# Multiscale Computations of Fluid Flows Using an Adaptive Wavelet Method 

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## Introduction

Solutions of many physical problems, formulated as PDEs, may contain sharp local variations in space, whose location may vary with time, in otherwise smooth solutions.

Since high resolution is needed to resolve such features, accurate numerical simulations using uniform grids require a large number of degrees of freedoms (DOFs).
The number of DOFs for a uniform grid discretization is $O\left(N^{d}\right)$ for problems in $d$ spatial dimensions.
To reduce the DOFs required, while maintaining solution accuracy, adaptive discretization becomes necessary.

Le Such task may be accomplished by use of AMR or adaptive FEM, where the refinement is based upon some error estimators/indicators.
Alternatively, we tackle such task by using an adaptive wavelet method. The method makes use of a wavelet multiscale basis in the design of the refinement strategy.

## Wavelet Approximation in Domain $[0,1]^{d}$

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

$$
u(\mathbf{x}) \approx u^{J}(\mathbf{x})=\sum_{\mathbf{k}} u_{J_{0}, \mathbf{k}} \Phi_{J_{0}, \mathbf{k}}(\mathbf{x})+\sum_{j=J_{0}}^{J-1} \sum_{\boldsymbol{\lambda}} d_{j, \boldsymbol{\lambda}} \Psi_{j, \boldsymbol{\lambda}}(\mathbf{x})
$$

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

- Scaling function:

$$
\Phi_{j, \mathbf{k}}(\mathbf{x})=\prod_{i=1}^{d} \phi_{j, \mathbf{k}}\left(x_{i}\right), k_{i} \in \kappa_{j}^{0}
$$

- Wavelet function:

$$
\Psi_{j, \mathbf{k}}^{\mathrm{e}}(\mathbf{x})=\prod_{i=1}^{d} \psi_{j, \mathbf{k}}^{e_{i}}\left(x_{i}\right), k_{i} \in \kappa_{j}^{e_{i}},
$$

where $\mathbf{e} \in\{0,1\}^{d} \backslash \mathbf{0}, \psi_{j, k}^{0}(x) \equiv \phi_{j, k}(x)$ and $\psi_{j, k}^{1}(x) \equiv \psi_{j, k}(x)$, and $\kappa_{j}^{0}=$ $\left\{0, \ldots, 2^{j}\right\}$ and $\kappa_{j}^{1}=\left\{0, \ldots, 2^{j}-1\right\}$.

## 1-D Interpolating Scaling Function and Wavelet

Some properties of $\phi_{j, k}$ and $\psi_{j, k}$ of order $p(p \in \mathbf{N}$, even):
$\phi_{j, k}$ is defined through $\phi\left(2^{j} x-k\right)$ where $\phi(x)=\int \varphi_{p}(y) \varphi_{p}(y-x) d y$, the auto-correlation of the Daubechies scaling function $\varphi_{p}(x)$.

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

## Wavelet Amplitudes

- Wavelet amplitude, $\left|d_{j, \boldsymbol{\lambda}}\right|$, measures the approximation error of $f(\mathbf{x})$ by a local polynomial approximation at the point $\mathbf{x}_{j, \boldsymbol{\lambda}}$.
- In other words, wavelet amplitudes, $d_{j, \boldsymbol{\lambda}}$, indicate the local regularity of a function.

Example: Consider $u(x, y)=$ 0.2/(|0.4- $\left.x^{2}-y^{2} \mid+0.2\right)$




Grid points correspond to wavelet amplitudes that are larger than $\varepsilon=5 \times 10^{-3}$.

## Sparse Wavelet Representation (SWR) and Irregular Sparse Grid

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

$$
\begin{gathered}
u^{J}(\mathbf{x})=\sum_{\mathbf{k}} u_{J_{0}, \mathbf{k}} \Phi_{J_{0}, \mathbf{k}}(\mathbf{x})+\sum_{j=J_{0}}^{J-1} \sum_{\left\{\boldsymbol{\lambda}:\left|d_{j, \boldsymbol{\lambda}}\right| \geq \varepsilon\right\}} d_{j, \boldsymbol{\lambda}} \Psi_{j, \boldsymbol{\lambda}}(\mathbf{x}) \\
+\underbrace{\sum_{j=J_{0}\left\{\boldsymbol{\lambda}:\left|d_{j, \boldsymbol{\lambda}}\right|<\varepsilon\right\}}^{J-1} d_{j, \boldsymbol{\lambda}} \Psi_{j, \boldsymbol{\lambda}}(\mathbf{x})}_{R_{\varepsilon}^{J}} .
\end{gathered}
$$

The Sparse Wavelet Representation (SWR) is obtained by discarding the term $R_{\varepsilon}^{J}$ :

$$
u_{\varepsilon}^{J}(\mathbf{x})=\sum_{\mathbf{k}} u_{J_{0}, \mathbf{k}} \Phi_{J_{0}, \mathbf{k}}(\mathbf{x})+\sum_{j=J_{0}}^{J-1} \sum_{\left\{\boldsymbol{\lambda}:\left|d_{j, \boldsymbol{\lambda}}\right| \geq \varepsilon\right\}} d_{j, \boldsymbol{\lambda}} \Psi_{j, \boldsymbol{\lambda}}(\mathbf{x})
$$

## SWR and Irregular Sparse Grid (continued)

In the context of interpolating wavelets, each basis function is associated with one dyadic grid point, i.e.

$$
\begin{aligned}
& \Phi_{j, \mathbf{k}}(\mathbf{x}) \quad \text { with } \quad \mathbf{x}_{j, \mathbf{k}}=\left(k_{1} 2^{-j}, \ldots, k_{d} 2^{-j}\right) \\
& \Psi_{j, \boldsymbol{\lambda}}(\mathbf{x}) \quad \text { with } \quad \mathbf{x}_{j, \boldsymbol{\lambda}}=\mathbf{x}_{j+1,2 \mathbf{k}+\mathbf{e}}
\end{aligned}
$$

Thus, for a given SWR, one can establish an associated grid of irregular points

$$
\mathcal{V}=\left\{\mathbf{x}_{J_{0}, \mathbf{k}}, \cup_{j \geq J_{0}} \mathbf{x}_{j, \boldsymbol{\lambda}}: \boldsymbol{\lambda} \in \boldsymbol{\Lambda}_{j}\right\}, \quad \boldsymbol{\Lambda}_{j}=\left\{\boldsymbol{\lambda}:\left|d_{j, \boldsymbol{\lambda}}\right| \geq \varepsilon\right\}
$$

Due to the interpolation property of the basis, there exists a fast wavelet transform $(A F W T)$, with $O(N)$ operations, $N=\operatorname{dim}\{\mathcal{V}\}$, that maps function values on the irregular grid $\mathcal{V}$ to associated wavelet coefficients and vice-versa:

$$
A F W T(\{u(\mathbf{x}): \mathbf{x} \in \mathcal{V}\}) \rightarrow \mathcal{D}=\left\{\left\{u_{J_{0}, \mathbf{k}}\right\},\left\{d_{j, \boldsymbol{\lambda}}, \boldsymbol{\lambda} \in \boldsymbol{\Lambda}_{j}\right\}\right\}
$$

## SWR and Irregular Sparse grid (continued)

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

$$
\left\|u-u_{\varepsilon}^{J}\right\|_{\infty} \leq C_{1} \varepsilon .
$$

Furthermore, for a function that is sufficiently smooth, the number of basis functions $N=\operatorname{dim}\left\{u_{\varepsilon}^{J}\right\}$ required for a given $\varepsilon$ satisfies

$$
N \leq C_{2} \varepsilon^{-d / p}
$$

so that we also have

$$
\left\|u-u_{\varepsilon}^{J}\right\|_{\infty} \leq C_{2} N^{-p / d} .
$$

## Dynamically Adaptive Algorithm for Solving Time-dependent PDEs

Numerical algorithm:

$$
\begin{aligned}
\frac{\partial u}{\partial t} & =F\left(t, u, u_{x}, u_{x x}, \ldots\right) \\
\Longrightarrow \mathcal{A}^{m+1} u^{m+1} & =\mathcal{F}^{m+1}\left(t^{m+1}, t^{m-q}, u^{m-q}, \ldots\right), q=0, \ldots, m(1)
\end{aligned}
$$

(1) Solve (1) to obtain the approximate solution $u^{m+1}$ on the irregular grid $\mathcal{V}^{m}$ by using the solution from the previous time step, $u^{m}$, as initial condition.
(2) Obtain the new sparse grid, $\mathcal{V}^{m+1}$, based on the thresholding of the magnitudes of wavelet amplitudes of the new solution, $u^{m+1}$.
(3) Assign $\mathcal{V}^{m+1} \rightarrow \mathcal{V}^{m}$ and $u^{m+1-q} \rightarrow u^{m-q}, q=0, \ldots, m$ and go back to step ${ }^{(1)}$.

Note: The initial sparse grid set, $\mathcal{V}^{0}$, is obtained from initial conditions.

## Grid Adaption Strategy

In each refinement step, determine the essential grid points, which are points whose associated wavelet amplitudes are larger than the threshold parameter $\varepsilon$ :

$$
\widehat{\mathcal{V}}_{e}=\left\{\mathbf{x}_{j, \boldsymbol{\lambda}}: j \geq J_{0}, \boldsymbol{\lambda} \in \boldsymbol{\Lambda}_{j},\left|d_{j, \boldsymbol{\lambda}}\right| \geq \varepsilon\right\}
$$

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

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

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

$$
\mathcal{V}=\left\{\mathrm{x}_{J_{0}, \mathrm{k}}\right\} \cup \widehat{\mathcal{V}}_{e} \cup \widehat{\mathcal{V}}_{b} .
$$

## Applications to Reactive Compressible Navier-Stokes Equations

Governing Equations (1-D):

$$
\begin{gathered}
\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x}(\rho u)=0 \\
\frac{\partial}{\partial t}(\rho u)+\frac{\partial}{\partial x}\left(\rho u^{2}+P-\tau\right)=0 \\
\frac{\partial}{\partial t}\left(\rho\left(e+\frac{u^{2}}{2}\right)\right)+\frac{\partial}{\partial x}\left(\rho u\left(e+\frac{u^{2}}{2}\right)+u(P-\tau)+q\right)=0 \\
\frac{\partial}{\partial t}\left(\rho Y_{i}\right)+\frac{\partial}{\partial x}\left(\rho u Y_{i}+j_{i}\right)=\dot{\omega}_{i}
\end{gathered}
$$

## Applications to Reactive Compressible Navier-Stokes Equations (continued)

Constitutive Equations:

$$
\begin{aligned}
P & =\rho \Re T \sum_{i=1}^{N} \frac{Y_{i}}{M_{i}} \quad \text { (thermal equation of state) } \\
e & =\sum_{i=1}^{N} Y_{i}\left(h_{i}^{o}+\int_{T_{o}}^{T} c_{p i}(\hat{T}) d \hat{T}\right)-\frac{P}{\rho} \quad \text { (caloric equation of state) } \\
\tau & =\frac{4}{3} \mu \frac{\partial u}{\partial x} \quad \text { (Newtonian gas with Stokes' assumption) } \\
j_{i} & =-\rho \sum_{j=1}^{N} \mathcal{D}_{i j} \frac{\partial Y_{j}}{\partial x} \quad \text { (Fick's law) } \\
q & =-k \frac{\partial T}{\partial x}+\sum_{i=1}^{N} j_{i}\left(h_{i}^{o}+\int_{T_{o}}^{T} c_{p i}(\hat{T}) d \hat{T}\right) \quad \text { (augmented Fourier's law) } \\
\dot{\omega}_{i} & =\sum_{j=1}^{M} a_{j} T^{\alpha_{j}} \exp \left(\frac{-E_{j}}{\Re T}\right) \nu_{i j} M_{i} \prod_{k=1}^{N}\left(\frac{\rho Y_{k}}{M_{k}}\right)^{\nu_{k j}} \quad \text { (reaction rate) }
\end{aligned}
$$

## Operator Splitting

## SYSTEM OF EQUATIONS:

$$
\mathbf{q}_{t}(x, t)+\mathbf{f}_{x}(\mathbf{q}(x, t))=\mathbf{r}(\mathbf{q}(x, t)),
$$

where $\mathbf{q}=\left(\rho, \rho u, \rho\left(e+\frac{u^{2}}{2}\right), \rho Y_{i}\right)^{T}$. Note that $\mathbf{f}$ models convection and diffusion, while $\mathbf{r}$ models the reaction source terms.

Strang Splitting:

Inert convection-diffusion integration (AB2):

$$
\mathbf{q}_{t}(x, t)=-\mathbf{f}_{x}(\mathbf{q}(x, t))=\mathcal{S}_{c}(\mathbf{q}(x, t)),
$$

Reaction source integration (BD2):

$$
\mathbf{q}_{t}(x, t)=\mathbf{r}(\mathbf{q}(x, t))=\mathcal{S}_{r} .
$$

(T) Time integration:

$$
\mathbf{q}(x, t+\Delta t)=\mathcal{S}_{r}(\Delta t / 2) \mathcal{S}_{c}(\Delta t) \mathcal{S}_{r}(\Delta t / 2) \mathbf{q}(x, t)
$$

## Operator Splitting (Continued)

The Reaction source step

$$
\frac{\partial}{\partial t}\left(\begin{array}{c}
\rho \\
\rho u \\
\rho\left(e+\frac{u^{2}}{2}\right) \\
\rho Y_{i}
\end{array}\right)=\left(\begin{array}{l}
0 \\
0 \\
0 \\
\omega
\end{array}\right)
$$

Reduces to

$$
\rho=\rho_{o}, \quad u=u_{o}, \quad e=e_{o}, \quad \frac{\partial Y_{i}}{\partial t}=\frac{\omega}{\rho_{o}} .
$$

Note:

』q9 $\omega$ HAS DEPENDENCY ON $\rho, e$, AND $Y_{i}$.
ODES FOR $Y_{i}$ CAN BE SOLVED POINTWISE.

## IgNition delay problem

## Premixed $H_{2}-O_{2}-A r$ in $2 / 1 / 7$ molar ratio

9 SPECIES: $\mathrm{H}_{2}, \mathrm{O}_{2}, \mathrm{H}, \mathrm{O}, \mathrm{OH}, \mathrm{H}_{2} \mathrm{O}_{2}, \mathrm{H}_{2} \mathrm{O}, \mathrm{HO}_{2}$, Ar

## 37 REACTIONS:

| $j$ | Reaction | $a_{j}$ | $\beta_{j}$ | $\mathrm{E}_{\mathrm{j}}$ |
| :--- | :--- | :--- | ---: | ---: |
| 1 | $\mathrm{O}_{2}+\mathrm{H} \rightarrow \mathrm{OH}+\mathrm{O}$ | $2.00 \times 10^{14}$ | 0.00 | 70.30 |
| 2 | $\mathrm{OH}+\mathrm{O} \rightarrow \mathrm{O}_{2}+\mathrm{H}$ | $1.46 \times 10^{13}$ | 0.00 | 2.08 |
| 3 | $\mathrm{H}_{2}+\mathrm{O} \rightarrow \mathrm{OH}+\mathrm{H}$ | $5.06 \times 10^{4}$ | 2.67 | 26.30 |
| 4 | $\mathrm{OH}+\mathrm{H} \rightarrow \mathrm{H}_{2}+\mathrm{O}$ | $2.24 \times 10^{4}$ | 2.67 | 18.40 |
| 5 | $\mathrm{H}_{2}+\mathrm{OH} \rightarrow \mathrm{H}_{2} \mathrm{O}+\mathrm{H}$ | $1.00 \times 10^{8}$ | 1.60 | 13.80 |
| 6 | $\mathrm{H}_{2} \mathrm{O}+\mathrm{H} \rightarrow \mathrm{H}_{2}+\mathrm{OH}$ | $4.45 \times 10^{8}$ | 1.60 | 77.13 |
| 7 | $\mathrm{OH}+\mathrm{OH} \rightarrow \mathrm{H}_{2} \mathrm{O}+\mathrm{O}$ | $1.50 \times 10^{9}$ | 1.14 | 0.42 |
| 8 | $\mathrm{H}_{2} \mathrm{O}+\mathrm{O} \rightarrow \mathrm{OH}+\mathrm{OH}$ | $1.51 \times 10^{10}$ | 1.14 | 71.64 |
| 9 | $\mathrm{H}+\mathrm{H}+\mathrm{M} \rightarrow \mathrm{H}_{2}+\mathrm{M}$ | $1.80 \times 10^{18}$ | -1.00 | 0.00 |
| 10 | $\mathrm{H}_{2}+\mathrm{M} \rightarrow \mathrm{H}+\mathrm{H}+\mathrm{M}$ | $6.99 \times 10^{18}$ | -1.00 | 436.08 |
| 11 | $\mathrm{H}+\mathrm{OH}+\mathrm{M} \rightarrow \mathrm{H}_{2} \mathrm{O}+\mathrm{M}$ | $2.20 \times 10^{22}$ | -2.00 | 0.00 |
| 12 | $\mathrm{H}_{2} \mathrm{O}+\mathrm{M} \rightarrow \mathrm{H}+\mathrm{OH}+\mathrm{M}$ | $3.80 \times 10^{23}$ | -2.00 | 499.41 |
| 13 | $\mathrm{O}+\mathrm{O}+\mathrm{M} \rightarrow \mathrm{O}_{2}+\mathrm{M}$ | $2.90 \times 10^{17}$ | -1.00 | 0.00 |
| 14 | $\mathrm{O}_{2}+\mathrm{M} \rightarrow \mathrm{O}+\mathrm{O}+\mathrm{M}$ | $6.81 \times 10^{18}$ | -1.00 | 496.41 |
| 15 | $\mathrm{H}+\mathrm{O}_{2}+\mathrm{M} \rightarrow \mathrm{HO}+\mathrm{M}$ | $2.30 \times 10^{18}$ | -0.80 | 0.00 |
| 16 | $\mathrm{HO}+\mathrm{M} \rightarrow \mathrm{H}_{2}+\mathrm{O}_{2}+\mathrm{M}$ | $3.26 \times 10^{18}$ | -0.80 | 195.88 |
| 17 | $\mathrm{HO}_{2}+\mathrm{H} \rightarrow \mathrm{OH}+\mathrm{OH}$ | $1.50 \times 10^{14}$ | 0.00 | 4.20 |
| 18 | ${\mathrm{OH}+\mathrm{OH} \rightarrow \mathrm{HO}_{2}+\mathrm{H}}^{1.33 \times 10^{13}}$ | 0.00 | 168.30 |  |
| 19 | $\mathrm{HO}_{2}+\mathrm{H} \rightarrow \mathrm{H}_{2}+\mathrm{O}_{2}$ | $2.50 \times 10^{13}$ | 0.00 | 2.90 |


| j | Reaction | $\mathrm{a}_{\mathrm{j}}$ | $\beta_{j}$ | $E_{j}$ |
| :---: | :---: | :---: | :---: | :---: |
| 20 | $\mathrm{H}_{2}+\mathrm{O}_{2} \rightarrow \mathrm{HO}_{2}+\mathrm{H}$ | $6.84 \times 10^{13}$ | 0.00 | 243.10 |
| 21 | $\mathrm{HO}_{2}+\mathrm{H} \rightarrow \mathrm{H}_{2} \mathrm{O}+\mathrm{O}$ | $3.00 \times 10^{13}$ | 0.00 | 7.20 |
| 22 | $\mathrm{H}_{2} \mathrm{O}+\mathrm{O} \rightarrow \mathrm{HO}_{2}+\mathrm{H}$ | $2.67 \times 10^{13}$ | 0.00 | 242.52 |
| 23 | $\mathrm{HO}_{2}+\mathrm{O} \rightarrow \mathrm{OH}+\mathrm{O}_{2}$ | $1.80 \times 10^{13}$ | 0.00 | -1.70 |
| 24 | $\mathrm{OH}+\mathrm{O}_{2} \rightarrow \mathrm{HO}_{2}+\mathrm{O}$ | $2.18 \times 10^{13}$ | 0.00 | 230.61 |
| 25 | $\mathrm{HO}_{2}+\mathrm{OH} \rightarrow \mathrm{H}_{2} \mathrm{O}+\mathrm{O}_{2}$ | $6.00 \times 10^{13}$ | 0.00 | 0.00 |
| 26 | $\mathrm{H}_{2} \mathrm{O}+\mathrm{O}_{2} \rightarrow \mathrm{HO}_{2}+\mathrm{OH}$ | $7.31 \times 10^{14}$ | 0.00 | 303.53 |
| 27 | $\mathrm{HO}_{2}+\mathrm{HO}_{2} \rightarrow \mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{O}_{2}$ | $2.50 \times 10^{11}$ | 0.00 | -5.20 |
| 28 | $\mathrm{OH}+\mathrm{OH}+\mathrm{M} \rightarrow \mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{M}$ | $3.25 \times 10^{22}$ | -2.00 | 0.00 |
| 29 | $\mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{M} \rightarrow \mathrm{OH}+\mathrm{OH}+\mathrm{M}$ | $2.10 \times 10^{24}$ | -2.00 | 206.80 |
| 30 | $\mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{H} \rightarrow \mathrm{H}_{2}+\mathrm{HO}_{2}$ | $1.70 \times 10^{12}$ | 0.00 | 15.70 |
| 31 | $\mathrm{H}_{2}+\mathrm{HO}_{2} \rightarrow \mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{H}$ | $1.15 \times 10^{12}$ | 0.00 | 80.88 |
| 32 | $\mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{H} \longrightarrow \mathrm{H}_{2} \mathrm{O}+\mathrm{OH}$ | $1.00 \times 10^{13}$ | 0.00 | 15.00 |
| 33 | $\mathrm{H}_{2} \mathrm{O}+\mathrm{OH} \rightarrow \mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{H}$ | $2.67 \times 10^{12}$ | 0.00 | 307.51 |
| 34 | $\mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{O} \rightarrow \mathrm{OH}+\mathrm{HO}_{2}$ | $2.80 \times 10^{13}$ | 0.00 | 26.80 |
| 35 | $\mathrm{OH}+\mathrm{HO}_{2} \rightarrow \mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{O}$ | $8.40 \times 10^{12}$ | 0.00 | 84.09 |
| 36 | $\mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{OH} \rightarrow \mathrm{H}_{2} \mathrm{O}+\mathrm{HO}_{2}$ | $5.40 \times 10^{12}$ | 0.00 | 4.20 |
| 37 | $\mathrm{H}_{2} \mathrm{O}+\mathrm{HO}_{2} \rightarrow \mathrm{H}_{2} \mathrm{O}_{2}+\mathrm{OH}$ | $1.63 \times 10^{13}$ | 0.00 | 132.71 |

Table Nine-species, 37-step reaction mechanism for a hydrogen-oxygen-argon mixture [25] with corrected $\mathrm{f}_{\mathrm{H}_{2}}$ from [3], also utilized by Fedkiw et al [16]. Units of $\mathrm{a}_{\mathrm{j}}$ are in appropriate combinations of cm , mol, s and K so that $\dot{\omega}_{\mathrm{i}}$ has units of mol cm ${ }^{-3} \mathrm{~s}^{-1}$; units of $\mathrm{E}_{\mathrm{j}}$ are $\mathrm{kJ} \mathrm{mol}^{-1}$. Third-body collision efficiencies with $M$ are $f_{\mathrm{H}_{2}}=1.00, \mathrm{f}_{\mathrm{O}_{2}}=0.35$ and $\mathrm{f}_{\mathrm{H}_{2} \mathrm{O}}=6.5$.

$$
t=230 \mu \mathrm{~s}
$$






$$
t=180,190,200,230 \mu \mathrm{~s}
$$



## Large and small scale structures at $t=230 \mu \mathrm{~s}$



Fine Scale Structure


## Instantaneous distribution of collocation points

UsED AT MOST 300 POINTS AND 15 SCALE LEVELS
$t=180 \mu \mathrm{~s}$ TWO-SHOCKS AND AT $t=230 \mu \mathrm{~S}$ ONE-SHOCK (DETONATION).


## Applications to Incompressible Navier-Stokes Equations

Governing Equations:

$$
\begin{aligned}
\nabla \cdot \mathbf{u} & =0, \\
\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u} \cdot \nabla \mathbf{u} & =-\nabla p+\frac{1}{R e} \nabla^{2} \mathbf{u}-\frac{G r}{R e^{2}} T \mathbf{n}, \\
\frac{\partial T}{\partial t}+\mathbf{u} \cdot \nabla T & =\frac{1}{\operatorname{RePr}} \nabla^{2} T,
\end{aligned}
$$

WITH APPROPRIATE BOUNDARY AND INITIAL CONDITIONS.
n is The unit vector in the direction of gravity.
$\operatorname{Re}=U L / \nu, G r=g \beta \Delta T L^{3} / \nu^{2}$, AND $\operatorname{Pr}=\nu / \alpha$.

Note: $L, U, L / U$, and $\Delta T$ are Reference length, velocity, TIME, AND TEMPERATURE SCALES, AND $T=\left(T^{*}-T_{r}\right) / \Delta T$.

## 2nd order Fractional Step Method

(1) Step (1). Compute the temperature field:

$$
\frac{T^{m+1}-T^{m}}{\Delta t}+\frac{1}{2}(\widetilde{\mathbf{u}} \cdot \nabla)\left(T^{m+1}+T^{m}\right)=\frac{1}{2 \operatorname{RePr}} \nabla^{2}\left(T^{m+1}+T^{m}\right)
$$

WHERE $\widetilde{\mathbf{u}}=(1+r) \mathbf{u}^{m}-r \mathbf{u}^{m-1}$ WITH $r=\frac{\Delta \tau}{\Delta t}, \Delta t=t^{m+1}-t^{m}, \Delta \tau=t^{m}-t^{m-1}$.
STEP (2). SOLVE FOR THE INTERMEDIATE VELOCITY $\widehat{\mathbf{u}}$ :

$$
\frac{\widehat{\mathbf{u}}-\mathbf{u}^{m}}{\Delta t}+\frac{1}{2}\left(\widetilde{\mathbf{u}} \cdot \nabla \widehat{\mathbf{u}}+\mathbf{u}^{m}\right) \cdot \nabla \mathbf{u}^{m}=-\nabla \tilde{p}+\frac{1}{2 R e} \nabla^{2}\left(\widehat{\mathbf{u}}+\mathbf{u}^{m}\right)-\frac{G r \mathbf{n}}{2 R e^{2}}\left(T^{m+1}+T^{m}\right) .
$$

Step (3). Determine the true velocity u $\mathbf{u}^{m+1}$ :

$$
\left.\begin{array}{l}
\mathbf{u}^{m+1}-\widehat{\mathbf{u}}=-\Delta t \nabla \phi, \\
\nabla \cdot \mathbf{u}^{m+1}=0,
\end{array}\right\} \Longrightarrow \quad \nabla^{2} \phi=(\nabla \cdot \widehat{\mathbf{u}}) / \Delta t
$$

Step (4). When needed, COMpute the pressure field:

$$
p^{m+1}=\widetilde{p}+\phi-1 / 2 \sqrt{R a / \operatorname{Pr}} \Delta t \nabla^{2} \phi
$$

## 2-D Differentially Heated Cavity



- $\Delta T \equiv T_{h}-T_{c}$ AND $T_{r} \equiv\left(T_{h}+T_{c}\right) / 2$, $T_{h}>T_{c}$.
- $H, U=\sqrt{\beta g \Delta T H}, \quad \Delta T, ~ A N D$ $H / U$ are used as reference LENGTH, VELOCITY, TEMPERATURE, and time scales.
- $R e^{2}=G r=R a / P r$, where the Rayleigh number $R a=$ $\beta g \Delta T H^{3} / \nu^{2}$.
- For a square cavity, $H=L, \Omega=(0,1)^{2}$ and BCs are given BY

$$
\begin{gathered}
\mathbf{u}=\mathbf{0}, \quad \text { ON } \quad x=0,1 \quad \text { AND } \quad y=0,1, \\
T=\frac{1}{2}-x, \quad \text { ON } x=0,1 \quad \text { AND } \quad \frac{\partial T}{\partial y}=0 \quad \text { ON } y=0,1 .
\end{gathered}
$$

## Numerical Simulations

The adaptive wavelet method is Applied to compute the flow OF AIR $(\operatorname{Pr}=0.71)$ IN A SQUARE CAVITY FOR $R a=10^{6}$ TO $5 \times 10^{8}$.

If In EACH CASE, THE INITIAL CONDITION IS CHOSEN TO BE THAT OF THE PURE CONDUCTING QUIESCENT STATE (i.e. $T(\mathbf{x}, 0)=1 / 2-x$ AND $\mathbf{u}(\mathbf{x}, 0)=\mathbf{0})$.

The steady state, If it exists, IS Reached through unsteady INTEGRATION IN TIME SATISFYING

$$
\frac{\left\|f^{m+1}-f^{m}\right\|_{\mathcal{V}^{m}, \infty}}{\left\|f^{m+1}\right\|_{\mathcal{V}^{m}, \infty}} \leq 5 \times 10^{-5}
$$

WHERE $f=\{\mathbf{u}, T\}$.
Parameters of the adaptive method:

$$
\begin{array}{ll}
\hline \text { INTERPOLATING WAVELET } & : p=6 \text { WITH } n=4 . \\
\text { RESOLUTION } & : J_{0}=3, J-J_{0}=6 . \\
\text { THRESHOLD } & : \varepsilon=\mathbf{1 0}^{-\mathbf{3}} \text { AND } \mathbf{5} \times \mathbf{1 0}^{-\mathbf{3}} .
\end{array}
$$

## Results for $R a=10^{8}$

Steady state solution for $\varepsilon=\mathbf{1 0}^{\mathbf{- 3}}, N=8791$


## Results for $R a=10^{8}$ <br> Evolution of DOFs



In THE EARLY PART OF THE SIMULATION, THE SOLUTION IS QUITE COMPLICATED AND REQUIRES A RELATIVELY LARGE NUMBER OF DOFS.
[罗 AS $\varepsilon$ IS DECREASED, THE NUMBER OF DOFS, $N$, GENERATED BY ALGORITHM INCREASES AUTOMATICALLY.
$R a=5 \times 10^{8}$ AT EARLY TIME WITH $\varepsilon=\left\{10^{-3}, 4 \times 10^{-3}, 4 \times 10^{-3}\right\}$

$$
t=33.33, N=42906
$$



$$
t=55.55, N=29335
$$



Velocity \& Temperature

$R a=5 \times 10^{8}$ AFTER LONG TIME WITH $\varepsilon=\left\{10^{-3}, 4 \times 10^{-3}, 4 \times 10^{-3}\right\}$

$$
t=418.89, N=9897
$$



$t=439.72, N=9281$


Velocity \& Temperature


Adaptive Grid

## Results for $R a=5 \times 10^{8}$


aqs IN THE EARLY PART OF SIMULATION, THE SOLUTION IS QUITE COMPLICATED AND REQUIRES A RELATIVELY LARGE NUMBER OF DOF.
ne QUIESCENT REGION IN THE CORE OF THE CAVITY, WITH A REQUIRED NUMBER OF DOF THAT IS SUBSTANTIALLY SMALLER.

## Conclusions

An adaptive wavelet algorithm for solving PDEs in $d$ dimensions has been described. The algorithm is based on $d$-DIMENSIONAL INTERPOLATING WAVELETS.

Numerical Results indicate that the adaptive Algorithm BEHAVES APPROXIMATELY LIKE

$$
\left\|u_{\text {exact }}-u_{\varepsilon}^{J}\right\|_{\mathcal{V}, \infty}=O\left(\varepsilon^{\min (p-2, n) / p}\right), \quad N=O\left(\varepsilon^{-d / p}\right)
$$

The method has been applied to solve compressible and INCOMPRESSIBLE FLOWS DESCRIBED BY THE NAVIER-STOKES EQUATIONS IN PRIMITIVE VARIABLES IN 1-D, 2-D, AND 3-D GEOMETRIES.

Solutions obtained agree well with accurate benchmark RESULTS (OBTAINED WITH MUCH LARGER NUMBER OF DOFs) AVAILABLE IN THE LITERATURE.

