet transform to obtain the function values at the associated irregular points.
  2. 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:

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

Dynamically Adaptive Algorithm for Solving Time-Dependent PDEs

Given the set of PDEs

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

with initial conditions

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

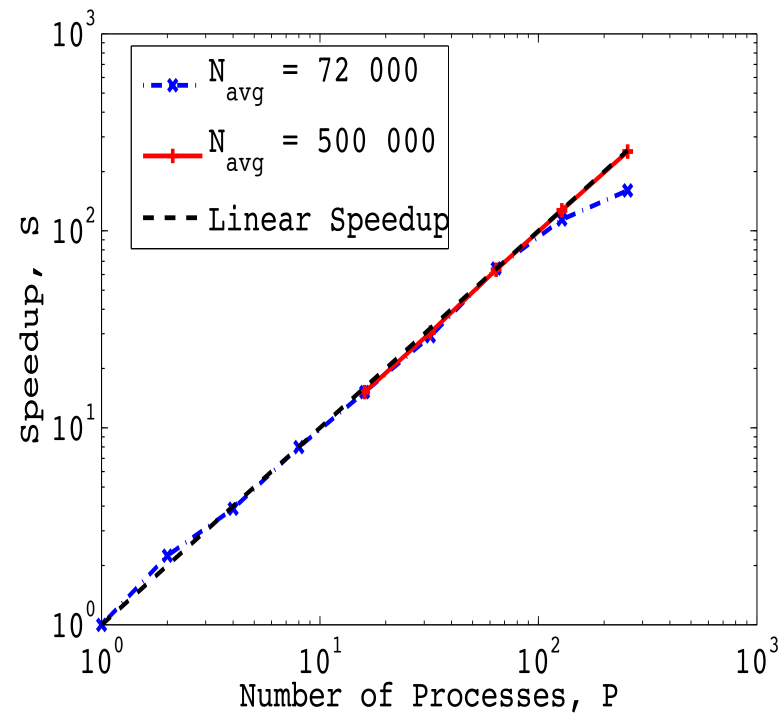
❶ Obtain sparse grid, $\boldsymbol{\mathcal{V}}^m$, based on thresholding of magnitudes of wavelet amplitudes of the approximate solution u^m.

❷ Integrate in time using an explicit time integrator with error control to obtain the new solution u^{m+1}.

❸ Assign $u^{m+1} \to u^m$ and return to step ❶.

Parallelization

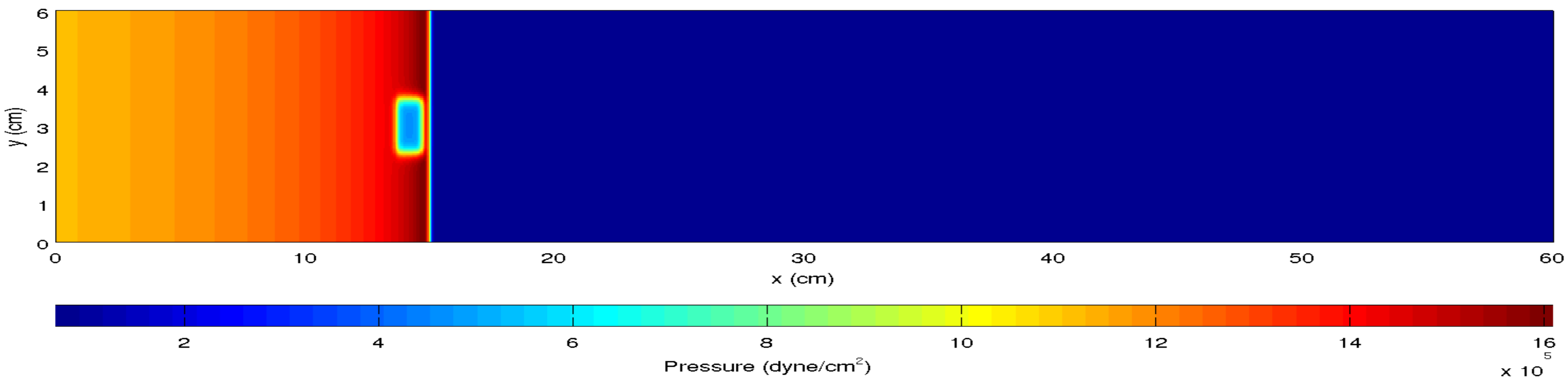
- Parallel algorithm uses an MPI-based domain decomposition.
- Hilbert space-filling curve used for partitioning and load-balancing.
- Strong scaling up to 256 cores with $> 90\%$ parallel efficiency.
- Chemkin-II and Transport Libraries used for evaluation of thermodynamics, transport properties, and reaction source terms.



Dual Quad-Core, 2.7 GHz L5520 Intel Nehalem nodes (8 cores/node), 12 GB RAM, Infiniband interconnect

2-D Viscous Detonation

Initial Conditions:



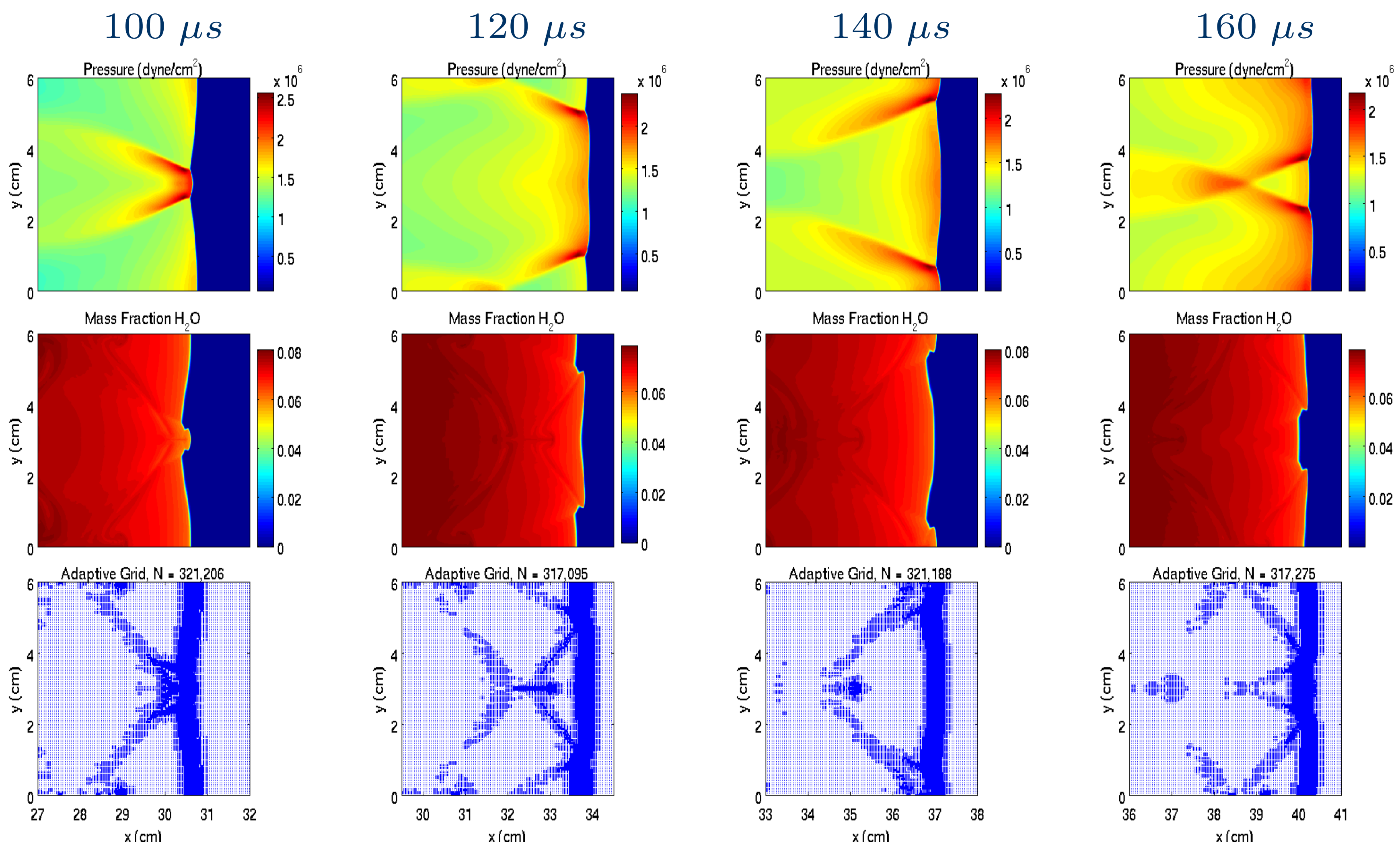
Domain: $[0, 60] \times [0, 6]$ cm
Front: $x = 15.0$ cm
Unreacted pocket:
$[1.05 \times 1.43]$ cm
at $x = 14.7$ cm
$P = 4.7 \times 10^5$ dyne/cm^2
$T = 2100$ K
128 cores
391 hrs runtime

$2H_2 : O_2 : 7Ar$ mixture
9 species, 37 reactions

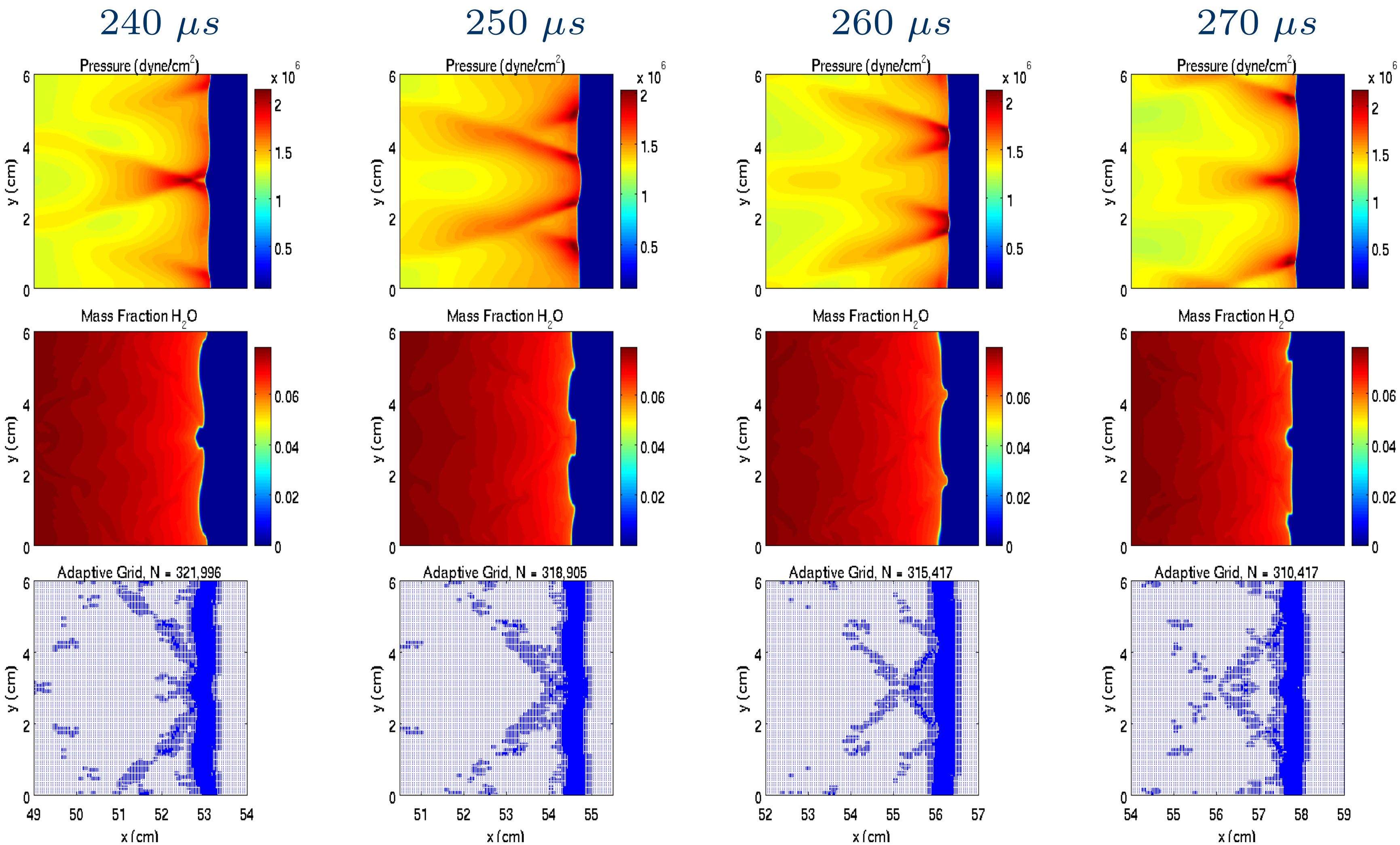
Wavelet parameters:

$\epsilon = 1 \times 10^{-3}$
$p = 6, \quad n = 5$
$[N_x \times N_y]_{j_0} = [600 \times 60]$
$J - j_0 = 10$

2-D Viscous Detonation (cont.)

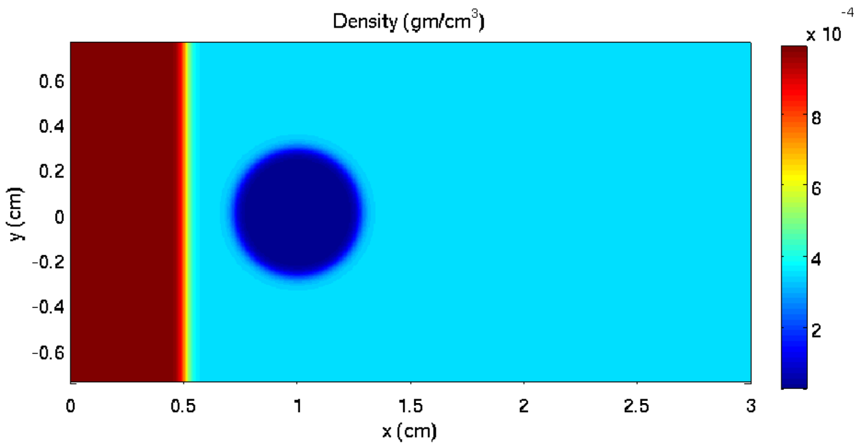


2-D Viscous Detonation (cont.)



Shock/H_2-Bubble Interaction

Initial Conditions:



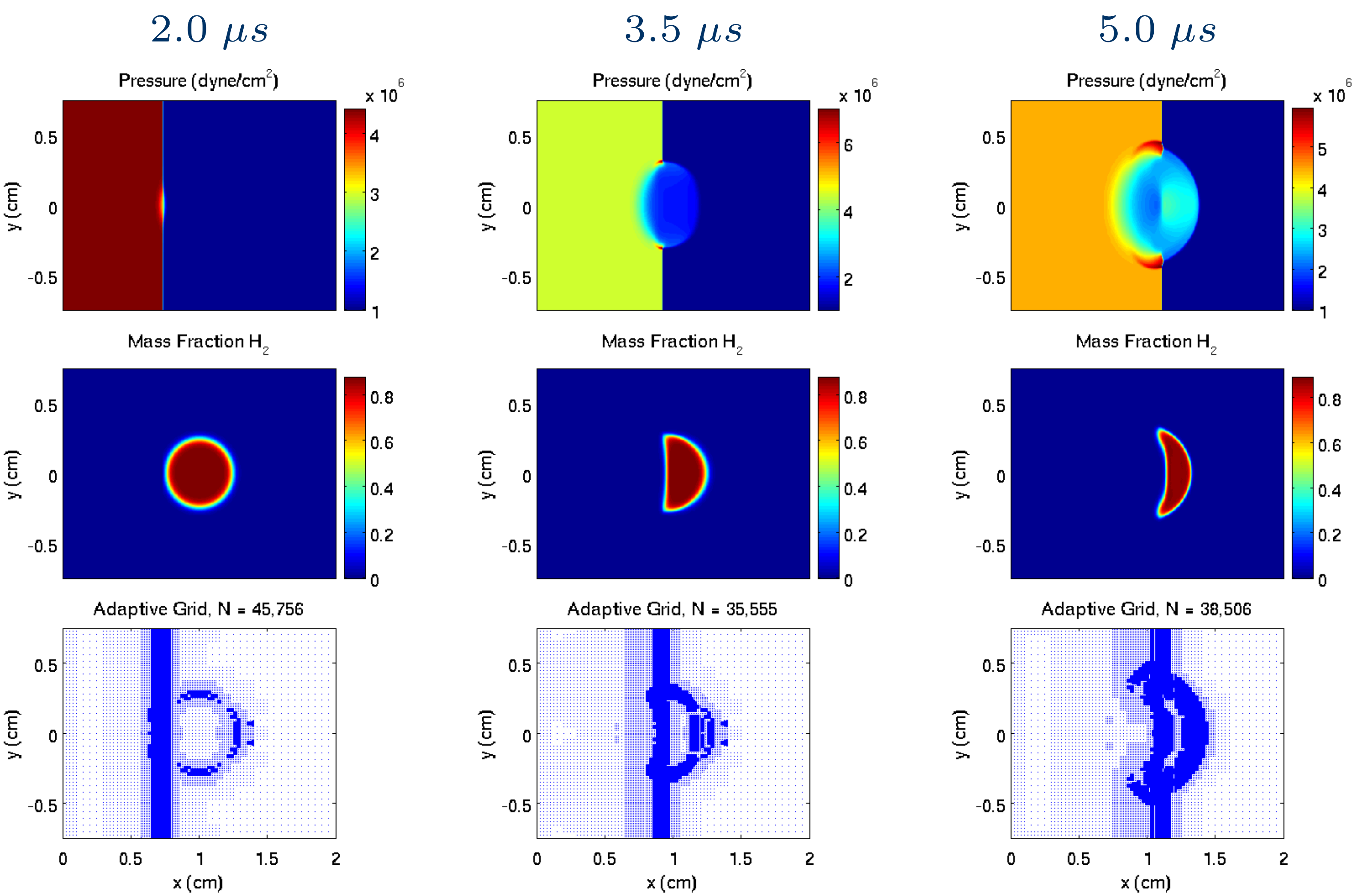
Domain: $[0,3] \times [0,0.75]$ cm
Mach 2 shock: $x = 0.5$ cm
$P_\infty = 1.0 \times 10^6$ dyne/cm^2
$T_\infty = 1000$ K
$r = \sqrt{(x-1)^2 + y^2}$
$r < 0.28$ cm: $83H_2 : 17N_2$
$r > 0.28$ cm: $22O_2 : 78N_2$
64 cores
runtime

$H_2 : O_2 : N_2$ mixture
9 species, 37 reactions

Wavelet parameters:

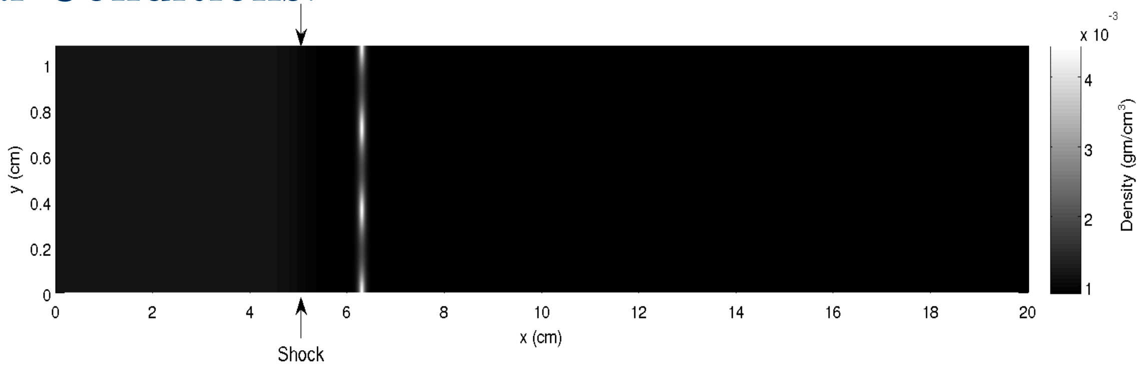
$\epsilon = 1 \times 10^{-3}$
$p = 6, \quad n = 5$
$[N_x \times N_y]_{j_0} = [30 \times 8]$
$J - j_0 = 10$

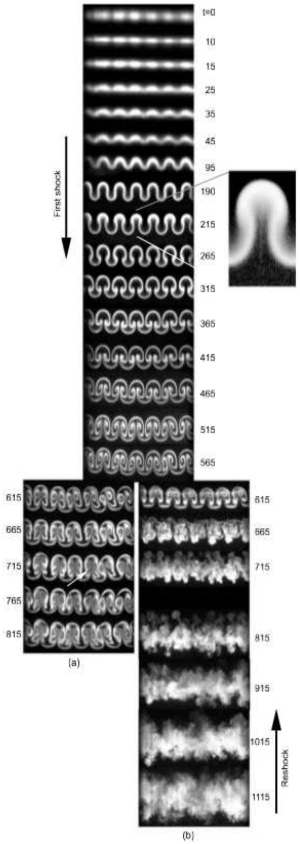
SHOCK/H_2-BUBBLE INTERACTION (CONT.)



Richtmeyer-Meshkov Instability

Initial Conditions:





Domain:

$[0, 20] \times [0, 1.08]$ cm

Ambient mixture:

$Y_{N_2} = 0.99, \; Y_{SF_6} = 0.01$

$P = 79.5$ kPa

$T = 300$ K

$M_s = 1.2$ shock

at $x = 5.0$ cm

64 cores

118 hrs runtime

Varicose sheet at $x = 6.3$ cm

$Y_{N_2} = 0.01, \; Y_{SF_6} = 0.99$

Balakumar *et al.*

Phys. Fluids **20**, 2008

Wavelet parameters:

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

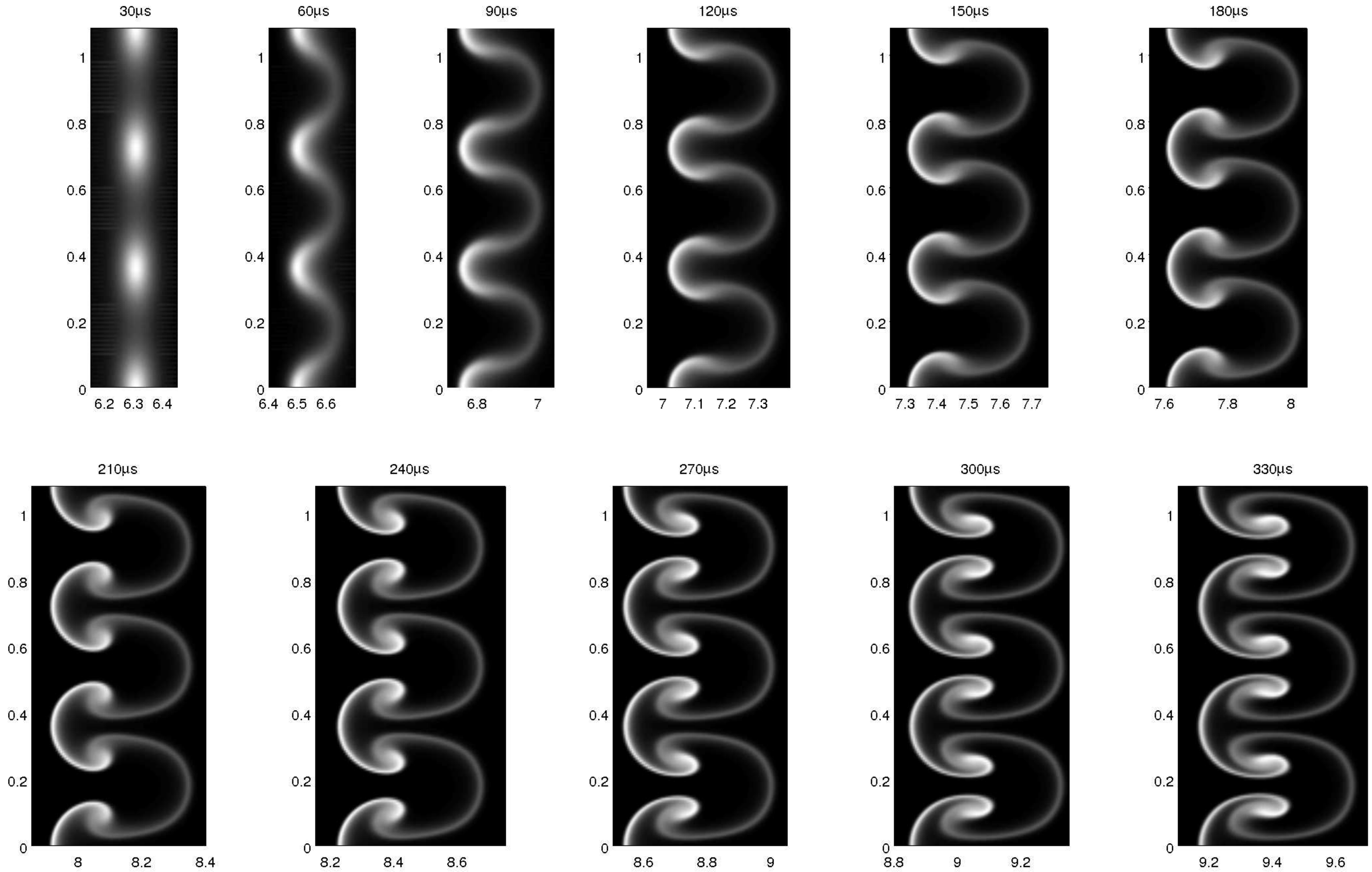
$p = 6, \quad n = 5$

$[N_x \times N_y]_{j_0} = [200 \times 10]$

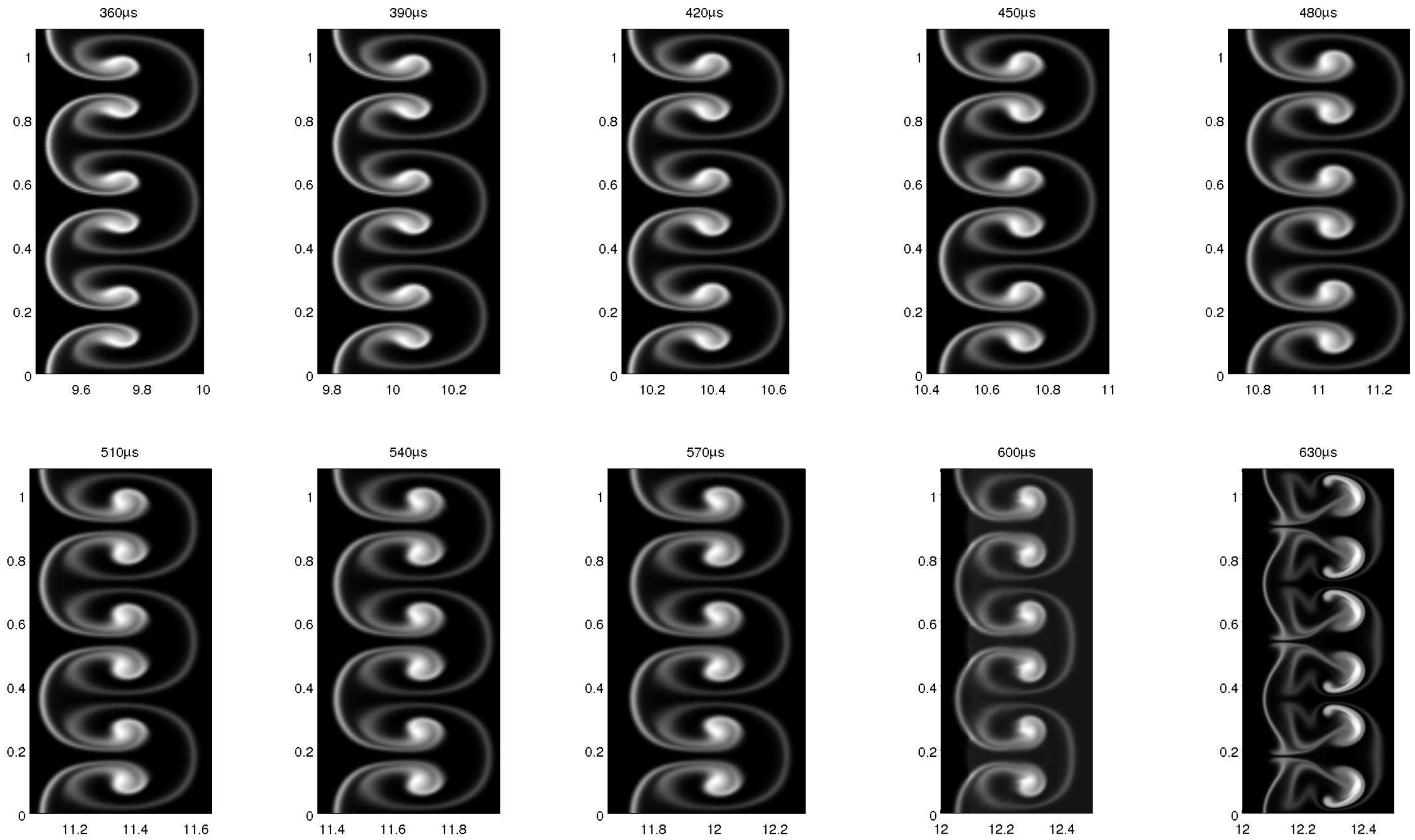
$J - j_0 = 10$

Richtmeyer-Meshkov Instability (cont.)

$\Longrightarrow$ Shock Direction $\Longrightarrow$



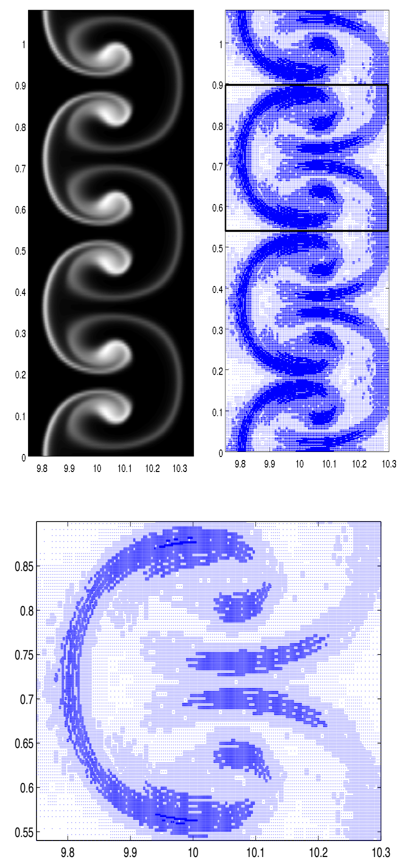
Richtmeyer-Meshkov Instability (cont.)



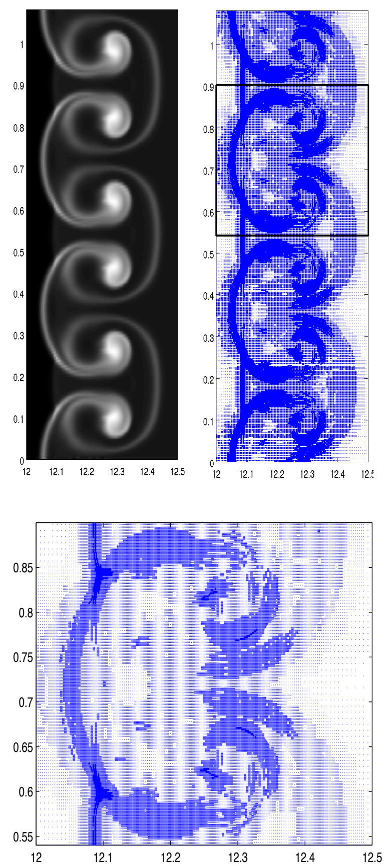
$\Leftarrow$ Reshock $\Leftarrow$

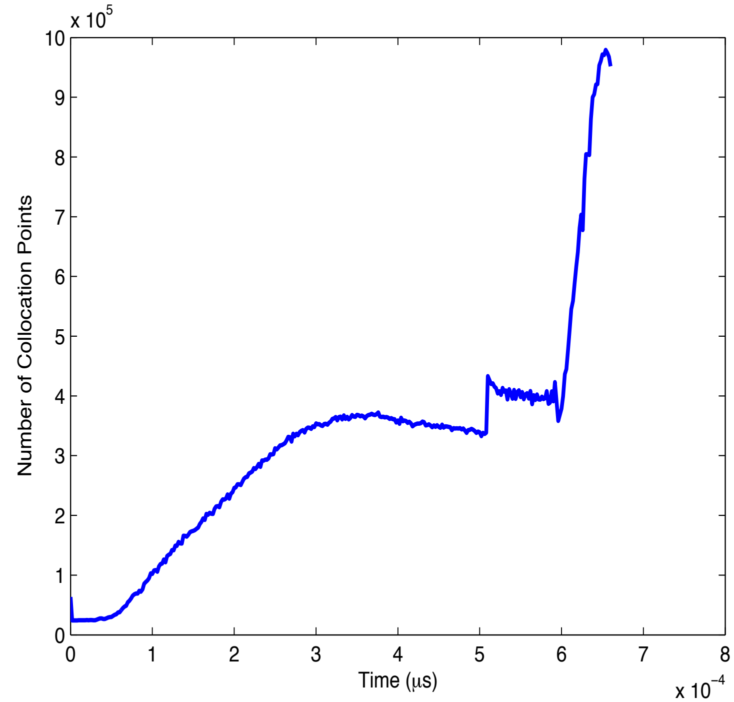
Richtmeyer-Meshkov Instability – Grid

$t = 390\ \mu s$



$t = 600\ \mu s$





Summary

- The wavelet adaptive multiresolution method provides a means to capture a wide range of scales present in multidimensional reactive compressible flows.
- The parallel algorithm shows excellent scaling up to the maximum number of cores tested.
- Resolved (verified) solutions in large geometries require large computational resources even with an adaptive method.

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.* $\mathrm{supp}\{\phi_{j,k}\} \sim |O(2^{-j})|$.
- $\phi_{j,k}(x_{j,n} = n2^{-j}) = \delta_{k,n}$, *i.e.* satisfies the *interpolation property.*
- $\psi_{j,k} = \phi_{j+1,2k+1}$.
- $\mathrm{span}\{\phi_{j,k}\} = \mathrm{span}\{\{\phi_{j-1,k}\},\{\psi_{j-1,k}\}\}$.
- $\{1, x, \cdots, x^{p-1}\}$, for $x \in [0,1]$, can be written as a linear combination of $\{\phi_{j,k},\ k = 0, \cdots, 2^j\}$.
- $\{\{\phi_{J_0,k}\},\{\psi_{j,k}\}_{j=J_0}^{\infty}\}$ forms a basis of a continuous 1-D function on the unit interval $[0,1]$.