Adaptive high-resolution methods for simulating shock-induced hydrogen-air combustion

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Outline

Introduction
   Governing equations

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Collaboration with

- Georg Bader (BTU Cottbus)
- Bok Jik Lee (King Abdullah University of Science and Technology)
- Jack Ziegler (now National Renewable Energy Laboratory)
- Dale Pullin, Joe Shepherd (Graduate Aeronautical Laboratory, California Institute of Technology)
- Daniel Meiron, Sean Mauch (Computational and Applied Mathematics, California Institute of Technology)
Axisymmetric Navier-Stokes equations with chemical reaction

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

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

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

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

\[
\mathbf{f}_v = \begin{bmatrix} \rho D_i \frac{\partial Y_i}{\partial x} \\ \tau_{xx} \\ \tau_{xy} \end{bmatrix} + \rho \sum \left( h_j D_j \frac{\partial Y_j}{\partial x} + u \tau_{xx} + \nu \tau_{xy} \right)
\]

\[
\mathbf{g}_v = \begin{bmatrix} \rho D_i \frac{\partial Y_i}{\partial y} \\ \tau_{xy} \\ \tau_{yy} \end{bmatrix} + \rho \sum \left( h_j D_j \frac{\partial Y_j}{\partial y} + u \tau_{xy} + \nu \tau_{yy} \right)
\]

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

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

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

\[
\tau_{xy} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)
\]

\[
\nabla \cdot \mathbf{v} = \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\nu}{y} \right)
\]
Equation of state

Ideal gas law and Dalton’s law for gas-mixtures

\[ p(\rho_1, \ldots, \rho_K, T) = \sum_{i=1}^{K} p_i = \sum_{i=1}^{K} \rho_i \frac{R}{W_i} T = \rho \frac{R}{W} T \]

with \( \sum_{i=1}^{K} \rho_i = \rho \), \( Y_i = \frac{\rho_i}{\rho} \).
Equation of state

Ideal gas law and Dalton’s law for gas-mixtures

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p(\rho_1, \ldots, \rho_K, T) = \sum_{i=1}^{K} p_i = \sum_{i=1}^{K} \rho_i \frac{R}{W_i} T = \rho \frac{R}{W} T \quad \text{with} \quad \sum_{i=1}^{K} \rho_i = \rho, \quad Y_i = \frac{\rho_i}{\rho}
\]

Caloric equation

\[
h(Y_1, \ldots, Y_K, T) = \sum_{i=1}^{K} Y_i h_i(T) \quad \text{with} \quad h_i(T) = h_i^0 + \int_0^T c_{pi}(s) ds
\]
Equation of state

Ideal gas law and Dalton’s law for gas-mixtures

\[ p(\rho_1, \ldots, \rho_K, T) = \sum_{i=1}^{K} p_i = \sum_{i=1}^{K} \rho_i \frac{R}{W_i} T = \rho \frac{R}{W} T \quad \text{with} \quad \sum_{i=1}^{K} \rho_i = \rho, \; Y_i = \frac{\rho_i}{\rho} \]

Caloric equation

\[ h(Y_1, \ldots, Y_K, T) = \sum_{i=1}^{K} Y_i h_i(T) \quad \text{with} \quad h_i(T) = h_i^0 + \int_0^T c_{pi}(s) ds \]

Computation of \( T = T(\rho_1, \ldots, \rho_K, e) \) from implicit equation

\[ \sum_{i=1}^{K} \rho_i h_i(T) - R T \sum_{i=1}^{K} \frac{\rho_i}{W_i} - \rho e = 0 \]

for thermally perfect gases with \( \gamma_i(T) = c_{pi}(T)/c_{vi}(T) \) using an iterative Newton or bisection method.
Chemistry and transport properties

Arrhenius-kinetics:

\[
\dot{\omega}_i = \sum_{j=1}^{M} (\nu^r_{ji} - \nu^f_{ji}) \left[ k^f_j \prod_{n=1}^{K} \left( \frac{\rho_n}{W_n} \right)^{\nu^f_{jn}} - k^r_j \prod_{n=1}^{K} \left( \frac{\rho_n}{W_n} \right)^{\nu^r_{jn}} \right] \quad i = 1, \ldots, K
\]
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

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\]

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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

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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:

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

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

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

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

- Evaluation with Chemkin-II Transport library
Splitting methods

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

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

Dimensional splitting for PDE

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

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

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

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

Treat right-hand side as source term

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

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

Dimensional splitting for PDE

\( \mathcal{X}(\Delta t) : \quad \partial_t \mathbf{q} + \partial_x (f(q) - f_v(q)) = 0 \), \quad IC: \quad Q(t_m) \quad \Delta t \rightarrow \tilde{Q}^{1/2} \\
\mathcal{Y}(\Delta t) : \quad \partial_t \mathbf{q} + \partial_y (g(q) - g_v(q)) = 0 \), \quad IC: \quad \tilde{Q}^{1/2} \quad \Delta t \rightarrow \tilde{Q} \\

Treat right-hand side as source term

\( \mathcal{C}(\Delta t) : \quad \partial_t \mathbf{q} = \frac{\alpha}{\gamma} (c(q) - g(q) + g_v(q)) \), \quad IC: \quad \bar{Q} \quad \Delta t \rightarrow \bar{Q} \\

Chemical source term

\( \mathcal{S}(\Delta t) : \quad \partial_t \mathbf{q} = s(q) \), \quad IC: \quad \bar{Q} \quad \Delta t \rightarrow Q(t_m + \Delta t) \)
Splitting methods

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

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

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

Chemical source term
\[ \mathcal{S}(\Delta t) : \quad \partial_t q = s(q) , \quad \text{IC: } \bar{Q} \xrightarrow{\Delta t} Q(t_m + \Delta t) \]

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 schemes

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

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

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

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 $I_{jk} = [x_j - \frac{1}{2}\Delta x, x_j + \frac{1}{2}\Delta x[\times[y_k - \frac{1}{2}\Delta y, y_k + \frac{1}{2}\Delta y[\times =: [x_{j-1/2}, x_{j+1/2}[\times[y_{k-1/2}, y_{k+1/2}[$

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

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

yield (for simplicity)

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

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

▶ 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 $I_{jk} = [x_j - \frac{1}{2}\Delta x, x_j + \frac{1}{2}\Delta x][y_k - \frac{1}{2}\Delta y, y_k + \frac{1}{2}\Delta y[\times =: [x_{j-1/2}, x_{j+1/2}][y_{k-1/2}, y_{k+1/2}[$

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

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

- 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 ($\ast$)

Stability condition used:

$$\max_{i,j,k} \left\{ \frac{\Delta t}{\Delta x} (|u_{jk}| + c_{jk}) + \frac{8}{3} \frac{\mu_{jk} \Delta t}{\rho_{jk} \Delta x^2}, \frac{\Delta t}{\Delta x} (|u_{jk}| + c_{jk}) + \frac{2k_j \Delta t}{c_{v,jk} \rho_j \Delta x^2}, \frac{\Delta t}{\Delta x} (|u_{jk}| + c_{jk}) + D_{i,jk} \frac{\Delta t}{\Delta x^2} \right\} \leq 1$$
Finite volume discretization – cont.

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

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

within explicit 2nd-order accurate Runge-Kutta method

- Gives 2nd-order central difference approximation of $G_v$
Finite volume schemes

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
Finite volume discretization – cont.

Symmetry source term \( C(\Delta t) \): Use

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

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!

\[
\partial_t \rho_i = W_i \dot{\omega}_i(\rho_1, \ldots, \rho_K, T) \quad i = 1, \ldots, K
\]
Flux difference splitting

Godunov-type scheme with \( \Delta Q^j_{j+1/2} = Q^j_{j+1} - Q^j_j \)

\[
Q^{n+1}_j = Q^n_j - \frac{\Delta t}{\Delta x} \left( A^- \Delta Q^n_{j+1/2} + A^+ \Delta Q^n_{j-1/2} \right)
\]
Flux difference splitting

Godunov-type scheme with $\Delta Q_{j+1/2}^n = Q_{j+1}^n - Q_j^n$

$$Q_{j}^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left( A^- \Delta Q_{j+1/2}^n + A^+ \Delta Q_{j-1/2}^n \right)$$

Use linearization $\tilde{f}(\bar{q}) = \hat{A}(q_L, q_R)\bar{q}$ and construct scheme for nonlinear problem as

$$Q_{j}^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left( \hat{A}^- (Q_j^n, Q_{j+1}^n) \Delta Q_{j+1/2}^n + \hat{A}^+ (Q_{j-1}^n, Q_j^n) \Delta Q_{j-1/2}^n \right)$$
Flux difference splitting

Godunov-type scheme with $\Delta Q_{j+1/2}^n = Q_{j+1}^n - Q_j^n$

$$Q_{j+1}^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left( A_- \Delta Q_{j+1/2}^n + A_+ \Delta Q_{j-1/2}^n \right)$$

Use linearization $\bar{f}(\bar{q}) = \hat{A}(q_L, q_R) \bar{q}$ and construct scheme for nonlinear problem as

$$Q_{j+1}^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x} \left( \hat{A}^-(Q_j^n, Q_{j+1}^n) \Delta Q_{j+1/2}^n + \hat{A}^+(Q_{j-1}^n, Q_j^n) \Delta Q_{j-1/2}^n \right)$$

stability condition

$$\max_{j \in \mathbb{Z}} |\hat{\lambda}_{m,j+1/2}| \frac{\Delta t}{\Delta x} \leq 1 , \quad \text{for all } m = 1, \ldots, M$$

[LeVeque, 1992]
Roe’s approximate Riemann solver

Choosing \( \hat{A}(q_L, q_R) \) [Roe, 1981]:

\[
\hat{A}(q_L, q_R) \text{ has real eigenvalues}
\]

\[
\hat{A}(q_L, q_R) \rightarrow \partial f(q) / \partial q \text{ as } q_L, q_R \rightarrow q
\]

\[
\hat{A}(q_L, q_R) \Delta q = f(q_R) - f(q_L)
\]

For Euler equations:

\[
\hat{\rho} = \sqrt{\rho_L \rho_R + \sqrt{\rho_R \rho_L}} \sqrt{\rho_L + \sqrt{\rho_R}}
\]

\[
\hat{v} = \sqrt{\rho_L v_L + \sqrt{\rho_R v_R}} \sqrt{\rho_L + \sqrt{\rho_R}}
\]

for \( v = u, H \)

Wave decomposition:

\[
\Delta q = q_r - q_l = \sum m a_m \hat{r}_m F(q_L, q_R) = f(q_L) + \sum \hat{\lambda}_m < 0 a_m \hat{r}_m = f(q_R) - \sum \hat{\lambda}_m \geq 0 a_m \hat{r}_m = \frac{1}{2} f(q_L) + f(q_R) - \sum |\hat{\lambda}_m| a_m \hat{r}_m
\]
Roe’s approximate Riemann solver

Choosing \( \hat{A}(q_L, q_R) \) [Roe, 1981]:

(i) \( \hat{A}(q_L, q_R) \) has real eigenvalues

\[
\begin{align*}
\hat{\rho} & = \sqrt{\rho_L \rho_R + \sqrt{\rho_R \rho_L}} \\
\sqrt{\rho_L} & = \frac{\hat{\rho}}{\sqrt{\rho_R}} \\
\sqrt{\rho_R} & = \frac{\hat{\rho}}{\sqrt{\rho_L}}
\end{align*}
\]

for \( v = u \).

Wave decomposition:

\[
\Delta q = q_r - q_l = \sum_m a_m \hat{r}_m F(q_L, q_R) = f(q_L) + \sum \hat{\lambda}_m < 0 a_m \hat{r}_m = f(q_R) - \sum \hat{\lambda}_m \geq 0 a_m \hat{r}_m = \frac{1}{2} f(q_L) + f(q_R) - \sum |\hat{\lambda}_m| a_m \hat{r}_m
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(i) $\hat{A}(q_L, q_R)$ has real eigenvalues

(ii) $\hat{A}(q_L, q_R) \to \frac{\partial f(q)}{\partial q}$ as $q_L, q_R \to q$
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For Euler equations:

$$\hat{\rho} = \frac{\sqrt{\rho_L \rho_R} + \sqrt{\rho_R \rho_L}}{\sqrt{\rho_L} + \sqrt{\rho_R}} = \sqrt{\rho_L \rho_R} \quad \text{and} \quad \hat{v} = \frac{\sqrt{\rho_L v_L} + \sqrt{\rho_R v_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad \text{for} \quad v = u_n, H$$
Roe’s approximate Riemann solver

Choosing \( \hat{A}(q_L, q_R) \) [Roe, 1981]:

(i) \( \hat{A}(q_L, q_R) \) has real eigenvalues

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For Euler equations:

\[
\hat{\rho} = \frac{\sqrt{\rho_L \rho_R} + \sqrt{\rho_R \rho_L}}{\sqrt{\rho_L} + \sqrt{\rho_R}} = \sqrt{\rho_L \rho_R} \quad \text{and} \quad \hat{v} = \frac{\sqrt{\rho_L v_L} + \sqrt{\rho_R v_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad \text{for} \ v = u, H
\]

Wave decomposition: \( \Delta q = q_r - q_l = \sum_m a_m \hat{r}_m \)

\[
F(q_L, q_R) = f(q_L) + \sum_{\lambda_m < 0} \hat{\lambda}_m a_m \hat{r}_m = f(q_R) - \sum_{\lambda_m \geq 0} \hat{\lambda}_m a_m \hat{r}_m
\]

\[
= \frac{1}{2} \left( f(q_L) + f(q_R) - \sum_m |\hat{\lambda}_m| a_m \hat{r}_m \right)
\]
Riemann solver for combustion

(S1) Calculate standard Roe-averages $\hat{\rho}, \hat{u}, \hat{v}, \hat{H}, \hat{Y}_i, \hat{T}$.

(S2) Compute $\hat{\gamma} := \hat{c}_p/\hat{c}_v$ with $\hat{c}_{\{p/v\}}_i = \frac{1}{\hat{T}_R - \hat{T}_L} \int_{\hat{T}_L}^{\hat{T}_R} c_{\{p,v\}}(\tau) d\tau$.

(S3) Calculate $\hat{\phi}_i := (\hat{\gamma} - 1) \left( \frac{\hat{u}_i^2}{2} - \hat{h}_i \right) + \hat{\gamma} R \hat{T}$ with standard Roe-averages $\hat{e}_i$ or $\hat{h}_i$.

(S4) Calculate $\hat{c} := \left( \sum_{i=1}^{K} \hat{Y}_i \hat{\phi}_i - (\hat{\gamma} - 1)\hat{u}^2 + (\hat{\gamma} - 1)\hat{H} \right)^{1/2}$.

(S5) Use $\Delta q = q_R - q_L$ and $\Delta p$ to compute the wave strengths $a_m$.

(S6) Calculate $W_1 = a_1 \hat{r}_1, W_2 = \sum_{\ell=2}^{K+d} a_\ell \hat{r}_\ell, W_3 = a_{K+d+1} \hat{r}_{K+d+1}$.

(S7) Evaluate $s_1 = \hat{u} - \hat{c}, s_2 = \hat{u}, s_3 = \hat{u} + \hat{c}$. 

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R. Deiterding – Adaptive high-resolution methods for simulating shock-induced hydrogen-air combustion
Riemann solver for combustion

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(S2) Compute $\hat{\gamma} := \hat{c}_p/\hat{c}_v$ with $\hat{c}_{\{p/v\}}_i = \frac{1}{\hat{T}_R - \hat{T}_L} \int_{\hat{T}_L}^{\hat{T}_R} c_{\{p,v\}}_i(\tau) \, d\tau$.

(S3) Calculate $\hat{\phi}_i := (\hat{\gamma} - 1) \left( \frac{\hat{u}^2}{2} - \hat{h}_i \right) + \hat{\gamma} R_i \hat{T}$ with standard Roe-averages $\hat{e}_i$ or $\hat{h}_i$.

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(S7) Evaluate $s_1 = \hat{u} - \hat{c}$, $s_2 = \hat{u}$, $s_3 = \hat{u} + \hat{c}$.

(S8) Evaluate $\rho^*_{L/R}, u^*_{L/R}, e^*_{L/R}, c^*_{L/R}$ from $q^*_L = q_L + \mathcal{W}_1$ and $q^*_R = q_R - \mathcal{W}_3$.

(S9) If $\rho^*_{L/R} \leq 0$ or $e^*_{L/R} \leq 0$ use $F_{HLL}(q_L, q_R)$ and go to (S12).
Riemann solver for combustion

(S1) Calculate standard Roe-averages \( \hat{\rho}, \hat{u}, \hat{v}, \hat{H}, \hat{Y}_i, \hat{T} \).

(S2) Compute \( \hat{\gamma} := \frac{c_p}{c_v} \) with \( c_{i\{p/v\}} = \frac{1}{T_R - T_L} \int_{T_L}^{T_R} c_{i\{p,v\}}(\tau) d\tau. \)

(S3) Calculate \( \hat{\phi}_i := (\hat{\gamma} - 1) \left( \frac{u_i^2}{2} - h_i \right) + \hat{\gamma} R_i \hat{T} \) with standard Roe-averages \( \hat{\rho}_i \) or \( \hat{h}_i \).

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(S10) Entropy correction: Evaluate \( |\tilde{s}_l| \).

\[
F_{Roe}(q_L, q_R) = \frac{1}{2} \left( f(q_L) + f(q_R) - \sum_{l=1}^{3} |\tilde{s}_l| W_l \right)
\]
Riemann solver for combustion

(S1) Calculate standard Roe-averages \( \hat{\rho}, \hat{u}, \hat{v}, \hat{H}, \hat{Y}_i, \hat{T} \).

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(S3) Calculate \( \hat{\phi}_i := (\hat{\gamma} - 1) \left( \frac{u_i^2}{2} - \hat{h}_i \right) + \hat{\gamma} R_i \hat{T} \) with standard Roe-averages \( \hat{e}_i \) or \( \hat{h}_i \).

(S4) Calculate \( \hat{c} := \left( \sum_{i=1}^{K} \hat{\gamma}_i \hat{\phi}_i - (\hat{\gamma} - 1) \hat{u}^2 + (\hat{\gamma} - 1) \hat{H} \right)^{1/2} \).

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(S8) Evaluate \( \rho^*_L/R, u^*_L/R, e^*_L/R, c^*_L/R \) from \( q^*_L = q_L + W_1 \) and \( q^*_R = q_R - W_3 \).

(S9) If \( \rho^*_L/R \leq 0 \) or \( e^*_L/R \leq 0 \) use \( F_{HLL}(q_L, q_R) \) and go to (S12).

(S10) Entropy correction: Evaluate \( |\bar{s}_l| \). \( F_{\text{Roe}}(q_L, q_R) = \frac{1}{2} \left( f(q_L) + f(q_R) - \sum_{l=1}^{3} |\bar{s}_l| W_l \right) \)

(S11) Positivity correction: Replace \( F_i \) by \( F^*_i = F^* \rho \cdot \left\{ \begin{array}{ll} Y_i^l, & F^* \rho \geq 0, \\ Y_i^r, & F^* \rho < 0. \end{array} \right. \)

(S12) Evaluate maximal signal speed by \( S = \max(|s_1|, |s_3|) \).
Riemann solver for combustion: carbuncle fix

Entropy corrections
Riemann solver for combustion: carbuncle fix

Entropy corrections [Harten, 1983]

1. \[ |\tilde{s}_l| = \begin{cases} |s_l| & \text{if } |s_l| \geq 2\eta \\ \frac{|s_l^2|}{4\eta} + \eta & \text{otherwise} \end{cases} \]

\[ \eta = \frac{1}{2} \max_l \{ |s_l(q_R) - s_l(q_L)| \} \]
Riemann solver for combustion: carbuncle fix

Entropy corrections [Harten, 1983]  
[Harten and Hyman, 1983]

1. $|\tilde{s}_i| = \begin{cases} 
|s_i| & \text{if } |s_i| \geq 2\eta \\
\frac{|s_i^2|}{4\eta} + \eta & \text{otherwise}
\end{cases}$

$\eta = \frac{1}{2} \max_i \{|s_i(q_R) - s_i(q_L)|\}$

2. Replace $|s_i|$ by $|\tilde{s}_i|$ only if $s_i(q_L) < 0 < s_i(q_R)$
Riemann solver for combustion: carbuncle fix

Entropy corrections [Harten, 1983] [Harten and Hyman, 1983]

1. \[ |\tilde{s}_t| = \begin{cases} |s_t| & \text{if } |s_t| \geq 2\eta \\ \frac{|s_t|^2}{4\eta} + \eta & \text{otherwise} \end{cases} \]

\[ \eta = \frac{1}{2} \max_t \{|s_t(q_R) - s_t(q_L)|\} \]

2. Replace \(|s_t|\) by \(|\tilde{s}_t|\) only if

\[ s_t(q_L) < 0 < s_t(q_R) \]

\[ \tilde{\eta}_{j+1/2,k} = \max \{ \eta_{j+1/2,k}, \eta_{j,k-1/2}, \eta_{j,k+1/2}, \eta_{j+1,k-1/2}, \eta_{j+1,k+1/2} \} \]
Riemann solver for combustion: carbuncle fix

Entropy corrections [Harten, 1983] [Harten and Hyman, 1983]

1. $|\tilde{s}_l| = \begin{cases} |s_l| & \text{if } |s_l| \geq 2\eta \\ \frac{|s_l^2|}{4\eta} + \eta & \text{otherwise} \end{cases}$

$\eta = \frac{1}{2} \max_l \{|s_l(q_R) - s_l(q_L)|\}$

2. Replace $|s_l|$ by $|\tilde{s}_l|$ only if $s_l(q_L) < 0 < s_l(q_R)$

$\tilde{\eta}_{j+1/2,k} = \max \{\eta_{j+1/2,k}, \eta_{j,k-1/2}, \eta_{j+1,k-1/2}, \eta_{j+1,k+1/2}\}$

2D modification of entropy correction [Sanders et al., 1998]:

Carbuncle phenomenon

▶ [Quirk, 1994]

▶ Test from [Deiterding, 2003]
Block-structured adaptive mesh refinement (SAMR)

For simplicity $\partial_t q(x, t) + \nabla \cdot f(q(x, t)) = 0$

- Refined blocks overlay coarser ones
Block-structured adaptive mesh refinement (SAMR)

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Block-structured adaptive mesh refinement (SAMR)

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- Refined blocks overlay coarser ones
- Refinement in space and time by factor $r_l$
- Block (aka patch) based data structures

Numerical scheme

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

$$- \frac{\Delta t}{\Delta y} \left[ G_{j, k+\frac{1}{2}} - G_{j, k-\frac{1}{2}} \right]$$

only for single patch necessary
Block-structured adaptive mesh refinement (SAMR)

For simplicity $\partial_t q(x, t) + \nabla \cdot f(q(x, t)) = 0$

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Numerical scheme

$$Q_{jk}^{n+1} = Q_{jk}^n - \frac{\Delta t}{\Delta x} \left[ F_{j+\frac{1}{2},k} - F_{j-\frac{1}{2},k} \right]$$
$$- \frac{\Delta t}{\Delta y} \left[ G_{j,k+\frac{1}{2}} - G_{j,k-\frac{1}{2}} \right]$$

only for single patch necessary

- Efficient cache-reuse / vectorization possible
  - Cluster-algorithm necessary
Level transfer / setting of ghost cells

Conservative averaging (restriction):

\[
\hat{Q}_{jk} := \frac{1}{(r_l+1)^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} Q_{v+\kappa, w+\iota}^{l+1}
\]
Level transfer / setting of ghost cells

Conservative averaging (restriction):

\[
\hat{Q}_{jk}^{l} := \frac{1}{(r_{l+1})^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} Q_{v+\kappa,w+\iota}^{l+1}
\]
Conservative averaging (restriction):

\[ q'_{jk} := \frac{1}{(n+1)^2} \sum_{\kappa=0}^{n+1} \sum_{\ell=0}^{n+1-1} q_{\ell+k, \ell+\kappa, l} \]

Synchronization:

For boundary conditions: linear time interpolation

\[ \tilde{q}_l(t + \kappa \Delta t) := (1 - \kappa) \tilde{q}_l(t) + \kappa \tilde{q}_l(t + \Delta t) \text{ for } \kappa = 0, \ldots, n+1 \]
Level transfer / setting of ghost cells

Conservative averaging (restriction):

\[ \hat{Q}_{jk} := \frac{1}{(r_{l+1})^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\nu=0}^{r_{l+1}-1} Q_{\nu+\kappa, w+\nu}^{l+1} \]

\[ \hat{Q}_{jk} \] represents the conservative averaging of the variables from the fine grid to the coarse grid. The formula uses bilinear interpolation for prolongation (restriction) and linear time interpolation for synchronization.

Synchronization
Physical boundary conditions
Level transfer / setting of ghost cells

Conservative averaging (restriction):

\[ \hat{Q}_{jk}^{l} := \frac{1}{(r_{l+1})^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} Q_{v+\kappa, w+\iota}^{l+1} \]
Level transfer / setting of ghost cells

Conservative averaging (restriction):

\[ \hat{Q}_{jk} := \frac{1}{(r_{l+1})^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} Q^{l+1}_{v+\kappa, w+\iota} \]

Bilinear interpolation (prolongation):

\[ \tilde{Q}_{vw}^{l+1} := (1 - f_1)(1 - f_2) Q_{j-1,k-1}^l + f_1(1 - f_2) Q_{j,k-1}^l + (1 - f_1)f_2 Q_{j-1,k}^l + f_1f_2 Q_{jk}^l \]
Level transfer / setting of ghost cells

Conservative averaging (restriction):

\[ \hat{Q}_{jk}^l := \frac{1}{(r_{l+1})^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\nu=0}^{r_{l+1}-1} Q_{v+\kappa,w+\nu}^{l+1} \]

Bilinear interpolation (prolongation):

\[ \tilde{Q}_{vw}^{l+1} := (1 - f_1)(1 - f_2) Q_{j-1,k-1}^l + f_1(1 - f_2) Q_{j,k-1}^l + (1 - f_1)f_2 Q_{j-1,k}^l + f_1f_2 Q_{jk}^l \]

For boundary conditions: linear time interpolation

\[ \tilde{Q}_{l+1}^{l+1} (t + \kappa \Delta t_{l+1}) := \left( 1 - \frac{\kappa}{r_{l+1}} \right) \tilde{Q}_{l+1}^{l+1} (t) + \frac{\kappa}{r_{l+1}} \tilde{Q}_{l+1}^{l+1} (t + \Delta t_{l}) \quad \text{for} \quad \kappa = 0, \ldots, r_{l+1} \]
Conservative flux correction

Example: Cell $j, k$

\[
\dot{Q}_{jk}(t + \Delta t_l) = Q_{jk}(t) - \frac{\Delta t_l}{\Delta x_l} \left( F^{1,l}_{j+\frac{1}{2},k} - \frac{1}{r^{l+1}_k} \sum_{\kappa=0}^{r^{l+1}_k} \sum_{\iota=0}^{r^{l+1}_k-1} F^{1,l+1}_{v+\frac{1}{2},w+\iota} (t + \kappa \Delta t_{l+1}) \right) \\
- \frac{\Delta t_l}{\Delta y_l} \left( F^{2,l}_{j,k+\frac{1}{2}} - F^{2,l}_{j,k-\frac{1}{2}} \right)
\]

Correction pass:
Conservative flux correction

Example: Cell \( j, k \)

\[
\dot{Q}_{jk}(t + \Delta t_l) = Q_{jk}(t) - \frac{\Delta t_l}{\Delta x_l} \left( F_{1,l}^{1,1,}, j+\frac{1}{2}, k - \frac{1}{r_{l+1}} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{\nu_{l+1}-1} F_{1,l+1,\nu+\frac{1}{2},w+\iota} (t + \kappa \Delta t_{l+1}) \right) 
- \frac{\Delta t_l}{\Delta y_l} \left( F_{2,l}^{2,1,}, j, k+\frac{1}{2} - F_{2,l}^{2,1,}, j, k-\frac{1}{2} \right)
\]

Correction pass:

1. \( \delta F_{1,l+1,}^{1,1}, j-\frac{1}{2}, k := -F_{1,l}, j-\frac{1}{2}, k \)
Conservative flux correction

Example: Cell $j, k$

\[
\dot{Q}_{jk}(t + \Delta t_l) = Q_{jk}(t) - \frac{\Delta t_l}{\Delta x_l} \left( \mathbf{F}_{j+\frac{1}{2},k}^{1,l} - \sum_{\kappa=0}^{r_l+1-1} \sum_{\nu=0}^{r_{l+1}-1} \mathbf{F}_{\nu+\frac{1}{2},w+\kappa}^{1,l+1}(t + \kappa \Delta t_{l+1}) \right) \\
- \frac{\Delta t_l}{\Delta y_l} \left( \mathbf{F}_{j,k+\frac{1}{2}}^{2,l} - \mathbf{F}_{j,k-\frac{1}{2}}^{2,l} \right)
\]

Correction pass:

1. \( \delta \mathbf{F}_{j-\frac{1}{2},k}^{1,l+1} := -\mathbf{F}_{j-\frac{1}{2},k}^{1,l} \)

2. \( \delta \mathbf{F}_{j-\frac{1}{2},k}^{1,l+1} := \delta \mathbf{F}_{j-\frac{1}{2},k}^{1,l+1} + \frac{1}{r_{l+1}^2} \sum_{\nu=0}^{r_{l+1}-1} \mathbf{F}_{\nu+\frac{1}{2},w+\kappa}^{1,l+1}(t + \kappa \Delta t_{l+1}) \)
Conservative flux correction

Example: Cell \(j, k\)

\[
\begin{align*}
\bar{Q}_{jk}^l(t + \Delta t_l) &= Q_{jk}^l(t) - \frac{\Delta t_l}{\Delta x_l} \left( F_{j+\frac{1}{2},k}^{1,l} - \frac{1}{r_{l+1}^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} F_{v+\frac{1}{2},w+\iota}^{1,l+1} \left( t + \kappa \Delta t_{l+1} \right) \right) \\
&\hspace{1cm} - \frac{\Delta t_l}{\Delta y_l} \left( F_{j,k+\frac{1}{2}}^{2,l} - F_{j,k-\frac{1}{2}}^{2,l} \right)
\end{align*}
\]

Correction pass:

1. \(\delta F_{j-\frac{1}{2},k}^{1,l+1} := -F_{j-\frac{1}{2},k}^{1,l}\)

2. \(\delta F_{j-\frac{1}{2},k}^{1,l+1} := \delta F_{j-\frac{1}{2},k}^{1,l+1} + \frac{1}{r_{l+1}^2} \sum_{\iota=0}^{r_{l+1}-1} F_{v+\frac{1}{2},w+\iota}^{1,l+1} \left( t + \kappa \Delta t_{l+1} \right)\)

3. \(\bar{Q}_{jk}^l(t + \Delta t_l) := Q_{jk}^l(t + \Delta t_l) + \frac{\Delta t_l}{\Delta x_l} \delta F_{j-\frac{1}{2},k}^{1,l+1}\)
Heuristic error estimation for FV methods

1. Error estimation on interior cells
Heuristic error estimation for FV methods

1. Error estimation on interior cells

\[ \mathcal{H}^{t_l} Q'(t_l - \Delta t_l) \]
Heuristic error estimation for FV methods

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\[ \mathcal{H}^{\Delta t_l} Q^l(t_l - \Delta t_l) \]
Heurisitic error estimation for FV methods

1. Error estimation on interior cells

\[ H^{\Delta t_i} Q'_i(t_i - \Delta t_i) \]

\[ = H^{\Delta t_i} (H^{\Delta t_i} Q'_i(t_i - \Delta t_i)) \]

\[ = H^2_{t_i} Q'_i(t_i - \Delta t_i) \]
Heuristic error estimation for FV methods

1. Error estimation on interior cells

2. Create temporary Grid coarsened by factor 2
   Initialize with fine-grid-values of preceding time step

\[ H^{\Delta t_l} Q^l(t_l - \Delta t_l) = H^{\Delta t_l} (H^{\Delta t_l} Q^l(t_l - \Delta t_l)) = H^{\Delta t_l} Q^l(t_l - \Delta t_l) \]
Heuristic error estimation for FV methods

1. Error estimation on interior cells
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\[
\mathcal{H}^{\Delta t_i} \mathbf{Q}_i^l(t_l - \Delta t_l) = \mathcal{H}^{\Delta t_i} (\mathcal{H}^{\Delta t_i} \mathbf{Q}_i^l(t_l - \Delta t_l)) = \mathcal{H}^{2\Delta t_i} \bar{\mathbf{Q}}_i^l(t_l - \Delta t_l)
\]
Heuristic error estimation for FV methods

1. Error estimation on interior cells
2. Create temporary Grid coarsened by factor 2
   Initialize with fine-grid-values of preceding time step
3. Compare temporary solutions

\[ \mathcal{H}^{\Delta t_t} Q^l(t_l - \Delta t_t) = \mathcal{H}^{\Delta t_t} (\mathcal{H}^{\Delta t_t} Q^l(t_l - \Delta t_t)) = \mathcal{H}^{\Delta t_t} \bar{Q}^l(t_l - \Delta t_t) \]
Refinement criteria

Scaled gradient of scalar quantity \( w \)

\[
|w(Q_{j+1,k})-w(Q_{jk})| > \epsilon_w ,
|w(Q_{j,k+1})-w(Q_{jk})| > \epsilon_w ,
|w(Q_{j+1,k+1})-w(Q_{jk})| > \epsilon_w
\]
Refinement criteria

Scaled gradient of scalar quantity $w$

$$|w(Q_{j+1,k}) - w(Q_{jk})| > \epsilon_w, \quad |w(Q_{j,k+1}) - w(Q_{jk})| > \epsilon_w, \quad |w(Q_{j+1,k+1}) - w(Q_{jk})| > \epsilon_w$$

Usage of heuristic error estimation:
Current solution integrated tentatively 1 step with $\Delta t_l$ and coarsened

$$\tilde{Q}(t_l + \Delta t_l) := \text{Restrict}\left(\mathcal{H}_2^{\Delta t_l} Q(t_l - \Delta t_l)\right)$$

Previous solution coarsened and integrated 1 step with $2\Delta t_l$

$$Q(t_l + \Delta t_l) := \mathcal{H}_{2\Delta t_l} \text{Restrict}\left(Q(t_l - \Delta t_l)\right)$$
Refinement criteria

Scaled gradient of scalar quantity $w$

$$|w(Q_{j+1,k})-w(Q_{jk})| > \epsilon_w, \quad |w(Q_{j,k+1})-w(Q_{jk})| > \epsilon_w, \quad |w(Q_{j+1,k+1})-w(Q_{jk})| > \epsilon_w$$

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$$\bar{Q}(t_l + \Delta t_l) := \text{Restrict} \left( H_{2}^{\Delta t_l} Q'^{(t_l - \Delta t_l)} \right)$$

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$$Q(t_l + \Delta t_l) := H_{2}^{2\Delta t_l} \text{Restrict} \left( Q'^{(t_l - \Delta t_l)} \right)$$

Local error estimation of scalar quantity $w$

$$\tau_{jk}^w := \frac{|w(\bar{Q}_{jk}(t + \Delta t)) - w(Q_{jk}(t + \Delta t))|}{2^{o+1} - 2}$$
Refinement criteria

Scaled gradient of scalar quantity $w$

$$|w(Q_{j+1,k}) - w(Q_{jk})| > \epsilon_w, \quad |w(Q_{j,k+1}) - w(Q_{jk})| > \epsilon_w, \quad |w(Q_{j+1,k+1}) - w(Q_{jk})| > \epsilon_w$$

Usage of heuristic error estimation:
Current solution integrated tentatively 1 step with $\Delta t_I$ and coarsened

$$\bar{Q}(t_I + \Delta t_I) := \text{Restrict} \left( \mathcal{H}^{\Delta t_I} Q_I(t_I - \Delta t_I) \right)$$

Previous solution coarsened and integrated 1 step with $2\Delta t_I$

$$Q(t_I + \Delta t_I) := \mathcal{H}^{2\Delta t_I} \text{Restrict} \left( Q_I(t_I - \Delta t_I) \right)$$

Local error estimation of scalar quantity $w$

$$\tau_{jk}^w := \frac{|w(\bar{Q}_{jk}(t + \Delta t)) - w(Q_{jk}(t + \Delta t))|}{2^{o+1} - 2}$$

In practice [Deiterding, 2003] use

$$\frac{\tau_{jk}^w}{\max(|w(Q_{jk}(t + \Delta t)), S_w|)} > \eta_{w}^r$$
Non-Cartesian boundaries

Level-set method for boundary embedding

- Implicit boundary representation via distance function $\varphi$, normal $\mathbf{n} = \nabla \varphi / |\nabla \varphi|$
Level-set method for boundary embedding

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- Construction of values in embedded boundary cells by interpolation / extrapolation
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$$\hat{x} = x + 2\varphi \mathbf{n}$$
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Interpolate / constant value extrapolate values at

$$\tilde{x} = x + 2\varphi \mathbf{n}$$

Velocity in ghost cells – slip BC:

$$\mathbf{u}' = (2\mathbf{w} \cdot \mathbf{n} - \mathbf{u} \cdot \mathbf{n})\mathbf{n} + (\mathbf{u} \cdot \mathbf{t})\mathbf{t}$$

$$= 2((\mathbf{w} - \mathbf{u}) \cdot \mathbf{n})\mathbf{n} + \mathbf{u}$$

No-slip BC: $\mathbf{u}' = 2\mathbf{w} - \mathbf{u}$
Verification: shock reflection

- Reflection of a Mach 2.38 shock in nitrogen at 43° wedge
- 2nd order MUSCL scheme with Roe solver, 2nd order multidimensional wave propagation method
Verification: shock reflection

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- 2nd order MUSCL scheme with Roe solver, 2nd order multidimensional wave propagation method

Cartesian base grid $360 \times 160$ cells on domain of $36\text{ mm} \times 16\text{ mm}$ with up to 3 refinement levels with $r_l = 2, 4, 4$ and $\Delta x_{1,2} = 3.125\mu m$, 38 h CPU
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GFM base grid $390 \times 330$ cells on domain of $26 \text{ mm} \times 22 \text{ mm}$ with up to 3 refinement levels with $r_l = 2, 4, 4$ and $\Delta x_{e,1,2} = 2.849 \mu m$, 200 h CPU
Verification: Shock reflection for Euler equations

\[ \Delta x = 25 \text{ mm} \]
\[ \Delta x = 12.5 \text{ mm} \]
\[ \Delta x = 3.125 \text{ mm} \]
Verification: Shock reflection for Euler equations

\[ \Delta x = 25 \text{ mm} \]
\[ \Delta x = 12.5 \text{ mm} \]
\[ \Delta x = 3.125 \text{ mm} \]
\[ \Delta x_e = 22.8 \text{ mm} \]
\[ \Delta x_e = 11.4 \text{ mm} \]
\[ \Delta x_e = 2.849 \text{ mm} \]
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2nd order MUSCL scheme with Van Leer FVS, dimensional splitting

\[ \Delta x = 12.5 \text{ mm} \]
\[ \Delta x = 3.125 \text{ mm} \]
Shock reflection: solution for Navier-Stokes equations

- Convergence to correct solution but rather high boundary resolution required with this approach
Shock reflection: solution for Navier-Stokes equations

Convergence to correct solution but rather high boundary resolution required with this approach

- $\Delta x = 50 \text{ mm}$
- $\Delta x = 25 \text{ mm}$
- $\Delta x = 12.5 \text{ mm}$, SAMR
Shock reflection: solution for Navier-Stokes equations

- Convergence to correct solution but rather high boundary resolution required with this approach

\[ \Delta x = 50 \text{ mm} \]
\[ \Delta x = 25 \text{ mm} \]
\[ \Delta x = 12.5 \text{ mm, SAMR} \]
\[ \Delta x_e = 45.6 \text{ mm} \]
\[ \Delta x_e = 22.8 \text{ mm} \]
\[ \Delta x_e = 11.4 \text{ mm, SAMR} \]
Parallelization

Rigorous domain decomposition

- Data of all levels resides on same node
- Grid hierarchy defines unique "floor-plan"
- Workload estimation

\[
\mathcal{W}(\Omega) = \sum_{l=0}^{l_{\text{max}}} \left[ \mathcal{N}_{l}(G_l \cap \Omega) \prod_{\kappa=0}^{l} r_{\kappa} \right]
\]
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  - Redistribution of data blocks within regridding operation
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Outline

Introduction
  Governing equations

Numerical methods
  Finite volume schemes
  Adaptive mesh refinement
  Non-Cartesian boundaries

Computational results
  Shock-induced combustion
  Combustion induced by projectiles
  Detonation propagation

Higher order schemes
  Hybrid methods

Summary
  Conclusions
Detonation ignition in a shock tube

- Shock-induced detonation ignition of H$_2$ : O$_2$ : Ar mixture at molar ratios 2:1:7 in closed 1d shock tube
- Insufficient resolution leads to inaccurate results
Detonation ignition in a shock tube

- Shock-induced detonation ignition of $\text{H}_2 : \text{O}_2 : \text{Ar}$ mixture at molar ratios 2:1:7 in closed 1d shock tube
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- Reflected shock is captured correctly by FV scheme, detonation is resolution dependent

Left: Comparison of pressure distribution $t = 170 \mu s$ after shock reflection.
Detonation ignition in a shock tube

- Shock-induced detonation ignition of H₂ : O₂ : Ar mixture at molar ratios 2:1:7 in closed 1d shock tube
- Insufficient resolution leads to inaccurate results
- Reflected shock is captured correctly by FV scheme, detonation is resolution dependent
- Fine mesh necessary in the induction zone at the head of the detonation

Left: Comparison of pressure distribution $t = 170 \mu s$ after shock reflection. Right: Domains of refinement levels.
Detonation ignition in 1d - adaptive vs. uniform

Uniformly refined vs. dynamic adaptive simulations (Intel Xeon 3.4 GHz CPU)

<table>
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<tr>
<th>$\Delta x_1 [\mu m]$</th>
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<th>Adaptive</th>
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$\sim 12 \text{ Pts} / l_{ig}$

R. Deiterding - Adaptive high-resolution methods for simulating shock-induced hydrogen-air combustion
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$\sim 12$ Pts/$l_{ig}$

Refinement criteria:

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<tr>
<th>$Y_i$</th>
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<td>$H$</td>
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$\epsilon_{\rho} = 0.07$ kg m$^{-3}$, $\epsilon_p = 50$ kPa
Shock-induced combustion around a sphere

- Spherical projectile of radius $1.5 \text{ mm}$ travels with constant velocity $v_I = 2170.6 \text{ m/s}$ through $\text{H}_2 : \text{O}_2 : \text{Ar}$ mixture (molar ratios 2:1:7) at 6.67 kPa and $T = 298 \text{ K}$
- Mechanism by [Westbrook, 1982]: 34 forward reactions, 9 species
- Axisymmetric Euler simulation on AMR base mesh of $70 \times 40$ cells
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Iso-contours of $p$ (black) and $Y_{\text{H}_2}$ (white) on refinement domains for 3-level (left) and 4-level computation (right)
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- Higher resolved computation captures combustion zone visibly better and at slightly different position (see below)

![Iso-contours of p (black) and $Y_{H_2}$ (white) on refinement domains for 3-level (left) and 4-level computation (right)]
Combustion around a sphere - adaptation

Refinement indicators on $l = 2$ at $t = 350 \mu s$.
Blue: $\epsilon_\rho$, light blue: $\epsilon_\rho$, green shades: $\eta_{Y_i}$,
red: embedded boundary

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$\epsilon_\rho = 0.02 \text{ kg m}^{-3}$, $\epsilon_\rho = 16 \text{ kPa}$
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Parallel performance

Scaling of different code portions
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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- Stagnation point location and pressure tracked in every time step

- All computations were on 32 cores requiring $\sim 1500 \, \text{h CPU each}$
**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](image)
Viscous case – $M = 4.79$ – mesh adaptation
Comparison of temperature field
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](image.png)
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

Pressure

Combustion induced by projectiles

R. Deiterding – Adaptive high-resolution methods for simulating shock-induced hydrogen-air combustion
Oscillation mechanism

Schlieren of density

Temperature

Mass fraction OH

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

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Combustion induced by projectiles
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Oscillation created by accelerated reaction due to slip line from previous triple point
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.
Combustion induced by projectiles

Perturbed oscillation mechanism

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Small perturbations can quickly create numerous triple points.
Detonation cell structure in 2D

Simulation of regular structures

- 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 1.6 cm

- Perturb 1d 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/lig

- Configuration similar to Oran et al., J. Combustion and Flame 113, 1998.
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Triple point analysis

Double Mach reflection structure shortly before the next collision

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<th>$p/p_0$</th>
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Shock polar analysis of triple points in detonations

\[\text{Neglect reaction, but consider } c(\rho(T))\]

Data extracted point-wise from simulation

\[\text{Primary triple point } T \text{ travels exactly at tip of Mach stem} \rightarrow \text{use oblique shock relations between } A \text{ and } B \]

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

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

\[\text{to evaluate inflow velocity as } u_A = \frac{1}{\sin \varphi_B} \frac{\rho_B (p_B - p_A)}{\rho_A (\rho_B - \rho_A)}\]

\[\text{Measure inflow angle } \varphi_B \text{ between Mach stem and triple point trajectory} \]

\[\text{Velocity } a \text{ of } T' \text{ relative to } T \text{ cannot be derived that easily: Oblique shock relations across } C \text{ and } D \text{ hold true both in frame of reference for } T \text{ and } T' \]

\[
\rho_C u_C, n = \rho_D u_D, n,
\]

\[
p_C + \rho_C u_C^2, n = p_D + \rho_D u_D^2, n,
\]

\[\text{Velocity } a \text{ of } T' \text{ can be estimated as arbitrary } \]

\[\text{Estimate } a_t = \text{arbitrary} \]

\[\text{R. Deiterding – Adaptive high-resolution methods for simulating shock-induced hydrogen-air combustion} \]
Shock polar analysis of triple points in detonations

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

\[
\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)
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To evaluate inflow velocity as $u_A = \frac{1}{\sin \phi_B} \sqrt{\frac{\rho_B(p_B - p_A)}{\rho_A(p_B - p_A)}}$
Shock polar analysis of triple points in detonations

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

- Neglect reaction, but consider $c_{pi}(T)$
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\[
\rho_C \left( u_{C,n} - a_n \right) = \rho_D \left( u_{D,n} - a_n \right)
\]
\[
p_C + \rho_C \left( u_{C,n} - a_n \right)^2 = p_D + \rho_D \left( u_{D,n} - a_n \right)^2
\]
\[
u_{C,t} - a_t = u_{D,t} - a_t
\]
\[
h_C + \frac{1}{2} \left( u_{C,n} - a_n \right)^2 = h_D + \frac{1}{2} \left( u_{D,n} - a_n \right)^2
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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 $T'$

$$\rho_C (u_{C,n} - a_n) = \rho_D (u_{D,n} - a_n)$$

$$p_C + \rho_C (u_{C,n} - a_n)^2 = p_D + \rho_D (u_{D,n} - a_n)^2 \quad \rightarrow a_n = 0, \ a_t \ \text{arbitrary}$$

Estimate $a_t = \frac{L_R}{t_{init}}$

$$u_{C,t} - a_t = u_{D,t} - a_t$$

$$h_C + \frac{1}{2} (u_{C,n} - a_n)^2 = h_D + \frac{1}{2} (u_{D,n} - a_n)^2$$
Detonation propagation through pipe bends

- 2D Simulation of CJ detonation for $\text{H}_2 : \text{O}_2 : \text{Ar}/2 : 1 : 7$ at $T_0 = 298$ K and $p_0 = 10$ kPa. Tube width of 5 detonation cells

- 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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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 – $\varphi = 15^\circ$
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 structures – $\varphi = 30^\circ$

▶ 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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▶ Here: Nonreactive $\text{H}_2 : \text{O}_2 : \text{Ar}$ mixture at initially 298 K and 10 kPa

For detonations:

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

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


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.
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 400x24x24, 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 $Y_{\text{OH}}$
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Hybrid methods

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}
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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:

\[ u_* = \frac{\sqrt{\rho_L u_L} + \sqrt{\rho_R u_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \quad a_* = \sqrt{(\gamma_* - 1)(h_* - \frac{1}{2} u_*^2)}, \ldots \]
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2. Limiter-inspired discontinuity test based on mapped normalized pressure gradient \(\theta_j\)

\[
\phi(\theta_j) = \frac{2\theta_j}{(1 + \theta_j)^2} \quad \text{with} \quad \theta_j = \frac{|p_{j+1} - p_j|}{|p_{j+1} + p_j|}, \quad \phi(\theta_j) > \alpha_{Map}
\]

R. Deiterding – Adaptive high-resolution methods for simulating shock-induced hydrogen-air combustion
SAMR flux correction for Runge-Kutta method

Recall Runge-Kutta temporal update

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

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rewrite scheme as

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

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Flux correction to be used

1. \[ \delta F_{i-1/2,j}^{1,l+1} := -\varphi_1 F_{i-1/2,j}^{1,l}(\bar{Q}^0), \quad \delta F_{i-1/2,j}^{1,l+1} := \delta F_{i-1/2,j}^{1,l+1} - \sum_{\nu=2}^r \varphi_\nu F_{i-1/2,j}^{1,l}(\bar{Q}^{\nu-1}) \]

2. \[ \delta F_{i-1/2,j}^{1,l+1} := \delta F_{i-1/2,j}^{1,l+1} + \frac{1}{r_{l+1}} \sum_{i=0}^{r_{l+1}-1} \sum_{\nu=1}^r \varphi_\nu F_{i-1/2,j}^{1,l+1}(\bar{Q}^{\nu-1}(t + \kappa \Delta t_{l+1})) \]

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Storage-efficient SSPRK(3,3):

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Hybrid methods

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 $\longrightarrow$ 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 $Re = \frac{\rho_0 a_0 L(t)}{\mu_0}$
- Viscous shear layer thickness, thermal heat conduction layer thickness, and mass diffusion layer thickness grow as $\delta_{\text{visc}} \approx \sqrt{\frac{\mu}{\rho}} t$, $\delta_{\text{cond}} \approx \sqrt{\frac{k_{\text{ref}}}{\rho c_p}} t$, $\delta_{\text{mass},i} \approx \sqrt{\frac{D_i}{\rho}} t$
- Only shock thickness not resolved $\longrightarrow$ “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
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Computational results for shear layer

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\[ \Delta x_{\text{min}} = 3.91 \cdot 10^{-6} \text{ m} \]
MUSCL - 7 levels
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WENO/CD - 7 levels
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- Gain in CPU time from higher-order scheme roughly one order
Conclusions

- For smaller mechanisms, detailed detonation structure simulations are nowadays possible for realistic 2d geometries.
- Accurate studies for idealized 3d configurations feasible.
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- Incorporation of higher order FV methods also possible. Future work will concentrate on higher order schemes with low numerical dissipation.
The Virtual Test Facility

- AMROC V2.0 plus solid mechanics solvers
- Implements explicit SAMR with different finite volume solvers
- Embedded boundary method, fluid-structure coupling
- \(~ \sim \) 430,000 lines of code total in C++, C, Fortran-77, Fortran-90
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- AMROC V3.0 presently in private repository, will be released eventually again on http://amroc.sourceforge.net
Detonation-driven plastic deformation

Chapman-Jouguet detonation in a tube filled with a stoichiometric ethylene and oxygen ($\text{C}_2\text{H}_4 + 3\text{ O}_2$, 295 K) mixture. Euler equations with single exothermic reaction $A \rightarrow B$

$$
\partial_t \rho + \partial_x (\rho u) = 0, \quad \partial_t (\rho u_k) + \partial_x (\rho u_k u + \delta_{kn} p) = 0, \quad k = 1, \ldots, d
$$

$$
\partial_t (\rho E) + \partial_x (u (\rho E + p)) = 0, \quad \partial_t (Y \rho) + \partial_x (Y \rho u) = \psi
$$

with

$$
p = (\gamma - 1)(\rho E - \frac{1}{2}\rho u^n u - \rho Y q_0) \quad \text{and} \quad \psi = -k Y \rho \exp \left(\frac{-E_A \rho}{p}\right)
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modeled with heuristic detonation model by [Mader, 1979]

\[
V := \rho^{-1}, \quad V_0 := \rho_0^{-1}, \quad V_{CJ} := \rho_{CJ}
\]

\[
Y' := 1 - (V - V_0)/(V_{CJ} - V_0)
\]

If $0 \leq Y' \leq 1$ and $Y > 10^{-8}$ then

- If $Y < Y'$ and $Y' < 0.9$ then $Y' := 0$
- If $Y' < 0.99$ then $p' := (1 - Y') p_{CJ}$
- else $p' := p$

\[
\rho_A := Y' \rho
\]

\[
E := p'/(\rho (\gamma - 1)) + Y' q_0 + \frac{1}{2} u u
\]
Detonation-driven plastic deformation

Chapman-Jouguet detonation in a tube filled with a stoichiometric ethylene and oxygen ($\text{C}_2\text{H}_4 + 3\text{O}_2$, 295 K) mixture. Euler equations with single exothermic reaction $A \rightarrow B$

$$\partial_t \rho + \partial_x (\rho u_n) = 0, \quad \partial_t (\rho u_k) + \partial_x (\rho u_k u_n + \delta_{kn} p) = 0, \quad k = 1, \ldots, d$$

$$\partial_t (\rho E) + \partial_x (u_n (\rho E + p)) = 0, \quad \partial_t (Y \rho) + \partial_x (Y \rho u_n) = \psi$$

with

$$p = (\gamma - 1)(\rho E - \frac{1}{2} \rho u_n u_n - \rho Y q_0) \quad \text{and} \quad \psi = -k Y \rho \exp \left( \frac{-E_A \rho}{p} \right)$$

modeled with heuristic detonation model by [Mader, 1979]

$$V := \rho^{-1}, \quad V_0 := \rho_0^{-1}, \quad V_{\text{CJ}} := \rho_{\text{CJ}}$$

$$Y' := 1 - (V - V_0)/(V_{\text{CJ}} - V_0)$$

If $0 \leq Y' \leq 1$ and $Y > 10^{-8}$ then

If $Y < Y'$ and $Y' < 0.9$ then $Y' := 0$

If $Y' < 0.99$ then $p' := (1 - Y') \rho_{\text{CJ}}$

else $p' := p$

$$\rho_A := Y' \rho$$

$$E := p'/(\rho (\gamma - 1)) + Y' q_0 + \frac{1}{2} u_n u_n$$

Comparison of the pressure traces in the experiment and in a 1d simulation
Tube with flaps

Fluid density and displacement in y-direction in solid

Schlieren plot of fluid density on refinement levels

64+8 processors 2.2 GHz AMD Opteron, PCI-X 4x Infiniband network, \( \sim 4320 \) h CPU to \( t_{end} = 450 \mu s \)


References II


