Accurate simulation of detonation phenomena

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Generalized Euler equations

The computation of inviscid flows with chemical reaction requires the usage of generalized Euler equations. In cartesian coordinates the following equations have to be applied:

K continuity equations for K different gaseous species:

$$\partial_t \rho_i + \sum_{n=1}^{N} \partial_{x_n}(\rho_i v_n) = \dot{m}_i \qquad \text{for } i = 1,\ldots,K$$

N momentum equations:

$$\partial_t(\rho v_m) + \sum_{n=1}^{N} \partial_{x_n}(\rho v_n v_m + \delta_{n,m}\, p) = 0 \qquad \text{for } m = 1,\ldots,N$$

Energy equation:

$$\partial_t(\rho E) + \sum_{n=1}^{N} \partial_{x_n}\left[v_n(\rho E + p)\right] = 0$$

Equation of state

The species are assumed to be ideal gases in thermal equilibrium. The ideal gas law and Dalton's law can be applied:

$$p(\boldsymbol{\rho}, T) = \sum_{i=1}^{K} p_i = \sum_{i=1}^{K} \rho_i \frac{\mathcal{R}}{W_i} T = \rho \frac{\mathcal{R}}{W} T \qquad \text{with} \quad \rho = \sum_{i=1}^{K} \rho_i$$

Ideal gases are *thermally perfect* and the specific heats are functions of the temperature:

$$c_{pi} = c_{pi}(T) \quad , \qquad c_{vi} = c_{vi}(T) \quad , \qquad \gamma_i(T) = c_{pi}(T) \,/\, c_{vi}(T)$$

Caloric equation:

$$h(\boldsymbol{\rho}, T) = \sum_{i=1}^{K} Y_i h_i(T) \quad \text{mit} \quad h_i(T) = h_i^0 + \int_0^T c_{pi}(s)ds$$

Evaluation of $p(\boldsymbol{\rho}, T)$ requires the computation of $T = T(\boldsymbol{\rho}, e)$ from the implicit equation:

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

Only in the case of *calorically perfect* gases with c_{pi}, c_{vi} const. $\Rightarrow \gamma = \gamma(\boldsymbol{\rho})$ the temperature T can be eliminated and an explicit equation of state can be derived:

$$p(\boldsymbol{\rho}, e) = (\gamma(\boldsymbol{\rho}) - 1)\left(\rho e - \sum_{i=1}^{K} \rho_i h_i^0\right)$$

Detailed chemistry

The chemical production rates $m_i(\rho_1,\ldots,\rho_K,T)$ are derived from a *reaction mechanism* that consists of M chemical reactions:

$$\sum_{i=1}^{K} \nu_{ji}^f S_i \rightleftharpoons \sum_{i=1}^{K} \nu_{ji}^r S_i \qquad\qquad j = 1,\ldots,M$$

The forward reaction rate $k_j^f(T)$ is calculated with an empirical Arrhenius law:

$$k_j^f(T) = A_j T^{\beta_j} \exp(-E_j/\mathcal{R}T)$$

Evaluation of the equilibrium constant $K_j^c(T)$ allows the calculation of the corresponding backward reaction rate $k_j^r(T) = k_j^f(T)/K_j^c(T)$.

Mass production rate of specie S_i:

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

ZND detonation model

An instructive model-problem is derived by assuming a stationary detonation wave with only one single irreversible reaction $A \longrightarrow B$ with normalized energy release $q_0 = -\Delta h^0$ and forward reaction rate $k^f(T) = \exp(-E^+/T)$.

Mass production rate of species A and B:

$$\dot{m}_A = -\rho_A \exp(-E^+/T)\,, \qquad \dot{m}_B = -\dot{m}_A$$

A and B are treated as calorically perfect gases with $\gamma_A = \gamma_B$. The equation of state therefore reads:

$$p(\boldsymbol{\rho}, e) = (\gamma - 1)\,(\rho e - \rho_A\, q_0)$$

The parameter $f = (D/D_{CJ})^2 \geq 1$ measures the degree of overdrive for a given ZND detonation traveling with speed D in respect to the minimal detonation velocity D_{CJ}. f determines the stability of a ZND wave.

Numerical Methods

Incorporation of source terms and extension to multiple dimensions via the method of fractional steps:

A sequence of N one-dimensional initial value problems for the homogeneous transport equations and the system of ordinary differential equations

$$\partial_t \rho_i = \dot{m}_i\,(\rho_1,\ldots,\rho_K,T) \qquad i = 1,\ldots,K$$

are solved successively within each time-step.

The following upwind schemes are employed to solve the homogeneous 1D transport equations:

- Godunov's method
- Roe's method with entropy correction only in sonic rarefactions (Roe) and with entropy enforcement by adding numerical viscosity (RoeV)
- Steger-Warming and van Leer's flux vector splitting methods
- Harten, Lax, van Leer's (HLL) method

Decoupled source term integration:

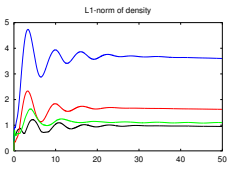
- Standard ODE-methods, e.g. semi-implicit Rosenbrock-Wanner method for detailed chemistry

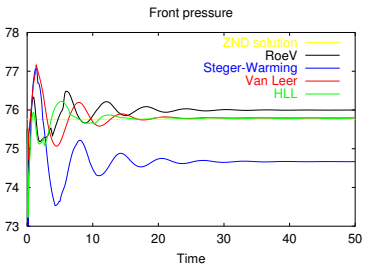
The integration of stiff source terms requires automatic stepsize adjustment in a single transport step.

Stable ZND detonation

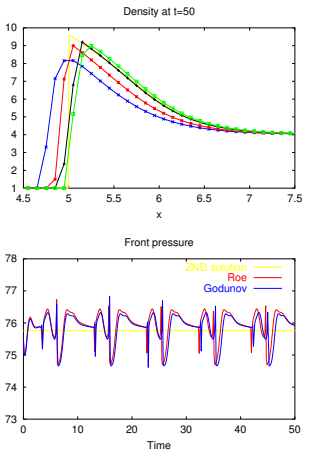
The computation of stable one-dimensional ZND detonations allows the quantitative comparison of solutions of different numerical schemes against the exact one. By applying an ODE solver of higher order different 1st order upwind schemes within the fractional-step method can be evaluated.

$\gamma = 1.2$, $E^+ = 50$, $q_0 = 50$, $f = 1.8$, $10\,pts/L_{1/2}$, $CFL = 0.9$





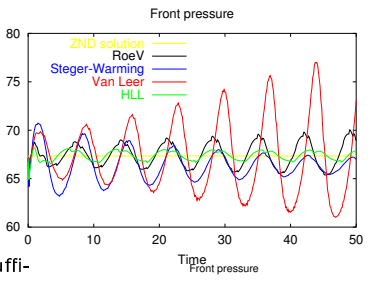
1. A sufficiently dissipative upwind scheme has to be employed to stabilize the splitting method: Stable detonations are computed with FVS methods, HLL and RoeV (upper right picture). The solution is qualitatively incorrect, if Roe's and Godunov's method are applied (lower right picture).
2. Van Leer's FVS and RoeV resolve the detonation front most sharply (middle left picture), but only Van Leer's FVS converges against the exact ZND front pressure (upper right picture).



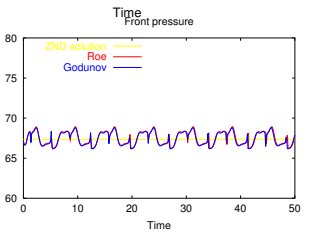
Unstable ZND detonation

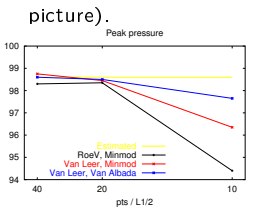
Linearized stability analysis for ZND waves predicts one unstable mode for $1.57 < f < 1.73$ and $\gamma = 1.2$, $E^+ = 50$, $q_0 = 50$. Starting from the unperturbed exact solution the numerical scheme should reproduce the unstable behavior.

$10\,pts/L_{1/2}$, $CFL = 0.9$



1. The instability is reproduced best with Van Leer's FVS. RoeV shows the unstable mode slightly. Steger-Warming FVS and HLL are to dissipative to resolve the detonation sufficiently at this resolution and do not reproduce the instability (upper right picture).
2. Numerical instabilities totally suppress the physical one when using Roe's or Godunov's method (lower right picture).





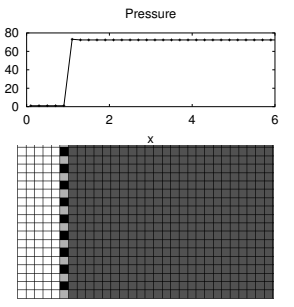
3. Higher order reconstruction technics within the upwind scheme can improve the solution significantly. (Compare maximal front pressures obtained with 2nd order MUSCL-Hancock in left picture to 1st order results).

Occurrence of the carbuncle phenomenon

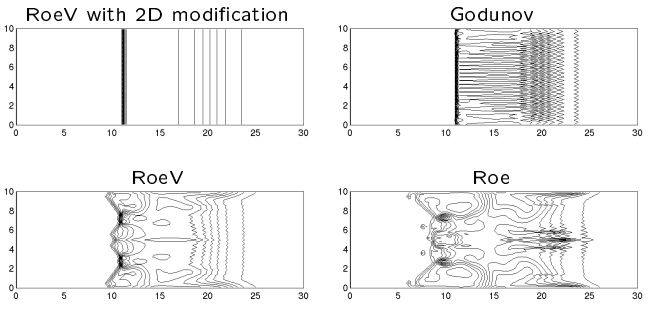
If a one-dimensional upwind scheme is used to solve the multidimensional Euler equations on a structured grid with a fractional-step method, strong shock or typical detonation wave solutions may become unstable. Sufficient crossflow dissipation is necessary to stabilize the solution.

A simple test for standard Euler equations can be derived by taking as Riemann initial data the values near the detonation front for $\gamma = 1.2$, $q_0 = 50$, $f = 2.0$ and disturbing the shock-pressure cellwise by $\pm 1\%$.

ρ	1.0	4.35
u	9.63	2.21
v	0.0	0.0
p	1.0	72.41



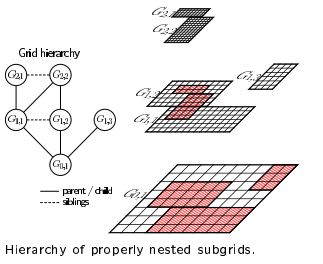
Van Leer, Steger-Warming, HLL, RoeV with 2D modification



Isolines of density at $t = 10$ for different 1st order schemes (CFL=0.5)

Generic framework for blockstructured AMR

A locally high resolution, which is essential for the accurate computation of detonation waves, is achieved by utilizing the most efficient adaptive method for hyperbolic conservation laws on blockstructured grids: The Berger and Oliger AMR algorithm.



Hierarchy of properly nested subgrids.

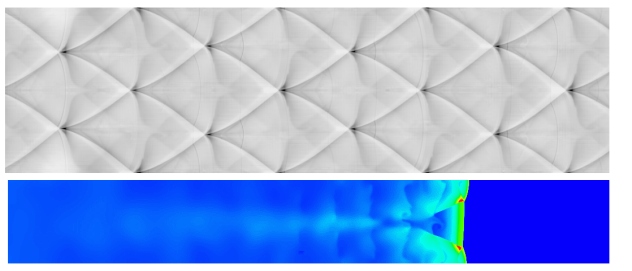
A generic and flexible framework for AMR has been developed. It consists of three abstraction levels:

1. Specific application. (Extended Clawpack supplied as demo application)
2. AMROC (Adaptive Mesh Refinement in Object-oriented C++).
3. Parallel hierarchical data structures that employ the MPI-library.

Typical benchmarks run on distributed memory machines show high parallel efficiency and a computational performance like purely Fortran-based codes. The framework and appropriate visualization tools can be obtained from *http://www.math.tu-cottbus.de/~deiter/amroc*

Planar detonation with transverse waves

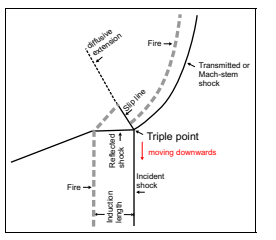
Experiments have shown that self-sustaining detonation waves are locally multidimensional and nonsteady. Triple-points may form, which enhance the local chemical reaction significantly. Equilibrium-configurations with regular detonation cells are possible in particular cases. The accurate numerical simulation of transverse wave phenomena in detonation waves requires extraordinarily high resolution.



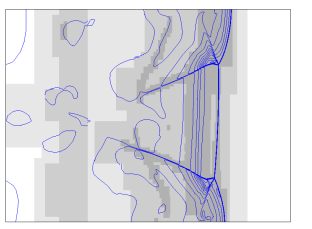
Top: The time history of the released chemical energy shows the detonation cells.
Bottom: Interacting transverse waves behind the detonation front.

Reaction mechanism: 34 elementary reactions for the 9 *thermally perfect* species H, O, OH, H_2, O_2, H_2O, HO_2, H_2O_2,Ar.
Configuration: Stoichiometric H_2-O_2-system with 70% Ar, at 6.7 kPa and 298 K.

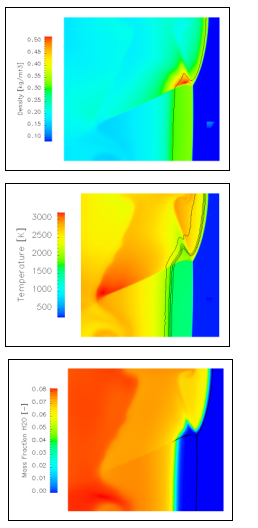
- 1044 time steps with 3 refinement levels (factors: 2,4,4). Finest level corresponds to 19840x640 grid (12.7 M cells).
- $\approx$ 32 cells within induction length.
- Adaptive computation uses 150k-200k cells.
- 121h real time on 7 nodes Pentium III-750 MHz.



Schematic diagram of the flow around a triple-point.



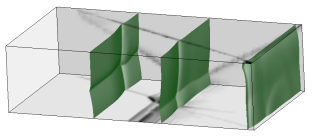
Isolines of density on refinement grids show the dynamic adaption of the detonation wave.



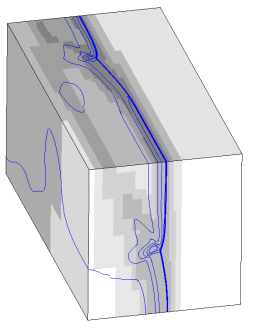
Detailed study of the flow around a triple-point. Additional isolines show the induction length.

Detonation with two orthogonal transverse waves

- Detonation front remains quasi-stationary, because unburned gas flows in with CJ-velocity.
- 264 time steps with 3 refinement levels (factors: 2,2,2). Finest level corresponds to 224x96x192 grid (4.1 M cells).
- $\approx$ 8 cells within induction length.
- Adaptive computation uses 800k-1.2M cells.
- 66h real time on 15 nodes Pentium III-750 and Pentium III-450 MHz.



Temporal development of the detonation front with two orthogonal triple-point lines.



Isolines of density on refinement grids.

Temporal development of the detonation front structure with coarse triple-point tracks.