Automatic Finite Volume Discretizations Through Symbolic Computations

Karl Rupp, Florian Rudolf, Josef Weinbub, Ansgar Jüngel, Tibor Grasser
TU Wien
rupp@iue.tuwien.ac.at, rudolf@iue.tuwien.ac.at,
weinbub@iue.tuwien.ac.at, juengel@asc.tuwien.ac.at,
grasser@iue.tuwien.ac.at

Abstract

The finite volume method is a popular method for the solution of systems of partial differential equations whenever local conservation properties are desired. However, engineering software usually does not reflect the underlying continuous mathematical formulation internally, but instead implements the discrete system directly, sacrificing a higher-level representation. As a consequence, the discretization code needs to be altered whenever the mathematical formulation changes. For modeling purposes, however, it is often desirable to only modify the mathematical formulation and let the software deal with the derivation of the discrete equations. In the context of computational fluid dynamics, OpenFOAM [1] has successfully demonstrated that such a goal can in principle be achieved.

We present results obtained from coupling the symbolic computation library ViennaMath [2] to a finite volume code to solve systems of PDEs on structured and unstructured grids in one, two, and three dimensions. As an example, a fully automatic Scharfetter-Gummel-like stabilization [3] of a finite volume method for a drift-diffusion system in the context of semiconductor device simulation is discussed. Nonlinear couplings are automatically handled through Picard iterations or a globalized Newton-Raphson scheme. Moreover, we demonstrate that the mathematical formulation can be easily changed to include additional details in the mathematical model. No recompilation of the source code is required, hence our approach is also suitable for graphical user interfaces as well as scripting languages such as Python, which are frequent requirements for engineering purposes.

References

1. OPENFOAM FOUNDATION. OpenFOAM. http://www.openfoam.com/.
2. K. RUPP ET AL.. ViennaMath. http://viennamath.sourceforge.net/.
3. D. L. SCHARFETTER AND H. K. GUMMEL. Large-Signal Analysis of a Silicon Read Diode Oscillator. IEEE Trans. El. Dev., 16:64-77, 1969.