Resolved Viscous Detonation in $H_2/O_2/Ar$ Using Intrinsic Low Dimensional Manifolds and Wavelet Adaptive Multilevel Representation

by

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presented to the

Second International Workshop on Combustion Modeling Instituto Tecnológico de Veracruz

 $22 \ {\rm February} \ 2001$

Support: NSF, AFOSR, LANL

Acknowledgments

Prof. Samuel Paolucci, Faculty, ND-AME, Mr. Sandeep Singh, Ph.D. Candidate, ND-AME, Mr. Yevgenii Rastigejev, Ph.D. Candidate, ND-AME.

Outline

- Motivation for Intrinsic Low Dimensional Manifold (ILDM) technique (Maas & Pope, 1992) for spatially homogeneous systems (ODEs, no convection-diffusion)
- Compressible Reactive Navier-Stokes equations
- Details of ILDM implementation in operator splitting method
- Wavelet Adaptive Multilevel Representation (WAMR) technique (Paolucci & Vasilyev) for spatial discretization
- Results for one-dimensional viscous $H_2/O_2/Ar$ detonation with detailed kinetics (Singh, Rastigejev, Paolucci, and Powers, *Combustion Theory and Modeling*, submitted 2001) using operator splitting for convection-diffusion
- Work in progress: systematic, center manifold-motivated correction for convection-diffusion using ILDMs
- Conclusions

Some Important Questions

- Do we have resolved, accurate solutions for systems with detailed kinetics?
- How can ILDM improve the calculation of systems with detailed kinetics?
- How can ILDM, derived for spatially homogeneous systems, be used rationally in systems in which convection and diffusion are important?

Motivation for ILDM

- Detailed finite rate kinetics critical in reactive fluid mechanics
- Common detailed kinetic models are computationally expensive.
- Expense increases with
 - number of species and reactions modeled (linear effect),
 - *stiffness*-ratio of slow to fast time scales, (geometric effect).
- chemical time scales typically more demanding than convectiondiffusion
- Reduced kinetics necessary given current computational resources.

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

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

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



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

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

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

Compressible Reactive Navier-Stokes Equations

$$\begin{split} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left(\rho u\right) &= 0, \quad \text{mass} \\ \frac{\partial}{\partial t} \left(\rho u\right) + \frac{\partial}{\partial x} \left(\rho u^2 + p - \tau\right) &= 0, \quad \text{momentum} \\ \frac{\partial}{\partial t} \left(\rho \left(c + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x} \left(\rho u \left(c + \frac{u^2}{2}\right) + u \left(p - \tau\right) + q\right) &= 0, \quad \text{cnergy} \\ \frac{\partial}{\partial t} \left(\rho V_i\right) + \frac{\partial}{\partial x} \left(\rho u Y_i + J_i^m\right) &= \dot{u}_i M_i, \quad (i = 1, \dots, N - L), \quad \text{species} \\ \tau &= \frac{4}{3} u \frac{\partial u}{\partial x}, \quad \text{Newtonian gas with Stokes' assumption} \\ J^q &= -k \frac{\partial T}{\partial x} + \sum_{i=1}^N J_i^m \left(h_i^q + \int_{T_i}^T c_{pi}(\hat{T}) d\hat{T}\right) - \Re T \sum_{i=1}^N \frac{\partial 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), \quad \text{Fourier's law} \\ J_i^m &= \rho \sum_{j=1, j \neq i}^N \frac{M_i}{M} Y_j 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^r \frac{1}{T} \frac{\partial T}{\partial x}, \quad (i = 1, \dots, N), \quad \text{Fick's law} \\ y_l &= m_l \sum_{i=1}^N \frac{\phi_{il}}{M_i} Y_i, \quad (l = 1, \dots, L - 1), \quad \text{element mass fraction} \\ M &= \sum_{i=1}^N M_i \chi_i, \quad (i = 1, \dots, N), \quad \text{mole fraction} \\ j_l &= m_l \sum_{i=1}^N \frac{\phi_{il}}{M_i} J_i, \quad (l = 1, \dots, L - 1), \quad \text{element mass flux} \\ \sum_{i=1}^N Y_i &= 1, \quad \text{element mass fraction constraint} \\ \sum_{i=1}^L y_i &= 1, \quad \text{element mass fraction constraint} \\ \frac{L}{\omega_i} &= \sum_{i=1}^J a_j T^{\mathcal{G}_i} \exp\left(\frac{-E_j}{\Re T}\right) (\nu_{ij}'' - \nu_{ij}') \prod_{i=1}^M \left(\frac{\rho Y_k}{M_k}\right)^{\nu_{kj}'}, \quad (i = 1, \dots, N - L) \quad \text{law of mass action} \\ 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^q + \int_{T_i}^T c_{\mu_i}(\hat{T}) d\hat{T} - \frac{\Re T}{M_i}\right). \quad \text{caloric equation of state} \end{split}$$

 ${\cal N}$ species, ${\cal L}$ elements, ${\cal J}$ reactions

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

Focus on element conservation

- L-1 element equations formed; N-L species equations, instead of the typical N-1 species equations,
- facilitates a proper use of ILDM in upcoming operator splitting,
- In general element mass fractions change due to mass diffusion

$$\rho \frac{dy_l}{dt} = -\frac{\partial j_l}{\partial x}.$$

- Assuming
 - Soret and DuFour effects are negligible, $D_i^T = 0$,
 - Deviations of molecular mass not large $M_i \sim M$,
 - Diffusion coefficients are equal, $\mathcal{D}_{ij} \sim \mathcal{D}$,
- Molecular mass diffusion reduces to $J_i^m = -\rho \mathcal{D} \frac{\partial Y_i}{\partial x}$.
- Elemental mass diffusion reduces to $j_l = -\rho \mathcal{D} \frac{\partial y_l}{\partial x}$.
- Evolution equation for element mass fraction becomes

$$ho rac{dy_l}{dt} = \mathcal{D} rac{\partial}{\partial x} \left(
ho rac{\partial y_l}{\partial x}
ight).$$

• In uniformly premixed problem with no boundary influences then, all element concentrations are constant for all time:

$$\frac{dy_l}{dt} = 0$$

Operator Splitting Technique for Convection-Diffusion

• Equations are of form

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t)) = \mathbf{g}(\mathbf{q}(x,t)), \qquad \mathbf{q}, \mathbf{f}, \mathbf{g} \in \Re^{N+2}.$$

where

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

- $\bullet~{\bf f}$ models convection-diffusion
- $\bullet~{\bf g}$ models reaction source terms
- Splitting
 - 1. Inert convection-diffusion step:

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

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

2. Reaction source term step:

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

• Operator splitting with implicit stiff source solution can induce nonphysical wave speeds! (LeVeque and Yee, *JCP* 1990)

ILDM Implementation in Operator Splitting

• Form of equations in source term step:

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

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

• Equations reduce to

- $\dot{\omega}_i$ 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 , ..., y_{L-1} parameterization.

Necessary Dimension of ILDM

- Spatial discretization of PDEs results in a set of adiabatic, isochoric spatially homogeneous reactors,
- N species with L elements at constant e and ρ gives rise to a (N L)-dimensional phase space (same as composition space),
- To resolve M slow time scales, we identify M-dimensional subspaces (manifolds), M < (N-L), embedded within the (N-L)dimensional phase space on which the M slow time scale events evolve,
 - Fast time scale events rapidly move to the manifold,
 - Slow time scale events move on the manifold,
 - Because of convection-diffusion, e, ρ , y_l vary, requiring a K = M + L + 1-dimensional manifold.
 - If y_l conserved (premixed with no preferential diffusion), dimension of manifold is reduced by L - 1.
 - e.g., for M = 1 in premixed $H_2/O_2/Ar$ with no preferential diffusion, small molecular mass deviation, and negligible Soret/DuFour diffusion, we need K = 3.

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 nonlinear ordinary differential equations:

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

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

• Equilibrium points defined by

$$\mathbf{x} = \mathbf{x}_{eq}$$
 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.)

- **Q** is an orthogonal matrix with real Schur vectors q_i in its columns.
- U is an upper triangular matrix with eigenvalues of $\mathbf{F}_{\mathbf{x}}$ 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 **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. $p(\rho, e, Y_{H_2O}), T(\rho, e, Y_{H_2O}), Y_H(\rho, e, Y_{H_2O}), \dots$
- Linear interpolation used for points not in table,
- Captures ~ 0.1 μs reaction events.



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.

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 convectiondiffusion time stepping, explicit (ILDM)/implicit (non-ILDM) reaction time stepping
- Viscous shocks, inductions zones, and entropy layers spatially resolved!



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

- $t = 195 \ \mu s$
- ILDM gives nearly identical results as full chemistry



Viscous $H_2 - O_2$ Ignition Delay with Wavelets Global and Fine Scale Structures

- $t = 230 \ \mu s$, Induction zone length: ~ 470 μm , Viscous shock thickness: ~ 50 μm (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.



Post Reflection Entropy Layer?: Viscous Wavelet Results

- No significant entropy layer evident on macroscale after shock reflection when resolved viscous terms considered,
- Inviscid codes with coarse gridding introduce a larger entropy layer due to numerical diffusion,
- Unless suppressed, unphysically accelerates reaction rate.



Post Reflection Entropy Layer: Viscous Wavelet Results

- small entropy layer evident on finer scale,
- temperature rise ~ 5 K; dissipates quickly,
- inviscid calculations before adjustment give persistent temperature rise of $\sim 20 \ K$; reaction acceleration small.



Center manifold-motivated correction for small convection-diffusion

• Consider system of Davis and Skodje, 1999, extended for diffusion

$$\frac{\partial y_1}{\partial t} = \underbrace{-y_1}_{\text{reaction}} + \underbrace{\epsilon \frac{\partial^2 y_1}{\partial x^2}}_{\text{diffusion}}, \\
\frac{\partial y_2}{\partial t} = \underbrace{-\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1 + y_1)^2}}_{\text{reaction}} + \underbrace{\epsilon \frac{\partial^2 y_2}{\partial x^2}}_{\text{diffusion}},$$

$$y_1(x,0) = x,$$
 $y_1(0,t) = 0,$ $y_1(1,t) = 1,$
 $y_2(x,0) = 0.55x$ $y_2(0,t) = 0,$ $y_2(1,t) = 0.55.$

- $\gamma >> 1$ for chemical stiffness; $\epsilon << 1$ for small diffusion
- Maas-Pope ILDM:

$$y_2 = \frac{y_1}{1+y_1} + \frac{2y_1^2}{\gamma(\gamma-1)(1+y_1)^3}.$$

- Purely reactive system has equilibrium point in phase space at $y_1 = 0, y_2 = 0$ at $t \to \infty$.
- System with convection-diffusion approaches steady state manifold, not ILDM, as $t \to \infty$ given by solution of ODEs:

$$0 = -y_1 + \epsilon \frac{d^2 y_1}{dx^2}; \quad y_1(0) = 0; \quad y_1(1) = 1,$$

$$0 = -\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1 + y_1)^2} + \epsilon \frac{d^2 y_2}{dx^2}; \quad y_2(0) = 0; \quad y_2(1) = 0.55.$$

Center manifold-motivated correction for small convection-diffusion

- Assume convection-diffusion acts as a small perturbation
- Define fast (w_f) and slow (w_s) variables based on analytic Jacobian of chemical source term:

$$\begin{pmatrix} w_s(x,t) \\ w_f(x,t) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\alpha(y_{10}(x)) & 1 \end{pmatrix} \cdot \begin{pmatrix} y_1(x,t) - y_{10}(x) \\ y_2(x,t) - h(y_{10}(x)) \end{pmatrix}$$

- $y_{10}(x)$ is solution for $y_1(x)$ at previous time step,
- $h(y_{10}(x))$ is the ILDM.
- Project original PDEs onto the slow and fast basis near ILDM to get

$$\frac{\partial w_s}{\partial t} = -y_{10}(x) - w_s + \underbrace{\epsilon \left(\frac{d^2 y_{10}}{dx^2} + \frac{\partial^2 w_s}{\partial x^2} \right)}_{\text{convection-diffusion correction}} + H.O.T.,$$

$$\frac{\partial w_f}{\partial t} = \underbrace{\text{Maas-Pope ILDM term}}_{=0} - \gamma w_f + \underbrace{\epsilon \left(g_1(y_{10}(x)) + w_s g_2(y_{10}(x)) + \frac{\partial w_s}{\partial x} g_3(y_{10}(x)) + \frac{\partial^2 w_f}{\partial x^2} \right)}_{\text{convection-diffusion correction}} + H.O.T.$$

Center manifold-motivated correction for small convection-diffusion

• equilibrate fast variables: $\frac{\partial w_f}{\partial t} = 0$, giving an elliptic equation

$$0 = -\gamma w_f + \underbrace{\epsilon \left(g_1(y_{10}(x)) + w_s g_2(y_{10}(x)) + \frac{\partial w_s}{\partial x} g_3(y_{10}(x)) + \frac{\partial^2 w_f}{\partial x^2}\right)}_{\text{convection-diffusion correction}} + H.O.T.$$

- Use method of lines, combined with simultaneous solution of elliptic equation, to advance slow variables using large time step,
- Analogous to solving elliptic equation for pressure when time advancing incompressible Navier-Stokes equations.

Center Manifold-Motivated Correction for Convection-Diffusion

- Long time solution does not approach Maas and Pope ILDM,
- Convection-diffusion correction gives more accurate predictions



- $H_2/O_2/Ar$ ILDM results accurate because restricted to near equilibrium regions
- arbitrary use of ILDM can give inaccurate results

Center Manifold-Motivated Correction for Convection-Diffusion

• The corrected method gives more accurate predictions of intermediate and long times.



Conclusions

- The WAMR method gives dramatic spatial resolution in viscous one-dimensional H_2/O_2 detonations with detailed kinetics; viscous shocks, entropy layers, and induction zones are resolved,
- 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,
- Work needed to better account for projection of initial conditions onto ILDM,
- Center manifold-motivated correction for convection and diffusion a promising improvement to ILDM method in some (not all) problems.