An Introduction to Multiscale Modeling with Applications

Preface

Obviously a collection of slides is not a traditional book, where an extensive elaboration and more detailed presentation of topics are typically requested. However, the goal of this material is two-fold. First of all, the present collection of slides is expected to be useful to our students, in order to have a more systematic overview on the different topics taught in our classes. Secondly, even though not all topics treated below are presented in the same class, students should now be able to more easily reconstruct the connections among different phenomena (and scales), build their own mind map and, eventually, find their own way of deepening the subjects they are more interested in. Even if a single student ever embarks in such an enterprise, this bunch of transparencies will then have fully reached its ultimate scope!

This collection comes by the merge of the teaching slides prepared for the course of *Advanced Engineering Thermodynamics* (offered within the Master of Science in Mechanical Engineering) and those for the course of *Multi-scale Modelling and Simulation of Molecular and Mesoscopic Dynamics* (offered within the PhD Program in Energetics) taught in English at Turin Polytechnic. Topics presented in these classes are complementary. Unfortunately, the two classes are quite heterogeneous, in the sense that they involve students with different backgrounds, different technical maturities and different expectations. For these reasons, the mathematical details have been kept at a minimum level in order to convey only the main messages and ideas behind modeling at different scales. Consequently, the technical language has been also adjusted for the Master of Science program.

Moreover, several engineering applications have been included (e.g. thermal transport in carbon nanotubes, gas particles dynamics towards local equilibrium, thermal-fluid dynamics, compact heat exchangers, louvered finned surfaces, local heat transfer coefficient, air-conditioning systems and combustion chemistry, just to mention a few).

This helps in stressing that very different phenomena are described by transport theory and obey the same underlying fundamentals of engineering thermodynamics. Engineering thermodynamics is a very wide topic and, because of time constraints, it is sometimes presented in undergraduate courses in a piecemeal way. This collection of slides tries to reconstruct the original broad vision of this discipline.

The latter point is essential when dealing with international students, who have different backgrounds but also different expectations about their future. For instance, local technical regulations might not be so interesting for international students who are still wondering in which country they are going to work. Therefore, here we make the effort of providing general notions about the studied subjects, and looking at engineering applications that do not depend on a special (or local) context. For similar reasons, we decided to use only open-source codes in the laboratories (Gromacs, Palabos, OpenFoam and Cantera).

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