Deciphering the Structure of Gaseous Detonations by Numerical Simulation

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6th Annual Symposium of the Burgers Program for Fluid Dynamics
University of Maryland, College Park, Nov 18, 2009

Work supported by DFG high priority research program “Analysis and Numerics of Conservation Laws”, grant Ba 840/3-3 and currently sponsored by the Office of Advanced Scientific Computing Research; U.S. Department of Energy (DOE) and was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725.
Outline of the talk

- Computational approach
  - Introduction
  - Governing equations
  - Finite volume method
    - Upwind scheme, embedded boundaries
    - Dynamic mesh adaptation, parallelization
  - Shock-induced combustion examples

- Mach reflection patterns in detonations
  - Qualitative description
  - Shock polar analysis for triple points in detonations
    - Oblique shock relations for real gases
    - Reflection type transition criteria
    - Construction of a transition diagram for low-pressure H$_2$:O$_2$:Ar
  - Weak and strong structures in detonations in 2D pipe bends
    - Classification of observed Mach reflection structures

- Short outlook: comparison 2D vs. 3D

- Conclusions
Difficulties in detonation simulations

1. Discontinuous solutions → high-resolution finite volume method with upwinding in all characteristic fields
2. Stiffness of reaction terms, $\Delta t_c << \Delta t$ → Numerical decoupling of time operators with method of fractional steps and local time steps $\Delta t_c$
3. Extremely high spatial resolution in reaction zone necessary. Discretization of an exact ZND detonation:
   - minimal spatial resolution: $7 - 8 \text{ Pts/}l_g \rightarrow \Delta x \approx 0.2 - 0.175\text{mm}$
   - Uniform grids for typical geometries: $> 10^7 \text{ Pts in 2D, } > 10^9 \text{ Pts in 3D}$ → Self-adaptive finite volume method (AMR)
4. Problem size even with AMR in 3D enormous → parallelization for massively parallel systems with distributed memory
Hydrodynamic equations

Euler equations for mixtures

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k}(\rho u_k) = 0
\]

\[
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho u_i u_k + \delta_{ik} p) = 0
\]

\[
\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_k}(u_k(E + p)) = 0
\]

\[
\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x_k}(\rho Y_i u_k) = \dot{m}_i
\]

Implicit equation of state

\[
\rho h - p - E + \frac{1}{2} \rho u_k u_k = 0
\]

Ideal gas law

\[
p = \rho RT \sum_{i=1}^{N} \frac{Y_i}{W_i}
\]

Caloric equation

\[
h = \sum_{i=1}^{N} h_i(T) Y_i \quad \text{with}
\]

\[
h_i(T) = h_i^0 + \int_{T_0}^{T} c_{pi}(T^*)dT^*
\]

Chemical kinetics with Arrhenius law

\[
\dot{m}_i = W_i \sum_{j=1}^{M} (\nu_{ji}^r - \nu_{ji}^f) [k_j^f \prod_{n=1}^{N} (\frac{\rho_n}{W_n})]^{\nu_{jn}^f - k_j^r} \prod_{n=1}^{N} (\frac{\rho_n}{W_n})^{\nu_{jn}^r}
\]
Finite volume scheme

- Method of fractional steps
  \[ \mathcal{H}(\Delta t) : \quad \partial_t q + \nabla \cdot f(q) = 0 \quad \text{IC: } Q(t_m) \xrightarrow{\Delta t} \bar{Q} \]
  \[ S(\Delta t) : \quad \partial_t q = s(q) \quad \text{IC: } \bar{Q} \xrightarrow{\Delta t} Q(t_m + \Delta t) \]
  1^{\text{st}}-order: \quad Q(t_m + \Delta t) = S(\Delta t) \mathcal{H}(\Delta t)(Q(t_m))
  2^{\text{nd}}-order: \quad Q(t_m + \Delta t) = S(\frac{1}{2} \Delta t) \mathcal{H}(\Delta t) S(\frac{1}{2} \Delta t)(Q(t_m))

- Hydrodynamics
  - Extension to 2d and 3d via dimensional splitting
  - Positivity-preserving
    - Switching to HLL for unphysical \( \rho, p \)
  - 2^{\text{nd}}-order MUSCL reconstruction

- Evaluation of \( T \) with Newton iteration / bisection

Reaction mechanism

- 4th-order semi-implicit Rosenbrock-Wanner ODE solver with stepsize adjustment
- Production rates evaluated with automatically generated F77 function (4x faster Chemkin)
- Jacobian approximated
- $c_p, h_i$ tabulated
- All subsequent computations for hydrogen-oxygen mechanism with 34 elementary reaction, 9 species $O_2, H_2, H_2O, H, O, OH, HO_2, H_2O_2, Ar$

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A$ [cm. mol.$^{-1}$ s.$^{-1}$]</th>
<th>$\beta$ [cal. mol.$^{-1}$ K.$^{-1}$]</th>
<th>$E_{act}$ [cal. mol.$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. $H + O_2$ $\rightarrow$ $O + OH$</td>
<td>$1.86 \times 10^{-14}$</td>
<td>0.00</td>
<td>1670</td>
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<tr>
<td>2. $O + OH$ $\rightarrow$ $H + O_2$</td>
<td>$1.48 \times 10^{-13}$</td>
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<td>658</td>
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<tr>
<td>3. $H_2 + O$ $\rightarrow$ $H + H_2O$</td>
<td>$1.92 \times 10^{-10}$</td>
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<td>4. $H + OH$ $\rightarrow$ $H_2 + O$</td>
<td>$8.22 \times 10^{-8}$</td>
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<td>8000</td>
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<tr>
<td>5. $H_2O + O$ $\rightarrow$ $OH + OH$</td>
<td>$3.39 \times 10^{-8}$</td>
<td>0.00</td>
<td>18350</td>
</tr>
<tr>
<td>6. $OH + OH$ $\rightarrow$ $H_2O + O$</td>
<td>$3.16 \times 10^{-8}$</td>
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<td>1100</td>
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<tr>
<td>7. $H_2O + H$ $\rightarrow$ $H_2 + OH$</td>
<td>$9.55 \times 10^{-7}$</td>
<td>0.00</td>
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<tr>
<td>8. $H_2 + OH$ $\rightarrow$ $H_2O + H$</td>
<td>$2.10 \times 10^{-5}$</td>
<td>0.00</td>
<td>5150</td>
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<tr>
<td>9. $H_2O_2 + OH$ $\rightarrow$ $H_2O + HO_2$</td>
<td>$1.00 \times 10^{-4}$</td>
<td>0.00</td>
<td>1900</td>
</tr>
<tr>
<td>10. $H_2O + HO_2$ $\rightarrow$ $H_2O_2 + OH$</td>
<td>$2.82 \times 10^{-3}$</td>
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<tr>
<td>11. $H_2O + O$ $\rightarrow$ $OH + O_2$</td>
<td>$5.61 \times 10^{-3}$</td>
<td>0.00</td>
<td>10000</td>
</tr>
<tr>
<td>12. $OH + O_2$ $\rightarrow$ $HO_2 + O$</td>
<td>$6.46 \times 10^{-3}$</td>
<td>0.00</td>
<td>50160</td>
</tr>
<tr>
<td>13. $HO_2 + O$ $\rightarrow$ $OH + OH$</td>
<td>$2.51 \times 10^{-4}$</td>
<td>0.00</td>
<td>1900</td>
</tr>
<tr>
<td>14. $OH + OH$ $\rightarrow$ $H_2O_2 + H$</td>
<td>$1.20 \times 10^{-5}$</td>
<td>0.00</td>
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<tr>
<td>15. $HO_2 + H$ $\rightarrow$ $HO_2 + H$</td>
<td>$2.51 \times 10^{-3}$</td>
<td>0.00</td>
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<tr>
<td>16. $H_2 + O_2$ $\rightarrow$ $H + O_2$</td>
<td>$5.50 \times 10^{-4}$</td>
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<tr>
<td>17. $H + O_2$ $\rightarrow$ $H_2O + O$</td>
<td>$5.01 \times 10^{-4}$</td>
<td>0.00</td>
<td>10000</td>
</tr>
<tr>
<td>18. $H + OH$ $\rightarrow$ $H_2O + O$</td>
<td>$6.41 \times 10^{-4}$</td>
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<tr>
<td>19. $H + O$ $\rightarrow$ $OH + H$</td>
<td>$2.33 \times 10^{-5}$</td>
<td>0.00</td>
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</tr>
<tr>
<td>20. $H_2 + H$ $\rightarrow$ $H_2O_2 + O_2$</td>
<td>$1.90 \times 10^{-3}$</td>
<td>0.00</td>
<td>1000</td>
</tr>
<tr>
<td>21. $H_2O + H$ $\rightarrow$ $H_2O + H$</td>
<td>$1.70 \times 10^{-2}$</td>
<td>0.00</td>
<td>37500</td>
</tr>
<tr>
<td>22. $H_2O + O$ $\rightarrow$ $H_2O_2 + H$</td>
<td>$7.30 \times 10^{-2}$</td>
<td>0.00</td>
<td>18700</td>
</tr>
<tr>
<td>23. $H_2O + M$ $\rightarrow$ $H + OH + M$</td>
<td>$2.19 \times 10^{-3}$</td>
<td>0.00</td>
<td>105000</td>
</tr>
<tr>
<td>24. $H + OH + M$ $\rightarrow$ $H_2O + O$</td>
<td>$1.41 \times 10^{-2}$</td>
<td>0.00</td>
<td>1400</td>
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<tr>
<td>25. $H + O + M$ $\rightarrow$ $H_2 + OH + M$</td>
<td>$1.06 \times 10^{-4}$</td>
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<td>1000</td>
</tr>
<tr>
<td>26. $H + M + M$ $\rightarrow$ $H + O_2 + M$</td>
<td>$2.29 \times 10^{-5}$</td>
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<td>45000</td>
</tr>
<tr>
<td>27. $H_2O_2 + M$ $\rightarrow$ $OH + OH + M$</td>
<td>$1.20 \times 10^{-3}$</td>
<td>0.00</td>
<td>45000</td>
</tr>
<tr>
<td>28. $OH + OH + M$ $\rightarrow$ $H_2O_2 + M$</td>
<td>$9.12 \times 10^{-4}$</td>
<td>0.00</td>
<td>50700</td>
</tr>
<tr>
<td>29. $O + O + M$ $\rightarrow$ $O_2 + M$</td>
<td>$1.00 \times 10^{-4}$</td>
<td>0.00</td>
<td>1000</td>
</tr>
<tr>
<td>30. $OH + M$ $\rightarrow$ $O + H + M$</td>
<td>$7.94 \times 10^{-4}$</td>
<td>0.00</td>
<td>10000</td>
</tr>
<tr>
<td>31. $O_2 + M$ $\rightarrow$ $O + O + M$</td>
<td>$5.13 \times 10^{-4}$</td>
<td>0.00</td>
<td>11000</td>
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<tr>
<td>32. $O + O + M$ $\rightarrow$ $O_2 + M$</td>
<td>$4.98 \times 10^{-4}$</td>
<td>0.00</td>
<td>800</td>
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<tr>
<td>33. $O + M + M$ $\rightarrow$ $O + H + M$</td>
<td>$2.10 \times 10^{-4}$</td>
<td>0.00</td>
<td>9000</td>
</tr>
<tr>
<td>34. $H + H + M$ $\rightarrow$ $H_2 + M$</td>
<td>$3.02 \times 10^{-4}$</td>
<td>0.00</td>
<td>0</td>
</tr>
</tbody>
</table>

Third body efficiencies: $f(O_2) = 0.40, f(H_2O) = 6.50$

Detonation ignition in a shock tube

- Shock-induced detonation ignition of H₂ : O₂ : Ar/2 : 1 : 7 in a 1d shock tube closed at the left end, domain simulated: 12 cm
- Insufficient resolution leads to inaccurate results
- Reflected shock is captured by the FV scheme correctly at all resolutions, but the detonation is resolution-dependent

Detonation ignition in a shock tube

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Structured AMR for hyperbolic problems

- Refined subgrids overlay coarser ones
- Computational decoupling of subgrids by using ghost cells
- Refinement in space and time
- Block-based data structures
- Cells without mark are refined
- Cluster-algorithm necessary
- Efficient cache-reuse / vectorization possible

Discretization

\[
Q_{jk}^{n+1} = Q_{jk}^n - \frac{\Delta t}{\Delta x_1} \left[ F_{j+1/2,k}^1 - F_{j-1/2,k}^1 \right] \\
- \frac{\Delta t}{\Delta x_2} \left[ F_{j,k+1/2}^2 - F_{j,k-1/2}^2 \right]
\]

is applied patch-wise

→ Inherently parallel approach

Parallelization strategy

- Data of all levels resides on same node → Interpolation and averaging remain strictly local
- Only parallel operations to be considered:
  - Parallel synchronization as part of ghost cell setting
  - Load-balanced repartitioning of data blocks as part of \( \text{Regrid}(l) \)
  - Application of flux correction terms on coarse-grid cells
- Partitioning at root level with generalized Hilbert space-filling curve defined in AMR index coordinate system by M. Parashar

\[
W(\Omega) = \sum_{l=0}^{l_{\text{max}}} \mathcal{N}_l(G_l \cap \Omega) \prod_{\nu=0}^{l} r_{\nu}
\]
Embedded boundary method

- Incorporate complex moving boundary/ interfaces into a Cartesian solver (extension of work by R. Fedkiw and T. Aslam)
- Implicit boundary representation via distance function $\varphi$, normal $n = \nabla \varphi / |\nabla \varphi|$
- Treat an interface as a moving rigid wall
- Method diffuses boundary and is therefore not conservative
- Construction of values in embedded boundary cells by interpolation / extrapolation

$\rho_{n,j}^F$ $\rho_{n,j-1}^F$ $2u_{n,j+1/2}^S - u_{n,j}^F$ $2u_{n,j+1/2}^S - u_{n,j-1}^F$
$u_{n,j}^F$ $u_{n,j-1}^F$ $u_{t,j}^F$ $u_{t,j-1}^F$
$p_{n,j}^F$ $p_{n,j-1}^F$ $p_{t,j}^F$ $p_{t,j-1}^F$

Velocity: $u_{Gh}^F = 2((u^S - u^M) \cdot n) n + u^M$

- Higher resolution at embedded boundary required than with first-order unstructured scheme
- Appropriate level-set-based refinement criteria are available to cure deficiencies

Shock-induced combustion around a sphere

- Spherical projectile of radius 1.5 mm travels with constant velocity $v_i=2170.6$ m/s through $\text{H}_2 : \text{O}_2 : \text{Ar}/2:1:7$ at 6.67 kPa and $T=298$ K
- Cylindrical symmetric simulation on AMR base mesh of 70x40 cells
- Comparison in quasi-steady state at $t=350$ $\mu$s

Setup from P. Hung, PhD thesis, GalCIT, 2003
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Distribution to 8 processors

4-level with factors 2,2,4 (~19 Pts/\text{i}_{g})

Setup from P. Hung, PhD thesis, GalCIT, 2003
Transverse detonation structure - Regular instability


Photo courtesy: J. Austen, F. Pintgen, J.E. Shepherd (GalCIT)
Simulation of regular cellular structures

- Regular Chapman-Jouguet detonation for $\text{H}_2 : \text{O}_2 : \text{Ar}/2 : 1 : 7$ at $T_0 = 298\text{K}$ and $p_0 = 10\text{kPa}$, cell width 1.6 cm.
- Perturb 1d solution with unreacted high-pressure pocket behind front.
- Triple point trajectories by tracking $\max|\omega|$ on auxiliary mesh.
- Adaptation criteria:
  - Scaled gradients of $\rho$ and $p$
  - Error estimation in $Y_i$ by Richardson extrapolation
- 67.6 Pts within induction length. 4 additional refinement levels $(2,2,2,4)$.
Simulation of regular cellular structures

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- Triple point trajectories by tracking $\max|\omega|$ on auxiliary mesh.

$$\omega = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}$$

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- 67.6 Pts within induction length. 4 additional refinement levels $(2,2,2,4)$.
Flow Around a Triple-point


See also: Hu et al., The structure and evolution of a two-dimensional H₂/O₂/Ar cellular detonation, Shock Waves, 2004.
Flow Around a Triple-point


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Oblique shock relations

Apply Rankine-Hugoniot condition \( \sigma(q - q_0) = \omega \cdot (f(q) - f(q_0)) \) to steady shock wave with \( \sigma = 0 \) described by the 2D Euler equations:

\[
\begin{align*}
\rho_0 u_{0,n} &= \rho u_n \\
p_0 + \rho_0 u_{0,n}^2 &= p + \rho u_n^2 \\
u_{0,t} &= u_t \\
h_0 + \frac{1}{2} u_{0,n}^2 &= h + \frac{1}{2} u_n^2
\end{align*}
\]

Commonly used:

\[
\begin{align*}
\rho_0 u_0 \sin \phi &= \rho u \sin(\phi - \theta) \\
p_0 + \rho_0 u_0^2 \sin^2 \phi &= p + \rho u^2 \sin^2(\phi - \theta) \\
\rho_0 \tan \phi &= \rho \tan(\phi - \theta) \\
h_0 + \frac{1}{2} u_0^2 \sin^2 \phi &= h + \frac{1}{2} u^2 \sin^2(\phi - \theta)
\end{align*}
\]
Oblique shock relations

Apply Rankine-Hugoniot condition $\sigma(q - q_0) = \omega \cdot (f(q) - f(q_0))$
to steady shock wave with $\sigma=0$
described by the 2D Euler equations:

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

For thermally perfect mixtures with $h_i(T) = h_i^0 + \int_{T_0}^{T} c_p(T^*)dT^*$
one solves

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

numerically
Irregular reflection (IR) to regular reflection (RR): $M_B^r = 1$ with $M_B^r > 1$ for RR

Triple point configurations & Transition criteria
Triple point configurations & Transition criteria

- Irregular reflection (IR) to regular reflection (RR): $M_B^T=1$ with $M_B^T>1$ for RR

In the IR regime:

- von Neumann reflection (NR) to Mach reflection (MR): $M_D^T=1$ with $M_D^T>1$ for MR
Irregular reflection (IR) to regular reflection (RR): $M_B^T=1$ with $M_B^T>1$ for RR

In the IR regime:

- von Neumann reflection (NR) to Mach reflection (MR): $M_D^T=1$ with $M_D^T>1$ for MR

- Single Mach reflection (SMR) to transitional or double Mach reflection (TMR/DMR): $M_C^T=1$ with $M_C^T>1$ for TMR/DMR
Triple point configurations & Transition criteria

- Irregular reflection (IR) to regular reflection (RR): $M_B^T = 1$ with $M_B^T > 1$ for RR

In the IR regime:

- von Neumann reflection (NR) to Mach reflection (MR): $M_D^T = 1$ with $M_D^T > 1$ for MR

- Single Mach reflection (SMR) to transitional or double Mach reflection (TMR/DMR): $M_C^T = 1$ with $M_C^T > 1$ for TMR/DMR

- Transitional (TMR) to double Mach reflection (DMR): $M_C^{T'} = 1$ with $M_C^{T'} > 1$ for DMR

Shock polar analysis for a DMR

\[ u_c = 943 \text{ m/s used for plot (} +2.2\% \text{)} \]

\[ a_i \approx 60 \text{ m/s used.} \]
Reflection types depending on transverse wave strength

$H_2 : O_2 : Ar/2 : 1 : 7$ at $T_0 = 298K$ and $p_0 = 10 \text{kPa}$

$$S := \frac{p_C - p_D}{p_D}$$
Transient conditions: Propagation through smooth pipe bends

- Regular Chapman-Jouguet detonation for H₂ : O₂ : Ar/2 : 1 : 7 at T₀ = 298K and p₀=10 kPa, cell width 1.6 cm, tube width of 5 detonation cells (8 cm)
- Pipe bend with same radius. Angle: 15°, 30°, 45°, 60°
- 56.2 Pts within induction length. 4 additional refinement levels (2,2,2,4)
- Adaptive computations use ≈ 7·10⁶ cells (≈ 5·10⁶ on highest level) instead of 1.2·10⁹ cells (uniform grid)
- ~70,000h CPU each on 128 CPUs Pentium-4 2.2GHz
Dynamic mesh adaptation (60°, 56.2 Pts/\(l_{ig}\))

~170 \(\mu s\)

Time after entering bend
Enlarged triple point tracks (56.2 Pts/\(l_{ig}\))

- Slight overdrive decreases cell size
- Marginal detonation
- Triple point compression, structure disappears
- Detonation failure
- Re-ignition with transverse detonation
Resolution comparison (15°)– triple point tracks

Resolution insufficient to capture high-energy release in triple points

Resolution sufficient: Number of triple points becomes approximately the same as before bend
Principal flow phenomena ($45^0, 56.2$ Pts/$l_{ig}$)

Unreacted pockets

Mach reflection

Detonation failure

Time after entering bend:

- $\sim 60 \mu s$
- $\sim 80 \mu s$
- $\sim 100 \mu s$
Principal flow phenomena \((45^0, 56.2 \text{ Pts/}l_{ig})\)

- Transverse detonation
- Shock reflection of transverse detonation

\(~120\mu s\)  \(~130\mu s\)  \(~140\mu s\)
Triple point analysis (15°)

Strengthening of double Mach reflection pattern, trajectory angle increases.
Triple point analysis (15°)

Transitional Mach reflection pattern, Straight trajectories
Formation of transverse wave with transitional Mach reflection, double Mach reflection after collision.
Triple point analysis ($30^0$)

Triple point quenching and failure with weakening transitional Mach reflection patterns
Triple point analysis (45°)

Transverse detonation with strong double Mach reflection pattern, triple point on transverse wave.
Outlook: Regular cellular structures in 3D

- Regular Chapman-Jouguet detonation for $\text{H}_2 : \text{O}_2 : \text{Ar}/2 : 1 : 7$ at $T_0 = 298K$ and $p_0=6.67 \text{ kPa}$, cell width 3 cm
- Unburned gas flows in with CJ velocity

Front view of the periodic solution

$t = 680 \mu s + 600 \mu s$ (Computation 1)

$t = 660 \mu s + 620 \mu s$ (Computation 2)
High-resolution simulation

- Simulation of only one quadrant
- 44.8 Pts within induction length
- AMR base grid 400x24x24, 2 additional refinement levels (2, 4)
- Simulation uses ~18M cells instead of 118M (unigrid)
- ~51,000h CPU on 128 CPU Compaq Alpha (LANL QSC)

<table>
<thead>
<tr>
<th>Task</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid Dynamics</td>
<td>37.6</td>
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<tr>
<td>Chemical Kinetics</td>
<td>25.1</td>
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<td>Boundary Setting</td>
<td>24.4</td>
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<td>Reorganization</td>
<td>6.6</td>
</tr>
<tr>
<td>Misc.</td>
<td>6.3</td>
</tr>
</tbody>
</table>
High-resolution simulation: Results

Schlieren plot of $Y_{OH}$, iso-surfaces of $Y_{OH}$ and $\rho$ visualize induction length, periodicity exploited for visualization

Transverse wave strength $S$ smaller than in 2D. TMR patterns do occur!
Conclusions

- For particular mixtures, detailed detonation structure simulations with detailed chemistry are possible nowadays in 2D realistic geometries
- Accurate studies for idealized 3D configurations
- Resolution down to the scale of secondary triple points can be provided on parallel capacity computing systems
  - Key components:
    - Operator splitting allows a cell-wise integration of stiff reaction terms
    - SAMR provides a sufficient spatial and temporal resolution, savings up to >250
- Unreactive, thermally perfect shock polar analysis is applicable to explain observed reflection patterns
  - Shock wave reflection theory is applicable to predict local triple point structure and stability
  - Triple point type is determined solely by S and M which can be derived from a single time step
  - Still missing: estimate for secondary triple point velocity $a_s$, tailored for detonations to rigorously TMR/DMR transition
- Observations:
  - Stable triple point structures in self-sustained detonations seem to exist only in the TMR and DMR, but not in the SMR regime
  - A change of the reflection type happens especially in triple point collisions
- Literature, links to software, papers, etc.: http://www.csm.ornl.gov/~r2v