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Review of Multiscale Modeling of Detonation

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Issues associated with modeling the multiscale nature of detonation are reviewed, and potential applications to detonation-driven propulsion systems are discussed. It is suggested that a failure of most existing computations to simultaneously capture the intrinsic microscales of the underlying continuum model along with engineering macroscales could in part explain existing discrepancies between numerical predictions and experimental observation. Mathematical and computational strategies for addressing general problems in multiscale physics are first examined, followed by focus on their application to detonation modeling. Results are given for a simple detonation with one-step kinetics, which undergoes a period-doubling transition to chaos; as activation energy is increased, such a system exhibits larger scales than are commonly considered. In contrast, for systems with detailed kinetics, scales finer than are commonly considered are revealed to be present in models typically used for detonation propulsion systems. Some modern computational strategies that have been recently applied to more efficiently capture the multiscale physics of detonation are discussed: intrinsic low-dimensional manifolds for rational filtering of fast chemistry modes, and a wavelet adaptive multilevel representation to filter small-amplitude fine-scale spatial modes. An example that shows the common strategy of relying upon numerical viscosity to filter fine-scale physics induces nonphysical structures downstream of a detonation is given.

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Nomenclature

$\boldsymbol{b}$	=	generic constant vector
$\boldsymbol{D}$	=	diagonal matrix
$\bar{D}$	=	dimensionless detonation wave speed
d	=	number of dimensions
$\bar{E}$	=	dimensionless activation energy
$\boldsymbol{f}$	=	generic convective and diffusive flux
$\boldsymbol{g}$	=	generic reaction source
$\boldsymbol{h}$	=	generic function for linear representation
$\boldsymbol{J}$	=	generic Jacobian matrix
L	=	generic length, m
ℓ	=	local reaction length scale, m
M	=	number of dependent variables
N	=	number of spatial discretization points
$\boldsymbol{P}$	=	matrix of eigenvectors
RAM	=	size of random access memory, byte
t	=	time, s
$\bar{t}$	=	dimensionless time
X	=	mole fraction
x	=	distance coordinate, m
$\boldsymbol{x}$	=	generic distance vector
$\bar{x}$	=	dimensionless distance coordinate
Y	=	mass fraction
$\bar{y}$	=	dimensionless distance coordinate
$\mathbf{\Lambda}$	=	eigenfunction amplitude
$\mathbf{\Lambda}$	=	diagonal matrix of eigenvalues
λ	=	eigenvalue, 1/s
ϕ	=	generic dependent variable
ψ	=	generic orthonormal basis function

Subscripts

i	=	eigenfunction counter, species counter
j	=	spatial discretization counter
max	=	maximum
min	=	minimum

Superscript

$*$	=	constant state

I. Introduction

OVER the past several years, revolutionary advances in computational modeling of multiscale physics[1–3] have prompted numerous numerical simulations of the subject of this special issue, detonation-driven propulsion devices.[4–62] Among the devices in which detonation physics plays a leading role are the ram accelerator, the hypothesized oblique detonation wave engine, and the pulse detonation engine. And whenever shocks are present in the vicinity of chemical reaction, as is the case for many rocket and airbreathing propulsion applications, detonation physics is relevant.

The computational advances are embodied in improved mathematical models, numerical solution algorithms, and computational hardware. Most critically, the improvements have enabled a more robust scientific design procedure in which the engineer can predict with greater precision the behavior of a device a priori. The key to past and future enhancements in prognostic ability lies in the increase in the engineer's capacity to describe physical events that evolve over a wide range of spatial and temporal scales. While in the popular imagination, the so-called Moore's law[63] effect, which

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describes the exponentially increasing speed of computational hardware, is celebrated as the chief enabler of these enhancements, although in actuality, a quieter, but no less important set of improvements in computational modeling techniques deserves as much credit. These gains range from more efficient compilers, new algorithms to better exploit massively parallel hardware architectures, improved fundamental algorithms for solution of large linear algebraic systems, advances in grid-generation methods, and improved algorithms for solving large sets of ordinary and partial differential equations.[1,2]

Although the gains of the past decades have been remarkable, this paper will demonstrate that in many respects certain problems in detonation propulsion have barely been dented; many more scales remain to be captured before one can claim true understanding. As will be shown, key physical phenomena involving unsteady and multidimensional effects, such as ignition, stability, transverse wave dynamics, detonation diffraction, detailed reaction zone structures, and diffusive structures, remain unresolved for most important engineering applications. As a result, it is argued that the aeropropulsion modeling community stands to benefit from more critical and skeptical examination of reactive flow calculations used in design than is employed at present. It will be recommended, then, that the community continue to nurture advances in algorithms and hardware, but to moderate its expectations so that they are consistent with the scientific limitations of both.

In short, the physics are sufficiently complex that accurate numerical prediction remains problematic. For example, a recent exercise[31] in which several computational algorithms were employed in an effort to reproduce results of a benchmark experiment of a ram accelerator produced, according to the authors, "widely different outcomes," with strong sensitivity to induction zone dynamics. Another recent study,[49] which included both computational predictions and observations of pulse detonation engines, concluded the important run-up distance to detonation to be "underpredicted" and that "simulation of the deflagration to detonation transition (DDT) process remains a challenge." Analogous difficulties in related fields are easily found. For example, Kadanoff[3] summarizes some notable recent failures in simulations of sonoluminescence, Rayleigh–Taylor instability, and wave breaking. He concludes "resolution matters."

It is speculated here that challenges associated with truly capturing the multiscale physics in such flows can provide an explanation as to why predictions do not always match data. This paper will review modeling strategies to capture multiscale physics, with attention given to problems that arise in shock-laden supersonic reactive flow such as exists in detonation-driven propulsion devices. It will not give a detailed discussion of individual studies of those devices, which have been discussed in other review articles,[5,8,28,30,41,48] or fundamentals of detonation theory, well covered, for example, by Fickett and Davis.[64] Nor is it intended for those already expert in multiscale modeling. Instead, it is offered as a summary for those of the general propulsion community who might want to know more about this topic and appreciate how the disciplines of reactive gas dynamics, mathematics, computer science, and aerospace engineering can come together with the goal of advancing propulsion technology.

The plan of this paper is to open with a brief review of how multiscale physics is endemic in nature, and in particular, in supersonic propulsion devices. A short discussion then follows of fundamental mathematical modeling strategies that can be used to capture the effects of the physical mechanisms which dominate at broadly different scales. An argument is made that continuum-based mathematical models in the form of partial differential equations will remain for some time the critical tool to describe the behavior of common propulsion devices. A description of popular computational strategies for modeling partial differential equations is then given, focusing on how the multiscale physics is manifested mathematically. The following section gives multiscale detonation modeling examples from previous work of the author and some of his colleagues describing how 1) a simple model of detonation can undergo a classical period-doubling process and transition to a chaotic state,[65] 2) detailed gas-phase kinetic models give rise to fine-scale structures orders of magnitude below those commonly used in present design analyses,[66] 3) a detailed gas-phase reaction kinetics model can be rationally reduced so as to filter all fine timescale phenomena below a given threshold,[67,68] 4) an adaptive-mesh-refinement (AMR) technique can be used to simultaneously capture fine and coarse structures in a viscous detonation with detailed kinetics,[67] and 5) the effects of artificial numerical viscosity can corrupt some postshock detonation flowfield structures predicted by models with simple kinetic schemes.[69] The paper is closed with some brief comments on engineering applications followed by a short set of conclusions.

II. General Issues and Strategies in Multiscale Modeling

Here, we give a general discussion of multiscale modeling; a more detailed complementary review is given by Oran and Boris.[2]

A. Multiscale Physics

Our universe has identifiable structures that span a tremendous breadth of length scales. The popular book of Morrison et al.,[70] which vividly illustrates the multiscale universe, describes scales ranging from a proton-based scale of 10^{-16} m to a universe diameter of 10^{25} m. Even more dramatic, physicists are now actively studying a hypothesized quantum gravitational scale of 10^{-35} m (Ref. 71). Moreover, observable phenomena are known to evolve on a broad range of timescales, ranging from 10^{-25} s for the time necessary for a photon to traverse a proton-based length, to 10^{17} s for the estimated age of the universe.[72] An overriding goal of much of science is to develop the most efficient explanation for the behavior of the universe, as well as its components, which spans as wide a set of scales as is practical. The whole being a consequence of the parts, it stands to reason that one path to understanding macrobehavior of the universe is by understanding its building blocks and how they interact. Generally, the wider breadth of scales, the more impractical this strategy becomes.

B. Mathematical Strategies

As the naive theoretical approach of simply describing phenomena at all scales holds little promise, a key to making progress in developing predictive science has been the wise employment of assumptions that decouple phenomena which evolve on one scale from those that evolve on others. The most direct approach to this end combines good intuition guided by experiment with mathematical analysis to either eliminate or rationally account for phenomena that evolve on dramatically different scales than those of the phenomena of interest. Science being ultimately empirical, the proof of the wisdom of such assumptions lies in comparing the predictions of such theories to experiments whose results were not known before the fact.

A famous example of such an approach is found in the development of the kinetic theory of gases in the late 19th century. This theory showed how systematic averaging of complex molecular collision processes gives rise to a set of progressively simpler theories, each of which captures fewer physical phenomena, but are often more than sufficient for the task at hand. In a series of analytical steps in which progressively more and more fine scales are removed via averaging, one proceeds from a Liouville to a Boltzmann to a Burnett to a Navier–Stokes model of reactive fluid mechanics.[73–76] This theory relates both equation of state and diffusive transport properties, valid at the macroscale, to the more fundamental theory based on microscale molecular collisions. For simple molecules, first principles estimates are available for the resulting constitutive equations that are really models for capturing the average effect of subcontinuum phenomena.

The success of this approach has sparked much research in the same analytic vein. One need only consult the recent literature[77,78] or any issue of the new journal *Multiscale Modeling and Simulation* to see that one common conception of multiscale physics is often closely linked to developing custom models for highly distinct

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physical problems in which multiscale coupling plays a large role. For many problems, this method of the modeling artisan is a useful approach. For others, the basic mathematical models are reasonably well established; however, their solution for general problems is not. Such problems demand the tools of the algorithm artisan to meet the challenges of multiscale physics, which are already intrinsic to the models. The key problems in aeropropulsion tend to recommend the latter approach, as most models for reacting gas dynamics are generally accepted. The main challenges intrinsic in these models arise from their highly nonlinear character, which admits complex multiscale solutions in which disparate scales are often strongly coupled.

When one confines consideration to continuum reactive fluid mechanics applicable to aeropropulsion devices, one nevertheless finds widespread analytical efforts to filter the scales that remain in the continuum. An estimate of the smallest length scale that is inherent in the resulting continuum models is related to the mean free-path distance between molecular collisions, typically on the order of 10^{-7} m. This minimum length scale of relevance is the foundation of length scales predicted by continuum models of mass, momentum, and energy diffusion, as well as elementary reaction kinetics.[75] Note further that for compressible flow, the so-called Kolmogorov scale of turbulence is one and the same with the scale of shock thicknesses, which itself is on the order of the mean free-path distance, as can be shown by simple scaling arguments.[79] Thus, for a compressible flow with elementary reactions, all finest scales are related to the mean free path. The common flamelet approach in which some fine-scale flame structures are not resolved in some low-Mach-number simulations of combustion loses its physical rationale for a direct numerical simulation[80] (DNS) of detonation. In contrast, the largest length scale is typically a small multiple of the device length, which can be 10^1 m. Within the span of these scales, Fig. 1 gives rough estimates of scales associated with common features in reactive fluid mechanics, such as boundary layers and coarse scale reaction zones. This span of eight orders of magnitude of length scale still represents a grand challenge to achieve quantitative predictions from any theory.

The list of mathematical strategies to reduce the span of these scales is long and includes methods for filtering both space and timescales: 1) employment of Euler equations so as to neglect all diffusion processes and their associated thin layers—notably, such theories then admit true shock and contact discontinuities which give rise to new problems when accurate numerical simulation is attempted; 2) use of formal averaging theories to encapsulate fine-scale behavior in a new constitutive model—such approaches are common in flows involving granules and droplets; 3) a wide variety of asymptotic techniques such as boundary layer theory or the method of multiple scales[81,82]; 4) analytic models for Kolmogorov-scale turbulent fluid interactions; and 5) intrinsic low-dimensional manifolds (ILDM)[67,83,84] to locally equilibrate fast chemical reaction modes.

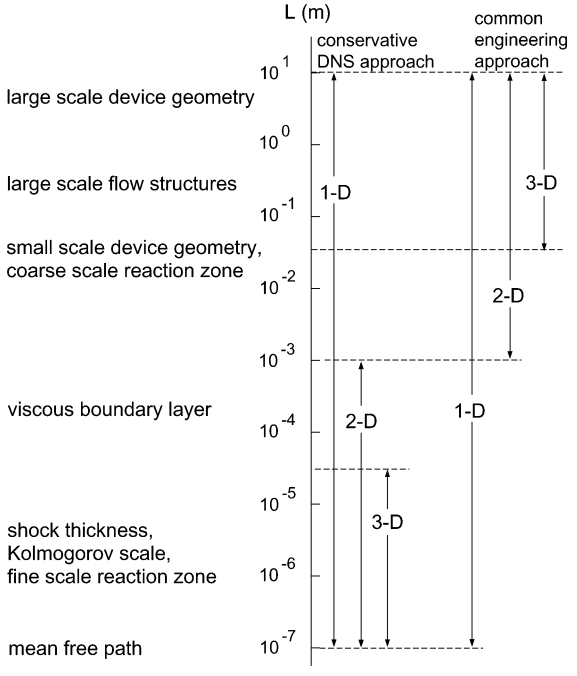

Fig. 1 Estimate of range of length scales for continuum model of compressible reactive flow with detailed kinetics in typical propulsion devices along with range of scales that can be loaded into desktop computer with 10^9 bytes *RAM* for one-, two-, and three-dimensional calculations with $M = 15$ variables per cell.

Whether or not any further mathematical filtering strategy is taken, the modeler is typically faced with a system of equations, which will be taken to be of the form

$$\frac{\partial \boldsymbol{\phi}}{\partial t} + \nabla \cdot \boldsymbol{f}(\boldsymbol{\phi}) = \boldsymbol{g}(\boldsymbol{\phi}) \tag{1}$$

Here, $\boldsymbol{\phi}$ is a generic set of M dependent variables, $\boldsymbol{f}$ is a nonlinear function embodying convective and diffusive fluxes, and $\boldsymbol{g}$ is a nonlinear reaction source term. These equations are solved on a spatial domain of $\boldsymbol{x} \in \mathbb{R}^d$, where $d = 1, 2, 3$ gives the dimension of the system and $\boldsymbol{x}$ is the spatial variable.

Much insight into general multiscale behavior can be gained by considering the special case in which Eq. (1) is linear. In such a case, one can define an infinite set of basis functions, $\psi_i(\boldsymbol{x}), i = 1, \ldots, \infty$, which in this linear case are eigenfunctions of the spatial derivative operator. For the linear system, one can always transform to the wave-attached frame so as to remove the convection and be left only with diffusion. Diffusion operators are typically self-adjoint and thus have an infinite set of real eigenvalues and orthonormal eigenfunctions. These eigenfunctions span the space, and thus any arbitrary set of initial conditions can be cast as an infinite series in terms of the eigenfunctions. The eigenfunctions are typically of a spatially oscillatory nature, whose wave number rises with increasing value of i. One then assumes that the dependent variables ϕ can be separated into spatial and temporal modes via the eigenfunction expansion

$$\boldsymbol{\phi} = \sum_{i=1}^{\infty} \boldsymbol{\alpha}_i(t) \psi_i(\boldsymbol{x}) \tag{2}$$

Here $\alpha_i(t)$ is the time-dependent amplitude of the ith eigenmode. Then, Eq. (1) can be cast as an infinite set of linear ordinary differential equations (ODEs) of the form

$$\frac{\mathrm{d}\boldsymbol{\alpha}_i}{\mathrm{d}t} = \lambda_i \boldsymbol{\alpha}_i, \qquad i = 1, \ldots, \infty \tag{3}$$

which describes the temporal evolution of the amplitude of each eigenmode. Here λ_i is the eigenvalue of the ith eigenmode. Critically, one notes that each ODE in Eq. (3) is uncoupled from all others and thus can be solved individually. Consequently, an analytic solution can be obtained for the amplitude of each mode; one typically finds, given that an entropy inequality is satisfied, that the amplitude of a given high-frequency mode decays to zero as the mode number increases to infinity. Thus, a finite series can accurately approximate the solution, and one can estimate the error incurred by the truncation. Such solutions formally have a multiscale character, but there is no coupling across scales, and the error of neglecting fine scales is small and quantifiable.

There is no robustly accurate way to segregate the effects of reaction and diffusion. Even in a purely linear version of Eq. (1), the eigenvalues λ_i are consequences of the combined effects of reaction and diffusion. An analysis of the related, operator-split, spatially homogeneous version of Eq. (1), $\mathrm{d}\boldsymbol{\phi}/\mathrm{d}t = \boldsymbol{g}(\boldsymbol{\phi})$, when $\boldsymbol{g}$ happens to be a linear operator, gives rise to a finite set of M eigenvalues, whose reciprocals give estimates of a finite set of reaction timescales. These scales can indeed be widely disparate and indicate that chemically induced stiffness is present. The stiffness however is finite and will

always be dominated by stiffness induced by the continuous differential diffusion operator when spatial inhomogeneity is included. In fact, only when enough modes are included so that $\lim_{i\to\infty}\lambda_i$ is dominated by diffusion, and so transcends the largest eigenvalue predicted by the spatially homogeneous model, are enough modes present for the solution's series to be in the asymptotically convergent region, so that one can claim the essence of the solution is spatially resolved. A discussion of the dangers of the common practice of splitting chemistry from convection and diffusion is given by LeVeque and Yee.[85] In fact, the artifice of operator splitting creates the illusion that chemical stiffness can be segregated from that of diffusion, when in fact the two are often highly coupled.

If Eq. (1) is nonlinear, one can still perform an expansion of ϕ in terms of an infinite set of orthonormal basis functions ψ_i, which no longer are eigenfunctions of the spatial operator. In this case one can, in principle, approximate the system by an infinite set of ODEs of the form

$$\frac{\mathrm{d}\boldsymbol{\alpha}_i}{\mathrm{d}t} = \boldsymbol{h}_i(\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_\infty), \qquad i = 1, \ldots, \infty \tag{4}$$

In the nonlinear case, there is coupling between modes, and it is difficult to determine a priori how strong that coupling is. In practice, it is often nearly impossible to form the exact representation given in Eq. (4), and one usually has to resort to discrete approximations. However, many spectral and pseudospectral methods, as well as low-order nonlinear stability analyses, do take as their starting points truncated versions of Eq. (4).

C. Computational Strategies

For nonlinear problems, exact solutions are typically not available, and the modeler most often turns to discretization of the underlying partial differential equations to enable an approximate numerical solution to be obtained. These equations contain their own challenges for which a summary of approaches will be summarized here. As the detonation-based aeropropulsion literature is beginning to contain more calculations based on Navier–Stokes models,[35,46,61,86–91] attention will be focused on them; similar arguments could be made for related models.

The ongoing development of the digital computer along with appropriate algorithms over the past decades has enabled a widening of the breadth of scales that can be modeled. However, it is often not appreciated still how narrow the band is at present. Consider a calculation to be performed in a one-, two-, and three-dimensional linear, square, and cubical box. Take $d = 1, 2, 3$, to be the dimension of the box and $L_{\max}$ to be its length. Take the minimum physical length scale to be $L_{\min}$ and M to be the number of dependent variables to be calculated at each computational node. Then it is easy to show the necessary size of the random access memory *RAM* is given by

$$RAM = M\left(\frac{L_{\max}}{L_{\min}}\right)^d \tag{5}$$

assuming a straightforward spatially uniform discretization of the geometric domain.

The most desirable calculation is one that has sufficient resolution to capture all of the relevant scales admitted by an underlying mathematical model. Such a calculation is a DNS. The real challenge associated with performing a DNS in a continuum calculation of flow in an aeropropulsion device, even on modern computational hardware, is evident on examination of Fig. 1. This figure presumes that $M = 15$ variables are associated with each cell, which is a reasonable estimate for calculation with detailed kinetics of, for example, a hydrogen-oxygen system. Estimating that a good desktop computer in the present day can have 10^9 bytes of *RAM*, it is seen that such a machine can perform simulations that span a ratio of scales $L_{\max}/L_{\min} = 10^8, 10^4$, and 10^2 for one-, two-, and three-dimensional calculations, respectively. Only the one-dimensional calculation approaches the breadth of physical scales admitted by a continuum model for aeropropulsion engineering devices.

Figure 1 also shows the results of two distinct approaches to modeling. The purpose of the conservative DNS approach, whose predictions are easier defended, is to always capture the finest scales. In this approach then, the largest one-, two-, and three-dimensional aeropropulsion problems, which can be loaded onto a 10^9 bytes computer, have characteristic lengths of 10^1 m, 10^{-3} m, and 10^{-5} m, respectively. This conservative approach is rarely adopted because it cannot capture the macroscopic scales of interest in typical engineering applications. In the more common, as well as more risky, approach, the engineering scale is taken as the largest scale, and as fine a discretization as is practical is used for a simulation. Assuming the largest device geometric scale is 10^1 m, a modern desktop computer with 10^9 bytes *RAM* can at best capture scales down to 10^{-7} m, 10^{-3} m, and 10^{-1} m in a given one-, two-, and three-dimensional calculation. Phenomena that evolve below these scales are not captured in any detail and are typically overwhelmed by nonphysical numerical diffusion.

Considering now supercomputers, recently developed massively parallel systems have achieved as much as 3.2×10^{13} bytes *RAM*.[92] Even then, the ability to span scales is not what is required for a first principles scientific design. For such a machine, the ratios of scales that can be spanned are 2×10^{12}, 1×10^6, and 1×10^4 for one-, two-, and three-dimensional calculations, respectively. The resolution of the necessary ratio of scales of $L_{\max}/L_{\min} = 10^8$ requires 1.5×10^9 bytes *RAM*, 1.5×10^{17} bytes *RAM*, and 1.5×10^{25} bytes *RAM* for a one-, two-, and three-dimensional calculation, respectively. Moreover, these estimates only speak to the necessary ability to load the problem into *RAM* but ignore the critical issue of speed of the actual computation, which increases dramatically with the fineness of the discretization. An indication of the the range of scales that can be resolved by such a DNS as a function of available *RAM* is given in Fig. 2.

With some notion of the range of length scales that can or should be modeled, the numerical analyst typically performs some class of spatial discretization of Eq. (1) in which the solution is only calculated at N discrete points. This allows the spatial differential operators to be replaced by discrete counterparts and transforms the coupled set of partial differential equations into a large set of differential algebraic equations (DAEs) of the form

$$\boldsymbol{D}\cdot\frac{\mathrm{d}\phi_j}{\mathrm{d}t} = -\nabla_j[\boldsymbol{f}(\phi_1, \ldots, \phi_N)] + \boldsymbol{g}(\phi_j) \qquad j = 1, \ldots, N \tag{6}$$

Here ∇_j is a discrete counterpart to the continuous gradient operator, and $\boldsymbol{D}$ is a diagonal matrix whose diagonal is composed of zeros or ones. It arises because some methods give rise to purely algebraic relations at some points. If $\boldsymbol{A} = \boldsymbol{I}$, the identity matrix, as it is for several methods, the set of N DAEs becomes a set of N ODEs.

There is a wide choice of spatial discretizations in common use. Among them are 1) finite difference/finite volume, 2) finite element, 3) spectral, 4) wavelet, and 5) manifold. There is a large body of literature on the first three discretizations, nicely summarized by Iserles[93]; for the hyperbolic equations used commonly for inviscid detonation simulations, LeVeque[94] gives a modern discussion. The

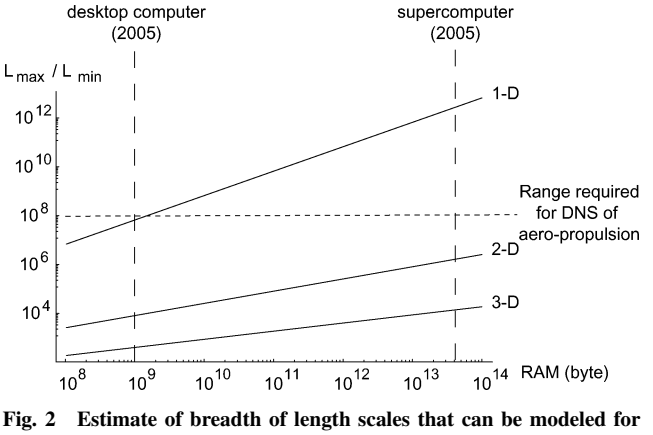

Fig. 2 Estimate of breadth of length scales that can be modeled for a typical continuum calculation of compressible reactive flow with detailed kinetics as a function of available random access memory (*RAM*).

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first two classes are related in that both involve a discretization in which a small number of points in the neighborhood of point j are used to estimate the spatial derivatives. Such discretizations have a low order of spatial accuracy. Spectral methods[95,96] involve discretizations in which all points in the domain are used to estimate local values of spatial derivatives; at the expense of additional complexity, these have a high order of accuracy for smooth problems. The wavelet discretization is a relatively new class whose use admits several advantages,[67] especially in developing computational grids that dynamically adapt to evolving flow structures. The manifold discretization, described for reactive systems recently,[68] is another relatively new approach, which gives rise to a set of DAEs. The algebraic relations force the solution to lie on specified manifolds and amount to equilibrating fast timescale events.

Considering from this point on the case where $\boldsymbol{D} = \boldsymbol{I}$, Eq. (6) is a large set of nonlinear ODEs in time of the form

$$\frac{\mathrm{d}\phi_j}{\mathrm{d}t} = -\nabla_j[\boldsymbol{f}(\phi_1, \ldots, \phi_N)] + \boldsymbol{g}(\phi_j) \qquad j = 1, \ldots, N \tag{7}$$

Spatial variables do not explicitly appear in Eq. (7). Consequently, one can apply notions from the well-developed theory of nonlinear dynamic systems[97] to understand behavior of the spatially discretized system. In particular, Eq. (7) for $N \geq 3$ contains the essential general property of nonlinearity so that one might expect to achieve a chaotic solution in time. In fact, such behavior is shown explicitly in detonation systems in a recent study.[65] Such solutions formally admit an infinite number of timescales, and none can be neglected. If a nonlinear system becomes chaotic, then small-scale events, which could safely be neglected if the system were linear, can no longer be simply dismissed. This is the fundamental conundrum of chaos: for such systems, even low-amplitude disturbances at fine scales have the potential to cascade up to induce large disturbances at coarse scales. In such cases, similar to homogeneous turbulence, one must perform more specialized studies to determine what meaningful statistically averaged information can be extracted from the nonlinear system and not expect to recover deterministic predictions at all scales.

Even if the solution to the ODEs of Eq. (7) were known to infinite precision, the solution might or might not represent well the solution of the corresponding continuous system, Eq. (1). How well the solution to Eq. (1) is approximated depends upon whether the spatial discretization was chosen to be fine enough to capture the intrinsic spatial scales of Eq. (1). This issue can only be resolved in general by systematic study of if and how the approximate solution is converging as the spatial discretization is refined. One can usually be confident in a solution if it is converging at a rate consistent with the order of accuracy of the spatial discretization; however, in the absence of an exact solution one cannot have absolute certainty that one is converging to a correct, physically meaningful solution. Imagine, as a counterexample, a sensitive nonlinear system with multiple stable equilibria. Some equilibria can be physical and some nonphysical. A small error at an intermediate stage of the computation can shift the solution path in phase space and send the solution to an incorrect, and perhaps nonphysical, albeit stable, equilibrium point. Fortunately, experience shows convergence to an incorrect solution is rare for models that are mathematically well posed and whose intrinsic scales have been computationally resolved. Lastly, one notes that 1) a solution is never "converged," but only can be converging at an appropriate rate; and 2) only when a solution is converging appropriately is it proper to ask the even more important question for precision engineering of just how computationally accurate is that solution.

Important information regarding the nonlinear temporal behavior of a spatially discretized system can often be gleaned from a local linearization, which when applied to Eq. (7) at a generic time and state t^*, ϕ_j^* gives rise to the linear system of ODEs of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\phi_j - \phi_j^*\right) = \boldsymbol{J} \cdot \left(\phi_j - \phi_j^*\right) + \boldsymbol{b}, \qquad \phi_j(t^*) = \phi_j^* \qquad j = 1, \ldots, N \tag{8}$$

Here $\boldsymbol{J}$ is the locally constant Jacobian matrix, and $\boldsymbol{b}$ is a locally constant vector. Standard linear systems analysis[98] shows that each local eigenmode of Eq. (8) evolves at a rate dictated by the eigenvalues of $\boldsymbol{J}$ and that local solutions take the form

$$\phi_j(t) = \phi_j^* + \{\boldsymbol{P} \cdot \exp[\boldsymbol{\Lambda}(t - t^*)] \cdot \boldsymbol{P}^{-1} - \boldsymbol{I}\} \cdot \boldsymbol{J}^{-1} \cdot \boldsymbol{b} \tag{9}$$

Here $\boldsymbol{P}$ is the matrix whose columns are populated by the right eigenvectors of $\boldsymbol{J}$, and $\boldsymbol{\Lambda}$ is the diagonal matrix whose diagonal is composed of the eigenvalues λ_j, $j = 1, \ldots, N$, of $\boldsymbol{J}$. This solution presumes that $\boldsymbol{J}$ can be diagonalized; if this is not possible, a related Jordan decomposition can be performed. The reciprocal of the real part of each eigenvalue λ_j gives the local timescale of evolution of each local eigenmode. Importantly, it can be shown that increasing the spatial resolution, thus increasing N, has the effect of introducing larger eigenvalues so as to increase their disparity, and thus the stiffness. Consequently, there are more timescales to resolve in a numerical solution.

It is Eq. (7) that is the departure point for a wide array of multiscale methods found in the scientific computing literature. It is well known that so-called time-explicit and time-implicit methods can be used to solve such systems. Both require a second discretization, here in time, with explicit methods using known values of ϕ_j to evaluate the right side of Eq. (7) and implicit methods using unknown values of ϕ_j to evaluate the same term. Explicit methods can be employed via relatively simple algorithms and do not place excessive demands on storage, but for numerical stability require that the discrete time step be of the order of the reciprocal of the largest eigenvalue of $\boldsymbol{J}$. For fine grids, this can become prohibitively expensive.

Implicit methods require more complicated solution algorithms, typically involving the iterative solution of a set of nonlinear algebraic equations, which places high demands on storage, with the advantage that much larger time steps can be used while retaining numerical stability. Most solution methods for nonlinear algebraic systems require repeated inversion of large matrices. The matrices that arise from stiff sets of ODEs have a large condition number, rendering their inversion computationally difficult. The matrices that arise from finite difference, finite element, or wavelet discretizations are usually sparse, which renders their inversion somewhat easier. In fact, the inversion of such sparse systems poses the critical computational multiscale challenge for a wide part of the scientific computing community. A large body of literature has arisen as a result.[99–102] Some of the key techniques are so-called Jacobi and successive-overrelaxation iterative techniques, Krylov subspace methods, and multigrid methods. As these methods often require iterative techniques that need to be truncated at some point, it is important to distinguish convergence of an intermediate iterative solver from convergence of the solution itself. For an approximate solution via a time-implicit technique to Eq. (1) to be converged, one must indeed have convergence of the iterative solver at each time step; in addition, one must use sufficient spatial resolution to insure the approximation to ϕ itself is converging.

Lastly, AMR methods must be mentioned. The literature on this is rapidly developing[103]; moreover, it is beginning to impact the combustion and detonation community.[67,88–90,104–108] The promise of these methods is that computational grids can be judiciously redistributed in such a fashion to maintain a small error of approximation. Precisely how to distinguish just what constitutes an error can pose challenges to an AMR strategy when no a priori knowledge of the exact solution exists. The idea is motivated by the fact that many flows have large regions of small variation, and, consequently, coarse discretizations can be tolerated in these regions. Likewise, in regions of steep gradients fine discretizations are necessary to capture the physics correctly. Unsteady detonation problems are challenging in that a dynamic adaptation is required in which the user cannot have a priori knowledge as to where to adapt. Thus, algorithms must be designed to automatically make decisions as to where to concentrate the discretization. This can pose serious challenges if the user wants to operate in a massively parallel environment. For flows with a small number of regions of steep gradients, AMR can be an effective tool to efficiently capture multiscale phenomena, with a

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potential gain of orders of magnitude in computational time relative to calculations performed on a uniformly fine grid. However, it is easy to imagine that in a complicated multidimensional detonation flowfield during which multiple reflections occur that the spatial domain could rapidly become saturated with interacting wavefronts, each of which would need to be resolved. Thus, for such problems, any AMR strategy would soon evolve into something close to a uniformly fine grid.

III. Sample Multiscale Detonation Results

This section will provide a compact review of some of the author's and coworkers' work in detonations that have a multiscale character. There is, of course, a wider literature on this topic, much of which is reviewed in the original source material.

A. Transition to Chaos with Simple Kinetics

Perhaps the simplest exposition of the multiscale character of detonations can be demonstrated with a classical model of unsteady one-dimensional detonation of a calorically perfect ideal gas whose irreversible exothermic reaction is described by one-step Arrhenius kinetics.[65] There is a long history of studying the linear[109,110] and nonlinear[111] stability of steady detonations predicted by this simple model; numerical studies of one-dimensional pulsating detonations are also beginning to appear for systems with detailed kinetics, although it is not clear that the finest scales have been resolved.[112]

Reference 65 considers the unsteady behavior of waves that have a Chapman–Jouguet (CJ) character when unsteady terms are neglected. Activation energy is taken as a bifurcation parameter. A standard case is considered in which the dimensionless heat release $q = 50$ and the ratio of specific heats $\gamma = \frac{6}{5}$. It is difficult to compactly describe the scaling parameters; a description is given in Ref. 65 and references therein. Results of unusually high accuracy are obtained by use of a novel shock-fitting scheme coupled with a new fifth-order spatial discretization.[113] In all cases, 20 points are taken to describe the so-called half-reaction zone length $L_{1/2}$, which is the length in the steady detonation structure at which the reaction progress variable takes on a value of $\frac{1}{2}$. Shock fitting is a viable method because only a single discontinuity ever appears in these flows. Consequently, there is no first-order corruption of the results as a result of shock-capturing effects of numerical viscosity, and the results have true fifth-order accuracy. This high-order accuracy enables the revelation of multiscale behavior in detonations, which is hidden in closely related studies done at lower order.[114,115]

For low activation energy, the steady detonation is hydrodynamically stable. As activation energy is increased, the detonation becomes unstable. While linear stability theory predicts more and more unstable modes at higher and higher frequencies as activation energy is increased, in this study the only cases considered are those for which the unstable behavior has as its origin a single unstable low-frequency mode as predicted by the linear stability theory. Within this confined range, interestingly, one finds a very different class of multiscale behavior: the dimensionless detonation wave speed $\bar{D}$ undergoes a classic period doubling behavior as activation energy is increased. That is to say, more and more low-frequency modes are exhibited. Consequently, to fully capture the behavior of the lowest frequency mode of oscillation, one must integrate for a long time over a large spatial domain; the largest scale admitted becomes ever larger with increasing activation energy, at least in the limited range studied.

This period doubling behavior is summarized in the bifurcation diagram of Fig. 3. This figure is qualitatively similar to bifurcation diagrams found in a wide variety of problems in nonlinear dynamics, for example, the famous logistics equation.[97] The bifurcation points accumulate with geometrically increasing frequency in the well-documented way of many chaotic systems. The Feigenbaum constant[116] for this accumulation rate is 4.66 ± 0.09, in close agreement to the known value of 4.669201. Moreover, for even greater values of activation energy there are windows of relative placidity, in that only a small number of oscillatory modes are present;

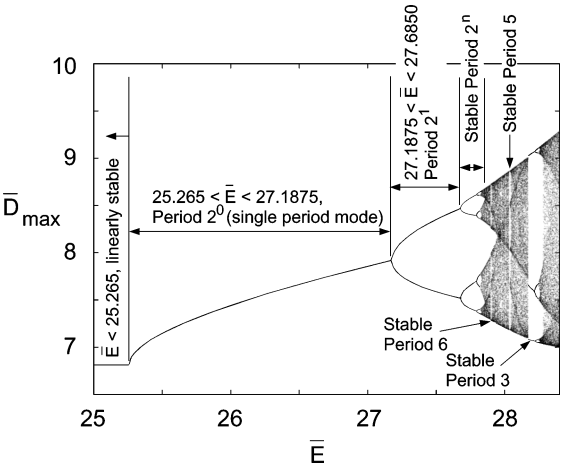

Fig. 3 Numerically generated bifurcation diagram $25 < \bar{E} < 28.4$ for one-dimensional inviscid detonation with one-step kinetics, adapted from Ref. 65.

again, this is entirely consistent with general theories of nonlinear dynamics. Figure 4 then shows numerical predictions of unsteady detonation wave speed $\bar{D}$ vs dimensionless time $\bar{t}$ for a variety of activation energies. For each of the activation energies, a different class of oscillation is predicted, including one that is chaotic.

B. Reaction Zone Length Scales for Steady Inviscid Models with Detailed Kinetics

Turing next to models with detailed kinetics, a recent study[66] has considered a standard one-dimensional model of steady inviscid CJ detonation in a hydrogen-air mixture using a model of nine molecular species and 19 elementary reactions. The model was identical in all respects to that used by Shepherd[117] as well as Mikolaitis,[118] and predictions were completely consistent with their results. The model was posed as a dynamic system of ODEs with the spatial coordinate x as the independent variable. A numerical solution of the ODEs gave a prediction of the reaction zone structure, shown in Fig. 5. In contrast to earlier results, Fig. 5 is plotted on a logarithmic scale, which better reveals the multiscale nature of this seemingly simple system. At small values of distance from the shock in the region known as the induction zone, the minor species are rapidly evolving over small length scales of less than 10^{-6} m. It is not surprising that this is similar to the length scale of molecular collisions as the constitutive theory for the detailed kinetics builds on a foundation from collision theory. The global effect of reaction evolves over a broader length scale of around 10^{-1} m. An eigenvalue analysis of the local Jacobian matrix, which characterizes the ODEs in space, reveals the precise values of the length scales in the steady detonation. Because the system has a finite number of ODEs, there are a finite number of length scales, each of finite value. These are plotted in Fig. 6. The smallest and largest, around 10^{-6} m and 10^{-1} m, respectively, predict well the small and largest scales seen in Fig. 5.

The implications of this study for unsteady modeling are disturbing. For the researcher to have full confidence in the predictions of a model with detailed kinetics, at a minimum a spatial grid resolution below that of the finest length scale must be captured. That is not the case in the bulk of the modern literature, and Ref. 66 lists recent calculations that are underresolved from one to five orders of magnitude. One must ask why the underresolved studies give results that at least seem plausible. We speculate that it is because combustion systems tend toward stable equilibria. Experience suggests that underresolved calculations approach the same equilibrium state as do resolved calculations, but at a rate dictated by numerical viscosity rather than the underlying mathematical physics model. It seems likely that a model that relies upon numerical viscosity to describe the finest scales runs the risk of improperly describing transient events such as ignition, DDT, and detonation instability. These issues remained to be explored fully.

This point is illustrated by the recent work of Fusina et al.,[91] which employs a Navier–Stokes model with detailed kinetics to

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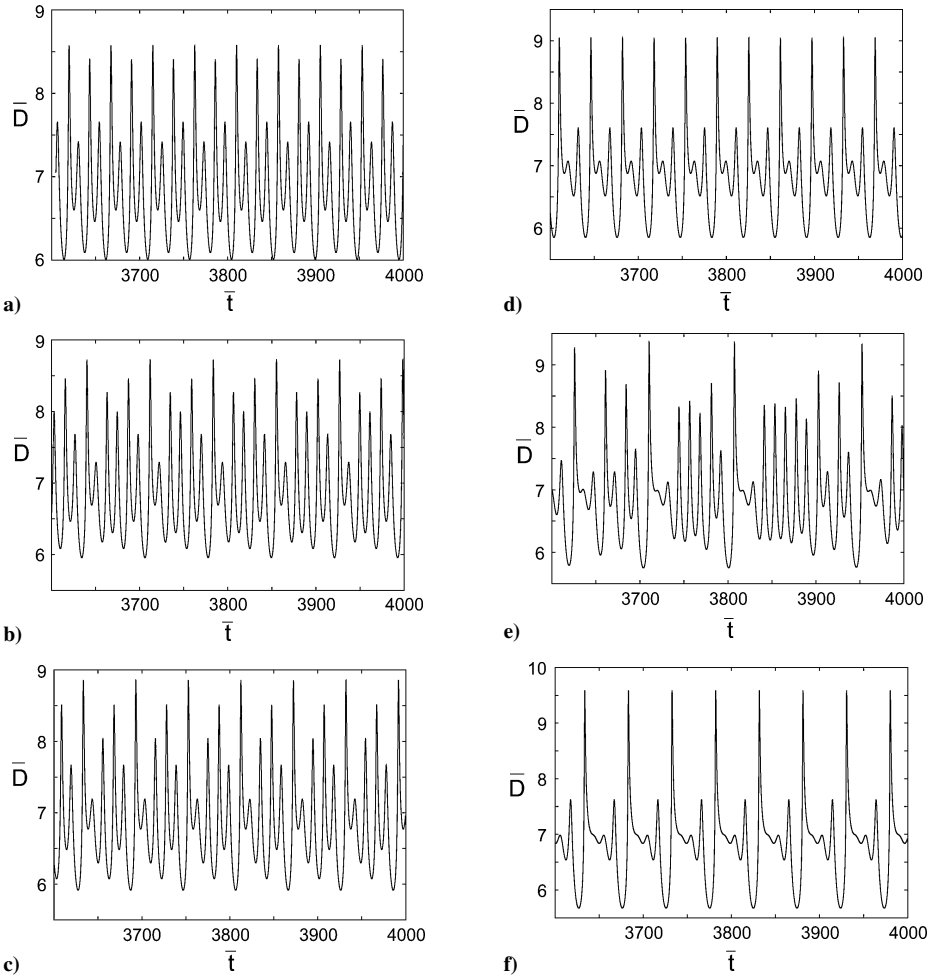

Fig. 4 Numerically generated detonation velocity $\bar{D}$ vs $\bar{t}$, using a fifth-order discretization coupled with shock fitting for one-dimensional inviscid detonation with one-step kinetics: a) $\bar{E} = 27.75$, period-4; b) $\bar{E} = 27.902$, period-6; c) $\bar{E} = 28.035$, period-5; d) $\bar{E} = 28.2$, period-3; e) $\bar{E} = 28.5$, chaotic; and f) $\bar{E} = 28.66$, period-3, adapted from Ref. 65.

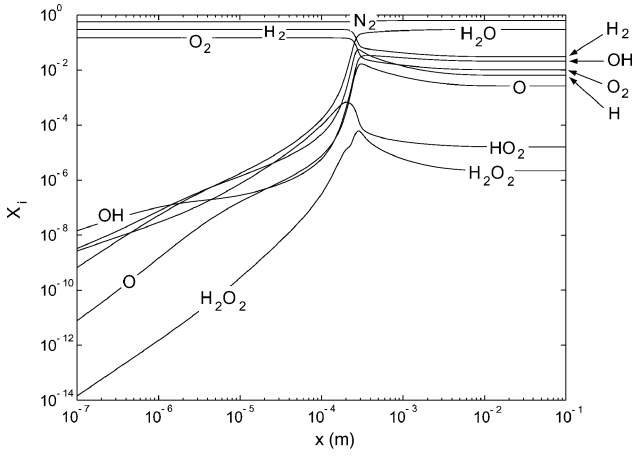

Fig. 5 Species mole fraction vs distance for steady CJ detonation in inviscid hydrogen-air mixture predicted by a one-dimensional steady model, adapted from Ref. 66.

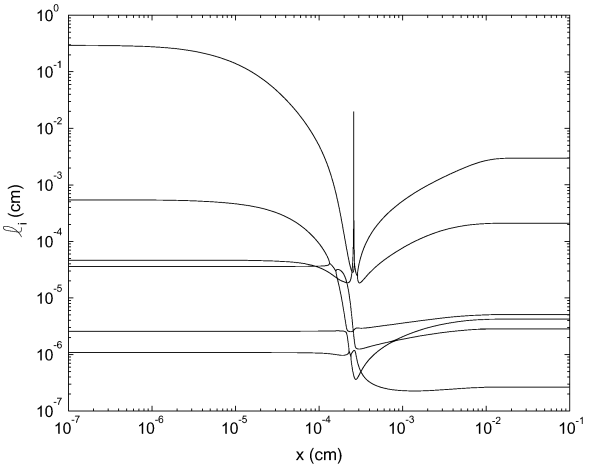

Fig. 6 Local length scales vs distance for steady CJ detonation in inviscid hydrogen-air mixture predicted by a one-dimensional steady model, adapted from Ref. 66.

study the stability of a two-dimensional Chapman–Jouguet oblique detonation wave (ODW). In their study, which is representative of the state of the art of detonation modeling for propulsion systems, the authors take the engineering approach of capturing device-length scales, but are not able to capture the finest viscous and reaction scales. In a detailed grid-resolution study, they conclude "The grid resolution ... is not fine enough to capture all the length scales present, such as the viscous shock thickness, but it is fine enough for determination of 'global' or macroscopic phenomena such as the ODW angle." Because determination of stability hinges upon proper resolution of length and timescales, it might be too early to conclude that such CJ waves are stable, and the authors are careful to qualify their conclusion on stability accordingly. Indeed, for flow of simpler fluid over the same geometry, resolved calculations of Grismer and Powers[119] show that a significant overdrive is necessary to stabilize inviscid oblique detonations predicted with one-step kinetics.

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C. Relaxation of Fast Timescale Kinetics with ILDM

When a fluid particle is both reacting and advecting, the length of the reaction zone is roughly given by the product of the advection velocity and the reaction time. The small reaction zones of the preceding section are direct consequences of fast reactions. One important strategy to reduce the multiscale challenges of reactive fluid mechanics is to develop reduced kinetic models. Unfortunately, most of the well-known methods, for instance, those involving so-called steady-state and partial equilibrium assumptions, come with no guarantee that they can robustly capture the results of the detailed kinetic models; that is to say, in such approaches there is no systematic way to adjust parameters so as to converge to the full kinetics solution. Moreover, even after these approaches have been applied, there is no guarantee that fast timescale events have truly been filtered from the system.

The relatively new ILDM[83] and the related computational singular perturbation[84] methods offer a rational approach to systematically reduce detailed kinetics models to simpler systems. The method is built around spatially homogeneous systems and thus focuses on filtering fast timescale events. The method relies on locally linearizing the ODEs that describe the temporal evolution of the reactive system so as to find a local Jacobian matrix. An eigendecomposition of the Jacobian matrix reveals an ordering of reactions from fastest to slowest along with the directions in composition space associated with fast and slow modes. A slow manifold is then constructed by forcing the manifold to lie orthogonal to all of the eigenvectors associated with the fast modes. The dimension of this manifold is chosen by the modeler.

One can then model the behavior of the spatially homogeneous reactive system by projecting from an arbitrary initial condition to a point on the manifold, thus avoiding the small time steps associated with the fast dynamics. One lets the system evolve only on the manifold, where the timescales are relatively slow, and inexpensive explicit methods can be used to calculate the time variation. A small error is introduced in neglecting the fast timescales; if the initial condition is too far from the ILDM, the error can be large, and special care must be taken to avoid this.

Figure 7 shows a projection of a composition space for the mass fraction Y of two of the species of a nine-species, 37-step mechanism that describes combustion in H_2-O_2-Ar systems.[67] Here, the equilibrium point, which can be thought of an ILDM of dimension zero, is calculated a priori as is a one-dimensional ILDM. Also shown are projections of several trajectories, each of which first relax to the one-dimensional ILDM and then to the equilibrium point. On each trajectory an $\times$ is plotted at equal time intervals. It is seen that these

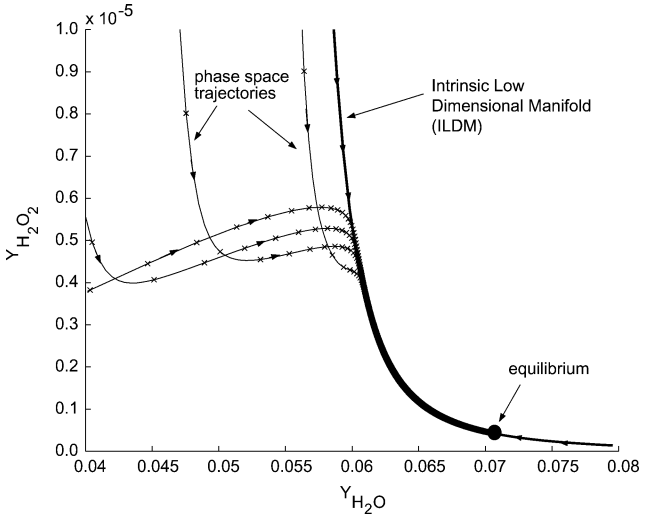

Fig. 7 ILDM projection for a nine-species, 37-step reaction mechanism of spatially homogeneous H_2-O_2-Ar combustion as a function of Y_{H_2O} along with trajectories from full time integration showing relaxation to the manifold and equilibrium. The symbol $\times$ denotes equally space 0.10-μs time intervals. Total time to relax to equilibrium is near 0.1 ms, adapted from Ref. 67.

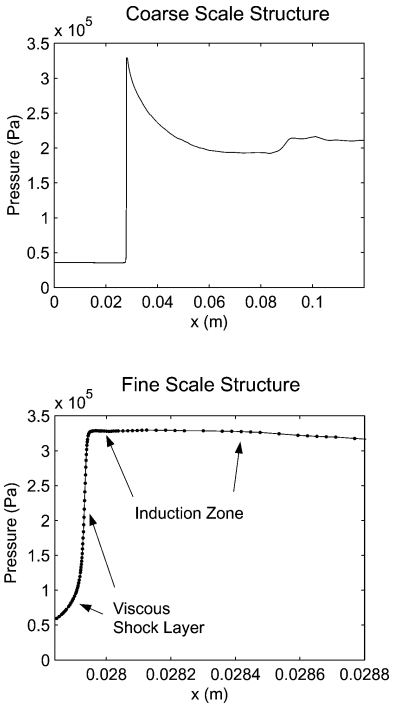

Fig. 8 Predictions of pressure vs distance at coarse and fine length scales for one-dimensional viscous detonation of H_2-O_2-Ar with detailed kinetics model, ILDM kinetics reduction, and wavelet adaptive multilevel representation, adapted from Ref. 67.

agglomerate near the ILDM, indicating that the bulk of the time is spent on the ILDM. The same approach can be used to generate ILDMs of higher dimension, which can capture progressively more timescales.

An a priori knowledge of the manifold can be employed in a spatiotemporal calculation to reduce computation time at the expense of a small error. This particular ILDM was used in a Navier–Stokes detonation calculation,[67] and the results are shown in Fig. 8, which gives a plot of pressure vs distance at two highly disparate spatial resolutions. In the fine-scale structure plot, the dots indicate the predictions utilizing the ILDM method, and the solid line gives the results of the full kinetic model. At this scale, they are indistinguishable, but there is a small difference. For this calculation, enough points were sufficiently close to the ILDM to enable a reduction in computational time of a factor of about two. For systems that were closer to equilibrium throughout the domain, this efficiency gain could be much larger.

D. Detonation for Unsteady Viscous Models with Detailed Kinetics

In addition to describing the ILDM method, Ref. 67 also exposes other multiscale features of detonations. This study considered a Navier–Stokes model and thus admitted shocks of finite thickness. Here the thickness was a function of the physical viscosity and not the numerical viscosity. The viscous layer associated with the shock is thin, as seen in Fig. 8, which shows in its bottom half a microscale portion of the macroscale given in the top half. The viscous layer actually overlaps with some of the finest reaction zone lengths but is distinct from the better understood induction zone.

These calculations were enabled by a relatively new adaptive method known as the wavelet adaptive multilevel representation (WAMR). To briefly summarize this complex method, a given set of initial conditions is projected onto a basis of wavelet functions. These functions have localization in both physical and wave-number space. Basis functions whose amplitude is below a threshold value are discarded, except for those in the near neighborhood of the threshold. For systems such as this one that contain a small number of zones with steep gradients, this projection and filtering greatly reduces the number of equations that need be solved, as well as the associated stiffness. The system is then evolved in time. If wavelet

amplitudes fall below the threshold value, they are discarded. Those in the near-threshold region whose amplitudes were calculated are checked to see if they cross the threshold, and if so, they are included in the next calculation. As a result of this WAMR method, the entire one-dimensional unsteady viscous detonation with detailed kinetics was represented by no more than 3×10^2 collocation points at any given time. Had the same calculation been performed on a spatially uniform grid, approximately 10^7 collocation points would have been required to achieve the same accuracy. Had a similar calculation been performed in multiple dimensions, the efficiency of the WAMR method, relative to a uniform mesh, would have been even greater.

E. Two-Dimensional Detonation Structures with Simple Kinetics

A common practice in detonation calculations is to ignore diffusion processes and only consider convection and reaction. In multidimensional detonation studies, such as those of Bourlioux and Majda[120] or Williams et al.[121] visually striking detonation structures have been predicted with reactive Euler models. Recent studies[122,123] have further highlighted the detailed spatiotemporal structures present in seemingly simple phenomena as detonation corner-turning predicted by inviscid one-step models.

However, as continuum models of reaction and diffusion both have molecular collision models as their foundation, and both models predict relaxation on the same length scales, it is difficult to physically justify neglecting diffusion without also neglecting reaction. Nevertheless, as it is commonly done, its consequences should be analyzed. One recent simplified analysis was given by Singh et al.[69] There, a simple one-step chemistry model for the unsteady two-dimensional behavior of a calorically perfect ideal gas nearly identical to that considered by Short and Stewart[124] was considered under the conditions found in Ref. 124 to contain one linearly unstable mode. In contrast to Ref. 124, Ref. 69 considered both viscous and inviscid models. The physical viscosity in the Navier–Stokes model was adjusted so that the viscous layers were roughly one-tenth the length of the global reaction zone length. Both the Euler and Navier–Stokes models were subjected to a grid-refinement study, and the results are summarized in Fig. 9. In the Euler calculations, intrinsic numerical viscosity, which depends on the size of the grid and the details of the particular numerical method chosen, always plays a large role in selecting the flow structures that evolve at and downstream of the shock. In the Navier–Stokes calculations at coarse resolutions, the same artificial viscosity dominates the physical viscosity, and the structures depend on the grid. As the grid is refined for the Euler calculations, the artificial viscosity decreases, and fewer downstream instabilities, such as the Kelvin–Helmholtz instability, are suppressed. Thus, it is possible to see ever-finer downstream structures in Fig. 9. At coarse resolutions in the Navier–Stokes model predicts similar results as the Euler model. In this case, the inherent numerical viscosity of the method dominates the physical viscosity. However, as the grid is refined in the Navier–Stokes calculations, the physical viscosity comes to dominate the numerical viscosity, and no finer scale structures are apparent. The sensitivity of our results to resolution is in general agreement with the recent related study of Tegnér and Sjögreen.[125]

Clearly, the downstream structures in detonations are influenced by the amount of viscosity, real or numerical present. Moreover, these difficulties are entirely analogous to those reported by Kadanoff,[3] which depend on a numerical viscosity in inviscid calculations of a Rayleigh–Taylor instability; Ref. 3 concludes, "The practical meaning is that we cannot promise different approximation approaches will converge to the same answer, and that any one of those will correspond to the experimental system." The most

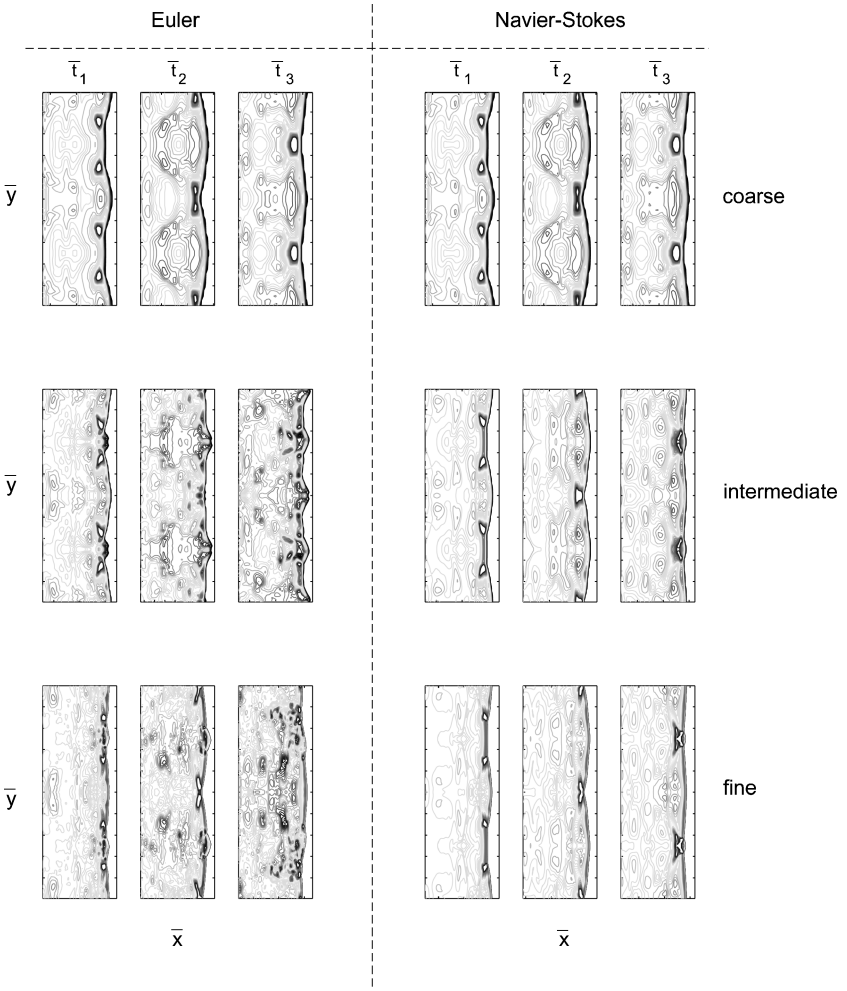

Fig. 9 Isochores at three different spatial resolutions at three different times, $\bar{t}_1, \bar{t}_2, \bar{t}_3$, for two-dimensional Euler and Navier–Stokes detonation with one-step Arrhenius kinetics. Domain for each simulation, $\bar{x} \in [0, 15]$, $\bar{y} \in [0, 20]$, adapted from Ref. 69.

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straightforward remedy is to employ physical viscosity and refine the grid so that it dominates over numerical viscosity. However, Ref. 126 has noted that the dynamics of the leading shock, which are those that determine the patterns etched on walls that have long been observed in experiment, seem to be insensitive to the magnitude of artificial viscosity in Euler calculations. Although fortuitous, there is no guarantee that this result will extend to other important issues. Also, as noted in Ref. 127, one will in very special cases find that numerical viscosity captures the effects of physical viscosity. However, with no a priori standard of what a viscous structure should be, it is unlikely that one could discern that grid resolution would lead to the correct calculation, and so this does not appear to be of great practical interest.

IV. Detonation Propulsion Implications

What then are the implications for detonation applications in propulsion? In the most general sense, the answer cannot be known with certainty until one has performed calculations that actually capture the full multiscale nature of the flow, from molecular collision scales to device scales. However, it is possible to offer some speculation. It must be said that many important parameters for system performance, such as steady detonation wave speed and final detonation pressure, do not have a strong dependence on multiscale dynamics and instead depend mainly on thermodynamic properties. However, whenever transient events are relevant, such as in ignition, a proper capturing of the multiscale space and timescales is critical to predict device performance.

Consider, for example, the pulse detonation engine.[41] This engine relies upon the successful initiation of a detonation at a rate of many cycles per second. In developing models for such devices, an understanding of the ignition and DDT behavior is critical. Models of actual reactive mixtures have heretofore not had great success in this prediction.[49] One cannot yet rule out a failure to capture the multiscale nature of the ignition/DDT process as a reason for this lack of success. In short, one must resolve the local timescales for chemical power deposition and radical generation relative to the local acoustic timescales in the spatial domain in which the transient events are evolving. One might expect inertial confinement for fast timescale events and wave generation for slower events. Many recent studies of pulse detonation engines have focused on the use of small geometric obstacles, such as Schelkin spirals, to enhance the DDT process. Modeling of how shocks and detonations diffract around such small-scale barriers so as to induce ignition is a process in which multiscale physics clearly play a large role. Successful transmission of a detonation from a large tube to a small tube without inducing extinction is an issue in pulse detonation engines. And once again, a proper numerical capture of this highly transient multidimensional effect represents a challenge for multiscale methods. Another issue relating to the pulse detonation engine is the issue of cellular detonation instability and transverse waves. Although such waves can be predicted with models of one-step kinetics, much uncertainty remains with regard to models of detailed kinetics to be able to match the well-known results of fundamental experiments. It is again likely that the present-day inability to capture fine-scale phenomena lies at the heart of our inability to correctly predict these structures. Certainly, one can say that grid-refinement studies in one-step kinetic models reveal that the structures are sensitive to a proper resolution of the reaction zones, and the same is likely true for models with detailed kinetics. As a pulse detonation engine relies for thrust on the axial transmission of impulse, any impulse diverted to transverse modes is that which cannot be used to generate thrust, and so any theory that can suggest how that impulse can be directed in a useful way will have value.

Similar comments could be made with regard to the ram accelerator, the oblique detonation wave engine, and other devices. In any device in that detonations must be initiated, where they can diffract, where the detonation becomes unstable, or where extinction could exist, an understanding of the fundamental science of multiscale detonations has direct ramifications for device performance.

All this said, it must be remembered that not all calculations are done for engineering design, and, as subtly argued by Kadanoff,[128] that some numerical solutions can be both "inaccurate and important." Such a notion, detailed in his article which highlights astrophysical detonation, is not inconsistent with that of Buckmaster,[129] who holds for more conventional systems, "Modelers write down false equations and extract useful, physically relevant information from them." Nor is it inconsistent with Williams'[130] trio of maxims: "Theory needn't be right to be good...Theory needn't be mathematical to be right...Theory needn't be incomprehensible to be mathematical." None are arguing for inaccurate design calculations relative to the highly desirable verified and validated prediction.[131,132] Instead, they remind the reader that if enhanced scientific insight is the goal of the calculation, that such an end can be achieved by making, what are for design purposes, inaccurate calculations.

V. Conclusions

It is clear that observable detonation physics is richly complicated with spatial and temporal structures evolving on a wide range of scales. It is also clear that the nonlinear continuum theories that are commonly used to mathematically model these physics have the ability to predict many of the basic observable quantifiable features, such as one-dimensional detonation wave speeds, as well as some qualitative details, such as cellular structures.

How to explain those differences that remain, in evidence in the "widely different outcomes" of Ref. 31, is a grand challenge. One plausible hypothesis is that the underlying continuum mathematical models are in fact correct and that it remains for us to devise better ways to truly capture all of the scales these models admit. Such is the nature of the mathematical exercise known as verification.[131,132] Only after a model has been verified is it appropriate to ask the deeper scientific question regarding validation: do the equations accurately predict what is observed in experiment? In short, verification considers if the equations were solved correctly, and validation considers if the correct equations were solved. And if a verified model cannot be validated, it is only then suitable to begin to question the modeling assumptions, constitutive theories, and material property values. The practice of harmonizing mathematically unverified calculations with experimental observation by tuning adjustable parameters is too common and often leads to models that are at best "postdictive" rather than the preferred "predictive." Such hasty calculations, when otherwise done carefully, occasionally serve immediate needs, but do little to further the progress of scientific aeropropulsion design, nor do they do much to advance fundamental science. At best they provide a useful tool to interpolate experimental results. At worst, calculations performed with intemperate attention to both verification and validation serve neither science nor engineering and can, in extreme cases, pose a real danger to those who rely on such calculations.

To conclude, the science-based engineering design process requires significant effort, as do most enterprises that seek to truly expand the frontiers of what can be achieved. Indeed, it will take some time and further advances in both hardware and algorithms before first principles models that are both verified and validated will be able to be used with confidence to quantitatively predict, with no a priori knowledge of the outcome, the detailed behavior of detonation-driven propulsion devices. At a minimum for the present, one can hope that the varied communities involved in this enterprise can appreciate the challenges and limitations imposed by the multiscale physics on both theories and computational methods. But it should also be realized that tremendous progress has been made in the past in expanding the spectrum of scales that can be modeled, and there is no reason why we should not continue to seek new ways to expand them even further.

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