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1 Major research accomplishments

1.1 A new shock-fitting algorithm for reactive Euler equations

We have developed a new shock-fitting algorithm that is based on a coordinate transformation to a shock attached frame. We derived a new evolution system for the shock dynamics from the analysis of the Rankine-Hugoniot conditions and used it coupled with the Euler equations behind the shock to solve for the dynamics of detonation with high accuracy. Our algorithm eliminates numerical errors due to shock capturing (i.e. Gibbs oscillations and shock smearing) at the lead shock and thus makes the order of accuracy of the method controlled purely by the discretization algorithm in the post-shock flow. Our present implementation is a high-order WENO shock-capturing method for the entire system. Most of the calculations reported in our main paper [17] use a third order spatial and temporal discretizations of the whole system and show overall third order accuracy.

The main idea of the proposed numerical approach is based on a coordinate transformation of the reactive Euler equations to a frame attached to the lead detonation shock with subsequent solution of the postshock flow as well as the evolution of the lead shock. A key advantage of the method is that the coordinate transformation is exactly the same as in the theories of detonation linear stability but without linearization. This allows for a simple and direct calculation of linear stability properties and their comparison with theoretical predictions.

The reactive Euler equations of inviscid gas dynamics ([17, 6]):

$$v_t + \mathbf{u} \cdot \nabla v - v \nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} + \nu \nabla p = 0, \tag{2}$$

$$p_t + \mathbf{u} \cdot \nabla p + \rho c^2 \nabla \cdot \mathbf{u} = \rho c^2 \sigma \omega, \tag{3}$$

$$\lambda_t + \mathbf{u} \cdot \nabla \lambda = \omega, \tag{4}$$

are coupled with the Rankine-Hugoniot conditions

$$M = -\rho_a D_n = \rho_s U_{ns},\tag{5}$$

$$P = p_a + M^2 v_a = p_s + M^2 v_s, (6)$$

$$D_{\tau 1} = U_{\tau 1s}, \qquad D_{\tau 2} = U_{\tau 2s}, \tag{7}$$

$$H = e_a + p_a v_a + \frac{1}{2} M^2 v_a^2 = e_s + p_s v_s + \frac{1}{2} U_{ns}^2,$$
(8)

where $D_n = Mv_a$ is the speed of the shock normal to itself, $D_{\tau 1}$ and $D_{\tau 2}$ are the tangential velocity components of the incoming flow for an observer moving with the shock, and U_n , $U_{\tau 1}$, $U_{\tau 2}$ are the components of the post-shock particle speed relative to the shock. Subscripts *a* and *s* identify the ambient state immediately ahead of the shock and the state immediately behind the shock, respectively. The shock state is completely determined by the normal mass flux *M* and the shock slope (which enters the definitions of the velocity components.) Therefore, the shock dynamics will be completely determined if we can solve for the postshock flow as well as the shock state, given by M and the shock slope.

If $\Phi(x, y, z, t) = 0$ is the equation of the shock surface, then the evolution of the surface in space-time is governed by the level-set equation

$$\Phi_t + \mathbf{D} \cdot \nabla \Phi = 0, \tag{9}$$

where **D** is the surface velocity vector. The unit outward normal to the surface is given by $\mathbf{n} = -\nabla \Phi / |\nabla \Phi|$, and with $\mathbf{D} = D_n \mathbf{n}$ the normal mass flux across the surface is

$$M = \rho_a \frac{\Phi_t}{|\nabla \Phi|}.\tag{10}$$

The second equation needed for the shock evolution calculation comes from differentiating the Rankine-Hugoniot conditions. We differentiate the post-shock state variables, p_s and \mathbf{u}_s , in time and relate their derivatives to the flow gradients at the shock by means of the Euler equations. We arrive at

$$\frac{\partial p_s}{\partial t} - \rho_s \mathbf{U}_s \cdot \frac{\partial \mathbf{u}_s}{\partial t} = \left[(\gamma - 1) Q \rho \omega - \rho c^2 \nabla \cdot \mathbf{u} + \rho \mathbf{U} \cdot (\mathbf{U} \cdot \nabla) \mathbf{u} \right] |_s, \tag{11}$$

where $\mathbf{u} - \mathbf{D} = \mathbf{U}$ is the particle velocity relative to the shock.

Equation (11) together with (10) can be solved for M and Φ provided the gradient of the postshock velocity vector is known. Once M and Φ are known, all the shock-state variables can be calculated through the Rankine-Hugoniot conditions. In principle, this idea can be applied in any geometry thus forming a foundation for a generalized DSD method, but so far the method has been implemented only in a channel geometry and a one-dimensional spherical/cylindrical geometries.

In channel geometry, the Euler equations with a one-step chemical reaction are

$$\frac{\partial \mathbf{Y}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{Y})}{\partial x} + \frac{\partial \mathbf{G}(\mathbf{Y})}{\partial y} = \mathbf{S}(\mathbf{Y}), \qquad (12)$$

where the vectors representing the state variables \mathbf{Y} , x-fluxes \mathbf{F} , y-fluxes \mathbf{G} , and the source term \mathbf{S} are

$$\mathbf{Y} = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho e_t \\ \rho \lambda \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \rho u_1 \\ p + \rho u_1^2 \\ \rho u_1 u_2 \\ u_1 (\rho e_t + p) \\ \rho u_1 \lambda \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} \rho u_2 \\ \rho u_1 u_2 \\ p + \rho u_2^2 \\ u_2 (\rho e_t + p) \\ \rho u_2 \lambda \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho \omega \end{bmatrix}.$$
(13)



Figure 1: Schematics of the mapping and coordinate transformation to the shock attached frame: (a) - the actual shock shape in the physical plane; (b) - the shock in the mapped computational domain.

In an ideal gas, the total energy e_t is the sum of the internal, chemical, and kinetic energies as $e_t = \frac{pv}{\gamma - 1} - \lambda Q + \frac{u_1^2 + u_2^2}{2}$. We also take one-step irreversible Arrhenius reaction rate law, $\omega = k(1 - \lambda) \exp\left(-\frac{E}{pv}\right)$.

After collecting all the terms in (11) and (10), we derive the following shock evolution system

 $\mathbf{y}_t + \mathbf{f}_y = \mathbf{s},\tag{14}$

where

$$\mathbf{y} = \begin{bmatrix} M \\ \psi \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} 0 \\ -\nu_a \sqrt{1 + \psi^2} M \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} s \\ 0 \end{bmatrix}, \quad (15)$$

and

$$s = s(M, \psi, \mathbf{q}) = \frac{1}{A_0} (R_s - A_s),$$
 (16)

$$A_0 = \frac{2}{\gamma + 1} M v_a \left(3 + \frac{i_a}{M^2} \right), \quad R_s = (\gamma - 1) Q \rho_s \omega_s, \tag{17}$$

$$A_{s} = \rho_{s} \left[\left(c_{s}^{2} - U_{s}^{2} \right) q_{11} + \left(c_{s}^{2} - V_{s}^{2} \right) \left(q_{22} + \psi q_{21} \right) - U_{s} V_{s} \left(q_{12} + q_{21} + \psi q_{11} \right) \right].$$
(18)

Here $q_{ij} = \partial u_i / \partial x_j$ are the components of the velocity-gradient tensor evaluated at the shock $((x_1, x_2) = (x, y))$. Importantly, (14) is exact. In general, **q** is not known in terms of y, but we approximate it based on a previous time step in a numerical algorithm. Away from the lead shock,

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we integrate the Euler equations in their conservative form, which is preserved under the coordinate transformation to the shock-attached frame:

$$\mathbf{Y}_{t} + \left[\mathbf{F} + M v_{a} \sqrt{1 + \psi^{2}} \mathbf{Y} + \psi \mathbf{G}\right]_{x} + \mathbf{G}_{y} = \mathbf{S}.$$
(19)

The algorithm has been implemented in parallel Fortran 90/95 with MPI. Most of the calculations have been carried out on an 88 core Linux cluster at UIUC and took 10-20 hours to complete. Despite the fact that the method computes only the regions of interest (i.e. does not calculate the unreacted state ahead of the shock or the completely burnt state far behind it,) the computational resources required for well-resolved simulations are still extensive. This is a well-known challenge in detonation simulations and is a reflection of a very complex dynamics of flow within the reaction zone. A typical plot of the computed detonation structure is shown in Figure 2.

1.2 Validation of theoretical predictions of two-dimensional detonation instability

So far, we have performed the first detailed testing of detonation stability theory in two dimensions. With moderate resolution of about 40 points per half-reaction zone, we have been able to compute the growth rates and frequencies of instability in excellent agreement with theoretical predictions based on the normal-mode analysis of Short and Stewart [14]; our main results appear in [17].

The governing equations for the flow variables in the shock attached frame and shock evolution equations were discretized on a two-dimensional finite volume grid and a one-dimensional finite volume grid, respectively. Spatial fluxes of the flow variables and the flux in the shock slope equation were computed using a fifth-order WENO scheme [15]. A third-order TVD Runge-Kutta scheme was used for temporal discretization. The numerical fluxes at the x-face nearest the shock require special treatment, as we do not want to compute the flux interpolants using data from ahead of the shock. In this case, the interpolant weights corresponding to the stencil that extends ahead of the shock are set to a very small value so that the reconstructed fluxes are based only on the solution within the computational domain.

The spatial discretization scheme is shown schematically in Figure 3. The figure illustrates that the shock mapping variables, M and ψ , are stored in a one-dimensional grid along the y direction. The velocity gradient tensor **q** in the mass flux equation is computed using one-sided and centered finite-differences in the x and y directions, respectively. The cell-centered grid points used to compute the velocity gradients in the shock-normal direction are indicated by filled black circles, while the points used to compute the velocity gradients in the shock-normal direction are indicated by filled black circles.

A weakly unstable two-dimensional detonation with particularly simple unstable behavior was one of the cases examined by Short and Stewart [14], and is used as a point of comparison here to verify the simulation results. The model parameters are $\gamma = 1.2$, Q = 0.4, f = 1.2, and E = 50. This case is one-dimensionally stable and two-dimensionally unstable over a small range of transverse disturbance wavenumbers, see Figure 4.

Simulations were performed in channels of width 2.1 to 7.8 with solid wall boundary conditions at a resolution of 30 grid cells per unit length. In each simulation, the longest admissible wavelength was perturbed(w = 2W). The resulting transverse disturbance wavenumbers cover the entire unstable range for this case. Dispersion relations can be constructed from the computed growth rates and frequencies, as shown in Figure 4. As can be seen from the figure, the agreement with linear stability theory is excellent. Another example, now with a more complex dispersion relation is shown in Figure 5.



Figure 3: Spatial discretization. Shock surface is gray. Finite difference stencils for x and y velocity derivatives at shock are denoted by black and white circles, respectively.



Figure 4: Dispersion relations. Linear stability (solid line), simulation (circles). Model parameters: $\gamma = 1.2, Q = 0.4, f = 1.2, E = 50.$

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Figure 5: Comparison of numerically computed spectra with linear stability results. Model parameters: $\gamma = 1.2$, Q = E = 50, f = 1.8.

1.3 Extension of the algorithm to complex chemistry

The algorithm can be extended to include multiple-step chemical mechanisms by replacing in the shock dynamic condition the energy release rate (product of thermicity and reaction rate) for the single reaction with the net energy release rate for several reactions (a sum of all thermicity and reaction rate products.) This multi-step reaction scheme was implemented in a modified version of SAF2D code and used to compute 2D linear stability results of a detonation model consisting of an ideal EOS and a three-step chain-braching reaction mechanism [13],

$$F \to X, \qquad \omega_1 = \exp\left(-E_I\left(\frac{1}{T_I} - \frac{1}{T}\right)\right),$$

$$F + X \to 2X, \qquad \omega_2 = \exp\left(-E_B\left(\frac{1}{T_B} - \frac{1}{T}\right)\right),$$

$$X \to P, \qquad \omega_3 = 1.$$

The shock dynamic condition for complex chemistry is generalized as follows

$$\frac{dp_s}{dt} - \rho_s \mathbf{U}_s \cdot \frac{d\mathbf{u}_s}{dt} = \left[\rho c^2 \sum \sigma_i \omega_i - \rho c^2 \nabla \cdot \mathbf{u} + \rho \mathbf{U} \cdot (\mathbf{U} \cdot \nabla) \mathbf{u}\right]_s, \\ \sigma_i = -e_{\lambda_i} / \left(\rho c^2 e_p\right),$$

while the kinematic condition is unchanged. Required modifications for the code are minimal.



Figure 6: Numerically computed spectra of linear instability for detonation with a model three-step chain branching chemistry with $E_I = 20$, $E_B = 10$, $\gamma = 1.2$, f = 1, Q = 3, $T_I/T_B = 3$, $T_B/T_s = 0.9$ [13].

A particular case is shown in Figure 6. These results have been presented at 2009 ICDERS meeting [11] and are being prepared for a journal publication. They are also a part of the doctoral thesis of B. Taylor [16].

1.4 Application to radially expanding detonations

For radially expanding detonations, we need to add a divergence term to the thermicity in the equation for the mass flux (16), so that s becomes now $s = (R_s - \rho_s c_s^2 u_s \kappa - A_s)/A_0$, where the shock curvature is $\kappa = j/r$ with j = 1,2 for cylindrical and spherical detonation, respectively. This modification was implemented in SAF1D and used to verify DSD results by taking the DSD solution as an initial condition for the direct simulation. For example, the simulation results have shown that $\dot{D} \sim 0$ on the D-kappa curve. The scheme was also used to study the instability of DSD solutions that have turning points. It was demostrated that the middle branch of a $D - \kappa$ curve with turning points is highly unstable and, in the case of an ideal EOS and one-step reaction mechanism, results in a rapid transition ("ignition") to a strong detonation on the upper branch, see Figure 7. This is the first calculation of such a solution using the DSD solution from the middle branch as an initial condition. Ongoing efforts, as part of B. Taylor's PhD thesis, include comparisons between the simulation results from unstable DSD solutions with linear stability theory of a curved



Figure 7: Calculations of the dynamics of a curved detonation with SAF1D and comparisons with DSD predictions. Simulations were started at the $D - \kappa$ curve and continued using SAF1D. Both ignition from the middle branch and stable settling to the CJ detonation from the upper branch of the $D - \kappa$ curve is observed.

detonation.

Our algorithm is ideally suited for direct calculations of detonation shock dynamics using the same variables as those used in DSD theories [2, 1, 8, 10], namely shock acceleration \dot{D} , speed D, and curvature κ of the front. This provides a useful tool for verification of results of DSD theories, which are otherwise hard to test.

1.5 Formulation for non-ideal equations of state

Our shock-attached frame formulation admits a generalization to a non-ideal equation of state as well and thus to realistic models of high explosives. Complications arise in the shock dynamic condition primarily because of the need to calculate the left-hand side, which involves time derivatives of the shock state variable. Now the left-hand side will be proportional to M_t with a factor that involves the terms dp_s/dM and du_s/dM , which cannot be computed analytically for a general EOS. Instead, the scheme implemented in SAF1D numerically approximates these derivatives using a central finite difference of solutions to the Rankine-Hugoniot relations. This scheme was tested against the analytical solution for an ideal EOS and yields results that are in very good agreement. Thus the only complications due to non-ideal EOS are of algebraic nature and require no new derivations of the shock evolution equations. This work is ongoing and is also a part of Brian



Figure 8: Computed modal content of the detonation shock perturbation showing the most unstable dominant mode together with the secondary modes. The linear stability results, namely the growth rate and frequency, are extracted from these data. Initially linear growth of perturbations evolves into a non-linear regime where mode interactions lead to changes in the modal growth rates [17].

Taylor's PhD dissertation [16]. The non-ideal EOS that is being implemented is the wide-ranging EOS of Wescott, Stewart, and Davis [18].

1.6 A method for direct calculation of detonation instability spectra

One of the most important achievements of our research is a new, direct method for calculation of detonation linear stability properties for arbitrary constitutive laws [11]. The kinematic condition (10) is independent of the details of chemistry and equation of state. At the same time, as described above, the dynamic condition can be easily generalized to arbitrary constitutive laws [16, 12, 3]. Thus the method can be used to compute linear growth of instability of any reactive system with any chemical reaction mechanism. Although computational demands will still be high, at present this is the only available general method for calculating detonation stability spectra. It must be pointed out that the detonation stability theory, first formulated by Erpenbeck in 1960s [4, 5], is still being developed for general constitutive laws 50 years later. There are major theoretical and numerical difficulties associated with the normal-mode formulation of detonation stability theory

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stemming from the complexity of the far-field radiation conditions and problems with stiff numerical ODE and root solvers. These problems are completely absent in the direct numerical solution of the stability problem, because our method computes the evolution of small perturbations of the *full* exact reactive Euler system employing the *exact* Rankine-Hugoniot conditions and requiring no radiation conditions. In contrast, the normal mode analysis computes the solutions of the *linearized* Euler equations and requires knowledge of the complicated behavior of the solution in the neighborhood of the frozen sonic state. Our ongoing research efforts are directed to creating a unified framework for calculation of the reactive Euler equations in the shock attached frame in 1,2, or 3 dimensions with subsequent postprocessing that analyzes the simulation results to extract the growth rates, frequencies, and eigenfunctions from the growth of small perturbations.

1.7 Development of detonation analogs

We have discovered that there exists a number of phenomena that are analogous to the Chapman-Jouguet detonation wave in terms their structure consisting of a shock followed by transonic flow. Two of such phenomena, a circular hydraulic jump [9] and a traffic jam [7], have been investigated in detail. It was shown that both in traffic jam and the hydraulic jump, the theory of the steady solution is similar to the Zel'dovich-von Neumann-Doering theory of detonation [6]. In both cases, the steady structure is found by solving the underlying hyperbolic system, imposing the shock conditions and sonic (CJ) conditions. Unlike the detonation wave, these phenomena are described by a system of two partial differential equations and is thus simpler to analyze. Nevertheless, going beyond the steady state solutions leads to serious challenges having to do with the behavior of solutions near the sonic locus. Our continuing efforts are directed towards understanding the formulation of the initial boundary value problems for such systems and the regularity of their solutions. This appears to be a major mathematical challenge with wide-ranging implications for a large number of applications where self-sustained shocks are possible, not only in shallow-water systems and traffic flows, but also in certain astrophysical flows (accretion shocks,) flows in flexible tubes, two-phase flows, and others.

The analogy is seen in the main properties of the shallow-water and traffic-flow systems [9, 7]:

$$\mathbf{u}_t + \mathbf{F}_x = \mathbf{s}.$$

In both cases, a traveling wave solution exists of the form, $\mathbf{u} = \mathbf{u} (x - st)$, and the resultant system of ordinary differential equations reduces to a single differential equation,

$$\frac{du}{d\xi} = \frac{f(u,\xi)}{c^2 - u^2},$$

where c is the local speed of small perturbations and u is the flow speed. This equation has a regular solution crossing the sonic point c = u provided f = 0 at the same point, which is precisely



Figure 9: Left - comparison between our theoretical prediction of the hydraulic jump structure [9] and experiment. Right - jamiton profile in the theory of traffic shocks [7].

the Chapman-Jouguet condition of detonation theory.

The discovery of the analogy allowed us to develop the first rational theory of a classical phenomenon in fluid mechanics, the hydraulic jump [9], and to find a simple analytical solution to another textbook problem in gasdynamics/partial differential equations, namely the traffic jam [7] described within the framework of a continuum model.

2 Personnel

- PI: Dr. Aslan R. Kasimov, MIT
- <u>Collaborators</u>: Brian D. Taylor, graduate student (UIUC,) Prof. D. Scott Stewart (UIUC,) Prof. Ruben R. Rosales (MIT,) B. Seibold (MIT,) J.-C. Nave (MIT,) and Prof. M. Flynn (University of Alberta.)

3 PhD Thesis

1. B. D. Taylor, Stability of Steady and Quasi-steady Detonations, University of Illinois at Urbana-Champaign. Co-advised with Prof. D.S. Stewart.

4 Publications

- 1. B. D. Taylor, A. R. Kasimov, and D. S. Stewart, Mode selection in unstable two-dimensional detonations, *Combustion Theory and Modelling*, Vol. 13, No. 6, 2009, 973-992.
- M.R. Flynn, A. R. Kasimov, J.-C. Nave, R.R. Rosales, B. Seibold, Self-sustained nonlinear waves in traffic flow, *Phys. Rev. E* 79, 056113 (2009).
- 3. A.R. Kasimov, A stationary circular hydraulic jump and its gasdynamic analogue, *Journal* of Fluid Mechanics, 601:189-198, 2008
- 4. A.R. Kasimov, Hyperbolic dynamics of weakly nonlinear detonation waves (in preparation).
- A.R. Kasimov, B. D. Taylor, D.S. Stewart, Accurate direct numerical computation of detonation instability, *ICDERS*, Minsk, 2009
- 6. A.R. Kasimov, Detonation analogs, ICDERS, Minsk, 2009

5 Invited presentations and talks

- 1. A.R. Kasimov, Accurate Simulation of Multi-Dimensional Detonation Waves in a Shock-Attached Frame, APS Division of Fluid Dynamics, Nov. 2008.
- 2. A.R. Kasimov, Detonation: Its Theory, Numerical Simulation, and a Hydraulic Analogue, (Seminar at GALCIT, Caltech, Jan 18, 2008).
- 3. A.R. Kasimov, Shocks and sonic points, MIT Physical Mathematics Seminar, May 13, 2008.
- A.R. Kasimov, The power of analogy: from traffic jams to black holes, MIT Applied Mathematics Colloquium, 2009.
- 5. A.R. Kasimov, Theory and simulation of shock dynamics: detonations and related phenomena, MIT Mechanical Engineering Seminar, 2009
- A.R. Kasimov, Theory and simulation of shock dynamics: detonations and related phenomena, NEU Mechanical Engineering Seminar, 2009
- A.R. Kasimov, Analysis and simulation of shock dynamics: detonations and related phenomena, U. of Alberta, 2009
- A.R. Kasimov, Analysis and simulation of shock dynamics: detonations and related phenomena, UMass Dartmouth, 2009

6 Conference talks

- R. Kasimov, Kinematics and dynamics of multi-dimensional shock waves with application to detonation simulation, 12th International Conference on Numerical Combustion, CA, April 2008
- 2. A.R. Kasimov, B. D. Taylor, and D. S. Stewart, Mode selection in unstable two-dimensional detonations, 12th International Conference on Numerical Combustion, CA, April 2008
- A.R. Kasimov, B. D. Taylor, D.S. Stewart, Accurate direct numerical computation of detonation instability, *ICDERS*, Minsk, 2009
- 4. A.R. Kasimov, Detonation analogs, ICDERS, Minsk, 2009
- Taylor, B. D., Kasimov, A. R., and Stewart, D. S., November 2009. "Axisymmetric Shock-Attached Frame Detonation Simulations." 62nd Annual Meeting of the American Physical Society Division of Fluid Mechanics, Minneapolis, Minnesota, 2009

7 New discoveries, inventions, or patent disclosures

- A new shock fitting numerical algorithm for the simulation of multi-dimensional detonation waves
- A new algorithm for calculation of detonation instability spectra
- Analogy between detonations, hydraulic jumps, and traffic jams

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