Juergen Geiser

Multicomponent and Multiscale Systems

Theory, Methods, and Applications in Engineering

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Juergen Geiser
Department of Electrical Engineering
Ruhr University of Bochum
Bochum
Germany

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First, I am grateful to my colleagues at the Ernst-Moritz Arndt University of Greifswald, Germany, and Ruhr-University of Bochum, Germany, for their support and ideas on modelling and computational sciences. Next, I have to thank my supporters and mentors in all modelling problems and splitting ideas. They helped me to be open and to be sensitive to rigorous analysis of the numerical methods, modelling of engineering problems and their applications.

My special thanks go to my wife Andrea and my daughter Lilli who have always supported and encouraged me.

Preface

I am glad to introduce *Multicomponent and Multiscale Systems: Theory, Methods and Applications in Engineering*.

When I started this book project, I proposed to write a book about my recent advances in mathematical modelling problems to multicomponent and multiscale systems. I considered the upcoming areas in material modelling, which include transport and reaction flow simulations and also electronic applications with electromagnetic fields.

I organized this book in combining theoretical and also application to practical problems. While multicomponent and multiscale systems are very new problems, the early stage of such a field needs such a book to explain in a theoretical and also a practical manner the tools and methods to solve such problems.

I have tried to fill the gap between numerical methods and the applications to real problems. I present rigorously the fundamental aspects of the numerical methods with their underlying analysis and applying such schemes to real-life.

This monograph is in the field of technical and physical simulation problems in engineering and sciences. Based on the theoretical framework in methods and structures of applied mathematics, it concludes with numerical approximations of multi-component and multi-scale problem. A main motivation of the book came from students and researchers in different lectures and research projects.

In this monograph, we describe the theoretical and practical aspects of solving complicated and multi-component and multi-scale systems, which are applied in engineering models and problems.

In the book, we are motivated to describe numerical receipts, based on different multi-scale and multi-component methods, that allow to apply truly working multi-scale and multi-component approaches. Nowadays, one of the main problems in multi-scale and multi-component systems is the gap between several models based on different time- and spatial-scales. Often the drawback of applying standard numerical methods, e.g. explicit time-discretization schemes, instead of working multi-scale approaches, e.g. multi-scale expansion methods, is, that we have a dramatic limiting factor, e.g. very small time- or spatial steps (due to resolving the

finest scale). Such limiting factors did not allow to solve engineering complexity and industrial advancement is impossible to obtain. Here, we fill the gap between numerical methods and their applications to engineering complexities of real-life problems.

Such engineering complexities are delicate and need extraordinary treatment with special solver and tools to overcome the difficulties and restrictions of time- and spatial steps.

Therefore, we discuss the ideas of solving such multi-component and multi-scale systems with the help of non-iterative and iterative methods. Often such methods can be related to splitting multi-scale methods to be taken into account to decompose such problems to simpler ones. Such decomposition allows to treat the complex systems in simpler ones and skip the restriction of the finest scale to the solver methods, while we can apply individual scale to the decomposed system.

We discuss analytical and numerical methods in time and space for evolution equations and also nonlinear evolution equations with respect to their linearization and relaxation schemes.

All problems are related to engineering problems and their applications. I have started from reactive flow and transport models, which are related to bioremediation, combustion and various CFD applications, to delicate electronic models, which are related to plasma transport and flow processes in technical apparatus.

The main motivation is to embed novel multiscale approaches to complex engineering problems such that it is possible to apply a model-reduction. Thus, it is possible that parts of the model can be reduced or for those based on multiscale or multicomponent approaches, the data-transfer between fine and coarse grid is done, in a way that each scale is considered.

The outline of the monograph is given as:

1. Introduction (outline of the book)
2. General principles for multi-component and multiscale systems
    a. Multi-component Analysis (separating of components)
    b. Multiscale analysis (separating of scales)
    c. Mathematical methods
3. Theoretical part: functional splitting:
    a. Decomposition of a global multi-component problem
    b. Decomposition of a global multiscale problem
4. Algorithmic part
    a. Iterative methods
    b. Additive methods
    c. Parallelization

5. Models and applications
   a. Multicomponent applications
      i. Application of multicomponent fluids
      ii. Application of multicomponent kinetics
      iii. Analytical methods for a multicomponent transport model
   b. Multiscale applications
      i. Additive splitting method for Maxwell-equations
      ii. Nonuniform grids for particle in cell methods
6. Engineering applications (real-life models)
   a. Multicomponent applications
      i. Application of a multicomponent model in a plasma-mixture problem
      ii. Application of a multicomponent model in a biological problem (glycolysis)
   b. Multiscale applications
      i. Application of a multiscale model in a stochastic problem
      ii. Application of a multiscale model in a code-coupling problem
      iii. Application of a multiscale model in a dynamical problem
      iv. Application of a multiscale model in a particle transport problem
      v. Application of a multiscale model in plasma applications
      vi. Application of a multiscale model in complex fluids
7. Conclusion (fields of application and future ideas)

Based on the outline of the book, we hope that we could increase the attention of both industry and scientists; theoretical and practical aspects are illustrated and considered in an equal way.

Dallgow-Doeberitz Juergen Geiser
June 2015

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I would like to thank Th. Zacher for programming MULTI-OPERA software and his help in the numerical experiments. I would also like to acknowledge my colleagues and students who helped me to write such a book and gave me hints with numerical and experimental results.

Contents

Acronyms

BCH	Baker-Campbell-Hausdorff formula
BDF	Backward differentiation formula
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy condition
CIC	Cloud-in-Cell function (see [1] and [2])
CVD	Chemical vapor deposition
CSP	Computational Singular Perturbation Method (see [3])
DD	Domain decomposition methods
FDTD	Finite Difference Finite Time method (see [4])
EFM	Equation Free Method (see [5])
HIPIMS	High Power Impulse Magnetron Sputtering
HMM	Heterogeneous Multiscale Method (see [6])
HPM	Homotopy Perturbation Method (see [7])
ICE-PIC	Invariant Constrained-equilibrium Edge Pre-Image Curve (see [8])
ILDM	Intrinsic Low Dimensional Manifold approach (see [9])
IOS	Iterative operator splitting methods
MAX-phase	Special material with metallic and ceramic behavior; see [10]
MD	Molecular dynamics
MIG	Method of Invariant Grid (see [11])
MIM	Method of Invariant Manifold
MISM	Multiscale Iterative Splitting Method (see [12])
MQ	Multiquadric bases functions (see [13])

MULTI-OPERA	Software package based on MATLAB, which solves multiscale problems with splitting methods
ODE	Ordinary differential equation
OFELI	Object finite element library
PDE	Partial differential equation
PECVD	Plasma-enhanced chemical vapor deposition
PIC	Particle in Cell (see [1])
PID	Proportional integral derivative controller
PM	Particle Method (see [1])
PVD	Physical vapor deposition
RBF	Radial basis function
REDIMs	Reaction–Diffusion Manifolds approach (see [14])
RRM	Relaxation Redistribution Method (see [15])
R^3T	Radioactive-reaction-retardation-transport software toolbox, done with the software package UG (unstructured grids)
SiC	Silicon carbide
Ti_3SiC_2	Special material used for thin-layer deposition; see [10]
SIM	Slow Invariant Manifold
SDE	Stochastic Differential Equation
SODE	Stochastic Ordinary Differential Equation
SPDE	Stochastic Partial differential equation
UG	Unstructured grid (software package; see [16])

Symbols

λ	Eigenvalue
A	In the following A is a matrix in $\mathbb{R}^m \times \mathbb{R}^m$, $m \in \mathbb{N}^+$ is the rank
λ_i	i-th eigenvalue of A
$\rho(A)$	Spectral radius of A
e_i	i-th eigenvector of matrix A
$\sigma(A)$	Spectrum of A
$Re(\lambda_i)$	i-th real eigenvalue of λ
$u_t = \frac{\partial u}{\partial t}$	First-order partial time derivative of c
$u_{tt} = \frac{\partial^2 u}{\partial t^2}$	Second-order partial time derivative of c
$u_{ttt} = \frac{\partial^3 u}{\partial t^3}$	Third-order partial time derivative of u
$u_{tttt} = \frac{\partial^4 u}{\partial t^4}$	Fourth-order partial time derivative of u
$u' = \frac{du}{dt}$	First-order time derivative of u
$u'' = \frac{d^2 u}{dt^2}$	Second-order time derivative of u
$\tau = \tau_n = t^{n+1} - t^n$	Time step

u^n	Approximated solution of u at time t^n
$\partial_t^+ u = \frac{u^{n+1}-u^n}{\tau_n}$	Forward finite difference of u in time
$\partial_t^- u = \frac{u^n-u^{n-1}}{\tau_n}$	Backward finite difference of u in time
$\partial_t^0 u = \frac{u^{n+1}-u^{n-1}}{2\tau_n}$	Central finite difference of u in time
$\partial_t^2 u = \partial_t^+ \partial_t^- u$	Second-order finite difference of u in time
∇u	Gradient of u
$\Delta u(x,t)$	Laplace operator of u
$\nabla \cdot \mathbf{u}$	Divergence of $\mathbf{u}$ (where $\mathbf{u}$ is a vector function)
n_m	Outer normal vector to Ω_m
$\partial_x^+ u$	Forward finite difference of u in space dimension x
$\partial_x^- u$	Backward finite difference of u in space dimension x
$\partial_x^0 u$	Central finite difference of u in space dimension x
$\partial_x^2 u$	Second-order finite difference of u in space dimension x
$\partial_y^+ u$	Forward finite difference of u in space dimension y
$\partial_y^- u$	Backward finite difference of u in space dimension y
$\partial_y^0 u$	Central finite difference of u in space dimension y
$\partial_y^2 u$	Second-order finite difference of u in space dimension y
$e_i(t) := u(t) - u_i(t)$	Local error function with approximated solution $u_i(t)$
err_{local}	Local error
err_{global}	Global error
$[A,B] = AB - BA$	Commutator of operators A and B

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Introduction

While engineering applications are becoming increasingly complicate, the underlying modelling problems are becoming more related with multi-modelling aspects. Such complexities arise due to multiscale and multicomponent approaches in the modelling-equations, which need rigorous numerical analysis for the underlying schemes. The main problems are the disparate time- and spatial scales, which have to be included into the models and their underlying numerical approaches.

In the next chapters, we like to solve such delicate problems with numerical schemes, which are improved multi-scale and multi-component methods.

We discuss the following items:

- General principles for multi-component and multiscale systems,
- Multi-component analysis (separating of components),
- Multiscale analysis (separating of scales),
- Mathematical and numerical methods.

While we start with classical multicomponent and multiscale methods, e.g. homogenization and asymptotic matching, we discuss their limits and application background. Such limits allow us to take into account the design of structure and algorithmical methods, which overcome the restriction of disparate scales and modify such methods to apply engineering problems with delicate complexities.

Here the main topic is related to splitting methods, which are nowadays applied to multi-scale and multi-component problems, while they are flexible in coupling different spatial and time scales.

We discuss additive and iterative methods, which can be embedded to standard discretization and solver schemes, such that the multiscales are respected in their modelling structures. Practical and theoretical tools are extended with scientific simulations of their underlying models, which allows revealing the deeper structures, for example multi-component and multi-scale structures, which are coupled in different time and spatial scales.

Based on the upcoming areas of multi-scale approaches for material modelling, see the framework of Horizon 2020,[1] it is important to link different models, e.g.,

- Multi-scaling: Different time- or spatial scales of the phenomena are modelled in different entities (e.g., micro- or macro model) and their results are transferred from one model to another.
- Multi-Modelling: Different physics and chemistry are coupled at the same scale, which means the models are applied to the same time- and spatial scale.

Such new modelling areas are nowadays important and we take into account the modification of our proposed multi-scale and multi-component methods to customize for practical engineering problems. One of the key motivation is to bridge the gap between the engineering application and the development of multi-scale methods for theoretical test applications, such that it is possible to adapt the theoretical tested schemes to real problems.

Here in our book, we concentrate on multi-scaling, which means, we can apply our models and methods to such problems, that different models (microscopic model or macroscopic model) are coupled via a method and therefore, we transfer the results from one to the other model.

We consider the following multi-scaling:

- Multi-scaling: Different time- or spatial scales of the phenomena are modelled in different entities (e.g., micro- or macro model) and their results are transferred from one model to another.
- Multi-Modelling: Different physics and chemistry is coupled at the same scale, which means the models are applied to the same time- and spatial scale.

Based on the first interpretation, we have in the book the following examples:

- Langevin-like equations (micro- and macro-time scale), see Sect. 5.1,
- Levitron Problem (micro- and macro-spatial scale), see Sect. 5.3,
- Glycolysis Problem (micro- and macro-time scale), see Sect. 5.6.

In Fig. 1, we present the first interpretation (same physics model to different spatial and time scales).

In Fig. 2, we present the second interpretation (linking models with different physics). Based on the second interpretation, we have in the book the following examples:

- Code-coupling (fluid dynamical and heat-transfer model), see Sect. 5.2,
- Adaptive Particle in Cell (molecular dynamical model and continuum model), see Sect. 5.4,
- Multicomponent Plasma (kinetic model and continuum model), see Sect. 5.5.

[1]European Commission, Research & Innovation-Key Enabling Technologies, Modelling Material, http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html.

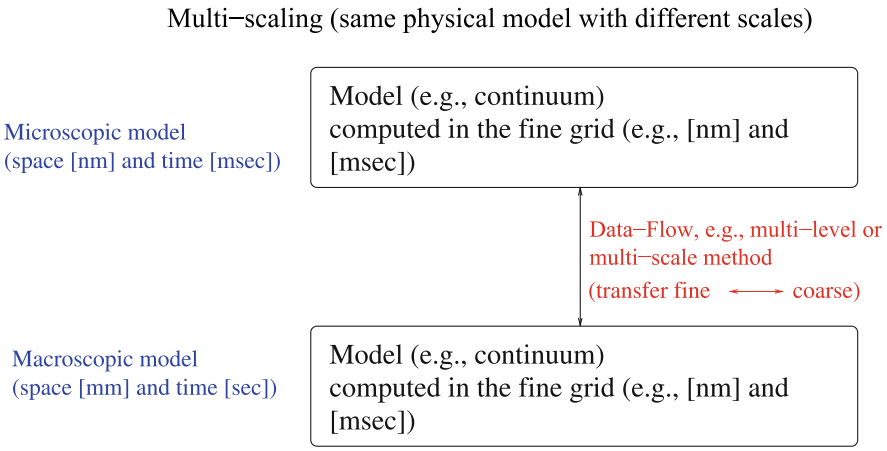

Fig. 1 First interpretation of multi-scaling (often in classical material engineering applied)

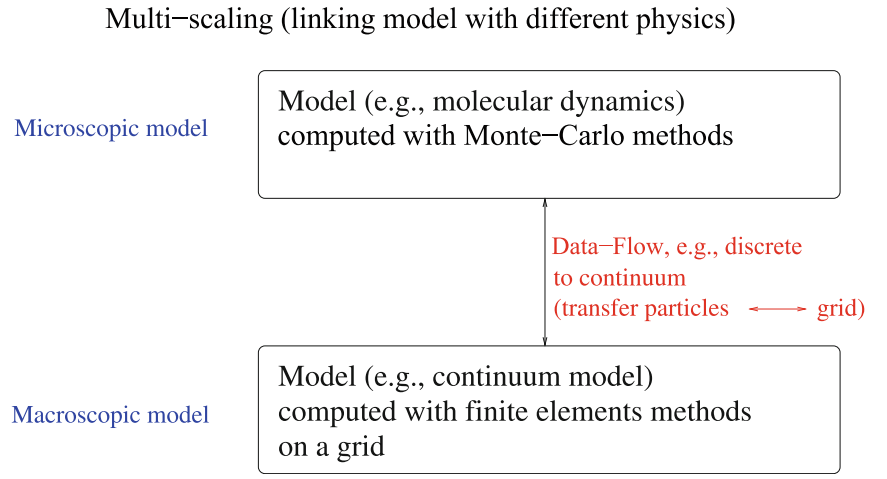

Fig. 2 Second interpretation of multi-scaling (in modern material engineering applied)

In the book, we try to close the gap between several available models, e.g. in material modelling, due to disparate time and spatial scales, and the possibility to apply multi-scale and multi-component methods to couple such scales.

The use of such truly working multi-scale approaches is important in the case of engineering complexity; in the book, we present such approaches. Nowadays, if such methods are not considered or well-studied in the applications, it is a dramatic limiting factor for today's industrial advancement, see [1].

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Chapter 1
General Principles

Abstract In the general principle, we give an overview of the recently used methods and schemes to solve multicomponent and multiscale systems. While multicomponent systems are evolution equations based on each single species, which are coupled with the other species, e.g. with reaction-, diffusion-processes, multiscale systems are evolution equations based on different scales for each species, e.g. macroscopic- or microscopic scale. We give the general criteria for practically performing the different splitting and multiscale methods, such that a modification to practical applications of the splitting schemes to a real-life problem can be done.

1.1 Multicomponent Systems

In the following, we deal with multicomponent systems. Multicomponent systems concentrate on disparate components in the underlying multiscale models, while they can be coupled by linear or nonlinear functions or differential systems, e.g. reactions or transport phenomena. Often, also different scales are important to resolve to understand the interactions of the different components. Here, we have to apply multicomponent schemes that are also related to disparate spatial and timescales to resolve such complexities, see algorithmic ideas of multicomponent problems in [1].

In the following sections, we concentrate on modelling or algorithmical aspects of multicomponent systems for the following applications:

- Multicomponent flows, see [2, 3].
- Multicomponent transport, see [1, 4].

We simulate the flow and transport systems based on their interactions with the different components. Hence, we allow to study weakly or strongly coupled components in the underlying modelling equation systems.

1.1.1 Multicomponent Flows

The class of multicomponent flows can be defined as a mixture of different chemical species on a molecular level, which are flown with the same velocity and temperature,

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see [5]. The chemical species are interacting by chemical reactions and such a result is a multicomponent reactive flow.

The modelling of such behaviours is important in engineering, e.g. reactor design (Chemical vapour deposition reactors, see [6]) in chemical engineering. Such processes are very complex, while different physical processes occur, e.g. injection, heating, mixturing, homogeneous and heterogeneous chemistry and further, see [7].

In the following, we present some typical problems in multicomponent flow problems:

- Ionized Species, e.g. plasma problems, see [4].
- Combustion of oil, coal or natural gas, see [8].
- Chemical reaction processes in chemical engineering, see [6, 9, 10].
- Atmospheric pollution, see [11].

Remark 1.1 In the different applications, the term multiphase flow is often used. Here, we define multiphase flows where the phases are immiscible and not chemically related, see [2, 12]. So each phase has a separately defined volume fraction and velocity field. Therefore, also the conservation equations for the flow of each species and their interchange between the phases are different from the multicomponent flow. Here, one is taken into account to define a common pressure field, while each phase is related to the gradient of this field and its volume fraction, see [13]. The applications are two-phase flow problems, Buckley Leverett problems and multiphase heat transfer, see [2].

1.1.2 Multicomponent Transport

We define the multicomponent transport in the direction of a computational aspect. If we deal in our description with multicomponent flow model, e.g. multicomponent plasma, multicomponent fluid, the interest is related in this item to the transport properties, e.g. of the chemical mixture.

The algorithmical aspect is important to deal with multicomponent systems; here often the idea of splitting into simpler and faster equation parts is important, e.g.:

- Multicomponent splitting of multicomponent flow problem, e.g. ocean modelling [14].
- Multicomponent transport algorithms, e.g. fluid modelling [4].
- Multicomponent transport modelling, e.g. plasma modelling [15].

All ideas are related to decompose the multicomponent model into simpler single-component models and solve them separately.

1.1.3 Application of Operator Splitting Methods to Multicomponent Flow and Transport Problems

The general criteria for a practical performing of the operator splitting methods to multicomponent systems are motivated by decomposing into simpler systems, which can be solved independently or with less computational amount, see [16, 17].

One of the main advantages of decoupling operators in multicomponent systems is the computational efficiency, while we decompose the operators in their different temporal and spatial scales. Such a decomposition allows to apply the most accurate discretization and solver methods.

A classical receipt of such a decomposition for multicomponent systems is given in Fig. 1.1.

Example 1.1 As an example, we deal with a multicomponent transport problem, a multi-diffusion-reaction equation. Such a multi-diffusion operator is decomposed into simpler diffusion operators. Each operator part can be solved with its accurate method (e.g. implicit time discretization for the fastest diffusion part to allow large time steps and higher order explicit Runge–Kutta methods for slowest diffusion part to obtain accurate results), see [18].

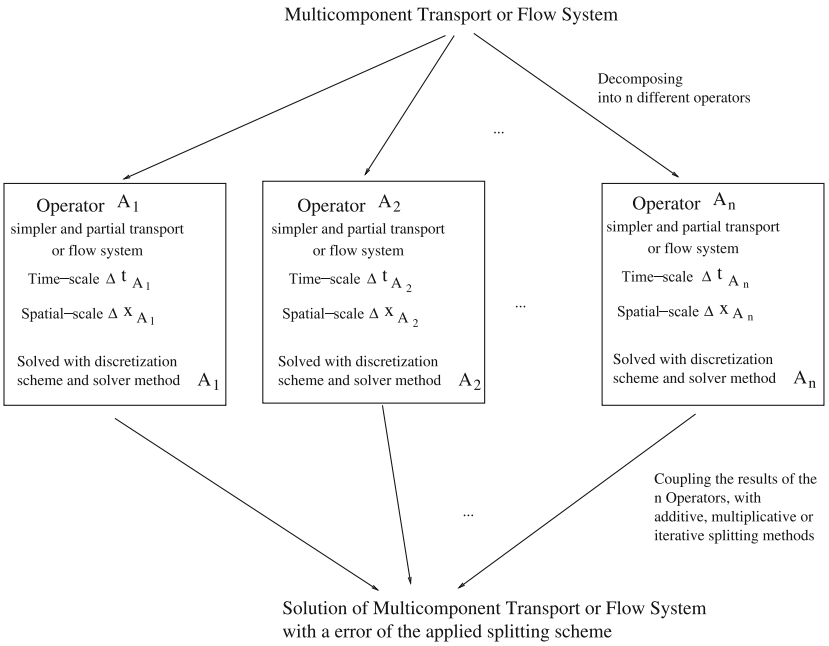

Fig. 1.1 Multicomponent systems and an operator splitting approach

1.2 Multiscale Systems

Multiscale systems deal with modelling equations of different time- and spatial behaviours. While different scale lengths, e.g. microscopic or macroscopic scales, in time and space are important, also the different models of the problem, e.g. microscopic or macroscopic model, are important to understand the complexity of the underlying system. Different hierarchies of models are important to see in each different time- or spatial scale the influence to the model problem or the influence to a lower or upper hierarchical model, see [19, 20].

We have to understand the related multiscale models, e.g. different scales or different models, and also the application of different multiscale methods, e.g. top–down or bottom–up methods, see [21].

In the following, we deal with multiscale systems and their modelling and algorithmical aspects.

We discuss the following topics:

- Multiscale Modelling, see [2, 3].
- Multiscale Methods, see [1, 4].

We take into account the different modelling types, type A and type B, and the practical implementation to adequate multiscale methods to close the gap between the influence of disparate time- and spatial schemes. We can accelerate the computational time while we solve upscaled microscopic equation into fast performing macroscopic equations or concentrate on embedding microscopic performance to important time- or spatial windows of the macroscopic equations, e.g. updating macroscopic parameters with microscopic computations.

1.2.1 Multiscale Modelling

In the past years, in many engineering applications, multiscale systems are important tools for solving engineering models which have multiple scales, e.g. spatial and/or temporal scales of different, see [22].

The modelling aspects concentrate on resolving the properties or system behaviour on each important level (e.g. microscale, mesoscale, macroscale) by using additional information from the other levels or scales (e.g. lower or higher levels).

While each level has its own specific behaviour, e.g. conservation or constraints, such a behaviour is important for a detailed description of the full system with all the levels.

Multiscale modelling is therefore important to understand the detailed information of an engineering model, e.g. the material and system behaviours. Such a detailed analysis allows to forecast the material or system behaviours.

1.2.2 Multiscale Methods

There are several different methods to solve multiscale problems.

Often, it is sufficient to deal with analytical methods, e.g. method of multiple-timescales (MMTS) see [23]. The next larger group is numerical methods, where we distinguish between different types of algorithms:

- Top–down.
- Bottom–up.

Further, we distinguish between classical and modern numerical schemes, while the classical schemes, e.g. multiscale methods, multiresolution methods, have linear scaling and modern schemes, e.g. heterogeneous multiscale method (HMM), equation free method (EFM), iterative multiscale methods (IMSM) have sublinear scaling of the computational time, see [22].

1.2.3 Application of Different Multiscale Methods to Multiscale Problems

In the following, we discuss three recipes of practical application of the following multiscale methods:

- HMM (Heterogeneous Multiscale Method), see [24].
- EFM (Equation free method), see [25].
- MISM (Multiscale Iterative Splitting Method), see [26].

For multiscale problems, a main motivation is also to reduce the computational amount, see [22].

To have a general criteria to apply to a real model, we can classify a multiscale problem into two types and apply each type to the appropriate method, see [20, 26].

- Multiscale Problem of Type A (top–down)
  The micro-model is only used for the regions where the microscopic laws are important, e.g. local defects or singularities, boundary-layers or interfaces. For all other regions it is sufficient to apply the macro-model (i.e. the macroscopic equations). Here, the examples are fluid–solid models or plasma-boundary models.
- Multiscale Problem of Type B (bottom–up)
  The microscale model is necessary for all the regions (e.g. globally) to derive the parameters for the macroscopic laws. The macroscopic model is extrapolated by the microscopic model, i.e. we reconstruct the macroscopic equations.

The methods for the different types are given in the following:

HMM: Top–down-method

Here, we have the HMM (Heterogeneous Multiscale Method), which embeds the microscale model into the macroscopic model. That is, the macroscopic model is extended by the information of the microscopic model.

We have the following steps of the HMM algorithm, see Algorithm 1.1.

We deal with the following multiscale equation:

$$\frac{dy}{dt} = \frac{1}{\varepsilon}(y - \phi(x)), \tag{1.1}$$

$$\frac{dx}{dt} = f(x, y), \tag{1.2}$$

where y is the fast and x is the slow variable. Further, we assume $\varepsilon \ll 1$ and f, ϕ are nonlinear functions and $t \in [0, T]$, where T is the end-time point.

Algorithm 1.1 • We solve the microscopic equation:

$$y^{n,m+1} = y^{n,m} - \frac{\delta t}{\varepsilon}(y^{n,m} - \phi(x^n)), \tag{1.3}$$

with $m = 0, 1, \ldots, M-1$, e.g. $\delta t \leq \Delta t/M$ as microscopic time-steps.

- We reconstruct or equilibrate the microscale operator:

$$F^n = \frac{1}{M}\sum_{m=1}^{M} f(x^n, y^{n,m}). \tag{1.4}$$

- We solve the macroscopic equation, with respect to the improved operator F^n:

$$x^{n+1} = x^n - \Delta t F^n. \tag{1.5}$$

with the macroscopic time-step Δt.

Remark 1.2 We solve only a few microscopic time-steps around a macroscopic time-point, such that we do not resolve the full macroscopic time-step, therefore we can reduce the microscopic computations.

MISM: Top–down-method

Here, we have a next top–down method, which deals with an underlying macroscopic equation with A as the macroscopic operator and the coarse timescale τ. Further, we assume a microscopic equation (e.g. material law) with the microscopic operator B and the fine timescale $\delta\tau$.

The different scales and the method is illustrated in Fig. 1.2.

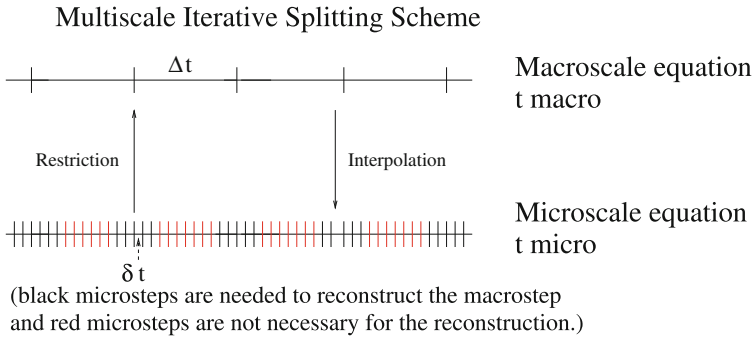

Fig. 1.2 Illustration of the MISM method

The idea is to embed the results of the microscopic equations around the macroscopic time-points, i.e. smaller time frame of microscopic steps as the full macroscopic time-step, such that we can save computational time. The finer scale is embedded into the coarser scale and it is sufficient to update a smaller time interval around the coarser time-steps to concentrate on the macroscopic equations, which can be solved much more efficiently than the microscopic equation.

The Algorithm 1.2 is given in the following.

Algorithm 1.2 We have the following parameters:

- The coarse time-step is τ.
- The fine time-step is $\delta\tau \leq \tau/M$, where M is the number of small time-steps around the coarse time-step.
- The macroscopic time interval is given as $[t^n, t^{n+1}]$.

The algorithm is given in the next steps:

- Initialization: $c_0(t^n) = c^n$, I is the number of iteration steps and we have N time intervals.
- We solve the macroscopic equation with one time-step τ:

$$\frac{\partial c_i(t)}{\partial t} = A(c_i(t)) \; + \; R(B(c_{i-1}(t)). \tag{1.6}$$

- Then we apply the interpolation, i.e. operator A is resolved in the finer scale, so we couple into the microscopic equation

$$I(A(c_i)(t)) = A(c(t^n)) + \frac{\partial A(c)}{\partial c}\frac{c_i(t) - c(t^n)}{c_i(t^{n+1}) - c(t^n)}, \; t \in [t^n, t^{n+1}]. \tag{1.7}$$

$$I(A(c_i)(t)) = A(c(t^n)) + \frac{A(c_i(t^{n+1})) - A(c(t^n))}{c_i(t^{n+1}) - c(t^n)}(c_i(t) - c(t^n)), \; t \in [t^n, t^{n+1}]. \tag{1.8}$$