DFG Proposal
Coupling hyperbolic PDEs with switched DAEs: Analysis, numerics and application to blood flow models

Within the Priority Programm SPP 1962: Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization
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Summary

In this project we study hyperbolic partial differential equations (PDEs) with boundary conditions driven by switched differential algebraic equations (DAEs). This class of systems is motivated by models of the human circulatory system. The flow of blood in the vessels is described by a hyperbolic PDE, its connection to the heart is represented by boundary conditions. The dynamics of the heart can be modeled by a combination of ordinary differential equations and algebraic constraints. The corresponding choice depends on the state of the valves (e.g. when the valves are closed the flow is zero) which results in a switched DAE model. Due to the possible change of algebraic constraints at switching instants, solutions of switched DAEs exhibit jumps. Additionally, solutions may also contain Dirac impulses or their derivatives. The coupling of these discontinuities and Dirac- impulses with PDEs needs a rigorous solution theory and novel numerical schemes. Furthermore, the developed high order numerical methods will allow for more accurate simulations of the blood flow taking rigorously into account discontinuous and impulsive effects.

Project description

1 State of the art and preliminary work

Motivation & Introduction

The human circulatory system has been subject to research since its discovery and many models have been developed to describe the flow of blood in the human body. With the ability of numerical simulations the complexity of such models increases constantly. Current representations consists of a hierarchy of 3D- ,1D- and 0D-descriptions [21]. Points of special interest are resolved in full detail by 3D-models, the main part of the circulatory network is treated with coupled 1D equations and often the large number of capillaries is represented by ODEs. Furthermore special components such as the ventricles of the heart or the venous valves can be described as a combination of ODEs and algebraic constraints.

In the human heart four valves help to establish the required blood pressure. In simplified models the flow through these valves follows an ODE driven by the local pressure gradient. But if the gradient points into the direction opposite to the desired orientation of the flow, the valve is closed and the flow is forced to be zero [11, 29, 23]. If the valves are closed the pressure build up is solely described by ODEs for the volumes of the four ventricles. This combination of ODEs and algebraic constraints leads to a description via differential-algebraic equations; furthermore the sudden qualitative changes of the description can be formulated in the switched systems framework. Thus the novel modeling framework of switched DAEs [26] is suitable for describing these switching processes in the dynamics of the heart. At the in- and outflow ends of the heart this switched DAE is coupled to the beginning or end points of arteries and veins, which can be modeled with 1D hyperbolic partial differential equations.

Such a coupling can be written in a mathematical framework as a coupled system of the following form

$$\begin{aligned} &\partial_t u(t,x) + \partial_x f(u(t,x)) = g(u(t,x)), && x > 0, \\ &b\left(u\left(t,0+\right)\right) = B\left(t, w(t)\right), && t \geq 0, \\ &D_{\sigma(t,w)} \dot{w}(t) = F_{\sigma(t,w)}\left(t, u\left(t, 0+\right), w(t)\right). && \end{aligned} \tag{1}$$

For the modeling of the blood flow, $u(t,x)$ describes the states in all the connected vessels, which is governed by a hyperbolic balance law (PDE). The function $t \mapsto w(t)$ contains the information of the four ventricles and the flow through their corresponding valves. The flux of w directly depends on the values of u at the boundary of the PDE-domain. There the information of w is partially assigned to u via boundary conditions (BC) given by the functions b and B. A schematic illustration of this coupling is given in the diagram (Figure 1).

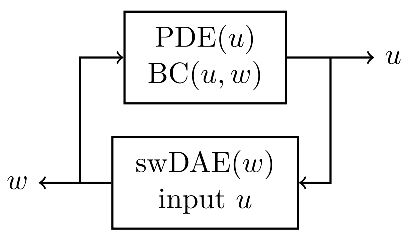

Figure 1: Coupling of a PDE with a switched DAE via boundary condition.

Applications for systems of the above structure are not restricted to the heart. A further occurrence of switched DAEs in the human circulatory system are the so called venous valves [13, 30]. These valves in the veins prevent the blood from flowing downwards if the person stands in an upright position and help in the transport of blood back to the heart.

Models of the type (1) also arise in the context of gas- or water-networks. Here valves and pumps can be operated externally, which can lead to a switching of differential and algebraic equations. Furthermore it is sometimes of interest to alter the level of detail in the modeling of the connected pipes [2]. If such a switching is between algebraic equations and ODEs it also can fit in the above framework.

State of the art

Although systems of the type (1) are used in different applications, they have not been subject to rigorous analytical investigations. Therefore especially considerations like the well-posedness of the coupled system remain as open questions. One of the major objective of the proposed project is to close this gap. The expertise of the two PIs in coupling of PDEs with ODEs on the one hand and a distributional solution theory of switched DAEs on the other hand (detailed in the following) perfectly complement each other to resolve the mathematical challenges posed by the system class given by (1).

Coupling PDEs with ODEs

A simplified version of (1) can be studied, if a hyperbolic balance law is coupled with an ODE. In this case the system of coupled equations read as

$$\begin{aligned} &\partial_t u(t,x) + \partial_x f(u(t,x)) = g(u(t,x)), && x > 0, \\ &b\left(u\left(t,0+\right)\right) = B\left(t, w(t)\right), && t \geq 0, \\ &\dot{w}(t) = F\left(t, u\left(t,0+\right), w(t)\right), && \end{aligned} \tag{2}$$

where $u(t,x) \in \Omega \subseteq \mathbb{R}^n$. The corresponding schematic representation is shown in Figure 2.

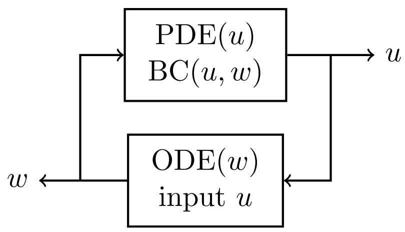

Figure 2: Coupling of a PDE with an ODE via boundary condition.

This system (2) has been subject to detailed investigations of the first PI. These include a detailed analysis of the coupled equations [4, 5] as well as the design of highly accurate numerical schemes [6, 7].

In [4, 5] it was shown that under certain assumptions and with appropriate initial conditions the problem (2) is well posed. For the hyperbolic flux function f and the source term g no special features are required, except that the speeds of the internal waves, i.e. the eigenvalues of the Jacobian of f, have to be non characteristic w.r.t. the boundary, i.e. $|\lambda_i| \geq c > 0$, $i = 1, \dots, n$. The correct number of boundary conditions ℓ, if $b \in \mathbf{C^1}(\Omega; \mathbb{R}^\ell)$, coincides with the number of waves which can enter the domain. This is a classical requirement for boundary values of hyperbolic conservation laws.

Regarding the ODE, the function $F\colon \mathbb{R}^+ \times \Omega \times \mathbb{R}^m \longrightarrow \mathbb{R}^m$ has to be Lipschitz-continuous w.r.t. both variables w and u and Lebesgue measurable w.r.t. t. Furthermore, it has to be bounded in the following way:

(F) There exists a function $C \in L^1_{loc}(\mathbb{R}^+;\mathbb{R}^+)$ such that for all $t > 0$, $u \in \Omega$ and $w \in \mathbb{R}^m$

$$\|F(t,u,w)\|_{\mathbb{R}^m} \leq C(t)\ (1 + \|w\|_{\mathbb{R}^m})\ .$$

Finally the function $B \in \mathbf{C^1}(\mathbb{R}^+ \times \mathbb{R}^m;\mathbb{R}^{n-\ell})$ assigning the values of w to the boundary of the PDE is locally Lipschitz in both variables. With these assumptions there exists locally in time a unique solution to the coupled problem (2). This solution depends Lipschitz continuously on the initial data for u and w.

Due to the mild assumption on F this result already allows for a piecewise-constant dependence on t, i.e. w may be governed by a time-dependent *switched* ODE. However, discontinuities in the solution w are not allowed and this continuity-requirement is too restrictive for the applications we want to study.

Analysis considering measure valued solutions for hyperbolic conservation laws can be found e.g. in [16, 12]. But these do not consider boundary values coupled to ODEs or even switched DAEs.

Switched DAEs

Switched DAEs are a novel modeling framework to describe dynamics governed by a a combination of ODEs and algebraic constraints in the presence of sudden structural changes (switches). This modeling framework for the linear case was proposed by the second PI in his PhD-thesis [24] and lead to numerous novel results in the area of mathematical systems theory (including two successful DFG-proposals). A key feature of switched DAEs is the presence of jumps or even Dirac-impulses in the solution. As an illustration consider the following simple academic example:

for t in $[0,1)$:

$$\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\dot{w} = \begin{bmatrix}0 & 1\\ 0 & 1\end{bmatrix} w + \begin{bmatrix}0\\ 1\end{bmatrix} u$$

for t in $[1,2)$:

$$\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\dot{w} = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} + \begin{bmatrix}0\\ 0\end{bmatrix} u$$

Under the assumption that u is constant, an ad hoc analysis of this switched DAE reveals the following properties: On the interval $[0,1)$ we have $w_2(t) = -u$ and from $\dot{w}_1 = w_2$ it follows that $w_1(t) = w_1(0) - t \cdot u$; on the open interval $(1,2)$ we have $w_1(t) = 0$. In particular, w_1 has a *jump* at the switching time $t = 1$ (unless $w_1(0) = u$). Furthermore, the relationship $\dot{w}_1 = w_2$ holds for all times, this means that w_2 has to be the *derivative of a discontinuous function*. This is only possible if the solution space is enlarged to the space of distributions (generalized functions) in the sense of Schwartz [20]. This introduces some technical problems, but these can be resolved by introducing the space of piecewise-smooth distributions [25]. In this solution space, the above switched DAE has a unique solution where w_2 contains a *Dirac impulse* at the switching time $t = 1$. It should be noted that the above example is actually based on the model of a simple electrical circuit composed of an inductor in series with a switch and a voltage source (c.f. [26, Example 6.1.1]), which indeed produces a voltage spark when the switch is opened , hence the presence of the *Dirac impulse is not just a mathematical artifact.*

So far a rigorous solution theory for switched DAEs is only available for the linear case with time-dependent switching. An extension to the nonlinear case in the context of stability theory are presented in [18], but the presence of Dirac-impulses is excluded.

State-dependent switching for switched DAEs has not been considered so far, however there is a strong similarity to the framework of complementarity systems [28, 14, 9, 1] and some preliminary results concerning the equivalence of the induced jump maps are presented in [10].

Numerical methods

In many numerical simulations of blood flow switched DAEs for valves are only considered in combination with pure ODE models [22]. Only a few realizations consider a coupling of hyperbolic conservation laws with ODEs and algebraic equations for the heart e.g. [19, 17]. These ad hoc couplings work for the considered numerical test cases, but no mathematically rigorous investigation of the coupling is performed. For the venous valves the coupling might be even more complex, since the venous blood flow itself is much more challenging compared to its aterial counterpart [19].

The coupling of hyperbolic PDEs and ODEs has been subject to intensive research of the first PI [8, 6, 7]. Note that a simple splitting of the PDE and the ODE can not guarantee desired properties of balance laws, e.g. the conservation of mass. Therefore both components of the system have to be solved simultaneously, i.e. the update of the ODE has to be incorporated into the treatment of the boundary values of the PDE [8]. For higher order schemes further techniques have to be considered in order to achieve the desired accuracy in the complete system [6, 7]. Here the switching in the DAE has to be handled with additional care.

Modeling valves for blood flow simulations

There exists a variety of possible models describing the flow passing valves in human circulatory system. The most detailed ones include a 3D fluid-structure interaction e.g. [15]. Many simplified models describing the human blood flow use an analogy to electrical circuits [11, 29, 23, 30]. In this context the four valves in the heart, as well as the venous valves, are represented as diodes. If a valve is open the flow through the valves is governed by an ODE depending on the pressure gradient of the two connected volumes. If the pressure gradient points into the direction opposite to the intended flow, the valve closes. The closing is described by switching to an algebraic constraint forcing the flow to zero.

There exist further alternative modeling approaches, e.g. by means of time-varying drag coefficients [31] or tracking for each valve a nominal leaflet opening angle which is governed by an ODE. Both approaches can not significantly improve the modeling and introduce further complications.

2 Objectives and work programme

2.1 Objectives

Objective 1: Solution theory for the coupled system (1) (Area 1 of SPP 1962)

The major goal of the proposed project is establishing an analytical foundation for coupled systems of the form (1). This overall goal is divided into partial objectives as follows.

Objective 1a: Distributional solution theory for linear case

Although the linear uncoupled case is well understood for each the PDE and the switched

DAE, the combination of both introduces some new challenges. A first goal of the proposed project is therefore the development of a rigorous solution theory of the linear version of (1) with special emphasis on distributional solutions. Explicit solution formulas shall be derived. This simplest model already captures important features of blood flow models as well as other applications like water networks.

Objective 1b: Solution theory for linear switched DAE coupled with nonlinear PDE

The linear solution theory shall be extended to the coupled system (1) with linear switched DAE but nonlinear PDE. This allows for more realistic models of blood flow coupled with simple impulsive dynamics (governed by a linear switched DAE). Some conditions on the evolution of Dirac impulses shall be constructed. Another important application for this case are models of gas networks.

Objective 1c: Solution theory for the fully nonlinear case

Finally, a solution theory for the general coupled system (1) shall be derived. Of special interest will be the case where only jumps (induced by the nonlinear switched DAE) enter the PDE via boundary conditions.

Objective 2: Numerical methods and robustness (Area 2 of SPP 1962)

Based on the analytical properties obtained in Objective 1 numerical methods for finding approximate solutions of the coupled system (1) shall be developed. Special emphasis will be on higher order schemes which will also be necessary to robustly approximate Dirac impulses.

Objective 3: Analysis of blood flow models (Area 3 of SPP 1962)

The analysis of the coupled models should provide conditions under which Dirac-free solutions can appear. This also includes investigations of the robustness of the above conditions w.r.t. parameters or modeling simplifications.

2.2 Work program incl. proposed research methods

The majority of the objectives shall be achieved by the work of a PhD-student (funded by the DFG) who will be jointly supervised by both PIs. Furthermore, the project will be supported by a student assistant, who will contribute to the implementation of the developed numerical methods and run simulations. The above objectives will be approached as follows.

Objective 1a: Distributional solution theory for linear case

In this part of the project the linear case of (1) will be studied, i.e.

$$\begin{aligned} \partial_t u(t,x) + J\partial_x u(t,x) &= g\,u(t,x), && x>0,\\ b\,u(t,0^+) &= Bw(t), && t\geq 0,\\ D_{\sigma(t)}\dot{w}(t) &= F_{\sigma(t)}w(t) + G_{\sigma(t)}u(t,0^+), && \end{aligned} \tag{3}$$

where $\sigma : [0,\infty) \to \{1,2,\dots,p\}$ is the time-varying switching signal and J, g, b, B, $D_1,\dots D_p$, $F_1,\dots,F_p$, $G_1,\dots,G_p$ are given matrices of appropriate size. As was established by the research of the second PI, classical solutions of the switched DAE cannot be expected and w must be viewed as an element of the space of piecewise-smooth distributions, which consists of distributions which can be expressed as the sum of a piecewise-smooth function and Dirac-impulses (and their derivatives). This space is closed under differentiation and a (non-commutative multiplication) is well defined. For coupling with the PDE it is necessary that the variable u is of a compatible type, i.e. measure valued solutions with piecewise-smooth distributions at the boundary have to be defined. Since certain DAEs may even produce derivatives of Dirac impulses in the solution, considering only measured valued solutions may not be sufficient as these only allow for the occurrence of Dirac impulses, but not their derivatives. Once the underlying solution space is specified, the coupled system can be analyzed with respect to solvability. Since for the uncoupled PDE and switched DAE explicit solution formulas exist, we aim at deriving explicit solution formulas for the coupled system. These solutions will in general contain jumps and Dirac impulses. Since Dirac impulses can be interpreted as infinite peaks, it may be desirable to find conditions such that these infinite peaks do not occur in the solutions (at least in some parts thereof); the same is true for certain jumps. The complete understanding of the nature of Dirac-impulses and jumps is also important for developing robust numerical methods later.

It is well known (see e.g. the survey [27]) that for existence and uniqueness of solutions for DAEs the involved matrix pairs must be regular. In the coupled situation (3) this regularity assumption may be too restrictive or not realistic and therefore singular DAEs have to studied as well. Here the quasi-Kronecker form derived by the second PI [3] may be utilized.

An important extension of (3) is allowing for state-depending switching signals $(t, w) \mapsto \sigma(t, w)$ instead of just time-depending switching signals. This introduces a mild nonlinearity to the system description. The underlying solution space remains the same, however, a complete solution theory even for the individual switched DAE is not available yet. Nevertheless, the linear methods for analyzing the coupled systems are expected to be similar to the ones used in the time-dependent switching case and conditions for solvability will be derived.

Objective 1b: Solution theory for linear switched DAE coupled with nonlinear PDE

The change from linear to nonlinear hyperbolic PDEs makes the structure of the solutions much more complex. Especially the notion of entropy-admissibility has to be introduced to single out multiple solutions. Since in [5] the solutions are based on u being of bounded variation, the occurrence of Dirac impulses in u (induced by Dirac impulses in w) are excluded. In fact, note that in this case even jumps in w are excluded. We therefore will extend the techniques used in [5] to first allow for discontinuities in w and secondly to combine them with approaches which allow for Dirac impulses in u. The first case is relevant, when the switched DAE is impulse free, for which simple algebraic test are available. Allowing Dirac impulses in a nonlinear context poses some challenges, because the evaluation of a nonlinear function of a Dirac impulse is not well defined in general (e.g. what is the sine of the Dirac delta?). However recent research of the second PI indicates that for bounded nonlinear functions an evaluation of Dirac impulses is indeed well defined (in fact $\sin(\delta) = \sin(0) = 0$) and these initial thoughts will be formalized and used to study the coupling of linear switched DAEs (which are not impulse-free) with nonlinear PDEs.

Similar as in Objective 1, the case of state-dependent switching will be investigated as well and it is expected that similar methods as developed in Objective 1 can be applied to obtain solvability characterizations also for the case of nonlinear PDEs.

Objective 1c: Solution theory for the fully nonlinear case

The impulse-free solution approach from [18] for nonlinear switched DAEs will be combined with the techniques from [5] in a similar way as in Objective 1b. Allowing for Dirac impulses also in the nonlinear switched DAE case needs to be investigated and the above mention observation that the evaluation of bounded nonlinear functions at Dirac impulses is well defined may be utilized.

Allowing for state-dependent switching presumably will not add significantly new difficulties and will be handled in a similar fashion as above.

Objective 2: Development of numerical algorithms

The development of simple algorithms for the coupled system will accompany the above steps. These can help to understand and illustrate the complex coupled behavior.

For the simulation of blood flow highly accurate numerical methods are required. Therefore we will develop high order methods for the coupled problem, similar to [6, 7]. Since a high order resolution is only possible away from discontinuities, robust methods have to capture accurately the switching of the DAEs in order to combine high accuracy and stability. Furthermore we will consider a high order coupling for stiff problems, as they occur in venous blood flow at the venous valves.

For general systems of type (1), the Dirac impulses can not be represented exactly and pose extreme challenges onto classical schemes. Here high order methods will help to resolve sufficiently the underlying dynamics.

Objective 3: Analysis of blood flow models

In blood flow models strong jumps or even Dirac impulses may not be desired. Therefore we will analyze if such peaked solution might occur in different models investigated in Objective 1. If possible, we aim to provide precise conditions and identify parameters for which the states in the coupled system remain bounded. In the case of linear systems analytical constraints seem to be reachable, whereas for complex nonlinear systems this likely will be investigated on a numerical level.

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