Detailed and reduced modeling of reacting fluid mechanics

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Environmental Fluid Dynamics Seminar Series

University of Notre Dame

21 April 2015

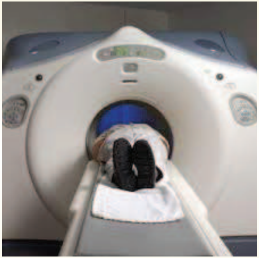
UNIVERSITY OF NOTRE DAME

Outline

1. Some semantics and some provocation
2. Some overly brief detonation discourse
3. A tangential discussion from astronomy's history
4. Back to the high Mach number future
5. Some modern high resolution (DNS) detonation calculations
6. Some DNS conclusions
7. Treatment: manifold reduction methods?
8. Broader conclusions

Some semantics: diagnosis or treatment?

- Engineers often both diagnose and treat problems.
- There are challenges in both!
- I will argue that many problems in reacting fluids are sufficiently complex that detailed diagnosis is a worthy problem.
- Detailed treatment will need more work!

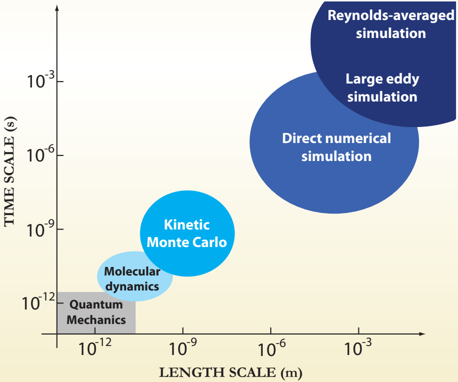


Diagnosis: MRI machine

Treatment: artificial hip

Some semantics....

- *Verification*: solving the equations right
- *Validation*: solving the right equations
- *Direct Numerical Simulation (DNS)*: a verified and validated computation that resolves *all* ranges of relevant continuum physical scales present

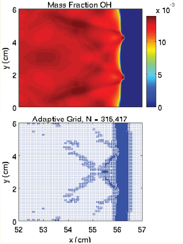


"Research needs for future internal combustion engines," *Physics Today*, Nov. 2008, pp. 47-52.

Some provocation....

- *Hypothesis*: DNS of fundamental detonation flow fields (thus, detailed kinetics, viscous shocks, multi-component diffusion, etc. are represented, verified, and validated) is on a trajectory toward realization via advances in
  - adaptive refinement algorithms, and
  - massively parallel architectures.
- *Corollary I*: A variety of modeling compromises, e.g.
  - shock-capturing (FCT, PPM, ENO, WENO, etc.),
  - implicit chemistry with operator splitting,
  - turbulence modeling (RANS, $k - \epsilon$, LES, etc.), or
  - reduced/simplified kinetics, flamelet models,

  could enjoy a graceful retirement *when and if* this difficult goal of DNS is realized.
- *Corollary II*: Macro-device-level DNS remains in the distant future; micro-device-level DNS is feasible.



C. E. Yeager, 1923-

Consultation with an expert

ELSEVIER
Available online at www.sciencedirect.com
ScienceDirect
Proceedings of the Combustion Institute 32 (2009) 83–98
Proceedings of the Combustion Institute
www.elsevier.com/locate/proci

Detonation in gases

J.E. Shepherd *

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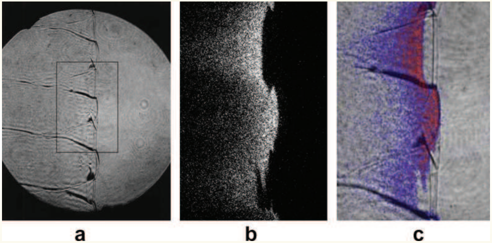
- Shepherd's 2009 review article identifies the key issue in verification and validation.

3. Simulating detonation fronts

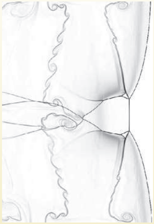
Examining Fig. 1a, we note that the characteristic propagation distance in typical laboratory experiments is 1–10 m, while the reaction zone shown in Fig. 1c and d exhibits significant spatial gradients on the order of 1–10 μm. Despite the widespread availability of software for adaptive mesh refinement, this range of 10^7 in length scales obviously poses a significant issue (see the discussions in [83,97–100]) for accurate direct numerical simulation of the reactive, viscous flow with detailed chemical reaction kinetics. Other considerations include the storage requirements for detailed chemical reaction mechanisms with 50–500 individual species needed for typical hydrocarbon fuels [101], the three-dimensional nature of the coherent structures and turbulent flow in the reaction zone, and the challenge of carrying out high-order simulations needed for turbulence modeling and simultaneously capturing shock waves [102].

Evidence of complexity in detonations



images from Shepherd, 2009;

$2H_2 + O_2 + 12Ar$ at 20 kPa
adopted from Austin, 2003.



Euler simulation of five-step model of hydrogen combustion, adopted from Liang, et al. 2007

- Because detonation physics is multiscale, both experimental and numerical characterization is challenging.

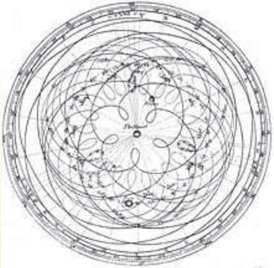
Midcourse diversion

- There's a lot of discussion about detonation theory (e.g. SWACER, turbulent flame brushes, explosions within explosions, etc.) that is difficult to verify and validate via computation today.
- Let's take a brief historical diversion to a see how some sister sciences, e.g. star-gazing, succeeded...

Supernova SN 2014J in the Meissier 82 galaxy from Chandra X-Ray Observatory, observed 21 January 2014

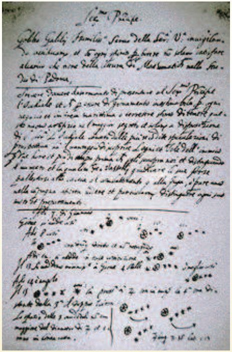
Appeal to an ancient

Ptolemy (90-168 AD)



- Science develops theory to predict behavior of nature, e.g. Ptolemy's epicylces to predict the motion of the planets.
- Theory of epicycles needs no verification; for many planetary motions, it is fully validated.

Renaissance revision



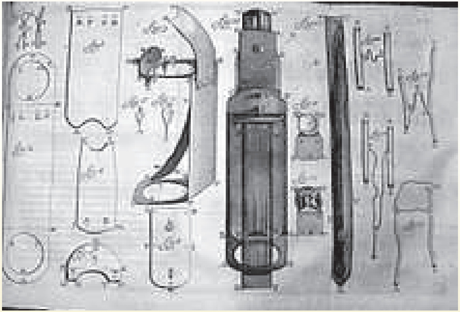
- Galileo, et al. invalidate the Ptolemaic theory with new data

Galileo Galilei (1564-1642)

Multiscale instrumentation

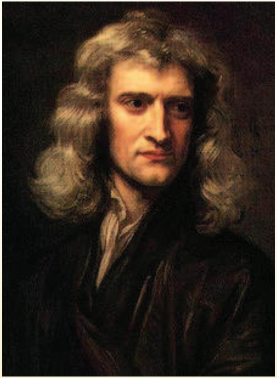
Telescope

Microscope



- Improvements of telescopes (Galileo, 1609) and microscopes (van Leeuwnehoek, 1670s) induced revolutions in astronomy and biology by use of optical instruments which clearly revealed more scales, large and small, in our *multiscale universe*.

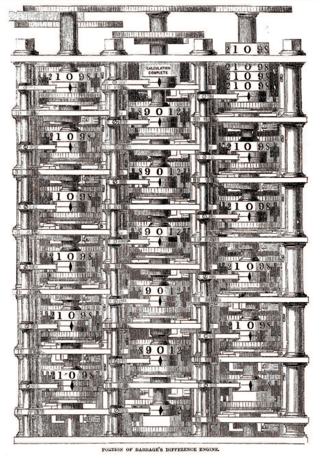
Enlightenment mathematization



Sir Isaac Newton (1643-1727)

- Newton's calculus gave an efficient mathematical tool to encapsulate predictive theories for the motion of heavenly bodies and better enable their validation.
- $$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$
- Since Newton insisted $\Delta x \to 0$, the theory is verified, *a priori*.
- Finite $\Delta x > 0$ introduces the need for verification!

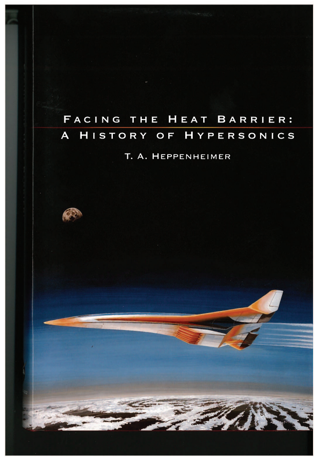
Victorian mechanization

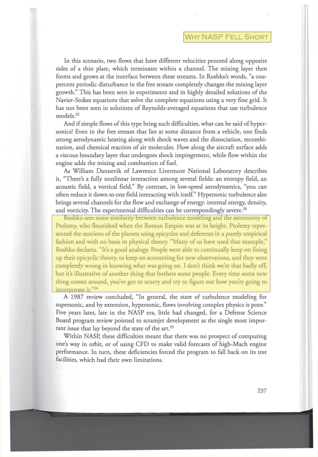


Schematic of difference engine of Babbage (1791-1871)

- The need to solve discrete approximate versions of continuous equations with no analytic solution motivated computing machinery.
- The discrete approximate nature of the solution introduces the new need for verification of the solution to see if it has essential fidelity with its mathematical analog.

Fast forward to a 2007 retrospective of the 1980s





In this scenario, two flows that have different velocities proceed along opposite sides of a thin plate, which terminates within a channel. The mixing layer then forms and grows at the interface between these streams. In Roshko's words, "a one-percent periodic disturbance in the free stream completely changes the mixing layer growth." This has been seen in experiments and in highly detailed solutions of the Navier-Stokes equations that solve the complete equations using a very fine grid. It has not been seen in solutions of Reynolds-averaged equations that use turbulence models.[22]

And if simple flows of this type bring such difficulties, what can be said of hypersonics? Even in the free stream that lies at some distance from a vehicle, one finds strong aerodynamic heating along with shock waves and the dissociation, recombination, and chemical reaction of air molecules. Flow along the aircraft surface adds a viscous boundary layer that undergoes shock impingement, while flow within the engine adds the mixing and combustion of fuel.

As William Dannevik of Lawrence Livermore National Laboratory describes it, "There's a fully nonlinear interaction among several fields: an entropy field, an acoustic field, a vortical field." By contrast, in low-speed aerodynamics, "you can often reduce it down to one field interacting with itself." Hypersonic turbulence also brings several channels for the flow and exchange of energy: internal energy, density, and vorticity. The experimental difficulties can be correspondingly severe.[23]

Roshko sees some similarity between turbulence modeling and the astronomy of Ptolemy, who flourished when the Roman Empire was at its height. Ptolemy represented the motions of the planets using epicycles and deferents in a purely empirical fashion and with no basis in physical theory. "Many of us have used that example," Roshko declares. "It's a good analogy. People were able to continually keep on fixing up their epicyclic theory, to keep on accounting for new observations, and they were completely wrong in knowing what was going on. I don't think we're that badly off, but it's illustrative of another thing that bothers some people. Every time some new thing comes around, you've got to scurry and try to figure out how you're going to incorporate it."[24]

A 1987 review concluded, "In general, the state of turbulence modeling for supersonic, and by extension, hypersonic, flows involving complex physics is poor." Five years later, late in the NASP era, little had changed, for a Defense Science Board program review pointed to scramjet development as the single most important issue that lay beyond the state of the art.[25]

Within NASP, these difficulties meant that there was no prospect of computing one's way in orbit, or of using CFD to make valid forecasts of high-Mach engine performance. In turn, these deficiencies forced the program to fall back on its test facilities, which had their own limitations.

Quotations from NASA's commissioned history:

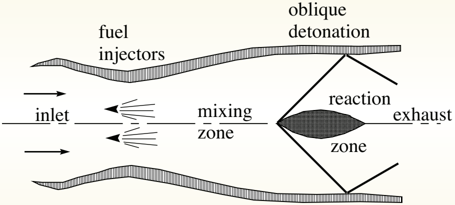
- *Still NASP fell short, and there were reasons. CFD proved not to be an exact science, particularly at high Mach.*
- *Roshko sees some similarity between turbulence modeling and the astronomy of Ptolemy, who flourished when the Roman Empire was at its height. Ptolemy represented the motions of the planets using epicycles and deferents in a purely empirical fashion and with no basis in physical theory. "Many of us have used that example," Roshko declares. "lt's a good analogy. People were able to continually keep on fixing up their epicyclic theory; to keep on accounting for new observations, and they were completely wrong in knowing what was going on. I don't think we're that badly off, but it's illustrative of another thing that bothers some people. Every time some new thing comes around, you've got to scurry and try to figure out how you're going to incorporate it."*

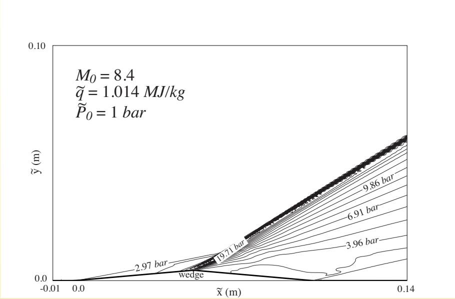
T. A. Heppenheimer, 2007, *Facing the Heat Barrier: A History of Hypersonics*, NASA SP-2007-4232, Washington DC.

Modern hardware: a computational "telescope/microscope" to circumvent the high Mach CFD problem?

- Today's Peta- and tomorrow's Exa-scale hardware enables heroic calculations,
- Tianhe-2, world's fastest computer, 33.86 PFLOP/s

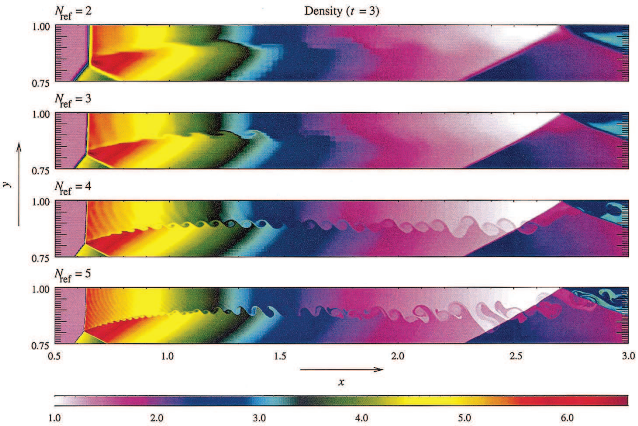
Some early inviscid detonation propulsion calculations





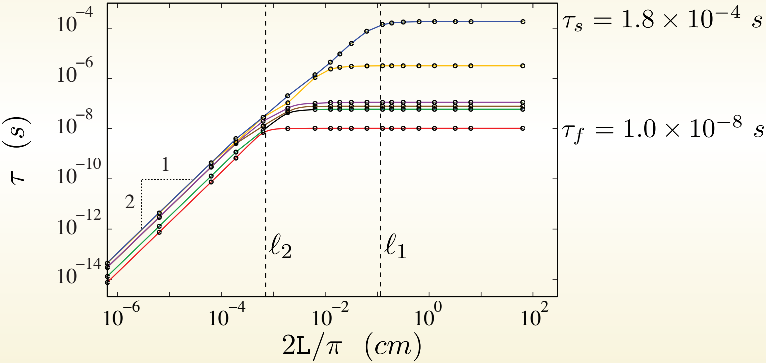
- Detonation wave engine design relies on predictive calculation
- Grisner and Powers, *Journal of Propulsion and Power*, 1995

Inviscid predictions do not converge!



- Fryxell, et al., 2000, *The Astrophysical Journal, Supplement Series*
- Multi-dimensional calculations of inviscid compressible flows are in general, *unverifiable* because of lack of a cutoff viscous length scale.

Calculation verifies fine reaction-diffusion length scales.



- H_2-air with detailed kinetics and multi-component diffusion
- $\ell_1 = \sqrt{D_{mix}\tau_s} = 1.1 \times 10^{-1}$ cm,
- $\ell_2 = \sqrt{D_{mix}\tau_f} = 8.0 \times 10^{-4}$ cm.
- see Al-Khateeb, Powers, & Paolucci, *Combustion Theory & Modeling*, 2013.

Scale necessary for verified calculation

- The simple length scale analysis dictates that $\Delta x < 8.0 \times 10^{-4}$ cm for a verified calculation for detailed kinetics simulations of $P = 1$ atm hydrogen-air combustion.
- This scale is consistent with Shepherd's 2009 discussion.
- This scale is equivalent to a few mean free paths.
- High order methods applied to under-resolved problems will not be verified, and may miss important dynamics.
- In other words, in a so-called $h - p$ refinement, one must *first and foremost* refine the grid (decrease h), and perhaps polish predictions via a refinement of order (increase p).

Compressible reactive Navier-Stokes model

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,$$
$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p\mathbf{I} - \boldsymbol{\tau}) = \mathbf{0},$$
$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{\mathbf{u}\cdot\mathbf{u}}{2}\right)\right) + \nabla \cdot \left(\rho \mathbf{u}\left(e + \frac{\mathbf{u}\cdot\mathbf{u}}{2}\right) + (p\mathbf{I} - \boldsymbol{\tau})\cdot \mathbf{u} + \mathbf{q}\right) = 0,$$
$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i + \mathbf{j}_i) = \overline{M_i}\dot{\omega}_i,$$

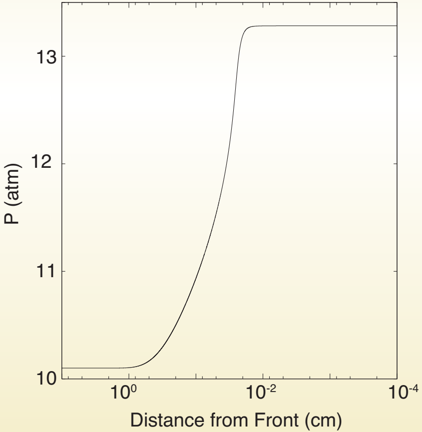
$$p = \mathcal{R}T \sum_{i=1}^{N} \frac{Y_i}{\overline{M_i}}, \qquad e = e\left(T, Y_i\right), \qquad \dot{\omega}_i = \dot{\omega}_i\left(T, Y_i\right),$$

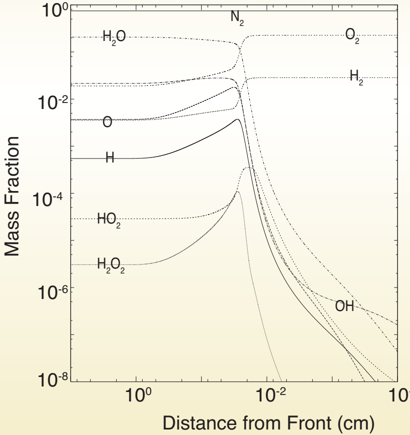
$$\mathbf{j}_i = \rho \sum_{\substack{k=1\\k\neq i}}^{N} \frac{\overline{M_i} D_{ik} Y_k}{\overline{M}} \left(\frac{\nabla y_k}{y_k} + \left(1 - \frac{\overline{M_k}}{\overline{M}}\right)\frac{\nabla p}{p}\right) - \frac{D_i^T \nabla T}{T},$$

$$\boldsymbol{\tau} = \mu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3}(\nabla \cdot \mathbf{u})\,\mathbf{I}\right),$$

$$\mathbf{q} = -k\nabla T + \sum_{i=1}^{N} \mathbf{j}_i h_i - \mathcal{R}T \sum_{i=1}^{N} \frac{D_i^T}{\overline{M_i}} \left(\frac{\nabla \overline{y}_i}{\overline{y}_i} + \left(1 - \frac{\overline{M_i}}{\overline{M}}\right)\frac{\nabla p}{p}\right).$$

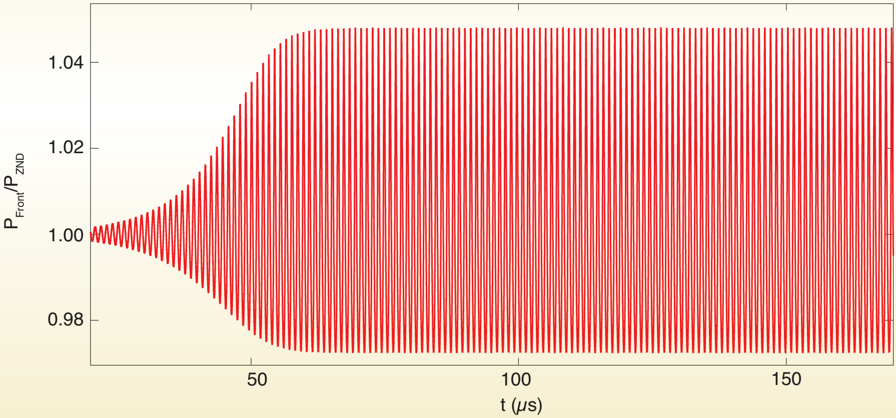
Steady wave profile for H_2-air detonation





See Powers and Paolucci, *AIAA Journal*, 2005.

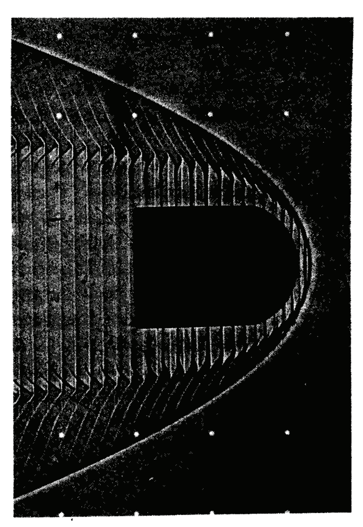
Such waves may be unstable



Predicted oscillation at 0.97 MHz.

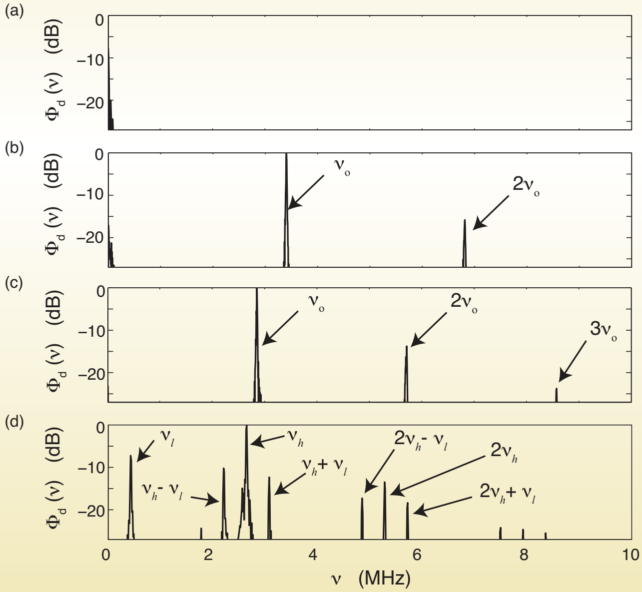
See Romick, Aslam, and Powers, *Journal of Fluid Mechanics*, 2015.

Prediction validated by experiment



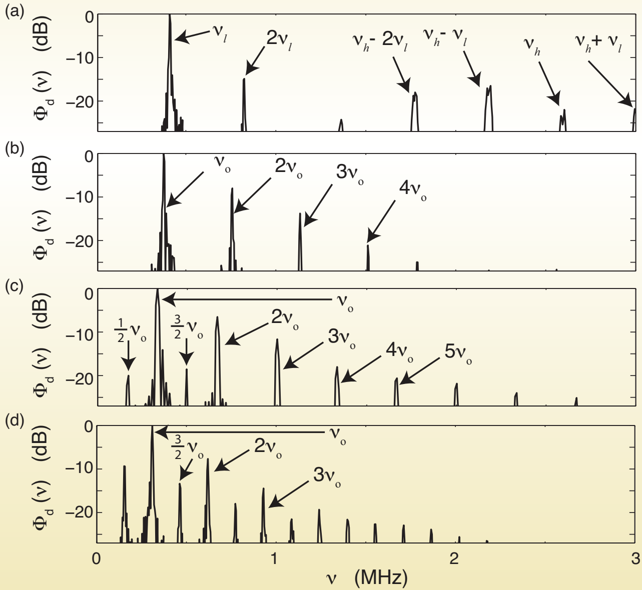
- Shock-induced combustion experiment (Lehr, *Astro. Acta*, 1972)
- Stoichiometric mixture of $2\mathsf{H}_2 + \mathsf{O}_2 + 3.76\mathsf{N}_2$ at 0.421 atm
- Observed frequency: 1.04 MHz
- Predicted frequency: 0.97 MHz

Galileo's telescope: FFT of unstable H_2-air detonation

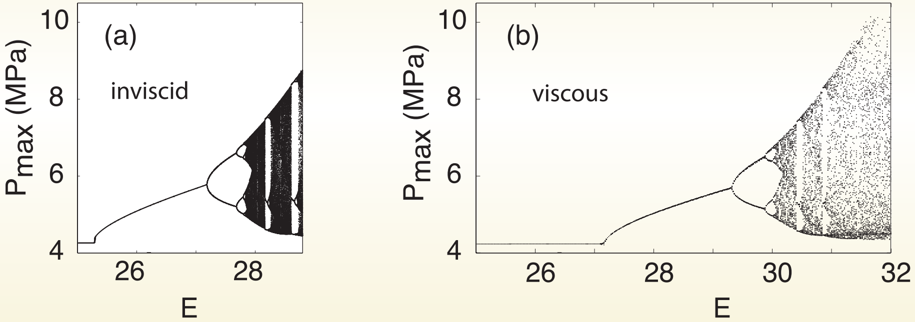


- The "music" of detonation is revealed.
- As over-drive is reduced, complexity increases.
- High over-drive: simple harmonics
- Low over-drive: sideband instabilities.

FFT of unstable H_2-air detonation



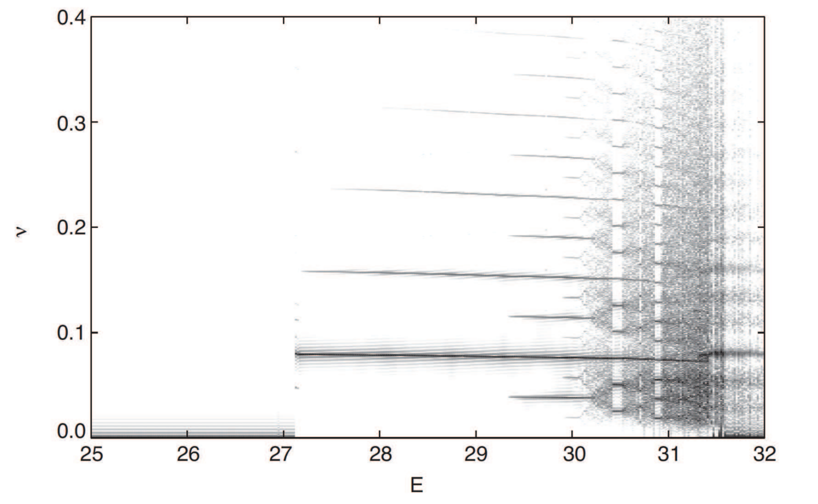
- Further reduction of over-drive concentrates energy in low frequency modes.
- Potentially more observable.



A route to chaos exists with a predicted Feigenbaum constant of 4.66, remarkably close to the known value of 4.669201...

Henrick, Aslam, Powers, *Journal of Computational Physics*, 2006,
Romick, Aslam, Powers, *Journal of Fluid Mechanics*, 2012.

Even simple kinetics yields a complicated diagnosis!



Some DNS conclusions

- Verified and validated detonation calculations for realistic reacting gas mixtures with detailed kinetics and multicomponent transport are possible.
- True validation of detonation flows against detailed unsteady calculations awaits three-dimensional extensions.
- Realization of verified and validated DNS calculation of detonation would remove the need for common, but problematic, modeling assumptions (shock-capturing, turbulence modeling, implicit chemistry with operator splitting, reduced kinetics).
- Such 3D V&V could be viable in an exascale environment; however, routine desktop DNS detonation calculations remain difficult to envision at macro-device scales.

Diagnosis and treatment

- Diagnosis: Reacting fluid mechanics is indeed fraught with multiscale complexities which require expensive (or presently impossible) DNS to fully expose.
- Treatment: Simplified models, based on rational reduction via so-called *manifold methods* could be sought which segregate the "signal" from the "noise."

Our goal is to use *rational reduction* that can be algorithmically achieved *a priori* and retain maximum fidelity to the more expensive DNS.

Treatment: manifold methods?

Advection, reaction, and diffusion are modeled by

$$\frac{\partial \mathbf{z}}{\partial t} = \underbrace{\mathbf{f}(\mathbf{z})}_{\text{reaction}} + \underbrace{\nabla \cdot (\mathbf{g}(\mathbf{z}) + \mathbf{h}(\mathbf{z}))}_{\text{advection/diffusion}}$$

Sufficiently fine spatial discretization or Galerkin projection yields ODEs:

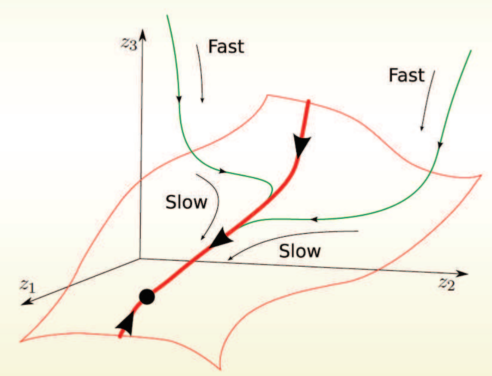
$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}) + \mathbf{G}(\mathbf{z}) + \mathbf{H}(\mathbf{z})$$

Lorenz and Temam's approach was to model these by low order systems whose dynamics is confined to a *low-dimensional manifold*. Their program fails when the spectral gap is not sufficiently large.

Some motivating questions...

Slow Attracting Canonial Invariant Manifold (SACIM)

- Just what is a SACIM?
- Does it exist?
- Is it easy to identify?
- Does it work?



See Powers, et al., *Journal of Chemical Physics*, 2009;
SIAM J. Appl. Dynamical Systems, 2013;
Journal of Mathematical Chemistry, 2015.

These are old questions....

VOL. 43, NO. 15 JOURNAL OF THE ATMOSPHERIC SCIENCES 1 AUGUST 1986

On the Existence of a Slow Manifold

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(Manuscript received and in final form 28 October 1985)

ABSTRACT

We identify the slow manifold of a primitive-equation system with the set of all solutions that are completely devoid of gravity-wave activity. We construct a five-variable model describing coupled Rossby waves and gravity waves. Successive-approximation schemes designed to determine the slow manifold fail to converge when applied to the model, although they sometimes appear to converge before finally diverging. A noniterative scheme which demands only that the fast variables be functions of the slow variables yields a "slowest invariant manifold," which, however, is not unequivocally slow. We question whether the complete absence of gravity waves can be logically defined, and we note that the existence or nonexistence of a slow manifold does not depend upon the convergence or nonconvergence of a power series or a succession of approximations.

(focused on the related topic of limit cycles)

on which understanding has varied with time....

2940 JOURNAL OF THE ATMOSPHERIC SCIENCES VOL. 44, NO. 20

On the Nonexistence of a Slow Manifold

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(Manuscript received 29 September 1986, in final form 13 April 1987)

ABSTRACT

We define the slow manifold S in the state space of a primitive-equation model as a hypothetical invariant manifold on which there is no gravity-wave activity, and on which unique velocity-potential and streamfunction fields correspond to each isobaric-height field. We introduce a five-variable forced damped model, and show that for this model the point H representing the Hadley circulation and the two orbits forming the unstable manifold of H must lie in S if S exists. We then show that in traveling along one of these orbits one eventually encounters gravity waves, whereupon it follows that S does not exist.

A measure G of gravity-wave activity is found to decrease very rapidly as the external forcing F decreases. An approximate formula is derived for G as a function of F.

We show that a particular nine-variable forced damped model with orography also fails to possess a slow manifold, and we speculate as to the existence of slow manifolds in larger and more realistic models.

and for which questions remain!

2450 JOURNAL OF THE ATMOSPHERIC SCIENCES VOL. 49, NO. 24

The Slow Manifold—What Is It?

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(Manuscript received 17 June 1991, in final form 17 March 1992)

ABSTRACT

Two studies that disagree as to whether a slow manifold is present in a particular low-order primitive equation model are compared. It is shown that the discrepancy occurs because of a difference of opinion as to what constitutes a slow manifold.

Taxonomy

- *Invariant Manifolds* (IMs) are sets of points which are invariant under the action of an underlying dynamic system.
- Any trajectory of a dynamic system is an IM.
- IMs may be locally or globally fast or slow, attracting or repelling.
- Slow or fast does not imply attracting or repelling and *vice versa*.
- We will evaluate the fast/slow and attracting/repelling nature of *Canonical Invariant Manifolds* (CIMs) constructed by connecting equilibria to determine *heteroclinic orbits* (Davis-Skodje, 1999).

Taxonomy, cont.

- It is relatively easy to construct CIMs by numerical integration.
- Many CIMs exist, but we are only interested in those that connect to physical equilibrium.
- It is desirable to identify those CIMs to which
  - dynamics are restricted to those which are *slow*, and
  - neighboring trajectories are rapidly *attracted*.

  We call such CIMs *Slow Attracting Canonical Invariant Manifolds* (SACIMs).
- A global SACIM may represent the *optimal reduction* potentially enabling dramatic computational accuracy and efficiency in multiscale problems.

Theoretical framework for spatially homogeneous combustion within a closed volume

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}), \qquad \mathbf{z}(0) = \mathbf{z}_o, \qquad \mathbf{z}, \mathbf{z}_o, \mathbf{f} \in \mathbb{R}^N.$$

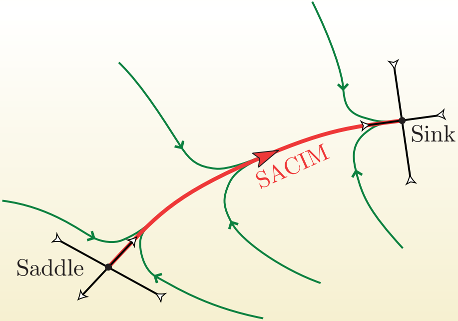
- $\mathbf{z}$ represents a set of N species concentrations, assuming all linear constraints have been removed.
- $\mathbf{f}(\mathbf{z})$ embodies the law of mass action and other thermochemistry.
- $\mathbf{f}(\mathbf{z}) = \mathbf{0}$ defines *multiple equilibria* within $\mathbb{R}^N$.
- $\mathbf{f}(\mathbf{z})$ is such that a *unique stable equilibrium* exists for physically realizable values of $\mathbf{z}$; the eigenvalues of the Jacobian

  $$\mathbf{J} = \frac{\partial \mathbf{f}}{\partial \mathbf{z}},$$

  are guaranteed real and negative at such an equilibrium (Powers & Paolucci, *American Journal of Physics*, 2008).

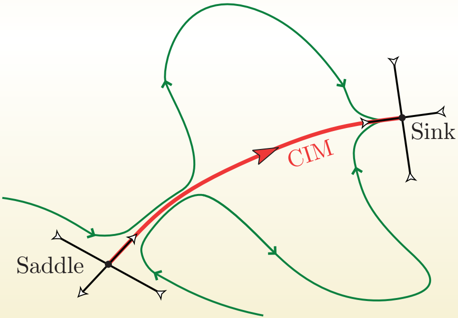
SACIM construction strategy: heteroclinic orbit connection

- Davis and Skodje suggested a CIM construction strategy.
- It employs numerical integration from a saddle to the sink.
- This guarantees a CIM.
- It *may* be a SACIM.

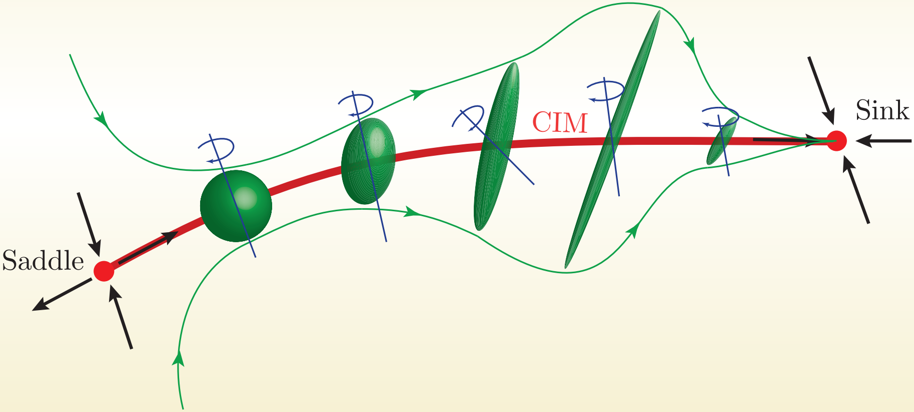


Failure of SACIM construction strategy

- It *may not* be a SACIM.
- The CIM will be attracting in the neighborhood of each equilibrium.
- The CIM need not be attractive away from either equilibrium.



Sketch of a volume locally traversing a nearby CIM



The local differential volume 1) translates, 2) stretches, and 3) rotates. Its magnitude can decrease as it travels, but elements can still be repelled from the CIM. All trajectories are ultimately attracted to the sink.

Local decomposition of "motion" in phase space

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}), \qquad \mathbf{z}(0) = \mathbf{z}_o, \qquad \mathbf{z}_o \in \text{CIM},$$

$$\frac{d}{dt}(\mathbf{z} - \mathbf{z}_o) = \underbrace{\mathbf{f}(\mathbf{z}_o)}_{\text{translation}} + \underbrace{\mathbf{J}_s\big|_{\mathbf{z}_o} \cdot (\mathbf{z} - \mathbf{z}_o)}_{\text{stretch}} + \underbrace{\mathbf{J}_a\big|_{\mathbf{z}_o} \cdot (\mathbf{z} - \mathbf{z}_o)}_{\text{rotation}} + \ldots.$$

Here, we have

$$\mathbf{J} = \frac{\partial \mathbf{f}}{\partial \mathbf{z}} = \mathbf{J}_s + \mathbf{J}_a,$$

$$\mathbf{J}_s = \frac{\mathbf{J} + \mathbf{J}^T}{2}, \quad \mathbf{J}_a = \frac{\mathbf{J} - \mathbf{J}^T}{2}.$$

The symmetry of $\mathbf{J}_s$ allows definition of a real orthonormal basis.

In 3d, the rotation vector $\boldsymbol{\omega}$ of the anti-symmetric $\mathbf{J}_a$ defines the axis of rotation; can be extended for higher dimensions.

Eigenvalue analysis, not shown, gives normal and tangential stretching rates for attraction/repulsion from CIM.

Example

- Model equations:

$$\begin{aligned}
\frac{dz_1}{dt} &= \frac{1}{20}(1 - z_1^2), \\
\frac{dz_2}{dt} &= -2z_2 - \frac{35}{16}z_3 + 2(1 - z_1^2)z_3, \\
\frac{dz_3}{dt} &= z_2 + z_3.
\end{aligned}$$

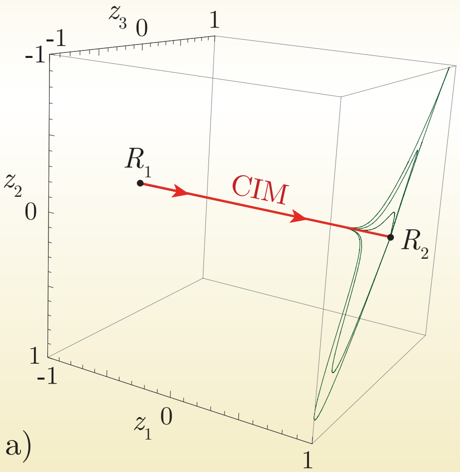
- Jacobian:

$$\mathbf{J} = \begin{pmatrix} -\frac{z_1}{10} & 0 & 0 \\ -4z_1 z_3 & -2 & -\frac{35}{16} + 2(1 - z_1^2) \\ 0 & 1 & 1 \end{pmatrix}.$$

- Two finite equilibria:
  - "non-physical" saddle at $R_1 : (z_1, z_2, z_3)^T = (-1, 0, 0)^T$, and a
  - "physical" sink at $R_2 : (z_1, z_2, z_3)^T = (1, 0, 0)^T$.

Example, cont.: CIM may not be a SACIM!

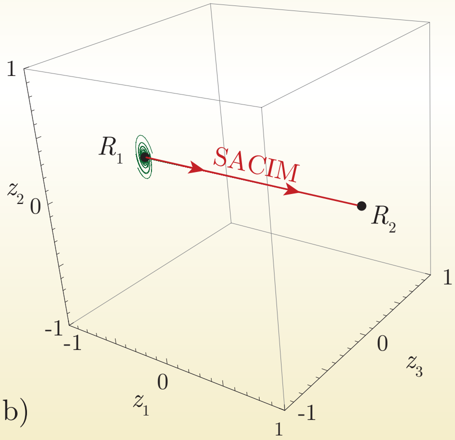
- There are regions of the CIM which do not attract nearby trajectories in the region far from equilibrium.
- This reflects the local influence of a positive normal stretching rate whose influence is realized due to modest local rotation.
- Projection onto the CIM in regions away from equilibrium would thus induce significant error in the prediction of certain state variables.



a)

Example, cont.: CIM may be a SACIM!

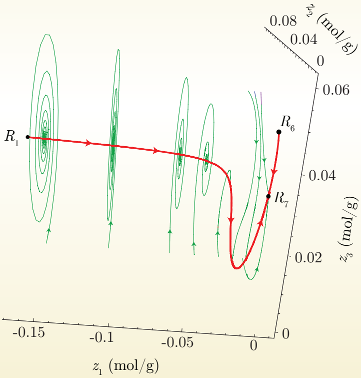
- A moderate change in **f** so as to increase the rotation rate renders the CIM to be a SACIM.
- Projection onto the CIM in regions away from equilibrium is a useful filter here.
- Analogs to "non-normality" in hydrodynamic stability and numerical methods considered by Trefathan (on campus this week).



Implications for combustion systems

- The example shares important features with combustion systems:
  - unique stable physical equilibrium, and
  - non-physical saddle equilibrium.
- The example may not share other important features with combustion systems:
  - no obvious imposed constraints from conserved variables, and
  - no clear entropy scalar guaranteed to be increasing on any physical path to equilibrium.

A limited result for H_2-air kinetics



SACIM obtained for isothermal, isochoric combustion of H_2-air. Local rotation overcomes any positive normal stretching.

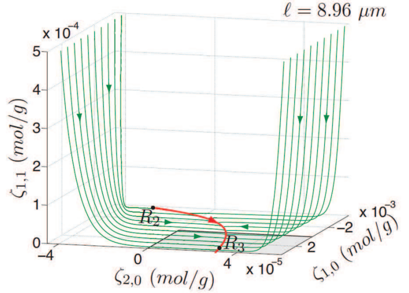
But, SACIM diagnosis for reaction systems is hard!

Reaction-diffusion manifolds?

- Effect of diffusion on reaction-based manifolds has been studied.
- In similar spirit as Lorenz's approach, we use Galerkin projection to write a low-order reaction-diffusion model as

$$\frac{d\mathbf{z}}{dt} = \mathbf{G}(\mathbf{z}) + \mathbf{f}(\mathbf{z})$$

- Meaningful SACIM exists only for micron-scale modes!
- SACIM diagnosis for reaction-diffusion systems is very hard!



A question which extends beyond combustion!

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The Slow Manifold—What Is It?

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(Manuscript received 17 June 1991, in final form 17 March 1992)

ABSTRACT

Two studies that disagree as to whether a slow manifold is present in a particular low-order primitive equation model are compared. It is shown that the discrepancy occurs because of a difference of opinion as to what constitutes a slow manifold.

3. Conclusions

The question as to just how the slow manifold ought to be defined seems to be presently unsettled. The procedure in J defines a unique manifold S that is slow but not strictly invariant, since orbits leave S when they leave the region of convergence. When S is extended to become S^*, it becomes invariant, but then it is no longer slow. Stated otherwise, a manifold that is locally invariant and locally slow exists but one that is globally invariant and globally slow does not. Whether such a statement would be true for other primitive equation systems presumably cannot be discovered without further work. We note, incidentally, that neither S nor S^* appears to be fuzzily defined.

More generally, Eqs. (1) are typical of innumerable systems encountered in fluid dynamics and other fields,

Note: attraction also needed!

Manifold conclusions and questions

- Lorenz asked and answered "The slow manifold–what is it?"
- The more fundamental question, "The slow manifold–where is it?," remains to be answered robustly.
- Stretching- and rotation-based diagnostics have utility in answering a related question, "When is a CIM a SACIM?"
- Our example showed for a problem with one universally positive normal stretching rate that local repulsion from a CIM was possible, overcome only near an equilibrium sink.
- Thus, heteroclinic orbit connection is *not guaranteed* to identify a SACIM.
- If the method of heteroclinic connection of equilibria cannot identify a SACIM, can any method do so?
- Open systems, multiple equilibria, and limit cycles, and raise further fundamental questions!

Broader editorial comments—Diagnosis: successful; Treatment: limited.

- Due to non-linearity and lack of spectral gaps, we should probably prefer DNS over reduction.
- We can do verified DNS, but it is hard, and our geometries must be small, at least today.
- DNS reveals ordered, validated harmonies in reacting fluids.
- DNS reveals tangled, unvalidated harmonies in reacting fluids.
- Prediction has value, *when it works*.
- Reduction has value, *when it works*.
- It is useful to recognize the frontier.
- That frontier is moving, not as fast as promised, but moving nonetheless!

Magritte's admonition:

(un)Scientific computing: a modern rabbit hole?

Scientific computing: a modern Galileo's telescope?