New Approaches for Simulating Complex Flows

When it comes to simulating the flow of material mixtures, classical CFD (computational fluid dynamics) methods reach their limits. For several years now, Sulzer has been pursuing a fundamentally new approach—the Lattice-Boltzmann method—working closely with an external research partner (FlowKit SA). Sulzer uses this method to simulate specific products, and this method makes it possible to develop technically superior solutions, both for pumps and for separation and mixing technology.

The Palabos open-source software is the result of collaboration between industry and academia, and it provides the basic building blocks for a wide range of flow simulations using the Lattice-Boltzmann method (see infobox). One advantage of Palabos is that, in contrast to traditional CFD methods, the computational grids are automatically generated; even very complex geometries do not need to be simplified at the expense of accuracy (for more information: www.palabos.org). One of the benefits of the Lattice-Boltzmann method is that the algorithm can be very easily parallelized (i.e., divided among several simultaneously ongoing subcalculations) and has an almost perfect scalability. A further advantage is the relatively easy implementation of models for complex physical phenomena, which is mainly of interest for simulations with multiphase fluids. The resulting mesh, which is finer than with traditional CFD methods, along with the restrictive time step size, however, leads to an increased need for hardware resources for the simulations. Sulzer has the required infrastructure: the high-performance cluster that is jointly used by Pumps Equipment and Chemtech. Three case studies that show the successful use of the Lattice-Boltzmann method at Sulzer are described below.

Pump simulations with Palabos

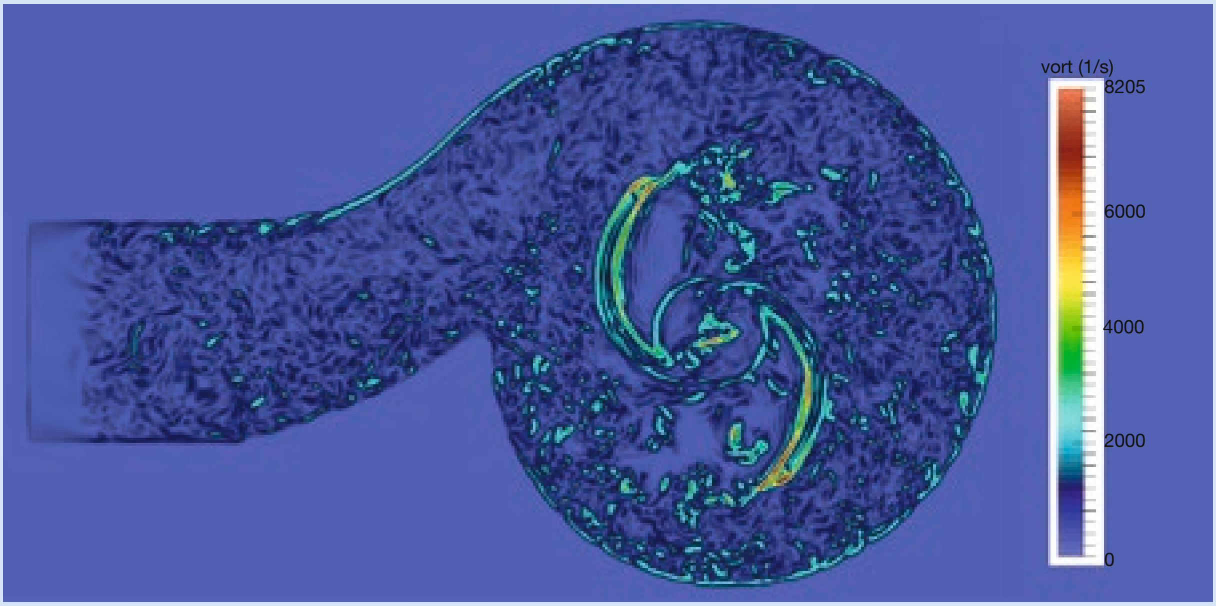
As a first step, Sulzer evaluated the Palabos software for pumps simulations with the aim of correctly predicting the target pump curves for single-phase flow. The programmers from FlowKit set up a code framework to read in pump geometries and operating data easily via an interface (in XML, extensible markup language).

Tracking the molecules with the Lattice-Boltzmann method

Classical CFD (computational fluid dynamics) codes are based on the Navier-Stokes equations, and they describe flow on the basis of macroscopic values, such as the velocity or the density of the fluids. The Lattice-Boltzmann method, on the other hand, is a microscopic simulation method in which flow is described through the transport and interaction of individual molecules. In doing this, it is not the molecules themselves, but their probability density f that is considered. It describes the probability of finding a particle with a specific particle velocity ξ at a given location at a specific time. The Boltzmann equation describes the temporal and spatial development of f:

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla f = C(f)$$

In this case, the flow simulation must model the collision operator $C(f)$. The macroscopic flow variables are obtained as statistical moments of f.[1]

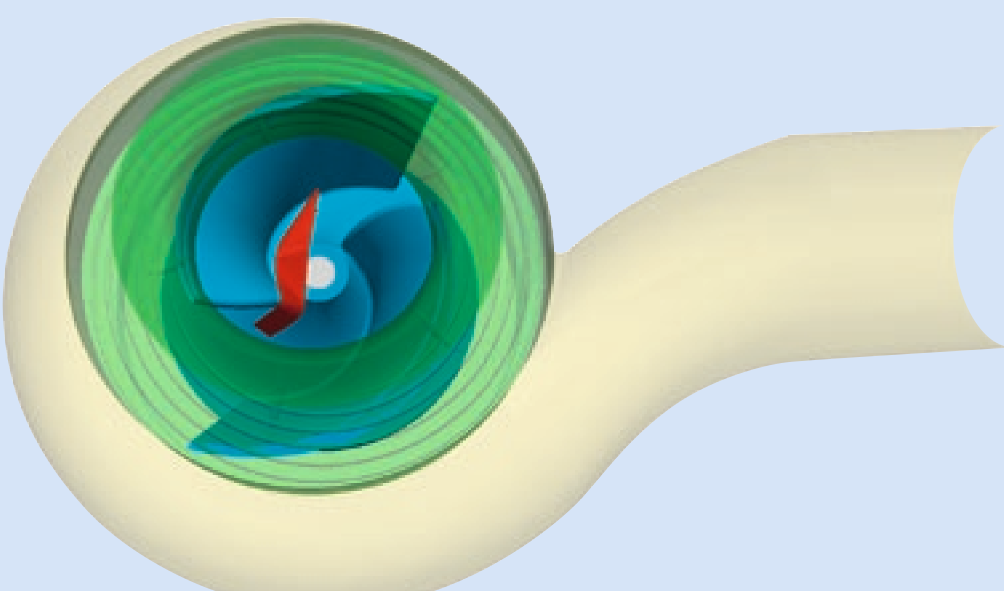


1 Vortex structures in a pump can be simulated very precisely with the Palabos software and the LES turbulence model.

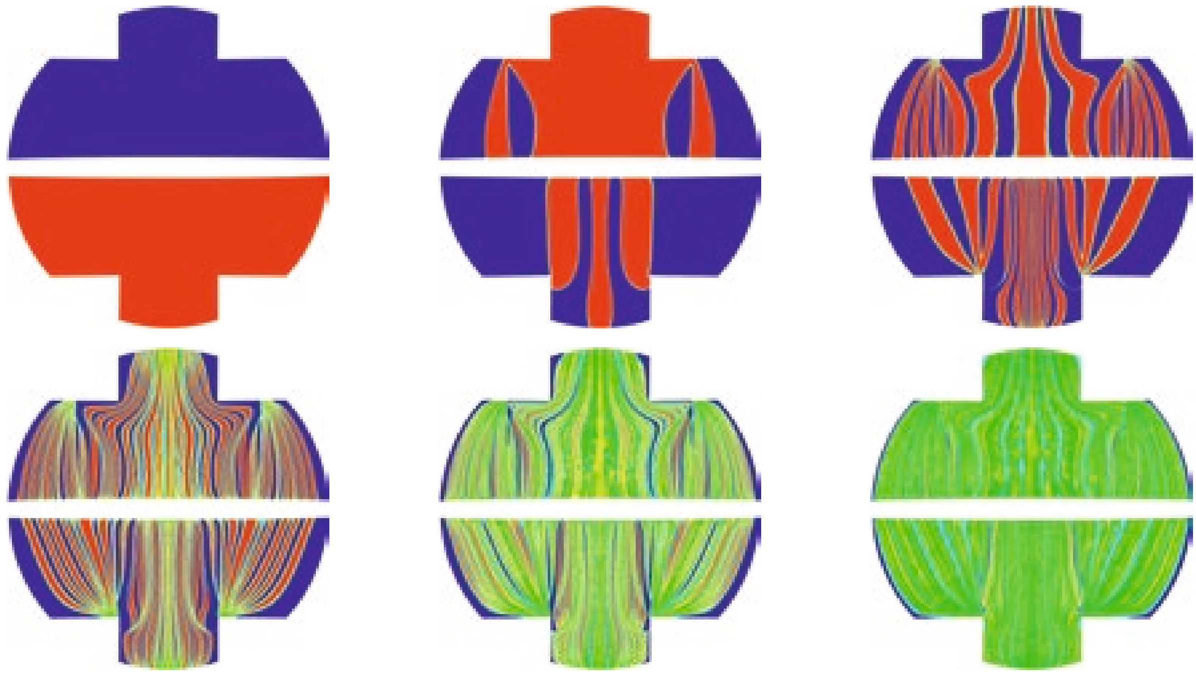
Because pump simulations with the Lattice-Boltzmann method are breaking new ground, a great deal of time was invested in the calibration of the method, to obtain accurate results. The choice of the boundary conditions at the outlet of the computational domain was particularly challenging because numerical pressure wave reflections occurred at certain settings. Fig. 1 shows how finely the turbulence structures in the pump could be resolved with the LES turbulence model (large eddy simulation).

Interaction with solids

Clogging means the blockage of a pump by solids such as rags. CFD analysis of the flow conditions close to the blades can be used only to a limited extent to estimate clogging behavior. Other possibilities, such as the simulation of a scalar or two-phase mixture with an extremely high viscosity component, are also of limited use because the interaction of solids with the pump impeller is physically not correctly modeled. Therefore, Sulzer used the Lattice-Boltzmann method to simulate



2 The simulation shows the interaction between a cloth (red) and the impeller (blue) of a wastewater pump.



3 The predicted mixing quality of the MIXPAC™ T-mixer is illustrated by means of the concentration distribution at several cross-sections along the mixer (inlet distribution followed by distributions after two, four, six, eight, and ten mixing elements). The colors red and blue denote the two components, and green areas describe regions that have been mixed through molecular diffusion.

a wastewater pump with a piece of cloth by means of coupled fluid-structure interactions. The difficulty here is to correctly simulate the deformation of the cloth and the detection and handling of the collisions with the pump surfaces. The elasticity of the cloth and the friction at the surfaces must also be calibrated according to realistic conditions. Fig. 2 shows a simulation example.

Mixing behavior of highly viscous fluids

Although the prediction of laminar flow is very reliable with classical CFD methods, the description of the mixing behavior of highly viscous fluid components involves certain risks with these procedures. In addition to the natural molecular diffusion, the steep concentration gradients can also be reduced in the simulation by numerical diffusion, due to the coarse computational grid. Passive particles thereby offer a sensible alternative for describing the mixing process because the particle trajectories are not bound by the numerical grid. The almost linear scalability of Palabos makes it possible to calculate a very large number of such particles efficiently. This leads to very detailed results within the entire laminar mixer.[2] Sulzer further optimized this general approach for the prediction of static laminar mixers with the same fluid properties. The component layers, which become thinner the more mixer elements there are, can be described in more detail using this method (Fig. 3).

Outlook

The case studies examined have shown that the open-source Lattice-Boltzmann-Palabos package is a promising option for the analysis of complex physical flow phenomena. Thanks to the use of specialized open-source simulation tools and the collaboration with external research partners, Sulzer can get involved in the development process of these tools and obtain specialized predictive applications at a reasonable cost.

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Literature

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