ANALYSIS of BIFURCATIONS in LOW-DIMENSIONAL MODELS of TURBULENT COMBUSTION

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**BACKGROUND**

- Low-Dimensional Models (LDMs) Widely Studied
  - Numerous methods for construction
  - Many different kinds of models

- Especially Appropriate for Use with LES
  - Resources needed for LES generally greater than required for RANS—but there is potential for far better results
  - Details likely to be missing in reduced models usually not resolved with LES

- Suggests Detailed Understanding of LDMs Could Be Helpful

- Because LDMs Represent Generally Nonlinear Phenomena, Can Be Expected to Exhibit Bifurcations of Behavior
**BACKGROUND (Cont.)**

- Bifurcations Widely Observed in Combustion Phenomena
  - Implies if particular LDM incapable displaying physical bifurcation sequences, it may be inappropriate
  - Use should be restricted to parameter ranges in which bifurcations do not occur

- Goals of Present Study
  - Briefly present new form of LES expected to be especially appropriate for use with LDMs
  - Outline derivation of subgrid-scale (SGS) equations corresponding to selected LDM
  - Demonstrate form of analysis that identifies bifurcation sequences
**ALTERNATIVE LES/LDM APPROACH**

- **Filter Solutions**—not equations
  - Mathematically equivalent to *mollification*
  - Provides *dissipation* needed to prevent aliasing of under-resolved solutions
  - Leads to *simpler SGS models*

- **Model Physical Variables**—not their statistics
  - Results in SGS models able to produce *DNS-like fluctuations*—but, clearly not at DNS spatial resolutions
  - Yields ability to model *SGS interactions of turbulence with other physics* (combustion in the present case)

- **Directly Use SGS Results**—don’t discard them
  - Corresponds (mathematically) to *multi-level formalism*
  - Hence, provides *rigorous foundation*, and availability of analysis tools
GOVERNING EQUATIONS

- **Usual Balance Equations**

\[ \rho_t + \nabla \cdot (\rho \mathbf{U}) = 0 \]

\[ \rho \frac{D \mathbf{U}}{Dt} = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{U}) + \rho \mathbf{g} \]

\[ \rho c_p \frac{D T}{Dt} = \nabla \cdot (\lambda \nabla T) + \sum_{i=1}^{N_s} c_{p,i} D_i W_i \nabla \left( \frac{\rho Y_i}{W_i} \right) \cdot \nabla T - \sum_{i=1}^{N_s} h_i \dot{w}_i \]

\[ \frac{D(\rho Y_i)}{Dt} = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{w}_i \quad i = 1, ..., N_s \]

with

\[ \dot{w}_i = W_i \sum_{j=1}^{N_r} (v_{i,j}'' - v_{i,j}') w_j \quad \text{and} \quad w_j = k_{f,j} \prod_{\ell=1}^{N_s} \left( \frac{\rho Y_{\ell}}{W_{\ell}} \right)^{v_{\ell,j}} - k_{b,j} \prod_{\ell=1}^{N_s} \left( \frac{\rho Y_{\ell}}{W_{\ell}} \right)^{v_{\ell,j}''} \]
SGS Models (temporal fluctuating part, only)

*Usual LES decomposition* of dependent variables

\[ q_i (x,t) = \tilde{q}_i (x,t) + q_i^*(x,t) \]

for \( i^{th} \) dependent variable

Assume *Fourier representation* of each dependent variable:

\[ q_i (x,t) = \sum_k a_{i,k} (t) \varphi_k (x) \]

Construct *Galerkin ODEs*

Decimate result to *single (relatively-high) wavevector* per equation—within part of series corresponding to \( q^* \)

Apply *simple numerical integration methods* (and some transformations) to obtain multi-dimensional discrete dynamical system (DDS)
THE DISCRETE DYNAMICAL SYSTEM


\[ a^{(n+1)} = \beta_u a^{(n)} (1-a^{(n)}) - \gamma_u a^{(n)} b^{(n)} \]

\[ b^{(n+1)} = \beta_v b^{(n)} (1-b^{(n)}) - \gamma_v a^{(n)} b^{(n)} + \alpha_T c^{(n)} \]

\[ c^{(n+1)} = \left[ \left( \sum_{i=1}^{N_s} \alpha_{T_d} d_i^{(n+1)} - \gamma_{u_Y} a^{(n+1)} - \gamma_{v_Y} b^{(n+1)} \right) c^{(n)} - \sum_{i=1}^{N_s} H_i \dot{\omega}_i \right] / (1+\beta_T) + c_0 \]

\[ d_i^{(n+1)} = -\left( \beta_{Y_i} + \gamma_{u_Y} a^{(n+1)} + \gamma_{v_Y} b^{(n+1)} \right) d_i^{(n)} + \dot{\omega}_i + d_{i,0}, \quad i = 1,2,...,N_s \]

\[ \dot{\omega}_i = \sum_{j=1}^{N_r} \left[ C_{f,ij} \prod_{\ell=1}^{N_s} d_{\ell}^{v_{j,\ell}} - C_{b,ij} \prod_{\ell=1}^{N_s} d_{\ell}^{v_{j,\ell}} \right] \]

- Produce temporal fluctuations for SGS model
- DDS very general—can be applied to any reaction mechanism—simplifies significantly for elementary reactions
- Contain numerous bifurcation parameters—all related to physics
General Features of LDM Based on DDSs
- DDS used for each product species of each elementary reaction
- Number of iterations of each DDS proportional to Kolmogorov-scale Damköhler number, $Da_K$
- Automatically provides subcycling during velocity time steps

Nine-Step Mechanism for $H_2$–$O_2$ Combustion
- At least one step each for initiation, propagation, chain branching, recombination
- Ordered such that species do not appear as reactants earlier than they have been produced
- Make following identifications

\[
\begin{align*}
  d_1 &\sim H_2 \\
  d_2 &\sim O_2 \\
  d_3 &\sim H_2O \\
  d_4 &\sim OH \\
  d_5 &\sim HO_2 \\
  d_6 &\sim H \\
  d_7 &\sim O \\
  d_8 &\sim N_2 \\
\end{align*}
\]
LDM (Cont.)

Example Equations

- Consider initiation step: contains two products: HO₂ and H, corresponding to \(d_7\) and \(d_5\), respectively

Results in following contributions to DDS

\[
d_7^{(n+1)} = -(\beta_{Y_7} + \gamma_{uY_7} + \gamma_{vY_7})d_7^{(n)} + \dot{w}_7 + d_{7,0}
\]

with

\[
\dot{w}_7 = C_{f,7,1} d_1 d_2
\]

and

\[
C_{f,7,1} = v''' \frac{W_7}{W_1 W_2} k_{f,1}
\]

- Similar equations hold for all species

- Computed results compared with experiments of Meier et al. (case H3) in figure at right
Recent Detailed Studies of Specific Reduced Mechanisms Further Illuminate Model Behaviors

For example, bifurcation diagrams display sequences of transitions accessible to model

- **part (a): temperature regimes**
  as functions of velocity strain rates

- **part (b): H₂O concentration**
  vs. velocity strain rate and Re

- **part (c): H₂O concentration**
  behaviors as function of H₂O concentration gradient

- table shows nominal values of bifurcation parameters not being varied
SOME STATISTICAL PROPERTIES OF MODEL

- Two Important Statistical Quantities: scalar dissipation and skewness of scalar derivatives:

\[ \chi = \left\langle D(\nabla \xi)^2 \right\rangle \]

\[ s = \frac{\left\langle (\partial T/\partial y)^3 \right\rangle}{\left\langle (\partial T/\partial y)^2 \right\rangle^{3/2}} \]

- \( \xi \) is elemental hydrogen mixture fraction:

\[ \xi = \frac{Y_H - Y_{H,o}}{Y_{H,f} - Y_{H,o}} \]

- Spatial derivatives obtained from time series using Taylor’s “frozen-flow” hypothesis

- Model Results Well Within Range of Expected Experimental Values for These Statistical Properties
SUMMARY/CONCLUSIONS

- Alternative Approach to Construction of LES/LDM Briefly Described
- Outline for Deriving DDS Providing Temporal Fluctuations on Sub-Grid Scales Presented
- Specific Example of LDM Based on DDS Corresponding to 9-Step H₂–O₂ Reduced Mechanism Analyzed Via Bifurcation Diagrams
- Results Display Many Different Bifurcation Sequences and Wide Range of Possible Bifurcation Parameters
- Statistics of Results Generated with DDS Consistent with Physical Observations
- Suggests Potential Use of DDS Form of LDM for SGS Models in LES of Turbulent Combustion, and Possibly in Real-Time Control Applications