1.3 Pressure-robust Flow Discretizations on General Polyhedral Meshes

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Computational fluid dynamics and quality meshes

Computational fluid dynamics (CFD) is a key technology of our modern society: It is of fundamental economic importance in weather forecasts for agriculture, air transportation, and emergency management, and can give substantial theoretical insight in various scientific disciplines like medicine, climate research, or astrophysics. Even hot topics like the spread of the Corona virus in aerosols or stability investigations of the gulf stream in relation to climate change are covered. What CFD simulations have in common is that they are based on a translation process: Physics describes the motion of fluids, e.g., water or air, by balance laws for their mass and momentum distribution. These laws are formulated in the language of mathematics, leading to the famous *Navier–Stokes equations*, which has continued to trigger challenging research questions since their discovery in the early nineteenth century. And finally, CFD translates these equations by a process called *discretization* into a language that is understood by modern computers. Like any translation process, also *discretization* is error-prone. And what makes the discretization even more challenging is that a reduction of the complexity, i.e., a *compression of information*, of the original problem is needed in order to make simulations computationally feasible in practice. In particular, a lack of *pressure-robustness* as discussed in this contribution can be a very important potential error source during this compression of information.

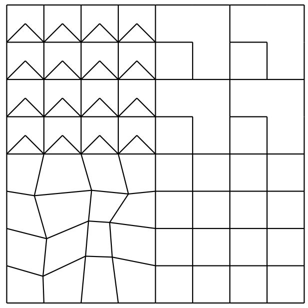

Fig. 1: *A square divided into various convex and non-convex polygons with hanging nodes showing the flexibility of polygonal meshes*

A starting point for the discretization of any CFD simulation is the availability of a *mesh*. A mesh serves several purposes. Basically, it delivers a partition called *triangulation* of the flow domain of interest, e.g., the outer space of an airplane. In every *control volume* of the mesh, a certain kind of *discrete physics* has to hold, which approximates the original balance laws for the mass and momentum distribution in the fluid. These control volumes are key for the simulation: On the one hand, the more control volumes are spent in the mesh, the more accurate the simulation results are. On the other hand, more control volumes mean more computing time and memory, hence, more electricity and money. But not only the pure number of control volumes, also the shape of the control volumes may help to approximate the physics of the flow. Thus, the availability of *quality meshes* is fundamental for CFD. Such quality meshes allow for appropriate unstructured, adaptive and anisotropic control volumes delivering an appropriate *compression of information*.

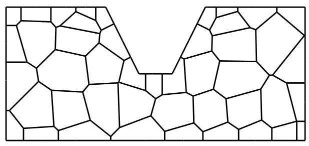

Fig. 2: *A Voronoi–Delaunay mesh as used, e.g., in WIAS electrochemistry simulations*

In the past, numerical mathematics required certain assumptions on the structure of the underlying mesh: Meshes should be built from simple geometrical objects like tetrahedra or hexahedra in three space dimensions, resp. triangle or quadrilaterals in two space dimensions, facilitating the algorithmic construction and the theoretical investigation of CFD considerably. In recent years, these assumptions have been questioned, though. Instead, *polyhedral meshes* have been proposed, where the flow domain of interest is decomposed into a partition of polyhedra in 3D, resp., general polygons in 2D, which has a great potential to simplify quality mesh generation; see Figures 1–2 for examples.

Indeed, *polyhedral meshes* facilitate:

- efficient local *mesh refinement*, wherever the physics of the flow locally requires a higher resolution, since *hanging nodes* can be incorporated naturally;
- anisotropic meshes, since anisotropic prismatic control volumes for challenging multiscale phenomena — like the resolution of boundary layers — are allowed;
- multi-physics, i.e., coupling with simulators for other subprocesses with specific mesh requirements is simplified, e.g., with WIAS electrochemistry finite volume solvers on Voronoi–Delaunay meshes.

However, a major challenge still remains: The *translation process of discretization* for challenging flow problems is much more error-prone on polyhedral and quality meshes than on simple (structured) grids. Especially, for incompressible flow problems recent WIAS research has recognized that only so-called *pressure-robust* flow solvers can be accurate and efficient in general. Thus, this article describes recent progress on the construction of *pressure-robust* flow solvers for *polyhedral grids*.

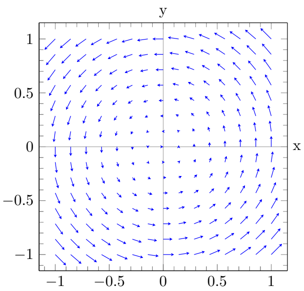

Fig. 3: *A divergence-free vector field. Thus, the* streamlines *of the flow field, indicating the path a fluid parcel will take, are closed loops.*

The incompressible Navier–Stokes equations

CFD as described above consists in the approximate solution of the Navier–Stokes equations (NSE). Mathematically, they form a challenging system of *partial differential equations*, whose solutions, i.e., *the output* of the simulation, are whole functions that model the mass density ρ of the fluid and the velocity distribution in the fluid $\mathbf{u}$. Since the physical quantities ρ and $\mathbf{u}$ depend on time and space, these functions depend actually on four variables: the time t and the position in space x, y, and z. It is important here to mention that the velocity $\mathbf{u} = (u, v, w)$ is represented as a *vector* of velocities, where u models the velocity of the fluid in x-direction at any point in the domain at any given time t, and v and w model the velocities in y- and z-direction.

Physically, the Navier–Stokes equations are a model that is based on classical Newtonian physics and a few simplifying assumptions valid for many relevant flows. These simplifications allow for a certain *compression of information* as mentioned above: i) in the absence of sources and sinks, *mass is conserved*, and ii) *momentum* changes only by the action of forces. Especially, the Navier–Stokes equations incorporate the *pressure gradient* as a driving force of the fluid and the *friction* force, which tends to decelerate and to homogenize the fluid velocity distribution as a whole. As a rule of thumb, high speed flows, so-called *high Reynolds number flows*, where the friction forces are negligible in large parts of the flow domain, are more difficult to simulate than low-speed flows, where comparably stronger friction forces simplify the simulations.

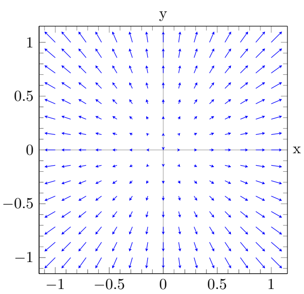

Fig. 4: *A gradient vector field. All streamlines start in the origin of the plot; hence, it is non-divergence-free.*

In the past, research at WIAS has focused on fluid flow in liquids as opposed to fluid flow in gases. Fluid flow in liquids is one — and not the only one — extreme case in fluid mechanics: Such flows are called *incompressible*, since the density of a liquid is practically independent of the pressure. Therefore, the balance law of *mass conservation* for the fluid mass *degenerates* to a *geometric constraint* for the velocity field: The velocity field $\mathbf{u}$ is *divergence-free*, i.e., at every time t, what flows into an arbitrary control volume has to flow out of the control volume, elsewhere. This geometric constraint is very strong and has some important consequences. Here, it matters most that the incompressible Navier–Stokes equations are truly vector-valued. Neither do they make much sense in a one-dimensional setting — under reasonable boundary conditions, the only one-dimensional, divergence-free velocity field is $\mathbf{u} = \mathbf{0}$ —, nor is it reasonable to decouple the equations for the velocity $\mathbf{u} = (u, v, w)$ into three, separate *scalar* equations for the velocity components u, v, and w.

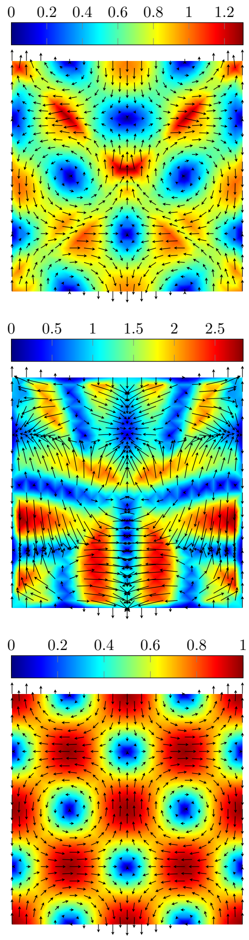

Fig. 5: *Velocity fields and their absolute values for a planar lattice flow for $\nu = 10^{-4}$ at time $t = 1$ (transient Stokes equations with exact convection term) calculated with different methods on the same mesh. The classical Taylor–Hood (top, 4771 unknowns) and Bernardi–Raugel (middle, 3682 unknowns) methods show large errors, whereas the pressure-robust Bernardi–Raugel method (bottom, 3682 unknowns) resolves the velocity better.*

Some history and WIAS research on pressure-robustness

According to the Helmholtz–Hodge decomposition, all the various forces of the vector-valued incompressible Navier–Stokes equations like the pressure gradient, the viscous forces, and the material derivative can each be split into sums of only two basic type of forces: *divergence-free forces* (closed streamlines as depicted in Figure 3) and *gradient field forces* (streamlines start and end in sources and sinks or at the boundary of the flow domain as shown in Figure 4), which is a remarkable difference to the one-dimensional case, where every force is a gradient, according to the fundamental theorem of calculus. It holds an important orthogonality property: Divergence-free vector fields $\mathbf{w}$ whose streamlines do not leave the flow domain and arbitrary gradient fields $\nabla\phi$ are perpendicular in the following sense:

$$\int \nabla\phi \cdot \mathbf{w} \, \mathrm{d}x = 0. \tag{1}$$

The WIAS research on *pressure-robustness* is essentially based on an improved understanding of how the orthogonality relation (1) can be exploited in a CFD algorithm. The term pressure-robustness indicates that the role of the pressure gradient is very special in the incompressible NSE: Only the divergence-free parts of forces like the friction force and the material derivative drive the flow; the gradient field parts of forces in the Navier–Stokes momentum balance are always balanced completely by the pressure gradient, which instantaneously adapts itself all the time for this purpose. This strange behavior of the pressure gradient is due to the degeneracy introduced by the divergence constraint.

Physically, this behavior leads to strong and complicated pressure gradients in fast and challenging vortex-dominated, e.g., hurricane-like, flows at high Reynolds numbers, since the centrifugal force, i.e., the nonlinear material derivative, in a rotating flow is nearly completely balanced by the pressure gradient. Recent WIAS research confirmed that *pressure-robustness* allows for more accurate simulation of such vortex-dominated flows at high Reynolds numbers [5].

Furthermore, the notion of *pressure-robustness* emanates from an improved understanding of the classical *theory of mixed methods* from the 1970ies, which is commonly viewed as a complete theory. This theory allows to construct CFD algorithms for the incompressible Navier–Stokes equations that converge to the exact flow solution if the mesh gets finer and finer. It proposes to relax the cumbersome divergence constraint in order to facilitate the construction of CFD algorithms. To this end, it introduces *discretely divergence-free* vector fields, for which (1) only holds in a certain *discrete sense*, i.e., not for arbitrary smooth ϕ. Unfortunately, this relaxation causes a lack of *pressure-robustness*, resulting in large discretization errors in case of high Reynolds number flows.

In a sense, the numerical analysis of partial differential equations since the 1970ies can be understood as the history of attempts to construct CFD algorithms that have less and less unnecessary constraints. On the one hand, these attempts concern the meshes, where first simplicial and hexahedral meshes were used and nowadays polyhedral meshes are exploited. On the other hand, they concern different kinds of continuity and differentiability constraints for the ansatz and test functions used in a CFD algorithm (H^1 -conforming finite elements, nonconforming finite element schemes, $\mathbf{L}^2$ -conforming Discontinuous Galerkin and finite volume schemes, ...).

In this context, past WIAS research on CFD algorithms on simplicial meshes has demonstrated that the sophisticated and efficient use of so-called $\mathbf{H}(\mathrm{div})$ *-conforming finite element schemes* allows to fulfill the orthogonality relation (1) exactly, leading to accurate simulation results for time-dependent vortex-dominated high Reynolds number flows [5]. At WIAS, researchers have revealed that pressure-robustness comes from divergence-free and $\mathbf{H}(\mathrm{div})$ -conforming discrete test functions, and not from trial functions [6].

As an outcome, novel pressure-robust low-order schemes like the pressure-robustly modified first-order Bernardi–Raugel scheme can be competitive, or on coarse unstructured meshes even superior, to higher-order schemes like a second-order Taylor–Hood method. An illustration with a time-dependent planar lattice flow $\mathbf{u}(x, y, t) = e^{-8\pi^2 \nu t}[\sin(2\pi x)\sin(2\pi y), \cos(2\pi x)\cos(2\pi y)]$ simulated in the time interval $(0, 1)$ is depicted in Figure 5. This illustration indicates that schemes of (formal) higher order are not enough for an efficient and accurate CFD simulation. Likewise, physical fidelity like pressure-robustness is important for the *translation process of discretization*.

In search for more flexible CFD algorithms, the extension of pressure-robust schemes to polyhedral meshes by exploiting $\mathbf{H}(\mathrm{div})$ conformity has naturally emerged as a research topic.

Pressure-robustness on polyhedral meshes

Methods allowing for polyhedral and polygonal meshes that were drawing enormous attention in the last decade are *hybrid high-order methods* (HHO) and *virtual element methods* (VEMs), besides, e.g., *discontinuous Galerkin methods*, *extended finite element methods*, or *mimetic finite difference methods*. HHO and VEMs work on general polyhedral meshes, but also give the possibility to respect physically relevant properties such as mass conservation.

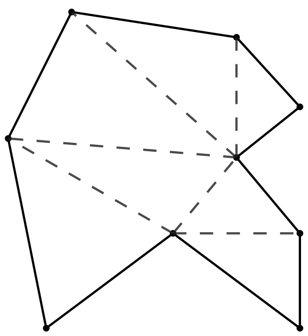

Fig. 6: *A polygon (solid lines) and a possible subtriangulation (dashed lines)*

In the case of VEMs, the divergence constraint mentioned above can be satisfied *exactly* and not only discretely by the design of the ansatz functions in the underlying discrete velocity and pressure space. However, here not only polynomials, but also other non-polynomial basis functions in the velocity space are required. Those basis functions are only defined implicitly, which is why the method is called *virtual* and, hence, have to be treated with care during the design of the discrete equations.

In general, exactly divergence-free methods are also pressure-robust since exactly divergence-free test functions are orthogonal in the sense of (1) to the gradient part of the force. However, this is not the case for the classical VEM, since the virtual test functions need to be projected to suitable polynomial functions that can be evaluated everywhere. Unfortunately, the *classically used* L^2 *best-approximation* does not preserve the divergence, i.e., the projection and the gradient part of the force are not orthogonal in the sense of (1). Therefore, gradient forces in the momentum balance might have a possibly enormous impact on the approximation of the velocity.

To repair the lack of pressure-robustness for the VEM in the spirit of the WIAS approach, another projection has to be used that preserves the divergence. This new and carefully designed *pressure-robust projection* is based on a subtriangulation of the polygons as in Figure 6, and thereon uses well-established ideas of $\mathbf{H}(\mathrm{div})$ -conforming interpolations. It ensures the continuity of the normal flux along the triangle boundaries and, hence, the divergence of the function is preserved, but now can be evaluated pointwise everywhere [4]. The superiority of the new pressure-robust variant compared to the classical VEM can also be seen in Figure 7 in practice for a high Reynolds number flow.

It can be noted that the subtriangulation is used only locally and that the total number of degrees of freedom stays the same. To conclude, this new *pressure-robust* VEM benefits from less computational cost and more flexibility due to polygonal meshes compared to simplicial methods on the corresponding subtriangulations, and reduces the computational cost dramatically in case of strong gradient field forces or high Reynolds number flows compared to the classical VEM.

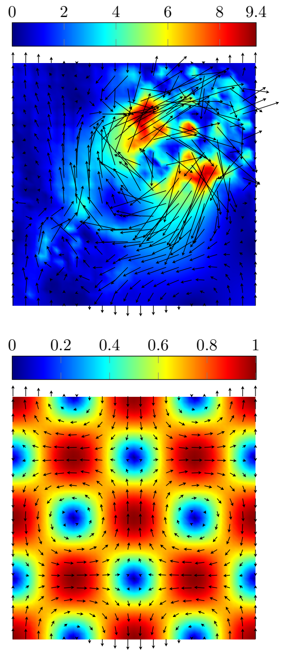

Fig. 7: *Velocity fields and their absolute values of the same velocity as in Figure 5 at fixed time $t = 0$ and $\nu = 10^{-4}$ (steady Stokes with exact convection term and exact time derivative) computed by different VEMs with 3426 unknowns. The classical VEM (top) shows large errors, whereas the pressure-robust VEM (bottom) resolves the velocity better.*

Outlook

Future research at WIAS on pressure-robust schemes has the following three main goals:

A first goal is to tap the full potential of pressure-robust methods on quality meshes. This goal concerns multi-physics and multi-scale real-world applications as in Czochralski crystal growth and in electro- or magneto-hydrodynamics. And it concerns the construction of CFD algorithms that deliver provably robust and accurate results on anisotropic three-dimensional meshes. First steps towards this goal for simplicial three-dimensional meshes can be found in [3].

A second goal is the construction of novel convection stabilizations for high Reynolds number flows that do not interfere with pressure-robustness. As a first result, the recent WIAS preprint [1] constructs the first $\mathbf{H}^1$ -conforming, convection-stabilized (LBB-stable) mixed method for the incompressible Oseen model problem that delivers provably optimal velocity convergence rates. Pressure-robustness is decisive to obtain the result.

Third, pressure-robustness extends nicely to novel well-balanced schemes for the compressible Navier–Stokes equations, where dominant gradient-field forces may also excite numerical errors at low Mach numbers [2]. In the future, WIAS research will investigate the case of compressible high Reynolds number flows at low — up to extremely low — Mach numbers.

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