Decomposition and approximation for PDE-constrained mixed-integer optimal control

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Abstract. Using partial outer convexification, we can reformulate MINLPs constrained by ODEs or PDEs such that all integer control variables are binaries. We can obtain the canonical continuous relaxation of such problems by replacing the binary control variables with $[0, 1]$-valued ones. The relaxation is generally easier to solve. The two-step approach of computing a relaxed solution and approximating it using binary controls afterwards is called Combinatorial Integral Approximation (CIA) decomposition. We survey recent developments concerning this methodology.

There are several well-behaved algorithmic approaches that approximate the relaxed controls with binary ones. For these algorithms, driving the mesh size of the rounding mesh to zero induces convergence of the binary control with the relaxed one in the weak-$*$ topology of L^∞. Such approximation results for one-dimensional domains transfer to multi-dimensional ones under a mild condition on the rounding mesh refinement. If the solution operator of the state equation exhibits sufficient regularity, i.e. compactness properties, the state vector corresponding to the rounded binary control converges in norm to the state vector of the relaxed problem. Variations of these algorithms allow additional pointwise constraints that involve the discrete controls without sacrificing these convergence properties.

As a test case, we present a multi-dimensional model problem that compares two recently investigated algorithmic approaches, which are transferred to the multi-dimensional setting using iterates of the Sierpinski curve.

Mathematics Subject Classification (2000). Primary 90C11; Secondary 49M20, 65K10.

Keywords. Mixed-integer optimal control, Approximation theory.

This work was completed with the support of DFG Priority Programme 1962.

1. Introduction

We consider *partial outer convexification* reformulations, see [21, 22], of optimal control problems with mixed control inputs, i.e. control problems of the form

$$\begin{aligned}
\min_{y,\omega}\ & J(y) \\
\text{s.t.}\quad & Ay = \sum_{i=1}^{M} \omega_i f_i(y), \\
& 0 \le \omega_i(s) c_i(y(s)) && \text{for a.a. } s \in \Omega_T, i \in \{1,\dots,M\}, \\
& \omega(s) \in \{0,1\}^M && \text{for a.a. } s \in \Omega_T, \\
& \sum_{i=1}^{M} \omega_i(s) = 1 && \text{for a.a. } s \in \Omega_T.
\end{aligned} \tag{BC}$$

Here, the quantity M denotes the number of different control realizations (or right-hand sides in the differential equation context), y denotes the state variable and ω the binary control input of the problem. $Ay = \sum_{i=1}^{M} \omega_i f_i(y)$ is the state equation of the optimized process. We assume that it is defined on a bounded domain or space-time cylinder Ω_T, A is a suitable differential operator and the f_i are suitable non-linearities. The functions c_i are pointwise a.e. defined constraint functions. The function $\omega : \Omega_T \to \{0,1\}^M$ activates the different right-hand sides $f_1, \dots, f_M$ of the state equation, i.e., $\omega_i(s) = 1$ for exactly one $i \in \{1,\dots,M\}$ and $\omega_j(s) = 0$ for $j \ne i$ a.e. The continuous relaxation of (BC) reads

$$\begin{aligned}
\min_{y,\alpha}\ & J(y) \\
\text{s.t.}\quad & Ay = \sum_{i=1}^{M} \alpha_i f_i(y), \\
& 0 \le \alpha_i(s) c_i(y(s)) && \text{for a.a. } s \in \Omega_T, i \in \{1,\dots,M\}, \\
& \alpha(s) \in [0,1]^M && \text{for a.a. } s \in \Omega_T, \\
& \sum_{i=1}^{M} \alpha_i(s) = 1 && \text{for a.a. } s \in \Omega_T.
\end{aligned} \tag{RC}$$

We note that additional continuous control inputs into J, the f_i and c_i would be possible here if we added additional assumptions. However, we omit them to keep the article concise. We note that the constraint $0 \le \alpha_i c_i(y)$ implies that versions of (RC) with discretized differential equations exhibit so-called *vanishing constraints*. For further information on optimality conditions and algorithmic approaches for the class of optimization problems exhibiting such constraints, *Mathematical Programs with Vanishing Constraints (MPVCs)*, we refer to the articles [1, 8, 9, 10].

Let Y be a Banach space that serves as the state space for the state equation. We will make use of the abbreviations

$$\mathcal{F}_{(\mathrm{BC})} \coloneqq \left\{(y,\omega) \in Y \times L^\infty(\Omega_T, \mathbb{R}^M) : (y,\omega) \text{ feasible for (BC)}\right\},$$
$$\mathcal{F}_{(\mathrm{RC})} \coloneqq \left\{(y,\alpha) \in Y \times L^\infty(\Omega_T, \mathbb{R}^M) : (y,\alpha) \text{ feasible for (RC)}\right\},$$

for the feasible sets of (BC) and (RC). The following definition applies the naming convention of relaxed and binary control to α and ω, see [15].

Definition 1.1 (Binary and relaxed control). Let $d \in \mathbb{N}$. Let $\Omega_T \subset \mathbb{R}^d$ be a bounded domain. We call a measurable function $\omega : \Omega_T \to \{0,1\}^M$ with $\sum_{i=1}^M \omega_i = 1$ a.e. in Ω_T a *binary control* and a measurable function $\alpha : \Omega_T \to [0,1]^M$ with $\sum_{i=1}^M \alpha_i = 1$ a.e. in Ω_T a *relaxed control.*

We split the process of solving (BC) into the following two steps:

1. solve the relaxation (RC) to obtain an optimal relaxed control α^*,
2. derive a binary control ω from α^* as an approximate solution for (BC).

We call the second step *rounding* and stress that this is different from pointwise rounding to the nearest integer. This splitting methodology is described in detail in [23] and sometimes called *Combinatorial Integral Approximation (CIA) decomposition.* Several algorithmic approaches exist to compute the binary control in the second step. For instance, Sum-Up Rounding (SUR) [20] and Next-Forced Rounding (NFR) [11] provide guaranteed bounds on the so-called *integrality gap*, $\sup_t \left\|\int_0^t \alpha - \omega\right\|$ in the one-dimensional case $\Omega_T = (0,T)$, which behave linearly with respect to the mesh size of the rounding mesh. Here, the term mesh size refers to the maximum cell volume of the mesh cells, which is different from its use in literature on PDE numerics. As the mesh size may be fixed prior to the solution process, it is also sometimes suggested to compute the binary control by directly minimizing the integrality gap for a given rounding mesh, see [23]. We later refer to the resulting optimization problem as the CIA problem.

As noted in [7, 14], similar convexification and approximation properties have been studied in the optimal control community in contexts other than mixed-integer optimization. We reference the important the Filippov-Ważewski theorem, see [6, 24]. This theorem states that the solutions of the differential inclusion

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} y(t) &\in F(y(t)), t \in [0,T],\\ y(0) &= y_0\end{aligned}$$

are dense in the solutions of the differential inclusion

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} y(t) &\in \overline{\operatorname{conv}\{F(y(t))\}}, t \in [0,T],\\ y(0) &= y_0\end{aligned}$$

for a Lipschitz continuous set-valued function F, which maps into compact subsets of a Euclidean space and a uniformly bounded solution set of the second differential inclusion.

Our rounding algorithms can be interpreted as constructive means to compute the approximation in a mixed-integer optimal control setting. We note that similar considerations are used for model order reduction using Koopman operators, see the recent publication [18].

1.1. Outline of the remaining sections

Section 2 summarizes sufficient conditions on the rounding meshes and algorithms as well as the approximation arguments to obtain norm convergence of the state vector associated with the rounded controls that are obtained in the second step of the CIA decomposition. Section 3 presents two algorithms that can be used in the second step of the CIA decomposition, i.e., both satisfy the prerequisites for the aforementioned convergence argument. The first is very resource efficient but not optimal with respect to the integrality gap. The second yields an optimal integrality gap and can be modified to incorporate additional combinatorial constraints on the control. Section 4 presents an algorithmic framework to perform the rounding step. Section 5 compares the two basic rounding algorithms computationally in terms of state vector and objective approximation error for an optimal control problem that is governed by an elliptic state equation on a two-dimensional domain. Finally, we summarize our findings in Section 6.

1.2. Notation

For an integer k, we use the abbreviating notation $[k] \coloneqq \{1, \ldots, k\}$. For a Banach space X, we denote its topological dual by X^*. As we have done up to this point, we use the abbreviated forms "a.e." and "for a.a." for "almost everywhere" and "for almost all" respectively.

2. Approximation arguments for the CIA decomposition

Independent of the actual rounding algorithms, this section summarizes the argument that a decaying integrality gap implies convergence of the control and state vectors. This later factors into the optimality and feasibility of the approximations. We begin by introducing required properties of rounding meshes and the output of the rounding algorithm. We continue by describing the convergence properties that result from these properties and show how they factor into optimality and feasibility. Finally, we point out the differences, i.e., our loss in approximation quality, if mixed constraints of the form $0 \leq \omega_i c_i(y)$ are present.

2.1. Properties of rounding meshes and algorithms

The rounding algorithms presented later operate on controls discretized on meshes. We refer to these as rounding meshes.

Definition 2.1 (Rounding mesh and mesh size). Let $d \in \mathbb{N}$. Let $\Omega_T \subset \mathbb{R}^d$ be a bounded domain. A set of mesh cells $\{\mathcal{T}_1, \ldots, \mathcal{T}_N\} \subset \mathcal{B}(\Omega_T)$ is called a *rounding mesh* if the cells make up a finite partition of Ω_T. The quantity N denotes the number of mesh cells and the quantity $h \coloneqq \max_{k\in[N]} \lambda(\mathcal{T}_k)$ denotes the *mesh size* of the rounding mesh.

We highlight again that, in contrast to PDE numerics literature, we have defined *mesh size* as the maximum cell volume and not as the maximum cell diameter of the mesh cells. Although these quantities are connected on the considered meshes, they are of course not equivalent.

The convergence results in this section require the following assumptions on the binary control vector ω produced during the rounding step. This will be justified for SUR in Section 3.1.

Assumption 2.2. There exists a constant $C > 0$ such that for all relaxed controls α and rounding meshes $\{\mathcal{T}_1, \dots, \mathcal{T}_N\}$ with mesh size h, the rounding ω satisfies

$$\max_{k\in[N]} \left\| \int_{\bigcup_{\ell=1}^{k} \mathcal{T}_\ell} \alpha(s) - \omega(s)\,\mathrm{d}s \right\|_\infty \le Ch. \tag{2.1}$$

2.2. Weak control approximation

Assumption 2.2 implies convergence of ω to α in the weak-$*$ topology of $L^\infty(\Omega_T, \mathbb{R}^M)$ by means of a density argument. We refer to [14] for the proof. In case Ω_T is one-dimensional, i.e., $\Omega_T = (0, T)$, this arises straightforwardly if the mesh cells are intervals.

Theorem 2.3. *Let $(\{\mathcal{T}_1^n, \dots, \mathcal{T}_{N_n}^n\})_n$ be a sequence of rounding meshes with the cells $\mathcal{T}_k^n$ being consecutive (closed, open and half-closed) intervals for all $n \in \mathbb{N}$ and $k \in [N_n]$. Let $(h_n)_n$ denote the corresponding sequence of mesh sizes and $(\omega^n)_n$ the corresponding sequence of binary controls by a rounding algorithm satisfying Assumption 2.2. Then,*

$$\sup_{t\in[0,T]} \left\| \int_0^t \alpha(s) - \omega^n(s)\,\mathrm{d}s \right\|_\infty \le Ch^n$$

If $h^n \to 0$, we have

$$\omega^n \rightharpoonup^* \alpha \text{ in } L^\infty((0,T), \mathbb{R}^M).$$

The density argument to prove Theorem 2.3 makes use of the one-dimensional domain of integration, namely the integration by parts formula before Assumption 2.2 is applied. This procedure does not generalize to the multi-dimensional setting as there is no multi-dimensional analog to the forward progression along the single coordinate axis in one-dimension. To overcome this, we impose a regularity condition on the refinement strategy of the sequence of rounding meshes to obtain weak-$*$ convergence of the sequence $(\omega^n)_n$.

Theorem 2.3 demonstrates that refining the meshes uniformly and satisfying a condition on the progression of the SUR algorithm through cells of consecutive meshes gives the desired convergence. This condition is satisfied by space-filling curves, e.g., the Hilbert curve. For a short proof, we refer to [16].

Fortunately, it is possible to obtain the weak-$*$ approximation property independently of chosen progressions through the mesh cells, i.e., independent of the indexing of the mesh cells in the estimate (2.1). However, we still require a regularity condition to avoid a degeneration of the eccentricity of the mesh cells during the successive refinement of the rounding meshes. The regularity condition is given in Definition 2.4 below and is introduced in [15].

Definition 2.4. Let $d \in \mathbb{N}$ and $\Omega_T \subset \mathbb{R}^d$ be a bounded domain. Let $(\{\mathcal{T}_1^n, \ldots, \mathcal{T}_{N^n}^n\})_n$ be a sequence of rounding meshes with corresponding sequence of mesh sizes $(h^n)_n$. Then, we call the sequence $(\{\mathcal{T}_1^n, \ldots, \mathcal{T}_{N^n}^n\})_n$ an *admissible sequence of refined rounding meshes* if

1. $h^n \to 0$,
2. for all $n \in \mathbb{N}$ and all $k \in [N^{n+1}]$, there exists $\ell \in [N^n]$ such that $\mathcal{T}_k^{n+1} \subset \mathcal{T}_\ell^n$,
3. the cells $\mathcal{T}_k^n$ *shrink regularly*, i.e. there exists $C > 0$ such that for each $\mathcal{T}_k^n$ there exists a ball B_k^n such that $\mathcal{T}_k^n \subset B_k^n$ and $\lambda(\mathcal{T}_k^n) \geq C\lambda(B_k^n)$.

As in [15], we note that the last condition, which limits the eccentricity of the cells along the refinements, is similar to requirements on finite element triangulations, namely refining with an isotropic strategy on quasi-uniform triangulations, see [3]. We state the weak-$*$ convergence, which is proven in [15].

Theorem 2.5. *Let $d \in \mathbb{N}$ and $\Omega_T \subset \mathbb{R}^d$ be a bounded domain. Let $(\{\mathcal{T}_1^n, \ldots, \mathcal{T}_{N^n}^n\})_n$ be an admissible sequence of refined rounding meshes and $(\omega^n)_n$ be the corresponding sequence of binary controls computed by means of a rounding algorithm satisfying Assumption 2.2. Then,*

$$\omega^n \rightharpoonup^* \alpha \text{ in } L^\infty(\Omega_T, \mathbb{R}^M).$$

2.3. State vector approximation

Let $y(\alpha)$ denote the solution of the state equation for the relaxed control α and $y(\omega^n)$ the solution of the state equation for the binary control ω^n. To obtain $y(\omega^n) \to y(\alpha)$ in the state space Y, we need compactness of the solution mapping to transform the weak-$*$ convergence into convergence in norm. We state two results. The first is for a class of semi-linear evolution equations with Lipschitz continuous non-linear part and unbounded linear part, which generates a strongly continuous semigroup. It is proven in [14] and extends the results in [7].

Theorem 2.6. *Let X be a Banach space. Let $\alpha : [0,T] \to \mathbb{R}^M$ be a relaxed control. Let $y \in Y \coloneqq C([0,T], X)$ solve*

$$\partial_t y + Ay = \sum_{i=1}^{M} \alpha_i f_i(y), \quad y(0) = y_0$$

with A being the generator of a strongly continuous semigroup on X and f_i being Lipschitz continuous with respect to y for $i \in [M]$. Let $(\omega^n)_n$ be a sequence of binary controls computed by means of a rounding algorithm satisfying Assumption 2.2 on a sequence of rounding meshes as demanded in Theorem 2.3 with $h^n \to 0$ and let

$(y^n)_n \subset Y$ be the sequence of state vectors that solve

$$\partial_t y + Ay = \sum_{i=1}^{M} \omega_i^n f_i(y), \quad y(0) = y_0$$

for $n \in \mathbb{N}$. Then,

$$y^n \to y \text{ in } Y.$$

The second result is developed in [15] for PDEs governed by elliptic operators of second order, for which it follows immediately from the Lax-Milgram theorem.

Theorem 2.7. *Let X and Y be Banach spaces satisfying the dense and compact embedding $X \hookrightarrow^c Y$. Let $\alpha : \Omega_T \to \mathbb{R}^M$ be a relaxed control. Let $y \in Y$ be the solution of*

$$Ay = \sum_{i=1}^{M} \alpha_i f_i(y)$$

with the restriction A having a bounded inverse $A^{-1} : X^* \to X$. Let $(\omega^n)_n$ be a sequence of binary controls computed by means of a rounding algorithm satisfying Assumption 2.2 on an admissible sequence of refined rounding meshes and let $(y^n)_n \subset X$ be the sequence of state vectors that solve

$$Ay = \sum_{i=1}^{M} \omega_i^n f_i(y)$$

for $n \in \mathbb{N}$. Let $\omega_i^n f_i(y) \rightharpoonup \alpha_i f(y^n)$ in Y^*. Then,

$$y^n \to y \text{ in } X.$$

One should have the Dirichlet-Laplacian with the Hilbert space setting $X = H_0^1(\Omega)$, $X^* = H^{-1}(\Omega)$ and $Y = Y^* = L^2(\Omega)$ in mind for this case. If the f_i do not depend on the state vector, the condition $\omega_i^n f_i(y^n) \rightharpoonup \alpha_i f(y^n)$ is trivially true in this case.

2.4. Optimality and feasibility in the absence of mixed constraints

Again, we denote the state space by the symbol Y. Regardless of the presence of the mixed constraint or not, we can deduce the following from continuity of the objective J with respect to the state vector.

Lemma 2.8. *Let (y, α) solve* (RC) *and let $(y^n, \omega^n)_n \subset Y \times L^\infty(\Omega_T)$ satisfy $y^n \to y$. Then,*

$$\lim J(y^n) = \min_{(y,\alpha)\in\mathcal{F}_{(\mathrm{RC})}} J(y).$$

Now assume, the mixed constraints c_i are not present, i.e., $c_i \equiv 0$ holds for all $i \in [M]$. Then we even obtain

Theorem 2.9. *Let the prerequisites of Lemma 2.8 hold. Then,*

$$\min_{(y,\alpha)\in\mathcal{F}_{(\mathrm{RC})}} J(y) = \inf_{(y,\omega)\in\mathcal{F}_{(\mathrm{BC})}} J(y).$$

These statements are proven in [15] and guarantee algorithmic well-definedness and finite termination if we refine the rounding mesh successively in the sense of Definition 2.4 until an acceptable approximation error between the objective value of the current iterate and the optimal objective value of (RC) is reached.

2.5. Optimality and feasibility in the presence of mixed constraints

As mentioned before, in the presence of mixed constraints, we need to take some extra care and unfortunately, the decomposition approach may not be able to produce a feasible point of (BC), in contrast to Theorem 2.9, but only one exhibiting an arbitrarily small constraint violation.

Applying a rounding algorithm in the presence of the constraints $0 \leq \alpha_i c_i(y)$ without any modifications might lead to arbitrary low values of the term $\omega_i c_i(y)$. To see this, let $i \in [M]$ be fixed and remember that the functions c_i are assumed to be continuous. The problem arises from the bilinear structure of the constraint $0 \leq \alpha_i c_i(y)$. If $\alpha_i = 0$ on a set of non-zero measure, the value of $c_i(y)$ may be arbitrarily low for $(y, \alpha) \in \mathcal{F}_{(\mathrm{RC})}$. If the algorithm does not prevent the rounding of ω_i^n to 1 on this particular set of non-zero measure, this may lead to an arbitrarily high violation of the constraint $0 \leq \omega_i^n c_i(y^n)$ on this particular set.

To overcome this problem, the following assumption restricts the indices that are admissible for rounding in a particular cell $\mathcal{T}_k^n$ to the ones satisfying $\int_{\mathcal{T}_k^n} \alpha_i > 0$.

Assumption 2.10. For all relaxed controls α and rounding meshes $\{\mathcal{T}_1, \ldots, \mathcal{T}_N\}$, the rounding ω satisfies

$$\int_{\mathcal{T}_k} \alpha_i = 0 \Rightarrow \int_{\mathcal{T}_k} \omega_i = 0$$

for all $k \in [N]$ and all $i \in [M]$.

Now, the continuity of the c_i and Assumption 2.10 yield the following result.

Theorem 2.11. *Let the prerequisites of Lemma 2.8 hold. Let the binary controls $(\omega^n)_n$ be computed by means of a rounding algorithm that satisfies Assumption 2.10. Then,*

$$\lim J(y^n) = \min_{(y,\alpha) \in \mathcal{F}_{(\mathrm{RC})}} J(y)$$

as well as

$$0 \leq \liminf \omega_i^n c_i(y^n) \text{ for all } i \in [M].$$

Note that the second asymptotics also hold for continuous path constraints (as a special case). Further classes of constraints on states and controls are discussed in [21].

3. Approximation quality of roundings

The rounding step of the CIA decomposition can be performed using different algorithmic approaches. Section 3.1 focuses on variants of the SUR algorithm, while the explicit minimization of the integrality gap using mixed-integer linear programs (MILPs) is the subject of Section 3.2. Note that other approaches like Next-Forced Rounding, see [11], exist for the second step of the CIA decomposition.

3.1. Sum-Up Rounding algorithms

We introduce two variants of the SUR algorithm, see [13, 20], below and discuss their basic properties and the difference between them.

Definition 3.1 (SUR algorithms). Let α be a relaxed control and let $\{\mathcal{T}_1, \dots, \mathcal{T}_N\}$ be a rounding mesh. We define the function ω iteratively for $k = 1, \dots, N$ as

$$\omega(s) \coloneqq \sum_{k=1}^{N} \chi_{\mathcal{T}_k}(s) W_k,$$

$$W_k(i) \coloneqq \begin{cases} 1 & \text{if } i = \operatorname*{arg\,max}_{j \in F_k} \int_{\mathcal{T}_k} \alpha_j - \int_{\bigcup_{\ell=1}^{k-1} \mathcal{T}_\ell} \alpha_j - \omega_j, \\ 0 & \text{else} \end{cases} \quad \text{for } i \in [M].$$

If a tie arises with respect to the maximizing index k, the smallest of the maximizing indices is chosen. We define the two variants, which differ in the sets of *admissible* indices for rounding in the cells of the rounding mesh:

$$F_k \coloneqq \{1, \dots, M\} \text{ for all } k \in [N], \tag{SUR}$$

$$F_k \coloneqq \left\{ i \in [M] : \int_{\mathcal{T}_k} \alpha_i > 0 \right\} \text{ for all } k \in [N]. \tag{SUR-VC}$$

The algorithm (SUR) is the original SUR algorithm introduced in [20] and the algorithm (SUR-VC) is a variant introduced in [13] that works properly in the presence of mixed constraints. We restate the approximation property that establishes Assumption 2.2 below. It is proven in [13, 22] for (SUR) and in [13, 17] for (SUR-VC).

Proposition 3.2. *The algorithms* (SUR) *and* (SUR-VC) *produce binary controls ω for all relaxed controls α and rounding meshes. There exists a constant $C > 0$ such that for a relaxed contro α and ω computed by means of* (SUR) *or* (SUR-VC) *on a rounding mesh with mesh size h, we have the estimate*

$$\max_{k \in [N]} \left\| \int_{\bigcup_{\ell=1}^{k} \mathcal{T}_\ell} \alpha(s) - \omega(s) \,\mathrm{d}s \right\|_\infty \leq Ch.$$

In particular, Assumption 2.2 holds true.

Due to the integration domain being an increasing union of rounding mesh cells, this estimate depends on the ordering of the mesh cells. However, if the sequence of mesh cells is constructed such that Definition 2.4 is satisfied, the reasoning in Section 2.2 guarantees convergence.

Example. We illustrate the necessity for making the rounding algorithm aware of the mixed constraint, see Section 2.5, for the algorithm (SUR). Let $M = 3$, $\Omega_T = (0, 2)$, let α be the relaxed control given by

$$\alpha_1 \coloneqq .5\chi_{[0,2]}, \quad \alpha_2 \coloneqq .5\chi_{[0,1]}, \quad \alpha_3 \coloneqq .5\chi_{[1,2]}.$$

Assume in mesh iteration n, Ω_T is discretized into $N_n = 2\cdot 3^n$ equidistant intervals, i.e., $h_n = 3^{-n}$. By applying (SUR), we obtain $\omega_1^n(s) = 1$ on the intervals with odd indices and $\omega_2^n(s) = 1$ on the intervals with even indices. This implies

$$\begin{aligned}
\textstyle\int_0^1 \alpha_1 - \omega_1^n &= \textstyle\int_{\bigcup_{k=1}^{3^n} \mathcal{T}_k^n} \alpha_1 - \omega_1^n &= -0.5 \cdot 3^{-n},\\
\textstyle\int_0^1 \alpha_2 - \omega_2^n &= \textstyle\int_{\bigcup_{k=1}^{3^n} \mathcal{T}_k^n} \alpha_2 - \omega_2^n &= 0.5 \cdot 3^{-n},\\
\textstyle\int_0^1 \alpha_3 - \omega_3^n &= \textstyle\int_{\bigcup_{k=1}^{3^n} \mathcal{T}_k^n} \alpha_3 - \omega_3^n &= 0.
\end{aligned}$$

Thus, for the $3^k + 1$-st interval, we have

$$\begin{aligned}
\textstyle\int_{\mathcal{T}^n_{3^n+1}} \alpha_1 + \int_{\bigcup_{k=1}^{3^n} \mathcal{T}_k^n} \alpha_1 - \omega_1^n &= 0.,\\
\textstyle\int_{\mathcal{T}^n_{3^n+1}} \alpha_2 + \int_{\bigcup_{k=1}^{3^n} \mathcal{T}_k^n} \alpha_2 - \omega_2^n &= 0.5 \cdot 3^{-n},\\
\textstyle\int_{\mathcal{T}^n_{3^n+1}} \alpha_3 + \int_{\bigcup_{k=1}^{3^n} \mathcal{T}_k^n} \alpha_3 - \omega_3^n &= 0.5 \cdot 3^{-n}
\end{aligned}$$

and (SUR) gives $\omega_2^n = 1$ on the interval $[1, 1 + h_n]$. Thus, $\|\omega_2^n|_{[1,2]}\|_{L^\infty} = 1$ for all $n \in \mathbb{N}$. Now, assume $c_2(y^n) \to c_2(y)$ and $c_2(y) \equiv -1$ on $[1, 2]$. Then,

$$\operatorname{ess\,inf} \omega_2^n c_2(y^n) \to -1 \text{ on } [1, 2].$$

The restriction of the set of admissible indices for rounding, F_k for $k \in [N]$, in the definition of (SUR-VC) ensures that Assumption 2.10 is satisfied as well and the problem illustrated above cannot occur, see [13].

Proposition 3.3. *Algorithm* (SUR-VC) *satisfies Assumption 2.10.*

We note that a similar modification is not possible for the algorithm Next-Forced Rounding (NFR) from [11] mentioned above as this may lead to an empty set of indices admissible for rounding.

3.2. Combinatorial Integral Approximation Problems

In this subsection, we discuss the minimization problem

$$\min_{\omega} \max_{k\in[N]} \left\| \int_{\bigcup_{\ell=1}^{k} \mathcal{T}_\ell} \alpha(s) - \omega(s)\, \mathrm{d}s \right\|_\infty ,$$

which defines binary controls ω that minimize the integrality gap. By introducing an additional variable $\theta \geq 0$ and adding inequality constraints for all control realizations and mesh cells, we are able to define an equivalent mixed-integer linear program (MILP) that aims at solving the above problem. We refer to the latter as *Combinatorial Integral Approximation Problem*, see [23], and provide its definition below.

Definition 3.4 (CIA-MILP). Let the prerequisites of Definition 3.1 hold. Based on the relaxed controls and the rounding mesh we introduce the average values

$$A_k(i) := \frac{1}{\lambda(\mathcal{T}_k)} \int_{\mathcal{T}_k} \alpha_i(s)\, \mathrm{d}s, \qquad \text{for } i \in [M],\ k \in [N].$$

We define further the CIA-MILP to be:

$$\min_{\theta,W} \theta \text{ s.t.} \tag{CIA-MILP}$$

$$\begin{aligned} \theta &\geq \pm \sum_{l\in[k]} (A_l(i) - W_l(i))\,\lambda(\mathcal{T}_l), && \text{for } i \in [M],\ k \in [N], \\ W_k(i) &\in \{0,1\} && \text{for } i \in [M],\ k \in [N], \\ 1 &= \sum_{i\in[M]} W_k(i) && \text{for } k \in [N]. \end{aligned}$$

The solution of (CIA-MILP) is used to construct a piecewise constant binary control function as already sketched in Definition 3.1:

$$\omega(s) := \sum_{k=1}^{N} \chi_{\mathcal{T}_k}(s) W_k, \quad s \in \Omega_T.$$

We note that the family of SUR algorithms has linear complexity in the total number of mesh cells N. In contrast, using an MILP in the rounding step increases the computational burden exponentially with N, but may construct solutions with smaller integrality gap. In fact, one can interpret SUR as a heuristic way to solve (CIA-MILP) or at least construct a feasible point. Since (SUR) provides a feasible point for (CIA-MILP), the following proposition which asserts Assumption 2.2, follows directly from Proposition 3.2.

Proposition 3.5. *The solution of* (CIA-MILP) *yields a binary control ω for all relaxed controls α and rounding meshes. There exists a constant $C > 0$ such that for α being a relaxed control and ω being computed by solving* (CIA-MILP) *on a mesh with mesh size h, we have the estimate*

$$\max_{k\in\{1,\dots,N\}} \left\| \int_{\bigcup_{\ell=1}^{k} \mathcal{T}_\ell} \alpha(s) - \omega(s)\,\mathrm{d}s \right\|_\infty \leq Ch.$$

In particular, Assumption 2.2 holds true.

(CIA-MILP) represents the CIA problem based on the ∞-norm, whereas there is a whole family of MILPs to carry out the binary approximation problem. A generalization of CIA problems with respect to different norms, the order of the accumulated control difference and different scaling of the latter is proposed in [25]. For instance, we may scale the approximation inequality for the CIA problem with the evaluated right hand side f_i after solving (RC).

Another aspect of using an MILP in the rounding step is the opportunity to include general combinatorial constraints on the binary controls. Real-world problems on a time domain, i.e., $\Omega_T \subset \mathbb{R}$, see e.g. [4, 19], often require a limited number of switches occurring between the system modes or the presence of so-called *minimum dwell time constraints* that describe the necessity of activating a control ω_i for at least a given minimal duration if at all. Similar constraints can be introduced for deactivation periods. To impose a maximum number of switches

$\sigma \in \mathbb{N}$ on the time horizon, we would add

$$\sigma \geq \frac{1}{2} \sum_{i \in [M]} \sum_{l \in [N-1]} |W_{l+1}(i) - W_l(i)| \tag{3.1}$$

to (CIA-MILP). The dwell time constraints for a given dwell time $C_D \in \mathbb{N}$, an assumed equidistant mesh, as well as $l \in [N-2]$, $k = l+1, \ldots, \min\{l+1+C_D, N\}$ would read

$$\begin{aligned} W_{k+1}(i) &\geq W_{l+1}(i) - W_l(i), \quad \text{for } i \in [M], \\ 1 - W_{k+1}(i) &\geq W_l(i) - W_{l+1}(i), \quad \text{for } i \in [M], \end{aligned}$$

and can also be addressed by (CIA-MILP). In contrast to the one-dimensional case, it is not immediately clear how to interpret such constraints on multi-dimensional domains. Here, the *total max-up constraint* is an example of a meaningful combinatorial condition, which limits the total number of activations on all mesh cells for certain controls by a constant $C_L(i) \in \mathbb{N}$:

$$C_L(i) \geq \sum_{l \in [N]} W_l(i), \quad \text{for } i \in [M].$$

Combinatorial conditions have in common that Assumption 2.2 can not generally be satisfied in their presence and hence the convergence argument in Section 2.2 may fail. The following example illustrates this issue.

Example. Let us again consider the case $\Omega_T = [0, 2]$ with two discrete control realizations, i.e. $M = 2$, and with the presence of the constraint (3.1) that limits the number of switches with the choice $\sigma = 1$. We further assume that the relaxed control is given by

$$\alpha_1 := .5\chi_{[0,2]}, \quad \alpha_2 := .5\chi_{[0,2]}.$$

Then, we recognize that the optimal solution of (CIA-MILP) approximates α by setting the values $W_l(1) = 1$ on a minimal set covering $\cup_l \mathcal{T}_l$ of $[0, 1]$ and $W_l(1) = 0$ else. Therefore, (CIA-MILP) exhibits an objective, i.e. an integrality gap, of at least $\frac{1}{2}$ *independent* of the discretization of Ω_T. In particular, Assumption 2.2 is not satisfied.

This example can be adapted analogously to cases where $\sigma > 1$ is given or $M > 2$ holds.

4. Solving the CIA problem

The open-source software package `pycombina`[1] contains an implementation for various rounding algorithms, e.g., for the presented SUR from Section 3. Sophisticated MILP solvers such as `Gurobi` struggle to solve (CIA-MILP) efficiently, see

[1]Available under `https://github.com/adbuerger/pycombina`

[11]. This may be due to the fact that its canonical linear programming relaxation, i.e. (CIA-MILP) with $W_k(i) \in [0,1]$, yields only trivial lower bounds in case of absent additional combinatorial constraints. (CIA-MILP) can be solved more efficiently by means of a tailored Branch and Bound scheme, see [23]; an efficient version is also implemented in `pycombina`. Algorithm 1 describes the main steps. The algorithm exploits that an evaluation of the objective function up to the current mesh cell yields a valid lower bound due to the maximization operator over all intermediate steps in the objective function. This lower bound is extremely cheap to compute and is tighter than canonical relaxations [12]. We select nodes from a queue Q until it is empty or a termination criterion is reached, such as a maximum number of iterations or a time limit (line 2). The selected node `n` is pruned if its lower bound θ is greater than the global upper bound UB (lines 4 - 5) or we update the currently best node $\texttt{n}^*$ to be `n`, if its depth equals the number of mesh cells N (lines 6 - 7). We branch forward with respect to the mesh index $k \in [N]$, whereby for each child node creation all control entries $W_k(i)$ become fixed with exactly one index set to be active (line 9). Nodes contain information on their depth, which is the mesh cell index, their so far largest accumulated control deviation θ and the accumulated deviation for each control realization θ_i. Depending on the imposed combinatorial constraints, we save also information about previous $W_k(i)$ values in the nodes and add their child nodes only if they satisfy these constraints (line 10). For further details and numerical examples benchmarking Algorithm 1 with MILP solvers, we refer to [4, 11].

5. Illustration of the multi-dimensional control approximation

As noted in Section 2.2, weak convergence of the control function can be ensured for elliptic PDEs with both algorithms, if we use an admissible sequence of refined rounding meshes. As shown in [16], this can be achieved by iterating over the mesh cells along approximants of a space-filling curve such as the Hilbert curve. In this section, we demonstrate the bare SUR algorithm and the MILP approach described above by applying them to a simple distributed inverse problem for the Poisson equation. We use a finite element method with continuous first-order Lagrange elements on a structured triangular mesh which we will iterate over according to the Sierpinski curve.

5.1. Test problem

Our test problem is based on the Poisson equation, which is an inhomogeneous, uniformly elliptic second-order linear PDE system used to find stationary solutions to diffusion and heating problems. Due to its theoretical simplicity, the Poisson equation is often used as a testbed for mixed-integer PDE-constrained optimization. We solve the Poisson equation in two dimensions on the unit square $\Omega = [0,1]^2$ using Robin boundary conditions, which guarantees the uniqueness and Fréchet differentiability of the PDE solution with respect to our controls, which select one

Algorithm 1: Branch and Bound for solving (CIA-MILP)

Input : Relaxed control values $A_k(i)$, mesh size volumes $\lambda(\mathcal{T}_k), k \in [N]$, termination criterion, parameters for combinatorial constraints.
Output: (Optimal) solution (θ^*, W^*) of (CIA-MILP).

Initialize node queue Q with empty node and set upper bound UB.
while *$Q \neq \emptyset$ and termination criterion not reached* **do**
  Choose $\mathtt{n} \in Q$ according to node selection strategy.
  if $n.\theta > UB$ **then**
    Prune node $\mathtt{n}$.
  else if $n.depth = N$ **then**
    Set new best node $\mathtt{n}^* \leftarrow \mathtt{n}$ and $UB = \mathtt{n}.\theta$
  else
    Create M child nodes $\mathtt{c}_i$ with

$$\mathtt{c}_i.depth \leftarrow d := \mathtt{n}.depth + 1,$$
$$W_{\mathtt{c}_i,d}(j) \leftarrow \begin{cases} 1 & \text{if } j = i \\ 0 & \text{otherwise} \end{cases},$$
$$\mathtt{c}_i.\theta_j \leftarrow \mathtt{n}.\theta_j + (A_d(j) - W_d(j)) \cdot \lambda(\mathcal{T}_d)$$
$$\mathtt{c}_i.\theta \leftarrow \max\Big(\{\mathtt{n}.\theta\} \cup \big\{|\mathtt{c}_i.\theta_j| \;\big|\; j \in [M]\big\}\Big).$$

    Add $\mathtt{c}_i$ to Q if and only if it satisfies all combinatorial constraints.
  end
end
return: $(\theta^*, W^*) = (\mathtt{n}^*.\theta, \mathtt{n}^*.W)$;

of five discrete source term values for each point in the domain. Our objective is an L^2 tracking objective. Thus, the problem can be stated as

$$\begin{aligned}
\min_{y,\omega}\ & \|y - \bar{y}\|^2_{L^2(\Omega)} & & \\
\text{s.t.}\quad & -\Delta y = \sum_{i=1}^{5} v_i \omega_i & & \text{a.e. in } \Omega, \\
& \frac{\partial y}{\partial \nu} - y = 0 & & \text{a.e. in } \partial\Omega, \\
& \sum_{i=1}^{5} \omega_i(x) = 1 & & \text{a.e. in } \Omega, \\
& \omega_i(x) \in \{0, 1\} & & \text{a.e. in } \Omega\ \forall i \in [5],
\end{aligned} \tag{P}$$

where $\nu\colon \partial\Omega \to \mathbb{R}^2$ is the outer unit normal of Ω and $\bar{y} \in L^2(\Omega)$ is the unique weak solution of the boundary value problem for the right-hand side given by

$$\bar{f}(x) \coloneqq \sum_{i=1}^{5} v_i \frac{\bar{\alpha}_i(x)}{\sum_{j=1}^{5} \bar{\alpha}_j(x)} \qquad \forall x \in \Omega$$

with a set of known control functions

$$\bar{\alpha}_i(x) \coloneqq \exp\left(-100(\min\{\|x - m_{*,1}\|, \|x - m_{*,2}\|\} - r_i)^2\right).$$

The additional parameters are

$$\begin{aligned} v &\coloneqq \left(-2, -\frac{1}{2}, \frac{1}{4}, 1, 2\right)^T, \\ r &\coloneqq (0.25, 0.2, 0.15, 0.1, 0.05)^T, \\ m &\coloneqq \begin{pmatrix} 0.25 & 0.75 \\ 0.25 & 0.75 \end{pmatrix}. \end{aligned}$$

After normalization, the functions $\bar{\alpha}$ sum up to one everywhere. Therefore, they are optimal controls for the relaxed problem with objective function value 0.

5.2. Mesh structure and Sierpinski curve

We use the finite-element package `FEniCS` [2] to generate meshes and solve the boundary value problem. Meshes are generated using a `RectangleMesh` with `crossed` diagonals, meaning that at refinement level $l \in \mathbb{N}_0$, the unit square is subdivided into 4^l equally sized squares, each of which is again subdivided into four congruent triangles along its diagonals. This is equivalent to subdividing each triangle into four congruent sub-triangles on each refinement level as illustrated in Fig. 1.

In order to generate an order approximating the Sierpinski curve, we generate the vertices of a Sierpinski curve at the l-th iteration, starting at the point $\left(\frac{1}{2^{l+1}}, \frac{\sqrt{2}-1}{2^{l+1}}\right)$ which is located in the leftmost triangle that has an edge contained entirely within the x_1 axis. The first step is made at an angle of $\frac{\pi}{4}$ and all steps have length $\frac{\sqrt{2}-1}{2^l}$. This produces one vertex within each triangle. We then iterate over the triangles in the mesh according to the order of the vertices.

For a more detailed description of the Sierpinski curve, we refer to [5, Section 2.10.3]. The procedure is illustrated for refinement levels $0, 1, 2$ in Fig. 2.

5.3. Numerical results obtained with the CIA decomposition

For practical problems we suggest to calculate optimal relaxed and derived binary controls iteratively on refined meshes. However, both the convergence of the relaxed solutions and of the rounding strategies have an impact and overlap, complicating the analysis of the overall convergence behavior. In our setting and due to the way the test problem is stated, the optimal relaxed control function is known in advance. This allows us to highlight the convergence of the rounded solutions to the optimal relaxed solution in function space. We use continuous first-order Lagrange elements to approximate weak PDE solutions and piecewise constant functions to

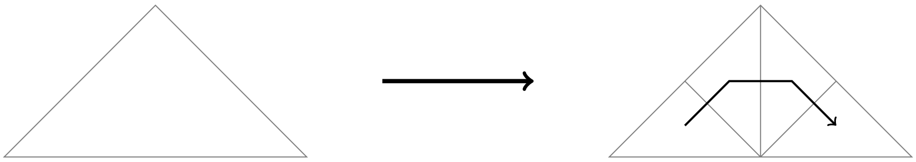

Figure 1. Refinement of a single triangle.

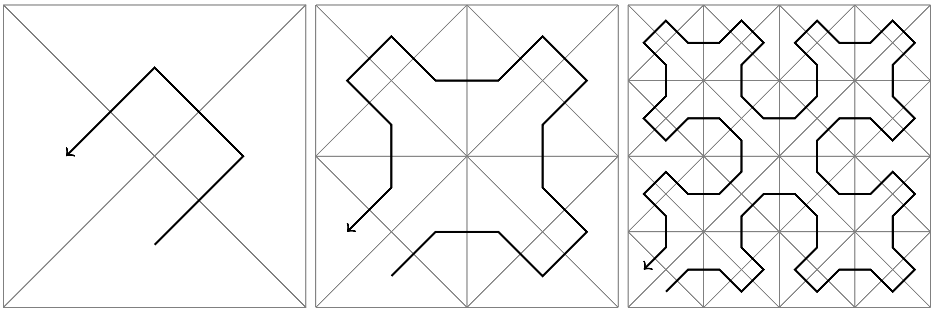

Figure 2. First three refinement levels in an admissible sequence of rounding meshes using the Sierpinski curve.

Table 1. Results of numerical experiments

Level	Cells	h	Abs. Err. SUR	Abs. Err. BnB	CIA Obj. SUR	CIA Obj. BnB
0	4	2.500000×10^{-1}	1.825637×10^{-3}	1.825637×10^{-3}	1.487897×10^{-1}	1.487897×10^{-1}
1	16	6.250000×10^{-2}	8.382177×10^{-4}	1.734637×10^{-4}	4.562038×10^{-2}	4.562038×10^{-2}
2	64	1.562500×10^{-2}	1.110449×10^{-5}	6.927478×10^{-6}	9.355154×10^{-3}	9.355154×10^{-3}
3	256	3.906250×10^{-3}	7.461304×10^{-6}	7.232266×10^{-6}	3.395206×10^{-3}	2.910952×10^{-3}
4	1024	9.765625×10^{-4}	2.725262×10^{-7}	3.082747×10^{-7}	8.505270×10^{-4}	7.388801×10^{-4}
5	4096	2.441406×10^{-4}	2.005071×10^{-8}	1.848401×10^{-8}	2.377537×10^{-4}	2.053501×10^{-4}
6	16384	6.103516×10^{-5}	2.574303×10^{-9}	4.133702×10^{-9}	7.280519×10^{-5}	7.280519×10^{-5}

approximate control functions. We coarsen the optimal relaxed control for lower refinement levels by taking a weighted average over each cell of the coarse mesh and approximate it using both sum up rounding and `pycombina`'s specialized branch-and-bound algorithm. The latter is limited to 10^8 explored nodes and up to one CPU hour of computation time. We compare both approximation methods using the absolute error in the objective function value as well as the objective they achieve in the CIA problem (CIA-MILP). The latter approaching zero indicates weak-$*$ convergence of the control function.

We note that `pycombina` terminates early on account of exceeding the explored node limit for levels 3, 4, 5, and 6. However, it does so in less than 20 CPU

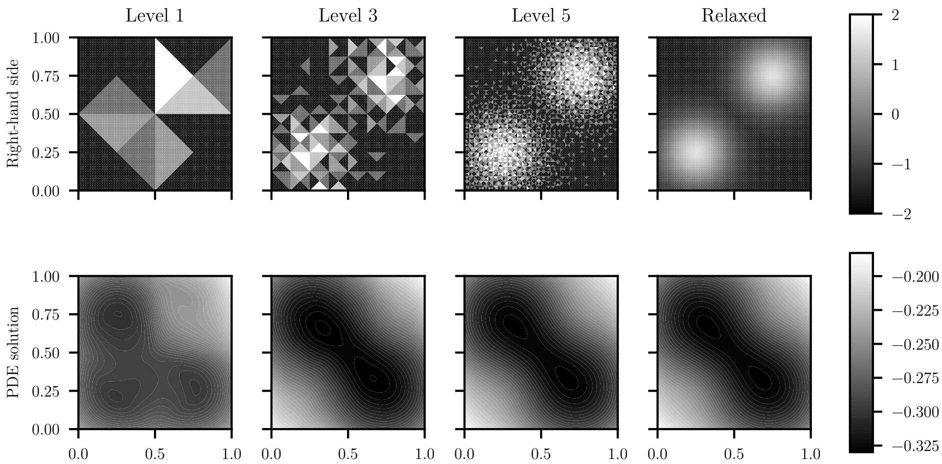

FIGURE 3. Solutions for SUR at levels 1, 3, and 5.

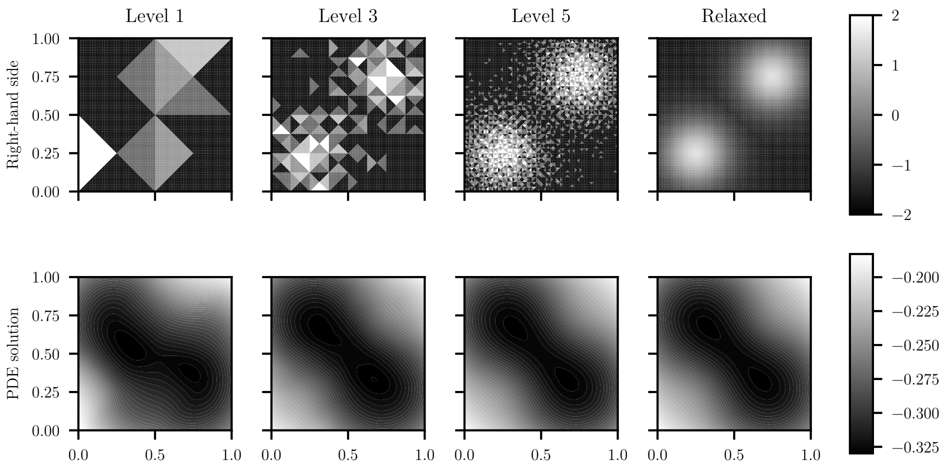

FIGURE 4. Solutions for branch-and-bound at levels 1, 3, and 5.

minutes in all cases. By contrast, if we try to solve the CIA problem (CIA-MILP) using `Gurobi`, the CPU time limit of one hour is already exceeded at level 3.

Table 1 summarizes the outcome of our experiment. Despite early and possibly suboptimal termination, we see that the branch-and-bound algorithm always achieves a CIA objective that is at least as good or better than that achieved by sum up rounding, though this does not always translate into a smaller error in the actual objective function value. For levels 1, 3, and 5, we plot the right-hand side function and PDE solution for sum up rounding and branch and bound alongside their relaxed counterparts in Figs. 3 and 4, respectively.

6. Conclusion

In this article, we surveyed recent improvements of the CIA decomposition for solving PDE-constrained mixed-integer optimal control problems. This approach consists of solving first the problem with relaxed controls before approximating these values with binary ones as part of a rounding problem. We summarized our findings with respect to convergence results in the weak-$*$ topology of L^∞ and discussed two rounding algorithms together with their efficient numerical implementation. Finally, these two algorithmic approaches were compared on a test problem based on the Poisson equation, where we used the space-filling Sierpinski curve to iterate over a structured triangular mesh.

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Acknowledgment

C. Kirches, S. Sager and P. Manns acknowledge funding by Deutsche Forschungsgemeinschaft through Priority Programme 1962, grant KI1839/1-1. C. Kirches acknowledges financial support by the German Federal Ministry of Education and Research, program "Mathematics for Innovations in Industry and Service", grants 05M17MBA-MOPhaPro, 05M18MBA-MOReNet, and program "IKT 2020: Software Engineering", grant 01/S17089C-ODINE. S. Sager, M. Hahn and C. Zeile have received funding from the European Research Council (ERC), grant agreement No 647573, from German Research Foundation – 314838170, GRK 2297 MathCoRe and from German Federal Ministry of Education and Research, program "Mathematics for Innovations", grant P2Chem.

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