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Research Statement

My primary research topic is the development of numerical methods for the approximation of solutions to the nonlinear partial differential equations that arise in computational fluid mechanics (CFD). I am particular interested in efficient and robust solution methods for flows in evolving domains that are directly applicable to real-world problems. The main tools of my research are Cartesian schemes with embedded boundary capability, block-structured hierarchical multilevel refinement and the idea of implicit geometry representation via level set functions. I want to utilize these principles to construct highly efficient numerical methods in all flow regimes and to combine the implementations in a unified, fully parallelized software framework. The resulting infrastructure would enable well-resolved simulations of very difficult flow problems, like multiphase or free-surface flows with fluid-structure interaction.

1 Background

The most appropriate discretization principle in CFD is the finite volume approach. Only finite-volume-type schemes satisfy essential physical properties like the global conservation of mass and momentum and are guaranteed to converge towards the correct solution in case the problem involves shock waves. Alternative discretization techniques such as particle methods or the Lattice-Boltzmann approach provide acceptable approximations only for certain types of problems in the subsonic regime and are typically only first-order accurate. On the other hand, finite volume or discontinuous Galerkin schemes are nowadays available for very high order (four or greater). While higher-order methods are computationally expensive on genuinely unstructured meshes, the computing costs are smallest when uniform Cartesian grids are employed [45, 46].

In order to consider complex, even moving boundaries on a Cartesian mesh, level set methods have recently become popular. The boundary is represented implicitly with a scalar function φ that stores the signed distance to the boundary surface and allows the direct evaluation of the boundary outer normal in every mesh point as $\mathbf{n} = \nabla\varphi/|\nabla\varphi|$ [39]. The level set function of a multiphase boundary for instance evolves according to

$$\varphi_t + \mathbf{a}\nabla\varphi = 0 \,, \tag{1}$$

where $\mathbf{a}$ denotes the interface velocity to be derived from the computation. Inherent problems are the effective numerical solution of Eq. (1) with significantly greater accuracy than that of the scheme for the underlying hydrodynamic equations and the efficient re-initialization of φ as a proper distance function. The most straightforward level set method directly uses some of the cells on the Cartesian mesh to enforce immersed boundary conditions [27] immediately before the original numerical update. This step involves interpolation and/or extrapolation operations to construct appropriate values in those internal "ghost cells" (compare Fig. 1). A cell is considered to be a valid fluid cell in the interior if the distance in the cell midpoint is positive and is treated as exterior otherwise. In a typical level set method, the numerical stencil itself is not modified, which causes a diffusion of the boundary location and results in an overall non-conservative scheme of only first-order accuracy. A possibility to alleviate the error is to use dynamic mesh adaptation.

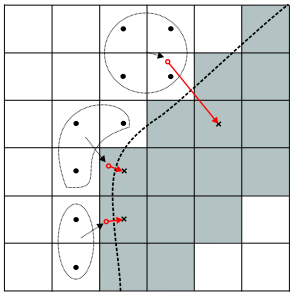


Figure 1: Interpolation stencils for the construction of values in interior ghost cells (gray) at an embedded rigid wall.

The idea of Structured Adaptive Mesh Refinement (SAMR) on purely Cartesian meshes has been pioneered by Berger and Collela in [2]. While originally developed for first-order hyperbolic conservation laws

$$\partial_t \mathbf{q}(\mathbf{x},t) + \nabla \cdot \mathbf{f}(\mathbf{q}(\mathbf{x},t)) = \mathbf{0} \tag{2}$$

with the compressible Euler equations in mind, the principle has been extended successfully to incompressible Navier-Stokes equations, incompressible and/or stationary Euler equations and magnetohydrodynamics.

Instead of replacing single cells by finer ones, the SAMR method follows a patch-oriented approach. Cells being flagged by error indicators (shaded in Fig. 2) are clustered into non-overlapping rectangular grids. Refinement grids are derived recursively from coarser ones and a hierarchy of successively embedded levels is thereby constructed (cf. Fig. 2). The regularity of the data allows high performance on vector and super-scalar processors and cache optimizations. The utilization of refinement both in time and in space is an important difference to usual unstructured adaptive strategies and is one of the main reasons for the high efficiency of the approach.

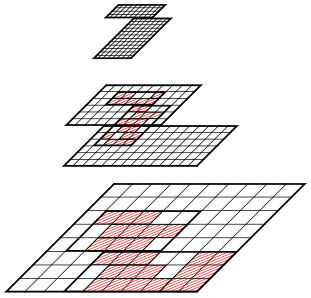


Figure 2: SAMR hierarchy.

2 Previous research

2.1 Shock-capturing methods for combustion

I have devoted my doctoral research to the construction of efficient numerical methods for the simulation of supersonic combustion phenomena, especially detonation waves [14]. The governing equations are the multi-component Euler equations

$$\begin{array}{rcl@{\qquad}rcl} \partial_t \rho + & \nabla\cdot(\rho\mathbf{u}) & = 0\,, & \partial_t(\rho\mathbf{u}) + & \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p & = 0\,, \\ \partial_t(\rho E) + & \nabla\cdot((\rho E + p)\mathbf{u}) & = 0\,, & \partial_t \rho_i + & \nabla\cdot(\rho_i\mathbf{u}) & = W_i\dot{\omega}_i\,, \end{array} \tag{3}$$

with ω_i denoting the production rate of species i derived from a detailed chemical reaction mechanism. The numerical solution of system (3) is considerable more difficult than in the standard case of a single ideal (and polytropic) gas, because an implicit equation of state for a mixture of real gases with different temperature-dependent transport properties needs to be considered.

The appropriate basic solution technique for transient supersonic combustion phenomena is the method of fractional steps that decouples the hydrodynamic transport and the chemical reaction numerically. In particular, this technique allows the utilization of a conventional time-implicit numerical solution method for ordinary differential equations local in every cell to advance the reactive source terms and the application of a time-explicit finite volume scheme for the homogeneous Euler equations. Beside other high-resolution shock capturing schemes, I derived a reliable second-order hybrid Roe-solver-based method for this purpose [22, 17]. The method is suited to eliminate several numerical uncertainties inherent to a large number of published detonation simulation results that have been obtained with recent methods, such as ENO or WENO.

Self-sustained detonations are characterized by a fragile balance between hydrodynamics and chemistry that can only be captured sufficiently by providing a very fine local resolution around the head of the detonation front. Especially, gaseous detonation waves genuinely exhibit highly oscillatory triple point patterns, a phenomenon that is not well understood and therefore the primary focus of experimental and theoretical detonation research [5]. By utilizing the above high-resolution scheme together with SAMR, I have been able to confirm computational results for regular oscillating triple point patterns in two and three space dimensions obtained on supercomputers only shortly earlier [29, 47] on conventional Linux-Beowulf clusters of moderate size [16, 19]. Recently, a series of large-scale computations has been conducted that investigates the evolution of similar structures under transient geometric conditions [20]. Complex boundaries are considered with a first-order level set method exactly as sketched in Section 1. Through extensive shock polar analysis it was found that even in transient situations, i.e. very high overdrive or marginal conditions close or even below the limit of detonability, the hydrodynamic wave configuration around a triple point corresponds to either a Double-Mach Reflection or a Transitional-Mach Reflection, but apparently never to the simpler Single-Mach Reflection case [21].

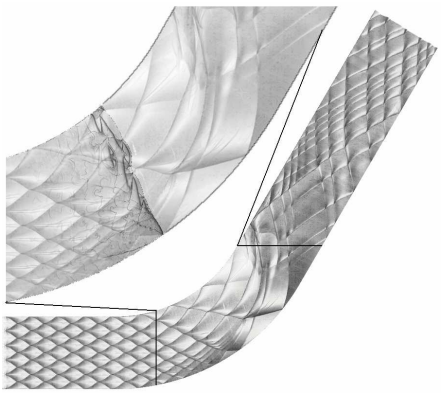


Figure 3: A trace of the maximal vorticity throughout the whole computation visualizes the triple point trajectories for a realistic 60^o pipe bend (lower). The enlarged upper graphic displays a snapshot of the detonation front on the trajectory picture.

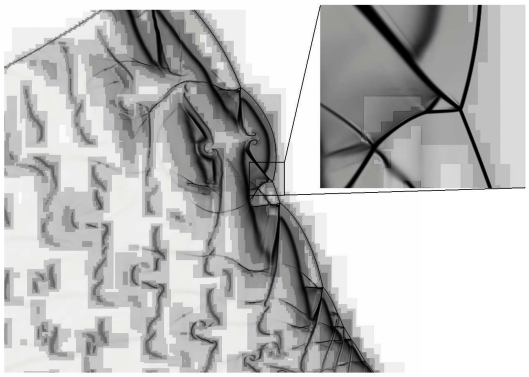


Figure 4: A Schlieren graphic of the detonation front snapshot overlying the domains of hierarchical mesh refinement (in different gray tones) visualizes the level of detail necessary for predictive detonation simulation.

2.2 Shock-driven fluid-driven structure interaction

As a postdoctoral scholar, I worked particularly on the development and application of level-set-based shock-capturing methods that can be employed for multi-physics fluid-structure interaction simulations. These ideas are implemented in the "Virtual Test Facility" (VTF) software [24], a fluid-structure interaction simulation environment that targets strong shock and detonation waves impinging dynamically on deforming solid materials [25]. Fluid-structure interaction (FSI) in the VTF is accomplished through a loosely coupled, partitioned approach with (basically) separated solvers that exchange boundary conditions at the interface after successive time steps. For this application, I developed a novel algorithmic extension of the hyperbolic SAMR method that incorporates the fluid-structure exchange smoothly into the recursive time step refinement pattern and allows very fine local resolutions to capture the near-body interaction at minimal computational costs [7, 23]. In coupled computations, the level set function φ, representing the solid surface, is updated after every boundary synchronization step by calling a specialized algorithm that computes the distance information for a triangulated surface mesh by utilizing characteristic geometric reconstruction and scan conversion [36]. By tailoring the level set computation to the case of multi-block meshes of identical resolution and by evaluating the distance information exactly only in a small band around the interface, we have been able to reduce the computational expense of the level set evaluation for typical surface meshes of several ten thousand triangles to less than 10 % of a typical explicit hydrodynamic update. Without frequent re-meshing and complicate mesh untangling the approach allows large plastic deformations, fracture and fragmentation.

Snapshots from two typical parallel VTF simulations are displayed in the Figs. 5 and 6. Figure 5 shows the deformation of a quasi-two-dimensional thin elastic steel panel under shock wave impact for which the FSI solution can be verified by considering the approximation of an Euler-Bernoulli beam under instantaneous loading [18]. Figure 6 shows the fracture of a thin copper plate at the end of a water shock tube [7, 23]. The later simulation utilizes a HLLC approximate Riemann solver. The strict positivity preservation of this scheme is essential for computing the splashing of the waterjet into the outside air. Further, it clearly illustrates the advantages of the level-set-based approach as the fluid solver handles major topology evolutions without problems.

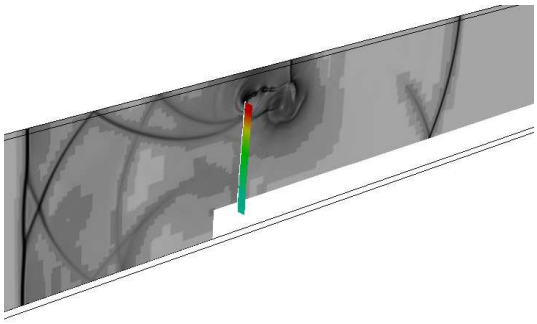


Figure 5: Deforming panel under shock wave impact. Mesh adaptation according to the flow field is shown in the backplane.

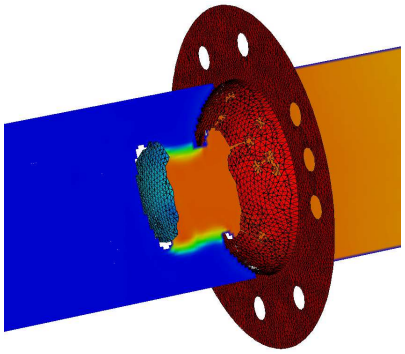


Figure 6: Thin copper plate ruptured by a pressure wave in a water shock tube. The fluid density in the midplane shows the water splash.

2.3 Block-structured adaptive mesh refinement

As generic framework for Cartesian finite volume methods, I developed the block-structured mesh refinement package AMROC (Adaptive Mesh Refinement in Object-oriented C++) [13] that allows the effective implementation of hierarchical multi-level algorithms, e.g., Berger-Collela SAMR for hyperbolic problems or geometric adaptive multigrid for parabolic and elliptic equations. A key feature of AMROC is the efficient distributed-memory parallelization of multi-level algorithms including the proper treatment of internal refinement boundaries that is indispensable to preserve the order of accuracy of higher-order discretizations [15].

The software encompasses already a very large number of approximate Riemann solvers and shock-capturing schemes, especially for the hyperbolic Euler equations with various equations of state. Beside the ones previously mentioned, further large-scale applications of AMROC include large-eddy simulation of compressible shock-driven turbulence with a hybrid centered finite-difference WENO method [40, 41] or shock wave interaction with blunt bodies [33].

As a prototype for implicit schemes on block-structured meshes, a dynamically adaptive solver for the Poisson equation has been implemented following the work of Martin and Collela [35]. The availability of multi-level hierarchical data in the regular SAMR approach suggests the application of adaptive geometric multigrid techniques. Note that the regularity of the data allows the implementation of very efficient matrix-free smoothing algorithms. This solver could be the basis for parallel adaptive methods for parabolic and elliptic equations, e.g., for the stationary and/or incompressible Euler or (Reynolds-averaged) Navier-Stokes equations.

3 Future Research

In my future research, I would like to address efficiency and general applicability of dynamically adaptive Cartesian methods. Cartesian methods with embedded boundaries automate the expensive step of volumetric mesh generation and are particularly suited for fluid-structure problems with large boundary movements. These properties make them a primary choice for computational-aided engineering applications. Among the large number of current research questions are the construction of conservative high-order discretizations, especially with additional constraints as they occur in the incompressible Navier-Stokes equations or the equations of magneto-hydrodynamics, the proper consideration of boundary-layer flows or effective parallelization strategies for hierarchical petascale architectures.

3.1 Discontinuous Galerkin methods for embedded boundaries

In the near future, I want to put special emphasis on the derivation of efficient Cartesian methods that are fully conservative and have an order of accuracy greater than two by applying the discontinuous Galerkin method (DGM). The DGM is a finite-element-type scheme that can be regarded as an extension of the finite volume method to arbitrary order [42]. A numerical solution of Eq. (2) is sought by discretizing the variational formulation

$$\frac{d}{dt}\int_{\Omega}\mathbf{q}(\mathbf{x},t)v(\mathbf{x})d\mathbf{x}+\int_{\partial\Omega}\mathbf{f}(\mathbf{q}(\mathbf{x},t))\cdot n_{\Omega}v(\mathbf{x})d\mathbf{s}-\int_{\Omega}\mathbf{f}(\mathbf{q}(\mathbf{x},t))\cdot\nabla v(\mathbf{x})d\mathbf{x}=\mathbf{0} \tag{4}$$

and solving for an approximation $\mathbf{Q}$ in the space of functions that are discontinuous at element boundaries and of polynomial degree r within cell k, i.e. $\mathbf{Q}_k=\sum_{i=0}^{R}\mathbf{c}_i^k p_i^k(\mathbf{x})$, where $\{p_i^k\}$ spans the local space of polynomials $P^r(\Omega_k)$ and $\mathbf{c}_i^k\in\mathbb{R}^n$. By using $v(\mathbf{x})\equiv p_i^k(\mathbf{x})$ as test functions and choosing an orthogonal set of polynomials, each element's mass matrix can be diagonalized, allowing the construction of fully explicit schemes (see [10, 45, 42] for details). The greatest strength of the DGM compared to conventional finite volume methods is the compactness of the discretization that requires neighboring information only to construct inter-element numerical fluxes to evaluate the surface integral in Eq. (4), for instance with an approximate Riemann solver (cf. Section 2.1). The DGM can be used on arbitrary triangulations, including those with hanging nodes, without problems and the polynomial basis in every cell can be decided locally, allowing for both spatial and polynomial adaptation. These properties make the DGM particularly interesting for embedded boundary methods that construct complex cut-cells (see Fig. 8 for a typical scenario) and might merge small cells with neighbors to reduce numerical stiffness, possibly leading to a non-conforming mesh (cf. right sketch of Fig. 9). Coirier and Powell [11] have demonstrated that small cell merging increases the local absolute error marginally, but leaves the overall order of a finite volume scheme unaffected. If required, local non-conformity can be eliminated by cell shape adjustment [43].

In principle, discretizing Eq. (4) on arbitrary cut-cells requires only Gaussian quadrature rules to evaluate the first and last integral and a loop over all cut-cell surfaces. Note that in general orthogonality of a given basis $\{p_i\}$ will be lost on arbitrary cell shapes resulting in a dense local element mass matrix. A first promising investigation for solving the Poisson equation with DGM on a two-dimensional Cartesian cut-cell mesh has been published by van Raalte [48]; Engwer and Bastian have recently applied the idea to simulate porous media flow with embedded solid obstacles [26]. When used with an explicit scheme, an embedded boundary DGM will involve solution of a dense $R\times R$ linear system with n right-hand sides in every cut-cell, which, given its small size, can be accomplished very effectively, e.g., by Cholesky decomposition. As an optimization, especially for explicit schemes, the derivation of a polynomial adaptive DGM that uses different orthonormal basis functions depending on the cut-cell type would also be of interest. Such sets of appropriately parameterized polynomial bases can be constructed by Gram-Schmidt orthonormalization (cf. [42]). If the boundary is specified as the iso-surface of a scalar field defined in the element corners, and a linear boundary approximation is assumed, only three fundamentally different cut-cell configurations can occur in two and 15 in three space dimensions [34].

3.2 Structured adaptive multi-level methods on petascale systems

The incorporation of an embedded boundary DGM into a SAMR framework, such as AMROC, is relatively straightforward. As the DGM has the communication pattern of a conventional finite volume method with extended vector of state, only a new single grid update routine with non-uniform workload and proper inter-level transfer operations for all degree of freedom are required. While the stencils of finite difference schemes increase with order [3], the DGM has always the stencil radius 1. This property together with the high local computational expense make the DGM very advantageous for distributed memory computers. Integrating the method into a block-structured mesh refinement system adds not only spatial and temporal adaptivity but combines single cells into larger cache-coherent compute entities in a natural way. Early investigations on multicore systems have

underscored that enforcing locality by data clustering is essential for exploiting multi-threaded shared memory parallelism [6]. Since the upcoming generation of petascale computers connects multi- and manycore shared memory compute nodes to hybrid distributed memory supercomputers, the overall approach provides an outline for utilizing such architectures effectively. It can be expected that, like for conventional finite volume methods, a block-structured adaptive DGM will outperform cell-based refinement approaches [3, 42]. In practice, the utilization of hybrid architectures requires an implementation that utilizes both MPI and OpenMP. The most immediate MPI/OpenMP parallelization would employ the existing MPI-based domain decomposition for distribution to nodes and OpenMP to parallelize the many loops over independent subgrids, characteristic for SAMR.

Further research is still required to develop multi-constraint domain decomposition methods directly applicable to hierarchical data structures that balance the work on every level, while keeping intra- and inter-level communication and data migration costs after repartitioning small. Figure 7 shows a representative AMROC scalability test with the currently employed strictly local domain decomposition method based on a space filling curve that partitions the hierarchy at the base level only [15]. The test uses a typical time-explicit finite volume scheme on a base grid with 32^3 cells and two additional levels with refinement factors 2, 4 and shows an ideal scale-up only for up to 128 nodes.

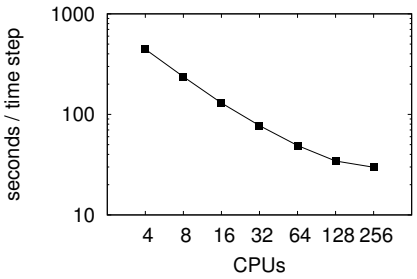
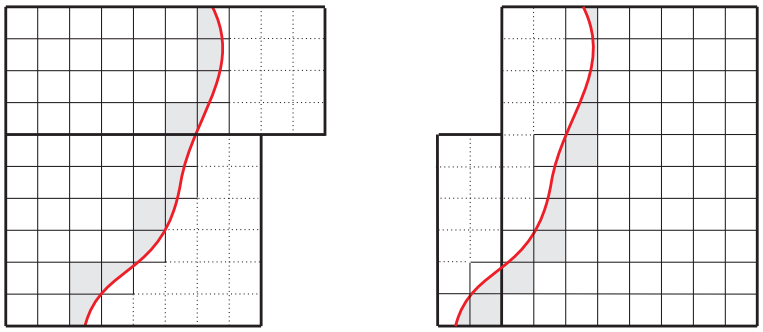


Figure 7: AMROC scalability test.

3.3 Multiphase and free surface problems

While an embedded boundary DGM can be developed most effectively for (moving) solid walls, a natural extension is the application of Eq. (1) to model dynamically evolving free surfaces or multiphase boundaries. Such problems can be solved with the "ghost-fluid" technique [27] similar in spirit to the method outlined in Section 1. Although this approach permits the unchanged utilization of higher-order finite difference schemes, it introduces a $O(h)$ conservation error and approximates the flux at the interface only crudely. Volume-of-fluid finite volume schemes on the other hand consider all volume changes and interfacial fluxes properly and are hence discretely conservative, but in practice use simplified reconstruction stencils near the boundary, reducing the order of accuracy at the boundary [12, 44]. Since such methods typically utilize a second-order accurate scheme away from the cut-cells, the global error often scales with $O(h^2)$, particularly when measured in the integral L_1 or L_2 norms. Nevertheless configurations can easily be constructed that exhibit a clear order reduction, especially in the L_∞ norm (cf. [12]). Since the DGM uses an entirely local higher-order interpolation, and values of the immediate neighbors are only required for numerical flux evaluation and limiting of discontinuous solutions (cf. [32, 10, 42]), a volume-of-fluid DGM will avoid all such problems elegantly.

The practical implementation of multiphase problems is complicated by the fact that the vector of state along the embedded boundary is multi-valued and a different numerical method might have to be employed for each phase. A naive solution would utilize a separate grid for every vector of



Grids for phase A Grids for phase B

Figure 8: Efficient application of Cartesian SAMR for multiphase problems. The shown meshes correspond to a higher refinement level. The actively used domains of cut-cells in an embedded boundary DGM are shaded gray.

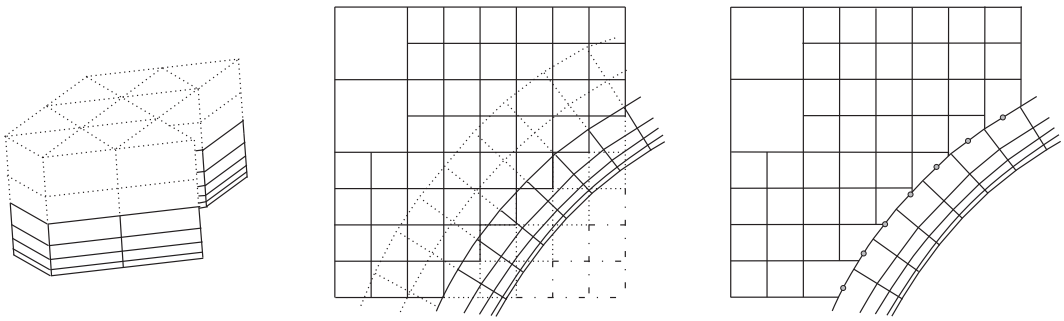


Figure 9: Left: Portion of a body-fitted triangular mesh tailored for boundary layer resolution. Center: Overlaying meshes in a Chimera approach. Ghost cells are displayed dotted. Right: The DG discretization allows the direct embedding of the body-fitted mesh into the Cartesian mesh. Small cut-cells have been merged with neighbors. The gray dots mark the location for evaluating the interfacial fluxes.

state covering the entire domain, but this approach is inappropriate for large-scale problems that are tractable only by mesh adaptation. I envision a novel memory- and computation-efficient solution to this problem that would use separate SAMR refinement hierarchies for every vector of state and multi-level scheme involved (cf. Fig. 8). By defining each SAMR hierarchy on the same base grid and using identical refinement factors, the boundary data exchange between hierarchies can be accomplished (as usual in SAMR methods) through integer-valued cell indices. As the AMROC core C++ data structures are already fully templatized, only additional communication routines would be required to enable the data exchange between distributed SAMR hierarchies in parallel.

3.4 Viscous boundary layer flows

When second-order problems, such as elliptic or convection-diffusion equations, are to be discretized with the DGM, the equations first need to be written as an extended first-order system [9]. While for instance the discretization of the compressible Navier-Stokes with such a "local DGM" is then straightforward [1], consideration of the solenoidal constraint in the incompressible Navier-Stokes equations can be accomplished for instance by specially chosen polynomial functions [30] or by applying a local projection operator in a post-processing step [8].

The practical computation of approximations of the Navier-Stokes equations becomes particularly challenging when boundary layers around objects influence the flow field considerably. Cartesian mesh adaptation is an inappropriate choice in this case since an exponential resolution reduction normal to the boundary is necessary to capture all flow features [28]. Providing the required resolution uniformly, i.e. with identical refinement in all three Cartesian directions, is highly inefficient. The best method currently available for computing boundary layer flows around moving objects is the adaptive Chimera approach developed by Meakin [37]. Communication between Cartesian and non-Cartesian meshes is accomplished via interpolation of ghost cell values after successive mesh updates. The approach uses the full stencil of a conventional finite volume method and is hence higher-order accurate, but the transfer operations between overlapping meshes are non-conservative. In order to cope with this fundamental problem I propose to utilize the local DGM instead. The properties of the DGM (compactness, tolerance to hanging nodes) allow the direct construction of a single mesh in which a small layer of non-Cartesian boundary-aligned cells near the body is directly embedded into the Cartesian background mesh and the method can be implemented as an extension of the embedded boundary DGM described in Section 3.1. In order to facilitate an on-the-fly generation of the boundary-fitted mesh and to allow arbitrary embedded geometries, three-dimensional bodies will be prescribed as a surface mesh of triangular elements, see left sketch of Fig. 9. The boundary-fitted mesh itself is then constructed by extension in the normal direction and a re-evaluation of the triangular vertices in every time step to consider surface mesh distortions and movements.

When extending the embedded boundary DGM sketched in Section 3.1 to hybrid meshes (like the one depicted in the right sketch of Fig. 9) only the discretization of the surface integral in Eq. (4) is non-obvious. An accurate coupling could be accomplished for instance as follows: 1. Compute all numerical fluxes $\mathbf{F}(\mathbf{Q}^+, \mathbf{Q}^-)$ in both meshes except at the mesh interface. 2. Evaluate $\mathbf{Q}_j$ in the midpoint of the jth boundary facet (marked by gray dots in Fig. 9) in the boundary-fitted (B) and the Cartesian (C) DG grid. 3. Use $\mathbf{F}(\mathbf{Q}_j^C, \mathbf{Q}^B)$ as jth boundary flux of the boundary-fitted mesh. 4. Distribute $\mathbf{F}(\mathbf{Q}_j^C, \mathbf{Q}_j^B)$ to the Cartesian cells in contact with facet j according to the area of intersection.

As the boundary layer mesh is small compared to the encompassing Cartesian mesh, it is reasonable to assume that non-Cartesian meshes have a tangential resolution comparable to the finest level of Cartesian mesh adaptation (cf. Fig. 9). This particular choice has several advantages: 1. In contrast to current existing Chimera implementations [38, 4] no dynamic mesh adaptation is necessary in non-Cartesian meshes. 2. Mesh adaptation can be implemented under the usual SAMR assumption of a global integer-valued index coordinate system without searching for neighboring grids in geometrical space. 3. Parallelization and especially load-balancing are straightforward, because additional to the current solution in AMROC only non-Cartesian meshes with regular topology have to be considered. The easiest solution is to parallelize these separately and, as communication with the DG approach is only necessary along the interface mesh, to utilize the same VTF communication routines that accomplish the boundary data synchronization between AMROC and a solid mechanics solver in the case of fluid-structure interaction, compare Section 2.2.

3.5 Lattice-Boltzmann methods with SAMR

Finally, as a very fast alternative for incompressible subsonic flows it would be interesting to extend the idea of block-structured mesh adaptation to grid-based Lattice-Boltzmann methods [31], which are currently used for approximately 2/3 of all exterior flow simulations in the automotive industry. To my best knowledge, all existing solutions use a cell-based refinement approach mandating expensive tree traversals that take in practice, due of the simplicity of the Boltzmann operators, more than 50 % of the overall compute time (private communication with M. Krafczyk). It can be expected that a block-structured solution can eliminate such overhead costs almost completely.

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