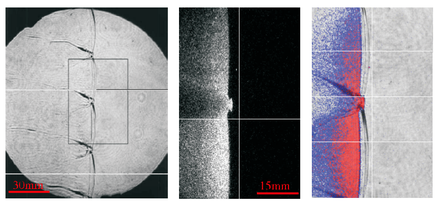
Analysis of weak and strong transverse-wave structures in gaseous detonations by large-scale simulation

Ralf Deiterding

Computer Science and Mathematics Division, Oak Ridge National Laboratory

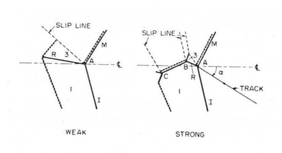
Cellular detonation and triple point structures

Self-sustaining detonations are inherently unstable and exhibit transverse pressure waves that propagate perpendicular to the detonation front. The transverse waves form evolving triple point patterns at the detonation front with severely enhanced pressure, temperature and thereby reaction. Despite considerable experimental efforts, a general model for the instability and the detailed flow field in triple points in detonations is not available yet.



Schlieren and PLIF images of a regularly oscillating detonation front in hydrogen-oxygen-argon (image courtesy J. E. Shepherd, Graduate Aeronautical Laboratory, California Institute of Technology).

Objective of this work is to decipher the detailed hydrodynamic flow conditions in triple point sub-structures under periodic and transient conditions. In experiments, basically two different configurations have been qualitatively distinguished.



Experimentally known triple point structures.

Governing equations

The governing equations for detonation wave simulation are the inhomogeneous Euler equations for multiple species

$$\begin{array}{rcrcl} \partial_t \rho_i & + & \nabla\cdot(\rho_i\vec{u}) & = & W_i\,\dot{\omega}_i\,, \\ \partial_t(\rho\vec{u}) & + & \nabla\cdot(\rho\vec{u}\otimes\vec{u})+\nabla p & = & 0\,, \\ \partial_t(\rho E) & + & \nabla\cdot((\rho E+p)\vec{u}) & = & 0\,. \end{array}$$

The equation of state follows the ideal gas law

$$p=\sum_{i=1}^{K} p_i = \mathcal{R}T\sum_{i=1}^{K}\frac{\rho_i}{W_i} \quad \text{with} \quad h_i(T)=h_i^0+\int_{T^0}^{T} c_{pi}(\sigma)d\sigma\,,$$

which requires computation of $T=T(\boldsymbol{\rho},e)$ from the implicit equation

$$\sum_{i=1}^{K}\rho_i\,h_i(T)-\rho e-\mathcal{R}T\sum_{i=1}^{K}\frac{\rho_i}{W_i}=0\,.$$

The reaction rates for detailed kinetics are

$$\dot{\omega}_i=\sum_{j=1}^{J}(\nu_{ji}^r-\nu_{ji}^f)\left[k_j^f\prod_{l=1}^{K}\left(\frac{\rho_l}{W_l}\right)^{\nu_{jl}^f}-k_j^r\prod_{l=1}^{K}\left(\frac{\rho_l}{W_l}\right)^{\nu_{jl}^r}\right].$$

In here, all results were obtained with a mechanism for H_2-O_2-Ar combustion with 34 elementary reactions and 9 species.

Numerical Methods

Numerical source term incorporation and extension to multiple dimensions with method of fractional steps. $\longrightarrow$ Numerical decoupling of hydrodynamic and chemical time steps.

Time-explicit 2nd order TVD shock-capturing method for thermally perfect gases:

- Upwinding with Roe-linearization for thermally perfect mixtures
- Avoids unphysical densities and energies by switching to HLL
- Preserves mass fraction positivity
- Entropy and carbuncle fix
- 2nd-order MUSCL reconstruction

Source term integration:

- Standard solver for stiff ODE's, e.g. semi-implicit Rosenbrock-Wanner method
- Automatic stepsize adjustment to allow for an efficient treatment of chemical time scales smaller than the global time-step

Embedding of complex domains:

- Implicit boundary representation with level-set signed distance function on Cartesian mesh
- Non-oscillating, 1st order accurate interpolation/extrapolation to construct ghost cell values
- Mirroring of the primitive values ρ_i, $\mathbf{u}$, p and inversion of normal velocity component by $\mathbf{u}'=(2\mathbf{w}\cdot\mathbf{n}-\mathbf{u}\cdot\mathbf{n})\mathbf{n}+(\mathbf{u}\cdot\mathbf{t})\mathbf{t}=2\,((\mathbf{w}-\mathbf{u})\cdot\mathbf{n})\,\mathbf{n}+\mathbf{u}$

Blockstructured AMR:

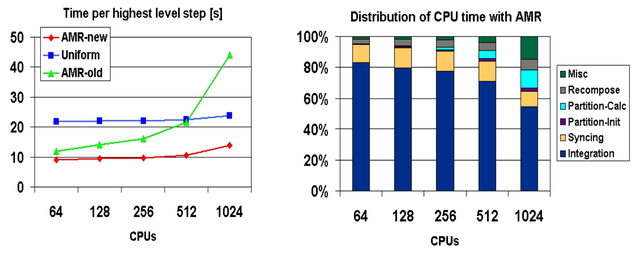
- Patch-based refinement of shock and reaction front, and embedded boundaries
- Spatial *and* temporal refinement
- Blockstructured data guarantees high computational performance

Our framework AMROC provides a generic MPI-parallel, object-oriented implementation of the blockstructured AMR method that is applicable to any explicit FV scheme.

- Data of all levels resides on same node $\rightarrow$ most AMR operations are local
- Distribution algorithm: generalization of Hilbert's space-filling curve

Recent scalability improvements for AMROC

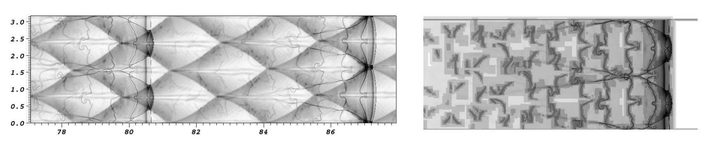
- Parallelization of space-filling curve computation
- Reduction of topological operations on global metadata to strictly local ones



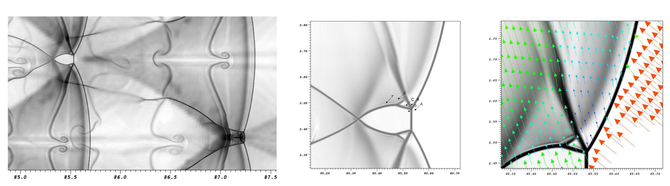
Weak scalability data for a typical non-reactive spherical shock expansion problem (periodically replicated). Two additional levels with refinement factors 2,4. Mesh adaptation and parallel re-distribution in every time step.

Regular detonation structures in 2d

- Mixture: $H_2:O_2:Ar$ at molar ratios 2:1:7 at initially 298 K and 10 kPA
- Initialization with Chapman-Jouguet ZND solution and an irregular pocket to quickly trigger symmetry breaking. Tube width 3.2 cm
- Simulation until a *single* perturbation has developed into *two* regularly oscillating cells with width $\lambda=1.6$ cm
- 67.6 Pts/l_{ig}. 4 additional refinement levels (2,2,2,4) on base mesh 2000×128
- Compute triple point trajectories by tracking the magnitude of the vorticity on a uniform mesh at level 1



Left: Oscillating detonation front on computed triple points tracks. Right: Schlieren plot on refinement levels.



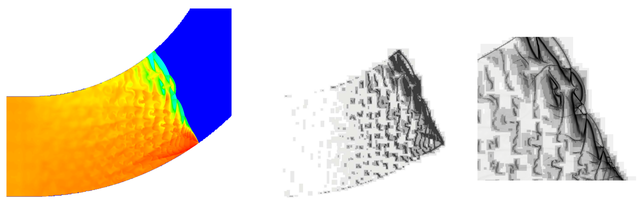
Left: Front on triple point tracks. 10 μs between snapshots (marked with stars in (M,S)-plane, cf. right column). Middle and right: Clearly established DMR pattern shortly before triple point collision.

	p/p_A	ρ/ρ_A	T [K]	v[m/s]	M
A	1.00	1.00	298	1775	5.078
B	31.45	4.17	2248	447	0.477
C	31.69	5.32	1775	965	1.153
D	19.17	3.84	1487	1178	1.533
E	35.61	5.72	1856	901	1.053
F	40.61	6.09	1987	777	0.880

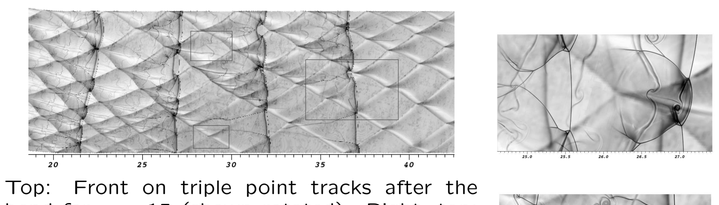
States and shock polar analysis for a DMR structure shortly before next collision. $a_t\approx 60$ m/s used.

Detonation structure in smooth pipe bends

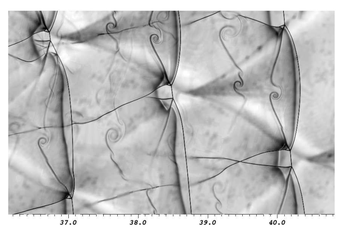
- Initialization with 5 regularly oscillating detonation cells, same mixture as above, tube with 8 cm
- Pipe bend with radius 8 cm. Angle $\alpha=\{15^o,30^o,45^o\}$
- 67.6 Pts/l_{ig}. 4 additional refinement levels with factors (2,2,2,4)
- Adaptive computations use $\sim 7\cdot 10^6$ cells ($\sim 5\cdot 10^6$ on highest level) instead of $\sim 1.2\cdot 10^9$ cells (uniform grid)
- $\sim 70,000$ h CPU each on 128 CPUs Pentium-4 2.2 GHz



Color plot of T and schlieren plot of ρ on triple point tracks and on refinement regions (middle, right) for $\alpha=45^o$ after $t=150\,\mu$s simulated time.

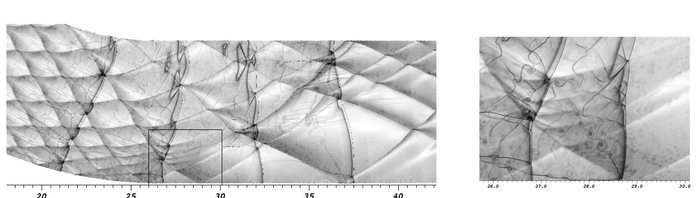


Top: Front on triple point tracks after the bend for $\alpha=15$ (shown rotated). Right, top: Strengthening of DMR pattern (open triangles) under expansion at 130 μs and 140 μs simulated time. Right, bottom: Weakening TMR in over-driven region (open squares) at 130 μs and 140 μs.



Triple point re-initiation with change from TMR to DMR (open circles) when the oscillation becomes regular again after the bend, $\alpha=15$ at 200 μs, 210 μs, and 220 μs.

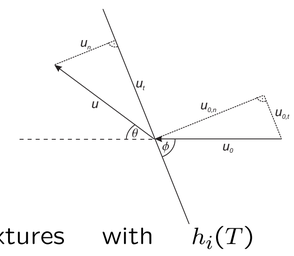
Bottom: Triple point quenching and failure as SMR in over-driven compression region for $\alpha=30$ at 140 μs, 150 μs (closed triangles)



Oblique shock relations

Apply jump conditions to steady shock wave described by 2D Euler equations.

$$\begin{array}{rcl} \rho_0 u_{0,n} & = & \rho u_n \\ p_0+\rho_0 u_{0,n}^2 & = & p+\rho u_n^2 \\ \rho_0 u_{0,n}u_{0,t} & = & \rho u_n u_t \\ h_0+\frac{1}{2}u_{0,n}^2 & = & h+\frac{1}{2}u_n^2 \end{array}$$



For thermally perfect mixtures with $h_i(T)=h_i^0+\int_{T^0}^{T}c_{pi}(T^\star)dT^\star$ one solves

$$\frac{RT_0}{u_{0,n}}+u_{0,n}-\frac{RT}{u_n}+u_n=0 \quad \text{with} \quad u_n=\sqrt{u_{0,n}^2-2\int_{T_0}^{T}c_p(\nu)d\nu}$$

numerically

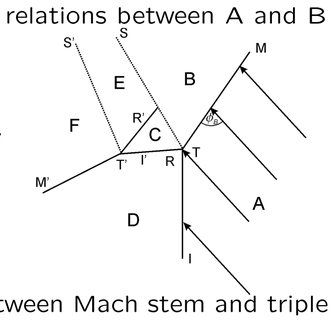
Shock polar analysis of triple points in detonations

- Neglect reaction, but consider $c_{pi}(T)$
- Data extracted point-wise from simulation
- Primary triple point T travels exactly at tip of Mach stem $\longrightarrow$ use oblique shock relations between A and B

$$\begin{array}{rcl} \rho_A u_A & = & \rho_B u_{B,n} \\ p_A+\rho_A u_A^2 & = & p_B+\rho_B u_B^2 \end{array}$$

to evaluate inflow velocity as

$$u_A=\sqrt{\frac{\rho_B(p_B-p_A)}{\rho_A(\rho_B-\rho_A)}}\Big/\sin\phi_B$$



- Measure inflow angle ϕ_B between Mach stem and triple point trajectory
- However, velocity a of T' relative to T cannot be derived easily. Oblique shock relations across C and D hold true both for T and T' $\longrightarrow a_n\equiv 0$, a_t arbitrary. Use estimate $a_t\approx L_R/\Delta t_{\text{init}}$

Transition criteria

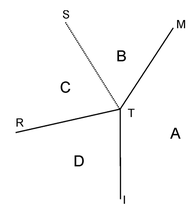
Transition between regular reflection (RR) and irregular reflection: $M_B^T=1$ with RR for $M_B^T>1$

Transition between single Mach reflection (SMR) and transitional or double Mach reflection (TMR/DMR): $M_C^T=1$ with TMR/DMR for $M_C^T>1$

Transition between TMR and DMR: $M_C^{T'}=1$ with DMR for $M_C^{T'}>1$

For now, we use $M_C^{T'}\equiv 1$ to find the TMR/DMR transition lines for given a_t numerically, i.e.

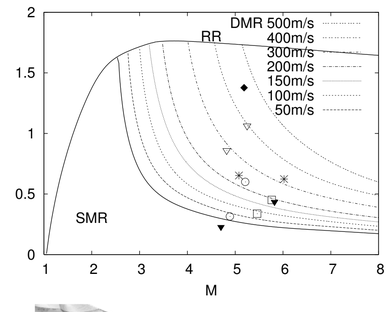
$$u_{C,n}^2+(u_{C,t}-a_t)^2=\gamma_C\frac{p_C}{\rho_C}$$

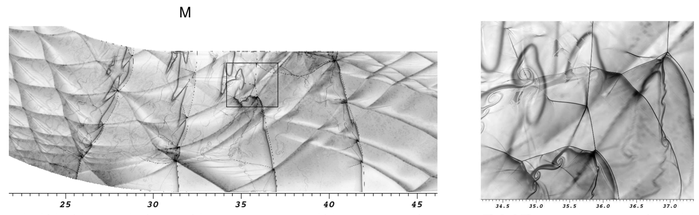


yields

$$a_t=u_{C,t}-\sqrt{\gamma_C\frac{p_C}{\rho_C}-u_{C,n}^2}\,.$$

Use oblique shock relations and transition criteria to numerically find transition boundaries of different shock wave reflection phenomena for non-reactive mixture $H_2:O_2:Ar$ $2:1:7$ at $T_0=298$ K and $p_0=10$ kPA. Specially geared to detonations, results are displayed (left) in the plane defined by the relative strength $S=\frac{p_C-p_D}{p_D}$ and the inflow Mach number M





Re-initiation detonation wave with very strong DMR and own triple point on reflected shock wave for $\alpha=45$ and 200 μs, 210 μs simulated time (closed diamond)

Conclusions

Non-reactive, thermally perfect shock wave reflection theory is applicable to explain observed reflection patterns in detonations

- Triple point type is determined solely by S and M
- Still missing: suitable estimate for a_t

Observations

- Stable structures exist only in the TMR/DMR, but not in the SMR regime
- TMR domain is rather small for typical values $50\,\text{m/s}<a_t<100\,\text{m/s}$
- A change of type happens especially in triple point collisions

References

RD. Parallel adaptive simulation of weak and strong detonation transverse-wave detonation structures in H_2-O_2 detonations. In R. Biswas et al., editors, *Parallel CFD 2009*, pages 519–534, DEStech Publications, Lancaster, 2010.

RD. A parallel adaptive method for simulating shock-induced combustion with detailed chemical kinetics in complex domains, *Computers & Structures*, 87: 769–783, 2009.