Adaptive High-Resolution Simulation of Shock-Induced Unsteady Hydrogen-Air Combustion

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Axisymmetric Navier-Stokes equations with chemical reaction

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

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

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

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

\[
f_v = \begin{bmatrix}
\rho D_i \frac{\partial Y_i}{\partial x} \\
\tau_{xx} \\
k \frac{\partial T}{\partial x} + \rho \sum h_j D_j \frac{\partial Y_j}{\partial x} + u \tau_{xx} + v \tau_{xy} \\
\tau_{xy}
\end{bmatrix}
\]

\[
g_v = \begin{bmatrix}
\rho D_i \frac{\partial Y_i}{\partial y} \\
\tau_{yy} \\
k \frac{\partial T}{\partial y} + \rho \sum h_j D_j \frac{\partial Y_j}{\partial y} + u \tau_{xy} + v \tau_{yy} \\
\tau_{xy}
\end{bmatrix}
\]

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

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

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

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

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

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

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

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

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

Caloric equation

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

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

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

Caloric equation

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

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

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

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:

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

Arrhenius-kinetics:

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

- 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:

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

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

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

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

Arrhenius-kinetics:

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

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

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

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

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

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

Arrhenius-kinetics:

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

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

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

\[
\mu = \sum_{i=1}^{K} \frac{Y_i \mu_i}{W_i \sum_{m=1}^{K} Y_m \Phi_{im}/W_m}
\]

with \( \Phi_{im} = \frac{1}{\sqrt{8}} \left( 1 + \frac{W_i}{W_m} \right)^{-\frac{1}{2}} \left( 1 + \left( \frac{\mu_i}{\mu_m} \right)^{\frac{1}{2}} \left( \frac{W_m}{W_j} \right)^{\frac{1}{4}} \right)^2 \)

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

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

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

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

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

Dimensional splitting for PDE

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

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

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

Dimensional splitting for PDE

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

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

Treat right-hand side as source term

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

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

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

Treat right-hand side as source term

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

Chemical source term

\[ S(\Delta t) : \partial_t \mathbf{q} = s(\mathbf{q}) , \quad \text{IC: } \bar{Q} \xrightarrow{\Delta t} Q(t_m + \Delta t) \]
Splitting methods

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

Dimensional splitting for PDE

\[ \chi^{(\Delta t)} : \partial_t q + \partial_x (f(q) - f_v(q)) = 0, \quad \text{IC: } Q(t_m) \xrightarrow{\Delta t} Q_1^{1/2} \]

\[ \gamma^{(\Delta t)} : \partial_t q + \partial_y (g(q) - g_v(q)) = 0, \quad \text{IC: } Q_1^{1/2} \xrightarrow{\Delta t} Q \]

Treat right-hand side as source term

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

Chemical source term

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

Formally 1st-order algorithm

\[ Q(t_m + \Delta t) = S^{(\Delta t)} C^{(\Delta t)} \gamma^{(\Delta t)} \chi^{(\Delta t)} (Q(t_m)) \]

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

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

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

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

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

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

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

- Riemann solver to approximate $F(Q_{jk}^n, Q_{j+1,k}^n)$
- 1st-order finite differences for $F_v(Q_{jk}^n, Q_{j+1,k}^n)$ yield 2nd-order accurate central differences in (*)
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

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

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

yield (for simplicity)

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

▶ 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 (*)

Stability condition used:

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

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

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

within explicit 2nd-order accurate Runge-Kutta method

- Gives 2nd-order central difference approximation of $G_v$
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 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 $G_v$
- 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 $\mathcal{C}(\Delta t)$: 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 $G_v$
- 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!

$$\partial_t \rho_i = W_i \dot{\omega}_i(\rho_1, \ldots, \rho_K, T) \quad i = 1, \ldots, K$$
Riemann solver for combustion

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

(S2) Compute $\mathbf{\hat{c}} : = \ddot{\mathbf{c}}_p / \ddot{\mathbf{c}}_v$ with $\ddot{\mathbf{c}}_{(p/v)i} = \frac{1}{T_R - T_L} \int_{T_L}^{T_R} c_{(p,v)i}(\tau) d\tau$.

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

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

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

(S6) Calculate $\mathbf{W}_1 = a_1 \hat{\mathbf{f}}_1$, $\mathbf{W}_2 = \sum_{i=2}^{K+d} a_i \hat{\mathbf{f}}_i$, $\mathbf{W}_3 = a_{K+d+1} \hat{\mathbf{f}}_{K+d+1}$.

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

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

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

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

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

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

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Riemann solver for combustion

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(S10) Entropy correction: Evaluate $|\mathfrak{s}_L|$.

$F_{Roe}(q_L, q_R) = \frac{1}{2} \left( f(q_L) + f(q_R) - \sum_{i=1}^{3} |\mathfrak{s}_L| W_i \right)$
Riemann solver for combustion

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

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(S11) Positivity correction: Replace $F_i$ by

$F_i^* = F_p \cdot \begin{cases} Y_i^f, & F_p \geq 0, \\ Y_i^f, & F_p < 0. \end{cases}$

(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]
[Harten and Hyman, 1983]

1. $|\bar{s}_i| = \begin{cases} |s_i| & \text{if } |s_i| \geq 2\eta \\ \frac{|s_i^2|}{4\eta} + \eta & \text{otherwise} \end{cases}$
\[\eta = \frac{1}{2} \max_k \{|s_k(q_R) - s_k(q_L)|\}\]

2. Replace $|s_i|$ by $|\bar{s}_i|$ only if $s_i(q_L) < 0 < s_i(q_R)$

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
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- Refined blocks overlay coarser ones
- Refinement in space and time by factor $r_t$
- 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
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only for single patch necessary

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

Conservative averaging (restriction):

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

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Level transfer / setting of ghost cells

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Bilinear interpolation (prolongation):

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

1. Error estimation on interior cells
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\[ H^{\Delta t_i} Q'(t_i - \Delta t_i) \]
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\[ \mathcal{H}^{\Delta t_i} Q'(t_i - \Delta t_i) = \mathcal{H}^{\Delta t_i}\left(\mathcal{H}^{\Delta t_i} Q'(t_i - \Delta t_i)\right) = \mathcal{H}^{\Delta t_i}_2 Q'(t_i - \Delta t_i) \]
Heuristic error estimation for FV methods

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

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Heuristic error estimation for FV methods

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\[
\mathcal{H}^{\Delta t_i} \dot{Q}'(t_i - \Delta t_i) = \mathcal{H}^{\Delta t_i} \left( \mathcal{H}^{\Delta t_i} \dot{Q}'(t_i - \Delta t_i) \right) = \mathcal{H}_2^{\Delta t_i} \dot{Q}'(t_i - \Delta t_i)
\]

\[
\mathcal{H}^{2\Delta t_i} \ddot{Q}'(t_i - \Delta t_i)
\]
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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Usage of heuristic error estimation:
Current solution integrated tentatively 1 step with $\Delta t_i$ and coarsened

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

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

$$Q(t_i + \Delta t_i) := H^{2\Delta t_i} \text{Restrict} \left( Q'(t_i - \Delta t_i) \right)$$
Refinement criteria

Scaled gradient of scalar quantity $w$

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

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$$Q(t_l + \Delta t_l) := H^{2\Delta t_l}_2 \text{Restrict} \left( Q'(t_l - \Delta t_l) \right)$$

Local error estimation of scalar quantity $w$

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

In practice [Deiterding, 2003] use

$$\frac{\tau^{w}_{jk}}{\max(|w(Q_{jk}(t + \Delta t)|, S_w)} > \eta^{r}_{w}$$
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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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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Cartesian base grid 360 × 160 cells on domain of 36 mm × 16 mm with up to 3 refinement levels with $n_l = 2, 4, 4$ and $\Delta x_{1,2} = 3.125\mu m$, 38 h CPU

GFM base grid 390 × 330 cells on domain of 26 mm × 22 mm with up to 3 refinement levels with $n_l = 2, 4, 4$ and $\Delta x_{e,1,2} = 2.849\mu m$, 200 h CPU
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

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- $\Delta x = 50 \text{ mm}$
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- $\Delta x = 12.5 \text{ mm, SAMR}$
- $\Delta x_e = 45.6 \text{ mm}$
- $\Delta x_e = 22.8 \text{ mm}$
- $\Delta x_e = 11.4 \text{ mm, SAMR}$
Outline

Introduction
  Governing equations

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

Computational results
  Combustion induced by projectiles
  Lehr’s configuration

Summary
  Conclusions / Outlook
Shock-induced combustion around a sphere

- Spherical projectile of radius 1.5 mm travels with constant velocity $v_f = 2170.6 \text{ m/s}$ 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 $Y_{H_2}$ (white) on refinement domains for 3-level (left) and 4-level computation (right)](image)
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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: $\epsilon_p$, green shades: $\eta_{Y_i}$,
red: embedded boundary

Refinement criteria:

<table>
<thead>
<tr>
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$\epsilon_{\rho} = 0.02 \text{ kg m}^{-3}$, $\epsilon_{\rho} = 16 \text{ kPa}$

Parallel performance

Scaling of different code portions

R. Deitering, B. J. Lee -- Adaptive High-Resolution Simulation of Shock-Induced Unsteady Hydrogen-Air Combustion
Lehr’s ballistic range experiments

- Spherical-nosed projectile of radius 1.5 mm travels with constant velocity through stoichiometric H₂ : O₂ : N₂ mixture (molar ratios 2:1:3.76) at 42.663 kPa and $T = 293$ K [Lehr, 1972]

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  - Velocity $v_I = 1806 \text{ m/s (M = 4.48), } \sim 60 \text{ Pts/}l_{ig}$
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- Stagnation point location and pressure tracked in every time step

R. Deiterding, B. J. Lee – Adaptive High-Resolution Simulation of Shock-Induced Unsteady Hydrogen-Air Combustion
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]
- Axisymmetric Navier-Stokes and Eulers simulations on AMR base mesh of $400 \times 200$ cells, physical domain size $6\text{ cm} \times 3\text{ cm}$
- 4-level computations with refinement factors 2,2,4 to final time $t = 170 \mu s$. Refinement downstream removed.
- Main configurations
  - Velocity $v_f = 1931$ m/s ($M = 4.79$), $\sim 40$ Pts/\text{ig}
  - Velocity $v_f = 1806$ m/s ($M = 4.48$), $\sim 60$ Pts/\text{ig}
- Various previous studies with not entirely consistent results. E.g. [Yungster and Radhakrishnan, 1996], [Axdahl et al., 2011]
- Stagnation point location and pressure tracked in every time step
- All computations were on 32 cores requiring $\sim 1500$ 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
- Experimental value: $\sim 720$ kHz

Schlieren plot of density
Viscous case – $M = 4.79$ – mesh adaptation
Inviscid case – $M = 4.79$

- 4158 iterations with CFL=0.9 to $t = 170\mu s$
- Oscillation frequency in last $20\mu s$: $\approx 737$ kHz
- Experimental value: $\approx 720$ kHz

Schlieren plot of density
Comparison of temperature field

Viscous
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
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 \( \mu s \): \( \sim 417 \text{ kHz} \)
- Experimental value: \( \sim 425 \text{ kHz} \)

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

$t=0.000151300$ sec
Inviscid case $- M = 4.79$

- 4158 iterations with CFL=0.9 to $t = 170 \mu s$
- Oscillation frequency in last 20 $\mu s$: $\sim 737$ kHz
- Experimental value: $\sim 720$ kHz

Schlieren plot of density
Oscillation mechanism

- Schlieren of density
- Temperature
- Mass fraction OH
- Pressure
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
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Conclusions / Outlook

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  - Stable oscillations also reported for $M = 5.03$ and $M = 5.11$ in experimental results.
  - But resolution requirements can increase significantly.
- Future computations will also consider higher-order and hybrid WENO schemes that are already available in AMROC.