Multi-scale simulations with complex automata: in-stent restenosis and suspension flow

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Publication date
2010

Chapter 6

Summary and Conclusions

The research presented in this thesis was motivated by the question how nature processes information. In the introduction this question was specified to the problem of the multi-scale character of natural processes now reading: How is information processed between structures on distinct scales?

In chapter 2 we have introduced a classification of multi-scale problems based on the position of a process on the scale separation map (SSM) and the relative position of another process which is coupled to it. We have also identified coupling templates based on this relative position on the SSM and whether the two processes share the same domain or only an interface between each other. This chapter also takes the step towards and works out an execution model which was implemented in a software framework based on these findings that allows to quickly set up multi-scale simulations. Applying the scale separation concept to two examples we could show that the actual area on the SSM can be very much reduced without causing significant errors but gaining a tremendous computational speedup compared to a full-scale simulation. We have therefore successfully identified the relevant aspects of the information processing in the sub-processes and the coupling between them.

In chapter 3 we could show that the CxA idea can be successfully applied in the challenging field of modeling cardiovascular diseases. Using the CxA tools like the SSM we identified the relevant processes involved in in-stent restenosis and the coupling between them. The multi-scale model of in-stent restenosis has been implemented employing the MUSCLE coupling library and the results, presented and compared to measurements in real systems, show that the approach is valid. Furthermore, preliminary results of a three-dimensional model are presented where the same scale separation and coupling concepts were used. Also, a model for the formation of thrombus could be successfully coupled in as an initial condition to the subsequent processes.

The multi-scale idea was also applied to the macroscopic flow of two-dimensional hard-sphere suspensions. In chapter 4 we discussed the single-scale processes involved in the formation of flow and particle concentration profiles. We identified the relevant scales of the sub-processes and made use of their separation in several aspects of the modeling. The micro-macro type of scale separation of the three sub-models for macroscopic non-Newtonian flow, macroscopic advection and diffusion of the particle concentration, and the micro-model involving the dynamics of both phases in a fully resolved fashion, and the fact that they all share the same spatial domain resulted in a multi-scale modeling approach in the sense of the Heterogeneous Multi-scale Method (HMM). We did not make use of the MUSCLE coupling environment as its current version does not support farming as a parallelization method which was intended in the initial planning of the modeling project. Instead, the HMM coupling was realized by implementing the micro-model in a subroutine fashion. However, we successfully analyzed the multi-scale model by means of the tools the CxA theory provides, discussed possible ways to implement the system as a CxA, and could estimate a very large speed-up obtained by the scale separation. The concept of CxA's were a great help categorizing the multi-scale problem, thinking about information flow between the scales and modeling approaches. Although the models introduced in this work could have been formulated independently each with the terminology of the field of application, the CxA concept served as a common language for multi-scale problems.

In the implementation of the multi-scale suspension model we made use of scale separations also in other aspects. We successfully exploited the temporal scale separation of the macroscopic flow and diffusion to accelerate the macroscopic dynamics and reduce the run-time of the simulations. Temporal scale-splitting was also applied to the dynamics of the fluid and particle phase in the micro-model to increase the stability of the numerical integration.

The concept of Chas, even if supported by the MUSCLE library, is not a specific method. It is a framework for designing multi-scale simulation methods. For any particular problem, there is usually a considerable amount of work to develop models and realize the coupling. For the CxA model of in-stent restenosis we developed a model for thrombus formation which particularly meets the aspects of its application in the ISR model.

During the work on the HMM suspension not only a Lagrangian particle advection-diffusion method has been implemented, and the mapping of relevant quantities between Lagrangian and Eulerian representation of the particle concentration has been discussed. We have also developed and implement a database to reduce the actually necessary runs of the computationally costly micro-model (which can be considered a smart conduit in the language of CxA's). Furthermore, the implementation of the submodels in a for the coupling optimized fashion have led to improvements of the methods used for it. To implement the micro-model by means of the Lattice-Boltzmann method for suspension flows based on the original idea of Ladd, Lees-Edwards boundary conditions (LEbc) have been developed to realize the shear flow of the micro-system in a quasi-infinite domain which corresponds well with the idea of HMM micro-models representing a sample of the micro-scale dynamics at a certain point of the macroscopic domain. Lees-Edwards boundary conditions could be shown to be able to remove the side-effects associated with the walls in a Couette type of shear flow. It could also be shown that using LEbc's the shear-thickening behavior of hard-sphere suspensions is prolonged in comparison to Couette-flow results. When implementing and validating LEbc's we found that the momentum exchange algorithm (MEA) used in commonly applied LBM suspension methods suffers from violation of Galileian invariance. With the help of an asymptotic analysis we could derive an appropriate correction to MEA to restore Galileian invariance. Also, a non-equilibrium refill method was found to produce more realistic particle dynamics than existing methods in situations where particles in close contact move together over the LBM lattice.