Verification and validation of detonation simulation: topical review

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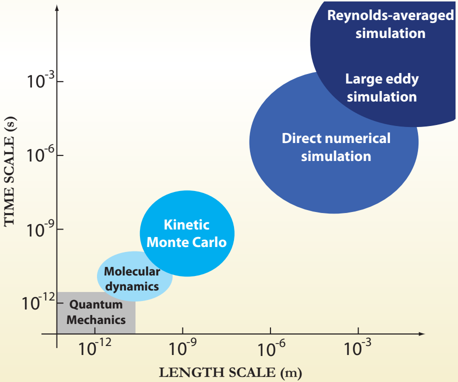
Outline

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 detonation calculations
6. Some conclusions

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

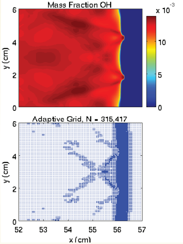


"Research needs for future internal combustion engines," *Physics Today*, Nov. 2008, pp. 47-52.

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 DNS is feasible.



C. E. Yeager, 1923-

Some present contributions...

This mini-symposium will highlight some recent work in detonation calculation relevant to exercises in V&V:

- *Bhattacharjee, Maines, Maley, & Radulescu*: Detonation wave attenuation by a cylinder and the subsequent re-initiation régimes
- *Ziegler, Deiterding, Shepherd, Pullin, & Blanquart*: Verification and direct numerical simulation of irregular hydrocarbon detonations
- *Mazaheri, Mahmoudi, & Radulescu*: Diffusion in gaseous detonations
- *Cole, Karagozian & Cambier*: Stability of flame-shock coupling in detonation waves: 1D dynamics
- *Papalexandris & Steisel*: Numerical study of detonation suppression with chemical inhibitors
- *Romick, Aslam & Powers*: Verified calculation of nonlinear dynamics of viscous detonation

Consultation with an expert

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Detonation in gases

J.E. Shepherd *

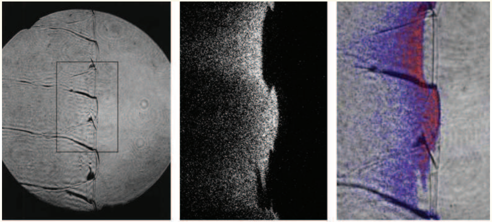
Aeronautics and Mechanical Engineering, California Institute of Technology, MS 105-50, Pasadena, CA 91125, USA

- 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].

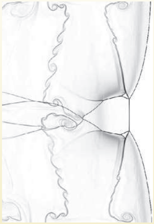
Evidence of complexity in detonations



a b c

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.

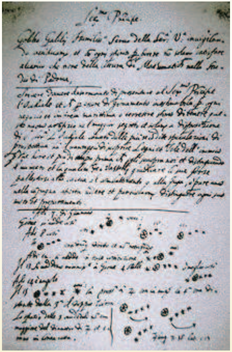
Midcourse diversion

- 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...

Abell 2744, "Pandora's Cluster," from Chandra X-Ray Observatory, released 22 June 2011

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.



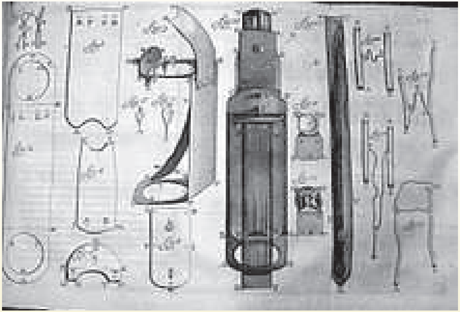
- Galileo, et al. invalidate the Ptolemaic theory with new data

Galileo Galilei (1564-1642)

Multiscale instrumentation

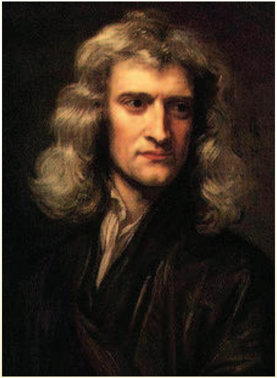
Telescope

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*.

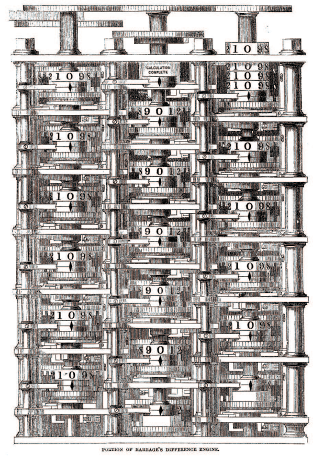
Enlightenment mathematization



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!

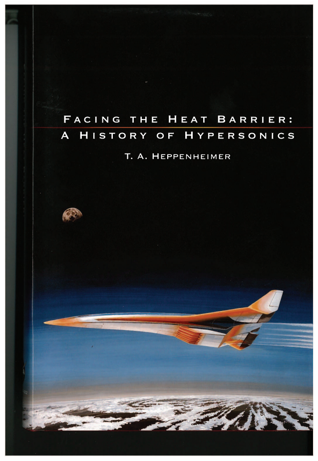
Victorian mechanization

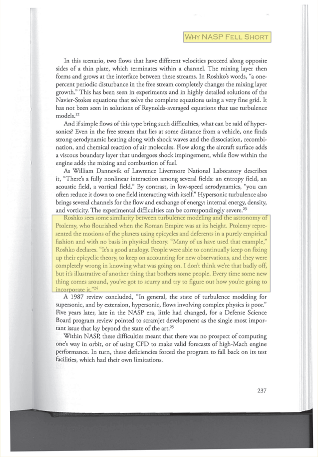


Schematic of difference engine of Babbage (1791-1871)

- 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





WHY NASP FELL SHORT

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.

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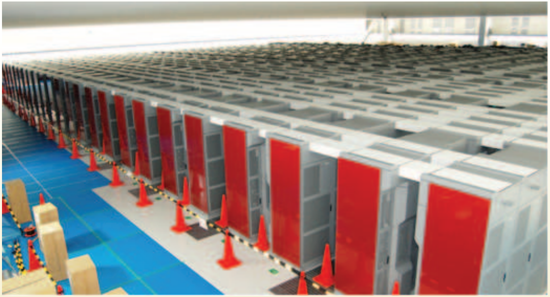
Quotations from NASA's commissioned history:

- *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?

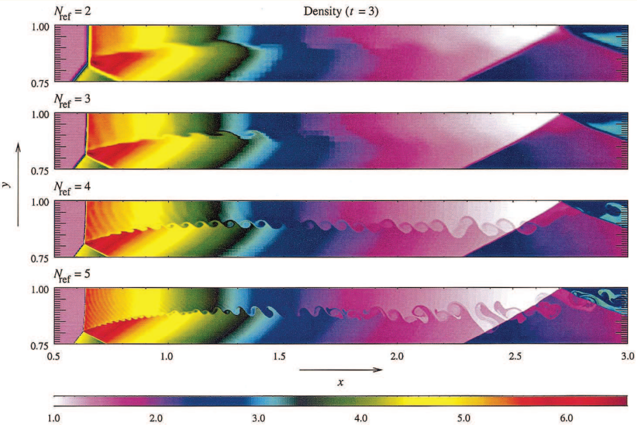


- Today's Peta- and tomorrow's Exa-scale hardware enables heroic calculations,
- RIKEN and Fujitsu's K, world's fastest computer, 8.162 $Pflop/s$

Let us look through the computational "telescope/microscope" at detonations and closely related phenomena

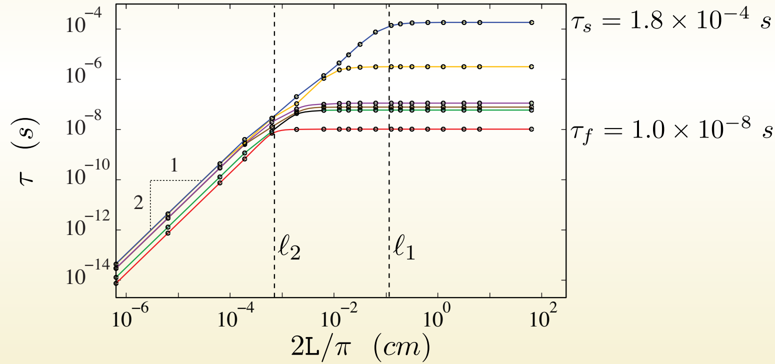
- This improved computational hardware and associated adaptive mesh refinement software provides a better "telescope" for observing nature.
- When seeking fundamental understanding, we should choose to look through this new "telescope" without clouding its images with de-focusing effects of shock-capturing, turbulence modeling, etc.

Results from University of Chicago's FLASH code



- 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.

Flame stability calculation verifies chemistry-induced fine length scales; Al-Khateeb & Powers, 2011.



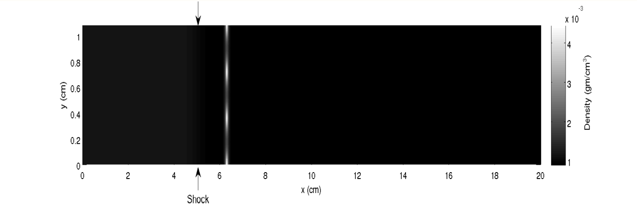
- $H_2 - air$ with detailed kinetics and multi-component diffusion
- $\ell_1 = \sqrt{D_{mix}\tau_s} = 1.1 \times 10^{-1}\ cm,$
- $\ell_2 = \sqrt{D_{mix}\tau_f} = 8.0 \times 10^{-4}\ cm.$

Scale necessary for verified calculation

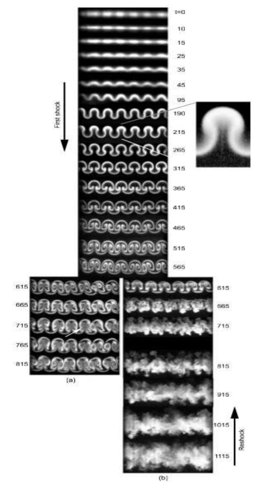
- The simple length scale analysis dictates that $\Delta x < 8.0 \times 10^{-4}\ cm$ for a verified calculation for detailed kinetics simulations of $P = 1\ atm$ hydrogen-air combustion.
- This scale is consistent with Shepherd's 2009 discussion.
- This scale is equivalent to a few mean free paths.
- High order methods applied to under-resolved problems will not be verified, and will likely 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).

Richtmyer-Meshkov instability; Zikoski, Paolucci, & Powers, 2010

Initial conditions:



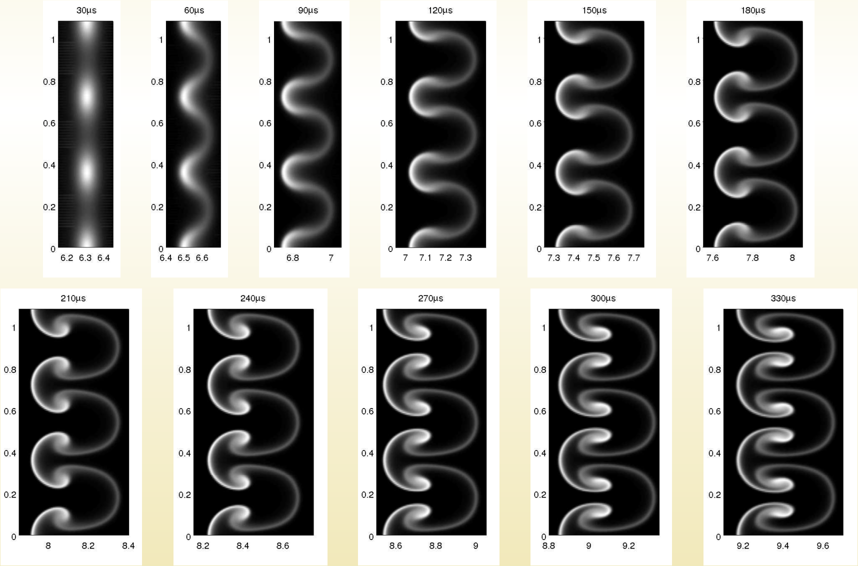
- 20 $cm \times 1.08$ cm
- $Y_{N_2} = 0.99$, $Y_{SF_6} = 0.01$, $P = 79.5$ kPa, $T = 300$ K, $M = 1.2$
- Calculations using an wavelet-based adaptive refinement method; finest scale $\sim 10^{-4}$ cm
- 64 cores, 118 hours computational time



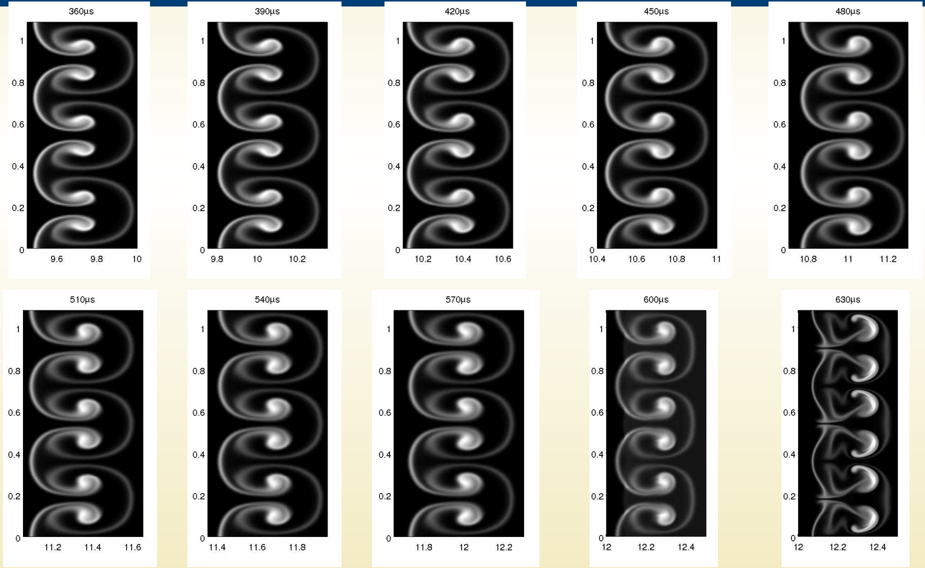
experimental image from Balakumar, *et al.*, 2008

Verified RM calculation with validated NS model

$\Longrightarrow$ Shock Direction $\Longrightarrow$



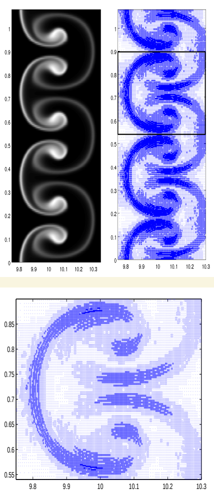
Verified RM calculation with validated NS model



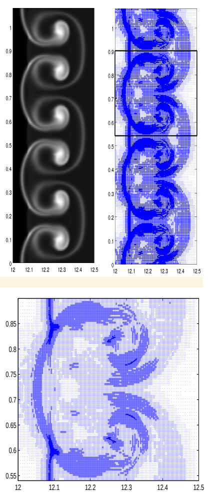
⇐ Reshock ⇐

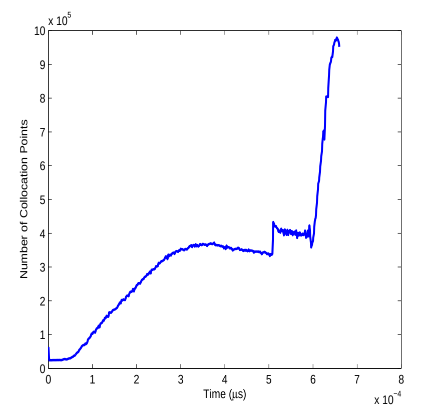
Verified RM calculation with validated NS model

$t = 390\ \mu s$



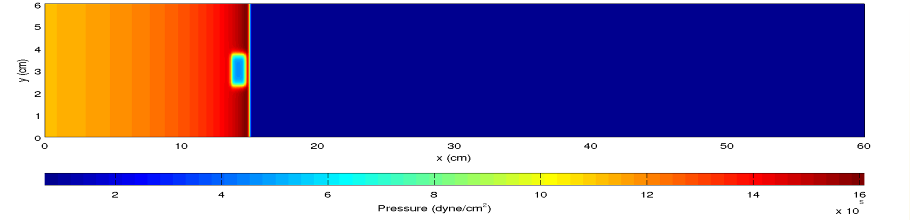
$t = 600\ \mu s$





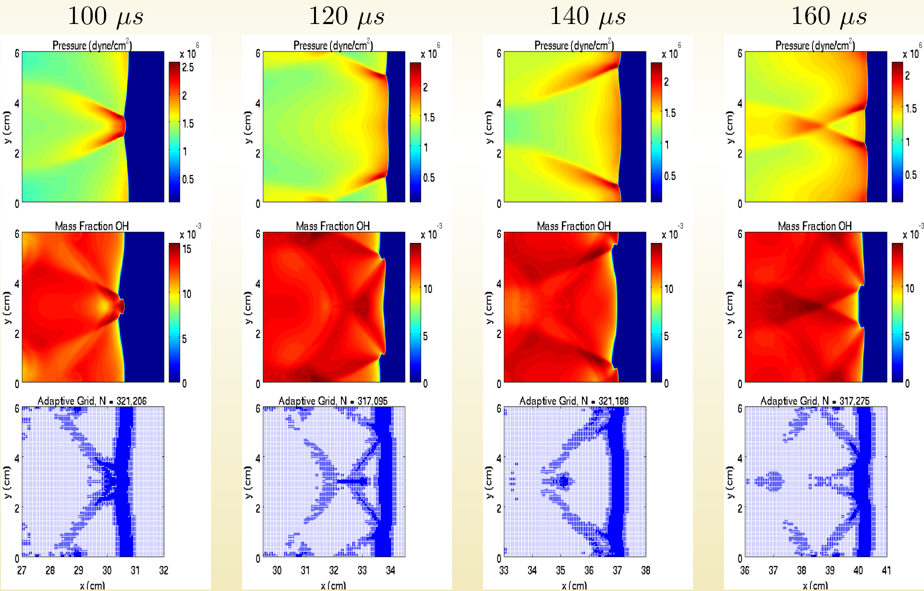
Wavelet adaptive detonation calculation gives verified multiscale structure (from 10^{-4} cm to 10 cm); Zikoski, Paolucci, & Powers, 2011

Initial Conditions, 1-D ZND detonation with 2-D perturbation:



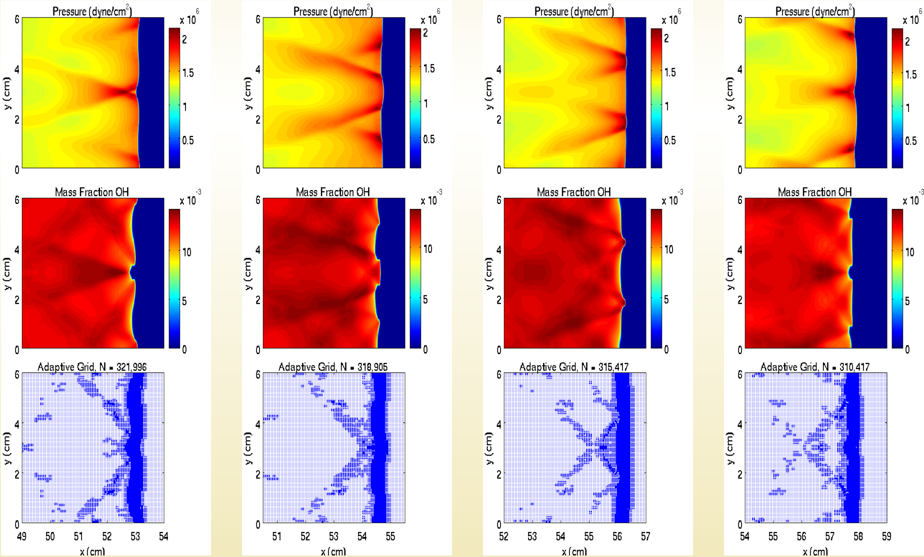
- $2H_2 + O_2 + 7Ar$, $P_o = 6.67\ kPa$, $T_o = 300\ K$
- 9 species, 37 reactions, multi-component diffusion
- 60 $cm \times 6$ cm spatial domain; finest scale $\sim 10^{-4}$ cm
- 128 cores, 391 hours run time

Verified multiscale detonation calculation



Verified multiscale detonation calculation

240 μs 250 μs 260 μs 270 μs



Conclusions

- Verified two-dimensional detonation calculations for realistic reacting gas mixtures with detailed kinetics and multicomponent transport are realizable with modern adaptive algorithms working within a massively parallel computing architecture.
- It is possible for 2D calculations to span over five orders of magnitude of length scale: ranging from near mean-free path scales (10^{-4} cm) to small scale device scales (10 cm).
- 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.


Workshop on
VERIFICATION &
VALIDATION
in Computational Science
October 17-19, 2011
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