Solving partial differential equations via sparse SDP relaxations

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Abstract.
To solve a partial differential equation (PDE) numerically, we formulate it as a polynomial optimization problem (POP) by discretizing it via a finite difference approximation. The resulting POP satisfies a structured sparsity, which we can exploit to apply the sparse SDP relaxation of Waki, Kim, Kojima and Muramatsu [20] to the POP to obtain a roughly approximate solution of the PDE. To compute a more accurate solution, we incorporate a grid-refining method with repeated applications of the sparse SDP relaxation or Newton's method. The main features of this approach are: (a) we can choose an appropriate objective function, and (b) we can add inequality constraints on the unknown variables and their derivatives. These features make it possible for us to compute a specific solution when the PDE has multiple solutions. Some numerical results on the proposed method applied to ordinary differential equations, PDEs, differential algebraic equations and an optimal control problem are reported.

Key words.
Partial differential equation, ordinary differential equation, differential algebraic equation, polynomial optimization, semidefinite programming relaxation, optimal control, sparsity

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1 Introduction

A vast number of problems arising from various areas, for instance physics, economics and engineering, can be expressed as partial differential equations (PDEs). Problems involving PDEs are often difficult to analyze, and therefore numerical methods to solve them are of particular interest. Though linear PDEs of second order are well studied and many numerical solvers for specific classes such as elliptic, parabolic and hyperbolic second order PDEs were developed, solvers for fairly general classes of nonlinear PDEs are in high demand and remain an active field of research.

Some ordinary and partial differential equations can be expressed as polynomial optimization problems (POPs) if they are approximated by finite differences. Presently POPs are in the focus of researchers of different background, involving fields such as semidefinite programming (SDP), moment theory, sum of squares, real algebra and operator theory. One of the fundamental contributions in polynomial optimization is the paper [10] by Lasserre. Lasserre introduced a sequence of SDP relaxation problems whose solutions converge to a global optimal solution of an unconstrained or constrained POP under moderate assumptions. In many POPs, the polynomials involved in objective functions and the constraints are sparse. A concept of structured sparsity for POPs was introduced in [8, 9]. Exploiting a structured sparsity of a POP, which is called the correlative sparsity, a sequence of sparse SDP relaxation problems was constructed by Waki, Kim, Kojima and Muramatsu in their paper [20]. Compared to the original SDP relaxation proposed by Lasserre, their sparse SDP relaxation provides stronger numerical results . Recently, Lasserre proved in his paper [11] the convergence of a sequence of sparse SDP relaxation problems. The observation that the POPs derived from certain PDE problems are equipped with some structured sparsity is the first motivation for our approach, as it enables us to apply the sparse SDP relaxations efficiently.

The purpose of this paper is to present a new numerical approach with the use of the sparse SDP relaxation of POPs to a class of nonlinear second order PDEs. Given a PDE with a boundary condition, (i) we discretize it into a system of polynomial equations, which forms equality constraints of the POP to be formulated, by applying a finite difference approximation, and (ii) we set up a polynomial objective function in the discretized variables, to formulate a POP. Also, (iii) we can add inequality constraints to impose lower and upper bounds on the unknown functions and their derivatives. As the resulting POP satisfies the correlative sparsity, the sparse SDP relaxation [20] works effectively in solving the POP. The features (ii) and (iii) are the main advantages of this approach; when the PDE has multiple solutions, we can pick up a specific solution by choosing an appropriate objective function in (ii) and adding inequality constraints in (iii) to restrict the unknown functions and their derivatives. It is an further advantage, that this approach covers ordinary differential equations (ODEs) and is extended to differential algebraic equations (DAEs) and optimal control problems. Our approach exploits, that these different classes of problems can be transformed to sparse POPs. To demonstrate its high potential we present some numerical results.

The correlative sparsity for POPs and the sparse SDP relaxation [20] are briefly recalled in Section 2. The new approach to solve a class of nonlinear PDEs using the sparse SDP relaxation for POPs is introduced in Section 3. We show there that POPs derived from discretized PDEs satisfy the correlative sparsity; hence we can effectively apply the sparse SDP relaxation to them. Section 4 discusses some numerical results on our approach applied to ODEs, PDEs, a DAE and an optimal control problem. An approach to solve first order PDEs was proposed recently in [5]. We discuss the performance of our approach for particular first order PDEs from [5].

2 Semidefinite program relaxations for sparse polynomial optimization problems

All partial differential equations, ordinary differential equations, differential algebraic equations and optimal control problems we will study in this paper can be expressed as **equality-inequality constrained POPs** satisfying the correlative sparsity. In this section, we briefly recall the concept of correlative sparsity of a POP and the SDP relaxation, which exploits the correlative sparsity, by Waki, Kim, Kojima and Muramatsu [20]. For simplicity of discussions here, we will consider only an inequality constrained POP. Basically, we could replace an equality constraint $h(x) = 0$ by two inequality constraints $h(x) \geq 0$ and $-h(x) \geq 0$, so that we could apply the discussions below to equality-inequality constrained POPs. For more direct and efficient handling of equality constraints and technical details of the sparse SDP relaxation, see [20].

Let $f_k \in \mathbb{R}[x]$ $(k = 0, 1, \ldots, m)$, where $\mathbb{R}[x]$ denotes the set of real-valued multivariate polynomials in $x \in \mathbb{R}^n$. Consider the following inequality constrained POP:

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_k(x) \quad \geq 0 \quad \forall\, k \in \{1, \ldots, m\}. \end{array} \tag{2.1}$$

Given a polynomial $f \in \mathbb{R}[x]$, $f(x) = \sum_{\alpha \in \mathbb{N}^n} c_\alpha(f) x^\alpha$ $(c_\alpha(f) \in \mathbb{R})$, we define its **support** by $supp(f) = \{\alpha \in \mathbb{N}^n \mid c_\alpha(f) \neq 0\}$. Then, let $\xi^\star = \inf\{f_0(x) : \ f_k(x) \geq 0 \ (k = 1, \ldots, m)\}$ and

$$F_k = \{i : \ \alpha_i \geq 1 \text{ for some } \alpha \in \text{supp}(f_k) \subset \mathbb{N}^n\},$$

the index set of variables x_i involved in the polynomial f_k. We define the $n \times n$ **correlative sparsity pattern matrix (csp matrix)** R of the POP (2.1) such that

$$R_{i,j} = \begin{cases} \star & \text{if} \quad i = j, \\ \star & \text{if} \quad \alpha_i \geq 1 \text{ and } \alpha_j \geq 1 \text{ for some } \alpha \in \text{supp}(f_0), \\ \star & \text{if} \quad i \in F_k \text{ and } j \in F_k \text{ for some } k \in \{1, 2, \ldots, m\}, \\ 0 & \text{otherwise.} \end{cases}$$

If R is sparse, the POP (2.1) is called **correlatively sparse**. The csp matrix R induces the **correlative sparsity pattern graph (csp graph)** $G(N, E)$. Its node set N and edge set E are defined as

$$N = \{1, 2, \ldots, n\} \quad \text{and } E = \{\{i, j\} : R_{i,j} = \star, \ i < j\},$$

respectively. Note that each edge $\{i, j\}$ corresponds to a nonzero off-diagonal element $R_{i,j} = \star$ of R. The sequence of SDP relaxations is defined via the maximal cliques of the csp graph $G(N, E)$. As it is an NP-hard problem to determine the maximal cliques of an arbitrary graph, we introduce a **chordal extension** $G(N, E')$ of the csp graph. (See the literature [1] for chordal graphs and their fundamental properties). Let $C_1, \ldots, C_p \subseteq N$ be the maximal cliques of $G(N, E')$. Since each $F_k \subseteq N$ forms a clique, it must be contained in some maximal C_q. Let $\hat{F}_k$ be such a maximal clique C_q. To construct a sequence of SDP relaxations, a nonnegative integer $\omega \geq \omega_{\max}$ is chosen for the **relaxation order**, where $\omega_{\max} = \max\{\omega_k : \ k = 0, 1, \ldots, m\}$ and $\omega_k = \lceil \frac{1}{2} \deg(f_k) \rceil$ $(k = 0, \ldots, m)$. In order to take the sparsity of R, i.e., the correlative sparsity of the POP, into account, we consider subsets $\mathcal{A}_\omega^{C_1}, \ldots, \mathcal{A}_\omega^{C_p}, \mathcal{A}_{\omega-\omega_1}^{\hat{F}_1}, \ldots, \mathcal{A}_{\omega-\omega_m}^{\hat{F}_m}$ of $\mathbb{Z}_+^n$, which are defined as $\mathcal{A}_\omega^C = \{\alpha \in \mathbb{Z}_+^n : \alpha_i = 0 \text{ if } i \notin C \text{ and } \sum_{j \in C} \alpha_j \leq \omega\}$. Then the POP (2.1) is equivalent to the problem

$$\begin{array}{ll} \min & f_0(x) \\ \text{s.t.} & u(x, \mathcal{A}_{\omega-\omega_k}^{\hat{F}_k}) u(x, \mathcal{A}_{\omega-\omega_k}^{\hat{F}_k})^T f_k(x) \succeq 0 \quad \forall\, k \in \{1, \ldots, m\}, \\ & u(x, \mathcal{A}_\omega^{C_l}) u(x, \mathcal{A}_\omega^{C_l})^T \succeq 0 \quad \forall\, l \in \{1, \ldots, p\}, \end{array} \tag{2.2}$$

where $u(x, \mathcal{G})$ is used for the $|\mathcal{G}|$-dimensional column vector consisting of the monomials x^α $(\alpha \in \mathcal{G})$. If we reform the $m + p$ matrix inequality constraints in (2.2) into a single matrix inequality and expand it with respect to the monomials x^α, we can write (2.2) as

$$\begin{array}{ll} \min & \sum_{\alpha \in \tilde{\mathcal{F}}} \tilde{c_0}(\alpha) x^\alpha \\ \text{s.t.} & M(0) + \sum_{\alpha \in \tilde{\mathcal{F}}} M(\alpha) x^\alpha \succeq 0, \end{array}$$

where $\tilde{\mathcal{F}} = \left(\cup_{l=1}^p \mathcal{A}_\omega^{C_l}\right) / \{0\}$. $M(0)$ and the $M(\alpha)$ are symmetric block diagonal matrices. If we replace each monomial x^α by a scalar variable y_α, we then derive an SDP relaxation of (2.1):

$$\begin{array}{ll} \min & \sum_{\alpha \in \tilde{\mathcal{F}}} \tilde{c_0}(\alpha) y_\alpha \\ \text{s.t.} & M(0) + \sum_{\alpha \in \tilde{\mathcal{F}}} M(\alpha) y_\alpha \succeq 0. \end{array}$$

The optimal objective value of this SDP relaxation problem is denoted by ξ_ω. For any feasible solution x of (2.1) and for $\omega_{\max} \leq \omega \leq \omega'$, the relation $\xi_\omega \leq \xi_{\omega'} \leq \xi^\star \leq f_0(x)$ holds. See [20] for more details. Lasserre [11] showed the convergence of this SDP relaxation under a moderate additional assumption.

Numerical experiments [20] show that it is usually sufficient to choose a $\omega \in \{\omega_{\max}, \ldots, \omega_{\max} + 3\}$ as relaxation order to approximate an optimal solution of the POP (2.1) accurately. In theory, however, it is not known a priori which relaxation order ω is necessary to obtain a sufficiently accurate solution. Moreover the size of the SDP relaxation increases as $\binom{n+\omega}{\omega}$ in ω.

3 Application of the sparse SDP relaxation to partial differential equations

In this section some methods of solving a certain class of partial differential equation (PDE) problems via SDP relaxations are introduced. They are based on the idea to derive a sparse polynomial optimization problem (POP) by taking a discretized PDE problem as constraint and choosing an appropriate objective function. The first method applies the software SparsePOP [17] to this POP directly. SparsePOP is an implementation of the SDP relaxation by Waki et al. [20]. For detailed information about SparsePOP, see [21]. This SDP relaxation method is improved by applying subsequently Newton's method with the SparsePOP solution as an initial guess. Finally a grid-refining method is proposed, which extends solutions found by SparsePOP (and Newton' s method) on a coarse grid to a finer grid by linear interpolation and subsequent iterations of SparsePOP or Newton's method. We demonstrate those three different methods to solve PDE problems in Section 4. Our grid-refining method shares a basic idea with the multigrid method for linear PDEs, where more sophisticated techniques such as a smoothing technique with the use of the weighted Jacobi iteration are used to get accurate approximate solutions on fine grids from rough approximate solutions on coarse grids. See [2, 19] for more details on the multigrid method.

In general we distinguish a **PDE**, which is an equation involving an unknown function $u : \Omega \to \mathbb{R}^m$ and its partial derivatives, and a **PDE problem**, which is a PDE equipped with additional conditions for the unknown function u on the boundary of the domain Ω. We restrict our attention to a certain class of PDE problems where Ω is given as a rectangular region $[x_l, x_u] \times [y_l, y_u]$ of $\mathbb{R}^2$. (Later we deal with ordinary differential equations where $\Omega = [x_l, x_u] \subset \mathbb{R}^1$). The target class of PDE problems is specified by the following definition.

Definition 1 *A PDE problem is called* ***polynomial second order in two variables (PSO)****, if it is a problem of finding an unknown function $u : \Omega \to \mathbb{R}^m$ of the form*

$$\begin{array}{rll} a(x,y,u)\frac{\partial^2 u}{\partial x^2}(x,y) + b(x,y,u)\frac{\partial^2 u}{\partial x \partial y}(x,y) + & & \\ c(x,y,u)\frac{\partial^2 u}{\partial y^2}(x,y) + d(x,y,u)\frac{\partial u}{\partial x}(x,y) + & & \\ e(x,y,u)\frac{\partial u}{\partial y}(x,y) + f(x,y,u) & = 0 & \forall\, (x,y) \in \Omega \subset \mathbb{R}^2, \\ r_l^x \frac{\partial u}{\partial n}(x_l,y) + s_l^x u(x_l,y) - o_u^x u(x_u,y) & = H(x_l,y) & \forall\, y \in [y_l,\, y_u], \\ r_u^x \frac{\partial u}{\partial n}(x_u,y) + s_u^x u(x_u,y) - o_l^x u(x_l,y) & = H(x_u,y) & \forall\, y \in [y_l,\, y_u], \\ r_l^y \frac{\partial u}{\partial n}(x,y_l) + s_l^y u(x,y_l) - o_u^y u(x,y_u) & = H(x,y_l) & \forall\, x \in [x_l,\, x_u], \\ r_u^y \frac{\partial u}{\partial n}(x,y_u) + s_u^y u(x,y_u) - o_l^y u(x,y_l) & = H(x,y_u) & \forall\, x \in [x_l,\, x_u]. \end{array} \tag{3.1}$$

Here a, b, c, d and e are diagonal functions $\Omega \times \mathbb{R}^m \to \mathbb{R}^{m \times m}$ polynomial in u, $f : \Omega \times \mathbb{R}^m \to \mathbb{R}^m$ is a function polynomial in u , the domain Ω is of the form $\Omega = [x_l, x_u] \times [y_l, y_u]$ and $H : \partial\Omega \to \mathbb{R}^m$. $\frac{\partial u}{\partial n}$ denotes the partial derivative of u in direction orthogonal to the boundary and $r_l^x,\ s_l^x,\ o_l^x,\ r_u^x,\ s_u^x,\ o_u^x,\ r_l^y,\ s_l^y,\ o_l^y,\ r_u^y,\ s_u^y,\ o_u^y \in \{0, 1\}$. The ***PSO discriminant D*** *is defined as*

$$\begin{aligned} & D : \mathbb{R}^2 \to \mathbb{R}^{m \times m}, \\ & D(x,y) = b(x,y,u(x,y))^2 - 4a(x,y,u(x,y))\, c(x,y,u(x,y)). \end{aligned}$$

In case D negative definite on Ω a PSO PDE is called ***elliptic****, in case D positive definite on Ω* ***hyperbolic*** *and in case $det(D) = 0$ on Ω* ***parabolic****.*

3.1 Discretization of PDEs and their formulation in terms of sparse POPs

Given a PSO PDE problem we induce a sparse POP in two steps. First we discretize the PDE and its boundary conditions into a system of polynomial equations. Next we choose an appropriate objective function, lower, upper and variational bounds for the discretized variables to construct a POP which we can apply SparsePOP to.

3.1.1 Discretization

Finite difference approximations: The rectangular domain $\Omega = [x_l, x_u] \times [y_l, y_u]$ of u is discretized with $N_x \times N_y$ grid points. In order to approximate the partial derivatives of u at each point in the grid, define

$$u_{i,j} = u\left(x_l + (i-1)\Delta x,\ y_l + (j-1)\Delta y\right)\ \forall i \in \{1,\ldots,N_x\},\ \forall j \in \{1,\ldots,N_y\},$$

where $\Delta x = \frac{1}{N_x-1}(x_u - x_l)$ and $\Delta y = \frac{1}{N_y-1}(y_u - y_l)$. We use the vector

$$u = (u_{i,j})_{i,j} = (u_{1,1},\ldots,u_{1,N_y},\ldots,u_{N_x,N_y})$$

to denote the unknown variables. With these variables $(u_{i,j})_{i,j}$ the partial derivatives in the PSO PDE problem are approximated by standard finite difference schemes. The finite difference approximations at a u_{i_0,j_0} are linear in $(u_{i,j})_{i,j}$, e.g. $\frac{\partial^2 u(x,y)}{\partial x^2}\ |_{u(x,y)=u_{i_0,j_0}} \approx \frac{\Delta^2 u_{i_0,j_0}}{(\Delta x)^2} := \frac{u_{i_0+1,j_0} - 2\,u_{i_0,j_0} + u_{i_0-1,j_0}}{(\Delta x)^2}$ and $\frac{\partial u(x,y)}{\partial x}\ |_{u(x,y)=u_{i_0,j_0}} \approx \frac{\Delta u_{i_0,j_0}}{\Delta x} := \frac{u_{i_0+1,j_0} - u_{i_0-1,j_0}}{2\Delta x}$. Note that derivatives exist at **interior grid points**, i.e. grid points $u_{i,j}$ with $i \in \{2, N_x - 1\}$ and $j \in \{2, N_y - 1\}$. Applying these finite difference approximations to the PDE problem (3.1), where a, b, c, d, e and f are polynomial in u, a system of polynomial equations $(p_{i,j}(u) = 0)_{i=2,j=2}^{N_x-1,N_y-1}$ in u is obtained, where $p_{i,j}(u)$ is given by

$$\begin{aligned} p_{i,j}(u) =& a(x_i,y_j,u_{i,j})\frac{\Delta^2 u_{i,j}}{\Delta x^2} + b(x_i,y_j,u_{i,j})\frac{\Delta^2 u_{i,j}}{\Delta x \Delta y} + c(x_i,y_j,u_{i,j})\frac{\Delta^2 u_{i,j}}{\Delta y^2} + \\ & d(x_i,y_j,u_{i,j})\frac{\Delta u_{i,j}}{\Delta x} + e(x_i,y_j,u_{i,j})\frac{\Delta u_{i.j}}{\Delta y} + f(x_i,y_j,u_{i,j}). \end{aligned}$$

There is no general theorem guaranteeing the convergence of a finite difference scheme's solution $(u_{i,j})_{i=1,\,j=1}^{N_x,\,N_y}$ to a solution u of the original PDE if $N_x, N_y \to \infty$. It may occur that more than one solution for the difference scheme exists. There are a lot of studies on the convergence. Among them, we note that Theorem 2.1 in [18] provides convergence for finite difference schemes of a certain class of parabolic PDE problems. Stable solutions of such a parabolic PDE problem will be discussed as one of our testing problems.

Additional polynomial inequality constraints: In order to apply POP solvers as SparsePOP, we are required to fix lower bounds $(\mathrm{lbd}_{i,j})_{i,j}$ and upper bounds $(\mathrm{ubd}_{i,j})_{i,j}$ for the $(u_{i,j})_{i,j}$. When choosing these bounds care has to be taken. A choice of lbd and ubd which is too tight may exclude solutions of the polynomial system, while a choice which is too loose may cause inaccurate results.

Beside those necessary constraints, it is also possible to impose additional inequality constraints of the form

$$g_l(u) \geq 0 \quad \forall\, l \in \{1,\ldots,k\}, \tag{3.2}$$

where the g_l are polynomial in $(u_{i,j})_{i,j}$. One possibility to obtain such bounds is derived by constraining the partial derivatives. We call bounds of this type **variation bounds**. For the derivative in $x-$direction they are given by

$$\left|\ \frac{\partial u(x_i,y_j)}{\partial x}\ \right| \leq M \qquad \forall i \in \{2,\ldots,N_x-1\},\ \forall j \in \{2,\ldots,N_y-1\}. \tag{3.3}$$

Expression (3.3) can be transformed into polynomial constraints easily. Choosing variation bounds (3.3) restricts the class of admissible functions in which we search for a PDE problem' s solution.

Choosing an objective function: To derive a POP, it remains to choose an appropriate objective function F that is polynomial in $u_{i,j}$ $(i = 1,\ldots,N_x,\ j = 1,\ldots,N_y)$. The choice of an appropriate objective function is dependent on the PDE problem we are aiming to solve. In case there is at most one solution of the PDE problem, we are interested in the feasibility of the POP we construct. Thus any objective is a priori acceptable for that purpose. However, the accuracy of obtained solutions may depend on the particular objective function. In case the solution of the PDE problem is not unique, the choice of the objective function determines a particular solution to be found. A large class of PDE's which occur in many applications can be written as Euler-Lagrange equations. A typical case is a stable state equation of reaction-diffusion type. In this case, a canonical choice is a discretization of the corresponding energy integral as we see in example 4.3.2.

With the definition of the objective function and the discretized PDE problem, we obtain the POP

$$
\begin{array}{lll}
\max & F((u_{i,j})_{i,j}) & \\
\text{s.t.} & p_{i,j}(u) = 0 & \forall i \in \{2,\ldots,N_x - 1\}, \\
 & & \forall j \in \{2,\ldots,N_y - 1\}, \\
 & -r_l^x \frac{\Delta u_{1,j}}{\Delta x} + s_l^x u_{1,j} - o_u^x u_{N_x,j} = H_{1,j} & \forall j \in \{1,\ldots,N_y\}, \\
 & r_u^x \frac{\Delta u_{N_x,j}}{\Delta x} + s_u^x u_{N_x,j} - o_l^x u_{1,j} = H_{N_x,j} & \forall j \in \{1,\ldots,N_y\}, \\
 & -r_l^y \frac{\Delta u_{i,1}}{\Delta y} + s_l^y u_{i,1} - o_u^y u_{i,N_y} = H_{i,1} & \forall i \in \{1,\ldots,N_x\}, \\
 & r_u^y \frac{\Delta u_{i,N_y}}{\Delta y} + s_u^y u_{i,N_y} - o_l^y u_{i,1} = H_{i,N_y} & \forall i \in \{1,\ldots,N_x\}, \\
 & \text{lbd}_{i,j} \leq u_{i,j} \leq \text{ubd}_{i,j} & \forall i \in \{1,\ldots,N_x\}, \\
 & & \forall j \in \{1,\ldots,N_y\}, \\
 & g_l\left((u_{i,j})_{i,j}\right) \geq 0 & \forall l \in \{1,\ldots,k\}.
\end{array}
\tag{3.4}
$$

We show in Section 3.4 that the POP (3.4) is correlatively sparse under some mild assumptions.

3.1.2 Note on boundary conditions

Beside the choice of the objective function and the discretization of the PDE in (3.4), the boundary conditions for the unknown function u have a crucial impact on the accuracy of numerical solutions obtained by SparsePOP. Recall the boundary condition of the PSO PDE (3.1). In our approach to solve PSO PDE we restricted ourselves to problems with boundary conditions of the types **Dirichlet, Neumann** or **periodic**.

Boundary conditions at $x = x_l$ or $x = x_u$ are called **Dirichlet**, if the values $u(x_l, y)$ or $u(x_u, y)$ are fixed for all $y \in [y_l, y_u]$. And they are called **Neumann**, if the values of the partial derivative $\frac{\partial u(x,y)}{\partial n}$ orthogonal to the domain's boundary are fixed at $x = x_l$ or $x = x_u$ for all $y \in [y_l, y_u]$. For instance the boundary conditions at $x = x_l$ and $x = x_u$ are of the form

$$
\begin{aligned}
-r_l^x \frac{\partial u(x_l, y)}{\partial x} + s_l^x\, u(x_l, y) &= H(x_l, y) \quad \forall\, y \in [y_l, y_u], \\
r_u^x \frac{\partial u(x_u, y)}{\partial x} + s_u^x\, u(x_u, y) &= H(x_u, y) \quad \forall\, y \in [y_l, y_u],
\end{aligned}
$$

with $r_l^x + s_l^x = 1$, $r_u^x + s_u^x = 1$. We discretize these equations by finite difference approximations.

In various PDE problems, the function $u(x_l, y)$ in $y \in [y_l, y_u]$ is sometimes identified with the function $u(x_u, y)$ in $y \in [y_l, y_u]$. In that case, the boundary condition is called **periodic**, it is written

$$
u(x_l, y) = u(x_u, y) \qquad \forall y \in [y_l, y_u],
$$

and is easily discretized to $u_{1,j} = u_{N_x,j}$ $(j = 1,\ldots,N_y)$. It corresponds to the general boundary condition in (3.1) at (x_l, y) with $H(x_l, \cdot) \equiv 0$, $r_l^x = 0$ and $s_l^x = o_u^x = 1$. Analogous expressions can be derived for boundary conditions in $y-$direction accordingly. Note that boundary conditions in x- and y-direction may be of different type.

3.1.3 Reducing the number of variables

In order to improve the numerical performance of the sparse SDP relaxation, we can simplify the POP (3.4). It is observed that by imposing Dirichlet or Neumann conditions on grid points at the boundary of the domain, the $u_{i,j}$ become either known or can be expressed in dependence of an adjacent interior grid point. For instance at x_l,

$$
u_{1,j} = H_{1,j} \qquad \text{or} \qquad u_{1,j} = H_{1,j}\,\Delta x + u_{2,j}. \tag{3.5}
$$

If we substitute the variables $u_{i,j}$ corresponding to boundary grid points by the expression (3.5), the number of grid points in x direction is reduced by 2. In case of periodic condition the number of grid points in that direction is reduced by 1. For instance under Dirichlet or Neumann condition for x and periodic condition for y the dimension n is reduced to $n = \hat{N}_x \hat{N}_y = (N_x - 2)(N_y - 1)$. These substitutions result in a POP where the constraints derived from discretized boundary conditions are eliminated:

$$
\begin{array}{lll}
\max & F(u) & \\
 & p_{i,j}(u) = 0 & \\
\text{s.t.} & \text{lbd}_{i,j} \leq u_{i,j} \leq \text{ubd}_{i,j} & \forall i \in \{1,\ldots,\hat{N}_x\},\ \forall j \in \{1,\ldots,\hat{N}_y\}, \\
 & g_\ell(u) \geq 0 & \forall \ell \in \{1,\ldots,k\}.
\end{array}
\tag{3.6}
$$

The finite difference approximations at boundary $u_{i,j}$ ($i \in \{1, \hat{N}_x\}$ or $j \in \{1, \hat{N}_y\}$) preserve the information given by the boundary conditions in POP (3.4).

3.2 SparsePOP and Newton's method

The optimal solution for a POP (3.6) obtained by the sparse SDP relaxation is often of inappropriate accuracy. Therefore, additional techniques are introduced to improve the solution's accuracy. Since the number of equality constraints in (3.6) coincides with the number n of unknown $u_{i,j}$, it is possible to apply the well known Newton's method for nonlinear systems of equations. It can be found in detail in [14] for example.

In our approach, we exploit the locally rapid convergence of Newton's method in combination with the global optimization property of SparsePOP [17]. At first, SparsePOP is applied to the POP (3.6) with an appropriate objective function and a sufficient **relaxation order** ω. In a second step Newton's method is applied to the system $(p_{k,l}(u) = 0)_{k,l}$ of dimension n with the SparsePOP solution as the initial guess u_0. Newton's method terminates after obtaining an appropriate accuracy or exceeding a maximum number N_N of iterations.

3.3 Grid-refining method

Even though SparsePOP is combined with Newton's method, still a high relaxation order ω is necessary in many examples, in order to obtain accurate solutions. Because the size of the SDP relaxation increases as $\binom{n+\omega}{\omega}$ in the relaxation order ω and in the number n of variables, those problems are solved for coarse discretization in appropriate time only.

In our grid-refining method a solution, which is obtained by SparsePOP and optional Newton's method for a coarse grid as a first step, is extended stepwise to a finer grid by subsequent interpolation, and applying SparsePOP or Newton' s method. The grid-refining method is implemented in the following algorithm:

Step 1 - Initialization	Apply SparsePOP, obj. $F(u)$, $\omega = \omega_1$. Apply Newton's method (optional).	obtain u^1
Step 2 - Extension	$N_x(k) = 2\ N_x(k-1) - 1$ or $N_y(k) = 2\ N_y(k-1) - 1$ Interpolation of u^{k-1}	obtain ${u^{k-1}}^\star$
Step 3a Step 3b	Apply SparsePOP, obj. $F_M(u)$, $\omega = \omega_2$. Apply Newton's method.	obtain u^k
Iterate	Step 2 and Step 3	

Step 1 - SparsePOP: Choose an objective function $F(u)$, a discretization grid size $(N_x(1), N_y(1))$, lower bounds $(\text{lbd}_i(1))_i$, upper bounds $(\text{ubd}_i(1))_i$ and an initial relaxation order ω_1. Apply SparsePOP with these parameters to a discretized PDE problem and obtain a solution u^1. To improve the accuracy of the SparsePOP solution u^1, Newton's method as stated in Section 3.2 may be applied to the same discretized PDE problem with the initial guess u^1.

Step 2 - Extension: Extend the *(k-1)*th iteration's solution u^{k-1} to a finer grid. Choose either x- or y-direction as the direction of refinement, i.e. choose either $N_x(k) = 2\ N_x(k-1)-1$ and $N_y(k) = N_y(k-1)$, or $N_x(k) = N_x(k-1)$ and $N_y(k) = 2\ N_y(k-1)-1$. In order to extend u^{k-1} to the new grid with the doubled number of grid points, assume without loss of generality the direction of extension is x. The interpolation of the solution u^{k-1} to ${u^{k-1}}^\star$ is given by the scheme

$$\begin{aligned}
{u^{k-1}_{2i-1,j}}^\star &= u^{k-1}_{i,j} \quad \forall i \in \{1,\dots,N_x(k-1)\},\ \forall j \in \{1,\dots,N_y(k)\}, \\
{u^{k-1}_{2i,j}}^\star &= \tfrac{1}{2}\left(u^{k-1}_{i+1,j} + u^{k-1}_{i,j}\right) \quad \forall i \in \{1,\dots,N_x(k-1)-1\},\ \forall j \in \{1,\dots,N_y(k)\}.
\end{aligned}$$

The interpolated solution ${u^{k-1}}^\star$ is a first approximation to the solution of POP (3.6) for the $N_x(k) \times N_y(k)$-grid.

Step 3a - Apply SparsePOP: We would like to be able to choose a new relaxation order $\omega_2 \leq \omega_1$ to apply SparsePOP with a new objective function F_M, defined as

$$F_M(u) = \sum_{i,j} (u_{i,j} - u_{i,j}^{k-1^{\star}})^2, \tag{3.7}$$

to POP (3.6) on the refined grid. We choose this objective function as we are interested in finding a feasible solution of the POP (3.6) with minimal Euclidean distance to the interpolated solution $u^{k-1^{\star}}$. To utilize the information given by $u^{k-1^{\star}}$ the lower and upper bounds are adapted by

$$\begin{aligned} \mathrm{lbd}_{i,j}(k) &= \max \left\{ \mathrm{lbd}_{i,j}(k-1),\ u_{i,j}^{k-1^{\star}} - \delta \right\} \quad \forall\, i,j, \\ \mathrm{ubd}_{i,j}(k) &= \min \left\{ \mathrm{ubd}_{i,j}(k-1),\ u_{i,j}^{k-1^{\star}} + \delta \right\} \quad \forall\, i,j, \end{aligned}$$

where $\delta > 0$. Apply SparsePOP to obtain a solution u^k.

Step 3b - Apply Newton's method: The SparsePOP solution u^k may be equipped with an inappropriate feasibility error ϵ_{feas}. Or it may occur that POP (3.6) for the finer grid is intractable, even when $\omega_2 < \omega_1$. In the first case Newton's method is applied with initial guess $u_0 = u^k$, in the second case it is applied with $u_0 = u^{k-1^{\star}}$.

The steps 2 and 3 are repeated until an accurate solution for a high resolution grid is obtained.

3.4 Sparsity of discretized PDE problems

The introduced SDP relaxations are desired to be deduced from a sparse POP in order to solve them efficiently. Due to the few variables $u_{i,j}$ involved in each equality constraint of POP (3.6), we expect POP (3.6) to be sparse. But it remains to confirm this expectation by showing the $n \times n$ csp matrix R is sparse, i.e. the number $n_z(R)$ of nonzero elements in R is of order $O(n)$. We distinguish the two cases:

1. $a \neq 0,\ b = 0$ and $c \neq 0$,
2. $a \neq 0,\ b \neq 0$ and $c \neq 0$,

where a, b and c the coefficients of u_{xx}, u_{xy} and u_{yy} in the PSO PDE (3.1). We derive bounds for $n_z(R)$ under the assumption that the objective function is linear in $u_{i,j}$. In case 1 there are at most 12 unknown $u_{k,l}$ that can occur in some equality constraint with a particular unknown $u_{i,j}$ as pictured in Figure 1. Hence the maximum number of nonzero elements in the row of R corresponding to $u_{i,j}$ is 13, which implies $n_z(R) \leq 13n$. Under the same argument it follows in case 2 that $n_z(R) \leq 25n$; see Figure 1. These bounds are tight; they are attained in case of periodic condition for x and y. Thus R is sparse and POP (3.6) is correlatively sparse.

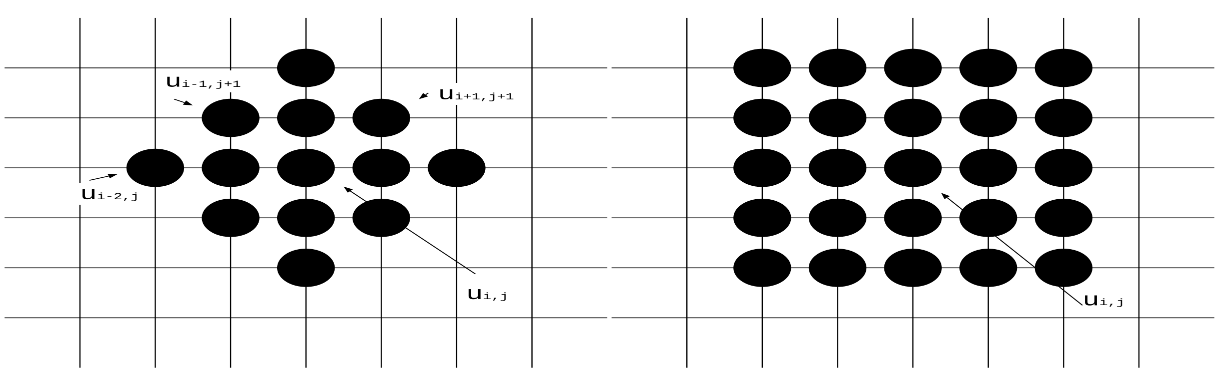

Figure 1: $u_{k,l}$ involved in some constraint with $u_{i,j}$ in case 1 (left) and case 2 (right)

Let R' denote the $n \times n$ matrix corresponding to the graph $G(N, E')$, which is a chordal extension of $G(N, E)$. For the computational effort it is also useful to know whether R' is sparse or not. $n_z(R')$ depends on the employed ordering method P for R, which is used to avoid fill-ins in the symbolic sparse Cholesky factorization LL^T of the ordered matrix PRP^T. R' is constructed as $R' = L + L^T$. We examine two different methods of ordering R, the **symmetric minimum degree (SMD) ordering** and **reverse Cuthill-McKee (RCM) ordering**. See [4] for details.

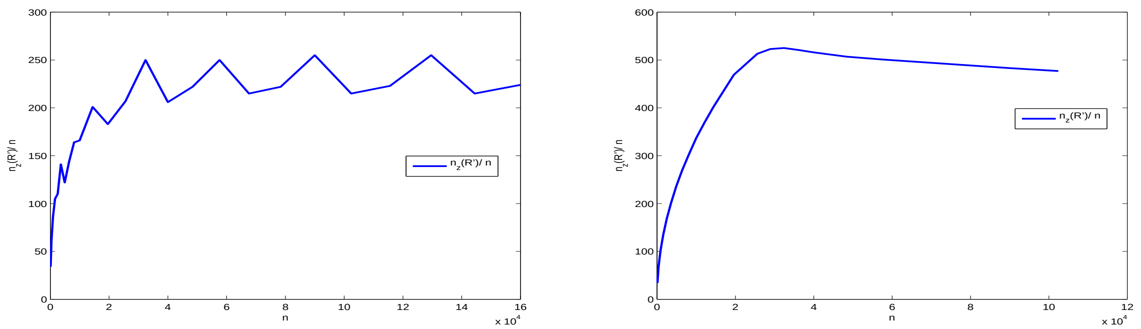

Figure 2: $\frac{n_z(R')}{n}$ for SMD (left) and RCM (right) ordering in case 1

We conduct some numerical experiments, in order to estimate the behavior of $n_z(R')$. Figure 3 shows examples of R' after SMD and RCM ordering, and Figure 2 shows $\frac{n_z(R')}{n}$ obtained by the SMD and RCM orderings for the $n \times n$-matrix R, respectively, in case 1 with Dirichlet or Neumann condition in x and periodic condition in y. For $n \in [100, 160000]$ it holds $\frac{n_z(R')}{n} \leq 300$ for SMD ordering and $\frac{n_z(R')}{n} \leq 600$ for RCM ordering, respectively. The behavior of $\frac{n_z(R')}{n}$ may suggest $n_z(R') = O(n)$ for both ordering methods. Hence we expect the numerical advantage of the sparse SDP relaxations. As the constants 300 and 600 are large, we can not expect a quick solution of the sparse SDP relaxation.

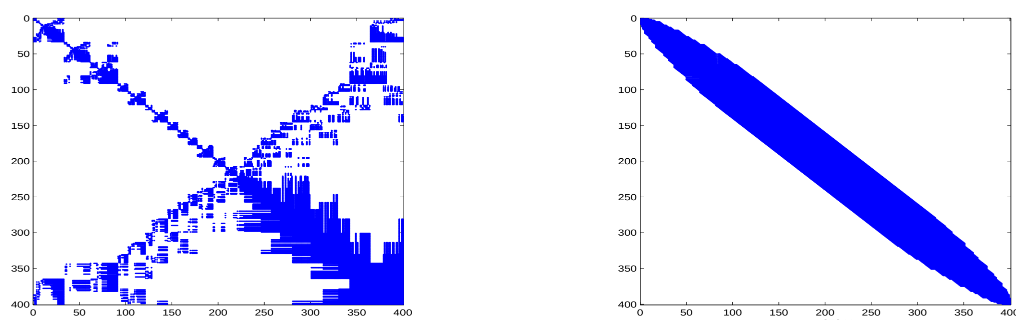

Figure 3: R' obtained by SMD (left) and RCM (right) orderings in case 1 with $n = 400$

4 Numerical results

In this section examples of ordinary differential equation, partial differential equation (PDE), differential algebraic equation and optimal control problems are solved via the methods proposed in Section 3. Before examining different PDE problems, we mention the most important parameters that have to be chosen to apply our approach. Apart from the objective function F, we choose the **relaxation order** ω for SparsePOP

[17]. In case we employ Newton' s method it is necessary to determine the **number N_N of Newton steps**, each time Newton's method is called. When the grid-refining method is applied with strategy 3a, instead of ω we have to choose two relaxation orders ω_1 and ω_2.

We used a Mac OS with CPU 2.5 GHz and 2 Gb Memory for all calculations. The **total processing time** is denoted as t_C.

4.1 Verification of results

After determining numerical solutions for discretized PDE problems by applying SparsePOP [17], Newton's method or the grid-refining method, the question arises, how to verify the accuracy of those results. Measures for feasibility and optimality of a numerical solution u of POP (3.6) are given by ϵ_{feas}, ϵ_{scaled} and ϵ_{obj}.

$$\epsilon_{\text{obj}} = \frac{|\text{the optimal value of SDP} - F(u)|}{\max\{1, |F(u)|\}}$$

denotes a **measure for the optimality** of the solution u. It is observed ϵ_{obj} is usually negligible if F is linear in u. Therefore ϵ_{obj} is documented in exemplary cases only. The **absolute feasibility error**

$$\epsilon_{\text{feas}} = \min\{- \mid p_{i,j}(u) \mid,\ \min\{g_l(u), 0\}\ \forall\, i, j, l\}$$

is the measure for feasibility of the numerical solution u. In case the problem is badly scaled, it is more suitable to consider the **scaled feasibility error**

$$\epsilon_{\text{scaled}} = \min\{- \mid p_{i,j}(u)/\sigma_{i,j}(u) \mid,\ \min\{g_l(u)/\hat{\sigma}_l(u), 0\}\ \forall\, i, j, l\},$$

where $\sigma_{i,j}$ and $\hat{\sigma}_l$ are the maxima of the monomials in the corresponding polynomials $p_{i,j}$ and g_l at u. In most examples we document ϵ_{feas}; if ϵ_{feas} and ϵ_{scaled} differ by some magnitudes, both are given.

Moreover, we define the **Jacobian** J of the system at a solution u as

$$J(u) = \left(\frac{\partial p_{i,j}}{\partial u_{k,l}}\right)_{i=1,j=1,k=1,l=1}^{\hat{N}_x,\hat{N}_y,\hat{N}_x,\hat{N}_y}.$$

The **maximal eigenvalue** of $J(u)$ is denoted as m_e. A solution u of POP (3.6) is called **stable** if m_e is nonpositive.

4.2 Ordinary differential equation problems

Simple ordinary differential equation (ODE) problems can be solved by a direct SparsePOP approach. Namely, highly accurate solutions on high resolution grids of ODE problems in one unknown function (PSO PDE with $m = 1$) under Dirichlet conditions are obtained by applying SparsePOP with a low relaxation order $\omega \in \{1, 2\}$.

4.2.1 A problem in Yokota's text book

An example of those easy solvable ODE problems is given by

$$\begin{array}{rll} \ddot{u}(x) + \frac{1}{8}u(x)\dot{u}(x) - 4 - \frac{1}{4}x^3 & = 0 & \forall\, x \in [1, 3], \\ u(1) & = 17, & \\ u(3) & = \frac{43}{3}, & \\ 10 \leq u(x) & \leq 20 & \forall\, x \in [1, 3]. \end{array} \tag{4.1}$$

For details about problem (4.1) see [22]. Choosing relaxation order $\omega = 2$ and objective function F, given by

$$F(u) = \sum_{i=1}^{N_x} u_i,$$

we obtain the highly accurate, stable solution, that is documented in Table 1 and pictured in Figure 4.

N_x	ϵ_{feas}	ϵ_{scaled}	ϵ_{obj}	m_e	t_C
200	1e-4	2e-9	-4e-11	-3	104

Table 1: results for problem (4.1)

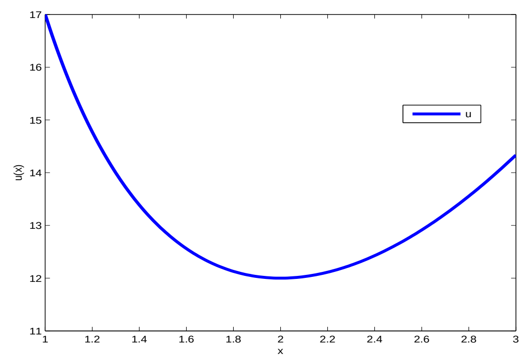

Figure 4: solution u for problem (4.1)

4.2.2 Mimura's problem

In the following we demonstrate the potential of our approach on a more difficult ODE example. An exciting and difficult ODE problem of two dependent functions is a problem by M. Mimura [13] which arises from the context of planktonic prey and predator models in biology. This problem is given below and is called **Mimura's problem**.

$$\begin{array}{ll} \frac{1}{20}\, u''(t) + \frac{1}{9}\left(35 + 16u(t) - u(t)^2\right)\, u(t) - u(t)\, v(t) & = 0, \\ 4\, v''(t) - \left(1 + \frac{2}{5}v(t)\right)\, v(t) + u(t)\, v(t) & = 0, \\ \dot{u}(0) = \dot{u}(5) = \dot{v}(0) = \dot{v}(5) = 0, & \\ 0 \leq u(t) \leq 14, & \\ 0 \leq v(t) \leq 14, & \\ \forall t \in [0, 5]\,. & \end{array} \tag{4.2}$$

In [13] the problem is analyzed, and the existence of continuous solutions is shown in [15]. This problem is obviously nonlinear in u and v, and various techniques introduced in Section 3 can be applied to it. Let N be the number of grid points in the interval [0, 5]. In order to construct a POP of the type (3.6), different **objective functions** are considered:

$$\begin{array}{l} F_1(u,v) = u_{\lceil \frac{N}{2} \rceil},\ F_2(u,v) = \sum_{i=1}^{N} u_i,\ F_3(u,v) = u_2, \\ F_4(u,v) = u_{N-1},\ F_5(u,v) = u_2 + u_{N-1}. \end{array} \tag{4.3}$$

At first, we apply SparsePOP with $\omega = 3$ and $N = 5$. In order to confirm the numerical results obtained for this coarse grid, we apply PHoM [7], which is a C++ implementation of the polyhedral homotopy continuation method for computing all isolated complex solutions of a polynomial system of equations, to the system of discretized PDEs. In that case the dimension n of the problem equals 6, as there are 2 unknown functions with 3 interior grid points each. PHoM finds 182 complex, 64 real and 11 nonnegative real solutions. Varying the upper and lower bounds for u_2 and u_4 and choosing one of the functions $F_1, \ldots, F_5$ as an objective function, all 11 solutions are detected by SparsePOP, as enlisted in Table 2.

The confirmation of our SparsePOP results by PHoM encourages us to solve Mimura's problem for a higher discretization. Relaxation order $\omega = 3$ is necessary to obtain an accurate solution in case $N = 7$ (Table 3, row 1). The upper bounds for u_2 and u_{N-1} are chosen to be 1. When we extended the grid size from 7 to 13, the solution obtained by SparsePOP got inaccurate, so that convergence of our algorithm was

u_2	u_3	u_4	v_2	v_3	v_4	obj	ubd_2	ubd_4	ϵ_{feas}
4.623	6.787	0.939	9.748	10.799	5.659	F_3	5	1.5	-2e-6
4.607	6.930	0.259	9.737	10.831	5.166	F_3	5	0.5	-3e-6
0.259	6.930	4.607	5.166	10.831	9.737	F_2	0.5	6	-5e-7
5.683	2.971	5.683	10.388	8.248	10.388	F_3	6	6	-1e-6
6.274	0.177	6.274	10.638	6.404	10.638	F_3	7	7	-7e-5
0.970	7.812	0.970	5.735	10.94	5.735	F_3	2	2	-2e-7
0.297	7.932	0.966	5.230	10.94	5.729	F_4	0.5	2	-1e-7
0.962	7.932	0.297	5.729	10.94	5.230	F_3	2	0.5	-2e-7
0.304	8.045	0.304	5.234	10.94	5.234	F_1	14	14	-5e-9
0.939	6.787	4.623	5.659	10.80	9.748	F_4	2	14	-1e-3
5.000	5.000	5.000	10.000	10.000	10.000	F_2	14	14	-2e-7

Table 2: SparsePOP solutions for (4.2) with discretization $N = 5$ grid points

strategy	N_N	N	solution	ϵ_{feas}	ϵ_{scaled}	m_e
init SPOP with F_2	10	7		-1e-8	-5e-9	-2.2
mGrid 3b	10	13		-1e+6	-2e+0	2.7
mGrid 3b	10	25		-6e-5	-2e-6	-0.9
mGrid 3b	10	49		-5e-11	-1e-12	0.1
mGrid 3b	10	97		-5e-10	-5e-12	0.2
mGrid 3b	10	193		-9e-2	-2e-4	0.3
mGrid 3b	10	385	2teeth	-1e-1	-5e-5	0.2
init SPOP with F_5	10	26		-3e+0	-1e-1	2.09
mGrid 3b	10	51		-8e-1	-5e-2	-0.18
mGrid 3b	10	101		-6e-12	-2e-15	-0.07
mGrid 3b	10	401	2,3peak	-1e-10	-6e-16	-0.07

Table 3: Results of grid-refining strategy 3b for solutions *2teeth* and *2,3peak*

lost. Also, if the initial SparsePOP is started with $\omega = 2$, or if Newton method is applied with another arbitrary starting point, or if we start for instance with $N = 5$ or $N = 9$, it is not possible to get an accurate solution. One possibility to overcome these difficulties is to start the grid-refining method with strategy 3b on a finer grid. We finally obtained a highly accurate stable solution *2teeth* when we started with $N = 7$ and the F_2 objective function, and a highly accurate stable solution *2,3peak* when we started with $N = 25$ and the F_5 objective function. See Table 3 and Figure 5. It seems reasonable to state that SparsePOP provides an appropriate initial guess for Newton' s method, which leads to accurate solutions for sufficiently high discretizations.

As the most powerful approach we apply the grid-refining method with strategy 3a/b, $\omega_1 = 3$ and $\omega_2 = 2$. We obtain the highly accurate stable solutions *3peak* and *4peak*, that are documented in Table 4 and pictured in Figure 6. As objective function for the iterated application of SparsePOP we choose the function F_M, which was introduced in (3.7).

4.3 Partial differential equation problems

4.3.1 Elliptic nonlinear PDE

For a PDE problem of two unknown functions in two variables, consider the following problem, where we distinguish two types of boundary conditions, Case I (Dirichlet condition) and Case II (Neumann condition).

$$\begin{array}{lll} u_{xx} + u_{yy} + u\ \left(1 - u^2 - v^2\right) & = 0, & \\ v_{xx} + v_{yy} + v\ \left(1 - u^2 - v^2\right) & = 0, & \forall\ (x, y) \in [0, 1]^2. \\ 0 \le u, v & \le 5, & \end{array} \tag{4.4}$$

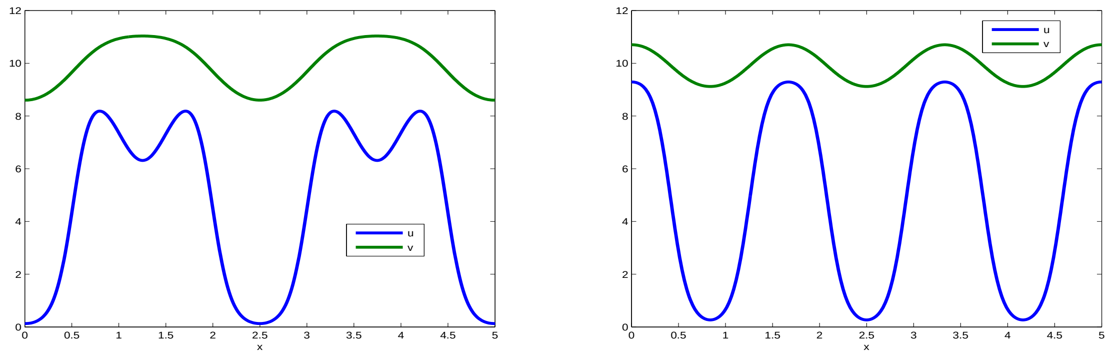

Figure 5: unstable solution *2teeth* (left) and stable solution *2,3peak* (right)

strategy	obj	N_N	N	solution	ϵ_{feas}	ϵ_{scaled}	m_e	t_C
init SPOP	F_5	10	26		-3e+1	-2e-1	2.09	203
mGrid 3a/b	F_M	10	51		-8e-1	-4e-2	-0.05	224
mGrid 3a/b	F_M	10	101		-3e-2	-4e-4	-0.02	383
mGrid 3a/b	F_M	10	201	4peak	-1e-8	-3e-11	-0.02	1082
init SPOP	F_1	10	26		-1e-1	-1e-3	-0.12	270
mGrid 3a/b	F_M	10	51		-1e-1	-4e-3	-0.08	348
mGrid 3a/b	F_M	10	101		-9e-12	-3e-16	-0.08	511
mGrid 3a/b	F_M	10	201	3peak	-5e-9	-2e-11	-0.07	1192

Table 4: Results for grid-refining strategy 3a/3b

$$
\begin{array}{llllll}
\text{Case I:} & & & & & \\
u(0,y) & = 0.5y + 0.3\sin(2\pi y), & u(1,y) & = 0.4 - 0.4y & \forall\, y \in [0,1], \\
u(x,0) & = 0.4x + 0.2\sin(2\pi x), & u(x,1) & = 0.5 - 0.5x & \forall\, x \in [0,1], \\
v(x,0) & = v(x,1) & = v(0,y) & = v(1,y) = 0 & \forall\, x \in [0,1] \\
 & & & & \forall\, y \in [0,1]. \\
\text{or} & & & & & \\
\text{Case II:} & & & & & \\
u_x(0,y) & = -1, & u_x(1,y) & = 1 & \forall\, y \in [0,1], \\
u_y(x,0) & = 2x, & u_y(x,1) & = x + 5\sin(\frac{\pi x}{2}) & \forall\, x \in [0,1], \\
v_x(0,y) & = 0, & v_x(1,y) & = 0 & \forall\, y \in [0,1], \\
v_y(x,0) & = -1, & v_y(x,1) & = 1 & \forall\, x \in [0,1].
\end{array}
$$

In both cases, we choose $F(u,v) = \sum_{i,j} u_{i,j}$ as an objective function.

Case I. SparsePOP is applied with the objective F and $\omega = 2$ to problem (4.4) under Dirichlet condition on a 9×9-grid. A highly accurate stable solution is found, which can be extended via grid-refining strategy 3b to a 65×65-grid. The numerical results are given in Table 5; the solution u is non-constant and pictured in Figure 7, and the solution v is zero on the entire domain.

boundary	strategy	N_N	N_x	N_y	ϵ_{feas}	m_e	t_C
I	init SparsePOP	5	9	9	-9e-9	-19	125
I	mGrid 3b	5	65	65	-1e-12	-19	12280

Table 5: Results for problem (4.4) in Case I, grid-refining strategy 3b

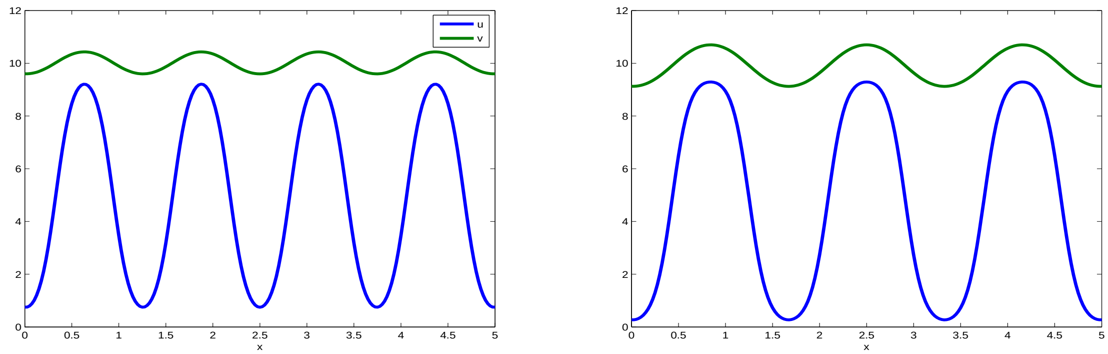

Figure 6: Stable solutions for grid-refining strategy 3a/b

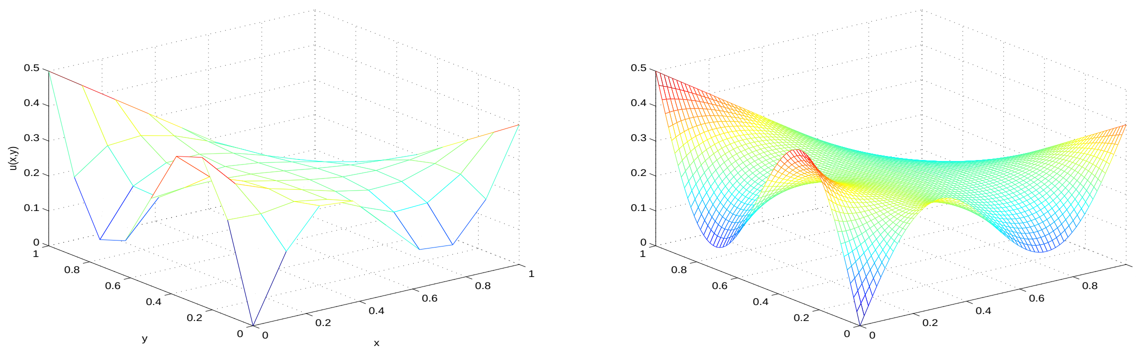

Figure 7: Stable solution u for problem (4.4) in Case I

Case II. SparsePOP is applied with the objective F and $\omega = 2$ to problem (4.4) under Neumann condition on a 6×6-grid. We obtain a non-constant stable solution for u and v, which we extend to a 41×41-grid via grid-refining strategy 3b. For the results see Table 6 and Figure 8.

boundary	strategy	N_N	N_x	N_y	ϵ_{feas}	m_e
II	init SparsePOP	5	6	6	-2e-14	-3
II	mGrid 3b	5	41	41	-4e-12	-3

Table 6: Results for problem (4.4) in Case II, grid-refining strategy 3b

4.3.2 Elliptic - Bifurcation

Consider another nonlinear elliptic PDE problem,

$$\begin{aligned} u_{xx}(x,y) + u_{yy}(x,y) + \lambda u(x,y)\ \left(1 - u(x,y)^2\right) &= 0 \quad \forall\,(x,y) \in [0,1]^2, \\ u(x,y) &= 0 \quad \forall\,(x,y) \in \partial[0,1]^2, \\ 0 \le u(x,y) &\le 1 \quad \forall\,(x,y) \in [0,1]^2, \end{aligned} \tag{4.5}$$

with parameter $\lambda > 0$. It is shown in [16], there exists a unique nontrivial solution for this problem if $\lambda > \lambda_0 = 2\pi^2 \approx 19.7392$, and there exists only the trivial zero solution if $\lambda \le \lambda_0$, where λ_0 is characterized as the smallest eigenvalue of the Laplacian Δ. At first we demonstrate the power of the grid-refining method for the case $\lambda = 22$. Beyond that, we apply a bisection algorithm to approximate λ_0.

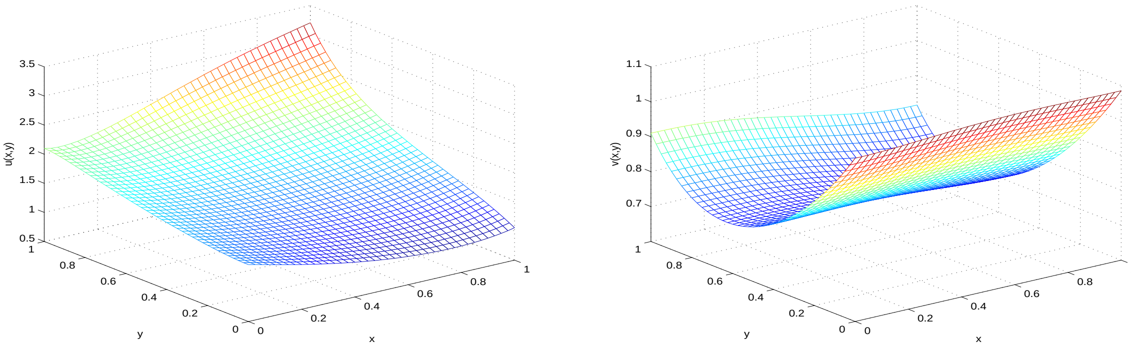

Figure 8: Solutions u (left) and v (right) for problem (4.4) in Case II

We take the objective function as $F(u) = \sum_{i,j} u_{i,j}$ and choose $\omega = 2$ and $N_x = N_y = 6$ for the initial SparsePOP and obtain a highly accurate stable solution on a 41×41-grid. The results are documented in Table 7 and pictured in Figure 9.

N_x	6	11	11	21	21	41	41
N_y	6	6	11	11	21	21	41
ϵ_{feas}	-6.4e-10	-6.2e-11	-1.2e-10	-8.3e-8	-8.9e-8	-3.7e-10	-3.8e-10
m_e	-5.61	-5.18	-4.74	-4.63	-4.51	-4.48	-4.46

Table 7: grid-refining strategy 3b for problem (4.5) in case $\lambda = 22$

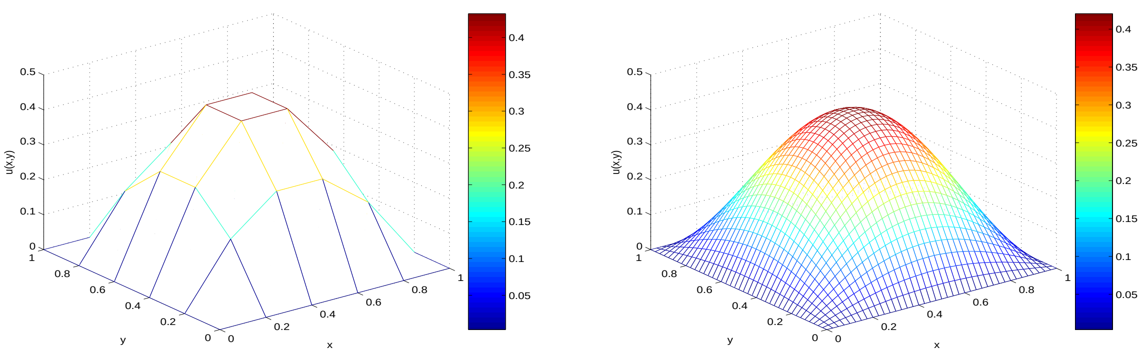

Figure 9: Solution for (4.5) if $\lambda = 22$, $(N_x, N_y) = (6, 6)$ and $(N_x, N_y) = (41, 41)$

To examine the uniqueness of the positive solution, we impose additional constraints

$$\begin{array}{ll} \mid u_x(x,y) \mid & \leq M \\ \mid u_y(x,y) \mid & \leq M \end{array} \qquad \forall\ (x,y) \in [0,1]^2. \tag{4.6}$$

We apply SparsePOP with $\omega = 2$ to problem (4.5) under (4.6) and $\lambda = 22$ on a 6×6-grid. For $M > 0.8$ we obtain a positive solution, as the one in the second column of Table 7. If we decrease M sufficiently, we obtain the zero solution. Hence, it seems there exists exactly one positive non-trivial solution to problem (4.5).

Next, we exploit a well known result for problem (4.5). As already shown in [3] a function $u: \ [0,1]^2 \rightarrow \mathbb{R}$

that is a minimizer of the optimization problem

$$
\begin{array}{lll}
\min_{u:\,[0,1]^2 \to \mathbb{R}} & \int_{[0,1]^2} u_x^2 + u_y^2 - 2\lambda \, \left(\frac{u^2}{2} - \frac{u^4}{4}\right) \, dx\, dy & \\
\text{s.t.} & u = 0 & \text{on } \partial[0,1]^2, \\
& 0 \leq u \leq 1 & \text{on } [0,1]^2.
\end{array}
\tag{4.7}
$$

is a solution to problem (4.5). The integral to be minimized in this problem is called the **energy integral**. In analogy to the discretization procedure for a polynomial second order PDE problem, problem (4.7) can be transformed into a polynomial optimization problem in case the partial derivatives are approximated by standard finite difference expressions:

$$
\begin{array}{lll}
\min & \sum_{i,j} \left[\left(\frac{\Delta u_{i,j}}{\Delta x}\right)^2 + \left(\frac{\Delta u_{i,j}}{\Delta y}\right)^2 - 2\lambda \left(\frac{u_{i,j}^2}{2} - \frac{u_{i,j}^4}{4}\right)\right] \, \Delta x \, \Delta y & \\
\text{s.t.} & 0 \leq u_{i,j} \leq 1, \quad \forall i \in \{1,\ldots,N_x\}, \, j \in \{1,\ldots,N_y\}, & \\
& u_{1,j} = u_{N_x,j} = 0 & \forall j \in \{1,\ldots,N_y\}, \\
& u_{i,1} = u_{i,N_y} = 0 & \forall i \in \{1,\ldots,N_x\}.
\end{array}
\tag{4.8}
$$

In opposite to the polynomial optimization problems that we derive from the class of polynomial second order PDE, the objective function of polynomial optimization problem (4.8) is not of free choice but canonically given by the discretization of the objective function in problem (4.7). We apply SparsePOP with relaxation order $\omega = 2$ to problem (4.5) and problem (4.7) on a 6×6- and a 10×10- grid and obtain an identical solution for both problems. These results are given in Table 8, where Δu, given by

$$\Delta u = \max_{i,j} \mid \tilde{u}_{i,j} - \hat{u}_{i,j} \mid,$$

evaluates the deviation of the SparsePOP solutions of both problems. $\tilde{u}_{i,j}$ denotes the SparsePOP solution to problem (4.5) and $\hat{u}_{i,j}$ the solution to problem (4.7).

Problem	N_x	N_y	t_C	ϵ_{obj}	ϵ_{feas}	Δu
(4.5)	6	6	5.4	2e-14	-3e-13	2e-6
(4.7)	6	6	2.1	1e-10	-	2e-6
(4.5)	10	10	131	4e-15	-4e-13	9e-7
(4.7)	10	10	98	2e-10	-	9e-7

Table 8: Computational results for problems (4.5) and (4.7)

The solutions to both problems are highly accurate and we note that the total computation time to minimize the energy integral is less than the time required to solve the polynomial optimization problem corresponding to (4.5).

Finally, we approximate the bifurcation point λ_0. Since a nontrivial solution is obtained for $\lambda = 20$ and the zero solution for $\lambda = 18$, we apply the bifurcation algorithm BISEC, which is given by

BISEC

initialize $\quad \lambda_l = \lambda_l^0, \ \lambda_u = \lambda_u^0$

repeat

$\quad \hat{\lambda} = \frac{1}{2}(\lambda_l + \lambda_u)$

$\quad$ if F $\left(u(\hat{\lambda})\right) > \epsilon_1$

$\quad\quad \lambda_u = \hat{\lambda}$

$\quad$ else

$\quad\quad \lambda_l = \hat{\lambda}$

until $\lambda_u - \lambda_l < \epsilon_2$,

with $\lambda_l^0 = 18$, $\lambda_u^0 = 20$ and $\epsilon_1 = \epsilon_2 =$ 1e-10. BISEC determines $\hat{\lambda}(N_x, N_y)$ to approximate λ_0, as reported in Table 9. The accuracy of $\hat{\lambda}(N_x, N_y)$ to approximate $\lambda_0 = 2\pi^2 \approx 19.7392$ increases in (N_x, N_y).

$N = N_x = N_y$	5	6	7	8	9	11	13
$\hat{\lambda}$	18.731	19.090	19.285	19.398	19.474	19.553	19.601

Table 9: Approximation $\hat{\lambda}$ of $\lambda_0 \approx 19.7392$ for different (N_x, N_y)

4.3.3 Hyperbolic - Nonlinear Wave equation

As an example of a hyperbolic PDE we study time periodic solutions of the **nonlinear wave equation**

$$\begin{array}{ll} -u_{xx} + u_{yy} + u\,(1-u) + 0.2\sin(2x) = 0 & \\ & \forall\ (x,y) \in [0,\pi] \times [0,2\pi], \\ u(0,y) = u(\pi,y) = 0 & \forall\ y \in [0,2\pi], \\ u(x,0) = u(x,2\pi) & \forall\ x \in [0,\pi], \\ -3 \leq u(x,y) \leq 3 & \forall\ (x,y) \in [0,\pi] \times [0,2\pi]. \end{array} \tag{4.9}$$

As far as we have checked on the mathsci data base, there is no mathematical proof of the existence of periodic solution of this system. However, our solver finds some periodic solutions. We observed the POP corresponding to problem (4.9) has various solutions. Therefore, the choice of the objective determines the solution found by the sparse SDP relaxation. We choose one of the functions

$$F_1(u) = \sum_{i,j} \sigma_{i,j} u_{i,j}, \qquad\qquad F_2(u) = \sum_{i,j} u_{i,j},$$

as objective, where $\sigma_{i,j}$ $(i = 1,\ldots,N_x,\ j = 1,\ldots,N_y)$ are random variables that are uniformly distributed on $[-0.5, 0.5]$. The results are enlisted in Table 10 and pictured in Figures 10 and 11.

strategy	ω	N_N	N_x	N_y	ϵ_{feas}	t_C	m_e
initial SPOP, obj. F_1	2	5	5	6	-3e-9	151	7
grid-refining 3b		5	33	40	-1e-6	427	415
initial SPOP, obj F_2	2	5	5	5	-5e-10	19	3
grid-refining 3b		5	33	33	-4e-9	86	411

Table 10: Results for nonlinear wave equation (4.9)

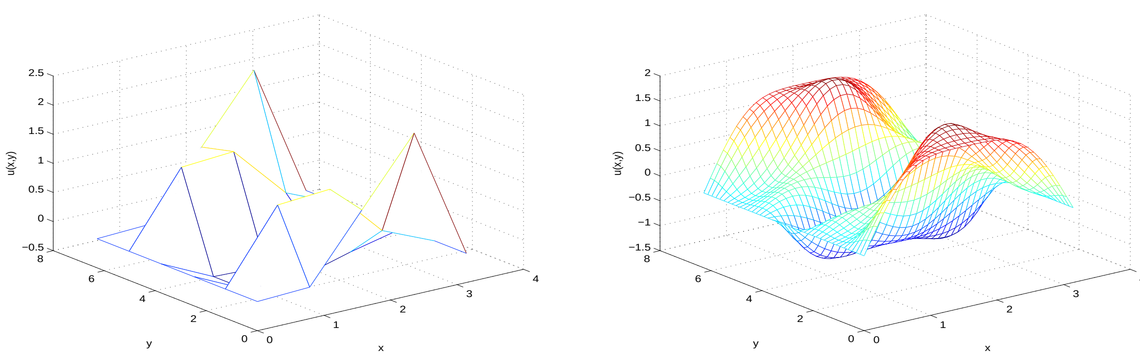

Figure 10: Solution for nonlinear wave equation (4.9), objective F_1

Variation bounds: As an extension of problem (4.9), we demonstrate the impact of additional polynomial inequality constraints in POP (3.6). We impose variation bounds w.r.t. $y-$direction, i.e.,

$$|\ u_y(x,y)\ | \leq 0.5 \quad \forall\ (x,y) \in (0,\pi) \times (0,2\pi). \tag{4.10}$$

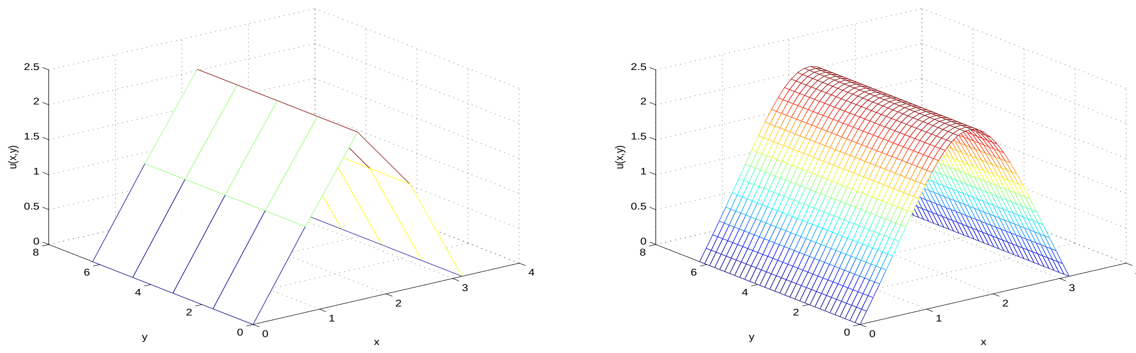

Figure 11: Solution for nonlinear wave equation (4.9), objective F_2

If SparsePOP is applied to (4.9) with additional condition (4.10) and objective function F_1, another solution of the PDE problem is obtained, which is documented in Table 11 and pictured in Figure 12. Thus several solutions of problem (4.9) are selected by changing the objective function of POP (3.6) and by enabling additional polynomial inequality constraints.

strategy	ω	N_N	N_x	N_y	ϵ_{feas}	t_C	m_e
initial SPOP, obj. F_1	2	5	5	6	-1e-14	437	7
grid-refining 3b		5	17	21	-7e-13	1710	104

Table 11: Results for nonlinear wave equation (4.9) under (4.10)

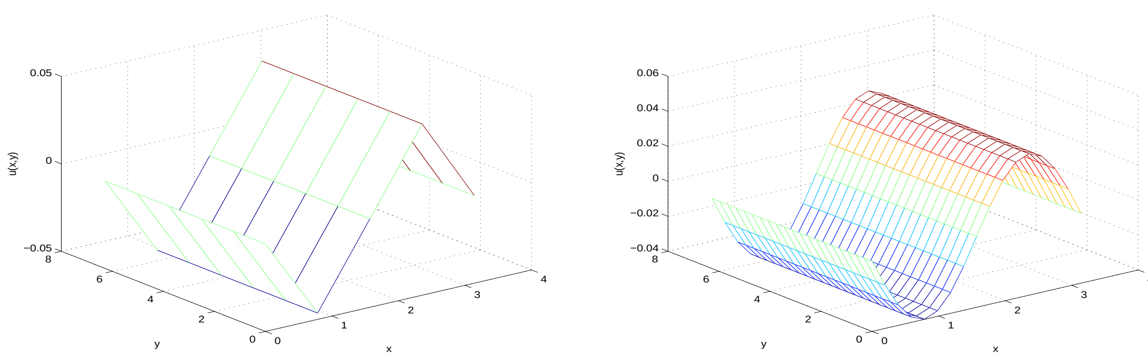

Figure 12: Solution for nonlinear wave equation (4.9) under (4.10), objective F_1

4.3.4 Parabolic - Diffusion

Consider a nonlinear parabolic PDE problem of two dependent scalar functions

$$\begin{array}{rll}
\frac{1}{50}u_{xx} - u_y + 1 + u^2\, v - 4u & = 0 & \forall x \in [0,1],\ y \geq 0, \\
\frac{1}{50}v_{xx} - v_y + 3u - u^2\, v & = 0 & \forall x \in [0,1],\ y \geq 0, \\
u(0,y) = u(1,y) & = 1 & \forall\, y \geq 0, \\
v(0,y) = v(1,y) & = 3 & \forall\, y \geq 0, \\
u(x,0) & = 1 + \sin(2\pi x) & \forall\, x \in [0,1], \\
v(x,0) & = 3 & \forall\, x \in [0,1].
\end{array} \tag{4.11}$$

In order to discretize the problem (4.11), y has to be cut at $y = T$. Since problem (4.11) is parabolic we know by [18], the solutions $((u_{i,j}, v_{i,j})(N_x, N_y))_{i,j}$ of the discretized problems converge to solutions (u, v) of (4.11). We apply the grid-refining method with strategy 3b, where objective F is given by $F(u, v) = \sum_{i,j} u_{i,j}$ and $\omega = 3$. Furthermore, lbd $\equiv 0$ and ubd $\equiv 5$ are chosen as bounds for u and v. Following this strategy we obtain highly accurate stable solutions on a 33×65-grid; see Table 12 and Figure 13.

strategy	N_x	N_y	m_e	ϵ_{feas}	ϵ_{abs}
init SparsePOP	5	9	-4.12	-7e-10	-2e-10
grid-refining 3b	33	65	-2.88	-3e-9	-5e-11

Table 12: Results for diffusion problem (4.11)

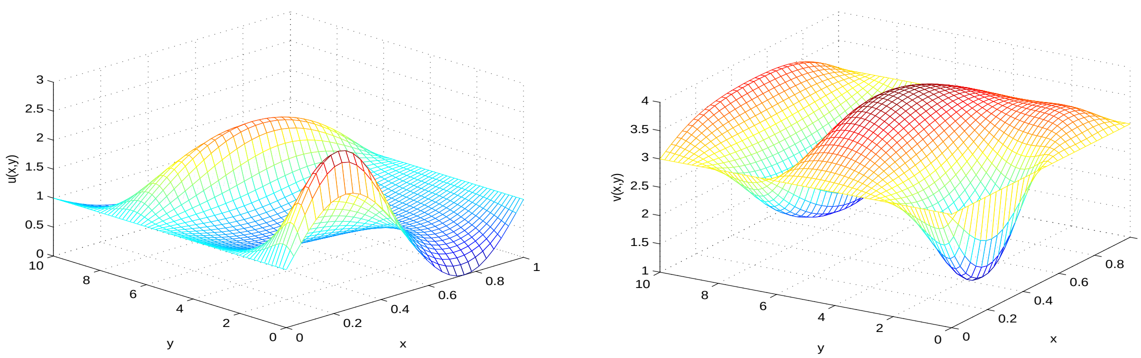

Figure 13: Solutions u (left) and v (right) for diffusion problem (4.11)

4.3.5 First order PDEs

An optimization based approach to attempt first order PDE was proposed recently by Guermond and Popov [5, 6]. In [5] the following example of an first order PDE with a discontinuous solution is solved on a $40 \times 40-$grid:

$$\begin{array}{lll} u_x(x, y) & = 0 & \forall\, (x, y) \in [0,\, 2] \times [0.2,\, 0.8], \\ u(0, y) & = 1 & \text{if } y \in [0.5,\, 0.8], \\ u(0, y) & = 0 & \text{if } y \in [0.2,\, 0.5[. \end{array} \tag{4.12}$$

Applying our approach with an forward or central difference approximation for the first derivative in (4.12) we detect the discontinuous solution

$$u(x, y) = \begin{cases} 1 \text{ if } y \geq 0.5 \\ 0 \text{ otherwise} \end{cases}$$

on a 40×40-grid.

A more difficult first order PDE problem is given by

$$\begin{array}{lll} u_x(x, y) + u(x, y) - 1 & = 0 & \forall\, (x, y) \in [0,\, 1]^2, \\ u(0, y) = u(1, y) & = 0 & \forall\, y \in [0,\, 1], \\ 0 \leq u(x, y) & \leq 1 & \forall\, (x, y) \in [0,\, 1]^2. \end{array} \tag{4.13}$$

As can be seen easily and was pointed out in [6], problem (4.13) is not well-posed since the outflow boundary condition is over-specified. Problem (4.13) is discussed in detail in [6] and the authors obtained an accurate approximation to the exact solution by L^1 approximation on a 10×10-grid. Applying our approach with relaxation order $\omega = 1$ and objective function $F(u) = \sum_{i,j} u_{i,j}$ on a 10×10 grid, we succeed in finding this solution in case we choose a forward difference approximation for the first derivative. In case of choosing central or backwards difference scheme the dual problem in the resulting SDP relaxation becomes infeasibe. Furthermore, by applying SparsePOP we are able to obtain a highly accurate solution to (4.13) on a 50×50-grid, as documented in Table 13 and pictured in Figure 14.

N_x	N_y	ϵ_{feas}	t_C
10	10	-4e-16	8
50	50	-3e-15	224

Table 13: Results for problem (4.13)

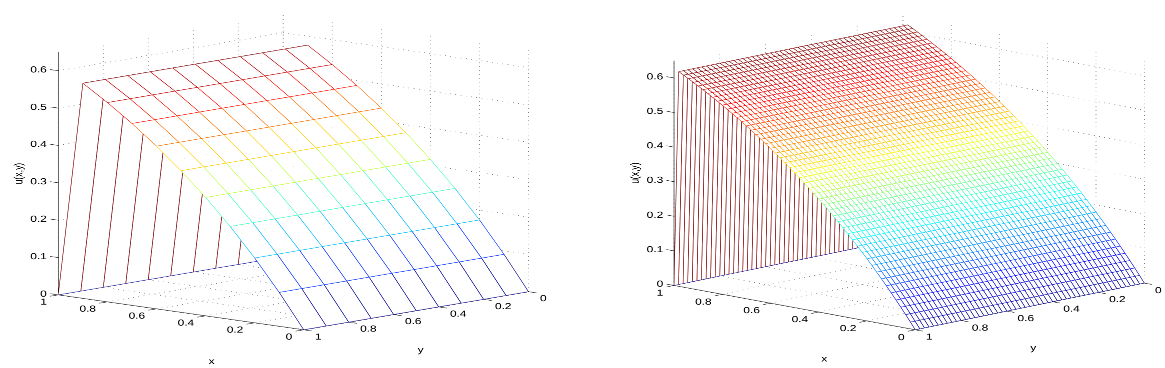

Figure 14: Solution u for problem (4.13)

4.4 Differential algebraic equation problem

The class of PSO PDE problems (3.1) includes the case of $m \geq 2$ and $n = 1$ with $a = b = c = e = 0$, $d = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $f = \begin{pmatrix} -f_1(x, u_1(x), u_2(x)) \\ f_2(x, u_1(x), u_2(x)) \end{pmatrix}$. Such a problem is called a **differential algebraic equation (DAE)**. It is an equation, where the derivatives of several unknown functions, in this case u_2, are not involved explicitly. As we will see in the following example, we are able to solve such problems with our approach.

Consider the DAE problem

$$\begin{aligned} \dot{u}_1(x) &= u_3(x), \\ 0 &= u_2(x)\,(1 - u_2(x))\,, \\ 0 &= u_1(x)\,u_2(x) + u_3(x)\,(1 - u_2(x)) - x, \\ u_1(0) &= u_0. \end{aligned} \qquad \forall\, x \in [0, T] \tag{4.14}$$

It is easy to see that two closed-form solutions u^1 and u^2 are given by

$$\begin{aligned} u^1(x) &= \left(u_0 + \tfrac{x^2}{2},\, 0,\, x\right)^T & x \in [0, T], \\ u^2(x) &= (x,\, 1,\, 1)^T & x \in [0, T]. \end{aligned}$$

To apply SparsePOP, we choose the bounds lbd $\equiv 0$ and ubd $\equiv 10$ for each function u_1, u_2 and u_3. We define as objective functions F_1 and F_2,

$$F_1(u) = \sum_{i=1}^{N_x} u_{1i}, \qquad F_2(u) = \sum_{i=1}^{N_x} u_{2i}.$$

First we choose $u_0 = 0$ and apply SparsePOP with F_2 as an objective function, and we obtain the highly accurate approximation of u^2, which is documented in Table 14 and Figure 15.

objective	ω	T	N_x	u_0	ϵ_{obj}	ϵ_{feas}	ϵ_{scaled}	t_C
F_2	2	2	100	0	4e-10	-7e-10	-4e-10	29
F_2	2	2	200	0	3e-9	-5e-9	-3e-9	122
F_1	2	2	200	1	8e-9	-5e-6	-2e-6	98
F_1	2	2	200	2	3e-10	-8e-8	-4e-8	107
F_1	2	2	10	0.5	3e-10	-5e-7	-3e-7	4
F_1	2	2	20	0.5	3e-10	-2e-5	-9e-6	9
F_1	2	2	30	0.5	8e-10	-6e-3	-3e-3	15
F_1	2	2	40	0.5	7e-8	-2e-1	-1e-1	24
F_1	3	2	30	0.5	9e-9	-4e-3	-2e-3	51
F_1	4	2	30	0.5	8e-9	-1e-3	-6e-4	210

Table 14: Results for DAE problem (4.14)

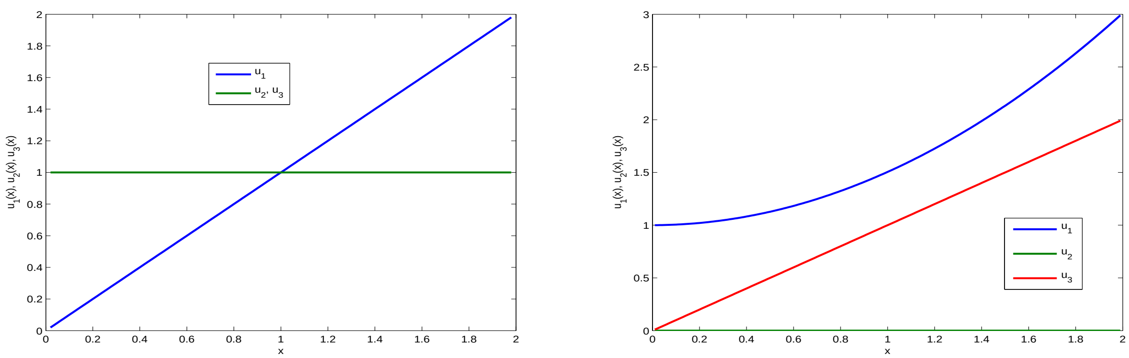

Figure 15: Solutions u^2 (left) and u^1 (right) of DAE problem (4.14)

Next the objective function is chosen to be F_1. For $u_0 \in \{1,\ 2\}$ highly accurate approximations of u^1 are obtained. An interesting phenomenon is observed in case u_0 is small. For instance, if we choose $u_0 = 0.5$ and $\omega = 2$, we get a highly accurate solution for $N_x = 10$. But, as we increase N_x stepwise to 40, the accuracy decreases, although the relaxation order remains constant. For numerical details see Table 14. This effect can be slightly compensated by increasing relaxation order ω, as demonstrated for the case $N_x = 30$. But due to the limited capacity of current SDP solvers it is not possible to increase ω until a high accuracy is reached.

4.5 Optimal Control problems

We can further apply the sparse SDP relaxation for PDE problems to certain optimal control problems. As an example, we consider a problem arising from the **control of reproductive strategies of social insects**.

$$\begin{array}{ll} \max\limits_{\alpha(\cdot)} & P(w(\cdot), q(\cdot), \alpha(\cdot)) = q(T) \\ \text{s.t.} & \dot{w}(t) = -\mu w(t) + b\, s(t)\alpha(t)\, w(t) \quad \forall\, t \in [0, T], \\ & w(0) = w^0, \\ & \dot{q}(t) = -\nu q(t) + c(1-\alpha(t))s(t)w(t) \quad \forall\, t \in [0, T], \\ & q(0) = q^0, \\ & 0 \le \alpha(t) \le 1 \quad \forall\, t \in [0, T], \end{array} \tag{4.15}$$

where $w(t)$ is the number of workers at time t, $q(t)$ the number of queens, $\alpha(t)$ the **control variable**, which denotes the fraction of the colony effort devoted to increasing work force, μ the workers death rate,

ν the queens death rate, $s(t)$ a known rate at which each worker contributes to the bee-economy, b and c constants.

The ordinary differential equation constraints are discretized as discussed in Section 3. In contrast to the previous examples the objective function F of the constructed POP is not of free choice anymore. Instead it is determined by the objective function $P(w(\cdot), q(\cdot), \alpha(\cdot)) = q(T)$ of the optimal control problem (4.15) as

$$F(w, q, \alpha) = q_{N_t}.$$

It follows from Pontryagin Maximum Principle [12] that the optimal control law α of problem (4.15) is a bang-bang control law for any rate $s(t)$, i.e., $\alpha(t) \in \{0, 1\}$ for all $t \in [0, 1]$. Table 15 and Figure 16 show the results on the application of SparsePOP to the discretized optimal control problem.

T	μ	b	w^0	ν	c	q^0	$s(t)$	ω	N_t	ϵ_{obj}	ϵ_{feas}	ϵ_{scaled}
3	0.8	1	10	0.3	1	1	1	2	300	2e-7	-1e-4	-2e-6
3	0.8	1	10	0.3	1	1	$\frac{1}{2}(\sin t + 1)$	2	300	1e-4	-2e-2	-4e-5

Table 15: Control of social insects (4.15) for two different rates $s(t)$

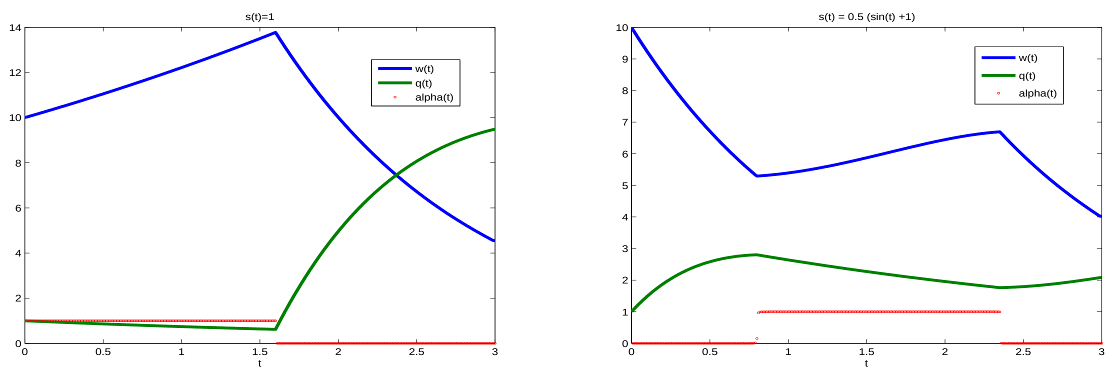

Figure 16: Control of social insects (4.15) for $s(t) = 1$ and $s(t) = 0.5(\sin(t) + 1)$

In the case of $s(t) = 1$, it is sufficient to choose $w(t)$, $q(t) \leq 20$ as upper bounds to get accurate results. For the more difficult problem with $s(t) = 0.5(\sin(t) + 1)$, it is necessary to tighten the upper bounds to $w(t) \leq 10$ and $q(t) \leq 3$, in order to obtain fairly accurate results. In both cases the bang-bang control law is obtained clearly.

5 Conclusion

Examining a class of polynomial second order partial differential equations (PSO PDE) in two variables, we were able to transform a PSO PDE problem into a sparse polynomial optimization problem (POP). The description is based on the discretization of a PDE problem, the approximation of its partial derivatives by finite differences and the choice of an appropriate objective function. Correlative sparsity was encountered and examined in POPs derived from PSO PDE problems, which enabled us to apply the sparse SDP relaxation [20] efficiently. Some additional techniques were introduced to obtain highly accurate solutions of sparse POPs derived from discretized PDE problems and effectively employed. Among others, we presented a grid-refining technique which applies the sparse SDP relaxation [20] on a coarse grid and extended the coarse grid solution by alternating interpolation and Newton's method to high resolution grids. This technique was shown to be very effective in solving PDE problems with a few unknown functions under Dirichlet, Neumann and periodic boundary conditions. As we have seen in case of Mimura' s problem (4.2) and the optimal control problem (4.15), it may be necessary to impose additional constraints on upper and lower bounds of the unknown functions to increase the solution's accuracy. Furthermore, it was demonstrated how to choose an objective function in (3.6), lower, upper and variation bounds on the unknown function, in order to detect particular solutions of a discretized PDE problem. In other words, one of the advantages of using the sparse SDP relaxation instead of several existing methods is that a function space to find solutions may be translated into natural constraints for a sparse SDP problem. In case we have certain information about a particular solution we want to find, this information is exploited by finding an appropriate initial guess for Newton's method by the sparse SDP relaxation. And even in case we have no information about the structure of a PDE's solution, applying the sparse SDP relaxation yields a reasonable initial solution for Newton's method. The possibility to attempt a broad class of PDE, including elliptic, parabolic and hyperbolic PDE, is another advantage of our approach. As we could transform a differential algebraic equation and an optimal control problem into a POP, we expect to be able to exploit this technique for other classes of problems.

Despite succeeding in many PSO PDE problems, we are facing several drawbacks. In the present state of the art, choices of objective functions are heuristic except the case of finding the global minimizer if a given equation is an Euler-Lagrange equation as we have seen in the example in 4.3.2. In this example in 4.3.2 the objective function is chosen canonically as a discretization of the energy integral. However this objective function finds only the stable solution standing for the global minimizer of the energy integral. As we have seen in the case of Mimura's problem in 4.2.2, suitable choices of objective functions yield unstable solutions, which are also interesting in order to understand a dynamical system. To take the sum or a sum with random coefficients of all unknown variables $u_{i,j}$ as the objective function of POP (3.6) turned out to be a good choice in order to find accurate solutions, but it is still an open question which objective function to choose for a POP derived from a particular PSO PDE. Furthermore, although we were able to solve some PDE problems with minimal relaxation order $\omega = \omega_{\max}$ in many cases, it is a priori not possible to predict the relaxation order ω which is necessary to attain an accurate solution. As the size of the sparse SDP relaxation increases polynomially in ω, the tractability of the SDP is limited by the capacity of current SDP solvers. Moreover, we observed the relaxation order ω to obtain an accurate solution for a PDE problem is sometimes increasing in the discretization grid size $(N_x,\, N_y)$. Defining the class of PSO PDEs, we restricted ourselves to second order PDEs of unknown functions in at most two independent variables. In theory, it is possible to apply the SDP relaxation method proposed in this paper to PDE problems of higher degree and in more independent variables as long as the derivatives' coefficients are polynomial in the unknown functions. But in such cases the necessary relaxation order ω can be too large and/or the resulting SDP relaxation problems can be too large to solve in practice. Nevertheless, we have succeeded in determining highly accurate solutions for some PSO PDE problems, a differential algebraic equation and an optimal control problem. It remains our aim to develop a numerical efficient solver for a class of PDE that is as general as possible. Applying a sequence of sparse SDP relaxations as presented in this paper may be seen as the first step to reach this aim.

References

[1] J.R.S. Blair, and B. Peyton, *An introduction to chordal graphs and clique trees*, Graph Theory and Sparse Matrix Computation, Springer Verlag (1993), pp. 1-29

[2] W.L. Briggs, V.E. Henson, and S.F. McCormick, *A Multigrid Tutorial*, SIAM (2000)

[3] R. Courant and D. Hilbert, *Methoden der Mathematischen Physik*, Vol 1 (1931), Chapter 4, *The method of variation*

[4] A. George, and J.W. Liu, *Computer Solution of Large Sparse Positive Definite Systems*, Prentice-Hall (1981).

[5] J.L. Guermond, *A finite element technique for solving first-order PDEs in L^P*, SIAM Journal Numerical Analysis, 42 (2004), No. 2, pp. 714-737

[6] J.L. Guermond, and B. Popov, *Linear advection with ill-posed boundary conditions via L^1-minimization*, International Journal of Numerical Analysis and Modeling, Vol. 4 (2007), No. 1, pp. 39-47

[7] T. Gunji, S. Kim, M. Kojima, A. Takeda, K. Fujisawa, and T. Mizutani, *PHoM - a Polyhedral Homotopy Continuation Method for Polynomial Systems*, Research Reports on Mathematical and Computing Sciences, Dept. of Math. and Comp. Sciences, Tokyo Inst. of Tech., B-386 (2003).

[8] S. Kim, M. Kojima, and H. Waki, *Generalized Lagrangian duals and sums of squares relaxations of sparse polynomial optimization problems*, SIAM Journal on Optimization, 15 (2005), pp. 697-719

[9] M. Kojima, S. Kim, and H. Waki, *Sparsity in sums of squares of polynomials*, Mathematical Programming, 103 (2005), pp. 45-62.

[10] J.B. Lasserre, *Global optimization with polynomials and the problem of moments*, SIAM Journal on Optimization, 11 (2001), pp. 796-817.

[11] J.B. Lasserre, *Convergent SDP-Relaxations in Polynomial Optimization with Sparsity*, SIAM Journal on Optimization, 17 (2006), No. 3, pp. 822-843.

[12] J. Macki, and A. Strauss, *Introduction to Optimal Control Theory*, Springer-Verlag (1982), pp. 108.

[13] M. Mimura, *Asymptotic Behaviors of a Parabolic System Related to a Planktonic Prey and Predator Model*, SIAM Journal on Applied Mathematics, 37 (1979), no. 3, pp. 499-512.

[14] J. Nocedal, and S.J. Wright, *Numerical Optimization*, Springer Series in Operations Research, (2006), pp. 270.

[15] J. Rauch, and J. Smoller, *Qualitative theory of the FitzHugh-Nagumo equations*, Advances in Mathematics, 27 (1978), pp. 12-44.

[16] J. Smoller, *Shock Waves and Reaction-Diffusion Equations*, Springer-Verlag (1983), pp. 106.

[17] SparsePOP HomePage, http://www.is.titech.ac.jp/∼kojima/SparsePOP.

[18] M. Tabata, *A finite difference approach to the number of peaks of solutions for semilinear parabolic problems*, J. Math. Soc. Japan, 32 (1980), pp. 171-192.

[19] U. Trottenberg, C.W. Oostelee, and A. Schüller, *Multigrid*, Academic Press, London (2001)

[20] H. Waki, S. Kim, M. Kojima, and M. Muramatsu, *Sums of Squares and Semidefinite Program Relaxations for Polynomial Optimization Problems with structured sparsity*, SIAM Journal on Optimization, 17 (2006), pp. 218-242.

[21] H. Waki, S. Kim, M. Kojima, and M. Muramatsu, *SparsePOP: a Sparse Semidefinite Programming Relaxation of Polynomial Optimization Problems*, Research Reports on Mathematical and Computing Sciences, Dept. of Math. and Comp. Sciences, Tokyo Inst. of Tech., B-414 (2005).

[22] Yokota, http://next1.cc.it-hiroshima.ac.jp/MULTIMEDIA/numeanal2/node24.html