Chapter 2
Theoretical Part: Functional Splitting

Abstract We describe a general method, which is based on a splitting approach and the knowledge of the exact solutions of some sub-problems. Such additional information is taken into account and has an important role in accelerating the computations. We apply a functional splitting idea to decompose the initial problem into several sub-problems where some of them are known with the analytical solutions. The sub-problems with unknown solutions are solved numerically by standard numerical methods, e.g. finite volume methods. This paper can be divided into four parts. In the first part, we introduce the model and its application. In the second part, we discuss the analytical solutions of coupled systems of convection-reaction equations. Functional splitting methods are developed in the third part.

2.1 Ideas of the Functional Splitting

The ideas of functional splitting are applied in different areas of decomposing multicomponent flow problems, see [1, 2].

The motivation is to reduce the problems of solving reacting flows whose complexity comes from the fact of a wide range of timescales.

Such complexity leads to numerical difficulties related, e.g. to stiffness of the reaction terms.

Here, the idea is to split the model equations additively into flow terms (e.g. advective transport, diffusive transport) and reaction terms (e.g. chemical transformations).

In the following, we discuss the different splitting techniques, that are applied in multi-component flow problem, see [3].

2.1.1 Flow Equations

We deal with a system of flow equations, which are coupled by the different flow operators, e.g. advection, diffusion, dispersion, etc. Here the main ideas are to decompose such delicate multi-operator equation into simpler one-operator equations.

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Therefore, we can treat each simpler one-operator equation with more adequate solver and discretization schemes and optimize their computational time. Splitting techniques allow to decompose the operators and couple the results of each simpler operator equation together to the full result, e.g. with overlaps in the initialization of each simpler operator equation (initial condition coupling).

2.1.1.1 Splitting of Physical Processes

So one splitting technique is based on the idea to decompose the discretized operator

$$\frac{\partial u}{\partial t} + Au = f, \; t \in [0, T], \tag{2.1}$$

where $A = \sum_{j=1}^{I} A_j$, $A_j \geq 0$ (A_j is positive definite) and $f = \sum_{j=1}^{I} f_i$ and $i = 1, 2, \ldots, I$.

The solution of the simpler equations are given as:

$$\frac{u^{j+1/I} - u^j}{\Delta t} + A_1(\alpha u^{j+1/I} + (1 - \alpha u^j)) = f_1, \; t \in [0, T], \tag{2.2}$$

$$\frac{u^{j+2/I} - u^{j+1/I}}{\Delta t} + A_1(\alpha u^{j+2/I} + (1 - \alpha u^{j+1/I})) = f_2, \; t \in [0, T], \tag{2.3}$$

$$\vdots \tag{2.4}$$

$$\frac{u^{j+1} - u^{j+(I-1)/I}}{\Delta t} + A_1(\alpha u^{j+1} + (1 - \alpha u^{j+(I-1)/I})) = f_I, \; t \in [0, T], \tag{2.5}$$

where for $\alpha = 1$ is an implicit scheme of first order, $\alpha = 0$ is an explicit scheme of first order and for $\alpha = 1/2$ we have a Crank–Nicolson scheme of second order, see [4].

2.1.1.2 Splitting of Physical Processes and Solution Components

Another splitting idea is based on splitting the components of the solutions with respect to their different scales, e.g. vertical and horizontal velocity in ocean circulation or decompose the velocity field into a time average motion and a turbulent fluctuation (Reynolds-averaging idea, see [5]).

The idea is based on two different velocity scales, i.e. a fast scale (turbulent fluctuation) and a slow scale (averaged motion), see Fig. 2.1.

We decompose the velocity into:

$$u = \overline{u} - u', \tag{2.6}$$

where $\overline{u} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} u(s) \, ds$ and $\Delta t = t^{n+1} - t^n$.

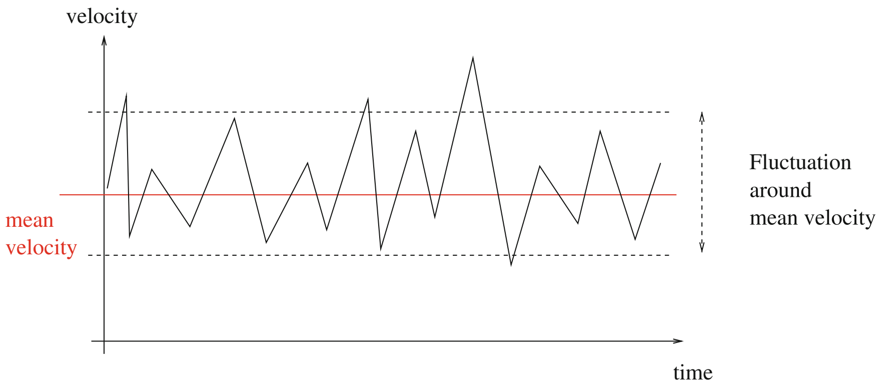

Fig. 2.1 Splitting approach to convection-diffusion-reaction equations

Example 2.1 Decomposition of a turbulent flow into an averaged flow and fluctuation flow. Such an application is known in the Navier–Stokes simulations, see [6].

We apply a flow-equation given with two flow variables u, v and have:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(uv) = Q_u, \tag{2.7}$$

where Q_u is a source of u and we have the following decomposition:

$$u = \overline{u} + u', \tag{2.8}$$

$$v = \overline{v} + v', \tag{2.9}$$

$$S_u = \overline{S_u} + S'_u, \tag{2.10}$$

and we decompose into

$$\frac{\partial(\overline{u} + u')}{\partial t} + \frac{\partial}{\partial x}((\overline{u} + u')(\overline{v} + v')) = \overline{Q_u} + Q'_u, \tag{2.11}$$

and we have:

$$\frac{\partial(\overline{u} + u')}{\partial t} + \frac{\partial}{\partial x}((\overline{uv} + \overline{u}v' + u'\overline{v} + u'v')) = \overline{Q_u} + Q'_u, \tag{2.12}$$

we apply the averaging operator and have:

$$\frac{\partial\overline{(\overline{u} + u')}}{\partial t} + \frac{\partial}{\partial x}((\overline{\overline{uv}} + \overline{\overline{u}v'} + \overline{u'\overline{v}} + \overline{u'v'})) = \overline{\overline{Q_u} + Q'_u}, \tag{2.13}$$

then, we skip the fast perturbations means $\overline{u'} = 0$, $\overline{S'_u}$ and obtain:

$$\frac{\partial \overline{u}}{\partial t} + \frac{\partial}{\partial x}((\overline{\overline{u}\overline{v}} + \overline{\overline{u}v'} + \overline{u'\overline{v}} + \overline{u'v'})) = \overline{Q_u}, \tag{2.14}$$

then based on the continuity equation we have $\frac{\partial \overline{u}}{\partial x} = 0$ and $\frac{\partial \overline{v}}{\partial x} = 0$ such that we can skip the mixed terms and we obtain:

$$\frac{\partial \overline{u}}{\partial t} + \frac{\partial}{\partial x}(\overline{u}\overline{v} + \overline{u'v'}) = \overline{Q_u}, \tag{2.15}$$

and by applying the operator parts of the equations, which splits the flow-field and the source-term (reaction part), we have:

$$\frac{\partial \overline{u}}{\partial t} = \overline{Q_u}, \tag{2.16}$$

and

$$\frac{\partial \overline{u}}{\partial t} + \frac{\partial}{\partial x}(\overline{u}\overline{v} + \overline{u'v'}) = 0, \tag{2.17}$$

Example 2.2 A next example in ocean modelling, here we have also different scales (horizontal and vertical velocities).

We assume the following linearized model, see [7], while we choose the adjustment equation given in a linearized form:

$$\frac{\partial u}{\partial t} - fv = -P_x, \frac{\partial v}{\partial t} + fu = -P_y, \tag{2.18}$$

where f is a function depending on time and space, $p = (P_x, P_y)^t$ is the pressure vector. We first decompose into the different physical processes (reaction and pressure part) and we have:

$$\frac{\partial u}{\partial t} = -P_x, \frac{\partial v}{\partial t} = -P_y, \tag{2.19}$$

and the second part:

$$\frac{\partial u}{\partial t} - fv = 0, \frac{\partial v}{\partial t} + fu = 0, \tag{2.20}$$

is further decomposed into:

$$u = \overline{u} + u', \tag{2.21}$$

$$v = \overline{v} + v', \tag{2.22}$$

and we get

$$\frac{\partial(\overline{u}+u')}{\partial t} - f(\overline{v}+v') = 0, \tag{2.23}$$

$$\frac{\partial(\overline{v}+v')}{\partial t} + f(\overline{u}+u') = 0, \tag{2.24}$$

and we apply the averaging and obtain:

$$\frac{\partial\overline{u}}{\partial t} - f\overline{v} = 0, \tag{2.25}$$

$$\frac{\partial\overline{v}}{\partial t} + f\overline{u} = 0. \tag{2.26}$$

Further, we can also solve the fluctuations or so-called inertia adjustments:

$$\frac{\partial u'}{\partial t} - f v' = 0, \tag{2.27}$$

$$\frac{\partial v'}{\partial t} + f u' = 0. \tag{2.28}$$

Here, we have decoupled the fast and slow velocities and also taken into account the different physical behaviours of the equation parts.

2.1.2 Decomposition of Convection-Diffusion-Reaction Problems

The motivation of decomposing convection-diffusion-reaction (CDR) problems are important, while time-consuming standard numerical approaches, e.g. Runge–Kutta methods for the the whole equation parts, have their drawbacks in resolving the finest scales. More and more complexities of coupling all the equations parts need to apply novel methods, that can overcome the restriction to time- and spatial steps, see [8]. Nowadays CDR problems are used to simulate delicate transport and reaction processes in engineering applications, e.g. chemical reactors [9], combustion flames [10], and bioremediation [11, 12].

Because of the drawback of losing accuracy or dealing with numerical artefacts with large time-steps to classical discretization and splitting schemes, we propose the following splitting strategies for global multiphase convection-diffusion-reaction equation, see [13].

- Time Splitting: Decoupling of convection-reaction and diffusion equation to solve them separately

- Dimensional Splitting: Exact solving of the 1D time-dependent systems of the convection-reaction equations
- Functional Splitting: Laplace transformation of the 1D time-dependent systems of convection-reaction equations and solving analytically the resulting systems of ordinary differential equations
- Iterative Splitting: Fix-point schemes, which couple the sub-problems of the global problem, which are then solved in advance independently using an analytical approach.

The technique called functional splitting has been tried as a means of solving decomposable problems, see [2]. Functional splitting is implemented in a splitting approach, where the knowledge of the exact solutions of some sub-problems has an important role in obtaining a-priori test-functions for solving the systems of differential equations. The solutions can be used as test-functions to improve the discretization schemes, e.g. finite volume schemes, or to solve analytically sub-problems which are coupled in the splitting approach, see [3].

Here are the Assumptions 2.1 of Functional Splitting approaches.

Assumption 2.1 In the following, we assume that our underlying problem has the following characteristics:

- Each sub-problem can be solved analytical or semi-analytical.
- The sub-problems can be coupled via splitting approaches, e.g. additive, multiplicative or iterative splitting methods.
- The underlying spatial discretization scheme, e.g. finite difference or finite volume method, can embed the one-dimensional analytical or semi-analytical solutions with a small splitting error, see Godunov's method [14, 15].
- Multiscale methods, e.g. multiscale expansion methods, can be applied and decompose to fine and coarse parts of the full model and apply multiscale splitting approaches, see [16].

In the following Fig. 2.2, we present the ideas of the this functional splitting approach to a coupled multiphase convection-diffusion-reaction (MCDR) equation. We start from the MCDR equation, while each parts, means the convection-, reaction-, diffusion- and multiphase- part (mobile and immobile parts) have their different spatial and time scales. In the step of the decomposition, we collect the different scales of equal or nearly equal part, so here in the Fig. 2.2, we can combine the convection and reaction part, immobile part. Now, we can concentrate on the four different model problems, e.g. convection-reaction equation, diffusion equation and mobile–immobile equations. In the next step, we apply the so-called Functional Splitting approach, see the Assumptions 2.1. Means, we can reconstruct one-dimensional solutions of each sub-problem, that has a highly accuracy, e.g., analytical or semi-analytical solution, and that the underlying spatial discretization scheme can embed such dimensional-splitted solutions. Further, we can concentrate on each simpler equation and apply multiscale approaches. In the final step, we couple the results of each sub-problem and apply the coupling approaches of the different splitting methods, see [17]. The errors of the applied methods, e.g. dimensional splitting error, time

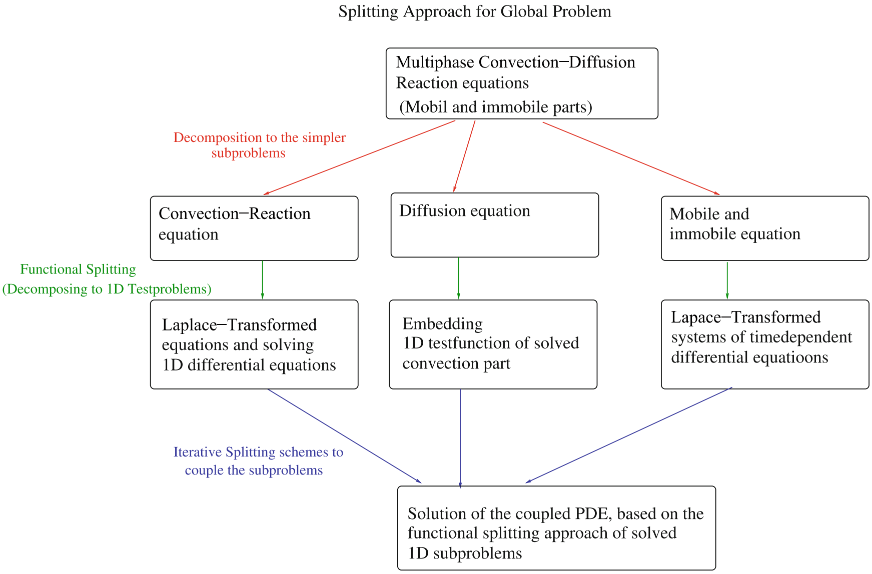

Fig. 2.2 Splitting approach to convection-diffusion-reaction equations

splitting error, can be reduced by applying higher order schemes of each underlying method.

Such splitting approaches allow of accelerating the solver process, so one can employ larger time-steps. Taking into account the different scales of these multiscale problems, one solves each singlescale problem with its optimal accuracy, see [8].

Our contribution is to derive the framework of a splitting approach to solve time-dependent coupled transport and reaction equations with different splitting schemes producing analytically solvable one-dimensional equations, whose solutions are then used as test-function. This framework is more economical since it uses only standard approaches such as finite volume schemes.

Remark 2.1 Furthermore, one could, hence, use more delicate chemical reaction terms and embed the semi-analytical solutions of their coupled convection-reaction systems into the schemes, or use iterative approaches to couple mixed mobile and immobile sub-models, which are delicate, to say the least, to solve only semi-analytical, see [17].

2.1.3 Functional Splitting with Respect to the Multiscale Approach

Often it is necessary to deal with a multiscale model with different underlying models, e.g., microscopic and macroscopic model.

Numerically, we deal with a multiscale method, that solves each individual model and couple the datatransfer between the different models, see [18].

Then, we deal with a hierarchical Decomposition of the underlying different models, means in each hierarchy, e.g. microscopic part or macroscopic part, we deal with different decomposition methods.

In the following Fig. 2.3, we present some recipes to apply a hierarchical splitting approach. Here, we apply in the different model hierarchies the optimal splitting approaches. Such that we can minimize the underlying splitting error and reduce optimal the computational time.

In the following example, we deal with a multi-flow problem based on a macroscopic and microscopic convection-diffusion-reaction equation, see Example 2.3.

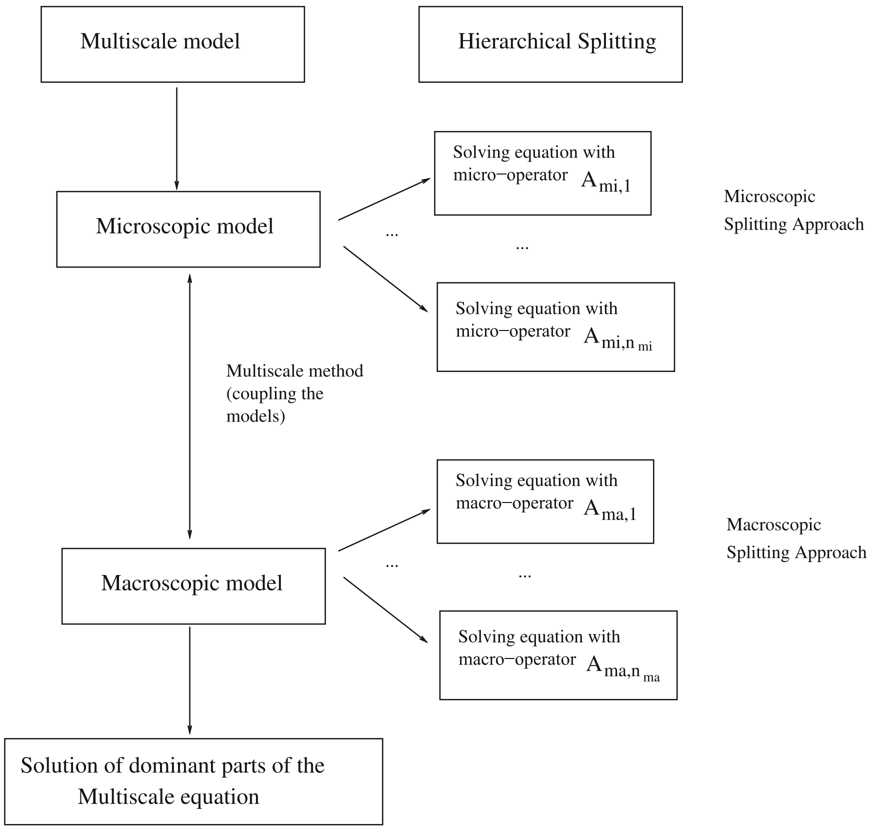

Fig. 2.3 Hierarchical splitting approach (Coupling of micro–macro and macro–micro)

Example 2.3 We have the following multi-flow problem, which is a coupled problem of fine- and coarse-scale CDR equations.

1. Macroscopic Equation:

$$\frac{du_{macro}}{dt} = F_1(u_{macro}, u_{micro}) + F_2(u_{macro}, u_{micro}). \tag{2.29}$$

   where F_1 is the convection-reaction operator and F_2 is diffusion operator.
2. Microscopic Equation:

$$\frac{du_{micro}}{dt} = -\frac{1}{\varepsilon}(\tilde{F}_1(u_{micro}) + \tilde{F}_2(u_{micro}) - \phi(u_{macro})). \tag{2.30}$$

   where $\tilde{F}_1$ is the convection-reaction operator and $\tilde{F}_2$ is diffusion operator. Further u_{macro} is the slow time-dependent and u_{micro} is the fast time-dependent variable.

In the following, we apply the HMM and the splitting of the different scale-dependent-equations in Algorithm 2.2.

Algorithm 2.2 We first apply the HMM algorithm.

- We solve the microscopic equation:

$$u_{micro}^{n,m+1} = u_{micro}^{n,m} - \frac{\delta t}{\varepsilon}((\tilde{F}_1 u_{micro} + \tilde{F}_2 u_{micro}^{n,m}) - \phi(u_{macro}^n)), \tag{2.31}$$

  where $m = 0, 1, \ldots, M-1$, z.B. $\delta t \leq \Delta t/M$ is applied as microscopic time-step.
- We apply the operator splitting method with respect to the microscopic equation:

$$u_{micro,1}^{n,m+1} = u_{micro,1}^{n,m} - \frac{\delta t}{\varepsilon}(\tilde{F}_1 u_{micro} - 0.5\phi(u_{macro}^n)), \text{ with } u_{micro,1}^{n,m} = u_{micro}^{n,m}, \tag{2.32}$$

$$u_{micro,2}^{n,m+1} = u_{micro,1}^{n,m+1} - \frac{\delta t}{\varepsilon}(\tilde{F}_2 u_{micro}^{n,m} - 0.5\phi(u_{macro}^n)), \text{ with } u_{micro,2}^{n,m} = u_{micro,1}^{n,m+1}, \tag{2.33}$$

  where $m = 0, 1, \ldots, M-1$, z.B. $\delta t \leq \Delta t/M$ is applied as microscopic time-step and next intermediate solution is given as $u_{micro}^{n,m+1} = u_{micro,2}^{n,m+1}$.
- Equilibration of the Microscopic operators (reconstruction):

$$\tilde{F}^n = \frac{1}{M}\sum_{m=1}^{M}(F_1(u_{macro}^n, u_{micro}^{n,m}) + F_2(u_{macro}^n, u_{micro}^{n,m})). \tag{2.34}$$

- Solving of the Macroscopic Equation:

$$u_{macro}^{n+1} = u_{macro}^{n} - \Delta t(\tilde{F}_1^n + \tilde{F}_2^n). \tag{2.35}$$

with Δt as macroscopic time-step.

- We apply the operator splitting method with respect to the macroscopic equation:

$$u_{macro,1}^{n+1} = u_{macro}^{n} - \Delta t \tilde{F}_1^n, \text{ with } u_{macro,1}^{n} = u_{macro}^{n}, \tag{2.36}$$

$$u_{macro,2}^{n+1} = u_{macro,1}^{n+1} - \Delta t \tilde{F}_2^n, \text{ with } u_{micro,2}^{n} = u_{macro,1}^{n+1}, \tag{2.37}$$

where the next intermediate solution is given as $u_{macro}^{n+1} = u_{macro,2}^{n+1}$.

- We apply the next microscopic step, till we have resolved the full time interval.

Remark 2.2 Here, we can apply the discrete macroscopic time-steps with respect to a fast splitting approach. Further also with the microscopic equation. The benefit is also to resolve only parts of the microscopic time interval such that we can also accelerate the multiscale computation.

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