Lecture 5

Detonation simulation

Course *Block-structured Adaptive Finite Volume Methods in C++*

Ralf Deiterding
University of Southampton
Engineering and the Environment
Highfield Campus, Southampton SO17 1BJ, UK

E-mail: r.deiterding@soton.ac.uk
Outline

Detonation simulation
  Detonation structures
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Detonation simulation
  Detonation structures

Combustion with viscous terms
  Combustion induced by projectiles
  Finite volume scheme
Outline

**Detonation simulation**
- Detonation structures

**Combustion with viscous terms**
- Combustion induced by projectiles
- Finite volume scheme

**Higher order schemes**
- Hybrid methods
Planar ZND Structure

Steady situation under Galilean transformation:

\[
\frac{\partial}{\partial x'} (\rho u') = 0
\]
\[
\frac{\partial}{\partial x'} (\rho u'^2 + p) = 0
\]
\[
\frac{\partial}{\partial x'} (u' \rho H) = 0
\]
\[
\frac{\partial Y_i}{\partial x'} = \frac{W_i \dot{\omega}_i (\rho \frac{Y_1}{W_1}, \ldots, \rho \frac{Y_K}{W_K}, T)}{\rho u'}
\]

CJ-detonation of H$_2$ : O$_2$ : Ar with molar ratios 2 : 1 : 7 at $T_0 = 298$ K and $p_0 = 6.67$ kPa, $d_{ CJ} \approx 1627$ m/s.

$t_{ig} \approx 3.55 \mu s$, $u'_{vN} \approx 395.5$ m/s, $l_{ig} \approx 0.14$ cm.

Cf. code/amroc/doc/html/apps/clawpack_2applications_2euler_2chem_21d_2ModelDetonation_2src_2Problem_8h_source.html
Planar ZND Structure

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CJ-detonation of $\text{H}_2 : \text{O}_2 : \text{Ar}$ with molar ratios $2 : 1 : 7$ at $T_0 = 298$ K and $p_0 = 6.67$ kPa, $d_{CJ} \approx 1627$ m/s.

$t_{ig} \approx 3.55$ $\mu$s, $u_{vN}' \approx 395.5$ m/s, $l_{ig} \approx 0.14$ cm.

Cf. code/amroc/doc/html/apps/clawpack_2applications_2euler_2chem_21d_2ModelDetonation_2src_2Problem_8h_source.html
Detonation cell structure in 2D - Regular instability

Transverse detonation structure - irregular instability
Simulation of regular structures

- CJ detonation for $\text{H}_2 : \text{O}_2 : \text{Ar}$ (2:1:7) at $T_0 = 298$ K and $p_0 = 10\,\text{kPa}$, cell width 1.6 cm

- Perturb 1d ZND solution with unreacted high-pressure pocket behind front

- Triple point trajectories by tracking $\max|\omega|$ on auxiliary mesh shifted through grid with CJ velocity. $\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$

- SAMR simulation with 4 additional levels (2,2,2,4), 67.6 Pts/$l_{ig}$

- Configuration similar to Oran et al., J. Combustion and Flame 113, 1998.
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Combustion with viscous terms

Higher order schemes

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Detonation structures

Detonation diffraction

- CJ 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 \( \lambda_c = 1.6 \text{ cm} \)

- Adaption criteria (similar as before):
  1. Scaled gradients of \( \rho \) and \( p \)
  2. Error estimation in \( Y_i \) by Richardson extrapolation

- \( 25 \text{ Pts} / l_{ig}. \) 5 refinement levels \((2,2,2,4)\).

- Adaptive computations use up to \( \sim 2.2 \text{ M} \) instead of \( \sim 150 \text{ M} \) cells 
  (uniform grid)

- \( \sim 3850 \text{ h CPU (\sim 80 h real time)} \) 
  on 48 nodes Athlon 1.4GHz

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Detonation diffraction - adaptation

Final distribution to 48 nodes and density distribution on four refinement levels
Detonation diffraction - adaptation

Final distribution to 48 nodes and density distribution on four refinement levels
Detonation simulation

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Final distribution to 48 nodes and density distribution on four refinement levels
Triple point analysis

Double Mach reflection structure shortly before the next collision

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Shock polar analysis of triple points in detonations

\[ \rho_A u_A \sin(\phi_B) = \rho_B u_B \sin(\phi_B - \theta_B) \]

\[ p_A + \rho_A u_A^2 \sin^2(\phi_B) = p_B + \rho_B u_B^2 \sin^2(\phi_B - \theta_B) \]

to evaluate inflow velocity as

\[ u_A = \frac{1}{\sin \phi_B} \sqrt{\frac{p_B - p_A}{\rho_A (\rho_B - \rho_A)}} \]

Measure inflow angle \( \phi_B \) between Mach stem and triple point trajectory

Velocity \( a \) of \( T' \) relative to \( T \) cannot be derived that easily: Oblique shock relations across \( C \) and \( D \) hold true both in frame of reference for \( T \) and \( T' \)
Shock polar analysis of triple points in detonations

- Neglect reaction, but consider $c_{pi}(T)$
- Data extracted point-wise from simulation

\[\rho_A u_A \sin(\phi_B) = \rho_B u_B \sin(\phi_B - \theta_B),\]
\[\rho_A u_A^2 \sin^2(\phi_B) = \rho_B u_B^2 \sin^2(\phi_B - \theta_B),\]
\[\rho_A u_A = \frac{\sin \phi_B \sqrt{\rho_B (p_B - p_A)}}{\rho_A (\rho_B - \rho_A)}\]

Measure inflow angle $\phi_B$ between Mach stem and triple point trajectory.

Velocity $a$ of $T'$ relative to $T$ cannot be derived that easily: Oblique shock relations across $C$ and $D$ hold true both in frame of reference for $T$ and $T'$. 

\[\rho_C u_C, n = \rho_D u_D, n,\]
\[p_C + \rho_C u_C^2, n = p_D + \rho_D u_D^2, n,\]
\[u_C, t = u_D, t, h,\]
\[\frac{1}{2} u_C^2, n = \frac{1}{2} u_D^2, n,\]
\[a, n = 0, a, t \text{ arbitrary}\]

Estimate $a, t = L_R t_{init}$
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 → use oblique shock relations between $A$ and $B$

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\rho_A u_A \sin(\phi_B) = \rho_B u_B \sin(\phi_B - \theta_B),
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p_A + \rho_A u_A^2 \sin^2(\phi_B) = p_B + \rho_B u_B^2 \sin^2(\phi_B - \theta_B)
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to evaluate inflow velocity as $u_A = \frac{1}{\sin \phi_B} \sqrt{\frac{\rho_B(p_B - p_A)}{\rho_A(p_B - p_A)}}$
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to evaluate inflow velocity as $u_A = \frac{1}{\sin \phi_B} \sqrt{\frac{\rho_B(p_B - p_A)}{\rho_A(p_B - p_A)}}$

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- Velocity $a$ of $T'$ relative to $T$ cannot be derived that easily: Oblique shock relations across $C$ and $D$ hold true both in frame of reference for $T$ and $T'$

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\begin{align*}
\rho_C u_{C,n} &= \rho_D u_{D,n} \\
p_C + \rho_C u_{C}^2 &= p_D + \rho_D u_{D}^2, \\
u_{C,t} &= u_{D,t} \\
h_C + \frac{1}{2} u_{C}^2 &= h_D + \frac{1}{2} u_{D}^2
\end{align*}
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Shock polar analysis of triple points in detonations

- Neglect reaction, but consider \( c_{pi}(T) \)
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- Velocity \( a \) of \( T' \) relative to \( T \) cannot be derived that easily: Oblique shock relations across \( C \) and \( D \) hold true both in frame of reference for \( T \) and \( T' \)

\[
\rho_C (u_C,n - a_n) = \rho_D (u_D,n - a_n)
\]
\[
p_C + \rho_C (u_C,n - a_n)^2 = p_D + \rho_D (u_D,n - a_n)^2
\]
\[
u_{C,t} - a_t = u_{D,t} - a_t
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h_C + \frac{1}{2} (u_C,n - a_n)^2 = h_D + \frac{1}{2} (u_D,n - a_n)^2
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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 \( \rightarrow \) use oblique shock relations between \( A \) and \( B \)

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\rho_A u_A \sin(\phi_B) = \rho_B u_B \sin(\phi_B - \theta_B),
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p_A + \rho_A u_A^2 \sin^2(\phi_B) = p_B + \rho_B u_B^2 \sin^2(\phi_B - \theta_B)
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p_C + \rho_C (u_{C,n} - a_n)^2 = p_D + \rho_D (u_{D,n} - a_n)^2
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\[
   u_{C,t} - a_t = u_{D,t} - a_t
\]
\[
h_C + \frac{1}{2} (u_{C,n} - a_n)^2 = h_D + \frac{1}{2} (u_{D,n} - a_n)^2
\]

\( \rightarrow a_n = 0, a_t \) arbitrary

Estimate \( a_t = \frac{L_R}{t_{\text{init}}} \)
Detonation simulation

Detonation propagation through pipe bends

- 2D Simulation of CJ detonation for $H_2 : O_2 : Ar/2 : 1 : 7$ at $T_0 = 298 \, \text{K}$ and $p_0 = 10 \, \text{kPa}$. Tube width of 5 detonation cells

- AMR base grid $1200 \times 992$. 4 additional refinement levels $(2,2,2,4)$. $67.6 \, \text{Pts/l}_i$g

- Adaptive computations use up to $7.1 \cdot 10^6$ cells ($4.8 \cdot 10^6$ on highest level) instead of $1.22 \cdot 10^9$ cells (uniform grid)

- $\sim 70,000 \, \text{h CPU on 128 CPUs}$ Pentium-4 2.2GHz
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Higher order schemes

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- AMR base grid \( 1200 \times 992 \). 4 additional refinement levels \((2,2,2,4)\). 67.6 Pts/\( l_{ig} \)
- Adaptive computations use up to \( 7.1 \cdot 10^6 \) cells (\( 4.8 \cdot 10^6 \) on highest level) instead of \( 1.22 \cdot 10^9 \) cells (uniform grid)
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- $\sim 70,000\,\text{h CPU}$ on 128 CPUs
  Pentium-4 2.2GHz
Triple point tracks

Slight overdrive decreases cell size

Marginal detonation

Mach reflection, high overdrive, structure disappears

Re-ignition with transverse detonation

Detonation failure

$\varphi = 15^\circ$ (left, top), $\varphi = 30^\circ$ (left, bottom), and $\varphi = 60^\circ$ (right)
Triple point structures – $\varphi = 15^\circ$
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- Triple point re-initiation after bend with change from transitional to Double Mach reflection
Triple point structures – $\varphi = 30^\circ$
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- Triple point quenching and failure as single Mach reflection
Transition criteria

Solve system of oblique shock relations numerically and determine transition boundaries [Ben-Dor, 2007].

- Regular reflection (RR): $M_B^T < 1$
- Single Mach reflection (SMR):
  $M_C^T < 1$ and $M_B^T > 1$
- Transitional Mach reflection:
  $M_C^{T'} < 1$ and $M_C^T > 1$
- Double Mach reflection: $M_C^{T'} > 1$ and $M_C^T > 1$
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Solve system of oblique shock relations numerically and determine transition boundaries [Ben-Dor, 2007].

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- Double Mach reflection: $M_C^{T'} > 1$ and $M_C^T > 1$

- Here: Nonreactive $H_2 : O_2 : Ar$ mixture at initially 298 K and 10 kPa

For detonations:

$$S := \frac{p_C - p_D}{p_D}$$
Transition criteria

Solve system of oblique shock relations numerically and determine transition boundaries [Ben-Dor, 2007].

- Regular reflection (RR): $M_B^T < 1$
- Single Mach reflection (SMR): $M_C^T < 1$ and $M_B^T > 1$
- Transitional Mach reflection: $M_C^{T'} < 1$ and $M_C^T > 1$
- Double Mach reflection: $M_C^{T'} > 1$ and $M_C^T > 1$

Here: Nonreactive H$_2$ : O$_2$ : Ar mixture at initially 298 K and 10 kPa

For detonations:

$$S := \frac{p_C - p_D}{p_D}$$

[Deiterding, 2011]

TMR/DMR transition for $a_t = 100$ m/s

- Non-reactive shock wave reflection theory seems applicable to predict local triple point structure and stability

- Triple point type is determined solely by $S$ and $M$. Useful to determine type in underresolved situations.
Triple point structures, $\varphi = 15$

Strong DMR structure in diffraction region behind bend, $S = 1.062$

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Triple point structures, $\varphi = 15$

Strong DMR structure in diffraction region behind bend, $S = 1.062$

TMR structure in compression region shortly behind bend, $S = 0.338$

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Triple point structures

TMR structure in marginal region near limit of detonability, $\varphi = 30$, $S = 0.338$

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<td>744</td>
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Re-ignition with strong DMR and transverse detonation, \( \varphi = 45, S = 1.377 \)

TMR structure in marginal region near limit of detonability, \( \varphi = 30, S = 0.338 \)

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Detonation cell structure in 3D

- Simulation of only one quadrant
- $44.8 \text{ Pts}/l_{ig}$ for $\text{H}_2 : \text{O}_2 : \text{Ar}$ CJ detonation
- SAMR base grid $400 \times 24 \times 24$, 2 additional refinement levels (2, 4)
- Simulation uses $\sim 18 \text{ M}$ cells instead of $\sim 118 \text{ M}$ (unigrid)
- $\sim 51,000 \text{ h CPU}$ on 128 CPU Compaq Alpha.
  $\mathcal{H}$: 37.6 %, $S$: 25.1 %

Schlieren and isosurface of $Y_{\text{OH}}$
Detonation cell structure in 3D

- Simulation of only one quadrant
- 44.8 Pts/$l_{ig}$ for H$_2$ : O$_2$ : Ar CJ detonation
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Schlieren and isosurface of $Y_{\text{OH}}$

Schlieren on refinement levels

Distribution to 128 processors
Detonation cell structure in 3D - II

Schematic front view of the periodic triple point line structure right plot at the same time.

Schlieren plots of density, mirrored for visualization

Schlieren plots of $Y_{OH}$

References

Detonation structures
Temporal Development of Detonation Velocity

Point-wise reinitiation along L1 (left) and L1' (right)

Simulation time [µs]
Temporal Development of Detonation Velocity

Point-wise reinitiation along L1 (left) and L1' (right)

Comparison with 2D Simulation
Axisymmetric Navier-Stokes equations with chemical reaction

\[ \frac{\partial \mathbf{q}}{\partial t} + \frac{\partial (\mathbf{f} - \mathbf{f}_v)}{\partial x} + \frac{\partial (\mathbf{g} - \mathbf{g}_v)}{\partial y} = \frac{\alpha}{y} (\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s} \]

\[
\begin{bmatrix}
\rho_i \\
\rho u \\
\rho v \\
\rho E
\end{bmatrix},
\begin{bmatrix}
\rho_i u \\
\rho u^2 + p \\
\rho uv \\
u(\rho E + p)
\end{bmatrix},
\begin{bmatrix}
\rho_i v \\
\rho uv \\
\rho v^2 + p \\
v(\rho E + p)
\end{bmatrix},
\begin{bmatrix}
0 \\
0 \\
p - \tau_{\theta\theta} \\
0
\end{bmatrix},
\begin{bmatrix}
\dot{\omega}_i \\
0 \\
0
\end{bmatrix}
\]
Axisymmetric Navier-Stokes equations with chemical reaction

\[
\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial (\mathbf{f} - \mathbf{f}_v)}{\partial x} + \frac{\partial (\mathbf{g} - \mathbf{g}_v)}{\partial y} = \frac{\alpha}{y} (\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s}
\]

\[
\mathbf{q} = \begin{bmatrix} \rho_i \\ \rho u \\ \rho v \\ \rho E \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \rho_i u \\ \rho u^2 + p \\ \rho uv \\ u(\rho E + p) \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} \rho_i v \\ \rho uv \\ \rho v^2 + p \\ v(\rho E + p) \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 0 \\ 0 \\ p - \tau_{\theta\theta} \\ 0 \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} \dot{\omega}_i \\ 0 \\ 0 \end{bmatrix}
\]

\[
\tau_{xx} = -\frac{2}{3} \mu (\nabla \cdot \mathbf{v}) + 2\mu \frac{\partial u}{\partial x}
\]

\[
\tau_{yy} = -\frac{2}{3} \mu (\nabla \cdot \mathbf{v}) + 2\mu \frac{\partial v}{\partial y}
\]

\[
\tau_{\theta\theta} = -\frac{2}{3} \mu (\nabla \cdot \mathbf{v}) + 2\mu \frac{v}{y}
\]

\[
\nabla \cdot \mathbf{v} = \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \alpha \frac{v}{y} \right)
\]
Chemistry and transport properties

Arrhenius-kinetics:

\[
\dot{\omega}_i = \sum_{j=1}^{M} (\nu_{ji}^r - \nu_{ji}^f) \left[ k_j^f \prod_{n=1}^{K} \left( \frac{\rho_n}{W_n} \right)^{\nu_{jn}^f} - k_j^r \prod_{n=1}^{K} \left( \frac{\rho_n}{W_n} \right)^{\nu_{jn}^r} \right] \quad i = 1, \ldots, K
\]
Chemistry and transport properties

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\]

- Parsing of mechanisms and evaluation of \( \dot{\omega}_i \) with Chemkin-II
- \( c_{pi}(T) \) and \( h_i(T) \) tabulated, linear interpolation between values
Chemistry and transport properties

Arrhenius-kinetics:

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- \( c_{pi}(T) \) and \( h_i(T) \) tabulated, linear interpolation between values

Mixture viscosity \( \mu = \mu(T, Y_i) \) with Wilke formula

\[
\mu = \sum_{i=1}^{K} \frac{Y_i \mu_i}{W_i \sum_{m=1}^{K} Y_m \Phi_{im}/W_m} \quad \text{with} \quad \Phi_{im} = \frac{1}{\sqrt{8}} \left( 1 + \frac{W_i}{W_m} \right)^{-\frac{1}{2}} \left( 1 + \left( \frac{\mu_i}{\mu_m} \right)^{\frac{1}{2}} \left( \frac{W_m}{W_j} \right)^{\frac{1}{4}} \right)^2
\]
Chemistry and transport properties

Arrhenius-kinetics:

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\]

Mixture thermal conductivity \( k = k(T, Y_i) \) following Mathur

\[
k = \frac{1}{2} \left( W \sum_{i=1}^{K} \frac{Y_i k_i}{W_i} + \frac{1}{W \sum_{i=1}^{K} Y_i/(W_i k_i)} \right)
\]
Chemistry and transport properties

Arrhenius-kinetics:

\[ \dot{\omega}_i = \sum_{j=1}^{M} (\nu_{ji}^r - \nu_{ji}^f) \left[ k_f \prod_{n=1}^{K} \left( \frac{\rho_n}{W_n} \right)^{\nu_{jn}^f} - k_r \prod_{n=1}^{K} \left( \frac{\rho_n}{W_n} \right)^{\nu_{jn}^r} \right] \quad i = 1, \ldots, K \]

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Mixture thermal conductivity \( k = k(T, Y_i) \) following Mathur

\[ k = \frac{1}{2} \left( W \sum_{i=1}^{K} \frac{Y_i k_i}{W_i} + \frac{1}{W \sum_{i=1}^{K} Y_i/(W_i k_i)} \right) \]

Mixture diffusion coefficients \( D_i = D_i(T, p, Y_i) \) from binary diffusion \( D_{mi}(T, p) \) as

\[ D_i = \frac{1 - Y_i}{W \sum_{m \neq i} Y_m/(W_m D_{mi})} \]

- Evaluation with Chemkin-II Transport library
Splitting method

\[ \partial_t q + \partial_x (f - f_v) + \partial_y (g - g_v) = \frac{\alpha}{y} (c - g + g_v) + s \]
Splitting method

\[ \partial_t q + \partial_x (f - f_v) + \partial_y (g - g_v) = \frac{\alpha}{y} (c - g + g_v) + s \]

Dimensional splitting for PDE

\[ \mathcal{X}(\Delta t) : \quad \partial_t q + \partial_x (f(q) - f_v(q)) = 0 , \quad \text{IC: } Q(t_m) \xrightarrow{\Delta t} \tilde{Q}^{1/2} \]

\[ \mathcal{Y}(\Delta t) : \quad \partial_t q + \partial_y (g(q) - g_v(q)) = 0 , \quad \text{IC: } \tilde{Q}^{1/2} \xrightarrow{\Delta t} \tilde{Q} \]
Splitting method

\[ \partial_t q + \partial_x (f - f_v) + \partial_y (g - g_v) = \frac{\alpha}{\gamma} (c - g + g_v) + s \]

Dimensional splitting for PDE

\[ \chi(\Delta t) : \quad \partial_t q + \partial_x (f(q) - f_v(q)) = 0 \quad , \quad \text{IC: } Q(t_m) \xrightarrow{\Delta t} \bar{Q}^{1/2} \]

\[ \gamma(\Delta t) : \quad \partial_t q + \partial_y (g(q) - g_v(q)) = 0 \quad , \quad \text{IC: } \bar{Q}^{1/2} \xrightarrow{\Delta t} \bar{Q} \]

Treat right-hand side as source term

\[ \mathcal{C}(\Delta t) : \quad \partial_t q = \frac{\alpha}{\gamma} (c(q) - g(q) + g_v(q)) , \quad \text{IC: } \bar{Q} \xrightarrow{\Delta t} \bar{Q} \]
Splitting method

\[ \partial_t q + \partial_x (f - f_v) + \partial_y (g - g_v) = \frac{\alpha}{y} (c - g + g_v) + s \]

Dimensional splitting for PDE

\( \mathcal{X}(\Delta t) : \quad \partial_t q + \partial_x (\mathcal{F}(q) - f_v(q)) = 0 \), \hspace{1cm} \text{IC: } Q(t_m) \xrightarrow{\Delta t} \tilde{Q}^{1/2} \\
\mathcal{Y}(\Delta t) : \quad \partial_t q + \partial_y (\mathcal{G}(q) - g_v(q)) = 0 \), \hspace{1cm} \text{IC: } \tilde{Q}^{1/2} \xrightarrow{\Delta t} \tilde{Q}

Treat right-hand side as source term

\( \mathcal{C}(\Delta t) : \quad \partial_t q = \frac{\alpha}{y} (c(q) - g(q) + g_v(q)) \), \hspace{1cm} \text{IC: } \tilde{Q} \xrightarrow{\Delta t} \bar{Q}

Chemical source term

\( \mathcal{S}(\Delta t) : \quad \partial_t q = s(q) \), \hspace{1cm} \text{IC: } \bar{Q} \xrightarrow{\Delta t} Q(t_m + \Delta t) \)
Splitting method

\[ \partial_t \mathbf{q} + \partial_x (f - f_v) + \partial_y (g - g_v) = \frac{\alpha}{y} (c - g + g_v) + s \]

Dimensional splitting for PDE

\[ \mathcal{X}(\Delta t) : \quad \partial_t \mathbf{q} + \partial_x (f(q) - f_v(q)) = 0 \quad \text{IC: } Q(t_m) \Rightarrow Q^{1/2} \]

\[ \mathcal{Y}(\Delta t) : \quad \partial_t \mathbf{q} + \partial_y (g(q) - g_v(q)) = 0 \quad \text{IC: } \tilde{Q}^{1/2} \Rightarrow \tilde{Q} \]

Treat right-hand side as source term

\[ \mathcal{C}(\Delta t) : \quad \partial_t \mathbf{q} = \frac{\alpha}{y} (c(q) - g(q) + g_v(q)) \quad \text{IC: } \tilde{Q} \Rightarrow \tilde{Q} \]

Chemical source term

\[ \mathcal{S}(\Delta t) : \quad \partial_t \mathbf{q} = s(q) \quad \text{IC: } \bar{Q} \Rightarrow Q(t_m + \Delta t) \]

Formally 1st-order algorithm

\[ Q(t_m + \Delta t) = S(\Delta t)C(\Delta t)Y(\Delta t)X(\Delta t)(Q(t_m)) \]

but all sub-operators 2nd-order accurate or higher.
Finite volume discretization

Time discretization $t_n = n\Delta t$, discrete volumes $I_{jk} = [x_j - \frac{1}{2} \Delta x, x_j + \frac{1}{2} \Delta x] \times [y_k - \frac{1}{2} \Delta y, y_k + \frac{1}{2} \Delta y] =: [x_{j-1/2}, x_{j+1/2}] \times [y_{k-1/2}, y_{k+1/2}]

Approximation $Q_{jk}(t) \approx \frac{1}{|I_{jk}|} \int_{I_{jk}} q(x, t) \, dx$ and numerical fluxes

$$F(Q_{jk}(t), Q_{j+1,k}(t)) \approx f(q(x_{j+1/2}, y_k, t)),$$

$$F_v(Q_{jk}(t), Q_{j+1,k}(t)) \approx f_v(q(x_{j+1/2}, y_k, t), \nabla q(x_{j+1/2}, y_k, t))$$

yield (for simplicity)

$$Q_{jk}^{n+1} = Q_{kj}^n - \frac{\Delta t}{\Delta x} \left[ F(Q_{jk}^n, Q_{j+1,k}^n) - F(Q_{j-1,k}^n, Q_{jk}^n) \right] + \frac{\Delta t}{\Delta x} \left[ F_v(Q_{jk}^n, Q_{j+1,k}^n) - F_v(Q_{j-1,k}^n, Q_{jk}^n) \right]$$
Finite volume discretization

Time discretization \( t_n = n \Delta t \), discrete volumes \( l_{jk} = [x_j - \frac{1}{2} \Delta x, x_j + \frac{1}{2} \Delta x] \times [y_k - \frac{1}{2} \Delta y, y_k + \frac{1}{2} \Delta y] =: [x_{j-1/2}, x_{j+1/2}] \times [y_{k-1/2}, y_{k+1/2}] \)

Approximation \( Q_{jk}(t) \approx \frac{1}{|l_{jk}|} \int_{l_{jk}} q(x, t) \, dx \) and numerical fluxes

\[
F \left( Q_{jk}(t), Q_{j+1,k}(t) \right) \approx f(q(x_{j+1/2}, y_k, t)),
\]

\[
F_v \left( Q_{jk}(t), Q_{j+1,k}(t) \right) \approx f_v(q(x_{j+1/2}, y_k, t), \nabla q(x_{j+1/2}, y_k, t))
\]

yield (for simplicity)

\[
Q_{jk}^{n+1} = Q_{kj}^n - \frac{\Delta t}{\Delta x} \left[ F \left( Q_{jk}^n, Q_{j+1,k}^n \right) - F \left( Q_{j-1,k}^n, Q_{jk}^n \right) \right] + \frac{\Delta t}{\Delta x} \left[ F_v \left( Q_{jk}^n, Q_{j+1,k}^n \right) - F_v \left( Q_{j-1,k}^n, Q_{jk}^n \right) \right]
\]

▶ Riemann solver to approximate \( F \left( Q_{jk}^n, Q_{j+1,k}^n \right) \)
Finite volume discretization

Time discretization $t_n = n\Delta t$, discrete volumes $I_{jk} = [x_j - \frac{1}{2}\Delta x, x_j + \frac{1}{2}\Delta x] \times [y_k - \frac{1}{2}\Delta y, y_k + \frac{1}{2}\Delta y] =: [x_{j-1/2}, x_{j+1/2}] \times [y_{k-1/2}, y_{k+1/2}]

Approximation $Q_{jk}(t) \approx \frac{1}{|I_{jk}|} \int_{I_{jk}} q(x,t) \, dx$ and numerical fluxes

$$F(Q_{jk}(t), Q_{j+1,k}(t)) \approx f(q(x_{j+1/2}, y_k, t)),$$

$$F_v(Q_{jk}(t), Q_{j+1,k}(t)) \approx f_v(q(x_{j+1/2}, y_k, t), \nabla q(x_{j+1/2}, y_k, t))$$

yield (for simplicity)

$$Q_{jk}^{n+1} = Q_{kj}^n - \frac{\Delta t}{\Delta x} \left[ F(Q_{jk}^n, Q_{j+1,k}^n) - F(Q_{j-1,k}^n, Q_{jk}^n) \right] + \frac{\Delta t}{\Delta x} \left[ F_v(Q_{jk}^n, Q_{j+1,k}^n) - F_v(Q_{j-1,k}^n, Q_{jk}^n) \right]$$

$\triangleright$ Riemann solver to approximate $F(Q_{jk}^n, Q_{j+1,k}^n)$

$\triangleright$ 1st-order finite differences for $F_v(Q_{jk}^n, Q_{j+1,k}^n)$ yield 2nd-order accurate central differences in ($\ast$)
Finite volume discretization

Time discretization \( t_n = n\Delta t \), discrete volumes \( l_{jk} = [x_j - \frac{1}{2}\Delta x, x_j + \frac{1}{2}\Delta x][y_k - \frac{1}{2}\Delta y, y_k + \frac{1}{2}\Delta y[\times =: [x_{j-1/2}, x_{j+1/2}][y_{k-1/2}, y_{k+1/2}]

Approximation \( Q_{jk}(t) \approx \frac{1}{|l_{jk}|} \int_{l_{jk}} q(x, t) \, dx \) and numerical fluxes

\[
F\left(Q_{jk}(t), Q_{j+1,k}(t)\right) \approx f(q(x_{j+1/2}, y_k, t)),
\]

\[
F_v\left(Q_{jk}(t), Q_{j+1,k}(t)\right) \approx f_v(q(x_{j+1/2}, y_k, t), \nabla q(x_{j+1/2}, y_k, t))
\]

yield (for simplicity)

\[
Q_{jk}^{n+1} = Q_{kj}^n - \frac{\Delta t}{\Delta x} \left[ F\left(Q_{jk}^n, Q_{j+1,k}^n\right) - F\left(Q_{j-1,k}^n, Q_{jk}^n\right) \right] + \frac{\Delta t}{\Delta x} \left[ F_v\left(Q_{jk}^n, Q_{j+1,k}^n\right) - F_v\left(Q_{j-1,k}^n, Q_{jk}^n\right) \right]
\]

- Riemann solver to approximate \( F\left(Q_{jk}^n, Q_{j+1,k}^n\right) \)

- 1st-order finite differences for \( F_v\left(Q_{jk}^n, Q_{j+1,k}^n\right) \) yield 2nd-order accurate central differences in (*)

Stability condition used:

\[
\max_{i,j,k} \left\{ \frac{\Delta t}{\Delta x} (|u_{jk}| + c_{jk}) + \frac{8}{3} \frac{\mu_{jk}\Delta t}{\rho_{jk}\Delta x^2}, \frac{\Delta t}{\Delta x} (|u_{jk}| + c_{jk}) + \frac{2k_j\Delta t}{c_{v,jk}\rho_f\Delta x^2}, \frac{\Delta t}{\Delta x} (|u_{jk}| + c_{jk}) + D_{i,jk} \frac{\Delta t}{\Delta x^2} \right\} \leq 1
\]
Finite volume scheme

Finite volume discretization – cont.

Symmetry source term $C^{(\Delta t)}$: Use

$$Q_{jk}^{n+1} = Q_{jk}^n + \Delta t \left( \frac{\alpha}{y} (c(Q_{jk}^n) - g(Q_{jk}^n) + \frac{1}{2} \left( G_v(Q_{jk}^n, Q_{j,k+1}^n) + G_v(Q_{j,k-1}^n, Q_{jk}^n) \right) \right)$$

within explicit 2nd-order accurate Runge-Kutta method

▶ Gives 2nd-order central difference approximation of $G_v$
Symmetry source term $C^{(\Delta t)}$: Use

$$Q_{jk}^{n+1} = Q_{jk}^n + \Delta t \left( \frac{\alpha}{\gamma} (c(Q_{jk}^n) - g(Q_{jk}^n)) + \frac{1}{2} \left( G_v(Q_{jk}^n, Q_{jk,k+1}^n) + G_v(Q_{jk,k-1}^n, Q_{jk}^n) \right) \right)$$

within explicit 2nd-order accurate Runge-Kutta method

- Gives 2nd-order central difference approximation of $G_v$
- Transport properties $\mu$, $k$, $D_i$ are stored in vector of state $Q$ and kept constant throughout entire time step
Finite volume discretization – cont.

Symmetry source term $C^{(\Delta t)}$: Use

$$Q_{jk}^{n+1} = Q_{jk}^n + \Delta t \left( \frac{\alpha}{\gamma} c(Q_{jk}^n) - g(Q_{jk}^n) + \frac{1}{2} \left( G_v (Q_{jk}^n, Q_{j,k+1}^n) + G_v (Q_{j,k-1}^n, Q_{jk}^n) \right) \right)$$

within explicit 2nd-order accurate Runge-Kutta method

- Gives 2nd-order central difference approximation of $G_v$
- Transport properties $\mu, k, D_i$ are stored in vector of state $Q$ and kept constant throughout entire time step

Chemical source term $S(\cdot)$:

- 4th-order accurate semi-implicit ODE-solver subcycles within each cell
- $\rho, e, u, v$ remain unchanged!

$$\partial_t \rho_i = W_i \dot{\omega}_i (\rho_1, \ldots, \rho_K, T) \quad i = 1, \ldots, K$$
Lehr’s ballistic range experiments

- Spherical-nosed projectile of radius 1.5 mm travels with constant velocity through stoichiometric $H_2 : O_2 : N_2$ mixture (molar ratios 2:1:3.76) at 42.663 kPa and $T = 293$ K [Lehr, 1972]

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- Axisymmetric Navier-Stokes and Euler’s simulations on AMR base mesh of 400 × 200 cells, physical domain size 6 cm × 3 cm

- 4-level computations with refinement factors 2,2,4 to final time t = 170 µs. Refinement downstream removed.
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- Main configurations
  - Velocity $v_I = 1931\, \text{m/s} \ (M = 4.79)$, $\sim 40\, \text{Pts/lig}$
  - Velocity $v_I = 1806\, \text{m/s} \ (M = 4.48)$, $\sim 60\, \text{Pts/lig}$
- Various previous studies with not entirely consistent results. E.g. [Yungster and Radhakrishnan, 1996], [Axdahl et al., 2011]
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▶ Stagnation point location and pressure tracked in every time step
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- Mechanism by [Jachimowski, 1988]: 19 equilibrium reactions, 9 species. Chapman Jouguet velocity \( \sim 1957 \text{ m/s} \).

- Axisymmetric Navier-Stokes and Eulers simulations on AMR base mesh of 400 \( \times \) 200 cells, physical domain size 6 cm \( \times \) 3 cm

- 4-level computations with refinement factors 2,2,4 to final time \( t = 170 \mu \text{s} \). Refinement downstream removed.

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- All computations were on 32 cores requiring \( \sim 1500 \text{ h CPU each} \)
Lehr’s ballistic range experiments

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  - Velocity v_I = 1931 m/s (M = 4.79), ∼ 40 Pts/lig
  - Velocity v_I = 1806 m/s (M = 4.48), ∼ 60 Pts/lig
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- Stagnation point location and pressure tracked in every time step
- All computations were on 32 cores requiring ∼ 1500 h CPU each
Viscous case – $M = 4.79$

- 5619 iterations with CFL=0.9 to $t = 170 \mu s$
- Oscillation frequency in last 20 $\mu s$: $\sim 722$ kHz (viscous), $\sim 737$ kHz (inviscid)
- Experimental value: $\sim 720$ kHz

Schlieren plot of density
Viscous case – $M = 4.79$ – mesh adaptation
Comparison of temperature field

Viscous
Comparison of temperature field

Inviscid
Viscous case – $M = 4.48$

- 5432 iterations with CFL=0.9 to $t = 170 \mu s$
- Oscillation frequency in last 20 $\mu s$: $\sim 417$ kHz
- Experimental value: $\sim 425$ kHz

Schlieren plot of density
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Oscillation created by accelerated reaction due to slip line from previous triple point.
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Oscillation created by accelerated reaction due to slip line from previous triple point.
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Oscillation created by accelerated reaction due to slip line from previous triple point.
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Detonation simulation

Combustion with viscous terms

Higher order schemes

References

Finite volume scheme
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

- Oscillation created by accelerated reaction due to slip line from previous triple point

Detonation simulation

Combustion with viscous terms

Higher order schemes

References
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Oscillation created by accelerated reaction due to slip line from previous triple point.
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Schlieren of density

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Schlieren of density

Temperature

Mass fraction OH

Pressure

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Schlieren of density

Temperature

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Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Detonation simulation

Combustion with viscous terms

Higher order schemes

References

Finite volume scheme
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Detonation simulation

Combustion with viscous terms

Higher order schemes

References

Finite volume scheme
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Oscillation created by accelerated reaction due to slip line from previous triple point.
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Detonation simulation

Combustion with viscous terms

Higher order schemes

Finite volume scheme

References
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Detonation simulation
Combustion with viscous terms
Higher order schemes
References

Finite volume scheme
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

$t=0.00105382\ \text{sec}$
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Oscillation created by accelerated reaction due to slip line from previous triple point
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Oscillation created by accelerated reaction due to slip line from previous triple point
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Detonation simulation

Combustion with viscous terms

Higher order schemes

References

Finite volume scheme
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Detonation simulation

Combustion with viscous terms

Higher order schemes

References
Oscillation mechanism

- Oscillation created by accelerated reaction due to slip line from previous triple point
Inviscid case – $M = 4.48$

- 4048 iterations with CFL=0.9 to $t = 170 \mu s$
- Oscillation frequency in last 20 $\mu s$: $\sim 395$ kHz
- Experimental value: $\sim 425$ kHz

Schlieren plot of density
Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Small perturbations can quickly create numerous triple points.
Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure
Detonation simulation

Combustion with viscous terms

Higher order schemes

References

Finite volume scheme

Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Small perturbations can quickly create numerous triple points
Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Small perturbations can quickly create numerous triple points
Perturbed oscillation mechanism

Schlieren of density
Temperature
Mass fraction OH
Pressure

Small perturbations can quickly create numerous triple points.
Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

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Perturbed oscillation mechanism

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Temperature

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Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Small perturbations can quickly create numerous triple points.
Perturbed oscillation mechanism
Perturbed oscillation mechanism

Schlieren of density, Temperature, Mass fraction OH, Pressure
Detonation simulation

Combustion with viscous terms

Higher order schemes

References

Finite volume scheme

Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Small perturbations can quickly create numerous triple points.
Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Small perturbations can quickly create numerous triple points

Detonation simulation

Combustion with viscous terms

Higher order schemes

References
Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

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Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure
Perturbed oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Small perturbations can quickly create numerous triple points.
Perturbed oscillation mechanism

Small perturbations can quickly create numerous triple points
Hybrid method

Convective numerical flux is defined as

\[ F_{inv}^n = \begin{cases} F_{inv-WENO}^n, & \text{in } C \\ F_{inv-CD}^n, & \text{in } \overline{C}, \end{cases} \]
Hybrid method

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- For LES: 3rd order WENO method, 2nd order TCD [Hill and Pullin, 2004]
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\end{cases}
\]

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Use WENO scheme to only capture shock waves but resolve interface between species.
Hybrid method

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Shock detection based on using two criteria together:

1. Lax-Liu entropy condition \( |u_R \pm a_R| < |u_* \pm a_*| < |u_L \pm a_L| \) tested with a threshold to eliminate weak acoustic waves. Used intermediate states at cell interfaces:

\[ u_* = \frac{\sqrt{\rho_L u_L} + \sqrt{\rho_R u_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \quad a_* = \sqrt{(\gamma_* - 1)\left(h_* - \frac{1}{2}u_*^2\right)}, \ldots \]
Hybrid method

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F^n_{inv-WENO}, & \text{in } C \\
F^n_{inv-CD}, & \text{in } \overline{C}, 
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u_* = \sqrt{\frac{\rho_L u_L + \sqrt{\rho_R u_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}}}, \quad a_* = \sqrt{(\gamma_* - 1)(h_* - \frac{1}{2} u_*^2)}, \ldots
\]

2. Limiter-inspired discontinuity test based on mapped normalized pressure gradient \( \theta_j \)

\[
\phi(\theta_j) = \frac{2\theta_j}{(1 + \theta_j)^2}, \quad \text{with} \quad \theta_j = \frac{|p_{j+1} - p_j|}{|p_{j+1} + p_j|}, \quad \phi(\theta_j) > \alpha_{Map}
\]
SAMR flux correction for Runge-Kutta method

Recall Runge-Kutta temporal update

\[ \tilde{Q}_j^\nu = \alpha_v Q_j^m + \beta_v \tilde{Q}_j^{\nu-1} + \gamma_v \frac{\Delta t}{\Delta x_n} \Delta F^n(\tilde{Q}_j^{\nu-1}) \]

[Pantano et al., 2007]
SAMR flux correction for Runge-Kutta method

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\tilde{Q}_j^\nu = \alpha_v Q_j^m + \beta_v \tilde{Q}_j^{\nu-1} + \gamma_v \frac{\Delta t}{\Delta x_n} \Delta F^n(\tilde{Q}^{\nu-1})
\]

rewrite scheme as

\[
Q^{m+1} = Q^m - \sum_{\nu=1}^{\tau} \varphi_\nu \frac{\Delta t}{\Delta x_n} \Delta F^n(\tilde{Q}^{\nu-1}) \quad \text{with} \quad \varphi_\nu = \gamma_\nu \prod_{\nu=\nu+1}^{\tau} \beta_\nu
\]

[Pantano et al., 2007]
SAMR flux correction for Runge-Kutta method

Recall Runge-Kutta temporal update

$$\tilde{Q}_j^\upsilon = \alpha_\upsilon Q^m_j + \beta_\upsilon \tilde{Q}_j^{\upsilon-1} + \gamma_\upsilon \frac{\Delta t}{\Delta x_n} \Delta F^n(\tilde{Q}^{\upsilon-1})$$

rewrite scheme as

$$Q^{m+1} = Q^m - \sum_{\upsilon=1}^{\tau} \varphi_\upsilon \frac{\Delta t}{\Delta x_n} \Delta F^n(\tilde{Q}^{\upsilon-1}) \quad \text{with} \quad \varphi_\upsilon = \gamma_\upsilon \prod_{\nu=\upsilon+1}^{\tau} \beta_\nu$$

Flux correction to be used

1. $$\delta F_{i-\frac{1}{2},j}^{1,l+1} := -\varphi_1 F_{i-\frac{1}{2},j}^{1,l}(\tilde{Q}^0), \quad \delta F_{i-\frac{1}{2},j}^{1,l+1} := \delta F_{i-\frac{1}{2},j}^{1,l+1} - \sum_{\nu=2}^{\tau} \varphi_\upsilon F_{i-\frac{1}{2},j}^{1,l}(\tilde{Q}^{\upsilon-1})$$

2. $$\delta F_{i-\frac{1}{2},j}^{1,l+1} := \delta F_{i-\frac{1}{2},j}^{1,l+1} + \frac{1}{r_{l+1}^2} \sum_{\nu=1}^{\tau} \varphi_\upsilon F_{v+\frac{1}{2},w+l}^{1,l+1} (\tilde{Q}^{\upsilon-1}(t + \kappa \Delta t_{l+1}))$$

[Pantano et al., 2007]
SAMR flux correction for Runge-Kutta method

Recall Runge-Kutta temporal update

\[
\tilde{Q}_j^v = \alpha_v Q_j^m + \beta_v \tilde{Q}_j^{v-1} + \gamma_v \frac{\Delta t}{\Delta x_n} \Delta F^n(\tilde{Q}_j^{v-1})
\]

rewrite scheme as

\[
Q^{m+1} = Q^m - \sum_{\nu=1}^{\tau} \varphi_\nu \frac{\Delta t}{\Delta x_n} \Delta F^n(\tilde{Q}_j^{v-1}) \quad \text{with} \quad \varphi_\nu = \gamma_\nu \prod_{\nu=\nu+1}^{\tau} \beta_\nu
\]

Flux correction to be used

1. \( \delta F_{i-\frac{1}{2},j}^{1,l+1} := -\varphi_1 F_{i-\frac{1}{2},j}^{1,l} (\tilde{Q}_j^0) \), \( \delta F_{i-\frac{1}{2},j}^{1,l+1} := \delta F_{i-\frac{1}{2},j}^{1,l+1} - \sum_{\nu=2}^{\tau} \varphi_\nu F_{i-\frac{1}{2},j}^{1,l} (\tilde{Q}_j^{v-1}) \)

2. \( \delta F_{i-\frac{1}{2},j}^{1,l+1} := \delta F_{i-\frac{1}{2},j}^{1,l+1} + \frac{1}{r_{l+1}^2} \sum_{\iota=0}^{r_{l+1}-1} \sum_{\nu=1}^{\tau} \varphi_\nu F_{i-\frac{1}{2},j}^{1,l+1} (\tilde{Q}_j^{v-1}(t + \kappa \Delta t_{l+1})) \)

Storage-efficient SSPRK(3,3):

\[
\begin{array}{c|cccc}
\nu & \alpha_\nu & \beta_\nu & \gamma_\nu & \varphi_\nu \\
\hline
1 & 1 & 0 & 1 & \frac{1}{2} \\
2 & \frac{4}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \\
3 & \frac{1}{2} & \frac{2}{3} & \frac{1}{4} & \frac{1}{3}
\end{array}
\]

[Pantano et al., 2007]
DNS of shear layer in detonation triple point

- Calorically perfect two-species model with $\gamma = 1.29499$ and $h_0 = 54,000$ J/mol and one-step Arrhenius reaction with parameters $E_a = 30,000$ J/mol, $A = 6 \cdot 10^5$ s$^{-1}$, $W = 0.029$ kg/mol $\rightarrow$ 1d ZND theory predicts $d_{CJ} = 1587.8$ m/s
- For dynamic viscosity, heat conductivity, and mass diffusion simple Sutherland models are used
- Distance $L(t) = d_{CJ} \sin(\theta)t$ is used to define a Reynolds number as $Re = \frac{\rho_0 a_0 L(t)}{\mu_0}$
- Visous shear layer thickness, thermal heat conduction layer thickness, and mass diffusion layer thickness grow as $\delta_{visc} \approx \sqrt{\frac{\mu}{\rho}} t$, $\delta_{cond} \approx \sqrt{\frac{k_{ref}}{\rho c_v}} t$, $\delta_{mass,i} \approx \sqrt{\frac{D_i}{\rho}} t$
- Only shock thickness not resolved $\rightarrow$ “pseudo-DNS”
- Computations with WENO/CD/RK3 use SAMR base mesh $320 \times 160$ and up to 8 levels refined by factor 2, domain: $40$ mm $\times$ $20$ mm
- Computations with MUSCL scheme use base mesh $590 \times 352$ and up to 7 levels refined by factor 2, domain: $40$ mm $\times$ $22$ mm

![Diagram](image.png)
DNS of shear layer in detonation triple point

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Computational results for shear layer

- **WENO/CD - 6 levels**
  - $\Delta x_{\text{min}} = 3.91 \cdot 10^{-6}$ m
  - MUSCL - 7 levels
  - $\Delta x_{\text{min}} = 1.05 \cdot 10^{-6}$ m

- **WENO/CD - 7 levels**
  - $\Delta x_{\text{min}} = 1.95 \cdot 10^{-6}$ m
  - MUSCL - 7 levels - Euler
  - $\Delta x_{\text{min}} = 1.05 \cdot 10^{-6}$ m

- **WENO/CD - 8 levels**
  - $\Delta x_{\text{min}} = 9.77 \cdot 10^{-7}$ m

Usage of WENO for WENO/CD - 8 levels

WENO/CD/RK3 gives results comparable to 4x finer resolved optimal 2nd-order scheme, but CPU times with SAMR 2-3x larger.
Computational results for shear layer

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\[ \Delta x_{\text{min}} = 3.91 \cdot 10^{-6} \text{ m} \]

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MUSCL - 7 levels - Euler
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- **WENO/CD/RK3**
  - Gives results comparable to 4x finer resolved optimal 2nd-order scheme, but CPU times with SAMR 2-3x larger

- **Gain in CPU time from higher-order scheme roughly one order**
References I


References II


