Wavelet Adaptive Multilevel Representation (WAMR) and Intrinsic Low Dimensional Manifold (ILDM) for Reactive Flows

by

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Outline

- Motivation
- Wavelet Adaptive Multilevel Representation (WAMR) technique (Paolucci & Vasilyev, 1997, *Journal of Computational Physics*) for spatial discretization
- Intrinsic Low Dimensional Manifold (ILDM) technique (Maas & Pope, 1992, *Combustion and Flame*) for reactive source terms
- One-dimensional results: viscous detonation in $H_2/O_2/Ar$ system (Singh, Rastigejev, Paolucci, & Powers, 2001, *Combustion Theory and Modeling*), and laminar ozone flame (Singh, Powers, & Paolucci, ICDERS, 2001)
- Two-dimensional results: lid-driven fluid in rectangular cavity at high Reynolds number
- Conclusions

General Motivation

- Combustion problems are among the most demanding computational problems solved in science and engineering (auto, jet, and rocket engines, atmospheric chemistry, fire safety,...)
- Combustion characterized by phenomena evolving on widely disparate space (1 nm to 10 m) and time (1 ns to 10 s) scales.
- Disparity of scales generated by
  - geometry
  - heterogeneities in material properties
  - diffusive boundary layers
  - fine and coarse reaction zones
  - interacting shock waves
  - intrinsic non-linear effects
- Solutions
  - faster and larger compuational hardware
  - more efficient software
- *Our focus: adaptive methods suited for parallel architectures*

Compressible Reactive Navier-Stokes Equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) = 0, \qquad \text{mass}$$

$$\frac{\partial}{\partial t}\left(\rho u\right) + \frac{\partial}{\partial x}\left(\rho u^2 + p - \tau\right) = 0, \qquad \text{momentum}$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{u^2}{2}\right) + u\left(p - \tau\right) + q\right) = 0, \qquad \text{energy}$$

$$\frac{\partial}{\partial t}\left(\rho y_l\right) + \frac{\partial}{\partial x}\left(\rho u y_l + j_l\right) = 0, \qquad \left(l = 1, \ldots, L-1\right), \qquad \text{elements}$$

$$\frac{\partial}{\partial t}\left(\rho Y_i\right) + \frac{\partial}{\partial x}\left(\rho u Y_i + J_i^m\right) = \dot{\omega}_i M_i, \qquad \left(i = 1, \ldots, N-L\right), \qquad \text{species}$$

$$\tau = \frac{4}{3}\mu\frac{\partial u}{\partial x}, \qquad \text{Newtonian gas with Stokes' assumption}$$

$$J^q = -k\frac{\partial T}{\partial x} + \sum_{i=1}^{N} J_i^m\left(h_i^o + \int_{T_o}^{T} c_{pi}(\hat{T})d\hat{T}\right) - \Re T\sum_{i=1}^{N}\frac{\mathcal{D}_i^T}{M_i}\left(\frac{1}{\chi_i}\frac{\partial \chi_i}{\partial x} + \left(1 - \frac{M_i}{M}\right)\frac{1}{p}\frac{\partial p}{\partial x}\right), \qquad \text{Fourier's law}$$

$$J_i^m = \rho\sum_{j=1, j\neq i}^{N}\frac{M_i}{M}Y_j\mathcal{D}_{ij}\left(\frac{1}{\chi_j}\frac{\partial \chi_j}{\partial x} + \left(1 - \frac{M_j}{M}\right)\frac{1}{p}\frac{\partial p}{\partial x}\right) - \mathcal{D}_i^T\frac{1}{T}\frac{\partial T}{\partial x}, \quad \left(i = 1, \ldots, N\right), \qquad \text{Fick's law}$$

$$y_l = m_l\sum_{i=1}^{N}\frac{\phi_{il}}{M_i}Y_i, \qquad \left(l = 1, \ldots, L-1\right), \qquad \text{element mass fraction}$$

$$M = \sum_{i=1}^{N} M_i\chi_i, \qquad \text{mean molecular mass}$$

$$\chi_i = \frac{M}{M_i}Y_i, \qquad (i = 1, \ldots, N), \qquad \text{mole fraction}$$

$$j_l = m_l\sum_{i=1}^{N}\frac{\phi_{il}}{M_i}J_i, \qquad \left(l = 1, \ldots, L-1\right), \qquad \text{element mass flux}$$

$$\sum_{i=1}^{N} Y_i = 1, \qquad \text{mass fraction constraint}$$

$$\sum_{l=1}^{L} y_l = 1, \qquad \text{element mass fraction constraint}$$

$$\dot{\omega}_i = \sum_{j=1}^{J} a_j T^{\beta_j}\exp\left(\frac{-E_j}{\Re T}\right)\left(\nu_{ij}'' - \nu_{ij}'\right)\prod_{k=1}^{N}\left(\frac{\rho Y_k}{M_k}\right)^{\nu_{kj}'}, \qquad (i = 1, \ldots, N-L) \qquad \text{law of mass action}$$

$$p = \rho\Re T\sum_{i=1}^{N}\frac{Y_i}{M_i}, \qquad \text{thermal equation of state}$$

$$e = \sum_{i=1}^{N} Y_i\left(h_i^o + \int_{T_o}^{T} c_{pi}(\hat{T})d\hat{T} - \frac{\Re T}{M_i}\right). \qquad \text{caloric equation of state}$$

N species, L elements, J reactions

$4N + L + 7$ equations in $4N + L + 7$ unknowns

Operator Splitting Technique

- Equations are of form

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \underbrace{\frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t))}_{\text{convection/diffusion}} = \underbrace{\mathbf{g}(\mathbf{q}(x,t))}_{\text{reaction}}, \qquad \mathbf{q},\mathbf{f},\mathbf{g} \in \Re^{N+2}.$$

where

$$\mathbf{q} = \left(\rho, \rho u, \rho\left(e + \frac{u^2}{2}\right), \rho y_l, \rho Y_i\right)^T.$$

- Splitting

1. Inert convection-diffusion step:

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t)) = 0,$$
$$\frac{d}{dt}\mathbf{q}_i(t) = -\Delta_x \mathbf{f}(\mathbf{q}_i(t)) \qquad \textit{WAMR.}$$

Δ_x is any spatial discretization operator, here a wavelet operator.

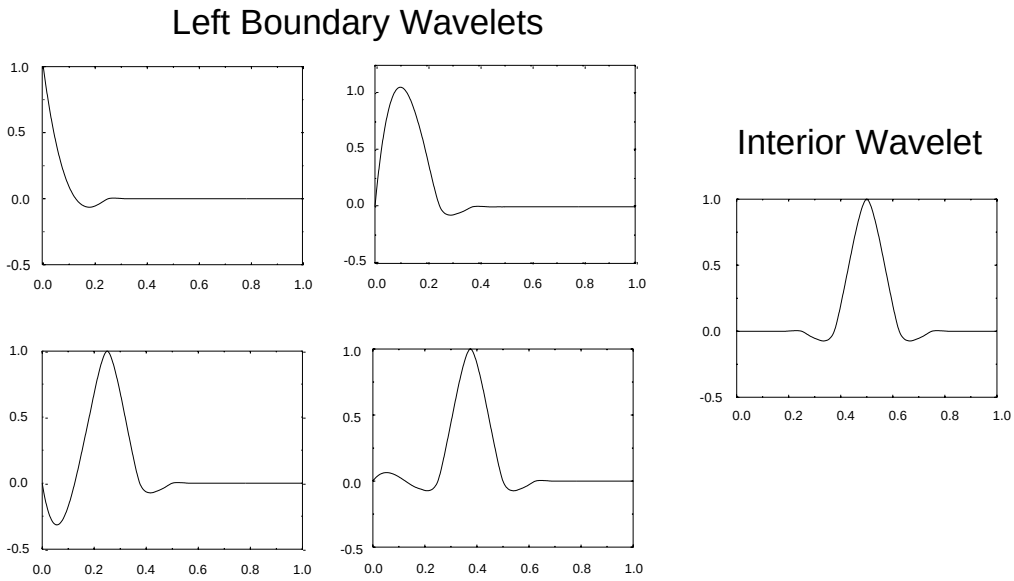
2. Reaction source term step:

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) = \mathbf{g}(\mathbf{q}(x,t)),$$
$$\frac{d}{dt}\mathbf{q}_i(t) = \mathbf{g}(\mathbf{q}_i(t)) \qquad \textit{ILDM.}$$

Wavelet Adaptive Multilevel Representation (WAMR) Technique

- Summary of standard spatial discretization techniques
  - Finite difference-good spatial localization, poor spectral localization, and slow convergence,
  - Finite element- good spatial localization, poor spectral localization, and slow convergence,
  - Spectral–good spectral localization, poor spatial localization, but fast convergence.
- Wavelet technique
  - See e.g. Vasilyev and Paolucci, "A Fast Adaptive Wavelet Collocation Algorithm for Multidimensional PDEs," *J. Comp. Phys.*, 1997,
  - Basis functions have compact support,
  - Well-suited for problems with widely disparate spatial scales,
  - Good spatial and spectral localization, and fast (spectral) convergence,
  - Easy adaptable to steep gradients via adding collocation points,
  - Spatial adaptation is automatic and dynamic to achieve prescribed error tolerance.

Wavelet Basis Functions



- Boundary-modified Daubechies autocorrelation functions and interior Daubechies autocorrelation function of order four
- Scaling function

$$\phi_{j,k}(x) = \phi(2^j x - k)$$

- Definition of the wavelet function on the first level

$$\psi_{1,0}(x) = \phi(2x - 1)$$

- Definition of the wavelet function on j level

$$\psi_{j,k+1}(x) = \psi(2^{j-1} x - k)$$

Algorithm Description

- Approximate initial function using wavelet basis,

$$\mathbf{P}^J u(x) = \sum_k u_{0,k}\phi_{0,k}(x) + \sum_{j=1}^{J}\sum_k d_{j,k}\psi_{j,k}(x)$$

- Discard non-essential wavelets if amplitude below threshold value (here we look only at P, T, u, and ρ, species could be included),

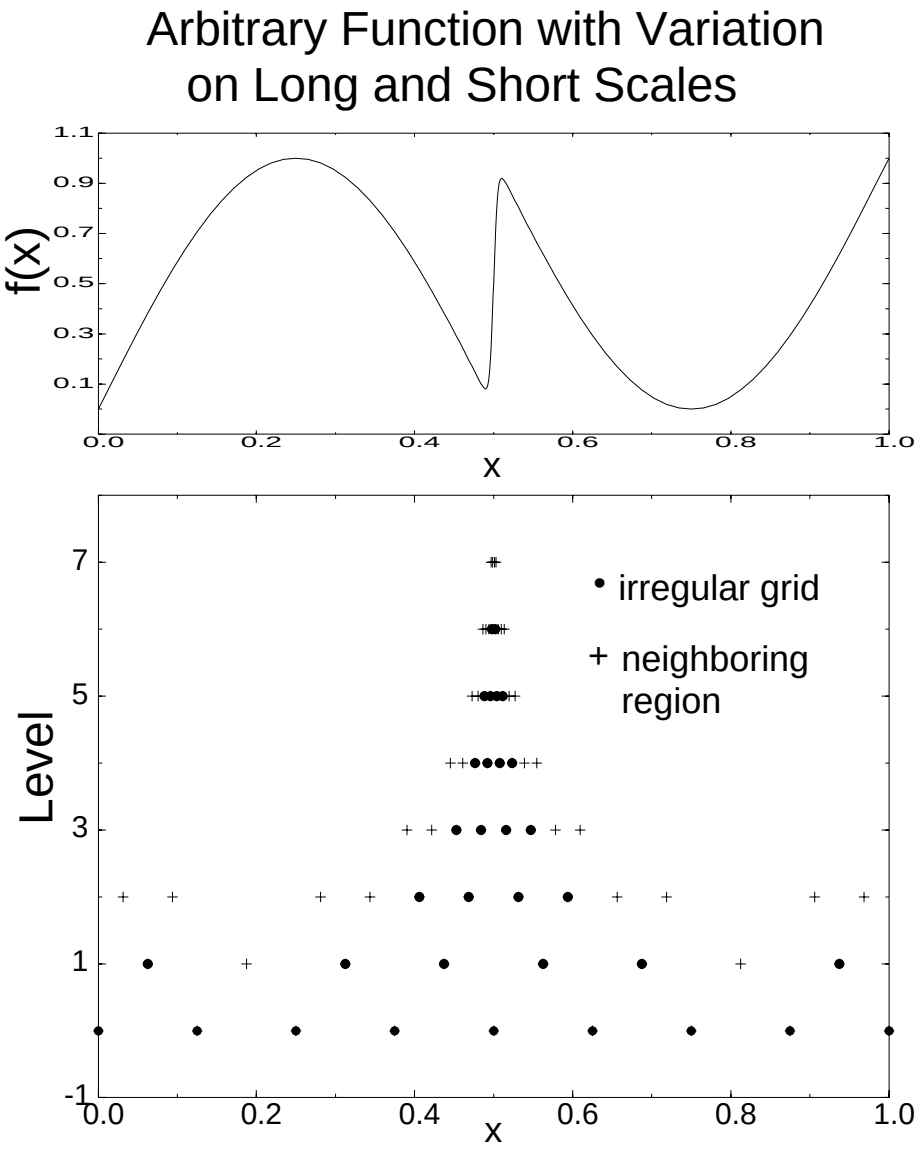
$$\mathbf{P}^J u(x) = u^J_{\geq}(x) + u^J_{<}(x)$$

$$u^J_{\geq}(x) = \sum_k u_{0,k}\phi_{0,k}(x) + \sum_{j=1}^{J}\sum_k d_{j,k}\psi_{j,k}(x), |d_{j,k}| \geq \epsilon$$

$$u^J_{<}(x) = \sum_{j=1}^{J}\sum_k d_{j,k}\psi_{j,k}(x), |d_{j,k}| < \epsilon$$

- Assign a collocation point to every essential wavelet,
- Establish a neighboring region of potentially essential wavelets,
- Discretize the spatial derivatives; five points used here (related to order of wavelet family),
- Integrate in time; linearized trapezoidal method (implicit) used here,
- Repeat

Sample Wavelet Approximation to Arbitrary Function



- Function shown has large and small length scale variation,
- Wavelets concentrated in regions of steep gradients.

Intrinsic Low-Dimensional Manifold Method (ILDM)

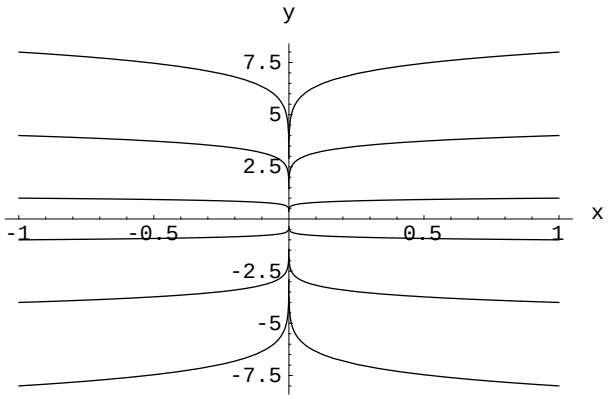
- Uses a dynamical systems approach,
- Most appropriate for spatially homogeneous systems (ODEs)
- Does not require imposition of *ad hoc* partial equilibrium or steady state assumptions,
- Fast time scale phenomena are systematically equilibrated,
- Slow time scale phenomena are resolved in time,
- Computation time reduced by factor of ~ 3 for non-trivial combustion problem considered here; manifold gives much better roadmap to find solution relative to general implicit solution techniques (Singh, *et al.*, 2001)
- Speed up factor depends on
  - initial conditions,
  - stiffness ratio
  - dimension of ILDM

Simplest Example

$$\frac{dx}{dt} = -10x, \qquad x(0) = x_o,$$
$$\frac{dy}{dt} = -y, \qquad y(0) = y_o.$$

- Stable equilibrium at $(x, y) = (0,0)$; stiffness ratio = 10.

- ILDM is $x = 0$



- Parameterization of manifold: $x(s) = 0; y(s) = s$.

$$\frac{dy}{dt} = \frac{dy}{ds}\,\frac{ds}{dt}, \qquad \text{chain rule}$$
$$-y(s) = \frac{dy}{ds}\,\frac{ds}{dt}, \qquad \text{substitute from ODE and manifold}$$
$$-s = (1)\frac{ds}{dt}, \qquad \text{no longer stiff!}$$
$$s = s_o e^{-t},$$
$$x(t) = 0; \qquad y(t) = s_o e^{-t}.$$

- Projection onto manifold for s_o, induces small phase error.

ILDM Implementation in Operator Splitting

- Form of equations in source term step:

$$\frac{d}{dt}\begin{pmatrix} \rho \\ \rho u \\ \rho\left(e+\frac{u^2}{2}\right) \\ \rho y_l \\ \rho Y_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_i M_i \end{pmatrix}.$$

$$l = 1, \ldots, L-1, \qquad i = 1, \ldots, N-L.$$

- Equations reduce to

$$\rho = \rho_o, \qquad u = u_o, \qquad e = e_o, \qquad y_l = y_{lo},$$

$$\frac{dY_i}{dt} = \frac{\dot{\omega}_i M_i}{\rho_o}, \qquad i = 1, \ldots, N-L$$

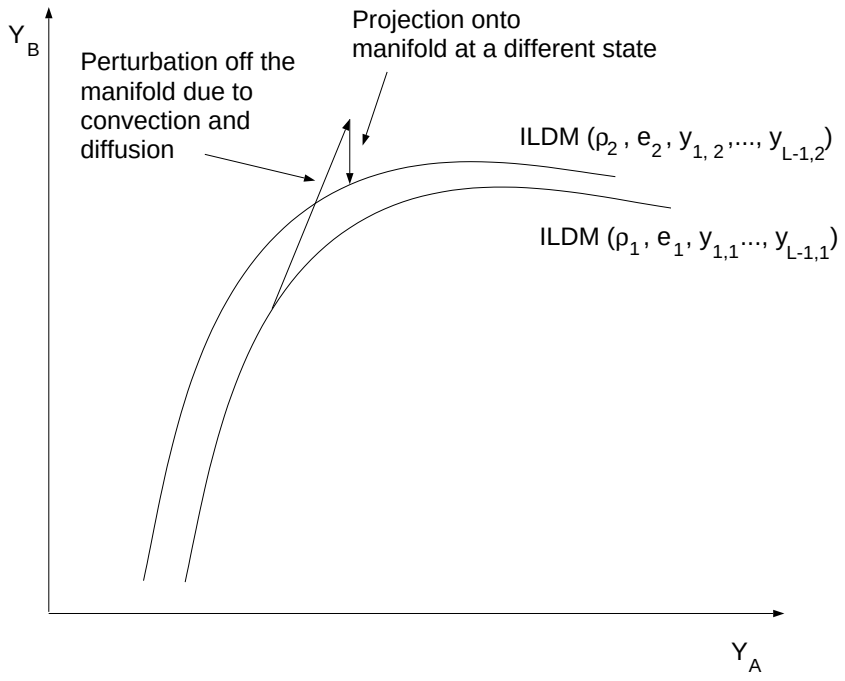
- $\dot{\omega}_i$ has dependency on ρ, e, y_l, and Y_i

- ODEs for Y_i are stiff, usually solved with implicit methods.

- ODEs for Y_i can be attacked with manifold methods to remove stiffness with ILDM with ρ, e, $y_l, \ldots, y_{L-1}$ parameterization.

Implementation of ILDMs with convection-diffusion and operator splitting

- To minimize phase error, must integrate full equations until sufficiently close to ILDM
- When near ILDM, M slow equations are integrated, other variables found by table lookup
- Convection-diffusion step *applied to all variables* perturbs system from ILDM
- In next reaction step, project to ILDM at *different* value of ρ, e, $y_1, \ldots, y_{N-1}$.



Formulation of General ILDMs

- A spatially homogeneous adiabatic, isochoric chemically reactive system of N species in L elements is modeled by a set of non-linear ordinary differential equations:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}), \qquad \mathbf{x}(0) = \mathbf{x}_o,$$

$$\mathbf{x}: \text{ species concentration}; \mathbf{x} \in \Re^{N-L}$$

- Equilibrium points defined by

$$\mathbf{x} = \mathbf{x}_{eq} \text{ such that } \mathbf{F}(\mathbf{x}_{eq}) = 0.$$

- Consider a system near equilibrium (the argument can and must be extended for systems away from equilibrium) with $\tilde{\mathbf{x}} = \mathbf{x} - \mathbf{x}_{eq}$.

- Linearization gives

$$\frac{d\tilde{\mathbf{x}}}{dt} = \mathbf{F}_{\mathbf{x}} \cdot \tilde{\mathbf{x}},$$

where $\mathbf{F}_{\mathbf{x}}$ is a *constant* Jacobian matrix.

- Schur decompose the Jacobian matrix:

$$\mathbf{F}_{\mathbf{x}} = \mathbf{Q} \cdot \mathbf{U} \cdot \mathbf{Q}^T$$

$$\mathbf{Q} = \begin{pmatrix} \vdots & \vdots & & \vdots \\ q_1 & q_2 & \cdots & q_{N-L} \\ \vdots & \vdots & & \vdots \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} \lambda_1 & u_{1,2} & \cdots & u_{1,N-L} \\ 0 & \lambda_2 & \cdots & u_{2,N-L} \\ 0 & \cdots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_{N-L} \end{pmatrix}, \quad \mathbf{Q}^T = \begin{pmatrix} \cdots & q_1^T & \cdots \\ \cdots & q_2^T & \cdots \\ & \vdots & \\ \cdots & q_{N-L}^T & \cdots \end{pmatrix}$$

Formulation of General Manifolds (cont.)

- $\mathbf{Q}$ is an orthogonal matrix with real Schur vectors q_i in its columns.
- $\mathbf{U}$ is an upper triangular matrix with eigenvalues of $\mathbf{F_x}$ on its diagonal, sometimes placed in order of decreasing magnitude.
- The Schur vectors q_i form an orthonormal basis which spans the phase space, $\Re^{N-L}$.
- We then define M slow time scales, $M < N - L$.
- Next define a non-square matrix $\mathbf{W}$ which has in its rows the Schur vectors associated with the fast time scales:

$$\mathbf{W} = \begin{pmatrix} \cdots & \cdots & q_{M+1}^T & \cdots & \cdots \\ \cdots & \cdots & q_{M+2}^T & \cdots & \cdots \\ & & \vdots & & \\ \cdots & \cdots & q_{N-L}^T & \cdots & \cdots \end{pmatrix}.$$

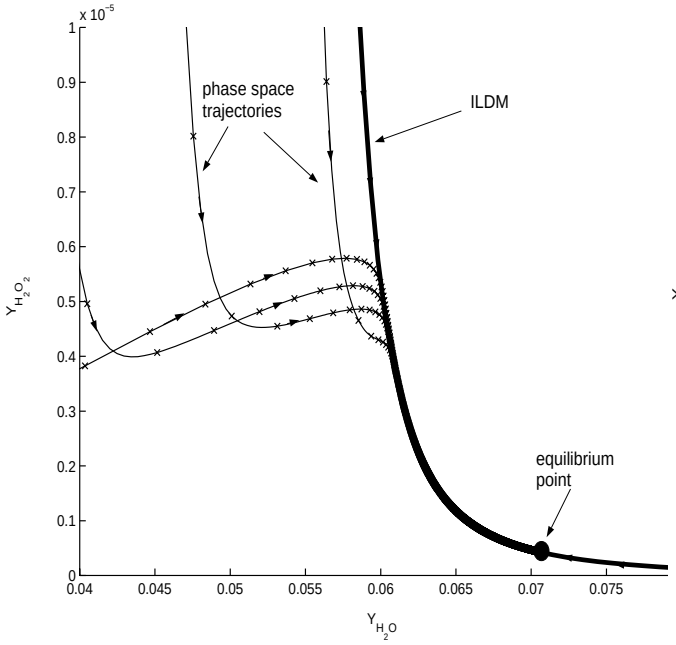
- Letting the fast time scale events equilibrate defines the manifold:

$$\mathbf{W} \cdot \mathbf{F}(\mathbf{x}) = 0.$$

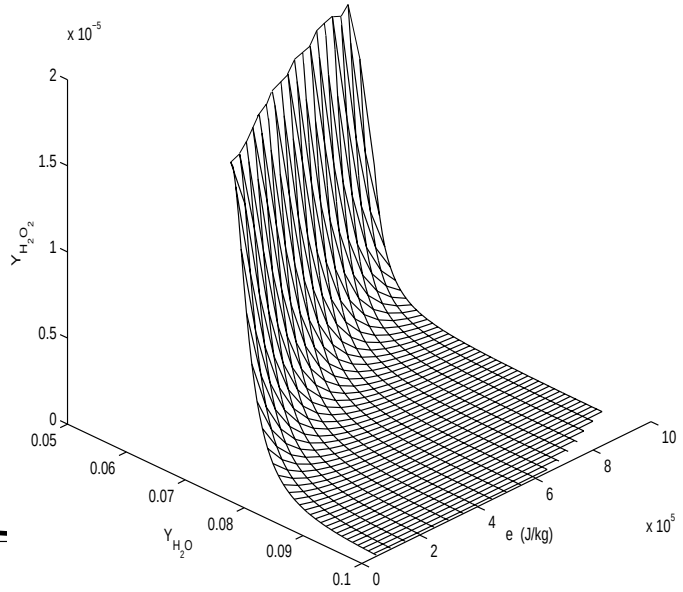
Sample ILDM for $H_2/O_2/Ar$

- Based on $N = 9$, $J = 37$ mechanism of Maas and Warnatz,
- Projection in Y_{H_2O}, $Y_{H_2O_2}$ plane and Y_{H_2O}, $Y_{H_2O_2}$, e space
- Adiabatic ($e = 8 \times 10^5\ J/kg$), isochoric ($\rho = 5.0 \times 10^{-4}\ kg/m^3$), $y_H = 0.01277$, $y_O = 0.10137$, $y_{Ar} = 0.88586$,
- We can get e.g. $p\left(\rho, e, Y_{H_2O}\right), T\left(\rho, e, Y_{H_2O}\right), Y_H\left(\rho, e, Y_{H_2O}\right), \ldots$
- Linear interpolation used for points not in table,
- Captures $\sim 0.1\ \mu s$ reaction events.

2-D projection



3-D projection

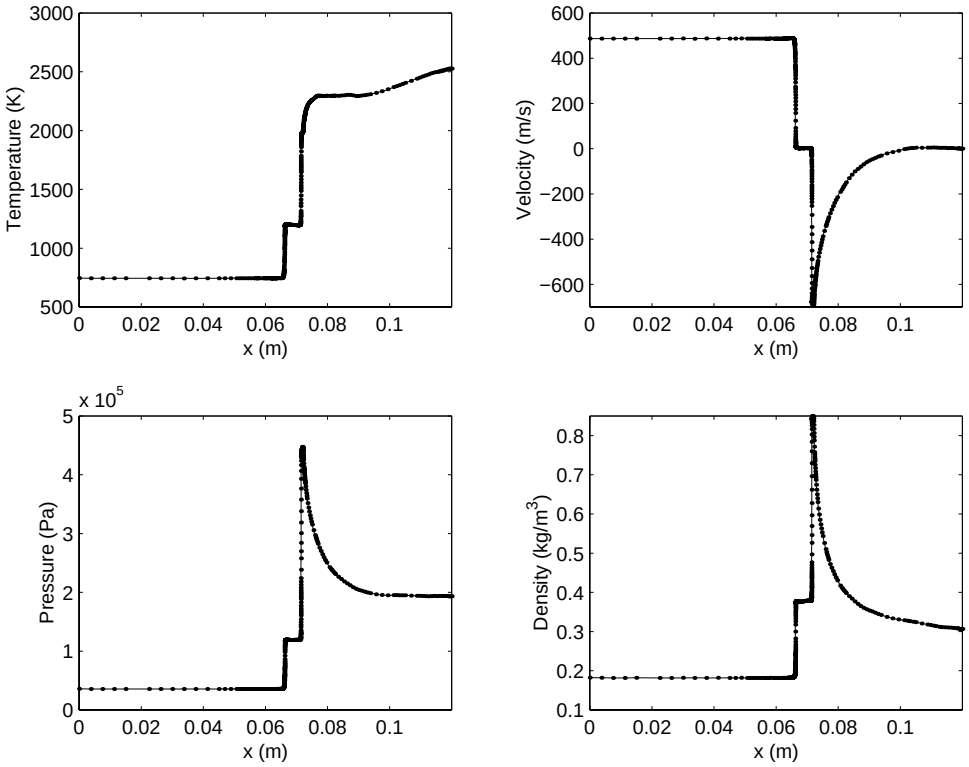


Ignition Delay in Premixed $H_2/O_2/Ar$

- Consider standard problem of Fedkiw, Merriman, and Osher, *J. Comp. Phys.*, 1996,
- Shock tube with premixed H_2, O_2, and Ar in 2/1/7 molar ratio,
- Initial inert shock propagating in tube,
- Reaction commences shortly after reflection off end wall,
- Detonation soon develops,
- Model assumptions
  - One-dimensional,
  - Mass, momentum, and energy diffusion,
  - Nine species, thirty-seven reactions,
  - Ideal gases with variable specific heats.

Viscous $H_2 - O_2$ Ignition Delay with Wavelets and ILDM

- $t = 195\ \mu s$, 300 collocation points, 15 wavelet scale levels
- ILDM gives nearly identical results as full chemistry
- WAMR spatial discretization, implicit linear trapezoidal convection-diffusion time stepping, explicit (ILDM)/implicit (non-ILDM) reaction time stepping
- *Viscous shocks, inductions zones, and entropy layers spatially resolved!*



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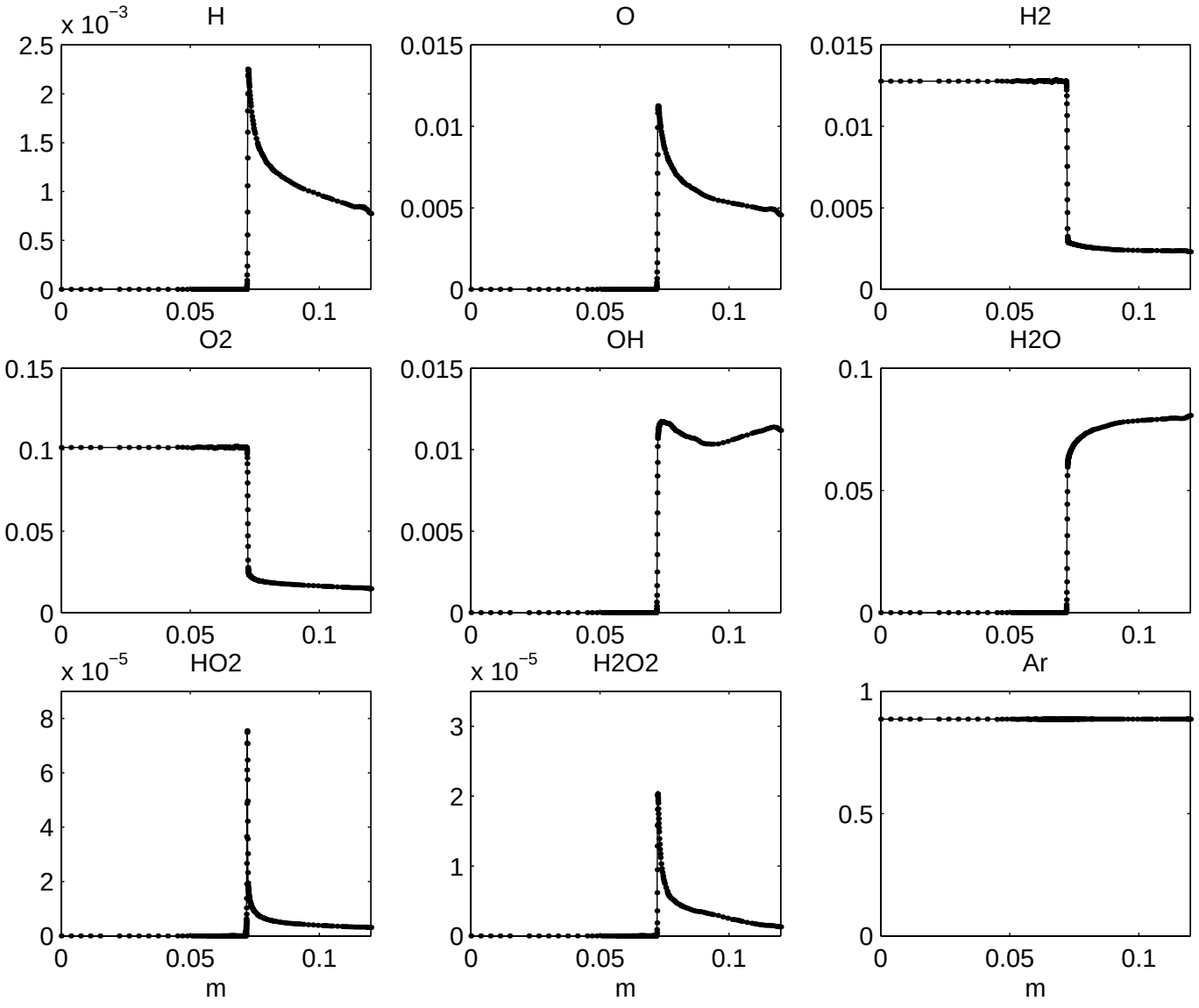
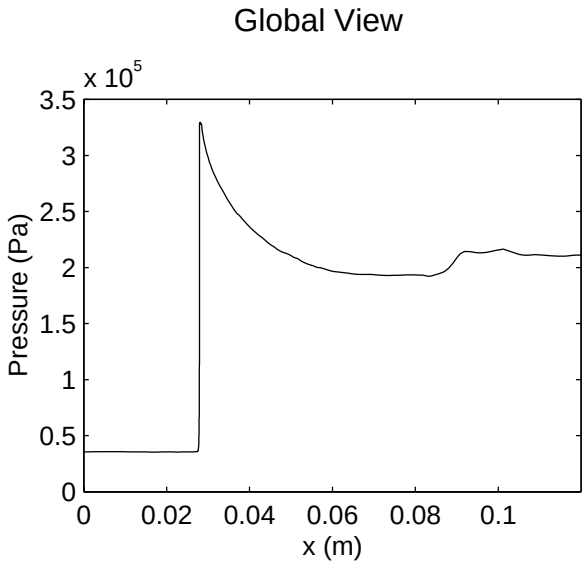
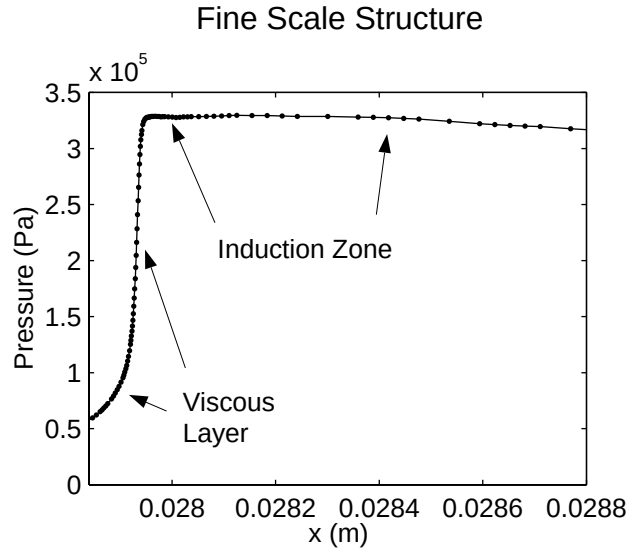


Viscous $H_2 - O_2$ Ignition Delay with Wavelets

Global and Fine Scale Structures

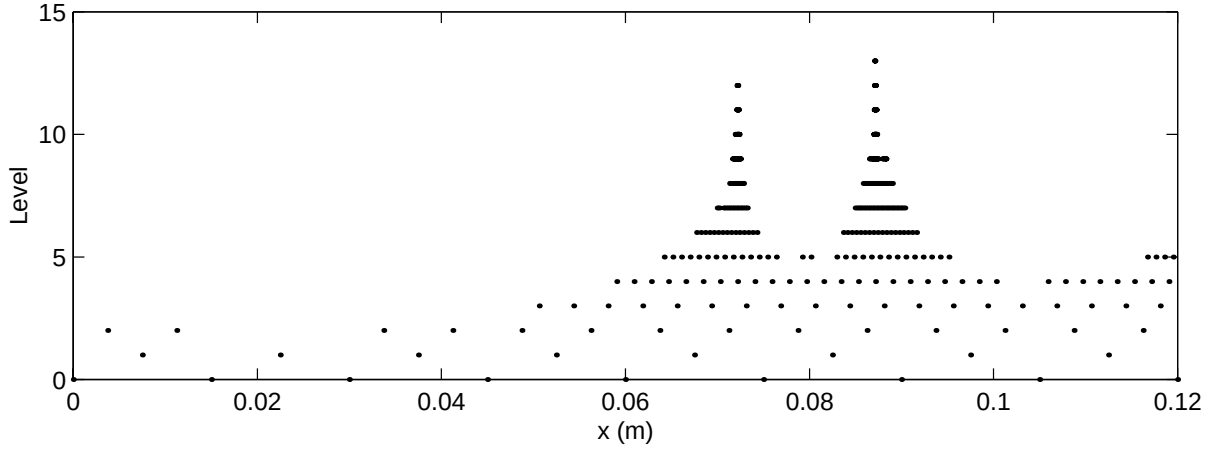
- $t = 230\ \mu s$, Induction zone length: $\sim 470\ \mu m$, Viscous shock thickness: $\sim 50\ \mu m$ (should use smaller μ),
- No significant reaction in viscous shock zone.

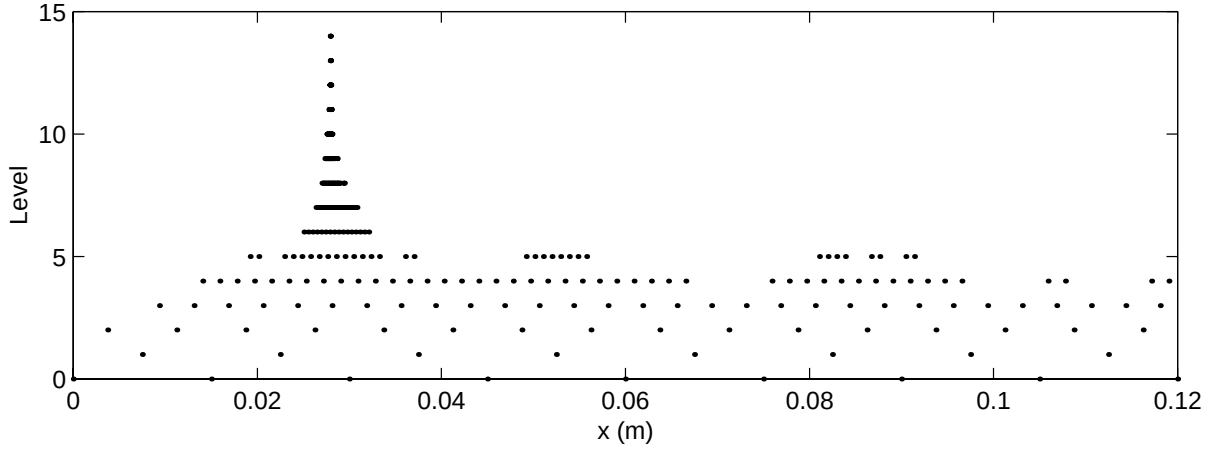




Viscous $H_2 - O_2$ Ignition Delay with Wavelets, Instantaneous Distributions of Collocation Points

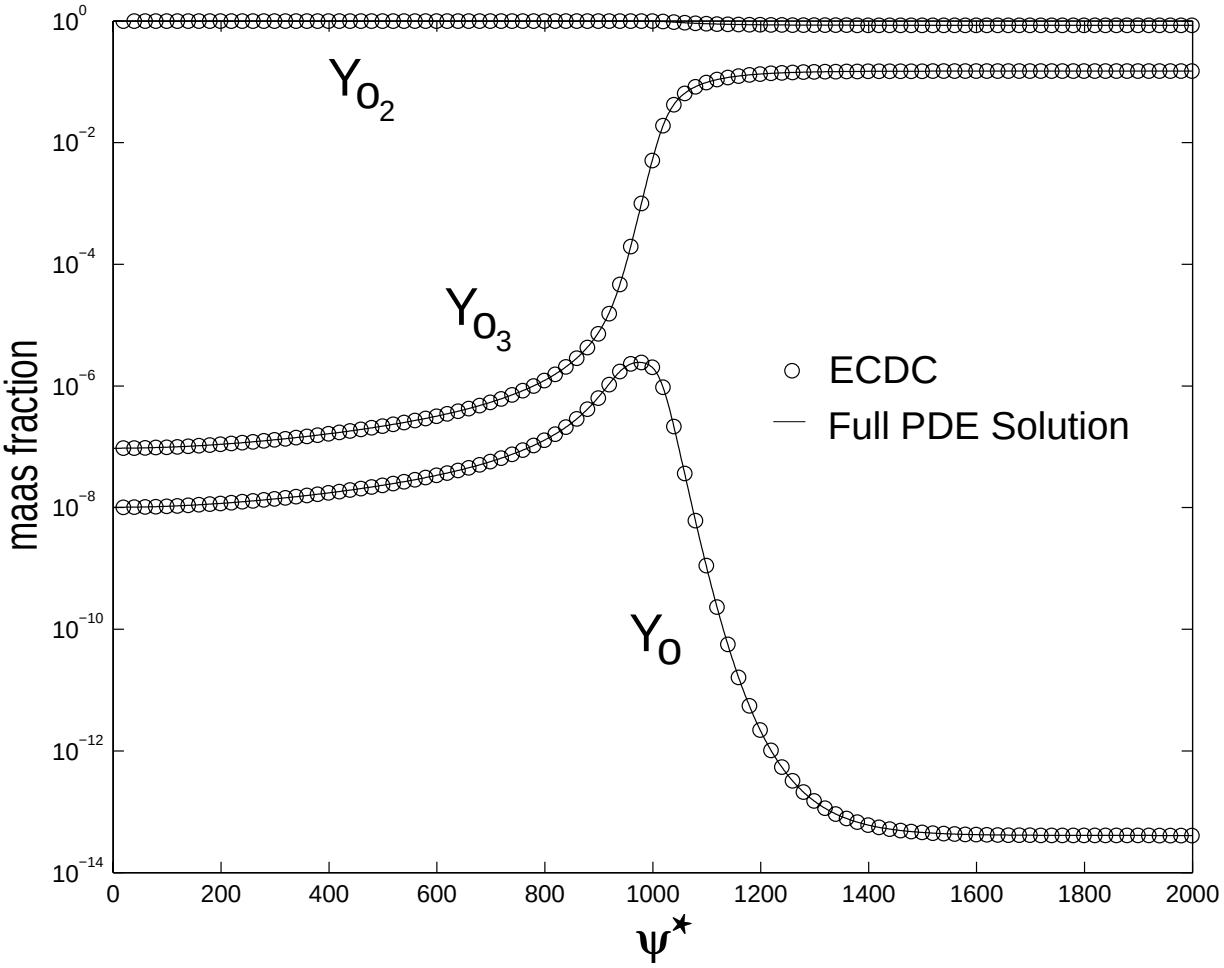
- $t = 180\ \mu s$, two-shock structure with consequent collocation point distribution,
- $t = 230\ \mu s$, one-shock structure with evolved collocation point distribution.





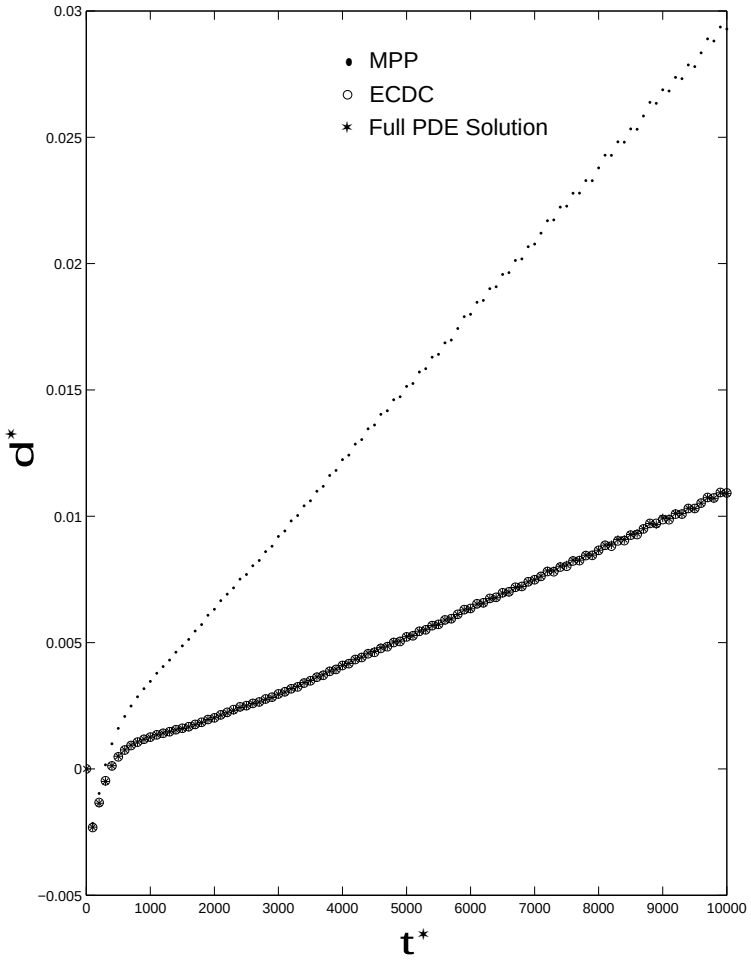
Laminar Ozone Flame with Improved ILDM

- One dimensional, low Mach number limit
- see Margolis, *J. Comp. Phys.*, 1978
- Classical ILDM for ODEs only
- Project PDEs onto fast and slow bases defined by ILDM.
- Solve slow PDEs and new elliptic equation: *Elliptic Convection-Diffusion Corrector*, ECDC



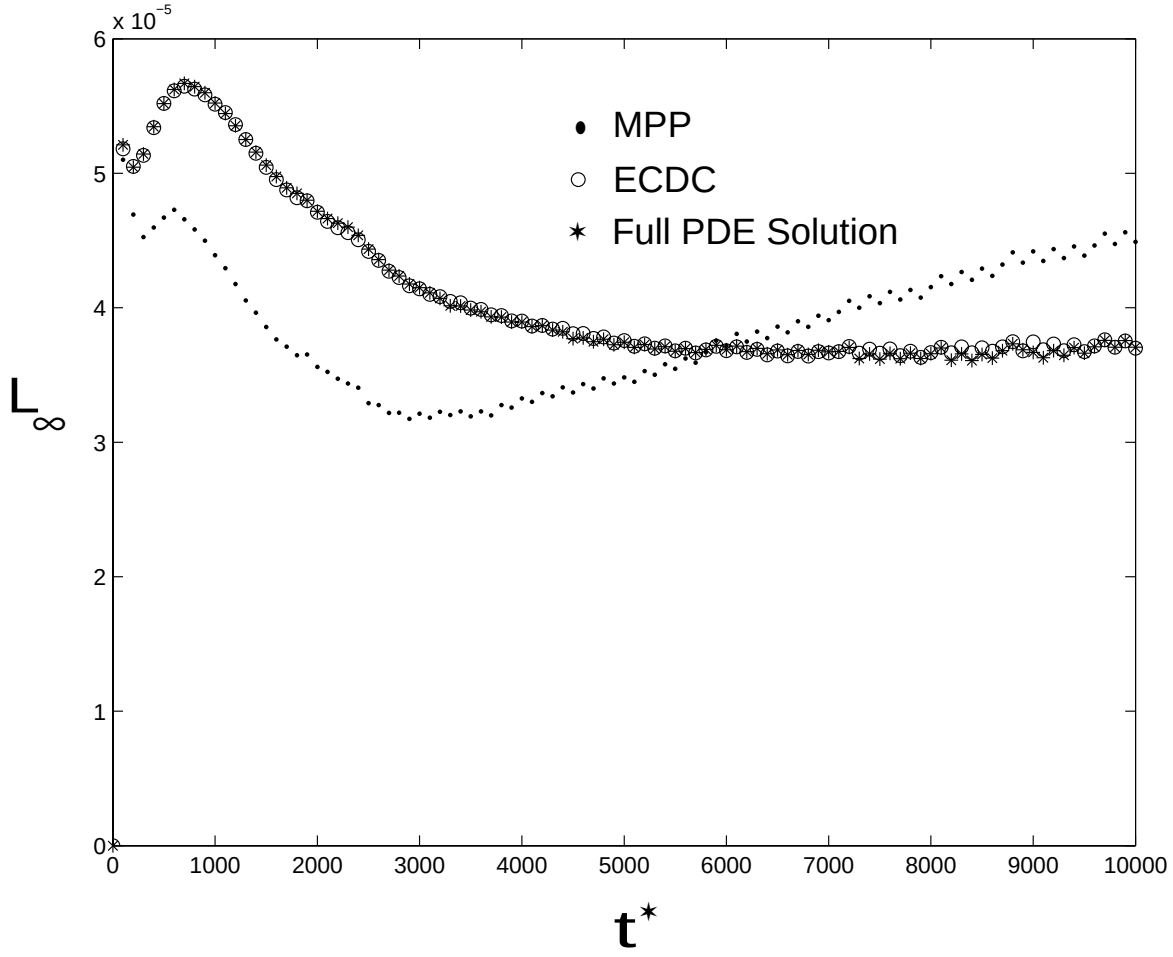
Laminar Ozone Flame with Improved ILDM: Phase Error

- ECDC gives improved accuracy in wave speed predictions relative to Maas-Pope projection.
- ECDC has stronger coupling with full equations.
- ECDC analagous to elliptic equation for pressure in incompressible Navier-Stokes, where fast acoustics have been filtered.



Laminar Ozone Flame with Improved ILDM: Amplitude Error

- ECDC gives improved accuracy in amplitude predictions at long time relative to Maas-Pope projection.



Lid-Driven Fluid in Rectangular Cavity

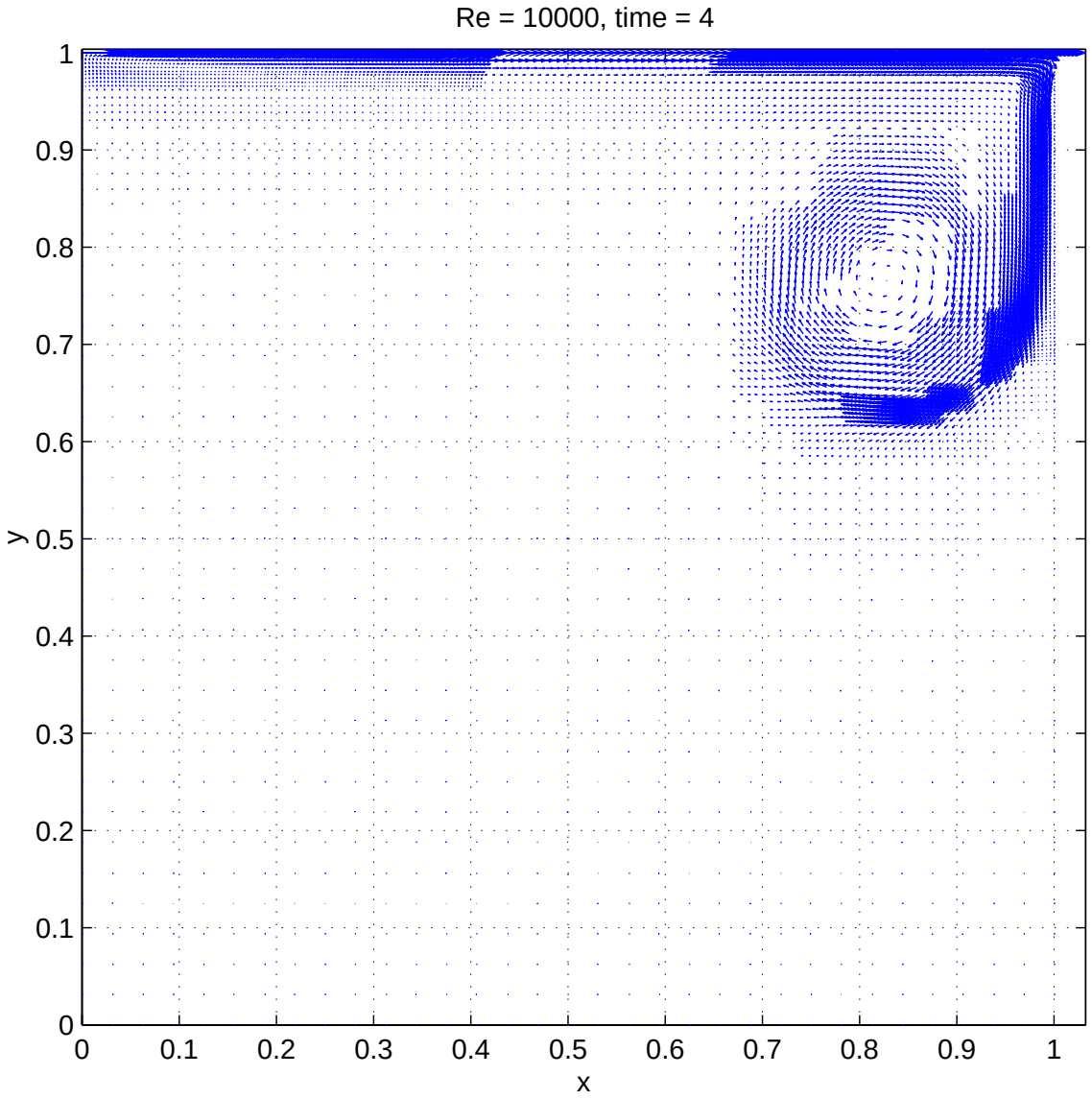
- Standard two-dimensional test problem (Ghia, *et al.*, *J. Comp. Phys.*, 1982)
- Consider incompressible Navier-Stokes equations

$$\begin{aligned}
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0, \\
\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} &= -\frac{\partial p}{\partial x} + \frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \\
\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} &= -\frac{\partial p}{\partial y} + \frac{1}{Re}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right).
\end{aligned}$$

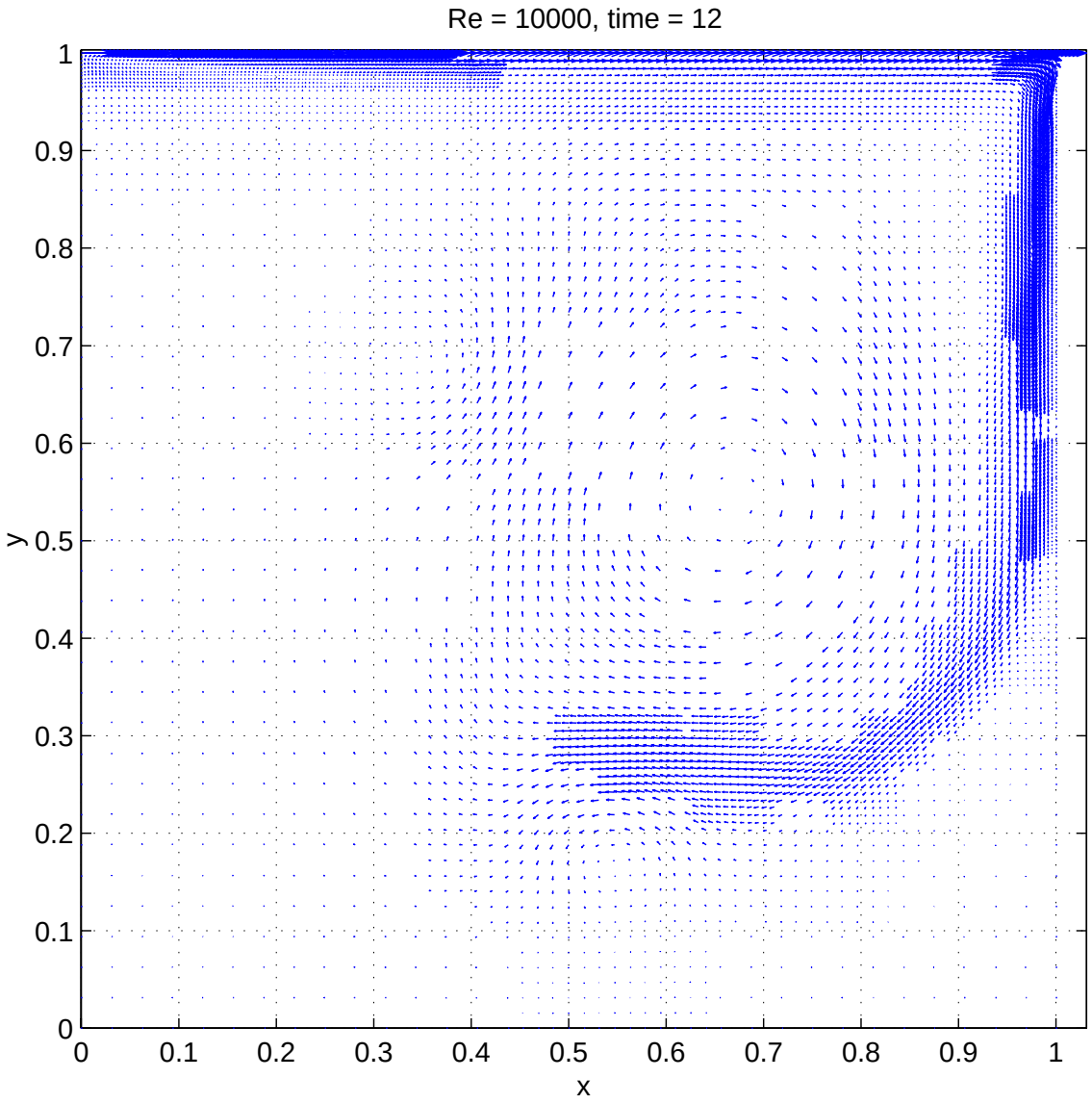
- Project dependent variables onto wavelet basis localized in two-dimensions.
- Fast Poisson solver developed for resulting equation for pressure.
- Dynamic memory allocation utilized for variable storage requirements.
- Adaptive nature of the method requires a robust computational technique for computing derivatives.
- Wavelets which are physically close may be far removed in memory storage.
- Method prepared to handle a wide variety of stencil combinations.

Velocity Vector Field, $Re = 10000$, $t = 4$

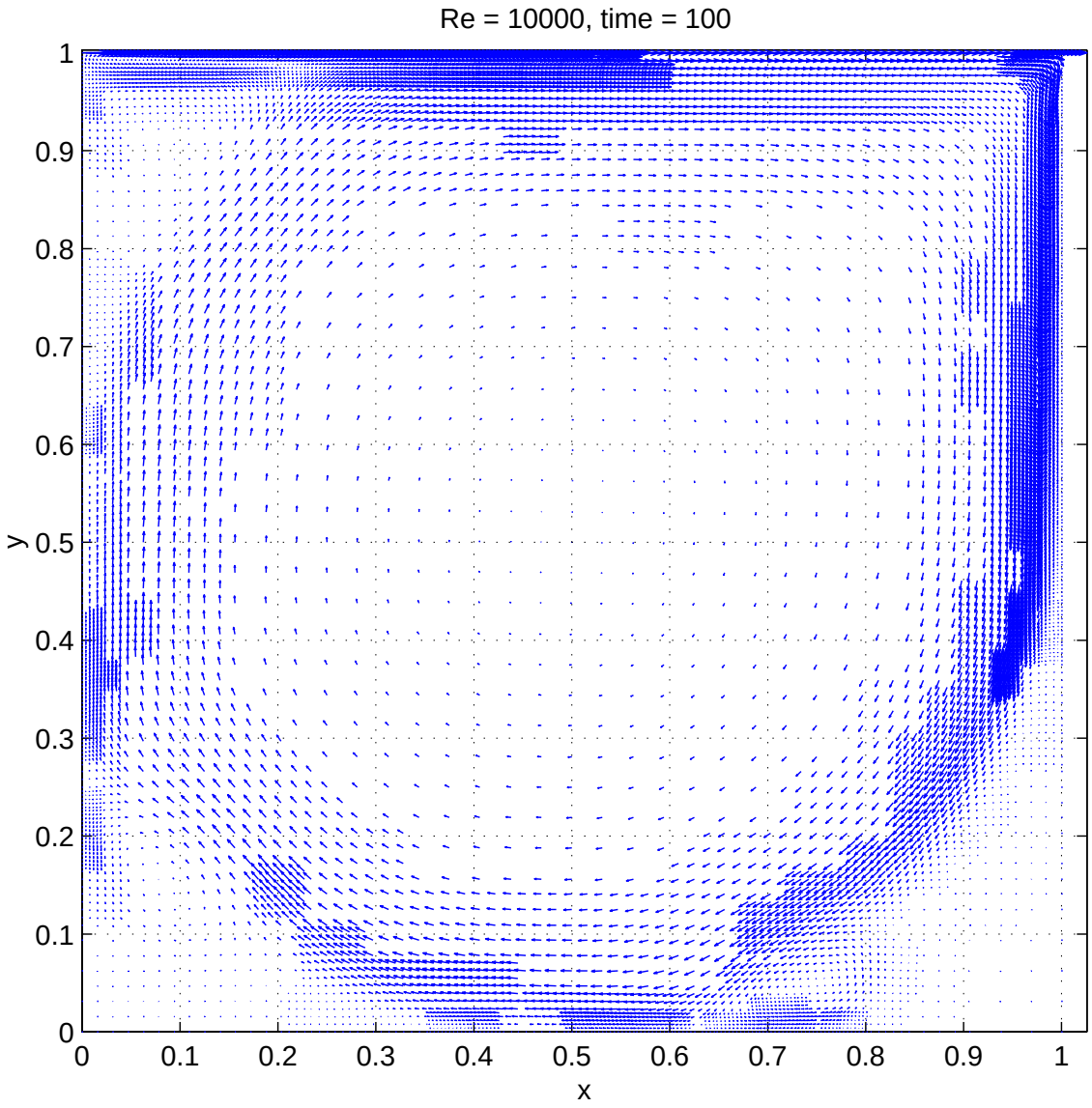
- $Re = 10000$ equivalent to highest Re for this problem in the published literature with long time steady results.
- Initial transients have not yet relaxed here.



Velocity Vector Field, $Re = 10000$**,** $t = 12$

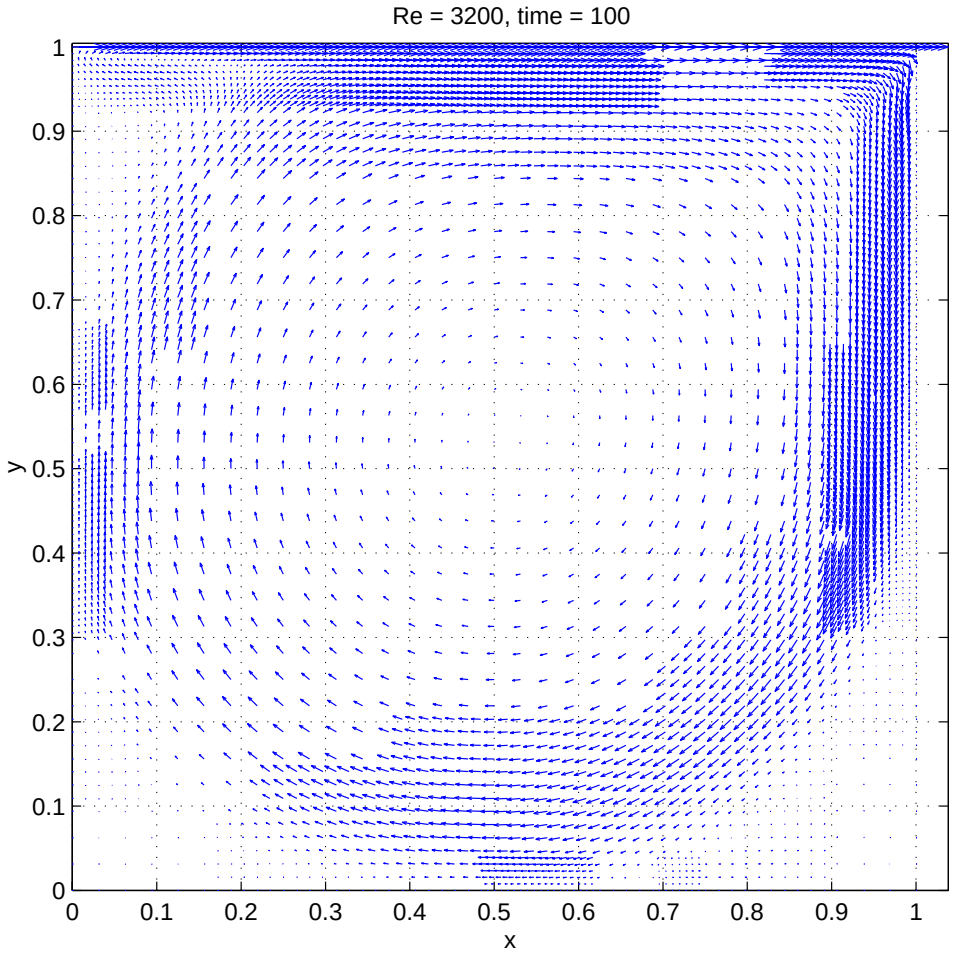


Velocity Vector Field, $Re = 10000$**,** $t = 100$



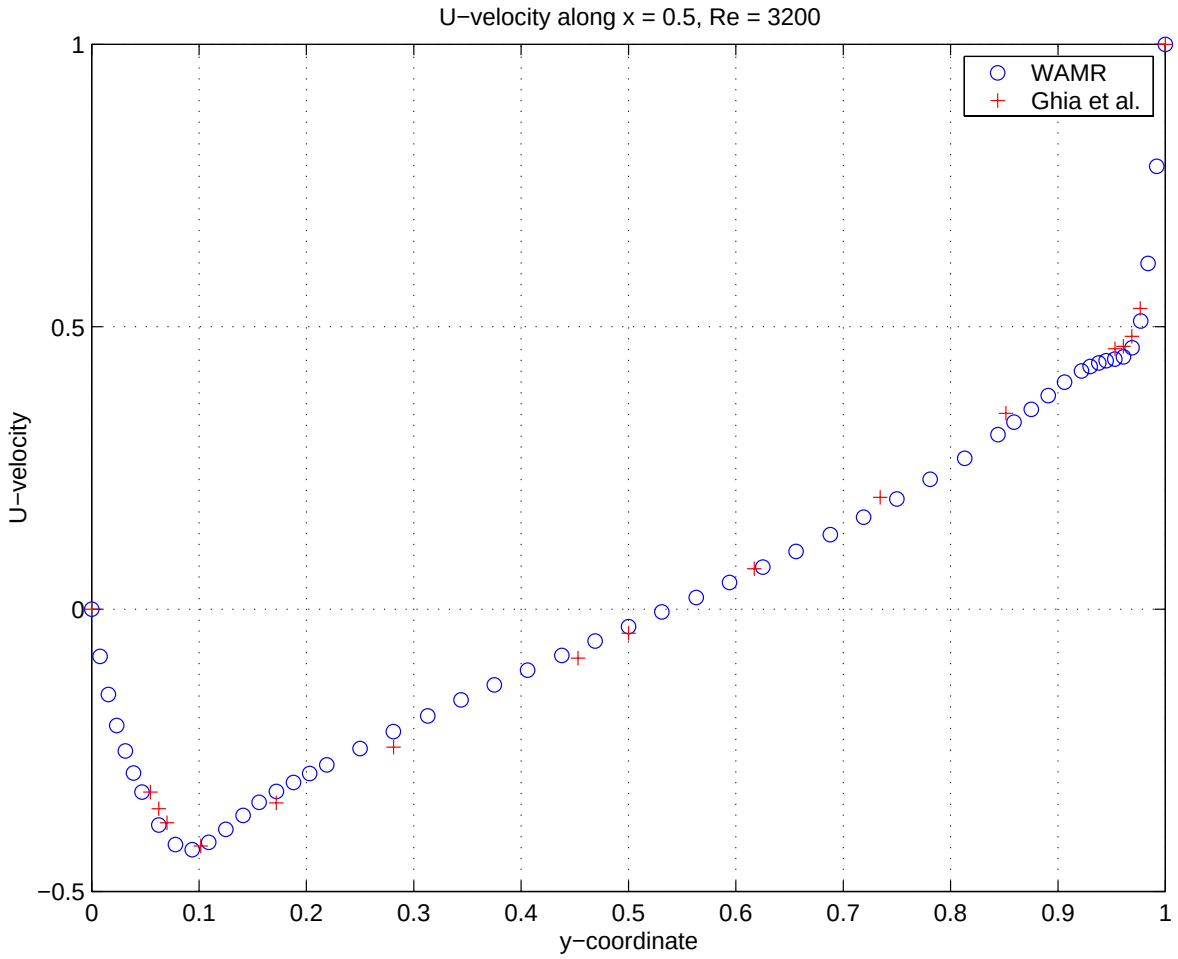
Velocity Vector Field, $Re = 3200$

- Long time results $t = 100$; initial transients have relaxed.
- Wavelets only present in regions of steep gradients.; $\epsilon = 0.01$.
- Five levels of wavelets: coarsest 16×16, finest 257×257; equivalent to Ghia's uniform grid.
- Results are more accurate than Ghia, as a higher order stencil was used on an equivalent grid.



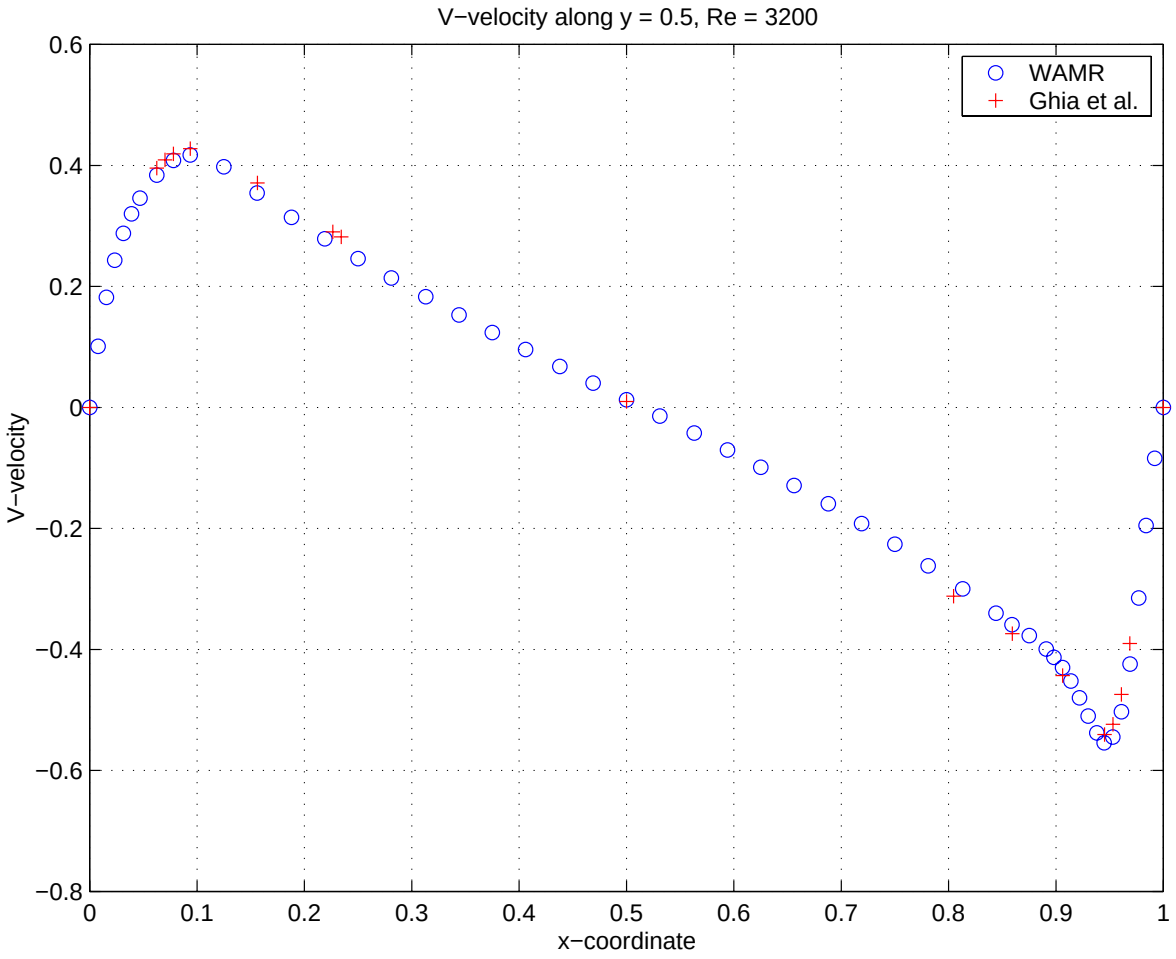
Comparison with Ghia's Results for u, $Re = 3200$

- Midplane predictions of long-time u velocity agree well with Ghia's predictions.



Comparison with Ghia's Results for v, $Re = 3200$

- Midplane predictions of long-time v velocity agree well with Ghia's predictions.



Conclusions

- The WAMR method gives dramatic spatial resolution in viscous one-dimensional $H_2/O_2/Ar$ detonations with detailed kinetics; viscous shocks, entropy layers, and induction zones are resolved,
- The ILDM method, coupled appropriate use of full integration, with operator spitting accurately recovers most results of full chemistry with decrease (factor of three for our case) in computational time,
- The ILDM method can be made more accurate at roughly the same computational cost by solving an elliptic equation for accounting for effects of convection and diffusion (ECDC)
- The WAMR method can be extended to multiple dimensions and can enable extremely detailed and accurate results on a challenging two-dimensional test problem.
- The extension to three-dimensional compressible reactive flows within complex geometries is underway.