Subproject B5

Title

Adaptive computing grids in space and time for efficient simulation of moving phase boundaries

Project management/-processing

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Task definition

The goal of subproject B5 in 2018 was the simulation of test cases to provide reliable time measurements and the efficiency aspects of the filling process of complex 3D shapes using adaptive time refinement.

Mold filling is an injection molding phase of great importance, since many defects of the plastic components can occur in this process step. It therefore plays an important role in determining the quality of the parts produced. Our goal is to provide temporal refinement close to the developing melt front within the framework of 4D simplex space-time grids.

This novel discretization method has an inherent flexibility to use completely unstructured grids with different levels of resolution in both spatial and temporal dimensions, allowing the use of local time steps during the simulations. This can lead to a higher simulation precision while maintaining the efficiency of the calculation.

The simulations are two-phase flow simulations [E1, E2], which include:

i. Injection molding of a three-dimensional plate-shaped geometry obtained from the Institute of Plastics Processing at the RWTH Aachen (IKV);

ii. Injection molding of a three-dimensional cavity with manifold (geometry obtained from Sandia National Laboratories).

Procedure

The main features of the mathematical model are:

i. Navier-Stokes equations for incompressible viscous Newtonian fluids or pseudoplastic fluids;

ii. the transient incompressible Navier-Stokes equations, are coupled with the heat conduction equation;

iii. an efficient and robust algorithm to capture the complex frontal movements (level set equation);

iv. the slip-type boundary conditions are a means of circumventing the "kinematic paradox" of a moving contact line at a slip-type boundary. A contact model is used in combination with a slip type boundary condition and the condition itself is restricted to a small zone in the immediate vicinity of the moving phase boundary;

v. Combining the Navier-Stokes equations and the level set methodology with novel unstructured space-time grids;

vi. temporal refinement in the area of the material front.

The numerical methods used for the simulation are:

vii. stabilized linear and square stabilized finite elements [Galerkin/Least-Squares];

viii. Space-time finite elements with time integration;

ix. in-house-Solver XNS in Fortran und C;

x. in-house mesh4d mesh generator in Fortran, C and Python for temporal design based on Delaunay triangulation (qhull code);

xi. Newton-Raphson-Iterationen with the linear GMRES Solver;

xii. ILU Preconditioning, scaled over several thousand processor cores.

Results

The filling of a plate-shaped geometry was simulated with the in-house solver XNS of the Chair for Computational Analysis of Technical Systems (CATS) [E1]. The Institute of Plastics Processing (IKV) supplied the geometry. A filling study was performed to illustrate the development of the flow front and the pressure distribution at different positions of the cavity and to analyse the simulation performance, while an adaptive temporal refinement was performed with XNS. To validate the proposed method, virtual experiments were conducted by the Institute of Plastics Processing (IKV) using the injection molding software Moldflow developed by Autodesk, San Rafael California, USA.

Next, we calculated the filling process of a three-dimensional cavity with manifold [E2]. Due to the symmetry of the geometry to the center plane, only half of the geometry was simulated, which saved time and resources. The same test case was simulated by Sandia National Laboratories using the ARIA software. In this benchmark we observed the temperature and viscosity profile and the shape of the developing interface. Although Sandia National Laboratories had assumed a Newtonian melt without temperature gradients, in our first calculation the effects of the structural viscosity were taken into account and represented using the Carreau-WLF model.

Summary and Conclusion

In 2018, the two-phase flow of highly viscous liquids was calculated using a novel discretization approach, which allows for arbitrary temporal refinement of the space-time plates near the developing front of the highly viscous melt during injection molding.

Future work includes the combination of arbitrary temporal refinement with arbitrary spatial refinement near the developing interface. The refinement criterion should be based on an appropriate a posteriori error estimation of local or global quantities of interest, such as front curvature, pressure discontinuities near the interface, material discontinuities and gradients in the viscosity field.

Publication

[E1] Karyofylli, V., Schmitz, M., Hopmann, C., & Behr, M. (2018, May). Adaptive temporal refinement in injection molding. In *AIP Conference Proceedings* (Vol. 1960, No. 1, p. 090008). AIP Publishing.

[E2] Karyofylli, V., Wendling, L., Make, M., Hosters, N., & Behr, M. (2019). Simplex space-time meshes in thermally coupled two-phase flow simulations of mold filling. *arXiv preprint arXiv:1903.08710*.

Other Publication:

[E3] Karyofylli, V. und andere, 2018. Stabilized FEM for Simplex Space-Time Meshes in 4D. In: *Curves & Surfaces Konferenz*. Arcachon, France, Juni – Juli 2018.

[E4] Karyofylli, V. und andere, 2019. Two-Phase Flow Simulations for Mold Filling on 4D Simplex Space-Time Meshes. In: *90. GAMM Jahrestagung*. Wien, Österreich, Februar 2019.