Lecture 3

Numerical methods for combustion research

Course *Block-structured Adaptive Finite Volume Methods for Shock-Induced Combustion Simulation*

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Outline

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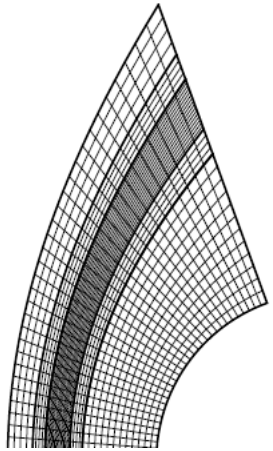
SAMR on boundary aligned meshes

Analytic or stored geometric mapping of the coordinates (graphic from [Yamaleev and Carpenter, 2002])

- Topology remains unchanged and thereby entire SAMR algorithm
- Patch solver and interpolation need to consider geometry transformation
- Handles boundary layers well



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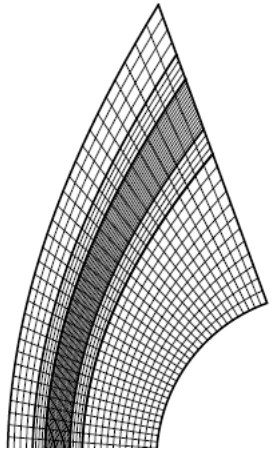

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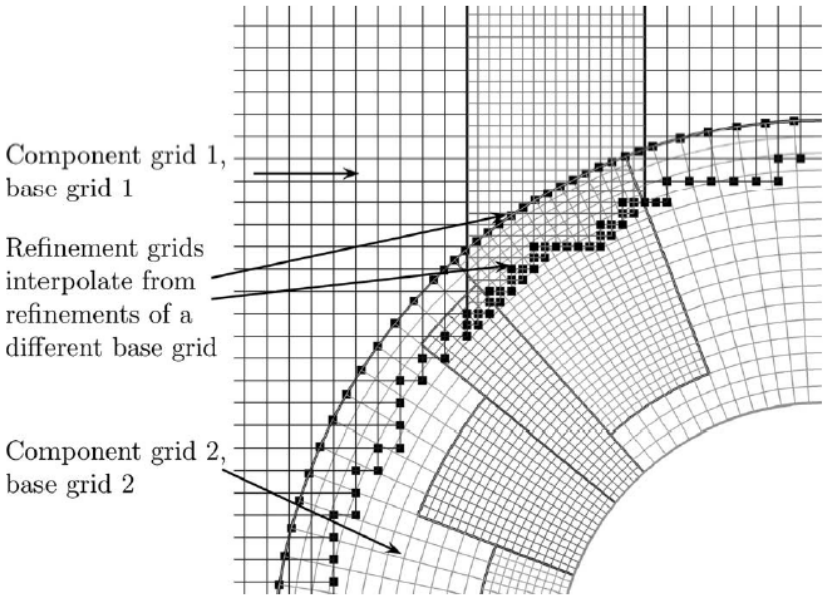


Overlapping adaptive meshes [Henshaw and Schwendeman, 2003], [Meakin, 1995]

- Idea is to use a non-Cartesian structured grids only near boundary
- Very suitable for moving objects with boundary layers
- Interpolation between meshes is usually non-conservative

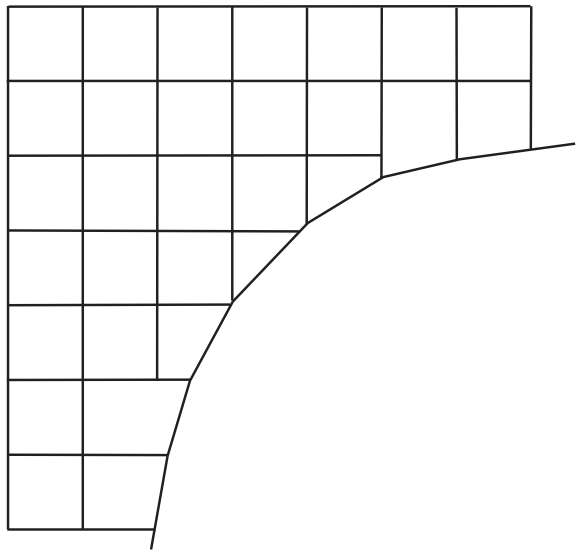
Cut-cell techniques

Accurate embedded boundary method

$$V_j^{n+1}\mathbf{Q}_j^{n+1} = V_j^n\mathbf{Q}_j^n - \Delta t \left(A_{j+1/2}^{n+1/2}\,\mathbf{F}(\mathbf{Q}, j) - A_{j-1/2}^{n+1/2}\,\mathbf{F}(\mathbf{Q}, j-1) \right)$$

Methods that represent the boundary sharply:

- Cut-cell approach constructs appropriate finite volumes
- Conservative by construction. Correct boundary flux



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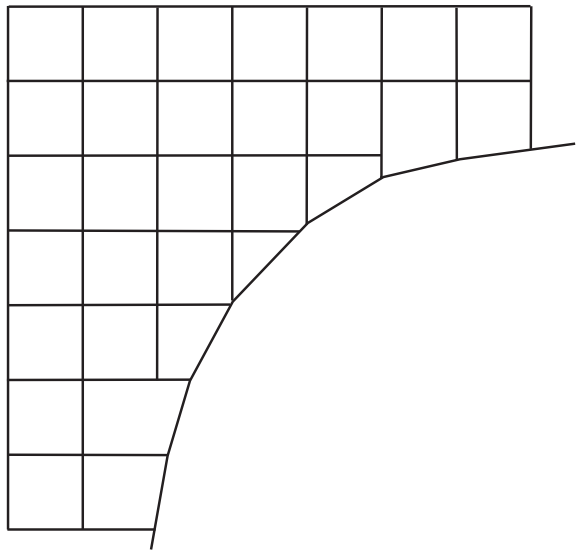

Methods that represent the boundary sharply:

- Cut-cell approach constructs appropriate finite volumes
- Conservative by construction. Correct boundary flux
- Key question: How to avoid small-cell time step restriction in explicit metyhods?
  - Cell merging: [Quirk, 1994a]
- Usually explicit geometry representation used [Aftosmis, 1997], but can also be implicit, cf. [Nourgaliev et al., 2003], [Murman et al., 2003]

Embedded boundary techniques

Volume of fluid methods that resemble a cut-cell technique on purely Cartesian mesh

- Redistribution of boundary flux achieves conservation and bypasses time step restriction: [Pember et al., 1999], [Berger and Helzel, 2002]

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Methods that diffuse the boundary in one cell (good overview in [Mittal and Iaccarino, 2005]):

- Related to the immersed boundary method by Peskin, cf. [Roma et al., 1999]
- Boundary prescription often by internal ghost cell values, cf. [Tseng and Ferziger, 2003]
- Not conservative by construction but conservative correction possible
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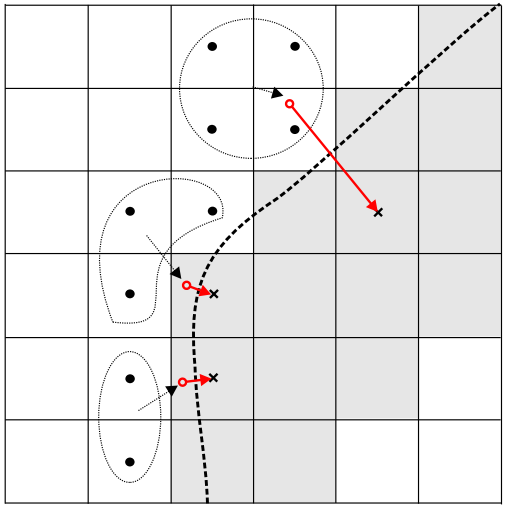
K. J. Richards et al., On the use of the immersed boundary method for engine modeling

Level-set method for boundary embedding



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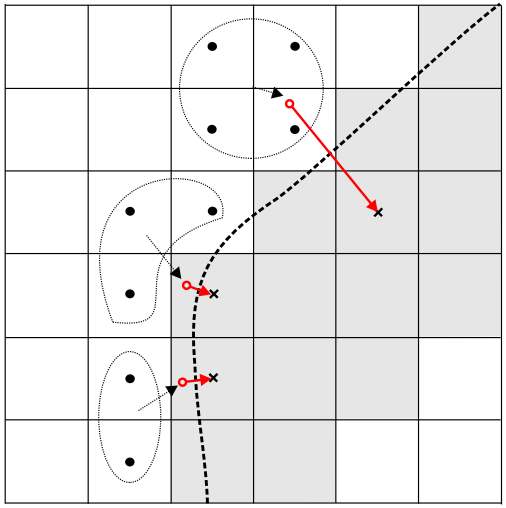

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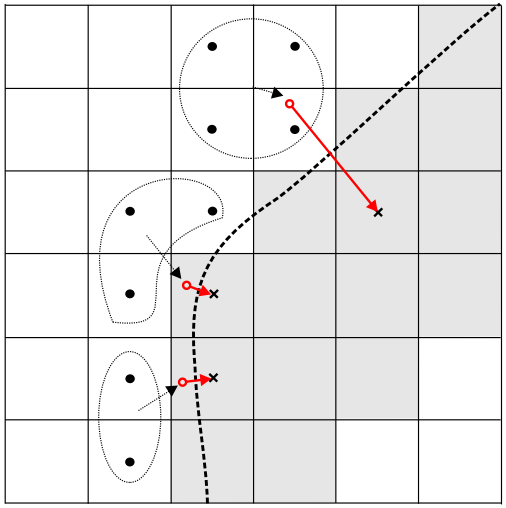

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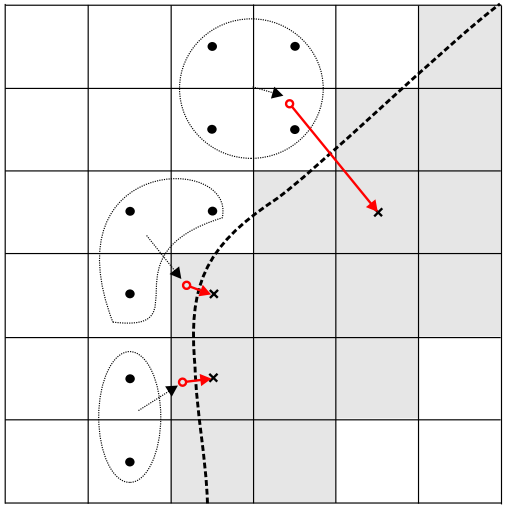

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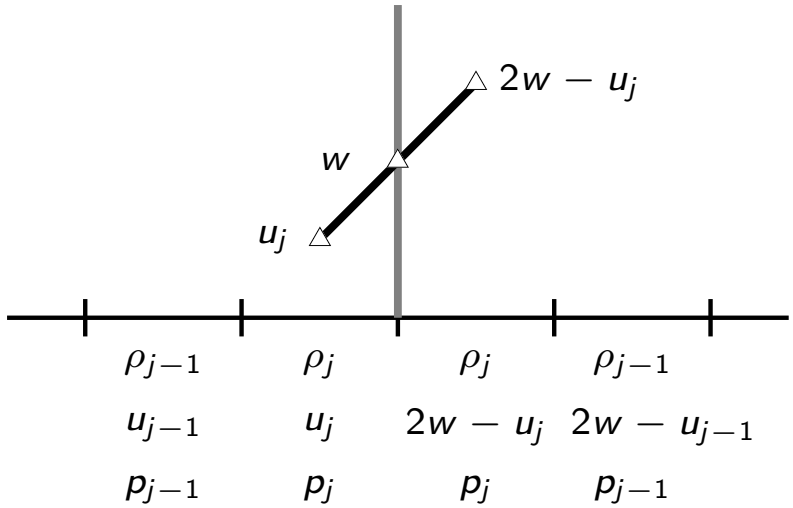
Interpolate / constant value extrapolate values at

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



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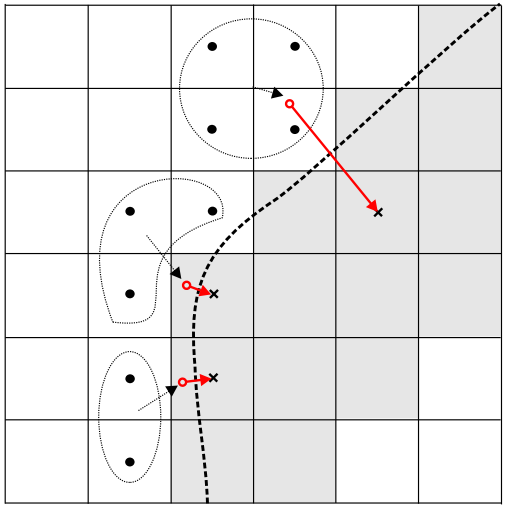

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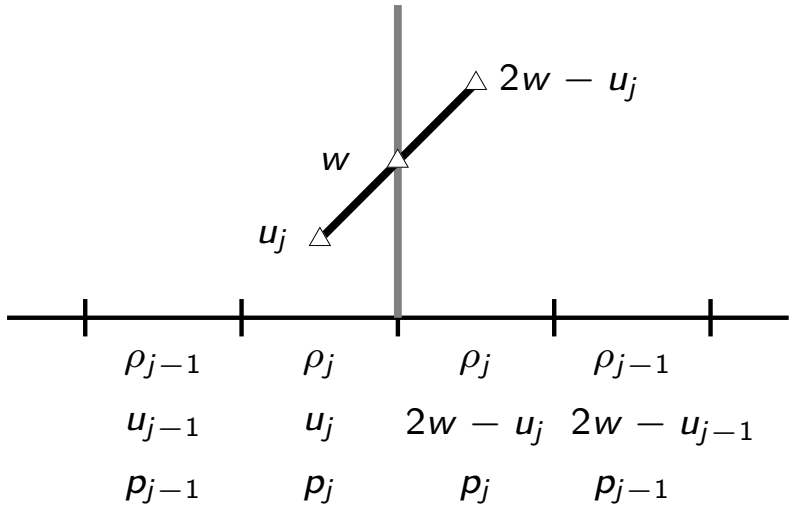
Velocity in ghost cells

$$\begin{aligned}\mathbf{u}' &= (2\mathbf{w}\cdot\mathbf{n} - \mathbf{u}\cdot\mathbf{n})\mathbf{n} + (\mathbf{u}\cdot\mathbf{t})\mathbf{t} \\ &= 2\left((\mathbf{w}-\mathbf{u})\cdot\mathbf{n}\right)\mathbf{n} + \mathbf{u}\end{aligned}$$



Closest point transform algorithm

The signed distance φ to a surface $\mathcal{I}$ satisfies the eikonal equation [Sethian, 1999]

$$|\nabla\varphi| = 1 \quad \text{with} \quad \varphi\big|_{\mathcal{I}} = 0$$

Solution smooth but non-diferentiable across characteristics.

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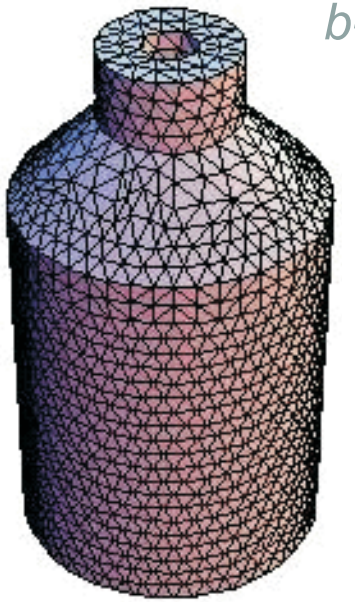
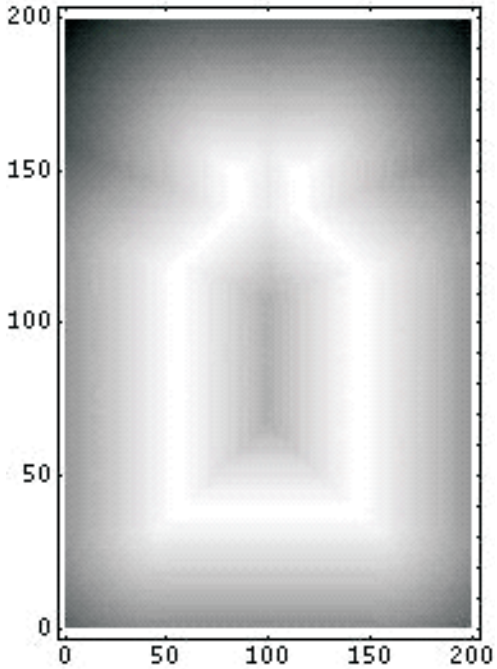
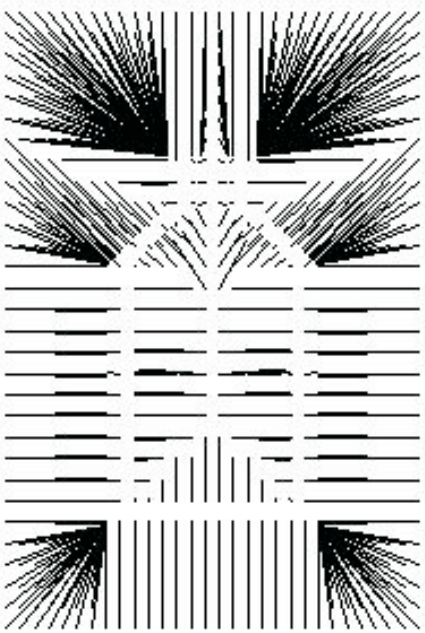


Surface mesh $\mathcal{I}$



Distance φ

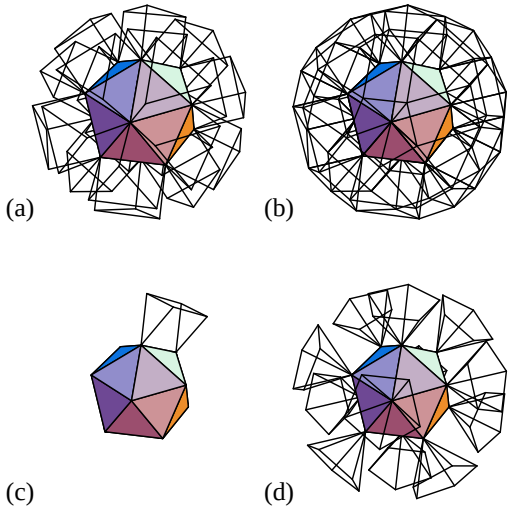


Normal to closest point

The characteristic / scan conversion algorithm

1. Build the characteristic polyhedrons for the surface mesh

Characteristic polyhedra for faces, edges, and vertices



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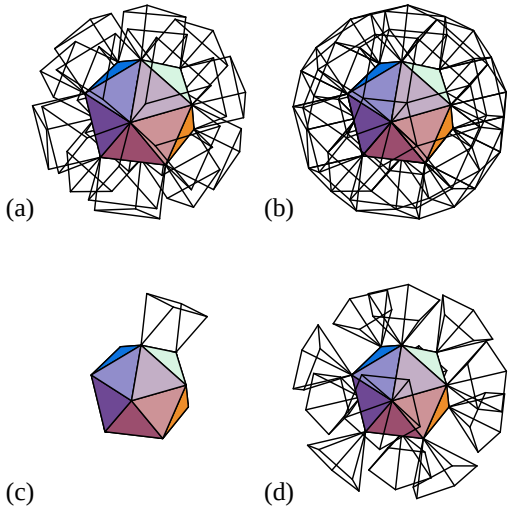
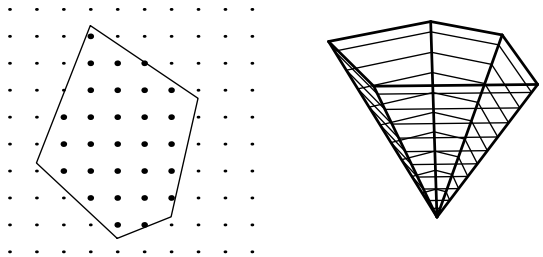


Slicing and scan conversion of apolygon



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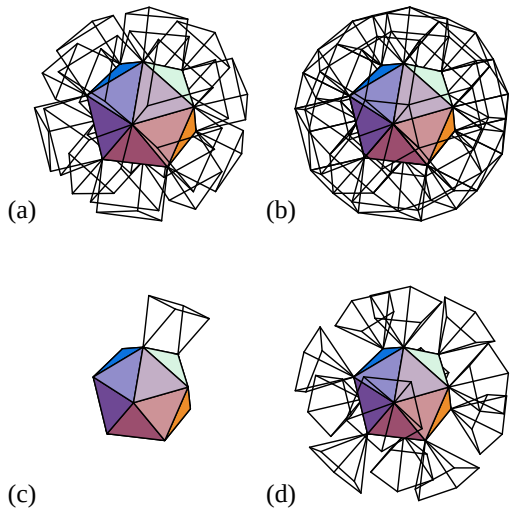

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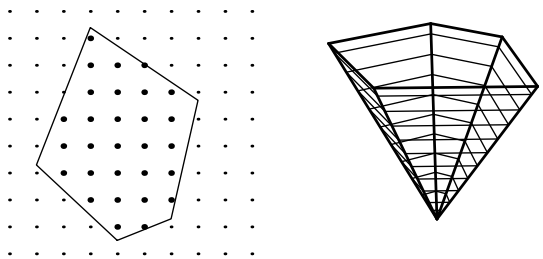

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   - $O(m)$ to build the b-rep and the polyhedra.
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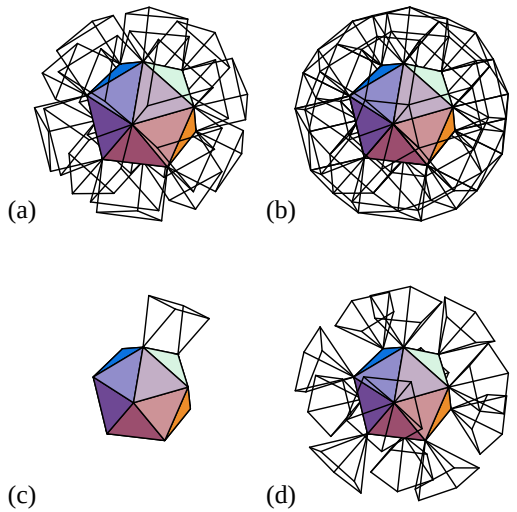

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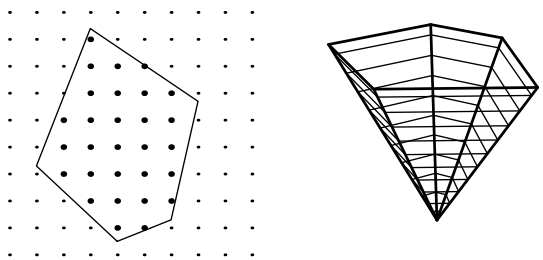

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4. Problem reduction by evaluation only within specified max. distance

[Mauch, 2003], see also
[Deiterding et al., 2006]

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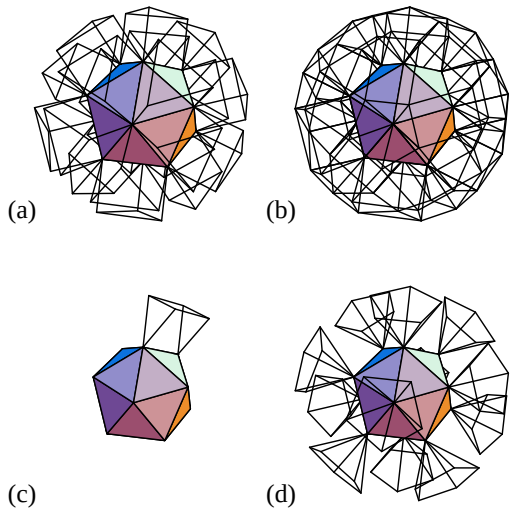

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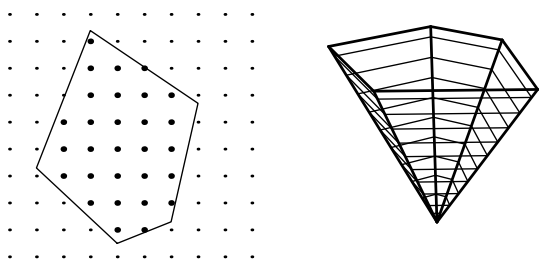


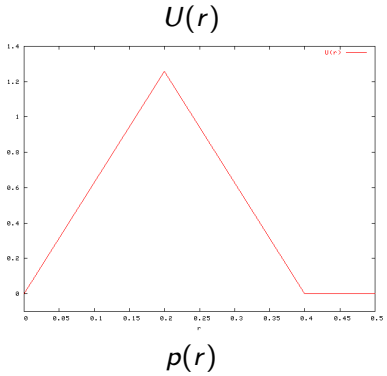
Accuracy test: stationary vortex

Construct non-trivial *radially symmetric* and *stationary* solution by balancing hydrodynamic pressure and centripetal force per volume element, i.e.

$$\frac{d}{dr}p(r) = \rho(r)\frac{U(r)^2}{r}$$

For $\rho_0 \equiv 1$ and the velocity field

$$U(r) = \alpha \cdot \begin{cases} 2r/R & \text{if } 0 < r < R/2, \\ 2(1 - r/R) & \text{if } R/2 \leq r \leq R, \\ 0 & \text{if } r > R, \end{cases}$$



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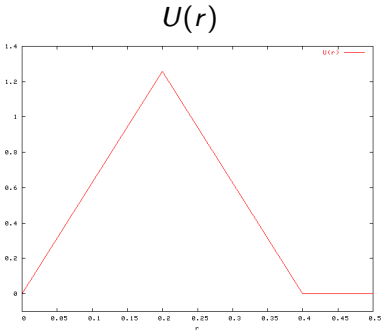

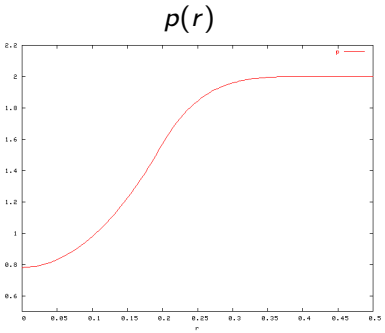

one gets with boundary condition $p(R) = p_0 \equiv 2$ the pressure distribution

$$p(r) = p_0 + 2\rho_0\alpha^2 \cdot \begin{cases} r^2/R^2 + 1 - 2\log 2 & \text{if } 0 < r < R/2, \\ r^2/R^2 + 3 - 4r/R + 2\log(r/R) & \text{if } R/2 \le r \le R, \\ 0 & \text{if } r > R. \end{cases}$$

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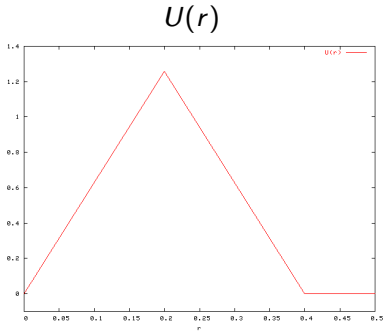

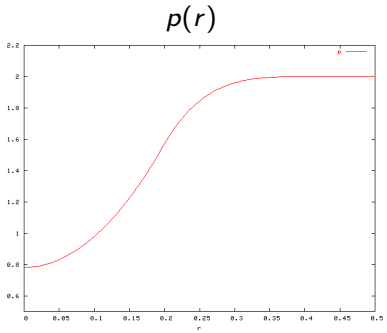

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Entire solution for Euler equations reads

$$\rho(x_1, x_2, t) = \rho_0,\ u_1(x_1, x_2, t) = -U(r)\sin\phi,\ u_2(x_1, x_2, t) = U(r)\cos\phi,\ p(x_1, x_2, t) = p(r)$$

for all $t \ge 0$ with $r = \sqrt{(x_1 - x_{1,c})^2 + (x_2 - x_{2,c})^2}$ and $\phi = \arctan\dfrac{x_2 - x_{2,c}}{x_1 - x_{1,c}}$

Stationary vortex: results

Compute one full rotation, Roe solver, embedded slip wall boundary conditions
$x_{1,c} = 0.5,\ x_{2,c} = 0.5,\ R = 0.4,\ t_{end} = 1,\ \Delta h = \Delta x_1 = \Delta x_2 = 1/N,\ \alpha = R\pi$

No embedded boundary

N	Wave Propagation		Godunov Splitting	
	Error	Order	Error	Order
20	0.0111235		0.0182218	
40	0.0037996	1.55	0.0090662	1.01
80	0.0013388	1.50	0.0046392	0.97
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Marginal shear flow along embedded boundary, $\alpha = R\pi,\ R_G = R,\ U_W = 0$

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80	0.0014193	1.31	0.0001588	0.0038401	0.93	-0.0001036
160	0.0005032	1.50	5.046e-05	0.0018988	1.02	-2.783e-06

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20	0.0120056		0.0079236	0.0144203		0.0020241
40	0.0035074	1.78	0.0011898	0.0073070	0.98	0.0001300
80	0.0014193	1.31	0.0001588	0.0038401	0.93	-0.0001036
160	0.0005032	1.50	5.046e-05	0.0018988	1.02	-2.783e-06

Major shear flow along embedded boundary, $\alpha = R\pi,\ R_G = R/2,\ U_W = 0$

N	Wave Propagation			Godunov Splitting		
	Error	Order	Mass loss	Error	Order	Mass loss
20	0.0423925		0.0423925	0.0271446		0.0271446
40	0.0358735	0.24	0.0358735	0.0242260	0.16	0.0242260
80	0.0212340	0.76	0.0212340	0.0128638	0.91	0.0128638
160	0.0121089	0.81	0.0121089	0.0070906	0.86	0.0070906

Verification: shock reflection

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

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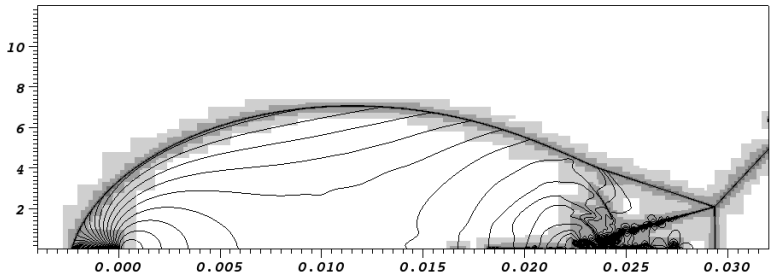

Cartesian base grid 360 $\times$ 160 cells on domain of $36\,\mathrm{mm} \times 16\,\mathrm{mm}$ with up to 3 refinement levels with $r_l = 2, 4, 4$ and $\Delta x_{1,2} = 3.125 \mu m$, $38\,\mathrm{h}$ CPU

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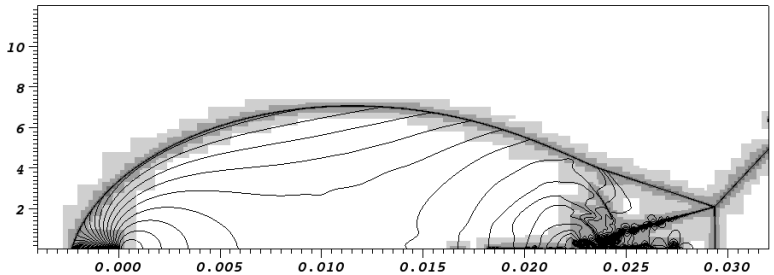
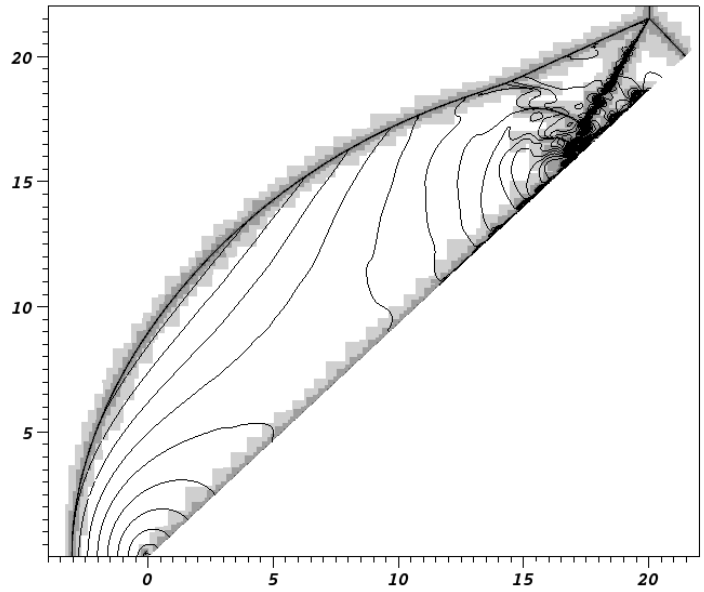


Cartesian base grid 360×160 cells on domain of $36\,\mathrm{mm} \times 16\,\mathrm{mm}$ with up to 3 refinement levels with $r_l = 2, 4, 4$ and $\Delta x_{1,2} = 3.125 \mu m$, 38 h CPU

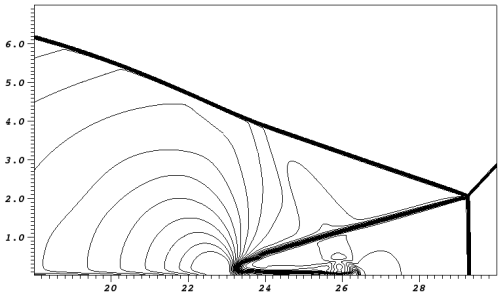


GFM base grid 390×330 cells on domain of $26\,\mathrm{mm} \times 22\,\mathrm{mm}$ with up to 3 refinement levels with $r_l = 2, 4, 4$ and $\Delta x_{e,1,2} = 2.849 \mu m$, 200 h CPU

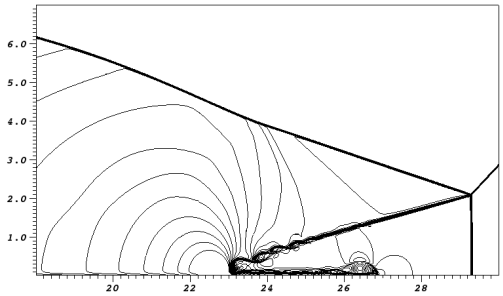
vtf/amroc/clawpack/applications/euler/2d/Ramp

vtf/amroc/clawpack/applications/euler/2d/RampGFM

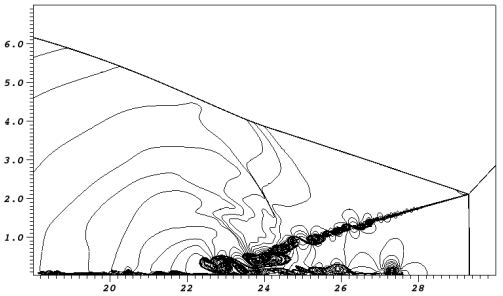
Shock reflection: SAMR solution for Euler equations



$\Delta x = 25\,\mathrm{mm}$

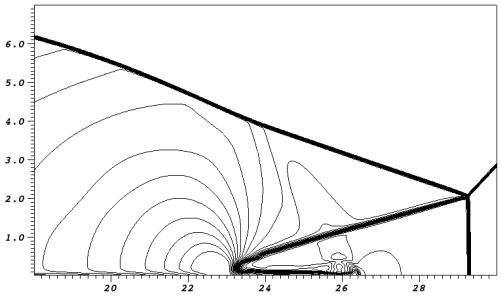


$\Delta x = 12.5\,\mathrm{mm}$



$\Delta x = 3.125\,\mathrm{mm}$

Shock reflection: SAMR solution for Euler equations



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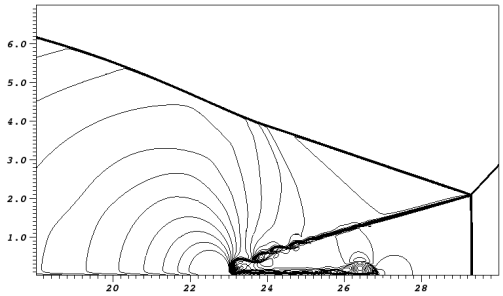

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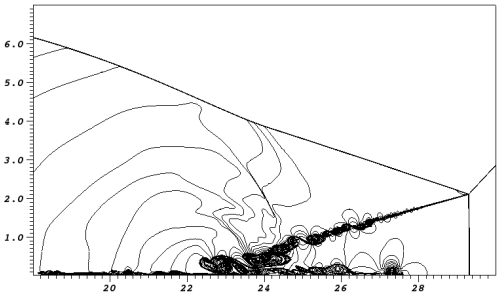

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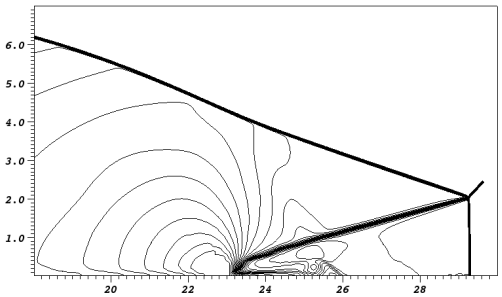
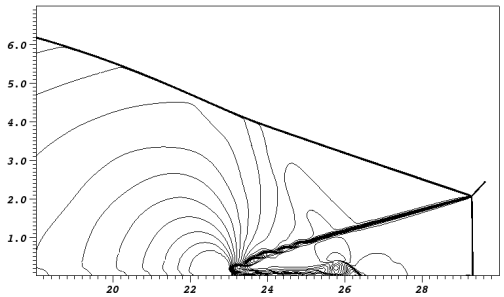
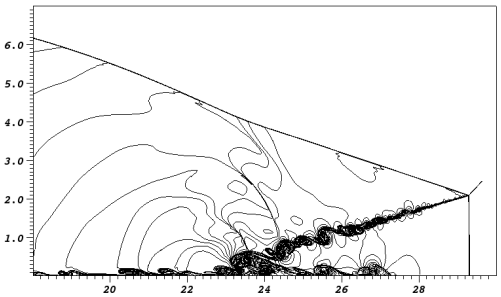


$\Delta x_e = 22.8\,\mathrm{mm}$

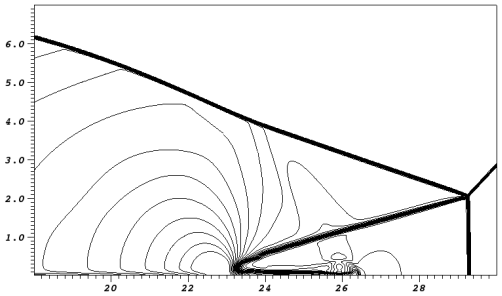


$\Delta x_e = 11.4\,\mathrm{mm}$



$\Delta x_e = 2.849\,\mathrm{mm}$

Shock reflection: SAMR solution for Euler equations



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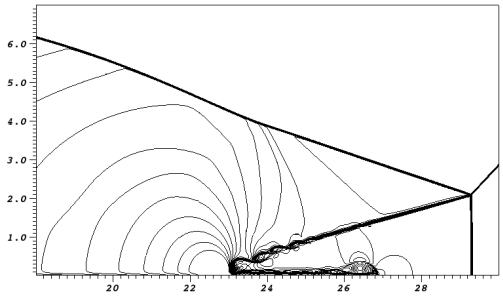

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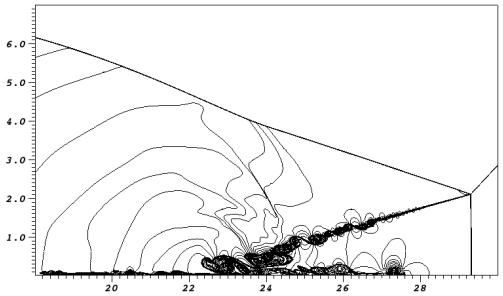

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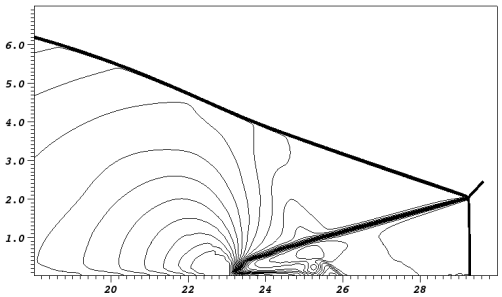

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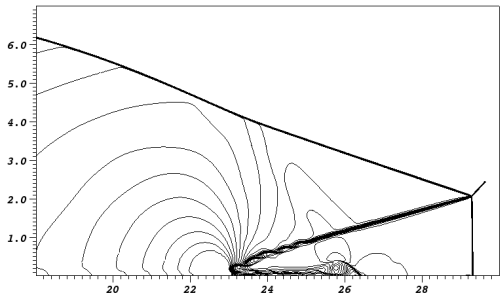

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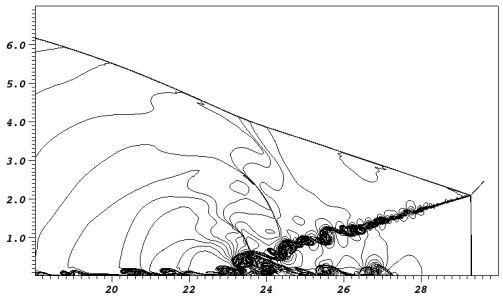

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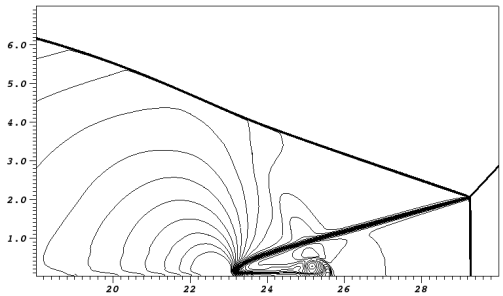
2nd order MUSCL scheme with Van Leer FVS, dimensional splitting



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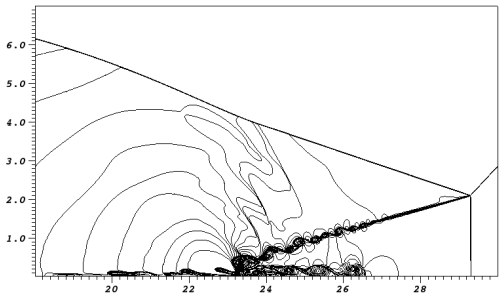

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Shock reflection: solution for Navier-Stokes equations

- No-slip boundary conditions enforced
- Conservative 2nd order centered differences to approximate stress tensor and heat flow

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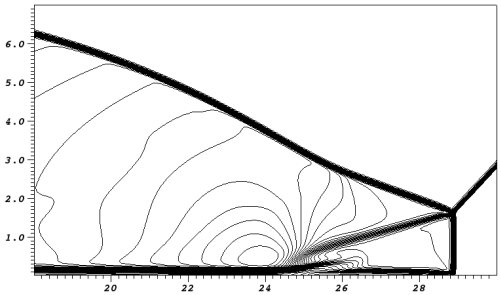
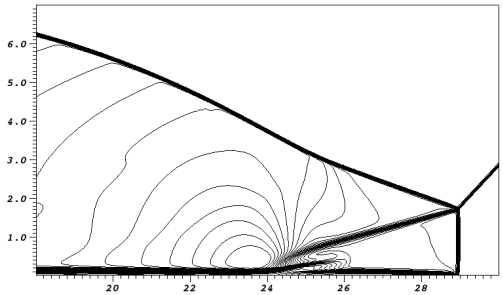
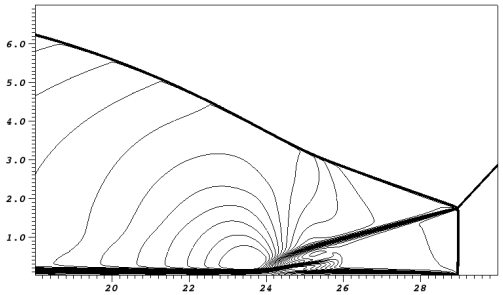


$\Delta x = 50\,\mathrm{mm}$



$\Delta x = 25\,\mathrm{mm}$



$\Delta x = 12.5\,\mathrm{mm}$, SAMR

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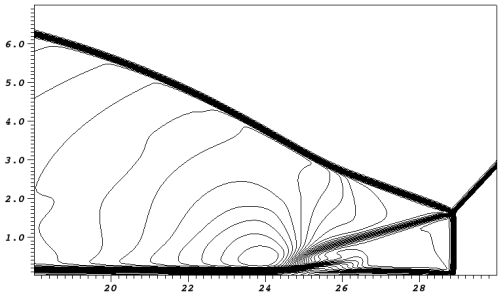

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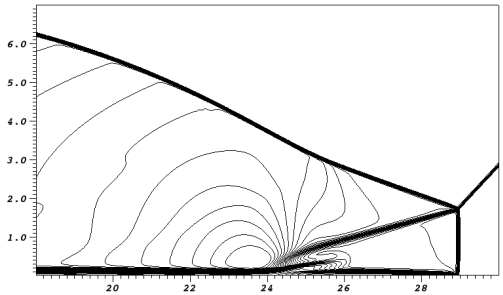

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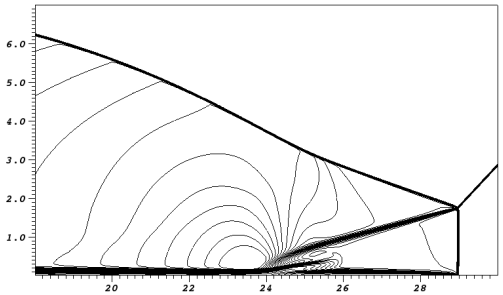

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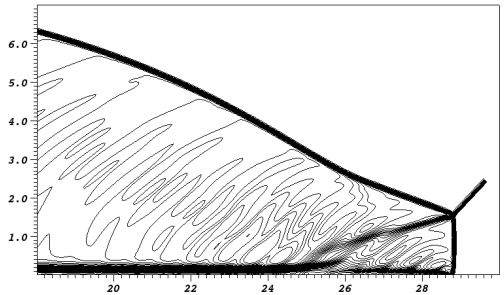
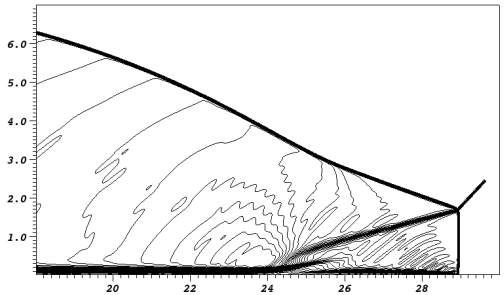
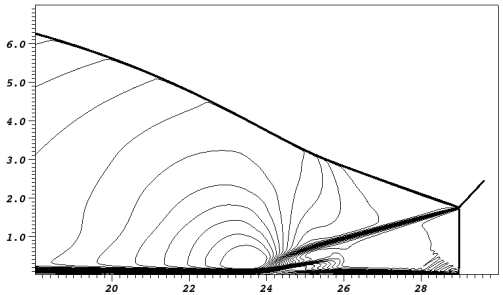


$\Delta x_e = 45.6\,\mathrm{mm}$



$\Delta x_e = 22.8\,\mathrm{mm}$



$\Delta x_e = 11.4\,\mathrm{mm}$, SAMR

Outline

Governing equations for premixed combustion

Euler equations with reaction terms

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial}{\partial x_n}\left(\rho_i u_n\right) = \dot{\omega}_i \ , \quad i = 1, \ldots, K$$

$$\frac{\partial}{\partial t}\left(\rho u_k\right) + \frac{\partial}{\partial x_n}\left(\rho u_k u_n + \delta_{kn} p\right) = 0 \ , \quad k = 1, \ldots, d$$

$$\frac{\partial}{\partial t}\left(\rho E\right) + \frac{\partial}{\partial x_n}\left(u_n(\rho E + p)\right) = 0$$

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

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

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Caloric equation

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

Governing equations for premixed combustion

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

Chemistry

Arrhenius-Kinetics:

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

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- Evalutation of $\dot{\omega}_i$ with automatically generated optimized Fortran-77 functions in the line of Chemkin-II

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- Parsing of mechanisms with Chemkin-II
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Integration of reaction rates: ODE integration in $\mathcal{S}^{(\cdot)}$ for Euler equations with chemical reaction

- Standard implicit or semi-implicit ODE-solver subcycles within each cell
- ρ, e, u_k remain unchanged!

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

Use Newton or bisection method to compute T iteratively.

Hyperbolicity of the homogeneous equations

Consider Jacobian $\mathbf{A}_1(\mathbf{q}) = \partial \mathbf{f}_1(\mathbf{q}) / \partial \mathbf{q}$

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$$\mathbf{A}_1(\mathbf{q}) = \begin{bmatrix} u_1(1-Y_1) & -u_1 Y_1 & \dots & -u_1 Y_1 & Y_1 & 0 & 0 \\ -u_1 Y_2 & u_1(1-Y_2) & \dots & -u_1 Y_2 & & & \\ \vdots & & \ddots & \vdots & \vdots & \vdots & \vdots \\ -u_1 Y_{K-1} & \dots & u_1(1-Y_{K-1}) & -u_1 Y_{K-1} & & & \\ -u_1 Y_K & \dots & -u_1 Y_K & u_1(1-Y_K) & Y_K & 0 & 0 \\ \phi_1 - u_1^2 & & \dots & \phi_K - u_1^2 & (3-\gamma)u_1 & -\tilde{\gamma} u_2 & \tilde{\gamma} \\ -u_1 u_2 & & \dots & -u_1 u_2 & u_2 & u_1 & 0 \\ u_1(\phi_1 - H) & & \dots & u_1(\phi_K - H) & H - \tilde{\gamma} u_1^2 & -\tilde{\gamma} u_1 u_2 & \gamma u_1 \end{bmatrix}$$

with

$$\frac{\partial p}{\partial \rho_i} = \tilde{\gamma}\left(\frac{\mathbf{u}^2}{2} - h_i\right) + \gamma R_i T =: \phi_i \quad \text{und} \quad \frac{\partial p}{\partial \tilde{E}} = \gamma - 1 =: \tilde{\gamma}$$

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Hyperbolicity of the homogeneous equations

Consider Jacobian $\mathbf{A}_1(\mathbf{q}) = \partial \mathbf{f}_1(\mathbf{q})/\partial \mathbf{q}$

$$\mathbf{A}_1(\mathbf{q}) = \begin{bmatrix} u_1(1-Y_1) & -u_1 Y_1 & & \dots & -u_1 Y_1 & Y_1 & 0 & 0 \\ -u_1 Y_2 & u_1(1-Y_2) & & \dots & -u_1 Y_2 & & & \\ \vdots & & \ddots & & \vdots & \vdots & \vdots & \vdots \\ -u_1 Y_{K-1} & \dots & & u_1(1-Y_{K-1}) & -u_1 Y_{K-1} & & & \\ -u_1 Y_K & \dots & & -u_1 Y_K & u_1(1-Y_K) & Y_K & 0 & 0 \\ \phi_1 - u_1^2 & & \dots & & \phi_K - u_1^2 & (3-\gamma)u_1 & -\tilde{\gamma} u_2 & \tilde{\gamma} \\ -u_1 u_2 & & \dots & & -u_1 u_2 & u_2 & u_1 & 0 \\ u_1(\phi_1 - H) & & \dots & & u_1(\phi_K - H) & H - \tilde{\gamma} u_1^2 & -\tilde{\gamma} u_1 u_2 & \gamma u_1 \end{bmatrix}$$

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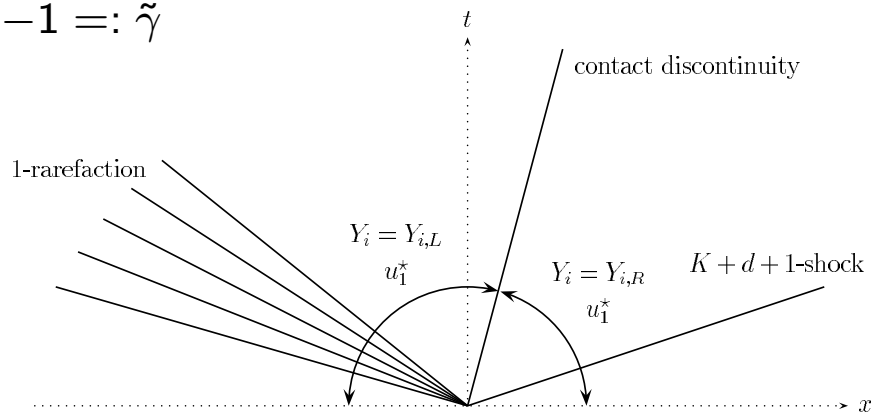

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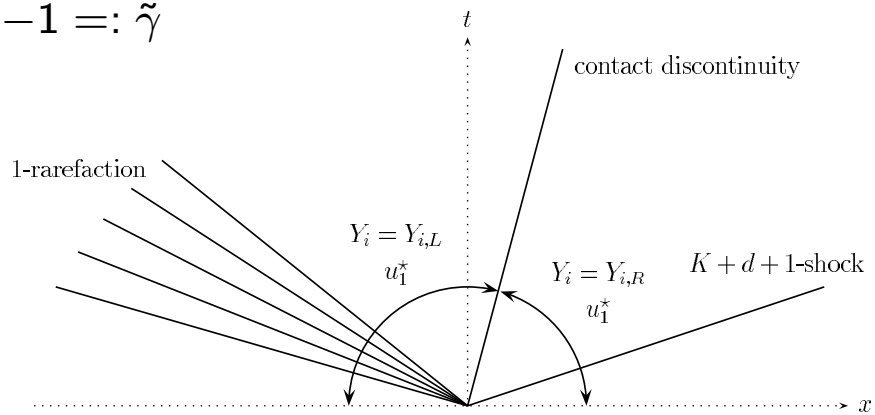

Empirical argument: $\partial_t Y_i + u_1\, \partial_x Y_i = 0$

Steger-Warming flux vector splitting

$$\mathbf{f}(\mathbf{q})^{+} = \mathbf{R}\mathbf{\Lambda}^{+}\mathbf{R}^{-1}\mathbf{q} \qquad \mathbf{f}(\mathbf{q})^{-} = \mathbf{R}\mathbf{\Lambda}^{-}\mathbf{R}^{-1}\mathbf{q}$$

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The corresponding stability condition is

$$C_{CFL}^{SW} := \max_{j\in\mathbb{Z}}(|u_{1,j}| + c_j) \leq 1$$

[Grossmann and Cinella, 1990, Larrouturou and Fezoui, 1989, Liu and Vinokur, 1989]

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vtf/amroc/clawpack/src/1d/equations/euler/rprhok/rp1eurhokswg.f

Van Leer flux vector splitting

$$\mathbf{f}^{\pm}(\mathbf{q}) = \pm\frac{\rho}{4c}(u_1 \pm c)^2 \begin{bmatrix} Y_1 \\ \vdots \\ Y_K \\ u_1 - (u_1 \mp 2c)/\gamma \\ u_2 \\ \vdots \\ u_d \\ H - \zeta(u_1 \mp c)^2 \end{bmatrix} \quad \text{with} \quad H = h + \frac{\mathbf{u}^2}{2}\,,$$

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Roe solver

Roe averages $\hat{\rho}$, $\hat{u}$, $\hat{v}$, $\hat{H}$, $\hat{W}$, $\hat{T}$, $\hat{h}_i$, $\hat{e}_i$, $\hat{Y}_i$

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With matrix of right eigenvectors

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Roe solver - fixes

Mass fraction positivity: Calculate numerical fluxes of partial densities by [Larrouturou, 1991]

$$\mathbf{F}_i^\star(\mathbf{q}_L, \mathbf{q}_R) = \mathbf{F}_\rho(\mathbf{q}_L, \mathbf{q}_R) \cdot \begin{cases} Y_{i,L}\,, & \mathbf{F}_\rho(\mathbf{q}_L, \mathbf{q}_R) > 0\,, \\ Y_{i,R}\,, & \mathbf{F}_\rho(\mathbf{q}_L, \mathbf{q}_R) < 0\,. \end{cases}$$

to ensure positivity of Y_i.

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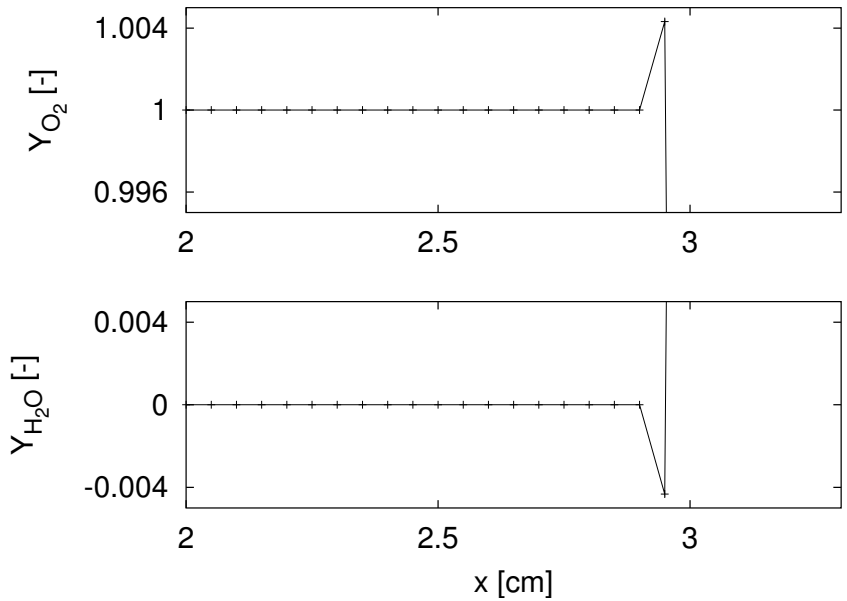
Example: Mass fraction for a typical Riemann problem after 1 time step with the Roe solver



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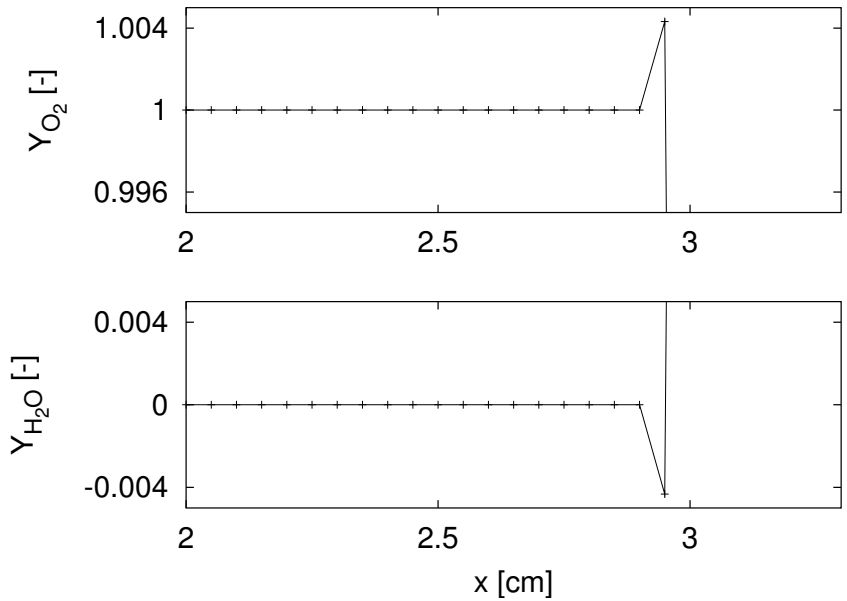

Further: Switch from Roe to HLL scheme near vacuum state to avoid unphysical values.

Roe solver - entropy and carbuncle fix

Entropy corrections

Roe solver - entropy and carbuncle fix

Entropy corrections [Harten, 1983]

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

$\eta = \frac{1}{2} \max_\iota \left\{ |s_\iota(\mathbf{q}_R) - s_\iota(\mathbf{q}_L)| \right\}$

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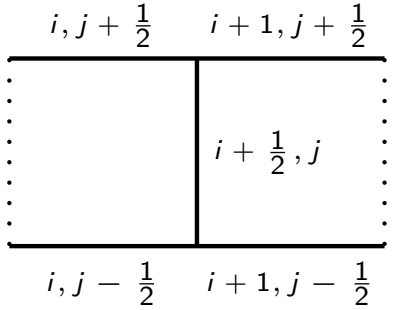
2D modification of entropy correction (here named EF 3) [Sanders et al., 1998]:



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

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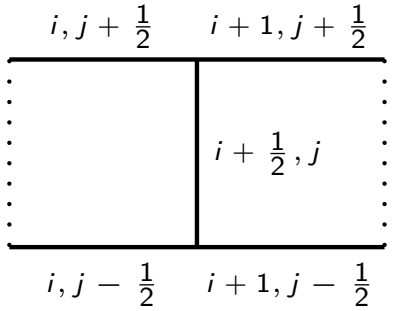
2D modification of entropy correction (here named EF 3) [Sanders et al., 1998]:



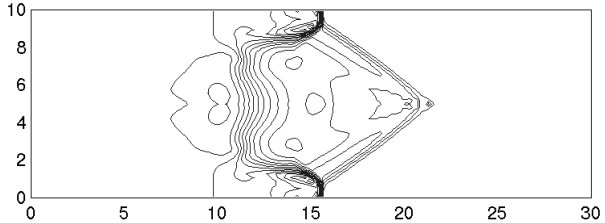
$$\tilde{\eta}_{i+1/2,j} = \max \left\{ \eta_{i+1/2,j}, \eta_{i,j-1/2}, \ \eta_{i,j+1/2}, \eta_{i+1,j-1/2}, \eta_{i+1,j+1/2} \right\}$$

Carbuncle phenomenon

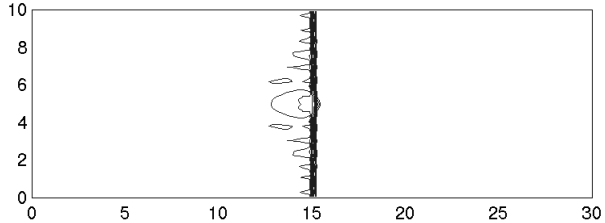
- [Quirk, 1994b]
- Test from [Deiterding, 2003]

clawpack/applications/euler_znd/ 2d/-Carbuncle

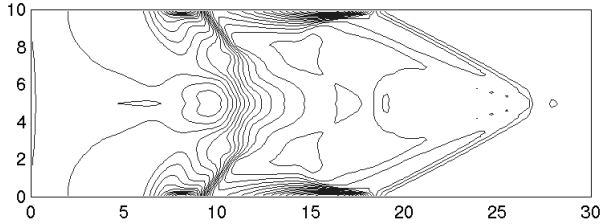
Roe + EF 1.



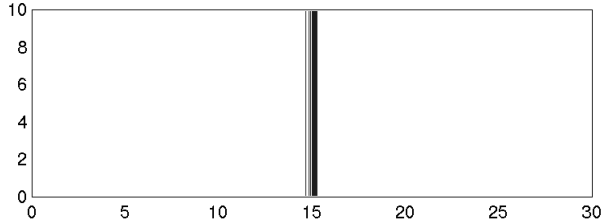
Exact Riemann solver



Roe + EF 2.



SW FVS, VL FVS, HLL, Roe + EF 3



Riemann solver for combustion

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

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

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

(S5) Use $\Delta\mathbf{q} = \mathbf{q}_R - \mathbf{q}_L$ and Δp to compute the wave strengths a_m.

(S6) Calculate $\mathcal{W}_1 = a_1 \hat{\mathbf{r}}_1$, $\mathcal{W}_2 = \displaystyle\sum_{\iota=2}^{K+d} a_\iota \hat{\mathbf{r}}_\iota$, $\mathcal{W}_3 = a_{K+d+1} \hat{\mathbf{r}}_{K+d+1}$.

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vtf/amroc/clawpack/src/1d/equations/euler/rprhok/rp1eurhokefix.f
vtf/amroc/clawpack/src/1d/equations/euler/rprhok/rp1eurhokefixg.f

ZND Detonation Model with Simplified Chemistry

Assume a stationary 1D detonation with irreversible reaction

$$A \longrightarrow B$$

with energy release $q_0 = -\Delta h^0$ and $k^f(T) = K \exp(-E_A/\mathcal{R}T)$.

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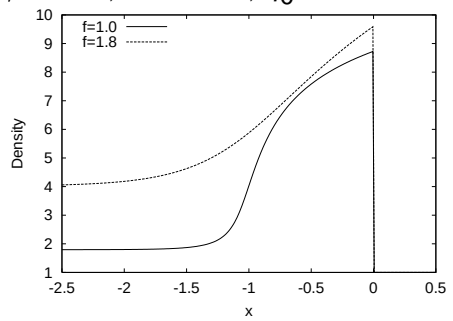
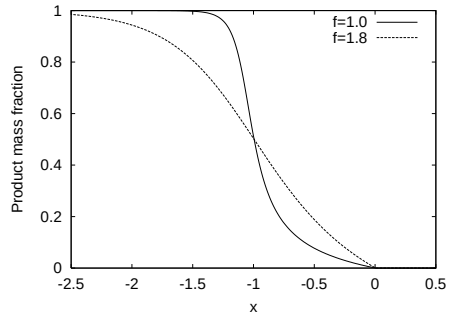
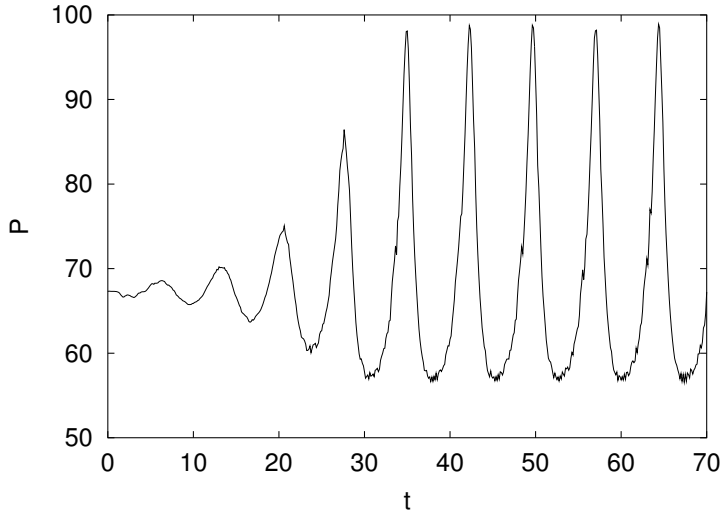




Unstable ZND Detonation

$\gamma = 1.2,\ E^+ = 50,\ q_0 = 50,\ f = 1.6,\ CFL = 0.9$

quasi-stationary



moving

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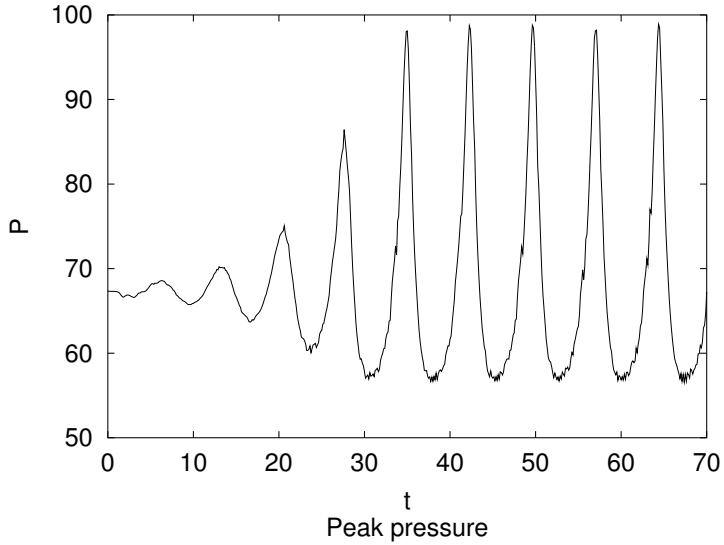
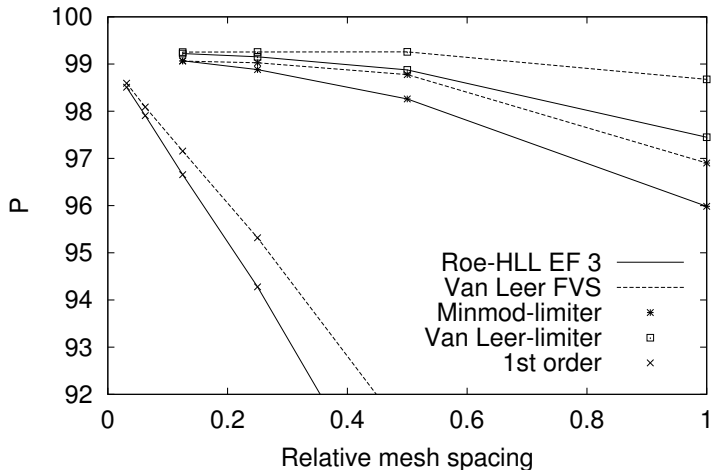


moving



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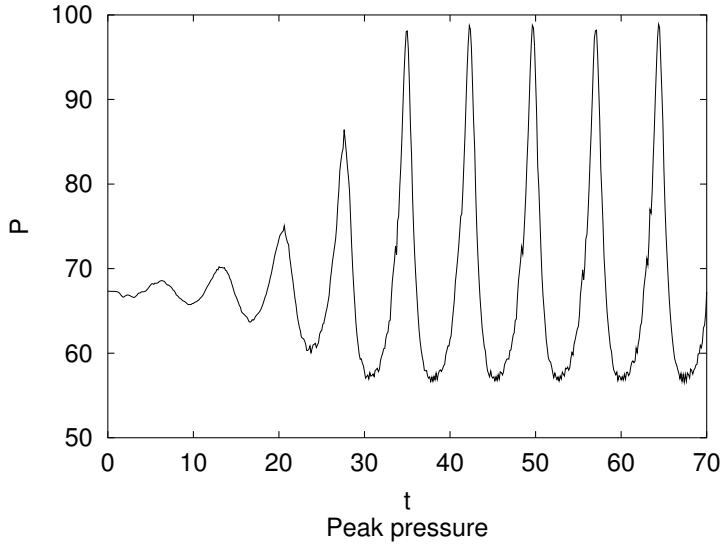

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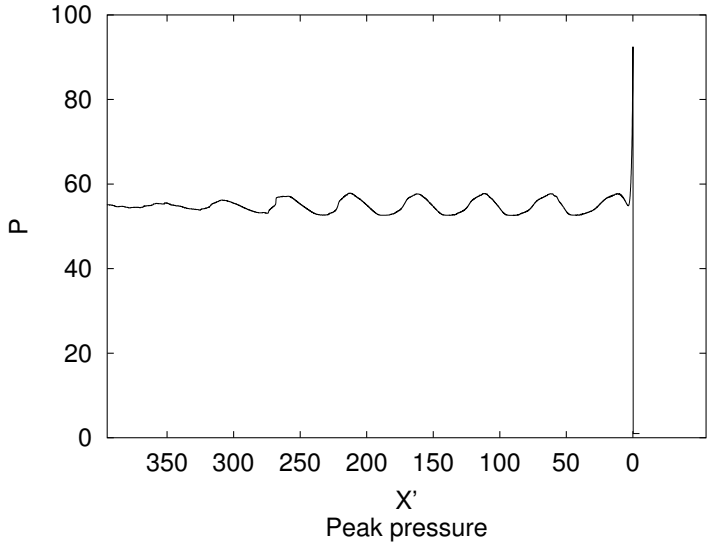
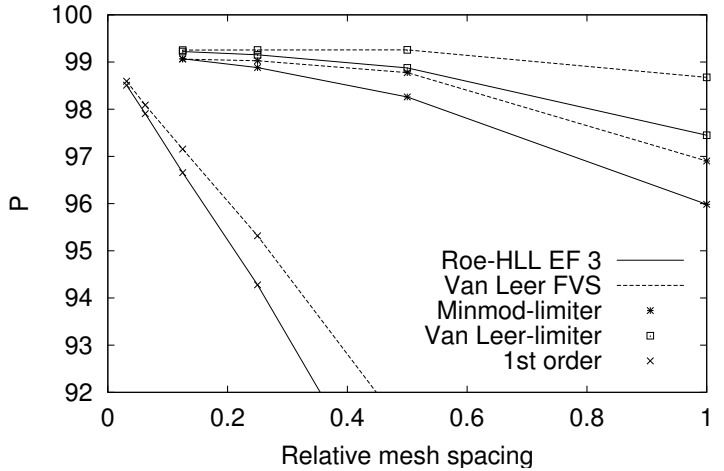
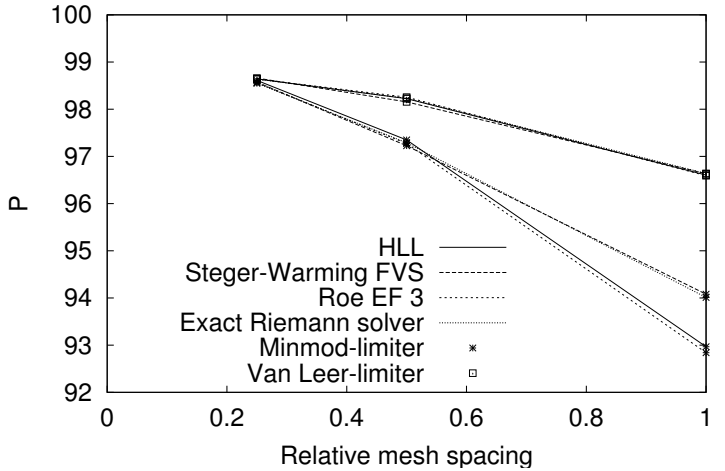






vtf/amroc/clawpack/applications/euler_znd/1d/StatDet

Comparison of FV Schemes: MUSCL, Van Albada-limiter

$\gamma = 1.2$, $E = 50$, $q_0 = 50$, $f = 3.0$, $40\,\mathrm{Pts}/L_{1/2}$

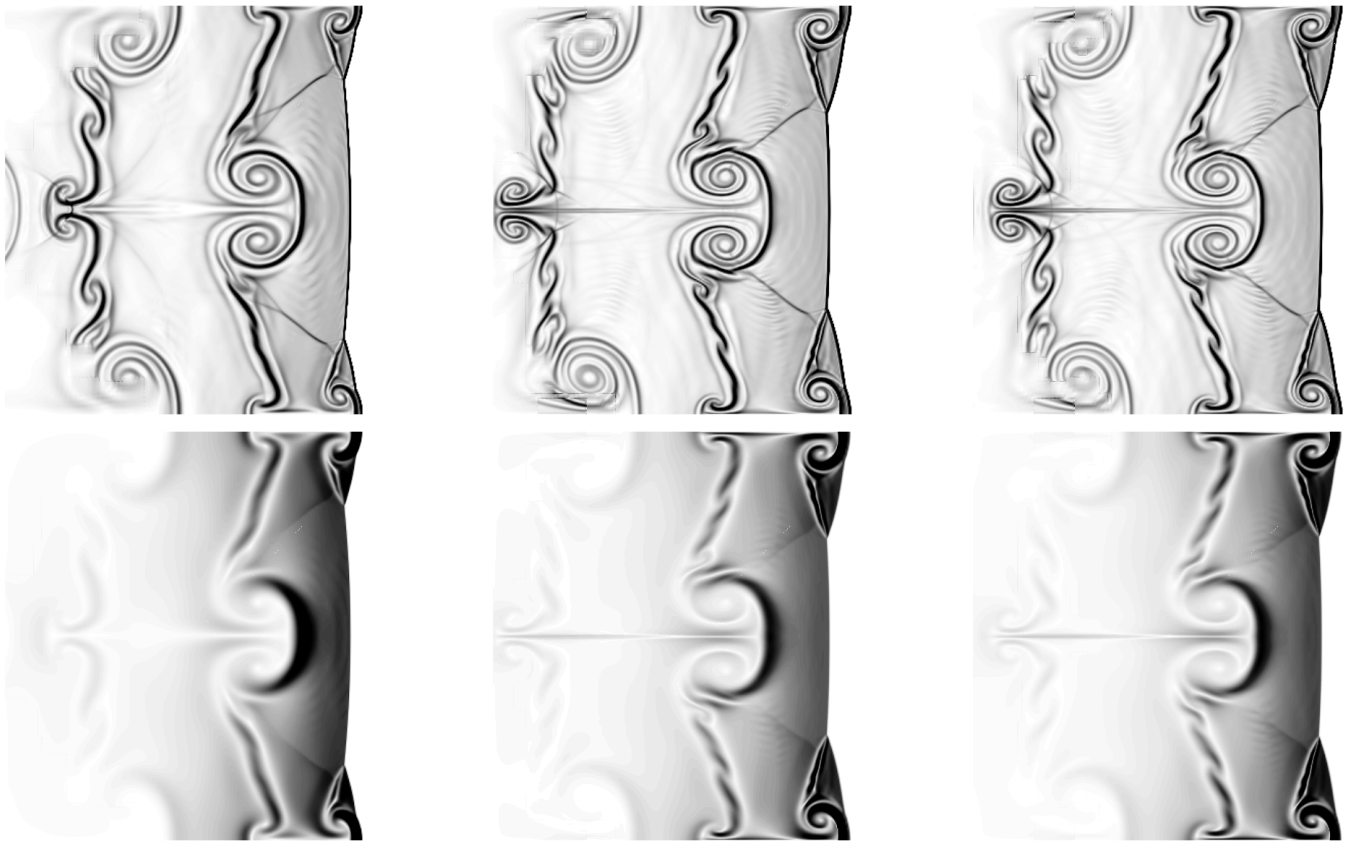
Van Leer FVS, DimSplit | Roe-HLL EF 3, DimSplit | Roe-HLL EF 3, WaveProp

Comparison of FV Schemes - II

$\gamma = 1.2,\ E = 10,\ q_0 = 50,\ f = 1.2,\ 40\,\mathrm{Pts}/L_{1/2}$

T

Z



Van Leer FVS, DimSplit

Roe-HLL EF $3^\star$-H, DimSplit

Roe-HLL EF $3^\star$-H, WaveProp

vtf/amroc/clawpack/applications/euler_znd/2d/StatDet

Detonations - motivation for SAMR

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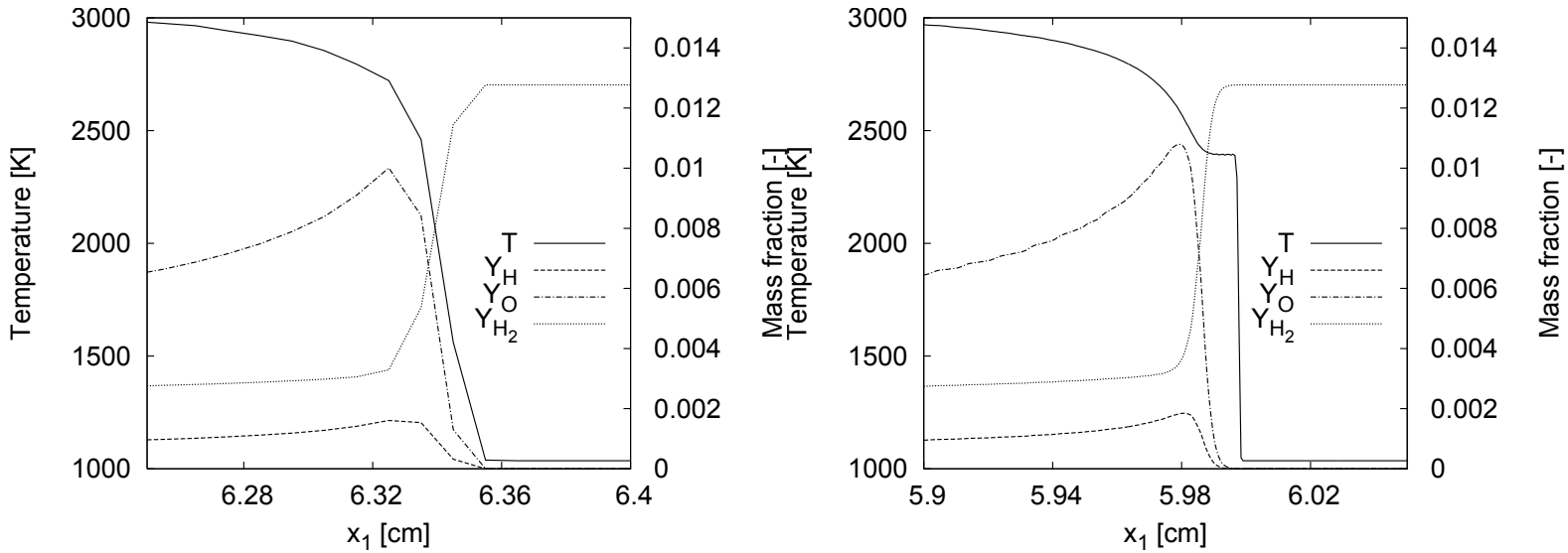

Approximation of $H_2 : O_2$ detonation at $\sim 1.5\,\mathrm{Pts}/l_{ig}$ (left) and $\sim 24\,\mathrm{Pts}/l_{ig}$ (right)

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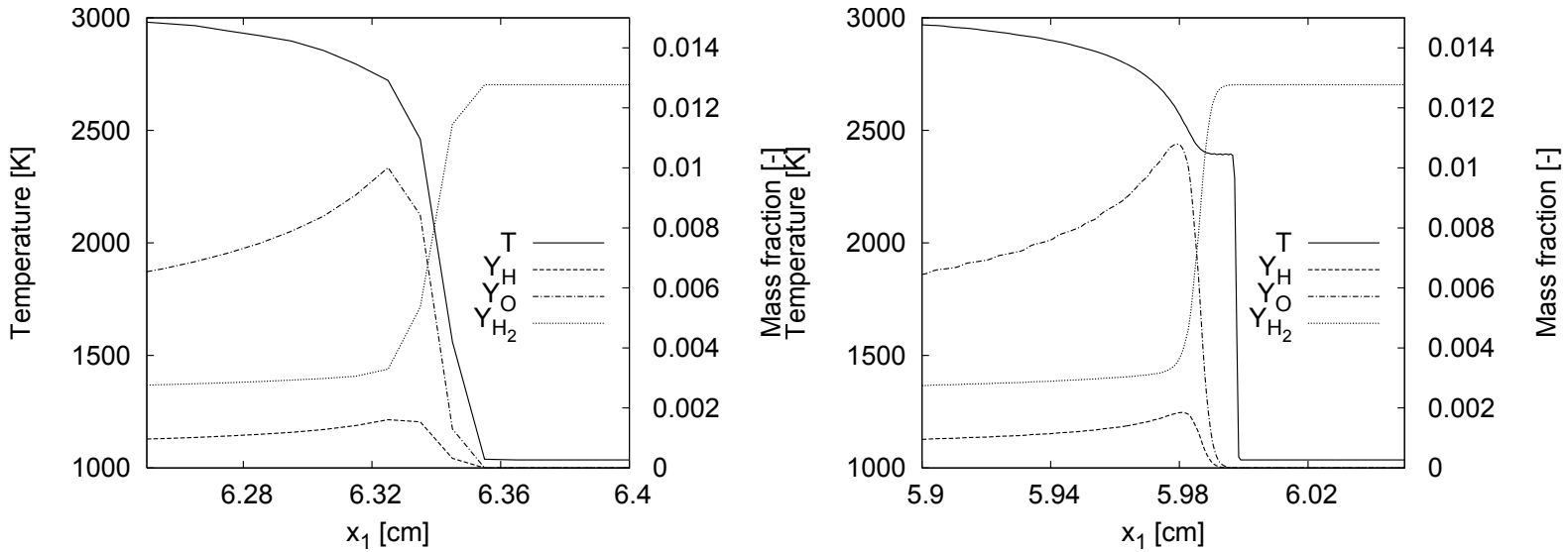
- Uniform grids for typical geometries: $> 10^7\,\mathrm{Pts}$ in 2D, $> 10^9\,\mathrm{Pts}$ in 3D $\longrightarrow$ Self-adaptive finite volume method (AMR)



Approximation of $H_2 : O_2$ detonation at $\sim 1.5\,\mathrm{Pts}/l_{ig}$ (left) and $\sim 24\,\mathrm{Pts}/l_{ig}$ (right)

Detonation ignition in a shock tube

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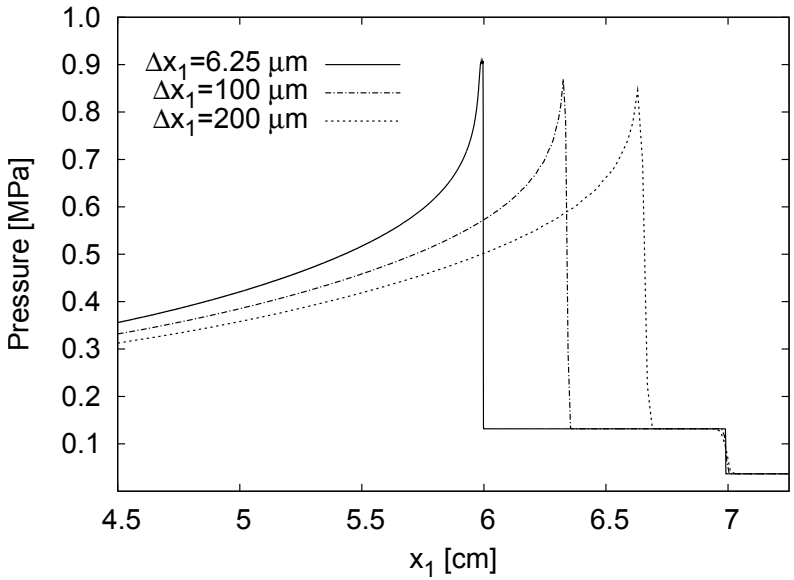

Left: Comparison of pressure distribution $t = 170\,\mu\mathrm{s}$ after shock reflection.

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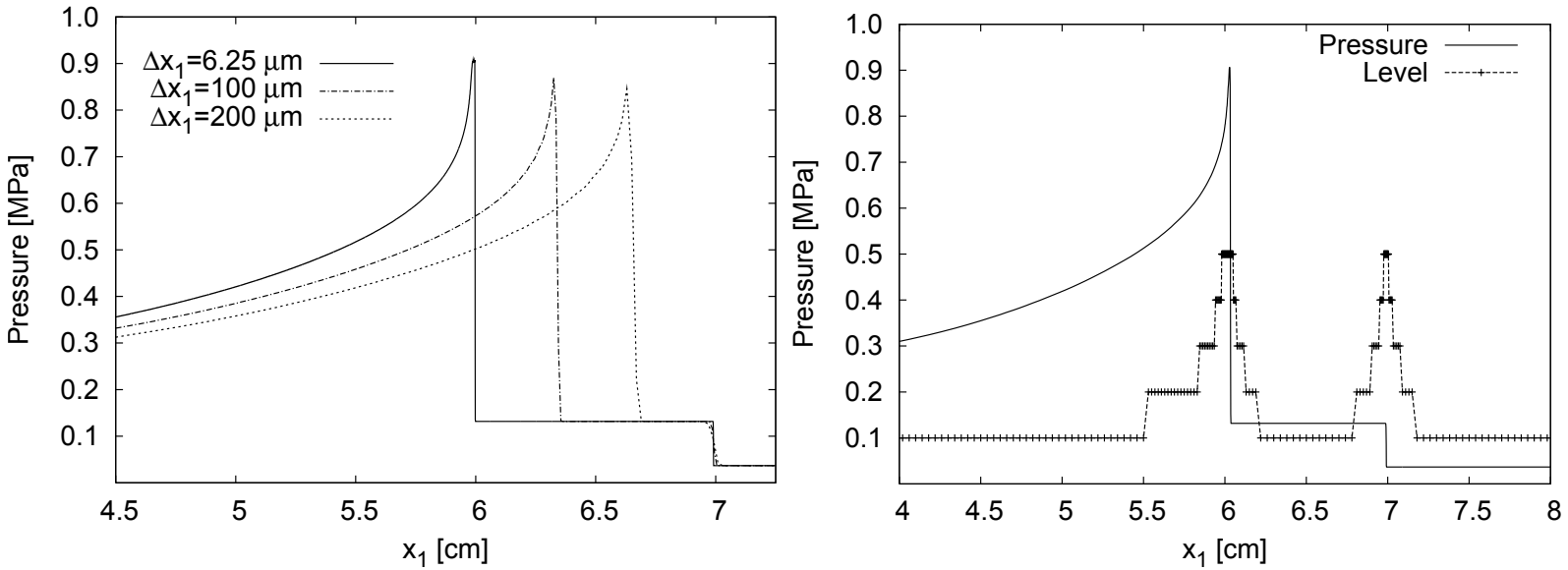
- Reflected shock is captured correctly by FV scheme, detonation is resolution dependent
- Fine mesh necessary in the induction zone at the head of the detonation



Left: Comparison of pressure distribution $t = 170\,\mu s$ after shock reflection.Right: Domains of refinement levels

Non-equilibrium mechanism for hydrogen-oxgen combustion

				A [cm, mol, s]	β	E_{act} [cal mol^{-1}]
1.	$H + O_2$	$\longrightarrow$	$O + OH$	1.86×10^{14}	0.00	16790.
2.	$O + OH$	$\longrightarrow$	$H + O_2$	1.48×10^{13}	0.00	680.
3.	$H_2 + O$	$\longrightarrow$	$H + OH$	1.82×10^{10}	1.00	8900.
4.	$H + OH$	$\longrightarrow$	$H_2 + O$	8.32×10^{09}	1.00	6950.
5.	$H_2O + O$	$\longrightarrow$	$OH + OH$	3.39×10^{13}	0.00	18350.
6.	$OH + OH$	$\longrightarrow$	$H_2O + O$	3.16×10^{12}	0.00	1100.
7.	$H_2O + H$	$\longrightarrow$	$H_2 + OH$	9.55×10^{13}	0.00	20300.
8.	$H_2 + OH$	$\longrightarrow$	$H_2O + H$	2.19×10^{13}	0.00	5150.
9.	$H_2O_2 + OH$	$\longrightarrow$	$H_2O + HO_2$	1.00×10^{13}	0.00	1800.
10.	$H_2O + HO_2$	$\longrightarrow$	$H_2O_2 + OH$	2.82×10^{13}	0.00	32790.
...	...		...	...	...	...
30.	$OH + M$	$\longrightarrow$	$O + H + M$	7.94×10^{19}	-1.00	103720.
31.	$O_2 + M$	$\longrightarrow$	$O + O + M$	5.13×10^{15}	0.00	115000.
32.	$O + O + M$	$\longrightarrow$	$O_2 + M$	4.68×10^{15}	-0.28	0.
33.	$H_2 + M$	$\longrightarrow$	$H + H + M$	2.19×10^{14}	0.00	96000.
34.	$H + H + M$	$\longrightarrow$	$H_2 + M$	3.02×10^{15}	0.00	0.

Third body efficiencies: $f(O_2) = 0.40$, $f(H_2O) = 6.50$

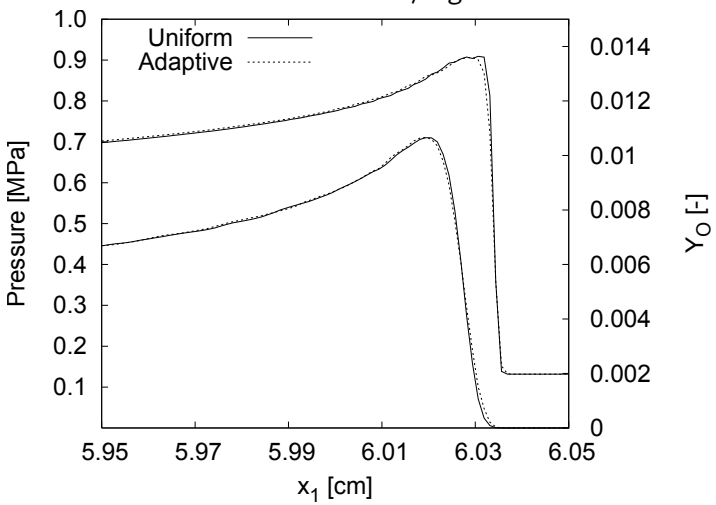
[Westbrook, 1982]

Detonation ignition in 1d - adaptive vs. uniform

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

	Uniform			Adaptive			
$\Delta x_1[\mu\mathrm{m}]$	Cells	$t_m[\mu\mathrm{s}]$	Time [s]	l_{max}	r_l	$t_m[\mu\mathrm{s}]$	Time [s]
400	300	166.1	31				
200	600	172.6	90	2	2	172.6	99
100	1200	175.5	277	3	2,2	175.8	167
50	2400	176.9	858	4	2,2,2	177.3	287
25	4800	177.8	2713	4	2,2,4	177.9	393
12.5	9600	178.3	9472	5	2,2,2,4	178.3	696
6.25	19200	178.6	35712	5	2,2,4,4	178.6	1370

$\sim 12\,\mathrm{Pts}/l_{ig}$



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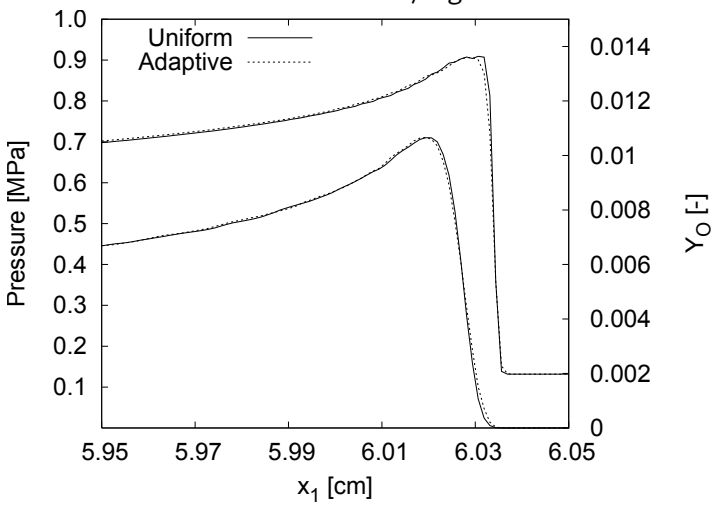

Refinement criteria:

Y_i	$S_{Y_i} \cdot 10^{-4}$	$\eta^r_{Y_i} \cdot 10^{-3}$
O_2	10.0	2.0
H_2O	7.8	8.0
H	0.16	5.0
O	1.0	5.0
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H_2	1.3	2.0

$\epsilon_\rho = 0.07\,\mathrm{kg\,m^{-3}}$, $\epsilon_p = 50\,\mathrm{kPa}$

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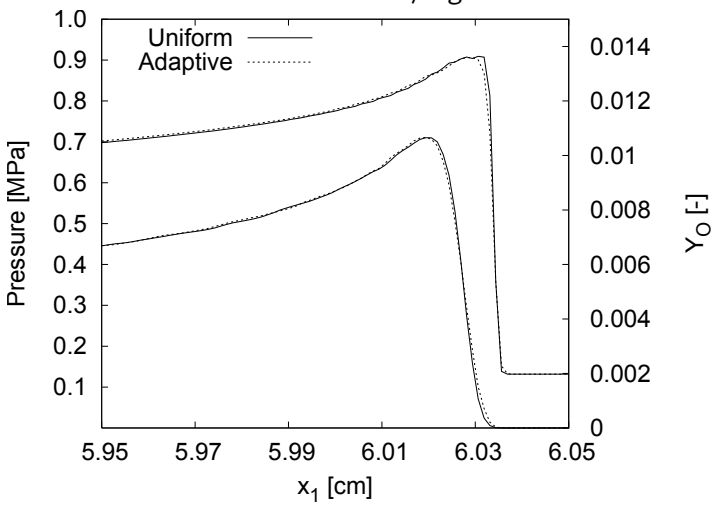

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vtf/amroc/clawpack/applications/euler_chem/1d/ReflecDet

Shock-induced combustion around a sphere

- Spherical projectile of radius $1.5\,\mathrm{mm}$ travels with constant velocity $v_l = 2170.6\,\mathrm{m/s}$ through $\mathrm{H_2} : \mathrm{O_2} : \mathrm{Ar}$ mixture (molar ratios 2:1:7) at $6.67\,\mathrm{kPa}$ and $T = 298\,\mathrm{K}$
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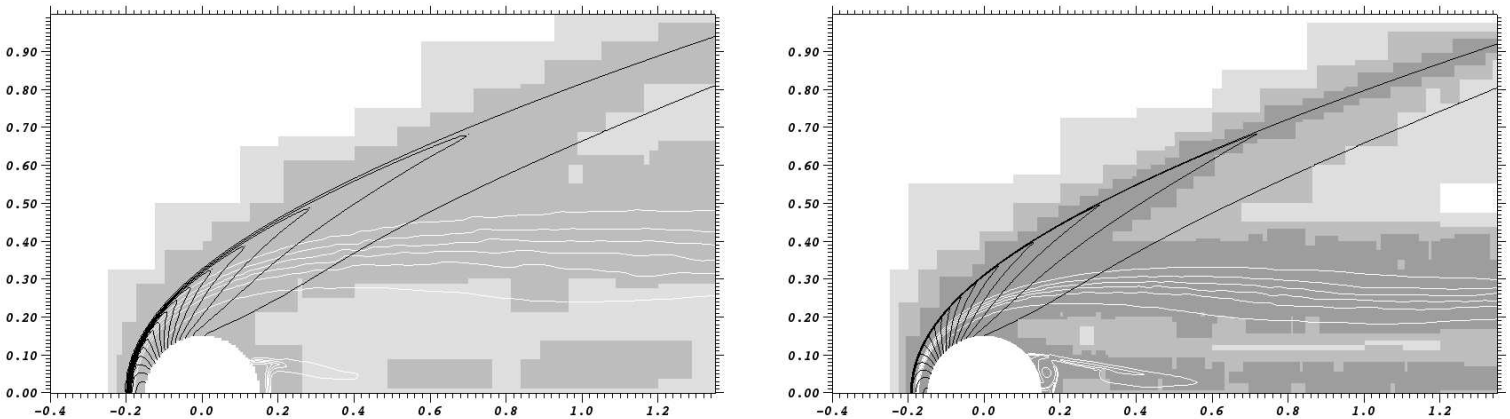
- Cylindrical symmetric simulation on AMR base mesh of 70×40 cells
- Comparison of 3-level computation with refinement factors 2,2 ($\sim 5\,\mathrm{Pts}/l_{ig}$) and a 4-level computation with refinement factors 2,2,4 ($\sim 19\,\mathrm{Pts}/l_{ig}$) at $t = 350\,\mu\mathrm{s}$



Iso-contours of p (black) and Y_{H_2} (white) on refinement domains for 3-level (left) and 4-level computation (right)

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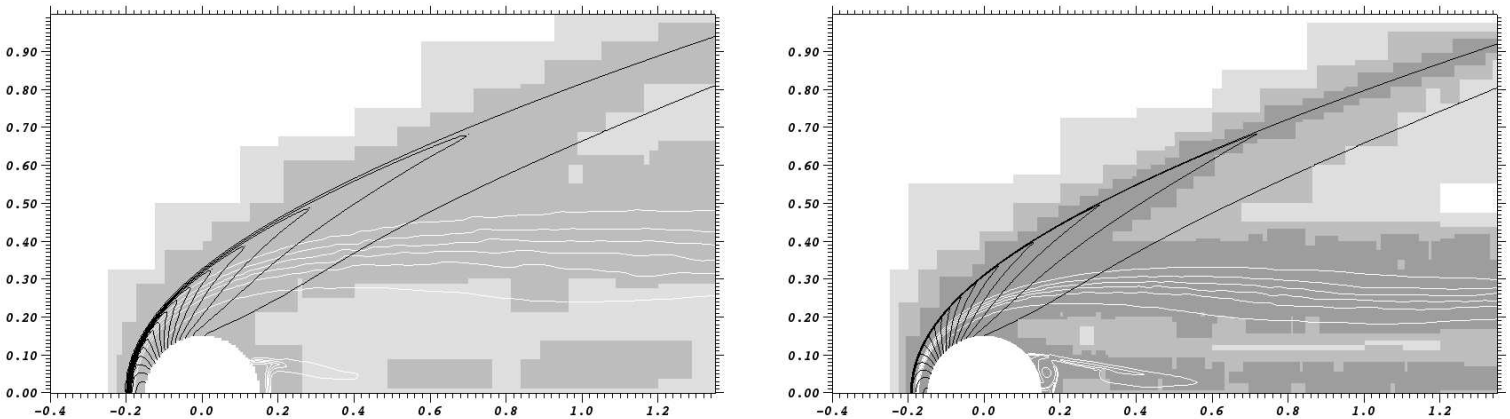
- Higher resolved computation captures combustion zone visibly better and at slightly different position (see below)



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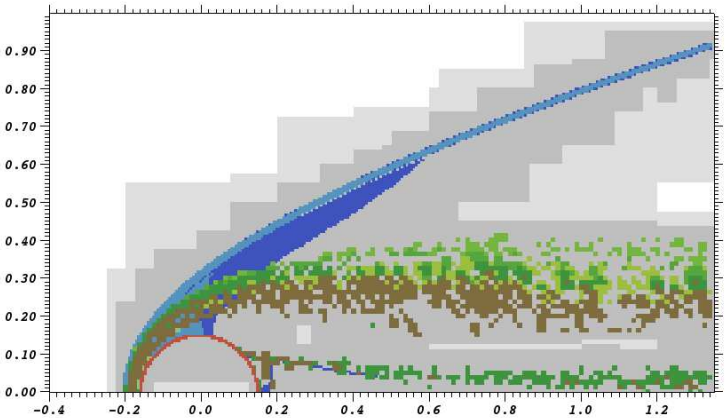
vtf/amroc/clawpack/applications/euler_chem/2d/Sphere

Combustion around a sphere - adaptation

Refinement indicators on $l = 2$ at $t = 350\,\mu\mathrm{s}$. Blue: ϵ_ρ, light blue: ϵ_p, green shades: $\eta^r_{Y_i}$, red: embedded boundary



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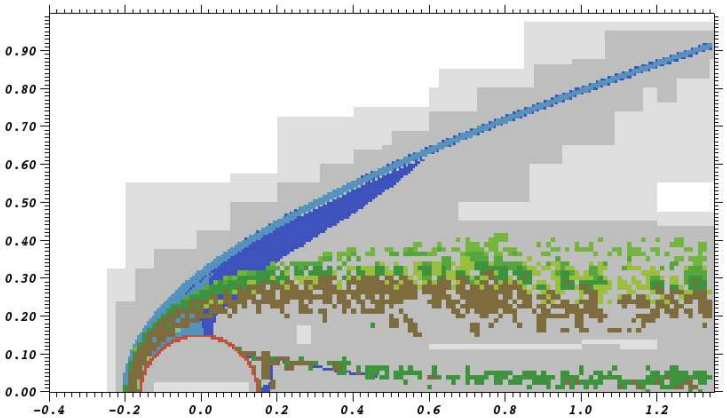

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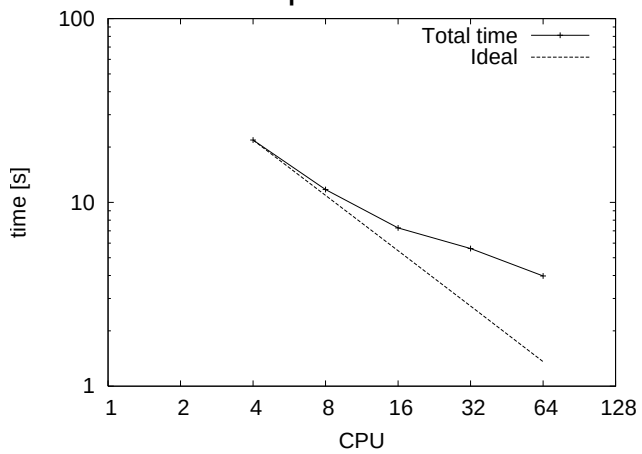
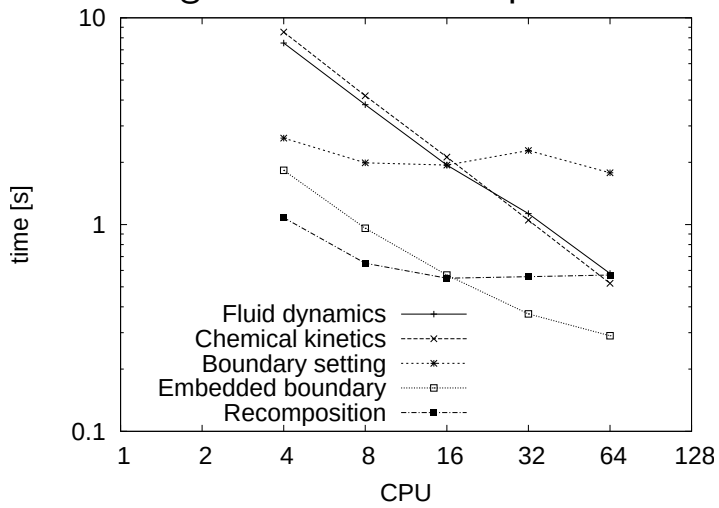
Parallel performance



Scaling of different code portions



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