Amroc - A Cartesian SAMR Framework for Compressible Gas Dynamics

Ralf Deiterding
Computer Science and Mathematics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee

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Collaboration with

- Sean Mauch and Daniel Meiron (Applied and Computational Mathematics Caltech)
- Fehmi Cirak (University of Cambridge)
- David Hill, Dale Pullin (Graduate Aeronautical Laboratories Caltech) and Carlos Pantano (University of Illinois at Urbana-Champaign)

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Outline of the talk

• Computation of compressible flows in Amroc
  – Currently supported equations and schemes
• Dynamically adaptive Cartesian meshes
  – Principles of hyperbolic SAMR, parallelization
  – Non-trivial examples
• Incorporation of complex boundaries
  – Level-set based ghost fluid approach
  – Verification and validation
• Incorporation of Lagrangian solid mechanics solvers
  – Fluid-structure coupling approach
  – Verification and validation
  – Multi-physics examples
• Framework design and realization of complex methods
• Conclusions
Hydrodynamic equations

Favre-averaged Navier-Stokes equations
\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_k} (\bar{\rho} \bar{u}_k) = 0
\]
\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i) + \frac{\partial}{\partial x_k} (\bar{\rho} \bar{u}_i \bar{u}_k + \delta_{ik} \bar{p} - \bar{\tau}_{ik} + \sigma_{ik}) = 0
\]
\[
\frac{\partial \bar{E}}{\partial t} + \frac{\partial}{\partial x_k} (\bar{u}_k (\bar{E} + \bar{p}) + \bar{q}_k - \bar{\tau}_{kj} \bar{u}_j + \sigma^e_k) = 0
\]
\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_i) + \frac{\partial}{\partial x_k} (\bar{\rho} \bar{Y}_i \bar{u}_k + \bar{J}^i_k + \sigma^i_k) = \bar{m}_i
\]
Implicit equation of state
\[
\bar{\rho} \bar{h} - \bar{p} - \bar{E} + \frac{1}{2} \bar{\rho} \bar{u}_k \bar{u}_k + \bar{p} k_{ss} = 0
\]
Ideal gas law
\[
\bar{p} = \bar{\rho} R (\bar{T} \sum_{i=1}^{N} \frac{\bar{Y}_i}{W_i} + w_s)
\]
Caloric equation
\[
\bar{h} = \sum_{i=1}^{N} h_i(\bar{T}) \bar{Y}_i + h_s \quad \text{with}
\]
\[
h_i(\bar{T}) = h_i^0 + \int_{T_0}^{\bar{T}} c_{pi}(T^*) dT^*
\]
Stress tensor and diffusion terms
\[
\bar{\tau}_{ik} = \bar{\mu} \left( \frac{\partial \bar{u}_k}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_k} - \frac{2}{3} \bar{\mu} \frac{\partial \bar{u}_j}{\partial x_j} \delta_{ik} \right)
\]
\[
\bar{q}_k = -\bar{\chi} \frac{\partial \bar{T}}{\partial x_k} \quad \bar{J}^i_k = -\bar{\rho} \bar{D_i} \frac{\partial \bar{Y}_i}{\partial x_k}
\]
Chemical kinetics with Arrhenius law
\[
\bar{m}_i = \bar{W}_i \sum_{j=1}^{M} (\nu_{ji}^r - \nu_{ji}^f) [k_j^f \prod_{n=1}^{N} \left( \frac{\rho_n}{W_n} \right)^{\nu_{jn}^f} - k_j^r \prod_{n=1}^{N} \left( \frac{\rho_n}{W_n} \right)^{\nu_{jn}^r}]
\]
Simulation of compressible flows

- **Convective part**
  - Conservative schemes with upwinding in all characteristic fields
  - Time-explicit treatment with Riemann solvers
  - Centered schemes in smooth solutions regions possible
  - Shock waves can not be resolved in practice → weak solutions of Euler equations are sought
  - Unique solution is determined by entropy condition

- **Diffusion terms**
  - Conservative centered differences

- **Source terms**
  - Fractional splitting method, typically with explicit or semi-implicit Runge-Kutta ODE schemes with automatic stepsize adjustment
  - With non-linear source terms the wave speeds become resolution-dependent, even with finite volume methods → very high local resolution necessary

- **Schemes are implemented in single grid routines, typically in F77/F90**
  - Clawpack version with extended higher-order capabilities and large number of Riemann solvers
  - Hydrid WENO-TCD method by D. Hill and C. Pantano with LES model for compressible flows by D. Pullin
  - Riemann Invariant Manifold Method by T. Lappas
  - Finite volume MHD solver by M. Torrilhon (only uniform for now)
Structured AMR for hyperbolic problems

- For simplicity
  \[ \partial_t q + \nabla \cdot f(q) = 0 \]
- Refined subgrids overlay coarser ones
- Computational decoupling of subgrids by using ghost cells
- Refinement in space \textit{and} time
- Block-based data structures
- Cells without mark are refined
- Cluster-algorithm necessary
- Efficient cache-reuse / vectorization possible
- Explicit finite volume scheme

\[
Q_{jk}^{n+1} = Q_{jk}^n - \frac{\Delta t}{\Delta x_1} \left[ F_{j+\frac{1}{2},k}^1 - F_{j-\frac{1}{2},k}^1 \right] - \frac{\Delta t}{\Delta x_2} \left[ F_{j,k+\frac{1}{2}}^2 - F_{j,k-\frac{1}{2}}^2 \right]
\]

only for single rectangular grid necessary

\[ \text{Root Level} \quad r_0 = 1 \]
\[ \text{Level 1} \quad r_1 = 4 \]
\[ \text{Level 2} \quad r_2 = 2 \]

\[ \text{Time} \]
- Regridding of finer levels.
- Base level (○) stays fixed.
Parallelization strategy

Domain decomposition: \( G_0 = \bigcup_{p=1}^{P} G_0^p \) with \( G_0^p \cap G_0^q = \emptyset \) for \( p \neq q \)

\[
G_0^p := \bigcup_{m=1}^{M_0^p} G_{0,m}^p \quad \rightarrow \quad G_l^p := G_l \cap G_0^p
\]

Workload: \( \mathcal{W}(\Omega) = \sum_{l=0}^{l_{\text{max}}} \left[ N_l(G_l \cap \Omega) \prod_{\kappa=0}^{l} r_{\kappa} \right] \), \( N_l(G) \) No. of cells on \( l \)

Load-balancing: \( \mathcal{L}^p := \frac{P \cdot \mathcal{W}(G_0^p)}{\mathcal{W}(G_0)} \approx 1 \) for all \( p = 1, \ldots, P \)

- Data of all levels resides on same node \( \rightarrow \) Interpolation and averaging remain strictly local
- Only parallel operations to be considered:
  - Parallel synchronization as part of ghost cell setting
  - Load-balanced repartitioning of data blocks as part of \( \text{Regrid}(l) \)
  - Application of flux correction terms on coarse-grid cells
- Partitioning at root level with generalized Hilbert space-filling curve by M. Parashar
• Classical framework approach with generic main program in C++
• Customization / modification in Problem.h include file by derivation from base classes and redefining virtual interface functions
• Predefined, scheme-specific classes (with F77 interfaces) provided for standard simulations
• Standard simulations require only linking to F77 functions for initial and boundary conditions, source terms. No C++ knowledge required.
• Interface mimics Clawpack
• Expert usage (algorithm modification, advanced output, etc.) in C++
Planar Richtmyer-Meshkov Instability

- Treat turbulent region in flow as a ‘feature’ to be refined
  - Containment of turbulence in refined zones
  - Turbulent base level resolution used as subgrid cutoff
- Perturbed Air-SF6 interface shocked and re-shocked by Mach 1.5 shock
- 96 CPUs IBM SP2-Power3 by D. Hill, C. Pantano
- WENO-TCD by D. Hill scheme with LES model by D. Pullin for Favre-averaged Navier-Stokes equations
  - AMR base grid 172x56x56, 2 additional levels with factors 2, 2
  - $9 \times 10^6$ cells in average instead of $34 \times 10^6$ (uniform)
Ghost fluid method

- Incorporate complex moving boundary/ interfaces into a Cartesian solver (extension of work by R. Fedkiw and T. Aslam)
- Implicit boundary representation via distance function $\varphi$, normal $n = \nabla \varphi / |\nabla \varphi|$
- Treat an interface as a moving rigid wall
- Method diffuses boundary and is therefore not conservative
- Construction of values in embedded boundary cells by interpolation / extrapolation

\[
\begin{align*}
\rho_F^{n,j-1} & \quad \rho_F^{n,j} & \quad \rho_F^{n,j} & \quad \rho_F^{n,j-1} \\
\mathbf{u}_F^{n,j-1} & \quad \mathbf{u}_F^{n,j} & \quad 2\mathbf{u}_S^{n,j+1/2} - \mathbf{u}_F^{n,j} & \quad 2\mathbf{u}_S^{n,j+1/2} - \mathbf{u}_F^{n,j-1} \\
\mathbf{u}_S^{t,j-1} & \quad \mathbf{u}_S^{t,j} & \quad \mathbf{u}_S^{t,j} & \quad \mathbf{u}_S^{t,j-1} \\
\rho_S^{n,j-1} & \quad \rho_S^{n,j} & \quad \rho_S^{n,j} & \quad \rho_S^{n,j-1} \\
p_F^{n,j-1} & \quad p_F^{n,j} & \quad p_F^{n,j} & \quad p_F^{n,j-1}
\end{align*}
\]

Velocity: $\mathbf{u}_{\text{Gh}}^{F} = 2((\mathbf{u}_S^{F} - \mathbf{u}_M^{F}) \cdot \mathbf{n}) \mathbf{n} + \mathbf{u}_M^{F}$

- Higher resolution at embedded boundary usually required than with first-order unstructured scheme
- Appropriate level-set-based refinement criteria are available
Ghost fluid method in Amroc

- Core algorithm implemented in derived HypSAMRSolver class
- Multiple independent EmbeddedBoundaryMethod objects possible
- Base classes are scheme-independent
- Specialization of GFM boundary conditions, level set description in scheme-specific F77 interface classes
Verification of GFM

**Double Mach reflection**
Overlay of two simulation of a double Mach reflection on a 800x400 grid with GFM and 2nd order accurate scheme

**Conical shocktube**
Cylindrical symmetric simulation by D. Hill of experiment by Setchel, Strom and Sturtevant (JFM 1972)
Mach 6 shock in Argon

Left: shock velocity along centerline in experiment and simulation (red)
Shock interaction at double-wedge geometry

- Simulation by D. Hill
- Mach 9 flow in air hitting a double-wedge (15° and 45°)
- Example from Olejniczak, Wright and Candler (JFM 1997)
- AMR base mesh 300x100, 3 additional levels with factor 2
- 3rd order WENO computation vs. 2nd order MUSCL with van Leer flux vector splitting

![Image of schematic diagram and computational results]

Figure 6. Schematic diagram of a Type V shock interaction with an enlargement of the interaction region.
Fluid-structure coupling

- Couple compressible Euler equations to Lagrangian structure mechanics
- Compatibility conditions between *inviscid* fluid and solid at a slip interface
  - Continuity of normal velocity: \( u^S_n = u^F_n \)
  - Continuity of normal stresses: \( \sigma^{S}_{nn} = -p^F \)
  - No shear stresses: \( \sigma^{S}_{n\tau} = \sigma^{S}_{n\omega} = 0 \)
- Time-splitting approach for coupling
  - **Fluid:**
    - Treat evolving solid surface with moving wall boundary conditions in fluid
    - Use solid surface mesh to calculate fluid level set
    - Use nearest velocity values \( u^S \) on surface facets to impose \( u^F_n \) in fluid
  - **Solid:**
    - Use interpolated hydro-pressure \( p^F \) to prescribe \( \sigma^{S}_{nn} \) on boundary facets
- Ad-hoc separation in dedicated fluid and solid processors
Algorithmic approach for coupling

- Fluid processors
  - Receive boundary from solid server
  - Compute level set via CPT and populate ghost fluid cells according to actual stage in AMR algorithm
  - AMR Fluid solve
  - Update boundary pressures using interpolation
  - Send boundary pressures
  - Compute next possible time step
- Efficient non-blocking boundary synchronization exchange (ELC)
- Solid processors
  - Update boundary
  - Send boundary location and velocity
  - Receive boundary pressures from fluid server
  - Apply pressure boundary conditions at solid boundaries
  - Solid solve
  - Do N Sub-iterations
  - Compute stable time step multiplied by N
  - Compute next time step

Efficient non-blocking boundary synchronization exchange (ELC)
Implicit representations of complex surfaces

- FEM Solid Solver
  - Explicit representation of the solid boundary, b-rep
  - Triangular facetted surface

- Cartesian FV Solver
  - Implicit level set representation
  - Need closest point on the surface at each grid point

→ Closest point transform algorithm (CPT) by S. Mauch
Amroc coupled to CSD solver (the VTF)

- Coupling algorithm implemented in further derived HypSAMRSolver class
- Level set evaluation always with CPT algorithm
- Parallel communication through efficient non-blocking communication module by S. Mauch
- Elastic motion of a thin steel plate when being hit by a Mach 1.21 shock wave, Giordano et al. Shock Waves (2005)
- Steel plate modeled with finite difference solver using the beam equation
\[ \rho h \frac{\partial^2 w}{\partial t^2} + EI \frac{\partial^4 w}{\partial x^4} = p(x, t) \]
- SAMR base mesh 320x64, 2 additional level with factors 2, 4
- Elastic motion of a thin steel plate when being hit by a Mach 1.21 shock wave, Giordano et al. Shock Waves (2005)
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- SAMR base mesh 320x64, 2 additional level with factors 2, 4
Validation example: detonation-driven fracture

- Experiments by T. Chao, J. C. Krok, J. Karnesky, F. Pintgen, J.E. Shepherd (GalCIT)
- Motivation: Validate VTF for complex fluid-structure interaction problem
- Interaction of detonation, ductile deformation, fracture
- Modeling of ethylene-oxygen detonation with constant volume burn detonation model

Treatment of shells/thin structures

- Thin boundary structures or lower-dimensional shells require “thickening” to apply ghost fluid method
  - Unsigned distance level set function $\varphi$
  - Treat cells with $0<\varphi<d$ as ghost fluid cells (indicated by green dots)
  - Leaving $\varphi$ unmodified ensures correctness of $\nabla \varphi$
  - Refinement criterion based on $\varphi$ ensures reliable mesh adaptation
  - Use face normal in shell element to evaluate in $\Delta p = p_u - p_l$
Fluid-structure interaction validation – tube with flaps

- C₂H₄+3 O₂ CJ detonation for \( p_0 = 100 \text{ kPa} \) drives plastic opening of pre-cut flaps
- Motivation:
  - Validate fluid-structure interaction method
  - Validate material model in plastic regime

**Fluid**
- Constant volume burn model
- AMR base level: 104x80x242, 3 additional levels, factors 2,2,4
- Approx. 4\( \cdot 10^7 \) cells instead of 7.9\( \cdot 10^9 \) cells (uniform)
- Tube and detonation fully refined
- Thickening of 2d mesh: 0.81 mm on both sides (real thickness on both sides 0.445 mm)

**Solid**
- Aluminum, J2 plasticity with hardening, rate sensitivity, and thermal softening
- Mesh: 8577 nodes, 17056 elements
- 16+2 nodes 2.2 GHz AMD Opteron quad processor, PCI-X 4x Infiniband network
- Ca. 4320h CPU to \( t = 450 \mu \text{s} \)
Tube with flaps – computational results

Simulated results at t=212 μs  Experimental results at t=210 μs
Tube with flaps - Results

Fluid density and displacement in y-direction in solid

Schlieren plot of fluid density on refinement levels
Plate deformation from water hammer

- 3d simulation of plastic deformation of thin copper plate attached to the end of a pipe due to water hammer
- Strong over-pressure wave in water is induced by rapid piston motion at end of tube
- Simulation by R. Deiterding, F. Cirak. Experiment by V.S. Deshpande et al. (U Cambridge)

Comparison of plate at end of simulation and experiment (middle and right). Left: Color of plate and lower half of plane shows the normal velocity.
Fluid
- Pressure wave generated by solving equation of motion for piston during fluid-structure simulation
- Modeling of water with stiffened gas equation of state
  \[ p = (\gamma - 1)(E - \frac{1}{2}u_k u_k) - \gamma p_\infty \]
  with \( \gamma = 7.415 \), \( p_\infty = 296.2 \) MPa
- Multi-dimensional 2nd order upwind finite volume scheme, negative pressures from cavitation eliminated by energy correction
- AMR base level: 350x20x20, 2 additional levels, refinement factor 2,2
- Approx. \( 1.2 \times 10^6 \) cells used in fluid on average instead of \( 9 \times 10^6 \) (uniform)

Solid
- Copper plate of 0.25 mm, J2 plasticity model with hardening, rate sensitivity, and thermal softening
- Solid mesh: 4675 nodes, 8896 elements
- 8 nodes 3.4 GHz Intel Xeon dual processor, Gigabit ethernet network, ca. 130h CPU

Levels of fluid mesh refinement (gray) ~197\( \mu \)s after wave impact onto plate.
Multi-physics examples with fracture

- Copper plate fracture demo simulation
- Two-component solver with stiffened gas EOS for water and ideal gas EOS for air
- 4+4 nodes 3.4 GHz Intel Xeon dual processor, ca. 550h CPU
Conclusions

- Amroc: general object-oriented framework for implementing Cartesian methods
- Applications shown for compressible flows, but any hyperbolic system can easily be considered (software can directly use Riemann solvers from Clawpack by R. LeVeque)
  - Advection
  - Acoustics
  - Shallow water
  - Elastic waves
  - Ideal magneto-hydrodynamics
- Generic ghost fluid implementation allows consideration of (possible moving) embedded boundaries
- Boundaries can be described directly through level set functions or arbitrary triangulated surface meshes
- Any Cartesian finite volume scheme can be used for real-world computations, mesh adaptivity provides necessary accuracy increase
- Fluid-structure interaction coupling routines available to incorporate solid mechanics solvers, e.g. coupling to serial LLNL Dyna3d recently completed by J. Cummings, P. Hung (Caltech)
- Most recent Amroc within VTF: [http://www.cacr.caltech.edu/asc](http://www.cacr.caltech.edu/asc)
Abbreviations

- Amroc: Adaptive mesh refinement in object-oriented C++
- GFM: Ghost fluid method
- CPT: Closest point transform
- CSD: Computational solid dynamics
- FEM: Finite element
- FV: Finite volume
- JFM: Journal of fluid mechanics
- MUSCL: Monotone upstream-centered schemes for conservation laws
- MHD: Magneto-hydrodynamics
- ODE: Ordinary differential equations
- SAMR: Structured adaptive mesh refinement
- TCD: Tuned central difference
- UML: Unified modeling language
- VTF: Virtual Test Facility
- WENO: Weighted essentially non-oscillatory