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Numerical solution of penalty formulations for constrained mechanical systems using heterogeneous multiscale methods

M.A. Köbis *, M. Arnold

Institute of Mathematics, Martin-Luther-University, Halle–Wittenberg, Theodor-Lieser-Str. 5, 06120, Halle (Saale), Germany

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ABSTRACT

The heterogeneous multiscale methods (HMM) extend the classical methods of averaging to a purely numerical approach for the solution of problems involving multiple scales. Especially for highly oscillatory ordinary differential equations HMM were recently seen to be competitive with usual time integration schemes. We study this hypothesis in the special case of penalty formulations for index-three differential-algebraic equations arising in multibody dynamics which have the particular property of solution-dependent oscillations with variable frequencies. First we motivate some additional assumptions on the structure of the proposed problems and give error estimates extending the results of Engquist et al. Limitations of the considered approach will be illustrated by means of the seven body mechanism benchmark.

1. Introduction

The heterogeneous multiscale methods (HMM) [1,2] provide a wide range of numerical methods in all branches of computational sciences. In the field of numerical treatment of ordinary differential equations (ODEs) and differential-algebraic equations (DAEs) they extend the rather analytical methods of averaging [3,4] to a stand-alone purely numerical approach for the solution of problems involving multiple scales.

They have proven to be competitive with state-of-the-art methods in the context of highly oscillatory ODE systems with monochromatic vibrations, see, e.g. [5–7]. Nevertheless the design and validation of methods for problems with solution dependent oscillatory perturbations appear to be more appealing for the investigation of many practical questions.

In this article we focus on the simulation of (preferably nonstiff) constrained mechanical systems represented by initial value problems for DAEs

$$\begin{aligned} &M(q)\cdot\ddot{q}(t) = f(t,q,\dot{q}) - G^{\top}(t,q)\cdot\lambda(t),\\ &g(t,q) = 0, \qquad q(t_0) = q_0, \qquad \dot{q}(t_0) = \dot{q}_0, \quad (t\in[t_0,t_{\text{end}}]), \end{aligned} \tag{1}$$

[8,9] where $q\colon \mathbb{R}\to\mathbb{R}^{n_q}$ indicates a set of generalized coordinates restricted to fulfill the rheonomic–holonomic constraints $g(t,q)=0\in\mathbb{R}^{n_\lambda}$. $\lambda\colon\mathbb{R}\to\mathbb{R}^{n_\lambda}$ denotes Lagrange multipliers and $G(t,q) := \partial_q g(t,q)$ is assumed to have full rank n_λ, such that the system (1) is of index three, assuming the mass matrix $M(q)$ to be symmetric positive definite [8].

The numerical solution of (1) requires implicit techniques which implies high computational effort for large space dimension $n_q \gg 1$ as one has to approximate and decompose the systems Jacobian in order to solve the emerging nonlinear algebraic systems [10]. So one aim of this article is to overcome the need of implicit solvers.

* Corresponding author. Tel.: +49 3455524656.
E-mail address: markus.koebis@mathematik.uni-halle.de (M.A. Köbis).

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System (1) is neither highly oscillatory nor does it reveal a multiscale character by nature. Contrarily we will give an asymptotically equivalent ODE formulation that enforces the constraints with the drawback of then being a vibrating system but permits explicit integrators.

We will then apply methods in the HMM framework to the systems showing a multiscale character with respect to time. Under weak additional assumptions convergence of the integration scheme will be shown and illustrated through numerical experiments.

The proposed strategy goes back to the work of Sanz-Serna et al. [11] and has recently been studied in more detail in [12]. The analysis therein is focused on a projection method to stabilize the integration and enhance the constraint enforcement. The main motivation lies in providing approximations to slow manifolds of stiff systems as well as initial values for a stable time integration.

On the contrary the main task of the algorithms proposed in the present paper is the direct integration of the DAEs of multibody dynamics and the analysis of those methods without additional stabilization techniques. The guiding principle of this analysis is the formulation of a certain set of assumptions to avoid linearization techniques as they are suggested in [12].

The paper is organized as follows: In Section 2 following [1,2] we introduce the concept of HMM focusing on the special case of highly oscillatory ODEs. We present the concept of penalty formulations in order to apply HMM to the differential-algebraic problems of multibody dynamics [13,14].

To prove convergence of the resulting time integration schemes some additional assumptions on the structure of these equations respectively their solution are beneficial which will be introduced and motivated in Section 3.

Based on this structure a rigorous proof of convergence of the penalty equations as well as the proposed multiscale schemes is given in Section 4 by means of deriving error bounds. Here we make use of the concepts of Rubin and Ungar [15], Lubich [16] and Engquist and Tsai [17].

Results of low dimensional test problems will be presented in Section 5 which underline the analytical results of Section 4 and show the potentials as well as possible limitations regarding the application to problems of practical interest.

2. The heterogeneous multiscale methods

HMM is not just a class of integration algorithms in a certain branch of computational sciences. It is neither a collection of specific methods nor is it actually new. Instead utilizing the concept of HMM one basically follows a very general framework which applies to almost every system obeying some kind of real, artificial or even just abstract scaling laws. Hence in place of providing the ground to new programs HMM hold a complete philosophy of program design, see [1,2] for a comprehensive description in a general setting.

2.1. HMM for ODEs

As outlined before there is not just one particular family of algorithms representing HMM for ODEs. Nonetheless in the context of highly oscillatory differential equations recent studies, e.g. [18,5,19], concentrate on the procedure now to be described.

Consider a highly oscillatory ODE

$$\dot{x}^\varepsilon(t) = \varphi(t, x^\varepsilon; \varepsilon), \qquad x^\varepsilon(t_0) = x_0 \in \mathbb{R}^{n_x}, \quad t \in [t_0, t_{\text{end}}] \tag{2}$$

depending on a small parameter $0 < \varepsilon \ll 1$ characterizing the systems vibrating behavior.

Often the main interest is in averaged values

$$X(t) \simeq \frac{1}{\eta} \int_{t-\frac{\eta}{2}}^{t+\frac{\eta}{2}} x^\varepsilon(\tau) \mathrm{d}\tau$$

for some $\eta > 0$ which is usually chosen to be comparable to ε and so we introduce an *averaged system*

$$\dot{X}(t) = \Phi(t, X; \varepsilon) \simeq \frac{1}{\eta} \cdot \int_{t-\frac{\eta}{2}}^{t+\frac{\eta}{2}} \left(\frac{\mathrm{d}}{\mathrm{d}\tau} x^\varepsilon(\tau) \right) \mathrm{d}\tau = \frac{1}{\eta} \cdot \int_{t-\frac{\eta}{2}}^{t+\frac{\eta}{2}} \varphi(\tau, x^\varepsilon(\tau); \varepsilon) \mathrm{d}\tau. \tag{3}$$

In the presence of more than one frequency it is more convenient to use a normalized smooth function $\mathcal{K}_\eta$, i.e.

$$\int_{-\frac{\eta}{2}}^{\frac{\eta}{2}} \mathcal{K}_\eta(\tau) \mathrm{d}\tau = 1 \tag{4}$$

and replace the basic averaging process in (3) by a convolution:

$$\Phi(t, X; \varepsilon) := \int_{t-\frac{\eta}{2}}^{t+\frac{\eta}{2}} \mathcal{K}_\eta(\tau - t) \cdot \varphi(\tau, x^\varepsilon(\tau); \varepsilon) \mathrm{d}\tau =: \mathcal{K}_\eta \circledast \varphi. \tag{5}$$

Of course in a practical implementation the data for the variables x^ε have to be computed through numerical integration and the convolution itself is also achieved by some quadrature rule. Subsequently we will refer to the functions $\mathcal{K}_\eta$ as