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DNS with a hybrid method 000 Summary 00

Recent examples of compressible aerodynamics simulation with the AMROC framework

Ralf Deiterding

Aerodynamics and Flight Mechanics Research Group University of Southampton Boldrewood Campus Southampton SO17 1BJ, UK Email: r.deiterding@soton.ac.uk

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Outline

Adaptive Cartesian finite volume methods

Block-structured AMR with complex boundaries Parallelization approach

Train-tunnel aerodynamics

Validation Passing trains in open space and in double-track tunnel

Two-temperature solver for high-enthalpy flows

Thermodynamic model Cartesian results Mapped mesh treatment Non-cartesian results and comparison

DNS with a hybrid method

Higher-order hybrid methods

Summary

Conclusions

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Collaboration with

- Train aerodynamics
 - Jose M. Garro Fernandez (now PhD student)
- High-enthalpy solver for AMROC
 - Chay Atkins (PhD student, Dstl)
- DNS for hypersonic boundary layers
 - Adriano Cerminara (now University of Wolverhampton)
 - Neil Sandham

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Block-structured AMR with complex boundaries

Block-structured adaptive mesh refinement (SAMR)

For simplicity $\partial_t \mathbf{q}(x, y, t) + \partial_x \mathbf{f}(\mathbf{q}(x, y, t)) + \partial_y \mathbf{g}(\mathbf{q}(x, y, t)) = 0$

Refined blocks overlay coarser ones



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- Refined blocks overlay coarser ones
- Refinement in space and time by factor r_l [Berger and Colella, 1988]
- Block (aka patch) based data structures
- + Numerical scheme

$$\begin{split} \mathbf{Q}_{jk}^{n+1} &= \mathbf{Q}_{jk}^{n} - \frac{\Delta t}{\Delta x} \left[\mathbf{F}_{j+\frac{1}{2},k} - \mathbf{F}_{j-\frac{1}{2},k} \right] \\ &- \frac{\Delta t}{\Delta y} \left[\mathbf{G}_{j,k+\frac{1}{2}} - \mathbf{G}_{j,k-\frac{1}{2}} \right] \end{split}$$

only for single patch necessary



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only for single patch necessary

- + Efficient cache-reuse / vectorization possible
- Cluster-algorithm necessary
- Papers: [Deiterding, 2011a, Deiterding et al., 2009b, Deiterding et al., 2007]



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Block-structured AMR with complex boundaries

Level transfer / setting of ghost cells

$$\hat{\mathbf{Q}}_{jk}^{\prime} := rac{1}{\left(r_{l+1}
ight)^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} \mathbf{Q}_{\nu+\kappa,w+\iota}^{\prime+1}$$



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Block-structured AMR with complex boundaries

Level transfer / setting of ghost cells

Conservative averaging (restriction):

$$\hat{\mathbf{Q}}'_{jk} := rac{1}{\left(r_{l+1}
ight)^2} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} \mathbf{Q}^{l+1}_{\nu+\kappa,w+\iota}$$

Bilinear interpolation (prolongation):

$$egin{aligned} \check{\mathbf{Q}}_{vw}^{\prime+1} &:= (1-f_1)(1-f_2)\,\mathbf{Q}_{j-1,k-1}^{\prime} \ &+ f_1(1-f_2)\,\mathbf{Q}_{j,k-1}^{\prime} + \ &(1-f_1)f_2\,\mathbf{Q}_{j-1,k}^{\prime} + f_1f_2\,\mathbf{Q}_{jk}^{\prime} \end{aligned}$$



For boundary conditions: linear time interpolation

$$\tilde{\mathbf{Q}}^{l+1}(t+\kappa\Delta t_{l+1}) := \left(1-\frac{\kappa}{r_{l+1}}\right)\,\check{\mathbf{Q}}^{l+1}(t) + \frac{\kappa}{r_{l+1}}\,\check{\mathbf{Q}}^{l+1}(t+\Delta t_l)\quad\text{for }\kappa=0,\ldots r_{l+1}$$

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Block-structured AMR with complex boundaries

Recursive integration order

• Space-time interpolation of coarse data to set I_l^s , l > 0



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Block-structured AMR with complex boundaries

Recursive integration order

- Space-time interpolation of coarse data to set I^s_l, l > 0
- Regridding:
 - Creation of new grids, copy existing cells on level l > 0
 - Spatial interpolation to initialize new cells on level I > 0



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Block-structured AMR with complex boundaries

Conservative flux correction

Example: Cell j, k

$$\begin{split} \check{\mathbf{Q}}_{jk}^{\prime}(t+\Delta t_{l}) &= \mathbf{Q}_{jk}^{\prime}(t) - \frac{\Delta t_{l}}{\Delta x_{1,l}} \left(\mathbf{F}_{j+\frac{1}{2},k}^{\prime} - \frac{1}{r_{l+1}^{2}} \sum_{\kappa=0}^{r_{l+1}-1} \sum_{\iota=0}^{r_{l+1}-1} \mathbf{F}_{\nu+\frac{1}{2},\nu+\iota}^{\prime+1}(t+\kappa\Delta t_{l+1}) \right) \\ &- \frac{\Delta t_{l}}{\Delta x_{2,l}} \left(\mathbf{G}_{j,k+\frac{1}{2}}^{\prime} - \mathbf{G}_{j,k-\frac{1}{2}}^{\prime} \right) \end{split}$$

Correction pass:



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Correction pass:

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



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Correction pass:

1. $\delta \mathbf{F}_{j-\frac{1}{2},k}^{l+1} := -\mathbf{F}_{j-\frac{1}{2},k}^{l}$ 2. $\delta \mathbf{F}_{j-\frac{1}{2},k}^{l+1} := \delta \mathbf{F}_{j-\frac{1}{2},k}^{l+1} + \frac{1}{r_{l+1}^2} \sum_{\iota=0}^{r_{l+1}-1} \mathbf{F}_{\nu+\frac{1}{2},\nu+\iota}^{l+1}(t+\kappa\Delta t_{l+1})$ 3. $\check{\mathbf{Q}}_{jk}^{l}(t+\Delta t_{l}) := \mathbf{Q}_{jk}^{l}(t+\Delta t_{l}) + \frac{\Delta t_{l}}{\Delta x_{1,l}} \delta \mathbf{F}_{j-\frac{1}{2},k}^{l+1}$



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Block-structured AMR with complex boundaries

Level-set method for boundary embedding



- Implicit boundary representation via distance function φ, normal n = ∇φ/|∇φ|
- Complex boundary moving with local velocity w, treat interface as moving rigid wall [Deiterding et al., 2007]
- Construction of values in embedded boundary cells by interpolation / extrapolation [Deiterding, 2009, Deiterding, 2011a]
- Creation of level set from triangulated surface data with closest-point-transform (CPT) algorithm [Mauch, 2003, Deiterding et al., 2006]

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Interpolate / constant value extrapolate values at

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

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

Velocity in ghost cells No-slip: $\mathbf{u}' = 2\mathbf{w} - \mathbf{u}$ Slip:

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

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arallelization approach				

Parallelization

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

$$\mathcal{W}(\Omega) = \sum_{l=0}^{l_{\max}} \left[\mathcal{N}_l(G_l \cap \Omega) \prod_{\kappa=0}^l r_{\kappa}
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Adaptive Cartesian methods 000000000 Parallelization approach

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Parallelization

Rigorous domain decomposition

- Data of all levels resides on same node
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[Deiterding, 2005, Deiterding, 2011a]



AMROC framework and most important patch solvers

- Implements described algorithms and facilitates easy exchange of the block-based numerical scheme
- Shock-induced combustion with detailed chemistry: [Deiterding, 2003, Deiterding and Bader, 2005, Deiterding, 2011b. Cai et al., 2016, Cai et al., 2018]
- Hybrid WENO methods for LES and DNS: [Pantano et al., 2007, Lombardini and Deiterding, 2010, Ziegler et al., 2011, Cerminara et al., 2018]
- Lattice Boltzmann method for LES: [Fragner and Deiterding, 2016, Feldhusen et al., 2016, Deiterding and Wood, 2016]
- FSI deformation from water hammer: [Cirak et al., 2007, Deiterding et al., 2009a, Perotti et al., 2013, Wan et al., 2017]
- Level-set method for Eulerian solid mechanics: [Barton et al., 2013]
- Ideal magneto-hydrodynamics: [Gomes et al., 2015, Souza Lopes et al., 2018] ►
- ► \sim 500,000 LOC in C++, C, Fortran-77, Fortran-90
- V2.0 plus FSI coupling routines as open source at http://www.vtf.website
- Used here V3.0 with significantly enhanced parallelization (V2.1 not released)

DNS with a hybrid method

Parallelization approach

AMROC strong scalability tests

3D wave propagation method with Roe scheme: spherical blast wave

Tests run IBM BG/P (mode VN)



 $64 \times 32 \times 32$ base grid, 2 additional levels with factors 2, 4; uniform $512 \times 256 \times 256 = 33.6 \cdot 10^6$ cells

Level	Grids	Cells
0	1709	65,536
1	1735	271,048
2	2210	7,190,208

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3D SRT-lattice Boltzmann scheme flow over rough surface of $19 \times 13 \times 2$ spheres





CPUs

 $360 \times 240 \times 108$ base grid, 2 additional levels with factors 2, 4; uniform $1440 \times 1920 \times 432 = 1.19 \cdot 10^9$ cells

Level	Grids	Cells
0	788	9,331,200
1	21367	24,844,504
2	1728	10,838,016

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Laboratory tunnel simulator [Zonglin et al., 2002]





Laboratory tunnel simulator [Zonglin et al., 2002]



Model solves the inviscid Euler equations

$$\begin{array}{l} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0\\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = 0\\ \partial_t (\rho E) + \nabla \cdot ((\rho E + p)\mathbf{u}) = 0 \end{array}$$

with $p = (\gamma - 1)(\rho E - \frac{1}{2}\rho \mathbf{u}^T \mathbf{u})$



Laboratory tunnel simulator [Zonglin et al., 2002]



Model solves the inviscid Euler equations

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with $p = (\gamma - 1)(\rho E - \frac{1}{2}\rho \mathbf{u}^T \mathbf{u})$

- Two-dimensional axi-symmetric computation
- $p_0 = 100 \, \text{kPa}, \, \rho_0 = 1.225 \, \text{kg/m}^3, \, \gamma = 1.4$
- Roe shock-capturing scheme blended with HLL
- 2nd order accuracy achieved with MUSCL-Hancock method
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|----------------------------|---------------------------|--|--------------------------|---------|
| Validation | | | | |
| | | 100 / | | |

Basic phenomena – $v_0 = 100 \,\mathrm{m/s}$

- $\blacktriangleright~800\times25$ mesh with Cartesian cut-out (200, 5) to (800, 25)
- 2 level of additional refinement by factor 2



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Comparison with experiment – I

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Pressure record at (1020 $\rm mm, 20\, \rm mm)$ for $v_0=75\,\rm m/s.$ Experiment (left) and AMROC (right)

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Summar

Comparison with experiment – I



Pressure record at (40 $\rm mm, 20 \ mm)$ for model velocity $v_0 = 100 \ \rm m/s.$ Experiment (left) and AMROC (right)

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Summar 00

Variation of velocity and nose half angle



• Dependence on v_0^2 is the dynamic pressure influence (left)

- For constant blockage ratio and body velocity, using more pointed noses alleviates the maximal pressure level (right, nose half angle varied)
- For $v_0 \approx 140 \text{ m/s}$ a shock wave (tunnel boom) can be observed. Sharper noses also delay this phenomenon.

Train-tunnel aerodynamics

Two-temperature solver for high-enthalpy flows

Passing trains in open space and in double-track tunnel

NGT2 prototype setup

- Next Generation Train 2 (NGT2) geometry by the German Aerospace Centre (DLR) [Fragner and Deiterding, 2016, Fragner and Deiterding, 2017]
- \blacktriangleright Mirrored train head of length $\sim 60\,{\rm m},$ no wheels or tracks, train models $0.17\,{\rm m}$ above ground above the ground level.
- $\blacktriangleright\,$ Train velocities 100 $\rm m/s$ and $-100\,\rm m/s,$ middle axis 6 $\rm m$ apart, initial distance between centers 200 $\rm m$
- $\blacktriangleright\,$ Base mesh of 360 \times 40 \times 30 for domain of 360 $\rm m \times$ 40 $\rm m \times$ 30 $\rm m$
- Two/three additional levels, refined by r_{1,2,3} = 2. Refinement based on pressure gradient and level set and regenerated at every coarse time step. Parallel redistribution at every level-0 time step.
- > On 96 cores Intel Xeon E5-2670 2.6 GHz a final $t_e = 3 \sec$ was reached after 12, 385 sec / 43, 395 sec wall time, i.e., 330 h and 1157 h CPU



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Passing in open space – AMR and dynamic distribution

Domains of three-level refinement



Distribution to 96 processors



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Passing in open space – AMR and dynamic distribution

Domains of three-level refinement



Distribution to 96 processors



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Pressure isosurfaces



Pressure (Pa) 98000.0 96500.0 99000.0 99500.0 100000.0 100500.0 101000.0 101500.0 102000.0 102500.0 103000.0 103500.0 104000.0 104500.0 105000.0



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R. Deiterding - Recent examples of compressible aerodynamics simulation with the AMROC framework







Passing trains in open space and in double-track tunnel Pressure isosurfaces

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X Axis (m)

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Passing trains in open space and in double-track tunnel

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Passing trains in open space and in double-track tunnel

Pressure transects



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Passing trains in open space and in double-track tunnel

Pressure transects



Passing trains in open space and in double-track tunnel

Pressure transects



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Train-tunnel aerodynamics

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DNS with a hybrid method S

Passing trains in open space and in double-track tunnel

Setup with realistic tunnel shape

- $\blacktriangleright\,$ Two NGT2 trains again at velocities 100 m/s and $-100\,m/s$
- Prototype straight double track tunnel of 640 m length, initial distance between centers of trains 820 m
- Base mesh of 1060 × 36 × 24 for domain of 1060 m × 36 m × 24 m, three levels refined by r_{1,2,3} = 2
- On 96 cores Intel Xeon E5-2670 2.6 GHz a final t_e = 5 sec was reached after 84, 651 sec wall time, i.e., 2257 h CPU



Tunnel shape

Train-tunnel aerodynamics

DNS with a hybrid method Summary

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Summary 00

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Tunnel shape



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Pressure transects





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Pressure transects





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Thermodynamic Model

The two temperature thermodynamic model is used to model the thermodynamic nonequilibrium,

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Thermodynamic Model

The two temperature thermodynamic model is used to model the thermodynamic nonequilibrium,

$$e_{s}(T_{tr}, T_{ve}) = e_{s}^{t}(T_{tr}) + e_{s}^{r}(T_{tr}) + e_{s}^{v}(T_{ve}) + e_{s}^{el}(T_{ve}) + e_{s}^{0}$$

Thermodynamic model

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- Computationally efficient,
- Widely used,
- Integrated into the open source library Mutation++ [Scoggins and Magin, 2014].

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- Computationally efficient,
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The internal energies are calculated within the Mutation++ library using the Rigid-Rotator Harmonic-Oscillator (RRHO) model.

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Thermodynamic model				
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Governing Equations

The two temperature thermodynamic model has been implemented using the equations,

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{W}$$

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Thermodynamic model				
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where,

$$\mathbf{Q} = \begin{bmatrix} \rho_{1} \\ \vdots \\ \rho_{N_{s}} \\ \rho_{u} \\ \rho_{v} \\ \rho_{e^{ve}} \\ \rho_{E} \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \rho_{1}u \\ \vdots \\ \rho_{N_{s}}u \\ \rho_{u^{2}} + p \\ \rho_{vu} \\ \rho_{e^{ve}u} \\ (\rho_{E} + p)u \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} \rho_{1}v \\ \vdots \\ \rho_{N_{s}}v \\ \rho_{uv} \\ \rho_{v^{2}} + p \\ \rho_{v^{e}v} \\ (\rho_{E} + p)v \end{bmatrix}, \quad \mathbf{W} = \begin{bmatrix} \dot{w}_{1} \\ \vdots \\ \dot{w}_{N_{s}} \\ 0 \\ 0 \\ Q_{ve} \\ 0 \end{bmatrix}$$

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Thermodynamic model							
Source Terms							

The net species production rates,

$$\begin{split} \dot{w}_{s} &= M_{s} \sum_{r=1}^{N_{r}} (\beta_{sr} - \alpha_{sr}) \left[k_{f,r} \prod_{i=1}^{N_{s}} \left(\frac{\rho_{i}}{M_{i}} \right)^{\alpha_{ir}} - k_{b,r} \prod_{i=1}^{N_{s}} \left(\frac{\rho_{i}}{M_{i}} \right)^{\beta_{ir}} \right] \text{, with} \\ k_{f,r}(T_{c}) &= A_{f,r} T_{c}^{\eta_{f,r}} \exp\left[-\theta_{r}/T_{c} \right] \text{, } T_{c} = \sqrt{T_{tr} T_{ve}} \end{split}$$

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Thermodynamic model	00000000000		000	00			
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and the energy transfer rate (neutral mixture),

$$\begin{split} Q_{ve} &= \sum_{s} Q_{s}^{T-V} + Q_{s}^{C-V} + Q_{s}^{C-el} , \\ Q_{s}^{T-V} &= \rho_{s} \frac{e_{s}^{v}(T_{tr}) - e_{s}^{v}}{\tau_{v,s}^{T-V}} , \\ Q_{s}^{C-V} &= c_{1} \dot{w}_{s} e_{s}^{v} , \quad Q_{s}^{C-el} = c_{1} \dot{w}_{s} e_{s}^{el} , \end{split}$$

are both calculated using the Mutation++ library.

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Numerical Integration

Finite volume method with two flux schemes implemented,

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Thermodynamic model

Numerical Integration

Finite volume method with two flux schemes implemented,

- Van Leer's flux vector splitting method [van Leer, 1982].
- The AUSM scheme [Liou and Steffen Jr, 1993].

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Thermodynamic model

Numerical Integration

Finite volume method with two flux schemes implemented,

- Van Leer's flux vector splitting method [van Leer, 1982].
- The AUSM scheme [Liou and Steffen Jr, 1993].

Second order in space and time.

- The MUSCL-Hancock scheme is used for the fluxes.
- Strang splitting is used to integrate the source term.

Double Wedge							
Cartesian results							
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Simulation of a double wedge in a high enthalpy flow of air [Pezzella et al., 2015].

$ au_\infty$	p_∞	U_∞	M_{∞}	L_1	θ_1	L_2	θ_2
$710\mathrm{K}$	$0.78\mathrm{kPa}$	$3812\mathrm{m/s}$	7.14	$50.8\mathrm{mm}$	30°	$25.4\mathrm{mm}$	55°

Table: Double wedge geometry and experimental conditions.

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Cartesian results							
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Table: Double wedge geometry and experimental conditions.

- Five species mixture of air.
- > Initial 200 \times 200 cell mesh, with 3 levels of refinement.
- Embedded boundary used to define geometry.
- Van Leer flux scheme.
- Physical time of 242 μ s.

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Dynamic load balancing distributes the cells across the processors.



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Adaptive Cartesian methods	Train-tunnel aerodynamics	Two-temperature solver for high-enthalpy flows	DNS with a hybrid method	Summary			



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The AMR enables the flow features to be captured in detail.



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Double Wedge							

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The schlieren image is taken from [Pezzella et al., 2015].

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Cartesian results

Hypersonic Sphere

Simulations of a half inch sphere travelling at hypersonic speeds in air [Lobb, 1964].

Mach number range between 8.4 and 16.1, with $p_{\infty} = 1333 \,\mathrm{Pa}$ and $\mathcal{T}_{\infty} = 293 \,\mathrm{K}.$

The shock standoff distance was measured at each condition.

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The shock standoff distance was measured at each condition.

The shock standoff distance is used to validate the non-equilibrium model.

Validation of the axi-symmetric source term.

$$\mathbf{W}_{\text{axi}} = -\frac{1}{y} \begin{bmatrix} \rho_1 v \\ \vdots \\ \rho_N v \\ \rho u v \\ \rho v^2 \\ (\rho E + p) v \end{bmatrix}$$

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Computed shock standoff distances compared with experimental data.





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Hypersonic Sphere



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Mapped Solution Update

Within the AMROC-Clawpack framework, the solution is stored in physical (x, y) space and the fluxes are mapped from computational (ξ, η) space.

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Using dimensional splitting the solution update is given by:

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Within the AMROC-Clawpack framework, the solution is stored in physical (x, y) space and the fluxes are mapped from computational (ξ, η) space.

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$$\mathbf{Q}_{i,j}^* = \mathbf{Q}_{i,j}^n - \frac{\Delta t}{\Delta \xi} \left[\left(\hat{\mathbf{F}} - \hat{\mathbf{F}}^{\nu} \right)_{i+1,j} - \left(\hat{\mathbf{F}} - \hat{\mathbf{F}}^{\nu} \right)_{i,j} \right] \frac{\Delta \eta \Delta \xi}{V_{i,j}} \,,$$

Adaptive Cartesian methods 00000000 Mapped mesh treatment Train-tunnel aerodynamics 00000000000

Mapped mesh treatment

Mapped Solution Update

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$$\mathbf{Q}_{i,j}^{n+1} = \mathbf{Q}_{i,j}^* - \frac{\Delta t}{\Delta \eta} \left[\left(\hat{\mathbf{G}} - \hat{\mathbf{G}}^v \right)_{i,j+1} - \left(\hat{\mathbf{G}} - \hat{\mathbf{G}}^v \right)_{i,j} \right] \frac{\Delta \eta \Delta \xi}{V_{i,j}} \,.$$

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where $V_{i,j}$ is the volume of cell *i*, *j* in physical space. $\hat{\mathbf{F}}$, $\hat{\mathbf{F}}^{\nu}$, $\hat{\mathbf{G}}$, $\hat{\mathbf{G}}^{\nu}$ are the physical fluxes per computational unit length.

Mapped Mesh Computation

In the mapped mesh computations, the flux is transformed to align with the cell face,

$$\hat{\mathbf{F}} = T^{-1} \mathbf{F}_n (T \mathbf{Q}_l, T \mathbf{Q}_r),$$

Mapped mesh treatment

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Mapped Mesh Computation

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$$\hat{\mathbf{F}} = \mathcal{T}^{-1} \mathbf{F}_n(\mathcal{T} \mathbf{Q}_l, \mathcal{T} \mathbf{Q}_r),$$

where T is the transformation matrix,

I

$$\mathcal{T} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{n}^{x} & \hat{n}^{y} & 0 & 0 \\ 0 & 0 & 0 & -\hat{n}^{y} & \hat{n}^{x} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

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Mapped Inviscid Fluxes

The inviscid fluxes per computational unit length are found by:

Mapped mesh treatment

Mapped Inviscid Fluxes

The inviscid fluxes per computational unit length are found by:

- Rotating the momentum components to be normal to the face,
- ► Calculating the flux with the rotated solution vectors,
- Rotating the solution vector back, ►
- Scaling the flux using the ratio of the computational face to the mapped face

Summary

Mapped mesh treatment

Mapped Inviscid Fluxes

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- Calculating the flux with the rotated solution vectors,
- Rotating the solution vector back,
- Scaling the flux using the ratio of the computational face to the mapped face

In the ξ directional sweep, this gives

$$\mathbf{F}_{i-1/2,j} = T_{i-1/2,j}^{-1} \mathbf{F}_n(T_{i-1/2,j} \mathbf{Q}_{i-1,j}, T_{i-1/2,j} \mathbf{Q}_{i,j}).$$

where T is the rotation matrix used to rotate the momentum components, and \mathbf{F}_n is the normal flux through the face.

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Mapped mesh treatment

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where T is the rotation matrix used to rotate the momentum components, and \mathbf{F}_n is the normal flux through the face. The scaling is given by:

$$\hat{\mathsf{F}}_{i,j} = \frac{|\mathbf{n}_{i-1/2,j}|}{\Delta \eta} \, \mathsf{F}_{i-1/2,j} \,,$$

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Non-cartesian results and comparison

Mapped Mesh Computation

Experiments of a cylinder in hypersonic flow [Hornung, 1972] were simulated with the mapping and initial conditions given by,

$$x = \xi \cos(\eta), \quad y = -\xi \sin(\eta).$$

Radius	Y_{N_2}	Y_N	T_∞	p_∞	U_∞	M_∞
$0.0127\mathrm{m}$	0.927	0.073	1833 K	$2.91\rm kPa$	$5590\mathrm{m/s}$	6.14

Table: Cylinder geometry and freestream conditions

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The implementation was verified by comparing a mapped computation with a embedded boundary computation.

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Mapped Mesh Computation



 $t = 100 \, \mu \mathrm{sec}$

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Viscous Computations

Preliminary results have been obtained for computations including the viscous flux vectors,

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \left(\mathbf{F} - \mathbf{F}^{\nu}\right)}{\partial x} + \frac{\partial \left(\mathbf{G} - \mathbf{G}^{\nu}\right)}{\partial y} = \mathbf{W}$$

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where,

$$\mathbf{F}^{\mathbf{v}} = \begin{bmatrix} -J_{x,1} \\ \vdots \\ -J_{x,N_s} \\ \tau_{x,x} \\ \tau_{y,x} \\ \kappa_{ve} \frac{\partial T_{ve}}{\partial x} - \sum_{s=1}^{N_s} J_{x,s} \mathbf{e}_{ve} \\ \kappa_{tr} \frac{\partial T_{tr}}{\partial x} + \kappa_{ve} \frac{\partial T_{ve}}{\partial x} + u\tau_{x,x} + v\tau_{y,x} - \sum_{s=1}^{N_s} J_{x,s} h_s \end{bmatrix}$$

and a similar expression is obtained for \mathbf{G}^{ν} .
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Non-cartesian results and comparison

Cylinder Heat Flux Computation

The mapped mesh solver has been validated by simulating a cylinder in a nonequilibrium, high enthalpy flow.

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The inflow conditions and results were taken from [Degrez et al., 2009].

T_∞	$ ho_{\infty}$	U_∞	Y_{N_2}	Y_N	Y_{O_2}	Y _O	Y _{NO}
$694\mathrm{K}$	$3.26\mathrm{g/m}^3$	$4776\mathrm{m/s}$	0.7356	0.0	0.1340	0.07955	0.0509

Table: Freestream conditions for the HEG cylinder simulation.

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Non-cartesian results and comparison

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A cylinder mesh was generated with hyperbolic tangent stretching away from the wall using a 1e-6 initial spacing.

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Cylinder Heat Flux Comparison

The simulated results show good agreement with the experimental results:



Figure: A comparison of the experimental and simulated surface pressures in the HEG cylinder experiment.

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Non-cartesian results and comparison

Cylinder Heat Flux Comparison

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Figure: A comparison of the experimental and simulated surface heat fluxes in the HEG cylinder experiment.

Adaptive Cartesian methods	Train-tunnel aerodynamics	Two-temperature solver for high-enthalpy flows	DNS with a hybrid method	
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Higher-order hybrid methods				

Convective numerical flux is defined as

$$\mathbf{F}_{inv}^{n} = \begin{cases} \mathbf{F}_{inv-WENO}^{n}, & \text{in } \mathcal{C} \\ \mathbf{F}_{inv-CD}^{n}, & \text{in } \mathcal{\overline{C}}, \end{cases}$$

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Adaptive Cartesian methods	Train-tunnel aerodynamics	Two-temperature solver for high-enthalpy flows	DNS with a hybrid method	Summary	
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Adaptive Cartesian methods	Train-tunnel aerodynamics	Two-temperature solver for high-enthalpy flows	DNS with a hybrid method	Summary
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Use WENO scheme to only capture shock waves but resolve interface between species.

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Use WENO scheme to only capture shock waves but resolve interface between species. Shock detection based on using two criteria together:

1. Lax-Liu entropy condition $|u_R \pm a_R| < |u_* \pm a_*| < |u_L \pm a_L|$ tested with a threshold to eliminate weak acoustic waves. Used intermediate states at cell interfaces:

$$u_* = rac{\sqrt{
ho_L u_L} + \sqrt{
ho_R u_R}}{\sqrt{
ho_L} + \sqrt{
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2. Limiter-inspired discontinuity test based on mapped normalized pressure gradient θ_{j}

$$\phi(heta_j) = rac{2 heta_j}{\left(1+ heta_j
ight)^2} \quad ext{with} \quad heta_j = rac{|m{p}_{j+1}-m{p}_j|}{|m{p}_{j+1}+m{p}_j|}, \quad \phi(heta_j) > lpha_{Map}$$

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Higher-order hybrid methods

Results for shear layer in Mach reflection pattern WENO/CD - 6 levels WENO/CD - 7 levels WENO/CD - 8 levels



 $\Delta x_{\rm min} = 3.91 \cdot 10^{-6}\,{\rm m}$

MUSCL - 7 levels



 $\Delta x_{\rm min} = 1.95 \cdot 10^{-6}\,{\rm m}$

MUSCL - 7 levels - Euler



 $\Delta x_{\rm min} = 1.05 \cdot 10^{-6} \, \mathrm{m}$



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Usage of WENO for WENO/CD - 8 levels



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 WENO/CD/RK3 gives results comparable to 4x finer resolved optimal 2nd-order scheme, but CPU times with SAMR 2-3x larger

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Higher-order hybrid methods

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- Gain in CPU time from higher-order scheme roughly one order

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Higher-order hybrid methods

Detonation ignition by hot jet in 2d



X. Cai, RD, J. Liang, Y. Mahmoudi, Proc. Combust. Institute 36(2): 2725-2733, 2017

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Adaptive Cartesian methods	Train-tunnel aerodynamics	Two-temperature solver for high-enthalpy flows	DNS with a hybrid method	Summary
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Conclusions				
Conclusions				

A Cartesian embedded boundary method for compressible flows with block-based adaptive mesh refinement is an efficient and scalable prediction tool for pressure and shock waves created by moving bodies

Conclusions			
Adaptive Cartesian methods	Train-tunnel aerodynamics	Two-temperature solver for high-enthalpy flows	DNS with a

NS with a hybrid method Summary

Conclusions

- A Cartesian embedded boundary method for compressible flows with block-based adaptive mesh refinement is an efficient and scalable prediction tool for pressure and shock waves created by moving bodies
- Multi-resolution and fluid-structure coupling problems can be tackled without expensive mesh regeneration
 - Level set approach easily handles large motions, element failure and removal
 - Dynamic adaptation ensures high resolution at embedded boundaries and essential flow features

Conclusions

- A Cartesian embedded boundary method for compressible flows with block-based adaptive mesh refinement is an efficient and scalable prediction tool for pressure and shock waves created by moving bodies
- Multi-resolution and fluid-structure coupling problems can be tackled without expensive mesh regeneration
 - Level set approach easily handles large motions, element failure and removal
 - Dynamic adaptation ensures high resolution at embedded boundaries and essential flow features
- Aerodynamics of bodies with large motion are easily accessible
 - Current inviscid approach predicts maximal overpressure in front of trains reliably
 - For predicting the flow around entire trains, the boundary layer growing over the train body needs to be considered.
 - AMROC solvers for the compressible Navier-Stokes equations and even LES are already available, however, for this particular application a turbulent wall function on the embedded boundary first needs to be implemented. Such a wall function is currently work-in-progress for the LBM-LES solver.

Summary

Conclusions – Hypersonics

- A two-temperature model solver that is suitable for very high temperatures, i.e., high enthalpy re-entry flows, has been developed.
- The Cartesian version is fully integrated into SAMR AMROC-Clawpack; structured non-Cartesian version runs also within AMROC-Clawpack but only on non-adaptive meshes so far
- SAMR framework can remain basically unchanged; however mapping needs to be considered in prolongation and restriction, flux correction, visualization (work in progress)

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- The Cartesian version is fully integrated into SAMR AMROC-Clawpack; structured non-Cartesian version runs also within AMROC-Clawpack but only on non-adaptive meshes so far
- SAMR framework can remain basically unchanged; however mapping needs to be considered in prolongation and restriction, flux correction, visualization (work in progress)
- For moving geometries, the goal is a Chimera-type approach that constructs non-Cartesian boundary layer meshes near the body and uses SAMR in the far field
- Incorporation of the methodology into the hybrid WENO/CD scheme for high enthalpy DNS in 3D is proposed within the next two years

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Clustering by signatures

			х	х	х	х	х	х	6
			х	х	х	х	х	х	6
		х	х	х					3
х	х	х							3
х	х								2
х	х								2
х	х								2
									0
х	х								2
х	х								2
6	6	2	3	2	2	2	2	2	

 $\begin{array}{ll} \Upsilon & \mbox{Flagged cells per row/column} \\ \Delta & \mbox{Second derivative of } \Upsilon, \ \Delta = \Upsilon_{\nu+1} - 2\,\Upsilon_{\nu} + \Upsilon_{\nu-1} \\ \mbox{Technique from image detection: [Bell et al., 1994], see also} \\ \mbox{[Berger and Rigoutsos, 1991], [Berger, 1986]} \end{array}$

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			х	х	х	х	х	х	6
			х	х	х	х	х	х	6
		х	х	х					3
х	х	х							3
х	х								2
х	х								2
х	х								2
									0
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R. Deiterding – Recent examples of compressible aerodynamics simulation with the AMROC framework

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Λ



- 1. 0 in Υ
- 2. Largest difference in Δ
- 3. Stop if ratio between flagged and unflagged cell $>\eta_{tol}$

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Closest point transform algorithm

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

$$|
abla arphi| = 1$$
 with $arphi \Big|_{\mathcal{T}} = 0$

Solution smooth but non-diferentiable across characteristics.

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 Geometric solution approach with plosest-point-transform algorithm [Mauch, 2003]

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1. Build the characteristic polyhedrons for the surface mesh

Characteristic polyhedra for faces, edges, and vertices



(c)

- 1. Build the characteristic polyhedrons for the surface mesh
- 2. For each face/edge/vertex
 - 2.1 Scan convert the polyhedron.





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 - O(m) to build the b-rep and the polyhedra.
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- 4. Problem reduction by evaluation only within specified max. distance

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



