**Governing Equations**

Multi-component reactive Euler equations for thermally perfect gases with general equation of state

\[
p(\rho, T) = \sum_{i=1}^{K} \frac{K}{\rho_i} = \sum_{i=1}^{K} \frac{R_i}{\rho_i} T.
\]

Caloric equation:

\[
h(\rho, T) = \sum_{i=1}^{K} Y_i h_i(T) \quad \text{with} \quad h_i(T) = \frac{\rho_i}{\rho} = \frac{\rho_i}{\rho} + \int_{0}^{T} \frac{\rho_i}{\rho} ds
\]

Evaluation of \( p(\rho, T) \) requires computation of \( T = T(\rho, c) \) from implicit equation

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

Non-equilibrium Arrhenius kinetics for \( H_2 : O_2 \) combustion:

- 34 elementary reactions.

**Numerical Methods**

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

Time-explicit finite volume shock-capturing method:

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

Source term integration:

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

Locally high resolution, which is essential for the accurate computation of detonation waves, is achieved by blockstructured adaptive mesh refinement (AMR).

- Discretization necessary only for single rectangular grid.
- Spatial and temporal refinement, no global time step restriction.
- Blockstructured data guarantees high computational performance.

**Cellular Structure Simulation in 2D**

Experiments have shown that self-sustaining detonation waves are locally multi-dimensional and nonsteady. Triple-points form, which enhance the local chemical reaction significantly.

- \( \approx 45 \) cells within induction length.
- Adaption criteria:
  1. Scaled gradients \( Q^m |_{\Delta x_{i+1}} - Q^m |_{\Delta x_i} \) of \( p \) and \( \rho \)
  2. Estimation of error in \( Y_i \) by Richardson extrapolation

\[
Q^m_1 = \frac{\Delta x_i \Delta t}{2 \Delta x_{i+1}} Q^m_1, \quad Q^m_1 = \frac{\Delta x_{i+1} \Delta t}{2 \Delta x_i} Q^m_1, \quad \tau = \frac{Q - Q^m_1}{2^{m+1} - 2}
\]

- Quasi-stationary computation. Symmetric in \( x_2 \)-direction.
- \( \approx 16.8 \) cells within induction length.
- Adaptive computation uses 1.0M-1.5M cells. (Nonadaptive 8.8M).

**Detonation Diffraction**

The simulation reproduces exactly the experimentally measured critical tube diameter of 10 detonation cells width.

- \( \approx 25 \) cells within induction length.
- Adaptive computation uses around 3M cells. (Nonadaptive 150 M)
- 4600h CPU time on 48 Athlon-1.4 GHz nodes.

**Mach Reflection of a Detonation**

For larger inflow angles a detonation wave is reflected in form of a Mach reflection. The higher overdrive factor in the Mach stem region suppresses the triple points (see left triple point track).

- \( \approx 20 \) cells within induction length.
- Adaptive computation uses around 1.2M cells. (Nonadaptive 59 M)
- 1200h CPU time on 16 Pentium-III-850 MHz nodes.