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Vorwort

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Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

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Report

POD-DEIM based model order reduction for a three-dimensional microscopic Li-Ion battery model

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Kaiserslautern

Abstract

Microscopic models for the processes occurring during charge and discharge of Li-ion batteries allow detailed studies of the occurring phenomena, but they often result in nonlinear, coupled diffusion-type PDE systems where the nonlinearities occur in the coefficients. Solving these models on microscopically resolved geometries of anode and cathode structures of Li-ion batteries is computationally very intensive. Model order reduction offers a possible remedy. We present a method based on Proper orthogonal decomposition (POD) and Discrete empirical interpolation method (DEIM) to solve the equations using Newton's Method in reduced space. Since the coefficients of the PDE system depend on the subdomain (i. e. anode, cathode or electrolyte) and the different terms of the system show different nonlinearities, special care needs to be taken to find the reduced basis and to use DEIM. We apply our approach to a simplified test problem.

Contents

1 Notation

1.1 Acronyms

DEIM Discrete empirical interpolation method
MOR Model order reduction
PDE Partial differential equation
POD Proper orthogonal decomposition

1.2 Table of symbols

Notation	Description
$\mathbf{u}^n = \begin{pmatrix} \mathbf{y}^n \\ \mathbf{z}^n \end{pmatrix}$	Unknowns $\mathbf{y}^n, \mathbf{z}^n \in \mathbb{R}^N$
$\mathbf{u}^n \in \mathbb{R}^{2N}$	Solution of the full system
$q \in \{\mathbf{y}, \mathbf{z}\}$	Unknown in the unknown vector $\mathbf{u}^n$
$\mathbf{c}$	Concentration
$\boldsymbol{\phi}$	Potential
$\tilde{\mathbf{u}}^n \in \mathbb{R}^n$	Solution of the reduced system
$\tilde{\mathbf{u}}^n = \begin{pmatrix} \tilde{\mathbf{y}}^n \\ \tilde{\mathbf{z}}^n \end{pmatrix}$	Unknowns $\tilde{\mathbf{y}}^n, \tilde{\mathbf{z}}^n$ in the reduced system
A, A_q	Matrices describing linear part
$F(\mathbf{u}), F_q(\mathbf{u})$	Nonlinear functions
$J(\mathbf{u})$	Jacobians corresponding to nonlinear functions
ε	Percentage of information in the reduced system compared to the one in the full system, see Section 3.1.2
N	Number of space points in the discretization of the full system
n	Size of the reduced basis for the solution $\mathbf{u}$
m	Size of the reduced basis for the nonlinear function $F(\mathbf{u})$ for DEIM
$m_{q,q}$	Componentwise size of the reduced basis for $F(\mathbf{u})$ for DEIM, i. e. size of $I_{\alpha,\beta}$
s	Number of snapshots
superscript $^{n,n+1}$	Old and new time step
superscript $^{k,k+1}$	Newton step
no superscript in k	Solution after Newton iterations
subscript $_i$	Unknowns in the mesh
$\{E, W, N, S, T, B\}$	Labels for neighbors, i. e. E east, W west, N north, S south, T top, B bottom (e. g. x_{i+E} is the unknown point of x_i's east neighbor)
p	Vector of integers whose i-th component p_i corresponds to the i-th interpolation index obtained via DEIM
$I, I_{\alpha,\beta}$	Index set containing indices needed for DEIM
$j \in I_{\alpha,\beta}$	Interpolation point index out of index set
$P, P_{\alpha,\beta} \in \mathbb{R}^{2N\times m}$	Matrix with unit vectors corresponding to I and $I_{\alpha,\beta}$, respectively
$X_u \in \mathbb{R}^{2N\times s}$	Matrix with snapshots as columns (i. e. column n is given by $\mathbf{u}^n$ after n time steps, $n = 1, \ldots, s$)
$K \in \mathbb{R}^{2N\times 2N}$	Correlation matrix given by $X_u X_u^T$
$V_u \in \mathbb{R}^{2N\times n}$	Transformation matrix whose columns are the POD modes corresponding to the n largest eigenvalues of $X_u X_u^T$
$V_F \in \mathbb{R}^{2N\times m}$	Transformation matrix whose columns are the POD modes obtained by applying POD to F evaluated at the snapshots $\mathbf{u}^1, \ldots, \mathbf{u}^s$
$\tilde{F}(\tilde{\mathbf{u}}^n)$	Approximation of the nonlinear term $V_u^T F(V_u \tilde{\mathbf{u}}^n)$
$\tilde{J}(\tilde{\mathbf{u}}^n)$	Approximation of the Jacobian of the nonlinear term $V_u^T F(V_u \tilde{\mathbf{u}}^n)$

1.3 Systems

As our notation depends on the systems for which the Model order reduction (MOR) methods are derived, we display them at this point and postpone further detailed system descriptions to later sections.

We aim to apply MOR to Partial differential equation (PDE) systems. However, the methods described herein were originally derived for dynamical systems of the forms, given in (1) and (2).

After semi-discretizing a PDE in space, we obtain a system of ordinary differential equations and therewith a dynamical system. Thus, it suffices to restrict ourselves to systems of the form

$$\frac{dy(t)}{dt} = A_y y(t) + F_y(y(t), z(t)) \tag{1a}$$

$$\frac{dz(t)}{dt} = A_z z(t) + F_z(y(t), z(t)). \tag{1b}$$

By setting $u(t) = \begin{pmatrix} y(t) \\ z(t) \end{pmatrix}$, we obtain the equation

$$\frac{du(t)}{dt} = A_u u(t) + F_u(u(t)) \tag{2}$$

for a matrix $A = \begin{pmatrix} A_y & \\ & A_z \end{pmatrix}$ describing the linear part and a function $F_u = \begin{pmatrix} F_y \\ F_z \end{pmatrix}$ for the nonlinear part.

Discretizing both in time and space yields a system of the form

$$A\mathbf{u}^n + F(\mathbf{u}^n) = 0.$$

after n time steps where the matrix $A \in \mathbb{R}^{2N,2N}$ and the nonlinear function F with $F(\mathbf{u}^n) \in \mathbb{R}^{2N}$ are chosen accordingly.

2 Introduction

Microscopic models for the processes occurring during charge and discharge of Li-ion batteries allow detailed studies of the occurring phenomena, but they often result in nonlinear, coupled diffusion-type PDE systems where the nonlinearities occur in the coefficients. Such a model is derived in [1, Pg. 139] for modeling the transport of Li-ions and the respective occuring potential for a microscopically resolved battery consisting of a porous anode, porous cathode and a separator. This Li-ion battery is modeled by the coupled, nonlinear PDE system

$$\frac{\partial c}{\partial t} - \nabla \cdot (\alpha(c,\phi)\nabla c + \beta(c,\phi)\nabla \phi) \quad = 0 \tag{3a}$$

$$-\nabla \cdot (\gamma(c,\phi)\nabla c + \delta(c,\phi)\nabla \phi) \quad = 0 \tag{3b}$$

for $c(x,t)$ the concentration of Li-ions in $\left[\frac{\text{mol}}{\text{cm}^3}\right]$ and $\phi(x,t)$ the electric potential in [V]. For details on the coefficients of (3) we refer to [1].

The discretization of results in a coupled, nonlinear DAE system, given in [2]. Solving this model on microscopically resolved geometries of anode and cathode structures of Li-ion batteries allows detailed insights into the distribution of concentration and potential (cp. [3]), but the computations are very intensive. Model order reduction offers a possible remedy. We present a POD-DEIM based method, extended from [4]. The basic concepts of the method are shown in Section 3 and applied to a simple, coupled system of diffusion equations with nonlinear coefficients. In Section 4, we derive the method for the actual system from [1] by extending [5] and solve the equations by a Newton method in reduced space. Besides, we discuss details of its implementation in the software BEST, based on the CoRheoS framework, described in [6]. As the coefficients of the PDE system depend on the subdomain - anode, cathode or electrolyte - and the different terms of the system show different nonlinearities, special care needs to be taken to find the reduced basis and to use DEIM. We show the basic applicability of the method by applying it to a simplified, pseudo-3D test problem.

3 Introduction to POD-DEIM for nonlinear PDE systems

DEIM has initially been introduced in [4] and is based on the Empirical interpolation method (EIM), introduced in [7]. For introductory purposes, we repeat the basics of DEIM. Since the reduced bases are found via POD, we firstly given an overview on the POD method which is a long-established method to compute a reduced basis for discretized PDE systems, given as a set of linear equations. Then, we describe the extension to DEIM for nonlinear contributions to the system.

3.1 Model reduction via POD

In this section we heavily rely on the description of MOR via POD in [8]. Since the time for computations and the data that needs to be stored grow with the size of the dynamical system, it is often necessary to approximate the full, high-dimensional, dynamical system by a low-dimensional system that describes the characteristic dynamic of the original system. A method for model reduction is POD, also known as total least-squares estimation. By using POD, we obtain an optimally ordered, orthonormal basis in the least-squares sense for the given data. Then, the constructed, optimal basis can be truncated in order to get a basis of the reduced system.

POD can also be seen as a method for data representation or as a projection method since the original dynamical system is projected onto a subspace of the original phase space. For this reason, we focus on the idea of finding a subspace that approximates a given data set in the least-squares sense.

3.1.1 Constructing a POD basis

In the following, it is described how to construct a POD basis for a finite dimensional vector space V. Let $V = \mathbb{R}^{2N}$ and assume that $U = \{u_1(t), \dots, u_k(t)\}$ is a given set of sampled data in V. The trajectories $u_i(t) \in \mathbb{R}^{2N}, i = 1, \dots, k, t \in [0, T]$ solve System (2) on the interval $[0, T]$ where T stands for the total time. We aim to find an n-dimensional subspace $W \subseteq V$ approximating the data in a least-squares sense. This means that we need to find an orthogonal projection $\Pi_n : V \to W$ minimizing

$$\|U - \Pi_n U\|^2 := \sum_{i=1}^{k} \int_0^T \|u_i(t) - \Pi_n u_i(t)\|^2 \, dt.$$

In order to solve this problem, we define the correlation matrix $K \in \mathbb{R}^{2N \times 2N}$ as

$$K := \sum_{i=1}^{k} \int_0^T u_i(t) u_i(t)^* dt \tag{4}$$

where $u_i(t)^*$ is obtained from $u_i(t)$ by taking the transposed and the complex conjugate for each entry. Note that K is a symmetric positive semidefinite matrix with real, ordered eigenvalues $\lambda_1 \geq \ldots \geq \lambda_{2N} \geq 0$. The corresponding eigenvectors $v_{u_j}, j = 1, \dots, 2N$, are given by

$$K v_{u_j} = \lambda_j v_{u_j}, \quad j = 1, \dots, 2N$$

and can be chosen such that $\{v_{u_1}, \dots, v_{u_{2N}}\}$ is an orthonormal basis of V. The eigenvectors $v_{u_j}, j = 1, \dots, 2N$, are then called the POD modes. It can be shown that under these assumptions the following equation holds:

$$\min_W \|U - \Pi_n U\| = \sum_{j=2N-n+1}^{2N} \lambda_j \tag{5}$$

where we take the minimum over all subspaces W of dimension n. The optimal orthogonal projection $\Pi_n : V \to W$ with $\Pi_n {\Pi_n}^* = I$ is given by

$$\Pi_n = \sum_{j=1}^{n} v_{u_j} {v_{u_j}}^*$$

and the optimal n-dimensional subspace W representing the data can be written as $W = span\{v_{u_1}, \dots, v_{u_n}\}$. Hence, the corresponding POD basis is given by $\{v_{u_1}, \dots, v_{u_n}\}$.

3.1.2 Choosing the dimension

In order to obtain the subspace W of V and the corresponding orthogonal projection Π_n, one can proceed as described in Section 3.1.1. Nevertheless, it remains to show how to choose the dimension n of W to get a good approximation of the data set. By Equation (5), there is a connection between the least-squares error and the eigenvalues of the correlation matrix K, defined in Equation (4). Large eigenvalues represent the main characteristics of a dynamical system while omitting smaller eigenvalues only leads to small perturbations of the system. Thus, the dimension n of the subspace W has to be chosen as small as possible such that the relative information content $I(n)$, defined by

$$I(n) := \frac{\sum_{i=1}^{n} \lambda_i}{\sum_{i=1}^{2N} \lambda_i},$$

is greater than a given bound that should be slightly smaller than one for good approximations. For a percentage ε of the information in V that is also contained in W the dimension n of the subspace W can be computed by

$$n = \text{argmin}\{I(n) : I(n) \geq \frac{\varepsilon}{100}\}.$$

3.1.3 Snapshots and POD

By definition of K in Equation (4), K is a square matrix of dimension $2N$ where N can be very large. Hence, a large eigenvalue problem for the matrix $K \in \mathbb{R}^{2N \times 2N}$ has to be solved for the computation of the POD modes. Instead of solving this high-dimensional eigenvalue problem, one can also consider the low-dimensional eigenvalue problem for a square matrix of dimension s with $s < 2N$ where s is the number of the so-called snapshots. That is why this method is called the method of snapshots.

In order to obtain snapshots, the trajectories of the dynamical system are evaluated at certain times $t_1, \dots, t_s \in [0, T]$. This means that the snapshots are given by $u_i = u(t_i) \in \mathbb{R}^{2N}$. The new correlation matrix K is defined by

$$K := \sum_{i=1}^{s} u(t_i) u(t_i)^*$$

In the following, we always refer to this definition of the correlation matrix. The matrix X_u, consisting of the snapshots $u(t_i) \in \mathbb{R}^{2N}, i = 1, \dots, s$, in the columns and of the trajectories of the system at discrete time events in the rows, is then given by

$$X_u = (u(t_1), \dots, u(t_s)) \in \mathbb{R}^{2N \times s}.$$

It holds that $K = X_u X_u^*$. Instead of considering $K \in \mathbb{R}^{2N \times 2N}$, the low-dimensional eigenvalue problem

$$X_u^* X_u v_j = \lambda_j v_j, \quad v_j \in \mathbb{R}^s, \quad j = 1, \dots, s,$$

for the matrix $X_u^* X_u \in \mathbb{R}^{s \times s}$ is solved in the method of snapshots. The eigenvectors $v_j, j = 1, \dots, s,$ can be chosen orthonormal and the POD modes are given by

$$v_{u_j} = \frac{1}{\sqrt{\lambda_j}} X_u v_j \in \mathbb{R}^{2N}, \quad j = 1, \dots, s.$$

3.2 Nonlinear model reduction via DEIM

This section describes how DEIM can be used for nonlinear model reduction. The method is described in [4]. We recapture major parts of this work in a more detailed fashion using our notation and extend it to systems of equations in Section 3.3.

As described in Section 1.3, we consider a system of nonlinear equations resulting from a discretized PDE of the form

$$A\mathbf{u}^n + F(\mathbf{u}^n) = 0 \tag{6}$$

where $A \in \mathbb{R}^{2N \times 2N}$ is a constant matrix, $\mathbf{u}^n = [u_1^n, \dots, u_{2N}^n]^T \in \mathbb{R}^{2N}$, $\mathbf{u}_i : [0, T] \to \mathbb{R}$, is a solution of the system, $t \in [0, T]$ denotes time and $F = [F_1(\mathbf{u}^n), \dots, F_{2N}(\mathbf{u}^n)]^T$, $F_i : \Omega \to \mathbb{R}$, for a continuous bounded domain $\Omega \subset \mathbb{R}^{2N}$, is a nonlinear function evaluated at $\mathbf{u}^n$. Here, the dimension $2N$ denotes the number of spatial grid points used for discretization. The corresponding Jacobian of System (6) is given by $A + J(\mathbf{u}^n)$. Since the dimension $2N$ can be very large, it is useful to approximate the full, high-dimensional system by a low-dimensional system that describes the characteristic dynamic of the original system. As described in Section 3.1.1, we need to construct a POD basis. Let $V_u \in \mathbb{R}^{2N \times n}$ the matrix whose columns are the (orthonormal) POD modes corresponding to the n largest eigenvalues of the correlation matrix. Given the matrix V_u, we have the following relation between the solution $\mathbf{u}^n \in \mathbb{R}^{2N}$ of the full system and the solution $\tilde{\mathbf{u}}^n \in \mathbb{R}^n$ of the reduced one:

$$\mathbf{u}^n = V_u \tilde{\mathbf{u}}^n \tag{7}$$

Thus, it also holds $V_u^T \mathbf{u}^n = \tilde{\mathbf{u}}^n$ for all $t \in [0, T]$. The reduced order system is obtained by multiplying (6) by V_u^T and inserting (7). Since we aim to apply a Newton method for solving the reduced system, the corresponding Jacobian is needed as well. The reduced order system and the corresponding Jacobian are given by

$$F_{Newton}(\tilde{\mathbf{u}}^n) := \underbrace{V_u^T A V_u}_{=:\tilde{A} \in \mathbb{R}^{n \times n}} \tilde{\mathbf{u}}^n + \underbrace{V_u^T}_{\in \mathbb{R}^{n \times 2N}} \underbrace{F(V_u \tilde{\mathbf{u}}^n)}_{\in \mathbb{R}^{2N \times 1}} = 0 \tag{8}$$

$$J_{Newton}(\tilde{\mathbf{u}}^n) := V_u^T A V_u + \underbrace{V_u^T}_{\in \mathbb{R}^{n \times 2N}} \underbrace{J(V_u \tilde{\mathbf{u}}^n)}_{\in \mathbb{R}^{2N \times 2N}} \underbrace{V_u}_{\in \mathbb{R}^{2N \times n}} = \tilde{A} + V_u^T J(V_u \tilde{\mathbf{u}}^n) V_u. \tag{9}$$

Although we have transformed the full system into a system of dimension n, we can see in Equations (8) and (9) that the nonlinear function F and its Jacobian are of dimension $2N$, i.e. they have the dimension of the high-dimensional system. Thus, these computations are inefficient, in particular because of the fact that we have to evaluate the high-dimensional Jacobian in every Newton iteration. To overcome this problem of high computational costs, DEIM can be used to reduce the number of rows of F that need to be evaluated. We firstly compute the POD basis for the nonlinear function F. This basis can be constructed by applying POD to F evaluated at the given snapshots $\mathbf{u}^1, \dots, \mathbf{u}^s$ where s is the number of snapshots. Let m be the dimension of the reduced system and let $v_{F_1}, \dots, v_{F_m} \in \mathbb{R}^{2N}$ be the vectors of the POD basis. Then, the corresponding transformation matrix V_F is given by $V_F = [v_{F_1}, \dots, v_{F_m}] \in \mathbb{R}^{2N \times m}$. Now, we construct a matrix $P = [e_{p_1}, \dots, e_{p_m}] \in \mathbb{R}^{2N \times m}$ where e_{p_i} is the p_i-th column of the $2N \times 2N$-identity matrix. Here, $p_i, i = 1, \dots m,$ denote the interpolation indices that can be determined by the following algorithm: In this algorithm, the notation $[|\rho|, p_l] = \max |r|$ denotes

Algorithm 1 Algorithm for interpolation indices $p = [p_1, \dots, p_m]^T \in \mathbb{R}^m$

Require: $v_{F_1}, \dots, v_{F_m} \in \mathbb{R}^{2N}$ linearly independent
  $[|\rho|, p_1] = \max |v_{F_1}|$
  $V_F = [v_{F_1}], P = [e_{p_1}], p = [p_1]$
  for $l = 2$ to m **do**
    Solve $(P^T V_F)c = P^T v_{F_l}$ for c
    $r = v_{F_l} - V_F c$
    $[|\rho|, p_l] = \max |r|$
    $V_F := [V_F, v_{F_l}], P := [P, e_{p_l}], p := [p^T, p_l]^T$
  end for

that $|\rho| = \max_{i=1,\dots,2N} |r_i| = |r_{p_l}|$ and p_l is the smallest index assuming the maximum of $|r|$. One can show that the following approximation holds for the nonlinear function F:

$$F(V_u \tilde{\mathbf{u}}^n) \approx V_F (P^T V_F)^{-1} P^T F(V_u \tilde{\mathbf{u}}^n)$$

Hence, we obtain the approximations for the nonlinear term $V_u^T F(V_u \tilde{\mathbf{u}}^n)$ in Equation (8) and its Jacobian $V_u^T J(V_u \tilde{\mathbf{u}}^n) V_u$, denoted by $\tilde{F}(\tilde{\mathbf{u}}^n)$ and $\tilde{J}(\tilde{\mathbf{u}}^n)$:

$$\tilde{F}(\tilde{\mathbf{u}}^n) := V_u^T V_F (P^T V_F)^{-1} P^T F(V_u \tilde{\mathbf{u}}^n) \approx V_u^T F(V_u \tilde{\mathbf{u}}^n) \tag{10}$$
$$\tilde{J}(\tilde{\mathbf{u}}^n) := V_u^T V_F (P^T V_F)^{-1} P^T J(V_u \tilde{\mathbf{u}}^n) V_u \approx V_u^T J(V_u \tilde{\mathbf{u}}^n) V_u \tag{11}$$

Since F in $\tilde{F}$ and J in $\tilde{J}$ are multiplied on the left by P^T whose rows are unit vectors, F and J only need to be evaluated in m distinguished rows p_i. By inserting Equations (10) and (11) into Equations (8) and (9) we obtain the approximations:

$$F_{Newton}(\tilde{\mathbf{u}}^n) \approx V_u^T A V_u \tilde{\mathbf{u}}^n + V_u^T V_F (P^T V_F)^{-1} P^T F(V_u \tilde{\mathbf{u}}^n) \stackrel{!}{=} 0 \tag{12}$$
$$J_{Newton}(\tilde{\mathbf{u}}^n) \approx V_u^T A V_u + V_u^T V_F (P^T V_F)^{-1} P^T J(V_u \tilde{\mathbf{u}}^n) V_u \tag{13}$$

Note that these equations describe the entire reduced system consisting of the linear term and an approximation of the nonlinear function. The solution $\tilde{\mathbf{u}}^n$ for the reduced system can be computed with the standard Newton method, given in Equation (14), using the reduced system formulation in Equation (12) and the corresponding Jacobian in Equation (13):

$$\text{Solve} \quad J_{Newton}\left(\tilde{\mathbf{u}}^{k,n}\right)\Delta\tilde{\mathbf{u}}^{k,n} = -F_{Newton}\left(\tilde{\mathbf{u}}^{k,n}\right) \quad \text{for} \quad \Delta\tilde{\mathbf{u}}^{k,n} \tag{14a}$$

$$\tilde{\mathbf{u}}^{k+1,n} = \tilde{\mathbf{u}}^{k,n} + \Delta\tilde{\mathbf{u}}^{k,n} \tag{14b}$$

$$\text{until a sufficiently accurate solution } \tilde{\mathbf{u}}^{n} \text{ is reached} \tag{14c}$$

The solution of the full (i. e. the original) system $\mathbf{u}^n$ after n time steps can easily be computed using the transformation in Equation (7).

3.3 Nonlinear model reduction via DEIM for systems of equations

The derivations given in [4] are applicable to PDE systems if the reduced basis is determined for the full coupled discretization. However, as each equation of the PDE system may show different properties and dynamics, we apply MOR for PDE systems by determining a POD basis for each equation separately. In this case, the approach in [4] needs to be extended which is shown in this section.

Consider a discretized system of the form

$$F(\mathbf{y},\mathbf{z}) = \begin{pmatrix} F_1(\mathbf{y},\mathbf{z}) \\ F_2(\mathbf{y},\mathbf{z}) \end{pmatrix} = \underline{0}$$

where $\mathbf{y}$ and $\mathbf{z}$ are the unknowns.

As before, we need to distinguish between linear and nonlinear terms. Thus, it holds

$$F_1(\mathbf{y},\mathbf{z}) = G_{11}(\mathbf{y},\mathbf{z}) + G_{12}(\mathbf{y},\mathbf{z}) \quad \text{and} \quad F_2(\mathbf{y},\mathbf{z}) = G_{21}(\mathbf{y},\mathbf{z}) + G_{22}(\mathbf{y},\mathbf{z})$$

with G_{11}, G_{21} nonlinear and G_{12}, G_{22} linear functions. Hence, we obtain:

$$F(\mathbf{y},\mathbf{z}) = \begin{pmatrix} F_1(\mathbf{y},\mathbf{z}) \\ F_2(\mathbf{y},\mathbf{z}) \end{pmatrix} = \begin{pmatrix} G_{11}(\mathbf{y},\mathbf{z}) + G_{12}(\mathbf{y},\mathbf{z}) \\ G_{21}(\mathbf{y},\mathbf{z}) + G_{22}(\mathbf{y},\mathbf{z}) \end{pmatrix} = \underbrace{\begin{pmatrix} G_{11}(\mathbf{y},\mathbf{z}) \\ G_{21}(\mathbf{y},\mathbf{z}) \end{pmatrix}}_{\tilde{F}_1(\mathbf{y},\mathbf{z})} + \underbrace{\begin{pmatrix} G_{12}(\mathbf{y},\mathbf{z}) \\ G_{22}(\mathbf{y},\mathbf{z}) \end{pmatrix}}_{\tilde{F}_2(\mathbf{y},\mathbf{z})}$$

where $\tilde{F}_1(\mathbf{y},\mathbf{z}) = \begin{pmatrix} G_{11}(\mathbf{y},\mathbf{z}) \\ G_{21}(\mathbf{y},\mathbf{z}) \end{pmatrix}$ is nonlinear and $\tilde{F}_2(\mathbf{y},\mathbf{z}) = \begin{pmatrix} G_{12}(\mathbf{y},\mathbf{z}) \\ G_{22}(\mathbf{y},\mathbf{z}) \end{pmatrix}$ is linear.

Let $\mathbf{u} = [\mathbf{y},\mathbf{z}]^T$ be the solution of the full system $F(\mathbf{y},\mathbf{z}) = \underline{0}$. As described in Section 3.2, $\mathbf{u}$ can be used in order to compute the POD basis as well as the interpolation indices. Thus, we construct the matrices V_1, V_{F1} and P_1 for the solution $\mathbf{y}$ by evaluating F_1 at the given snapshots. Analogously, the matrices V_2, V_{F2} and P_2 are constructed for $\mathbf{z}$. Hence, the reduced system that needs to be solved is given by

$$\begin{pmatrix} V_1^T V_{F1}(P_1^T V_{F1})^{-1} P_1^T G_{11}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) + V_1^T G_{12}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) \\ V_2^T V_{F2}(P_2^T V_{F2})^{-1} P_2^T G_{21}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) + V_2^T G_{22}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) \end{pmatrix} = \underline{0}$$

where $\tilde{\mathbf{u}} = [\tilde{\mathbf{y}}, \tilde{\mathbf{z}}]^T$ is the solution of the reduced system. This can be written in the following way:

$$\begin{pmatrix} V_1^T & 0 \\ 0 & V_2^T \end{pmatrix} \begin{pmatrix} V_{F1} & 0 \\ 0 & V_{F2} \end{pmatrix} \begin{pmatrix} (P_1^T V_{F1})^{-1} & 0 \\ 0 & (P_2^T V_{F2})^{-1} \end{pmatrix} \begin{pmatrix} P_1^T & 0 \\ 0 & P_2^T \end{pmatrix} \begin{pmatrix} G_{11}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) \\ G_{21}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) \end{pmatrix} + \begin{pmatrix} V_1^T & 0 \\ 0 & V_2^T \end{pmatrix} \begin{pmatrix} G_{12}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) \\ G_{22}(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) \end{pmatrix} = \underline{0}$$

Simplifying yields:

$$\begin{pmatrix} V_1^T & 0 \\ 0 & V_2^T \end{pmatrix} \begin{pmatrix} V_{F1} & 0 \\ 0 & V_{F2} \end{pmatrix} \left(\begin{pmatrix} P_1^T & 0 \\ 0 & P_2^T \end{pmatrix} \begin{pmatrix} V_{F1} & 0 \\ 0 & V_{F2} \end{pmatrix} \right)^{-1} \begin{pmatrix} P_1^T & 0 \\ 0 & P_2^T \end{pmatrix} \tilde{F}_1(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) + \begin{pmatrix} V_1^T & 0 \\ 0 & V_2^T \end{pmatrix} \tilde{F}_2(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) = \underline{0}$$

Hence, we obtain

$$V^T V_F \left(P^T V_F\right)^{-1} P^T \tilde{F}_1(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) + V^T \tilde{F}_2(V_1\tilde{\mathbf{y}}, V_2\tilde{\mathbf{z}}) = 0 \tag{15}$$

where $V := \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}$, $V_F := \begin{pmatrix} V_{F1} & 0 \\ 0 & V_{F2} \end{pmatrix}$ and $P := \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix}$.

3.4 An example: Solving the heat equation with nonlinear coefficients

As a simple example leading towards the actual problem, we want to solve in Section 4, we apply MOR to the scalar heat equation with a nonlinear coefficient and later, in Section 3.4.3, to a system of such coupled heat equations.

3.4.1 Description of the problem

In the following, we consider the one-dimensional heat equation given by

$$\frac{\partial u}{\partial t} = \lambda(u) \frac{\partial^2 u}{\partial x^2}$$

as in [9], where u is the temperature. Since the temperature u depends on space and time, $u(x,t)$ denotes the temperature at position x and time t. In our simulations, we consider the time interval (0,30] and a spatial range [0,1]. Besides, we assume the boundary conditions to be the following:

$$\frac{\partial u}{\partial x}(0,t) = q(t) \text{ with } q(t) = \begin{cases} 1, & t < 10 \\ 0, & t \geq 10 \end{cases}$$

$$\frac{\partial u}{\partial x}(1,t) = 0$$

The initial condition is set as $u(x,0) = 1$. The spatial distance between two discretization points Δx is assumed to be 0.01 and Δt denotes the size of one time step. By discretizing the PDE, we obtain:

$$\frac{\mathbf{u}_P^{n+1} - \mathbf{u}_P^n}{\Delta t}\Delta x = \lambda(\mathbf{u})\left(\frac{\mathbf{u}_E^{n+1} - \mathbf{u}_P^{n+1}}{\Delta x} - \frac{\mathbf{u}_P^{n+1} - \mathbf{u}_W^{n+1}}{\Delta x}\right) \tag{16}$$

This can be transformed into an equation of the form

$$F(\mathbf{u}^n) = 0 \tag{17}$$

where $\mathbf{u}^n$ is a vector whose component $\mathbf{u}_i^n$ denotes the temperature at discretization point i at time t.

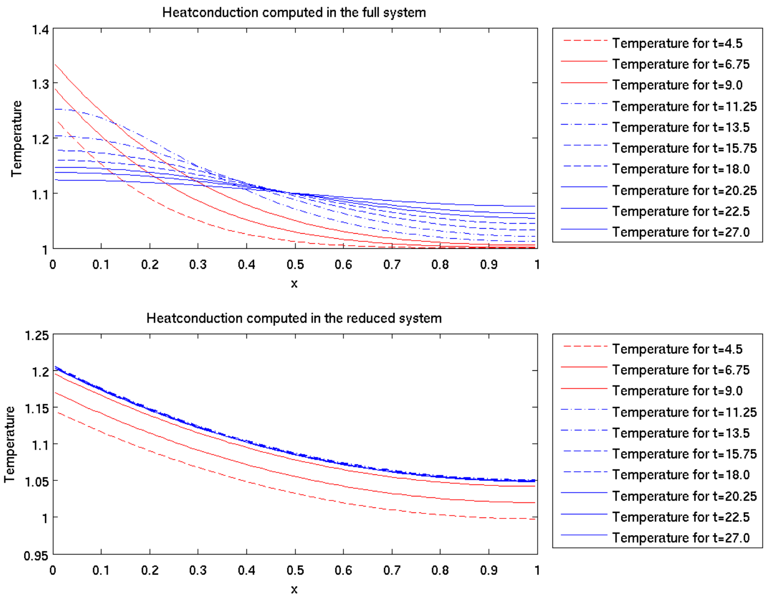

Figure 1:Comparison of the temperature computed in the full (top) and in the reduced system (bottom). The POD basis was of dimension 1, $\lambda(\mathbf{u}) = 0.01$.

Firstly, we assume $\lambda(\mathbf{u})$ to be constant for all $\mathbf{u}$, e. g. $\lambda(\mathbf{u}) = 0.01$. Thus, Equation (16) and therewith Equation (17) are linear. Hence, Equation (17) can easily be solved for all time events t. After computing the temperature $\mathbf{u}$ in the full system, the corresponding reduced system can be solved by using the snapshots, obtained from the full system, and by applying POD (cp. Section 3.1.1). The solution strongly depends on the chosen relative information content since it is responsible for the size of the chosen POD basis. Figures 1 and 2 show the solutions for the full system by applying POD with a POD basis of dimension 1 and of dimension 4. As expected the results for the POD basis of dimension 4 are much better and they are very similar to the results computed directly for the full system.

As a simple nonlinear case, we assume that $\lambda(\mathbf{u})$ is non-constant, i. e. $\lambda(\mathbf{u}) = 0.01\mathbf{u}$. Hence, the system that needs to be solved becomes nonlinear. The function F in Equation (17) can be written

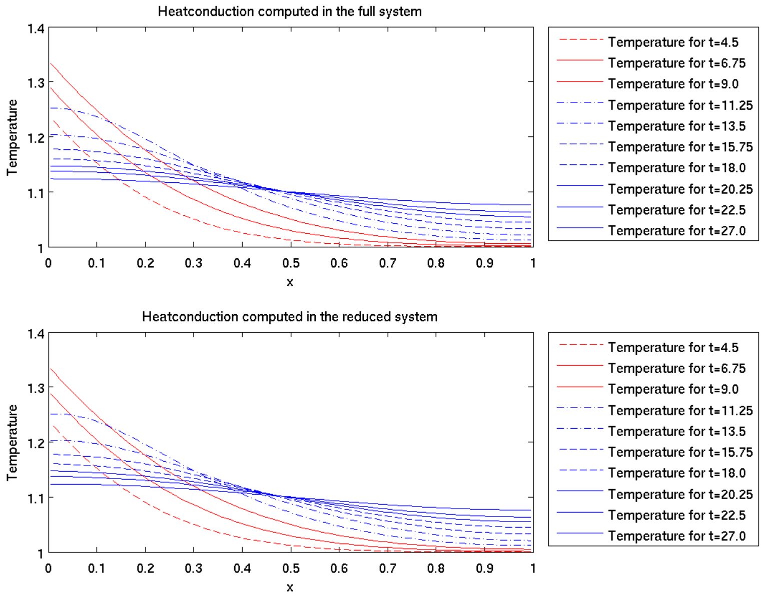

Figure 2:Comparison of the temperature computed in the full (top) and in the reduced system (bottom) . The POD basis was of dimension 4, $\lambda(\mathbf{u}) = 0.01$.

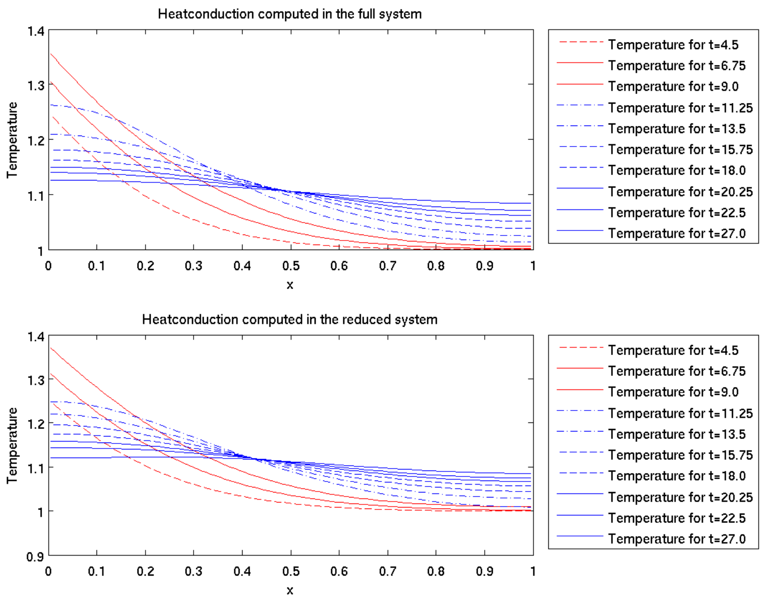

Figure 3:Comparison of the temperature computed in the full (top) and in the reduced system (bottom), $\lambda(\mathbf{u}) = 0.01\mathbf{u}$.

as

$$F(\mathbf{u}^n) = F_1(\mathbf{u}^n) + F_2(\mathbf{u}^n) = 0 \tag{18}$$

where F_1 contains the nonlinear terms (i. e. all terms of F depending on the function $\lambda(\mathbf{u})$) and F_2 the linear terms. In order to solve Equation (18) for certain times t, Newton's Method can be applied. As discussed earlier, it is often useful to solve a low-dimensional reduced system instead of solving the corresponding original system. Hence, we firstly compute the POD modes for the given snapshots by solving an eigenvalue problem as described in Sections 3.1.1 and 3.1.3. Then, we choose the dimension n of the reduced basis such that the relative information content of the reduced and the full system is larger than a given bound and the matrix V_u consisting of the POD modes corresponding to the n largest eigenvalues can be constructed. Analogously, another POD basis is computed for F_1, evaluated in the given snapshots, where F_1 denotes the nonlinear terms of function F. The corresponding matrix is called V_F. Then, the algorithm in Section 3.2 is applied in order to compute the interpolation indices and therewith the matrix P. By Equation (12), we obtain the following approximation for the heat equation and the corresponding Jacobian:

$$F_{Newton}(\tilde{\mathbf{u}}^n) \approx V_u^T F_2(V_u\tilde{\mathbf{u}}^n) + V_u^T V_F (P^T V_F)^{-1} P^T F_1(V_u\tilde{\mathbf{u}}^n)) \stackrel{!}{=} 0 \tag{19}$$

$$J_{Newton}(\tilde{\mathbf{u}}^n) \approx V_u^T J_{F_2}(V_u\tilde{\mathbf{u}}^n)V_u + V_u^T V_F (P^T V_F)^{-1} P^T J_{F_1}(V_u\tilde{\mathbf{u}}^n)V_u \tag{20}$$

The initial condition of the solution $\tilde{\mathbf{u}}$ of (19) is given by $\tilde{\mathbf{u}}(0) = V_u^T\mathbf{u}(0)$. Then, the solution can be computed by using Equation (20) as well as the initial condition and by applying Newton's Method that is formulated in (14). The solution of the full system is obtained from the solution of the reduced system for all time events t by using the transformation $\mathbf{u}^n = V_u\tilde{\mathbf{u}}^n$. The results for the temperature computed in the full and the reduced system are displayed in Figure 3.

3.4.2 Remarks

Our simulations have shown that it is necessary to distinguish between a linear and a nonlinear term instead of just evaluating F consisting of linear and nonlinear terms. This is of great importance for the computation of the POD basis for the nonlinear terms of F. Figure 4 shows the results for the case that the linear terms as well as the nonlinear terms are used for constructing the POD basis.

3.4.3 Solving a system of two coupled heat equations

In the following, we consider a system of equations of the form

$$\frac{\partial}{\partial t}\begin{pmatrix} y(x,t) \\ z(x,t) \end{pmatrix} = \begin{pmatrix} \lambda_1(y(x,t), z(x,t))\frac{\partial^2 y(x,t)}{\partial x^2} \\ \lambda_2(y(x,t), z(x,t))\frac{\partial^2 z(x,t)}{\partial x^2} \end{pmatrix} \tag{21}$$

Discretizing yields

$$\begin{pmatrix} \frac{\mathbf{y}^{k,n+1}-\mathbf{y}^{k,n}}{\Delta t}\Delta x \\ \frac{\mathbf{z}^{k,n+1}-\mathbf{z}^{k,n}}{\Delta t}\Delta x \end{pmatrix} = \begin{pmatrix} \lambda_1(\mathbf{y}^{k,n+1}, \mathbf{z}^{k,n+1})\left(\frac{\mathbf{y}^{k+1,n+1}-\mathbf{y}^{k,n+1}}{\Delta x} - \frac{\mathbf{y}^{k,n+1}-\mathbf{y}^{k-1,n+1}}{\Delta x}\right) \\ \lambda_2(\mathbf{y}^{k,n+1}, \mathbf{z}^{k,n+1})\left(\frac{\mathbf{z}^{k+1,n+1}-\mathbf{z}^{k,n+1}}{\Delta x} - \frac{\mathbf{z}^{k,n+1}-\mathbf{z}^{k-1,n+1}}{\Delta x}\right) \end{pmatrix}.$$

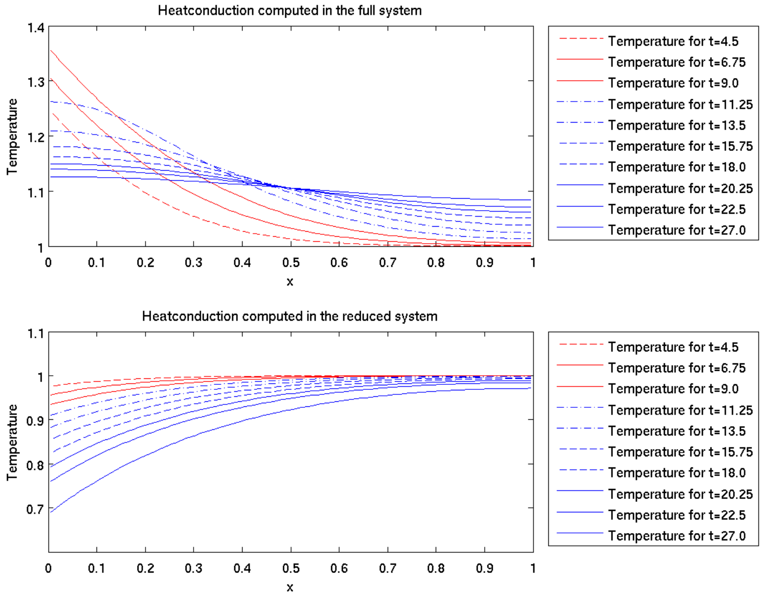

Figure 4:Comparison of the temperature computed in the full (top) and in the reduced system (bottom). No distinction between linear and nonlinear terms was used, $\lambda(u) = 0.01u$.

One can write the system of the form

$$F(\mathbf{y},\mathbf{z}) = \begin{pmatrix} F_1(\mathbf{y},\mathbf{z}) \\ F_2(\mathbf{y},\mathbf{z}) \end{pmatrix} = \underline{0} \tag{22}$$

where

$$F_1(\mathbf{y}) = \frac{\mathbf{y}^{k,n+1} - \mathbf{y}^{k,n}}{\Delta t}\Delta x - \lambda_1(\mathbf{y}^{k,n+1}, \mathbf{z}^{k,n+1}) \left(\frac{\mathbf{y}^{k+1,n+1} - \mathbf{y}^{k,n+1}}{\Delta x} - \frac{\mathbf{y}^{k,n+1} - \mathbf{y}^{k-1,n+1}}{\Delta x} \right)$$
$$F_2(\mathbf{z}) = \frac{\mathbf{z}^{k,n+1} - \mathbf{z}^{k,n}}{\Delta t}\Delta x - \lambda_2(\mathbf{y}^{k,n+1}, \mathbf{z}^{k,n+1}) \left(\frac{\mathbf{z}^{k+1,n+1} - \mathbf{z}^{k,n+1}}{\Delta x} - \frac{\mathbf{z}^{k,n+1} - \mathbf{z}^{k-1,n+1}}{\Delta x} \right).$$

Now, the system of equations can be solved via discrete empirical interpolation as described in Section 3.3.

Setting $\lambda_1(\mathbf{y}) = 0.01\mathbf{y}$ and $\lambda_2(\mathbf{z}) = 0.01\mathbf{z}$ results in a decoupled system. Therefore, the equations can be solved independently from each other. We obtain the same results for $\mathbf{y}$ and $\mathbf{z}$ since the same functions for λ_1 and λ_2 have been used. Besides, the results for solving a system of two equations in the full and the reduced system are very similar as expected. The results are displayed in Figure 5.

In a next step, the more general problem of a coupled system should be solved. Thus, the function F consists of $2N$ components and the corresponding Jacobian is a $2N \times 2N$-matrix. The reduced

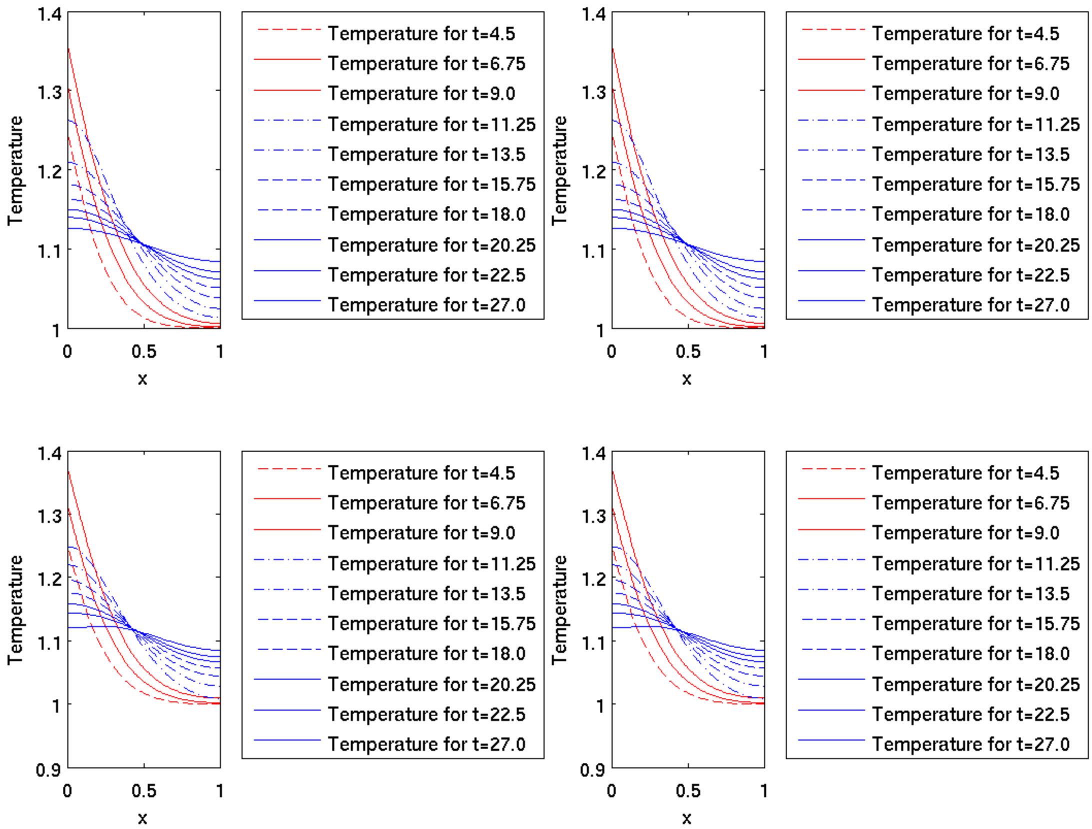

Figure 5: Comparison of the temperature computed for a system of equations in the full (top) and in the reduced (bottom) case with the first component on the left and the second on the right ($\lambda_1(\mathbf{y}) = 0.01\mathbf{y}, \lambda_2(\mathbf{z}) = 0.01\mathbf{z}$)

system that needs to be solved is given by (15) where the components of $\tilde{F}_1$ and $\tilde{F}_2$ might depend on the temperatures $\mathbf{y}$ and $\mathbf{z}$. The POD bases V_1 and V_{F_1} for system 1 as well as V_2 and V_{F_2} for system 2 can be computed separately from each other. The matrices P_1 and P_2 can be obtained by the algorithm in Section 3.2. Note that the indices for interpolation of the second system, i. e. the components of vector P_2, need to be shifted by N which corresponds to the definition of the blockdiagonal matrix P with matrices P_1 and P_2 as diagonal blocks because the i-th unit vector in P_2 corresponds to the $(N+i)$-th unit vector in P. By doing so, it is guaranteed that the correct components of the function $\tilde{F}_1$ are evaluated.

We set $\lambda_1(\mathbf{y}) = 0.01\mathbf{y}$ and $\lambda_2(\mathbf{z}) = 0.03\mathbf{z}$, so the system is still decoupled. Figure 6 shows the results for the temperature computed for systems 1 and 2 in the full and the reduced system using the approach for systems of equations as described in Section 3.3. For solving the coupled system with $\lambda_1(\mathbf{z}) = 0.01\mathbf{z}, \lambda_2(\mathbf{y}) = 0.03\mathbf{y}$, the results are displayed in Figure 7. For both simulations the values of the temperature for systems 1 and 2 computed for the full and the reduced system are very similar. Besides, one can see that the temperature of system 1 in the first simulation is slightly smaller than the temperature of system 1 in the second simulation whereas the temperature of system 2 in the first simulation is slightly larger than the corresponding temperature in the second simulation. This corresponds to the intuition: The constant in λ_1 is smaller than the one of λ_2 and thus the temperature of system 1 is smaller than the temperature of system 2 in general. Hence, the change of the dependence of λ results in a slightly changed total temperature.

4 POD-DEIM for the microscopic model in BEST

Using the method described in Section 3.3, we describe the details of applying an MOR method based on POD and DEIM to the model given in [1, Pg. 139]. It is essentially of the form:

$$\frac{\partial c}{\partial t} - \nabla \cdot (\alpha(c,\phi)\nabla c + \beta(c,\phi)\nabla\phi) = 0 \tag{23a}$$

$$-\nabla \cdot (\gamma(c,\phi)\nabla c + \delta(c,\phi)\nabla\phi) = 0 \tag{23b}$$

with different functions for $\alpha, \beta, \gamma, \delta$ in the different domains anode, cathode and electrolyte of a Li-ion battery.

The finite volume discretization of the full system is described in detail in [2]. We repeat it only in symbolic form here where we refer to the parts of the discretization corresponding to the terms in System (23). A method based on POD and DEIM has been exemplified for an one-dimensional mesoscopic model of the equations in [5]. We extend the approaches to the microscopic model and a three-dimensional discretization.

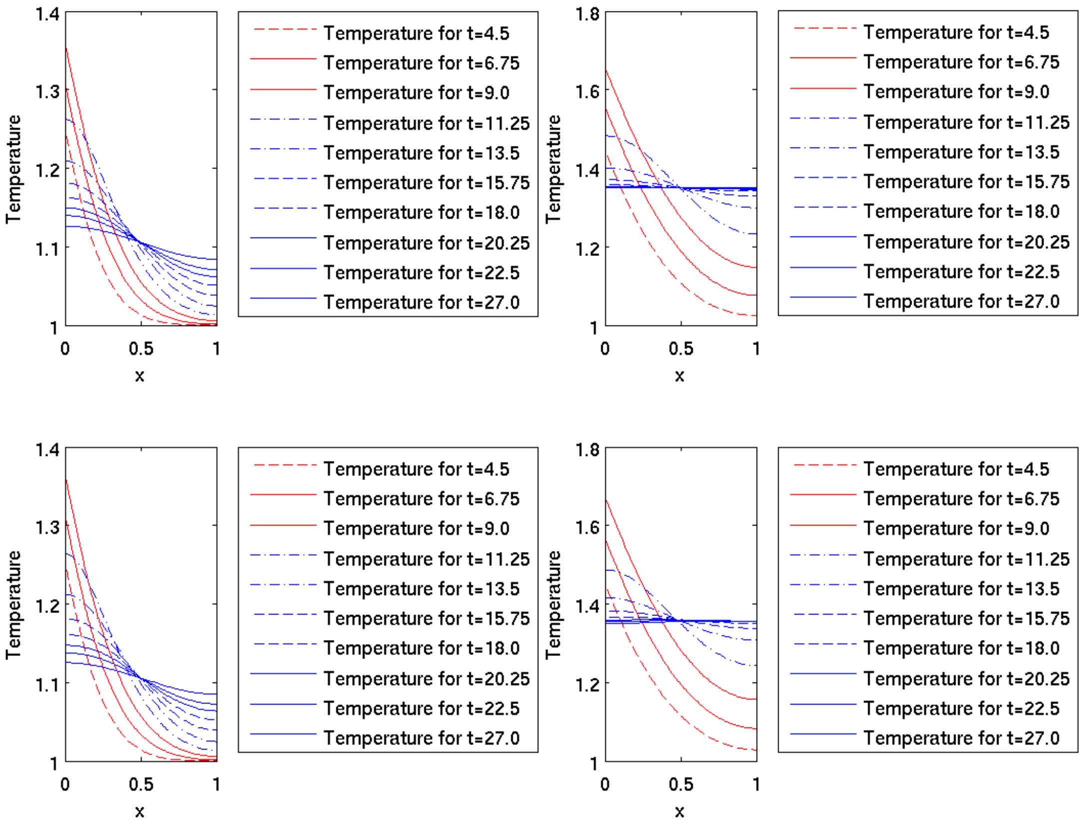

Figure 6: Comparison of the temperature computed for a system of equations in the full (top) and in the reduced (bottom) case with the first component on the left and the second on the right ($\lambda_1(y) = 0.01y, \lambda_2(z) = 0.03z$)

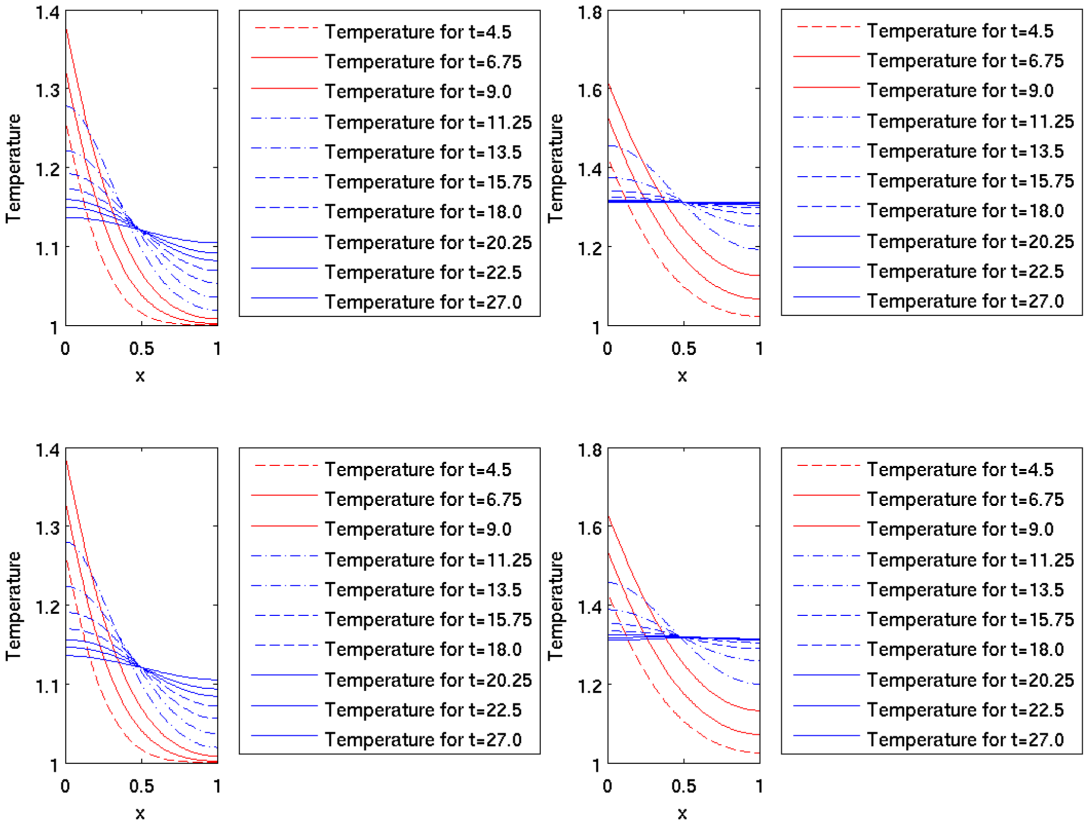

Figure 7:Comparison of the temperature computed for a system of equations in the full (top) and in the reduced (bottom) case with the first component on the left and the second on the right ($\lambda_1(z) = 0.01z, \lambda_2(y) = 0.03y$)

4.1 Newton's Method for the full system

Assuming a finite volume discretization of System (23) on N finite volumes, we write the discretized nonlinear system of equations as

$$F(\mathbf{u}) = 0, \quad \mathbf{u} = \begin{pmatrix} \mathbf{c} \\ \boldsymbol{\phi} \end{pmatrix} \in \mathbb{R}^{2N}.$$

where $F(\mathbf{u}) \in \mathbb{R}^{2N}$ and $\mathbf{c}, \boldsymbol{\phi} \in \mathbb{R}^N$.

Let $F_{\alpha,\beta}(\mathbf{u}) \in \mathbb{R}^N$ denote the discretization of the term in System (23) that is a function of the partial derivative of β with respect to α. Hence, the term $\frac{\partial c}{\partial t}$ in (23) can be discretized by

$$F_{t,c}(\mathbf{u}^{n+1}) = F_{t,c}(\mathbf{c}^{n+1}, \boldsymbol{\phi}^{n+1}) := \frac{1}{\Delta t} V(\mathbf{c}^{n+1} - \mathbf{c}^n) \tag{24}$$

where $V \in \mathbb{R}^{N \times N}$ is a diagonal matrix with the cell volumes V_i on the diagonal, i. e.

$$V = \begin{pmatrix} V_1 & & \\ & \ddots & \\ & & V_N \end{pmatrix}.$$

Analogously, we proceed for the other terms in System (23) and we obtain a discretized system, separated into terms according to the terms of System (23):

$$F(\mathbf{u}) = \begin{pmatrix} F_{t,c}(\mathbf{u}) + F_{x,c,c}(\mathbf{u}) + F_{x,c,\phi}(\mathbf{u}) \\ F_{x,\phi,c}(\mathbf{u}) + F_{x,\phi,\phi}(\mathbf{u}) \end{pmatrix} \tag{25}$$

Note that the term $F_{t,c}$ in (25) is a linear function. All the other terms F_* in Equation (25) might be nonlinear due to the definition of the system before discretization, given in (23). Thus, F can be written in the following form by using Equation (24):

$$\begin{aligned} F(\mathbf{u}) &= \begin{pmatrix} F_{t,c}(\mathbf{u}) \\ 0 \end{pmatrix} + \begin{pmatrix} F_{x,c,c}(\mathbf{u}) + F_{x,c,\phi}(\mathbf{u}) \\ F_{x,\phi,c}(\mathbf{u}) + F_{x,\phi,\phi}(\mathbf{u}) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{\Delta t} V(\mathbf{c}^{n+1} - \mathbf{c}^n) \\ 0 \end{pmatrix} + \begin{pmatrix} F_{x,c,c}(\mathbf{u}) + F_{x,c,\phi}(\mathbf{u}) \\ F_{x,\phi,c}(\mathbf{u}) + F_{x,\phi,\phi}(\mathbf{u}) \end{pmatrix} \\ &= \frac{1}{\Delta t} M(\mathbf{u}^{n+1} - \mathbf{u}^n) + \begin{pmatrix} F_{x,c,c}(\mathbf{u}) + F_{x,c,\phi}(\mathbf{u}) \\ F_{x,\phi,c}(\mathbf{u}) + F_{x,\phi,\phi}(\mathbf{u}) \end{pmatrix} \end{aligned} \tag{26}$$

where the matrix $M \in \mathbb{R}^{2N \times 2N}$ is defined by

$$M := \begin{pmatrix} V & 0 \\ 0 & 0 \end{pmatrix}. \tag{27}$$

Thus, the full system is given by

$$F(\mathbf{u}^{n+1}) = F_t(\mathbf{u}^{n+1}) + F_x(\mathbf{u}^{n+1}) = \frac{1}{\Delta t} M(\mathbf{u}^{n+1} - \mathbf{u}^n) + F_x(\mathbf{u}^{n+1})$$

where F_t is a linear and F_x is a nonlinear function with

$$F_x(\mathbf{u}) := \begin{pmatrix} F_{x,c,c}(\mathbf{u}) + F_{x,c,\phi}(\mathbf{u}) \\ F_{x,\phi,c}(\mathbf{u}) + F_{x,\phi,\phi}(\mathbf{u}) \end{pmatrix}. \tag{28}$$

By definition of F in Equation (25) we obtain

$$F(\mathbf{u}^{k,n+1}) = \begin{pmatrix} F_{t,c}(\mathbf{u}^{k,n+1}) + F_{x,c,c}(\mathbf{u}^{k,n+1}) + F_{x,c,\phi}(\mathbf{u}^{k,n+1}) \\ F_{x,\phi,c}(\mathbf{u}^{k,n+1}) + F_{x,\phi,\phi}(\mathbf{u}^{k,n+1}) \end{pmatrix}$$

and thus, the corresponding Jacobian $J(\mathbf{u}^{k,n+1}) \in \mathbb{R}^{2N \times 2N}$ can be computed by

$$\begin{aligned} J(\mathbf{u}^{k,n+1}) &= \begin{pmatrix} \frac{\partial F_{t,c}(\mathbf{u}^{k,n+1})}{\partial \mathbf{u}^{k,n+1}} + \frac{\partial F_{x,c,c}(\mathbf{u}^{k,n+1})}{\partial \mathbf{u}^{k,n+1}} + \frac{\partial F_{x,c,\phi}(\mathbf{u}^{k,n+1})}{\partial \mathbf{u}^{k,n+1}} \\ \frac{\partial F_{x,\phi,c}(\mathbf{u}^{k,n+1})}{\partial \mathbf{u}^{k,n+1}} + \frac{\partial F_{x,\phi,\phi}(\mathbf{u}^{k,n+1})}{\partial \mathbf{u}^{k,n+1}} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial F_{t,c}(\mathbf{u}^{k,n+1})}{\partial \mathbf{c}^{k,n+1}} + \frac{\partial F_{t,c}(\mathbf{u}^{k,n+1})}{\partial \boldsymbol{\phi}^{k,n+1}} \\ 0 \end{pmatrix} + \\ &\quad \begin{pmatrix} \frac{\partial F_{x,c,c}(\mathbf{u}^{k,n+1})}{\partial \mathbf{c}^{k,n+1}} + \frac{\partial F_{x,c,\phi}(\mathbf{u}^{k,n+1})}{\partial \mathbf{c}^{k,n+1}} & \frac{\partial F_{x,c,c}(\mathbf{u}^{k,n+1})}{\partial \boldsymbol{\phi}^{k,n+1}} + \frac{\partial F_{x,c,\phi}(\mathbf{u}^{k,n+1})}{\partial \boldsymbol{\phi}^{k,n+1}} \\ \frac{\partial F_{x,\phi,c}(\mathbf{u}^{k,n+1})}{\partial \mathbf{c}^{k,n+1}} + \frac{\partial F_{x,\phi,\phi}(\mathbf{u}^{k,n+1})}{\partial \mathbf{c}^{k,n+1}} & \frac{\partial F_{x,\phi,c}(\mathbf{u}^{k,n+1})}{\partial \boldsymbol{\phi}^{k,n+1}} + \frac{\partial F_{x,\phi,\phi}(\mathbf{u}^{k,n+1})}{\partial \boldsymbol{\phi}^{k,n+1}} \end{pmatrix} \end{aligned} \tag{29}$$

where $\frac{\partial F_*(\mathbf{u}^{k,n+1})}{\partial \mathbf{u}^{k,n+1}} \in \mathbb{R}^{N \times 2N}$.

Furthermore, we assume the existence of an initial condition for c and ϕ, given by

$$\mathbf{u}^0 = \theta$$

for a given vector $\theta \in \mathbb{R}^N$. Newton's Method can then be applied, given by the following algorithm:

Algorithm 2 Algorithm: Newton's Method in the full system

Let $\mathbf{u}^{k,n+1} \in \mathbb{R}^{2N}, J(\mathbf{u}) \in \mathbb{R}^{2N \times 2N}$
Solve
$J(\mathbf{u}^{k,n+1})\Delta\mathbf{u}^{k,n+1} = -F(\mathbf{u}^{k,n+1})$
$\mathbf{u}^{k+1,n+1} := \mathbf{u}^{k,n+1} + \Delta\mathbf{u}^{k,n+1}$
until solution $\mathbf{u}^{n+1}$ is found.

4.2 Newton's Method for the reduced system

The structure of Equation (28), where parts of a single equation are separated, extends the structures given in Section 3.2. Hence in this Section we extend the derivation of the Newton's Method for the reduced system initially given in Equation (10). The extension becomes apparent in the transformation and interpolation matrices in Equations (31) and (33).

The reduced system is fully solved in $\mathbb{R}^n$ instead of $\mathbb{R}^{2N}$. The solutions in $\mathbb{R}^n$ of the reduced space are denoted by $\tilde{\mathbf{u}}$ and the corresponding transformation matrix for transformations between the full and the reduced system is given by V_u.

Let the initial condition $\mathbf{u}^0 = \theta$ with $\theta \in \mathbb{R}^N$ be given. We aim to compute the solution $\mathbf{u}^{n+1}$ of the full system after $n+1$ time steps that can be obtained from the solution $\tilde{\mathbf{u}}^{n+1}$ of the reduced system after $n+1$ time steps because it holds $\mathbf{u}^{n+1} = V_u \tilde{\mathbf{u}}^{n+1}$. Since $\mathbf{u} = V_u \tilde{\mathbf{u}}, \mathbf{u} \in \mathbb{R}^{2N}, V_u \in \mathbb{R}^{2N \times n}, \tilde{\mathbf{u}} \in \mathbb{R}^n$, the relation $\mathbf{u}^0 = V_u \tilde{\mathbf{u}}^0$ implies that $\tilde{\mathbf{u}}^0 = V_u^T \mathbf{u}^0$ as it holds $V_u^T \mathbf{u} = V_u^T V_u \tilde{\mathbf{u}} = I \tilde{\mathbf{u}} = \tilde{\mathbf{u}}$. This is the first preparing step for the computations within the reduced system where some more transformation matrices are needed. The reduced system to be solved can be approximated by the following equation:

$$F_{Newton}(\tilde{\mathbf{u}}) = 0 \tag{30}$$

with $\tilde{\mathbf{u}}^{k,n+1} \in \mathbb{R}^n$ and $F_{Newton}(\tilde{\mathbf{u}}) \in \mathbb{R}^n$.

The function F_{Newton} can be obtained from F as described in Section 3.2 where the matrix $A \in \mathbb{R}^{2N \times 2N}$ is given by

$$A := \frac{1}{\Delta t} M$$

and $M \in \mathbb{R}^{2N \times 2N}$ is given by (27).

Let V_u be the transformation matrix created from the solution $\mathbf{u} = [\mathbf{c}, \boldsymbol{\phi}]^T$:

$$V_u = \begin{pmatrix} V_{uc} & 0 \\ 0 & V_{u\phi} \end{pmatrix} \in \mathbb{R}^{2N \times n}$$

where $V_{uc} \in \mathbb{R}^{N \times n_c}$ is obtained from $\mathbf{c}$ and $V_{u\phi} \in \mathbb{R}^{N \times n_\phi}$ from $\boldsymbol{\phi}$ with $n_c + n_\phi = n$.

Next, we construct the interpolation matrix V_F for DEIM given by

$$V_F = \begin{pmatrix} V_{F\,c,c} & 0 & 0 & 0 \\ 0 & V_{F\,c,\phi} & 0 & 0 \\ 0 & 0 & V_{F\,\phi,c} & 0 \\ 0 & 0 & 0 & V_{F\,\phi,\phi} \end{pmatrix} \in \mathbb{R}^{4N \times m} \tag{31}$$

where $V_{F\,c,c} \in \mathbb{R}^{N \times m_{c,c}}, \ldots, V_{F\,\phi,\phi} \in \mathbb{R}^{N \times m_{\phi,\phi}}$. Here, the matrices $V_{F\,\alpha,\beta}$ are obtained by applying POD to $F_{x,\alpha,\beta}$ evaluated at snapshots. Thus, we construct the interpolation matrix by creating interpolation matrices for each nonlinear term in F separately. Note that $m_{c,c} + \ldots + m_{\phi,\phi} = m$.

For the separate multiplication of all terms of Equation (28) with the interpolation matrices, the dimension of F_x is elevated from $\mathbb{R}^{2N}$ to $\mathbb{R}^{4N}$. Hence, in Equation (35), the separate interpolation of the terms in each equation needs to be summed again. This will be achieved by a dimensionwise-modified version of V_F which we call $\hat{V_F}$.

$$\hat{V_F} = \begin{pmatrix} V_{F\,c,c} & V_{F\,c,\phi} & 0 & 0 \\ 0 & 0 & V_{F\,\phi,c} & V_{F\,\phi,\phi} \end{pmatrix} \in \mathbb{R}^{2N \times m} \tag{32}$$

The matrix P consisting of unit vectors corresponding to the interpolation point index set is:

$$P = \begin{pmatrix} P_{c,c} & 0 & 0 & 0 \\ 0 & P_{c,\phi} & 0 & 0 \\ 0 & 0 & P_{\phi,c} & 0 \\ 0 & 0 & 0 & P_{\phi,\phi} \end{pmatrix} \in \mathbb{R}^{4N\times m} \tag{33}$$

with $P_{\alpha,\beta} \in \mathbb{R}^{N\times m_{\alpha,\beta}}$.

As $P^T V_F$ can be precomputed in the offline stage, let $C := P^T V_F \in \mathbb{R}^{m\times m}$ for ease of notation.

$$C := \begin{pmatrix} C_{c,c} & & & \\ & C_{c,\phi} & & \\ & & C_{\phi,c} & \\ & & & C_{\phi,\phi} \end{pmatrix} \in \mathbb{R}^{m\times m} \tag{34}$$

where

$$C_{c,c} \in \mathbb{R}^{m_{c,c}\times m_{c,c}}, \dots, C_{\phi,\phi} \in \mathbb{R}^{m_{\phi,\phi}\times m_{\phi,\phi}}$$

After constructing $V_u \in \mathbb{R}^{2N\times n}$, $V_F \in \mathbb{R}^{4N\times m}$ and $P \in \mathbb{R}^{4N\times m}$, an approximation of $F_{Newton}\left(\tilde{\mathbf{u}}^{n+1}\right) \in \mathbb{R}^n$, describing the reduced system, can be computed. Using Equation (8) and inserting the approximation of the nonlinear term in (10) yields:

$$\begin{aligned} F_{Newton}\left(\tilde{\mathbf{u}}^{n+1}\right) :&= V_u^T F_t(V_u\tilde{\mathbf{u}}^{n+1}) + V_u^T F_x(V_u\tilde{\mathbf{u}}^{n+1}) \\ &\approx V_u^T F_t(V_u\tilde{\mathbf{u}}^{n+1}) + V_u^T \hat{V}_F \left(P^T V_F\right)^{-1} P^T F_x\left(V_u\tilde{\mathbf{u}}^{n+1}\right) \\ &= \frac{1}{\Delta t} V_u^T M V_u \left(\tilde{\mathbf{u}}^{n+1} - \tilde{\mathbf{u}}^n\right) + V_u^T \hat{V}_F C^{-1} \tilde{F}_x\left(V_u\tilde{\mathbf{u}}^{n+1}\right) \end{aligned} \tag{35}$$

where $\tilde{F}_x\left(V_u\tilde{\mathbf{u}}^{n+1}\right) := P^T F_x\left(V_u\tilde{\mathbf{u}}^{n+1}\right) \in \mathbb{R}^m$. This corresponds to Equation (12) in the basic POD-DEIM derivation. Again, the approximation makes computations more efficient since only certain rows of F_x need to be evaluated.

Note that the way we solve the reduced system for the heat equation is completely analogous to solving the more general system above. Equation (19) corresponds to Equation (35) where $\frac{1}{\Delta t} V_u^T M V_u \left(\tilde{\mathbf{u}}^{n+1} - \tilde{\mathbf{u}}^n\right)$ is the linear term for the reduced system.

Let J_{Newton} with $J_{Newton}(\tilde{\mathbf{u}}) \in \mathbb{R}^{n\times n}$ denote the Jacobian corresponding to F_{Newton}. It can be approximated by:

$$\begin{aligned} J_{Newton}\left(\tilde{\mathbf{u}}^{n+1}\right) &\approx \frac{1}{\Delta t} V_u^T M V_u + V_u^T \hat{V}_F (P^T V_F)^{-1} \frac{\partial \tilde{F}_x\left(V_u\tilde{\mathbf{u}}^{n+1}\right)}{\partial \tilde{\mathbf{u}}^{n+1}} \\ &= \frac{1}{\Delta t} V_u^T M V_u + V_u^T \hat{V}_F (P^T V_F)^{-1} \begin{pmatrix} \frac{\partial \tilde{F}_{x,c,c}(V_u\tilde{\mathbf{u}}^{n+1})}{\partial \tilde{\mathbf{u}}^{n+1}} \\ \vdots \\ \frac{\partial \tilde{F}_{x,\phi,\phi}(V_u\tilde{\mathbf{u}}^{n+1})}{\partial \tilde{\mathbf{u}}^{n+1}} \end{pmatrix} \end{aligned} \tag{36}$$

where
$$\frac{\partial \tilde{F}_{x,c,c}(V_u \tilde{\mathbf{u}}^{n+1})}{\partial \tilde{\mathbf{u}}^{n+1}} \in \mathbb{R}^{m_{c,c} \times n}, \dots, \frac{\partial \tilde{F}_{x,\phi,\phi}(V_u \tilde{\mathbf{u}}^{n+1})}{\partial \tilde{\mathbf{u}}^{n+1}} \in \mathbb{R}^{m_{\phi,\phi} \times n}$$

Then, the reduced system, given in Equation (30), can be solved with Newton's Method:

Algorithm 3 Algorithm: Newton's Method in the reduced system

Solve
$J_{Newton}\left(\tilde{\mathbf{u}}^{k,n+1}\right) \Delta\tilde{\mathbf{u}}^{k,n+1} = -F_{Newton}\left(\tilde{\mathbf{u}}^{k,n+1}\right)$
$\tilde{\mathbf{u}}^{k+1,n+1} := \tilde{\mathbf{u}}^{k,n+1} + \Delta\tilde{\mathbf{u}}^{k,n+1}$
until the solution $\tilde{\mathbf{u}}^{n+1}$ is found.

4.3 Computation of the input argument, the nonlinear function and the Jacobian in the reduced system

For ease of reading $V_u\tilde{\mathbf{u}}^{n+1}$ is denoted by $V_u\tilde{\mathbf{u}}$ throughout this section. Since the computation of $V_u\tilde{\mathbf{u}} \in \mathbb{R}^{2N}$ is very inefficient $V_u\tilde{\mathbf{u}}$ should never be fully computed. Besides, $V_u\tilde{\mathbf{u}}$ is the only input of F_{Newton} and J_{Newton} where $J_{Newton} \in \mathbb{R}^{n\times n}$ is a sparse matrix. Thus, it suffices to compute $V_u\tilde{\mathbf{u}}$ only for the discretization point i and its neighbors.

Before discussing this in more detail, let us firstly look at $\tilde{F}_x$ and the corresponding Jacobian $\tilde{J}_x$ more closely:

$$\tilde{F}_x(V_u\tilde{\mathbf{u}}) = \begin{pmatrix} \left.\begin{matrix} F_{x,c,c}(V_u\tilde{\mathbf{u}})_{i_{c,c,1}} \\ \vdots \\ F_{x,c,c}(V_u\tilde{\mathbf{u}})_{i_{c,c,m_{c,c}}} \end{matrix}\right\} m_{c,c} \\ \left.\begin{matrix} F_{x,c,\phi}(V_u\tilde{\mathbf{u}})_{i_{c,\phi,1}} \\ \vdots \\ F_{x,c,\phi}(V_u\tilde{\mathbf{u}})_{i_{c,\phi,m_{c,\phi}}} \end{matrix}\right\} m_{c,\phi} \\ \vdots \\ \left.\begin{matrix} F_{x,\phi,\phi}(V_u\tilde{\mathbf{u}})_{i_{\phi,\phi,1}} \\ \vdots \\ F_{x,\phi,\phi}(V_u\tilde{\mathbf{u}})_{i\phi,\phi,m_{\phi,\phi}} \end{matrix}\right\} m_{\phi,\phi} \end{pmatrix} \in \mathbb{R}^m \tag{37}$$

So $\tilde{F}_x(V_u\tilde{\mathbf{u}})$ is the original F_x, evaluated at $V_u\tilde{\mathbf{u}}$ and only certain points $i_{c,c,1}, \dots, i_{c,c,m_{c,c}} \in I_{c,c}$ are picked. $\tilde{J}_x$ can be created in the same manner. It is given by:

$$\tilde{J}_x := \frac{\partial \tilde{F}_x(V_u\tilde{\mathbf{u}})}{\partial \tilde{\mathbf{u}}} = \begin{pmatrix} \left.\left[\frac{\partial F_{x,c,c}(V_u\tilde{\mathbf{u}})}{\partial \mathbf{u}} \cdot V_u\right]_{i_{c,c,1},\ldots,i_{c,c,m_{c,c}}} \right\} m_{c,c} \\ \vdots \\ \left.\left[\frac{\partial F_{x,\phi,\phi}(V_u\tilde{\mathbf{u}})}{\partial \mathbf{u}} \cdot V_u\right]_{i_{c,c,1},\ldots,i_{c,c,m_{c,c}}} \right\} m_{\phi,\phi} \end{pmatrix} \in \mathbb{R}^{m\times n} \tag{38}$$

because we obtain by chain rule with $\mathbf{u} = V_u\tilde{\mathbf{u}}$:

$$\frac{\partial \tilde{F}_x(V_u\tilde{\mathbf{u}})}{\partial \tilde{\mathbf{u}}} = \frac{\partial \tilde{F}_x(V_u\tilde{\mathbf{u}})}{\partial \mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial \tilde{\mathbf{u}}} = \frac{\partial \tilde{F}_x(V_u\tilde{\mathbf{u}})}{\partial \mathbf{u}} \cdot V_u$$

4.4 Efficient computation of the nonlinear function and the Jacobian

In this section, the efficient computation of

(1) the nonlinear function $[F_{x,c,c}(V_u\tilde{\mathbf{u}})]_{i_{c,c,1},\ldots i_{c,c,m_{c,c}}}$ and

(2) the Jacobian $\left[\frac{\partial F_{x,c,c}(V_u\tilde{\mathbf{u}})}{\partial \mathbf{u}} \cdot V_u\right]_{i_{c,c,1},\ldots i_{c,c,m_{c,c}}}$

are discussed.

4.4.1 Ad (1): Nonlinear function

It holds

$$[F_{x,c,c}(V_u\tilde{\mathbf{u}})]_{i_{c,c,1},\ldots i_{c,c,m_{c,c}}} = \begin{pmatrix} F_{x,c,c}(V_u\tilde{\mathbf{u}})_{i_{c,c,1}} \\ \vdots \\ F_{x,c,c}(V_u\tilde{\mathbf{u}})_{i_{c,c,m_{c,c}}} \end{pmatrix}, \tag{39}$$

meaning that we need to pick out the j-th entries of $F_{x,c,c}$, computed at $V_u\tilde{\mathbf{u}}$, with $j = i_{c,c,1}, \ldots, i_{c,c,m_{c,c}}$. Because of the underlying finite volume discretization stencil these values only depend on certain entries of $V_u\tilde{\mathbf{u}}$, namely those at the center node j and its neighbors for both variables $\mathbf{c}$ and $\boldsymbol{\phi}$ of the system.

Thus, we define

$$\tilde{V_u}\tilde{\mathbf{u}}_j := [V_u\tilde{\mathbf{u}}]_{\mathcal{N}_j=\{j,j+N,j_E,j_E+N,\ldots\}} \tag{40}$$

using only the indices in $\mathcal{N}_j$ which exist due to boundaries etc.

We also have:

$$[V_u\tilde{\mathbf{u}}]_{\mathcal{N}_j} = [V_u]_{\mathcal{N}_j}\,\tilde{\mathbf{u}} \tag{41}$$

where $[V_u]_{\mathcal{N}_j} \in \mathbb{R}^{\mathcal{N}_j \times n}$ is the matrix consisting only of those rows of V_u with indices in $\mathcal{N}_j$. Hence, $V_u\tilde{\mathbf{u}}_j$ as input for $F_{x,c,c}(V_u\tilde{\mathbf{u}})_j$ can be computed with very little cost by

$$V_u\tilde{\mathbf{u}}_j = \sum_{l\in\mathcal{N}_j} [V_u\tilde{\mathbf{u}}_j]_l \cdot e_l \tag{42}$$

i. e. putting the entries of $V_u\tilde{\mathbf{u}}_j$ into the right indices of the full vector $V_u\tilde{\mathbf{u}}$ and we can use the original discretization functions. This can be done for every $j \in \left\{i_{c,c,1,\ldots,i_{c,c,m_{c,c}}}\right\}$. The matrices $[V_u]_{\mathcal{N}_j} =: V_{uj}$ can and should be precomputed for all $j \in I_{c,c} \cup I_{c,\phi} \cup I_{\phi,c} \cup I_{\phi,\phi}$. $\tilde{F}$ is then built by writing all such computed entries of F in a column.

4.4.2 Ad (2): Jacobian

For preparing the input argument $V_u\tilde{\mathbf{u}}$ of

$$\left[\frac{\partial F_{x,c,c}(V_u\tilde{\mathbf{u}})}{\partial \mathbf{u}}\right]_{i_{c,c,1},\ldots i_{c,c,m_{c,c}}}$$

the method is identical to the one in ad 1. Again, we use the precomputed small matrices V_{uj} and the original discretization functions. The multiplication with V_u is then straightforward and can directly be done for each entry j of $\tilde{J}$ separately. We denote

$$\frac{\partial \tilde{F}_x(V_u\tilde{\mathbf{u}})}{\partial \tilde{\mathbf{u}}} = \left[\frac{\partial \tilde{F}_{x,q_1,q_2}(V_u\tilde{\mathbf{u}})}{\partial \tilde{\mathbf{u}}}\right]_{q_1,q_2\in\{c,\phi\}} \tag{43}$$

Now, we describe the computation of

$$\frac{\partial \tilde{F}_{x,q_1,q_2}(V_u\tilde{\mathbf{u}})}{\partial \tilde{\mathbf{u}}}$$

which is

$$\frac{\partial F_{x,q_1,q_2}(V_u\tilde{\mathbf{u}})}{\partial \mathbf{u}} \cdot V_u \tag{44}$$

Step 1 Assume V_{uj} has been created for each $j \in I_{q_1,q_2}$.

Step 2 For each $j \in I_{q_1,q_2}$
(1) Create input $V_u\tilde{\mathbf{u}}_j$ by the rule in Equation (42)

(2) Evaluate the j-th row of Equation (44) using input $V_u\tilde{\mathbf{u}}_j$ and get

$$\left[\frac{\partial F_{x,q_1,q_2}(V_u\tilde{\mathbf{u}}_j)}{\partial \mathbf{u}}\right]_j \tag{45}$$

(3) Multiply only the $\mathcal{N}_j$-th (see Equation (40)) columns of Equation (45) with $V_{uj} = [V_u]_{\mathcal{N}_j}$ to obtain the correct matrix row of $\frac{\partial \tilde{F}_x}{\partial \tilde{\mathbf{u}}}$:

$$\left[\frac{\partial \tilde{F}_{x,q_1,q_2}(V_u\tilde{\mathbf{u}})}{\partial \tilde{\mathbf{u}}}\right]_r = \left[\frac{\partial F_{x,q_1,q_2}(V_u\tilde{\mathbf{u}}_j)}{\partial \mathbf{u}}\right]_{j,\mathcal{N}_j} \cdot V_{uj}$$

for the r-th entry j of $\{i_{c,c,1}, \ldots, i_{c,c,m_{c,c}}\}$

4.5 Numerical results

4.5.1 Pseudo-3D test problem

In this section, we present some numerical results obtained with BEST. We restrict ourselves to a pseudo-3D test problem whose geometry is actually of dimension one due to periodicity and symmetry of the geometry.

Geometry For the Pseudo-3D case, the total size of the battery is given by $18 \cdot 10^{-3}cm \times 7 \cdot 10^{-3}cm \times 7 \cdot 10^{-3}cm$. Since the geometry should be very easy, both cathode and anode are set as $3 \cdot 10^{-3}cm \times 5 \cdot 10^{-3}cm \times 5 \cdot 10^{-3}cm$ and the separator between cathode and anode has a size of $4 \cdot 10^{-3}cm \times 5 \cdot 10^{-3}cm \times 5 \cdot 10^{-3}cm$, as illustrated in Figure 8.

In the following, lineouts through the center of different variables are displayed, i. e. the y- and z-component are assumed to be constantly $2.5 \cdot 10^{-3}cm$ whereas the concentration and the potential are shown as functions of the x-component.

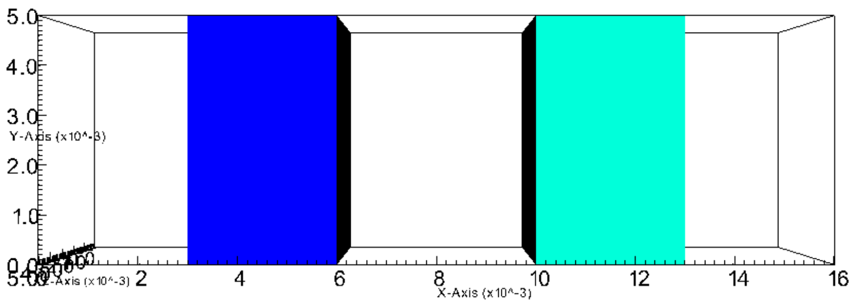

Figure 8:Geometry of the Pseudo-3D case. The geometry is made up of five domains: the current collector (leftmost and rightmost), the anode (left, blue), the cathode (right,turquoise) and the separator (transparent between anode and cathode)

Parameters The current density is set as 0.001 C = 0.0000190329 A/cm^2 and the total time is set as 205.000 s. Besides, it is important to set a suitable time step. In Figure 9, the concentration is plotted as a function of the x-coordinate using time steps 500 s and 9.000 s. Although 9.000 s is a very large time step, the results for the concentration are acceptable.

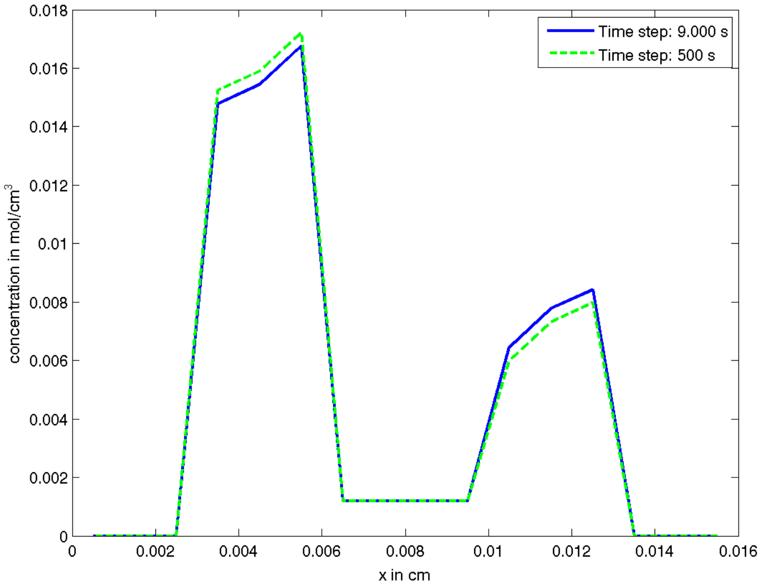

Figure 9:Pseudo-3D case: Concentration subject to time steps 500 s and 9.000 s for a full simulation

Results For the simulations in this section, we use Version 11 of BEST. The concentration in anode, cathode and electrolyte is computed separately for the full and the reduced system by applying POD to the three subdomains independent of each other. Furthermore, it is useful to compare the cell-potential as functions of time for a full and a reduced simulation. There results are displayed in Figure 10.

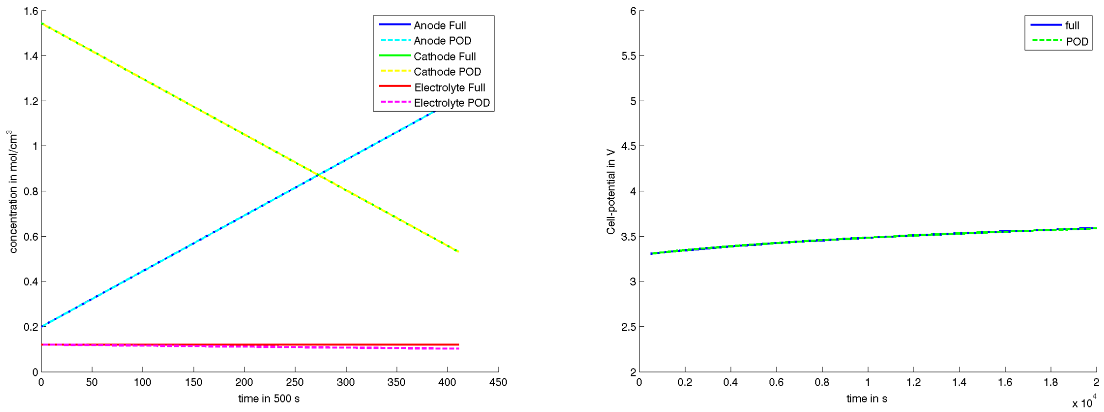

Figure 10:Pseudo-3D case: Left: Concentration plotted against time for a full and a POD simulation (time step: 500 s, output interval: 500 s). Right: Cell potential for a full and a reduced simulation (time step: 500 s, output interval: 500 s) using Version 11

5 Conclusion

We have shown the applicability of our method based on POD and DEIM for a complex coupled nonlinear PDE system resulting from the modeling of Li-ion battery charge transport. Determining a reduced basis for a simple geometry is possible. The solution, approximating the full system to the desired accuracy, can be found by applying a reduced Newton method. The possibility of solving the model with this MOR method on more complicated geometries requires more research on the careful choice and separation of the nonlinear terms used in the DEIM.

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