Regular and Singular Boundary Problems in Maple

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Abstract. We describe a new MAPLE package for treating boundary problems for linear ordinary differential equations, allowing two-/multipoint as well as Stieltjes boundary conditions. For expressing differential operators, boundary conditions, and Green's operators, we employ the algebra of integro-differential operators. The operations implemented for regular boundary problems include computing Green's operators as well as composing and factoring boundary problems. Our symbolic approach to singular boundary problems is new; it provides algorithms for computing compatibility conditions and generalized Green's operators.

Keywords: Linear boundary problem, Singular Boundary Problem, Generalized Green's operator, Green's function, Integro-Differential Operator, Ordinary Differential Equation.

1 Introduction

Although boundary problems clearly play an important role in applications and in Scientific Computing, there is no systematic support for solving them symbolically in current computer algebra systems. In this paper, we describe a MAPLE package with algorithms for regular as well as singular boundary problems for linear ordinary differential equations (LODEs). While a first version of the package with functions for regular boundary problems was presented in [1], the methods and the implementation for singular problems are new. A prototype implementation for regular boundary problems in the TH∃OREM∀ system was described in [2] as part of a general symbolic framework for boundary problems, including also some first steps towards linear partial differential equations (LPDEs).

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In Section 2, we recall the algebra of integro-differential operators providing the algebraic structure for computing with boundary problems. We describe its implementation in Maple, where we use a normal form approach in contrast to [2]. In Section 3, we outline our symbolic approach for solving boundary problems. For an analytic treatment of boundary problems for LODEs, see for example [3,4] or [5] for further applications. The functions we present include the computation of Green's operators and Green's functions as well as the factorization of boundary problems.

We introduce generalized boundary problems in Section 4 and develop an algorithm for computing generalized Green's operators. The main step of the algorithm is to determine compatibility conditions for arbitrary boundary problems in an algebraic setting; the special case of two-point boundary problems of second order is discussed in [6, Lecture 34]. For singular boundary problems and generalized or modified Green's functions in Analysis, we refer for example to [4] and [7], and in the context of generalized inverses to [8, Sect. 9.4], [9], and [10, Sect. H].

The Maple package *IntDiffOp* is available with an example worksheet at `http://www.risc.jku.at/people/akorpora/index.html`.

2 Integro-Differential Operators

We first recall the definition of integro-differential algebras and operators, see [11] and [12] for further details. For the similar notion of differential Rota-Baxter algebras, we refer to [13]. As a motivating example, consider the algebra $\mathcal{F} = C^\infty(\mathbb{R})$ with the usual derivation and the integral operator $\int \colon f \mapsto \int_a^x f(\xi)\, d\xi$ for a fixed $a \in \mathbb{R}$. The essential algebraic identities satisfied by the derivation and the integral operator are the Leibniz rule, the Fundamental Theorem of Calculus, and Integration by Parts. Note also that $f(a) = f - \int f'$, so the evaluation $\mathtt{E}_a \colon f \mapsto f(a)$ at the initialization point a of the integral can also be expressed in terms of the derivation and integral.

We call $(\mathcal{F}, \partial, \int)$ an *integro-differential algebra* if $(\mathcal{F}, \partial)$ is a commutative differential algebra over a commutative ring K and $\int$ is a K-linear right inverse (section) of $\partial = {}'$, meaning $(\int f)' = f$, such that the *differential Baxter axiom*

$$(\textstyle\int f')(\int g') + \int (fg)' = (\int f')g + f(\int g')$$

holds. We call $\mathtt{E} = 1 - \int \circ \partial$ the *evaluation* of $\mathcal{F}$. We say that an integro-differential algebra over a field K is ordinary if $\operatorname{Ker}(\partial) = K$. For an ordinary integro-differential algebra, the evaluation can be interpreted as a multiplicative linear functional (character) $\mathtt{E} \colon \mathcal{F} \to K$. This allows treating initial value problems, but for doing boundary problems we need additional characters $\varphi \colon \mathcal{F} \to K$ (in the above example, evaluations $\mathtt{E}_c \colon f \mapsto f(c)$ at various points $c \in \mathbb{R}$).

Let $(\mathcal{F}, \partial, \int)$ be an ordinary integro-differential algebra over a field K and let $\Phi \subseteq \mathcal{F}^*$ be a set of multiplicative linear functionals $\varphi \colon \mathcal{F} \to K$ including $\mathtt{E}$. The *integro-differential operators* $\mathcal{F}_\Phi[\partial, \int]$ are defined in [11] as the K-algebra

Table 1. Rewrite Rules for Integro-Differential Operators

$fg \to f \cdot g$	$\partial f \to f\partial + f'$	$\int f \int \to (\int f) \int - \int (\int f)$
$\varphi\psi \to \psi$	$\partial\varphi \to 0$	$\int f \partial \to f - \int f' - \mathrm{E}(f)\,\mathrm{E}$
$\varphi f \to \varphi(f)\,\varphi$	$\partial \int \to 1$	$\int f \varphi \to (\int f)\,\varphi$

generated by the symbols ∂ and $\int$, the "functions" $f \in \mathcal{F}$ and the "functionals" $\varphi \in \Phi$, modulo the Noetherian and confluent rewrite system of Table 1.

The representation of integro-differential operators in our Maple implementation is based on the fact that every integro-differential operator has a unique normal form as a sum of a differential, integral, and boundary operator. The normal forms of differential operators are as usual $\sum f_i \partial^i$, integral operators can be written uniquely (up to bilinearity) as sums of terms of the form $f \int g$, and the normal forms of *boundary operators* are given by

$$\sum_{\varphi \in \Phi} \Big(\sum_{i \in \mathbb{N}} f_{i,\varphi} \varphi \partial^i + \sum_{j \in \mathbb{N}} g_{j,\varphi} \varphi \int h_{j,\varphi} \Big), \tag{1}$$

with only finitely nonzero summands. Stieltjes *boundary conditions* are boundary operators where $f_{i,\varphi} = a_{\varphi,i} \in K$ and $g_{j,\varphi} = 1$. They act on $\mathcal{F}$ as linear functionals in the dual space $\mathcal{F}^*$. See [14] for Stieltjes boundary conditions in Analysis.

From Table 1 formulas can be derived for expressing the product of integro-differential operators directly in terms of normal forms; see [15] for the case $\Phi = \{\mathrm{E}\}$. Implementing these formulas leads to faster computations since we need not reduce in each step. In our package, we use for the underlying "integro-differential algebra" all the smooth functions in one variable representable in Maple, together with the usual derivation and the integral operator $\int = \int_0^x$, both computed by Maple . We take as characters $\Phi = \{\mathrm{E}_c \mid c \in \mathbb{R}\}$.

We created data types for the different kinds of operator, representing integro-differential operators as triples $\mathtt{INTDIFFOP}(a, b, c)$, where a is a differential operator, b an integral operator and c a boundary operator. Differential operators are represented as lists $\mathtt{DIFFOP}(f_0, f_1, \ldots)$ and integral operators as lists of pairs of the form $\mathtt{INTOP}(\mathtt{INTTERM}(f_1, g_1), \mathtt{INTTERM}(f_2, g_2), \ldots)$. In order to have a unique representation for integral operators, one would need a basis of the underlying integro-differential algebra and use only basis elements for the g_i. In our implementation, we use the following heuristic approach: We split sums in the g_i and move scalar factors to the coefficients f_i.

Due to (1), a boundary operator BOUNDOP contains a list of evaluations at different points. Each evaluation EVOP is a triple containing the evaluation point, the local part $\sum f_{i,\varphi} \varphi \partial^i$ and the global part $\sum g_{j,\varphi} \varphi \int h_{j,\varphi}$. Hence we use the expression $\mathtt{BOUNDOP}(\mathtt{EVOP}(c, \mathtt{EVDIFFOP}(f_0, \ldots), \mathtt{EVINTOP}(\mathtt{EVINTTERM}(g_1, h_1), \ldots), \ldots)$ for the representation of boundary operators.

In the following example, we first enter some operators of different types. For displaying the operators, we use D for ∂, A for $\int$ and E[c] for the evaluation E_c.

```
> T := DIFFOP(0,0,1);
```

$$T \ := \ \mathrm{D}^2$$

```
> G := INTOP(INTTERM(1,1));
```

$$G \ := \ \mathrm{A}$$

```
> B := BOUNDOP(EVOP(1, EVDIFFOP(1), EVINTOP(EVINTTERM(1,1))));
```

$$B \ := \ \mathrm{E}[1] \ + \ ((\mathrm{E}[1]) \ . \ A)$$

Now we show how to add and multiply integro-differential operators and how to apply them to a function $f \in \mathcal{F}$.

```
> ApplyOperator(G, f(x));
```

$$\int_0^x f(x)dx$$

```
> MultiplyOperator(G,G);
```

$$(x \ . \ A) \ - \ (A \ . \ x)$$

```
> MultiplyOperator(T,G,G);
```

$$1$$

```
> S := AddOperator(T, G, B);
```

$$S \ := \ \mathrm{D}^2 \ + \ A \ + \ \mathrm{E}[1] + \ ((\mathrm{E}[1]) \ . \ A)$$

```
> ApplyOperator(S, f(x));
```

$$\frac{\mathrm{d}^2}{\mathrm{dx}^2} f(x) + \int_0^x f(x)dx + f(1) + \int_0^1 f(x)dx$$

3 Regular Boundary Problems in Maple

In this section, we demonstrate how to compute with regular boundary problems in our MAPLE package. For an integro-differential algebra $\mathcal{F}$, a boundary problem is given by a monic differential operator $T = \partial^n + c_{n-1}\partial^{n-1} + \cdots + c_1\partial + c_0$ and boundary conditions $\beta_1, \ldots, \beta_m$. Given a forcing function $f \in \mathcal{F}$, we want to find $u \in \mathcal{F}$ such that

$$\boxed{\begin{array}{l} Tu = f, \\ \beta_1 u = \cdots = \beta_n u = 0. \end{array}} \tag{2}$$

A boundary problem is called regular if for each $f \in \mathcal{F}$ there is exactly one $u \in \mathcal{F}$ satisfying (2). We want to solve a boundary problem not only for a fixed f but to compute the Green's operator mapping each forcing function f to its unique solution u. In other words, we solve a whole family of inhomogeneous differential equations, parameterized by a "symbolic" right-hand side f. We restrict ourselves to homogeneous conditions because the general solution is then obtained by adding a particular solution satisfying the inhomogeneous conditions.

For convenience, we shortly recall the abstract linear algebra setting for boundary problems over a vector space $\mathcal{F}$ as described in [16]. For $U \leq \mathcal{F}$ we define the *orthogonal* as $U^\perp = \{\beta \in \mathcal{F}^* : \beta(u) = 0 \text{ for all } u \in U\} \leq \mathcal{F}^*$. Similarly, for $\mathcal{B} \leq \mathcal{F}^*$, we define $\mathcal{B}^\perp = \{v \in \mathcal{F} : \beta(v) = 0 \text{ for all } \beta \in \mathcal{B}\} \leq \mathcal{F}$. A subspace U (resp. $\mathcal{B}$) is *orthogonally closed* if $U = U^{\perp\perp}$ (resp. $\mathcal{B} = \mathcal{B}^{\perp\perp}$). Every subspace $U \leq \mathcal{F}$ is orthogonally closed and every finite dimensional subspace $\mathcal{B} \leq \mathcal{F}^*$ is orthogonally closed. For a linear map $T \colon \mathcal{F} \to \mathcal{G}$ between vector spaces, the transpose map $T^* \colon \mathcal{G}^* \to \mathcal{F}^*$ is defined by $\gamma \mapsto \gamma \circ T$. The image of an orthogonally closed space under the transpose map is orthogonally closed.

A *boundary problem* is given by a pair $(T, \mathcal{B})$, where T is a surjective linear map and $\mathcal{B} \leq \mathcal{F}^*$ is an orthogonally closed subspace of the dual space. We call $u \in \mathcal{F}$ a solution of $(T, \mathcal{B})$ for a given $f \in \mathcal{F}$ if $Tu = f$ and $u \in \mathcal{B}^\perp$. A boundary problem is *regular* if for each f there exists a unique solution u. The *Green's operator* of a regular problem maps each f to its unique solution u. We also write $(T, \mathcal{B})^{-1}$ for the Green's operator. A boundary problem is *regular* iff $\mathcal{B}^\perp$ is a complement of $\operatorname{Ker} T$ so that $\mathcal{F} = \operatorname{Ker} T \dotplus \mathcal{B}^\perp$ as a direct sum.

For $\mathcal{F} = C^\infty[a, b]$, a monic differential operator T is always surjective and $\dim \operatorname{Ker} T = n < \infty$. Moreover, variation of constants can be used to compute a distinguished right inverse: If T has order n and $u_1, \ldots, u_n$ is a fundamental system for it, the *fundamental right inverse* is given by

$$T^\blacklozenge = \sum_{i=1}^{n} u_i {\textstyle\int} d^{-1} d_i, \tag{3}$$

where d is the determinant of the Wronskian matrix W for $(u_1, \ldots, u_n)$ and d_i the determinant of the matrix W_i obtained from W by replacing the i-th column by the n-th unit vector. Equation (3) is valid in arbitrary integro-differential algebras provided the n-th order operator T has a fundamental system $(u_1, \ldots, u_n)$ with invertible Wronskian matrix; see [11] or [12]. This will be assumed from now on, together with the condition $\dim \mathcal{B} < \infty$ appropriate for LODEs.

Regularity of a boundary problem $(T, \mathcal{B})$ can be tested algorithmically as follows. If $(u_1, \ldots, u_n)$ is a basis for $\operatorname{Ker} T$ and $(\beta_1, \ldots, \beta_m)$ for $\mathcal{B}$, we have a regular problem iff the *evaluation matrix*

$$\beta(u) = \begin{pmatrix} \beta_1(u_1) & \ldots & \beta_1(u_n) \\ \vdots & \ddots & \vdots \\ \beta_m(u_1) & \ldots & \beta_m(u_n) \end{pmatrix} \tag{4}$$

is regular; see [16, Cor. A.17] or [17, p. 184] for the special case of two-point boundary conditions. Of course this implies $m = n$, but we will consider more general types of boundary problems in Section 4 where this is no longer the case. It will also be convenient to use the notation (4) for arbitrary $u_1, \ldots, u_n \in \mathcal{F}$ and boundary conditions $\beta_1, \ldots, \beta_m$.

The algorithm for computing the Green's operator is described in detail in [11]; see also [2]. The main steps consist in computing the fundamental right inverse $T^\blacklozenge \in \mathcal{F}[\partial, \int]$ from a given fundamental system as in (3) and the projector

$P \in \mathcal{F}[\partial, \int]$ onto $\operatorname{Ker} T$ along $\mathcal{B}^{\perp}$. Then the Green's operator is then computed as $G = (1 - P)T^{\blacklozenge}$.

For a boundary problem we need to enter a monic differential operator T and a list of boundary conditions $(b1, \ldots, bm)$ as described in Section 2 in the form $\text{BP}(T, \text{BC}(b1, \ldots, bm))$. We use the MAPLE function *dsolve* for computing a fundamental system of T. As an example, we compute the Green's operator for the simplest two-point boundary problem $u'' = f$, $u(0) = u(1) = 0$. From the Green's operator for two-point boundary problems, we can extract the Green's function [18], which is usually used in Analysis to represent the Green's operator.

```
> T := DIFFOP(0,0,1):
> b1 := BOUNDOP(EVOP(0, EVDIFFOP(1), EVINTOP())):
> b2 := BOUNDOP(EVOP(1, EVDIFFOP(1), EVINTOP())):
> Bp := BP(T, BC(b1, b2));
```

$$Bp \;:=\; \mathrm{BP}(\mathrm{D}^2,\; \mathrm{BC}(\mathrm{E}[0],\; \mathrm{E}[1]))$$

```
> IsRegular(Bp);
```

$$true$$

```
> GreensOperator(Bp);
```

$$(x \;.\; \mathrm{A}) \;-\; (\mathrm{A} \;.\; x) \;-\; ((x \;\; \mathrm{E}[1]) \;.\; \mathrm{A}) \;+\; ((x \;\; \mathrm{E}[1]) \;.\; \mathrm{A} \;.\; x)$$

```
> GreensFunction(%);
```

$$\begin{cases} -\xi + x\xi & 0 <= \xi \text{ and } \xi <= x \text{ and } x <= 1 \\ -x + x\xi & 0 <= x \text{ and } x <= \xi \text{ and } \xi <= 1 \end{cases}$$

For simplifying boundary problems, we can apply factorizations into lower order problems along given factorizations of the differential operators. Further details and proofs of the following results can be found in [16] and [11]. The composition of two boundary problems $(T_1, \mathcal{B}_1)$ and $(T_2, \mathcal{B}_2)$ is defined as

$$(T_1, \mathcal{B}_1) \circ (T_2, \mathcal{B}_2) = (T_1 T_2, T_2^*(\mathcal{B}_1) + \mathcal{B}_2). \tag{5}$$

The composition $(T_1, \mathcal{B}_1) \circ (T_2, \mathcal{B}_2)$ of two regular boundary problems is regular with Green's operator

$$((T_1, \mathcal{B}_1) \circ (T_2, \mathcal{B}_2))^{-1} = (T_2, \mathcal{B}_2)^{-1} (T_1, \mathcal{B}_1)^{-1}. \tag{6}$$

Given a regular boundary problem $(T, \mathcal{B})$, every factorization $T = T_1 T_2$ can be lifted to a factorization $(T, \mathcal{B}) = (T_1, \mathcal{B}_1) \circ (T_2, \mathcal{B}_2)$, where $(T_1, \mathcal{B}_1)$ and $(T_2, \mathcal{B}_2)$ are regular and $\mathcal{B}_2 \leq \mathcal{B}$. For factorizing a differential operator, we use the function *DFactor* in the MAPLE package *DEtools*. As an easy example, we show how to factor the boundary problem from above; more examples for solving and factoring boundary problems can be found in our example worksheet.

```
> Bp := BP(T, BC(b1, b2));
```

$$Bp := \mathrm{BP}(\mathrm{D}^2,\ \mathrm{BC}(\mathrm{E}[0],\ \mathrm{E}[1]))$$

```
> f1, f2 := FactorBoundaryProblem(Bp);
```

$$f1,\ f2 := \mathrm{BP}(\mathrm{D},\ \mathrm{BC}(\mathrm{E}[1]\ .\ \mathrm{A})),\ \mathrm{BP}(\mathrm{D},\ \mathrm{BC}(\mathrm{E}[0]))$$

4 Singular Boundary Problems

For illustrating the main issues with singular boundary problems, we consider the boundary problem

$$\boxed{\begin{array}{l} u'' = f, \\ u'(0) = u'(1) = 0; \end{array}} \tag{7}$$

see for example [4, Page 215] or [18, Section 3.5] from a Symbolic Computation perspective. This problem is singular since it is not solvable for all $f \in \mathcal{F}$. It can easily be seen that if $u'' = f$, then f has to fulfill the *compatibility condition* $u'(1) = \int_0^1 f(\xi)\, d\xi = 0$. Moreover, uniqueness fails as well: If a solution $u \in \mathcal{F}$ exists, then also $u + c$ solves the problem for all $c \in \mathbb{R}$.

Our goal here is to generalize the symbolic approach of the previous section to problems of the kind (7). Since we want to compute generalized Green's operators, we cannot give up uniqueness of solutions—but we no longer require existence. Of course, uniqueness of solutions can always be achieved by imposing additional boundary conditions. On the other hand, adding too many conditions introduces new compatibility conditions, which we want to avoid (see after Lemma 1 for the precise statement). For the boundary problem (7), we can add for example the condition $u(1) = 0$ and consider the problem

$$\boxed{\begin{array}{l} u'' = f, \\ u'(0) = u'(1) = u(1) = 0. \end{array}} \tag{8}$$

This does not introduce any new compatibility conditions as we will see later (see before Lemma 2).

A boundary problem has at most one solution for each forcing function f iff $\mathcal{B}^\perp \cap \operatorname{Ker} T = \{0\}$. We see that for (7) we have $\mathcal{B}^\perp \cap \operatorname{Ker} T = \mathbb{R}$ while in (8) the intersection is $\{0\}$. The regularity test for boundary problems in terms of the evaluation matrix (4) can be generalized from the setting in Section 3.

Lemma 1. *Let $U = [u_1, \ldots, u_n] \leq \mathcal{F}$ and $\mathcal{B} = [\beta_1, \ldots, \beta_m] \leq \mathcal{F}^*$ with β_i and u_j linearly independent. Then $U \cap \mathcal{B}^\perp = \{0\}$ iff the evaluation matrix $\beta(u)$ has full column rank.*

Proof. Let b_j denote the columns of $\beta(u)$. The evaluation matrix has deficient column rank iff there exists a linear combination $\sum_{j=1}^n \lambda_j b_j = 0$ with at least one $\lambda_j \neq 0$. This is the case iff there exist a nonzero $u = \sum_{j=1}^n \lambda_j u_j \in U \cap \mathcal{B}_1^\perp$. □

As mentioned for the example (8), singular boundary problems typically impose *compatibility conditions* on the admissible forcing functions. We can now make this precise: Clearly, a function f is admissible iff it is of the form Tu for a function u that satisfies the boundary conditions from $\mathcal{B}$, so the space of admissible functions is $T(\mathcal{B}^\perp)$. The compatibility conditions provide an implicit description of this space, comprising all those linear functionals that annihilate $T(\mathcal{B}^\perp)$. In other words, the compatibility conditions are the subspace $T(\mathcal{B}^\perp)^\perp$ of $\mathcal{F}^*$. This also makes precise what we mean by adding boundary conditions without imposing additional compatibility conditions: We enlarge $\mathcal{B}$ to $\tilde{\mathcal{B}}$ so as to ensure $\tilde{\mathcal{B}}^\perp \cap \operatorname{Ker} T = \{0\}$ despite retaining $T(\mathcal{B}^\perp) = T(\tilde{\mathcal{B}}^\perp)$.

For tackling the problem of existence, we modify the forcing function. In the example (8), this looks as follows: Since a solution exists only for forcing functions that fulfill $\int_0^1 f(\xi)\,d\xi = 0$, we consider the problem

$$\boxed{\begin{array}{l} u'' = f - \int_0^1 f(\xi)\,d\xi, \\ u'(0) = u'(1) = u(1) = 0, \end{array}} \tag{9}$$

which now always has a unique solution. For those f that fulfill the compatibility condition, problem (8) remains unchanged.

The general idea is that we project an arbitrary forcing function into the space of admissible functions. But this involves choosing those "exceptional functions" that we want to filter out. Even in the simple example (8), we might as well project f to $f - \frac{1}{2}x\int_0^1 f(\xi)\,d\xi$ instead of $f - \int_0^1 f(\xi)\,d\xi$. In the second case, we have filtered out the constant functions, in the first case the linear-homogeneous ones. The space $\mathcal{E}$ of exceptional functions can be any complement of the space $T(\mathcal{B}^\perp)$ of admissible functions, like $\mathcal{E} = [1]$ or $\mathcal{E} = [x]$ in this example.

Definition 1. *A* generalized boundary problem *is given by a triple* $(T, \mathcal{B}, \mathcal{E})$*, where* $(T, \mathcal{B})$ *is a boundary problem and* $\mathcal{E} \leq \mathcal{F}$*. A generalized boundary problem is called* regular *if*

$$\mathcal{B}^\perp \cap \operatorname{Ker} T = \{0\} \quad \textit{and} \quad \mathcal{F} = T(\mathcal{B}^\perp) \dotplus \mathcal{E}.$$

The generalized Green's operator *maps each forcing function* f *to the unique solution of the boundary problem*

$$\boxed{\begin{array}{l} Tu = Qf, \\ \beta_1 u = \ldots = \beta_m u = 0, \end{array}}$$

where $\mathcal{B} = [\beta_1, \ldots, \beta_m]$ *and* Q *is the projector onto* $T(\mathcal{B}^\perp)$ *along* $\mathcal{E}$*. We also write* $(T, \mathcal{B}, \mathcal{E})^{-1}$ *for the Green's operator.*

If $(T, \mathcal{B}, \mathcal{E})$ is regular, the restriction $T|_{\mathcal{B}^\perp} \colon \mathcal{B}^\perp \to T(\mathcal{B}^\perp)$ is bijective. So the generalized Green's operator is given by

$$G = T|_{\mathcal{B}^\perp}^{-1} Q. \tag{10}$$

We begin with computing the projector Q. For this we derive first an explicit description of the space of compatibility conditions.

Proposition 1. *Let $(T, \mathcal{B}, \mathcal{E})$ be a generalized boundary problem and let G be any right inverse of T. Then we have*

$$T(\mathcal{B}^\perp)^\perp = G^*(\mathcal{B} \cap (\operatorname{Ker} T)^\perp). \tag{11}$$

Moreover, $\dim T(\mathcal{B}^\perp)^\perp = \dim \mathcal{E}$ *for any complement* $\mathcal{E}$ *with* $\mathcal{F} = T(\mathcal{B}^\perp) \dotplus \mathcal{E}$.

Proof. With [16, Prop. A.6], we see that $T(\mathcal{B}^\perp)^\perp = (T^*)^{-1}(\mathcal{B})$. Since T is surjective, T^* is injective, and for any right inverse G of T, G^* is a left inverse of T^*. Hence $(T^*)^{-1}(\mathcal{B}) = G^*(\mathcal{B} \cap \operatorname{Im} T^*)$ by [16, Prop. A.13]. Again by [16, Prop. A.6], we have $\operatorname{Im} T^* = (\operatorname{Ker} T)^\perp$, and hence $T(\mathcal{B}^\perp)^\perp = G^*(\mathcal{B} \cap (\operatorname{Ker} T)^\perp)$.

Since $\dim \mathcal{B} < \infty$, by the first statement also $\dim T(\mathcal{B}^\perp)^\perp < \infty$. But $T(\mathcal{B}^\perp)$ is orthogonally closed; see for example [16, Section A.1]. Therefore we obtain

$$\dim T(\mathcal{B}^\perp)^\perp = \operatorname{codim} T(\mathcal{B}^\perp)^{\perp\perp} = \operatorname{codim} T(\mathcal{B}^\perp),$$

and the statement follows immediately from [16, Prop. A.14]. □

Note that $s = \dim \mathcal{E} = \operatorname{codim} T(\mathcal{B}^\perp)$ counts the number of (linearly independent) compatibility conditions. Equation (11) is the key for an algorithmic description of the projector Q onto $T(\mathcal{B}^\perp)$ along $\mathcal{E}$. The space $\mathcal{E}$ is given as part of the problem description, and it can be specified by a basis $(w_1, \ldots, w_s)$. Since the other space $T(\mathcal{B}^\perp)$ has finite codimension s, it can be specified in terms of s linearly independent compatibility conditions, and Equation (11) can be used to compute these in terms of T and $\mathcal{B}$. For that we just have to determine a basis of $\mathcal{B} \cap (\operatorname{Ker} T)^\perp$ and then apply any right inverse G of T, for example the fundamental right inverse $T^\blacklozenge$ defined in Section 3.

For determining a basis of $\mathcal{B} \cap (\operatorname{Ker} T)^\perp$ we first compute the kernel of the transpose of the evaluation matrix $\beta(u)$, where $(u_1, \ldots, u_n)$ is any basis of $\operatorname{Ker} T$ and $(\beta_1, \ldots, \beta_m)$ any basis of $\mathcal{B}$. If $w = (w_1, \ldots, w_m)^t \in \operatorname{Ker} \beta(u)^t$, then

$$w^t(\beta_1, \ldots, \beta_m)^t = \sum_{i=1}^m w_i \beta_i \in \mathcal{B} \cap (\operatorname{Ker} T)^\perp,$$

hence a basis of $\mathcal{B} \cap (\operatorname{Ker} T)^\perp$ can be obtained by computing the products $(v_1^t(\beta_1, \ldots, \beta_m)^t, \ldots, v_k^t(\beta_1, \ldots, \beta_m)^t)$, where $(v_1, \ldots, v_k)$ is a basis of $\operatorname{Ker} \beta(u)^t$.

Using Proposition 1, we can now verify that the compatibility conditions of the boundary problems (7) and (8) are the same. In both cases we have $T = \partial^2$, so we can choose the fundamental right inverse $\textstyle\int\!\int = x\int - \int x$ and $(1, x)$ as a basis of $\operatorname{Ker} T$. The evaluation matrices are given by

$$\beta(u) = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \beta(u) = \begin{pmatrix} 0 & 1 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}.$$

In the first case, a basis of $\beta(u)^t$ is given by $((-1, 1)^t)$, hence $(\mathrm{E}_1\partial - \mathrm{E}_0\partial)$ is a basis of $\mathcal{B} \cap (\operatorname{Ker} T)^\perp$. In the second case, a basis of $\beta(u)^t$ is given by $((-1, 1, 0)^t)$

and the basis of $\mathcal{B} \cap (\operatorname{Ker} T)^{\perp}$ is again $(\mathrm{E}_1\partial - \mathrm{E}_0\partial)$. Multiplying this basis by the right inverse of T, we get as a basis for the compatibility conditions

$$\begin{aligned}(\mathrm{E}_1\partial - \mathrm{E}_0\partial) \cdot (x{\textstyle\int} - {\textstyle\int} x) &= \mathrm{E}_1(x\partial + 1){\textstyle\int} - \mathrm{E}_0(x\partial + 1){\textstyle\int} - \mathrm{E}_1\partial{\textstyle\int} x + \mathrm{E}_0\partial{\textstyle\int} x\\ &= \mathrm{E}_1 x + \mathrm{E}_1{\textstyle\int} - \mathrm{E}_0 x - \mathrm{E}_0{\textstyle\int} - \mathrm{E}_1 x + \mathrm{E}_0 x = \mathrm{E}_1{\textstyle\int} = {\textstyle\int_0^1},\end{aligned}$$

which agrees with our heuristic considerations after (7).

We can now compute the projector Q just as the kernel projector P for standard boundary problems (mentioned in Section 3). If $(\kappa_1, \dots, \kappa_s)$ is a basis for the compatibility conditions $T(\mathcal{B}^{\perp})^{\perp}$ and $(w_1, \dots, w_s)$ a basis for $\mathcal{E}$, then the corresponding evaluation matrix $\kappa(w)$ is regular by Lemma 1, which can be applied to $\mathcal{F} = T(\mathcal{B}^{\perp}) \dotplus \mathcal{E} = T(\mathcal{B}^{\perp})^{\perp\perp} \dotplus \mathcal{E}$ since $T(\mathcal{B}^{\perp})$ is orthogonally closed. Hence we can compute the projector Q onto $T(\mathcal{B}^{\perp})$ along $\mathcal{E}$ as

$$Q = 1 - \sum_{i=1}^{s} w_i \tilde{\kappa}_i,$$

where $(\tilde{\kappa}_1, \dots, \tilde{\kappa}_s)^t = \kappa(w)^{-1} \cdot (\kappa_1, \dots, \kappa_s)^t$; see for example [16, Lemma A.1].

The final step for computing the generalized Green's operator (10) is to find the inverse function $T|_{\mathcal{B}^{\perp}}^{-1}$. In the regular case, we started with an arbitrary right inverse of T and multiplied with a projection onto $\mathcal{B}^{\perp}$ along $\operatorname{Ker} T$. But this step cannot be generalized to our setting. Our approach is to embed the generalized problem into a standard one in the following sense.

First note that the evaluation matrix of a regular generalized boundary problem has full column rank by Lemma 1, so it has a left inverse.

Lemma 2. *Let $(T, \mathcal{B}, \mathcal{E})$ be a regular generalized boundary problem. Let $\beta(u)^{-}$ be a left inverse of $\beta(u)$ and $(\tilde{\beta}_1, \dots, \tilde{\beta}_n)^t = \beta(u)^{-}(\beta_1, \dots, \beta_m)^t$. Then the boundary problem $(T, \tilde{\mathcal{B}})$ is regular, where $\tilde{\mathcal{B}} \leq \mathcal{B}$ is spanned by $\tilde{\beta}_1, \dots, \tilde{\beta}_n$.*

The proof of the statement is obvious, since the evaluation matrix $\tilde{\beta}(u)$ is given by $\beta(u)^{-}\beta(u) = 1_n$. Hence the problem $(T, \tilde{\mathcal{B}})$ is regular. In our package, we always choose the Moore-Penrose pseudoinverse as a left inverse $\beta(u)^{-}$ of the evaluation matrix $\beta(u)$. The generalized boundary problem (8) for example embeds into the standard boundary problem

$$\boxed{\begin{aligned}&u'' = f,\\ &u'(0) + u'(1) - 2\,u(1) = u'(0) + u'(1) = 0.\end{aligned}} \tag{12}$$

The Green's operator for this regular problem according to Section 3 is given by $x{\textstyle\int} - {\textstyle\int} x - \frac{1}{2}(x+1) + {\textstyle\int_0^1} x$. The next proposition tells us how to compute the generalized Green' s operator from it.

Proposition 2. *Let $(T, \mathcal{B}, \mathcal{E})$ be a regular generalized boundary problem and let $(T, \tilde{\mathcal{B}})$ be a regular boundary problem with $\tilde{\mathcal{B}} \leq \mathcal{B}$. Then*

$$(T, \mathcal{B}, \mathcal{E})^{-1} = (T, \tilde{\mathcal{B}})^{-1}\, Q,$$

where Q is the projector onto $T(\mathcal{B}^{\perp})$ along $\mathcal{E}$.

Proof. Since $\tilde{\mathcal{B}} \leq \mathcal{B}$, we have $\mathcal{B}^\perp \leq \tilde{\mathcal{B}}^\perp$. Hence the maps $T|_{\mathcal{B}^\perp}^{-1}$ and $\tilde{G} = (T, \tilde{\mathcal{B}})^{-1}$ coincide on $\mathcal{B}^\perp$. Since $T|_{\mathcal{B}^\perp} \colon \mathcal{B}^\perp \to T(\mathcal{B}^\perp)$ is a bijection, we can compute the restriction $T|_{\mathcal{B}^\perp}^{-1}$ by first applying a projector onto $T(\mathcal{B}^\perp)$ and then $\tilde{G}$. Hence $T|_{\mathcal{B}^\perp}^{-1} = \tilde{G}Q$, where Q is again the projection onto $T(\mathcal{B}^\perp)$ along $\mathcal{E}$. Hence the generalized Green's operator is given by $G = T|_{\mathcal{B}^\perp}^{-1} Q = \tilde{G}Q^2 = \tilde{G}Q$. □

Applying the previous proposition to Example (8) leads to the generalized Green's operator $x{\textstyle\int} - {\textstyle\int} x - \frac{1}{2}(x^2+1){\textstyle\int}_0^1 + {\textstyle\int}_0^1 x$. For a more involved example illustrating the Maple functions in our package, we refer to the Appendix.

5 Outlook

We are currently investigating in how far the composition of boundary problems (5) can be extended to generalized boundary problems such that an analog of the "reverse order law" (6) holds. We can see in the example below (13) that for such a generalization, we also have to modify the second component with the boundary conditions. The question under which conditions a reverse order law holds for different classes of generalized inverses—not necessarily related to integro-differential operators—is extensively studied in the literature, see for example [19] and the references therein.

The search for generalized composition laws is intimately connected with the question of "embedding" a singular boundary problem into a regular problem of higher order. For example in [18], the Green's operator G of the generalized boundary problem $(\partial^2, [\mathrm{E}_0\partial, \mathrm{E}_1\partial, {\textstyle\int}_0^1], [1])$ can be factored as $G = \tilde{G} \circ \partial$ where $\tilde{G}$ is the standard Green's operator of the boundary problem $(\partial^3, [\mathrm{E}_0\partial, \mathrm{E}_1\partial, {\textstyle\int}_0^1])$. Hence $\tilde{G} = G \circ {\textstyle\int}_0^x$ and, assuming (6) for the composition, also

$$(\partial^3, [\mathrm{E}_0\partial, \mathrm{E}_1\partial, {\textstyle\int}_0^1], [0]) = (\partial, [\mathrm{E}_0], [0]) \circ (\partial^2, [\mathrm{E}_0\partial, \mathrm{E}_1\partial, {\textstyle\int}_0^1], [1]), \qquad (13)$$

since ${\textstyle\int}_0^x$ is the Green's operator of the boundary problem $(\partial, [\mathrm{E}_0])$. The singular second-order problem is thus embedded into a regular third-order one.

Multi-point boundary problems can also be treated by our method, yielding a suitable Green's operator just as in the classical two-point setting. Generalizing the extraction procedure for Green's functions is future work, see [20] for an analytic description of Green's functions for multi-point boundary problems.

Going from LODEs to LPDEs, more drastic changes are necessary since geometry enters the picture. For example, the Green's operator of the inhomogeneous wave equation $u_{xx} - u_{tt} = f$ with homogeneous Dirichlet data on the x-axis integrates f over a certain triangle whose tip is at (x, t). In terms of the operator algebra, this means one must incorporate the chain and substitution rule along with explicit operators encoding change of variables. A first approach along these lines, for the very simple case of linear coordinate changes, was presented in [2] and is currently being refined. Studying singular boundary problems for LPDEs from a symbolic point of view is also very interesting; see for example [21] for a Gröbner bases approach to compute the (hierarchy of) compatibility conditions for elliptic boundary problems. It would be tempting to combine the tools of involutive systems used there with the setting of operator rings used here.

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A Example

Now we will give a detailed example for computations with generalized boundary problems. We introduced a new datatype $\texttt{GBP}(T, \texttt{BC}(b1,\dots,bm), \texttt{ES}(f1,\dots,fk))$, where T and $(b1,\dots,bm)$ again are a differential operator and boundary conditions and $(f1,\dots,fm)$ is a basis of the exceptional space. We added the new procedures *CompatibilityConditions, IsComplement* and *Projector*, which will be explained later and extended the procedures *GreensOperator* and *IsRegular*. The first one now also computes the Green's Operator for a generalized boundary problem and the second one tests the condition $\operatorname{Ker} T \cap \mathcal{B}^{\perp} = \{0\}$ also for generalized boundary problems.

We consider the more complicated example

$$\boxed{\begin{array}{l} u'''' + u'' = f \\ u'(0) = u''(0) = u''(\pi) = u'''(0) = u'''(\pi) = 0. \end{array}} \tag{14}$$

We enter the boundary problem stated above and compute a fundamental system for the differential operator $T = \mathrm{D}^4 + \mathrm{D}^2$.

```
> T := DIFFOP(0, 0, 1, 0, 1):
> b[1] := BOUNDOP(EVOP(0, EVDIFFOP(0, 1), EVINTOP())):
> b[2] := BOUNDOP(EVOP(0, EVDIFFOP(0, 0, 1), EVINTOP())):
> b[3] := BOUNDOP(EVOP(0, EVDIFFOP(0, 0, 0, 1), EVINTOP())):
> b[4] := BOUNDOP(EVOP(Pi, EVDIFFOP(0, 0, 1), EVINTOP())):
> b[5] := BOUNDOP(EVOP(Pi, EVDIFFOP(0, 0, 0, 1), EVINTOP())):
> Bp := BP(T, BC(b[1],b[2],b[3],b[4],b[5])):
> fs := FundamentalSystem(T);
```

$$[x,\ \sin(x),\ \cos(x),\ 1]$$

Now we add another boundary condition b[6] in order to achieve uniqueness of solutions. This can be checked by considering the column rank of the evaluation matrix. We further verify that the compatibility conditions of both problems are the same.

```
> b[6] := BOUNDOP(EVOP(Pi, ZEROEDOP, EVINTOP(EVINTTERM(1,1)))):
> BpA := BP(T, BC(b[1],b[2],b[3],b[4],b[5],b[6])):
> IsRegular(BpA);
```

$$true$$

```
> CompatibilityConditions(Bp);
```

$$\mathrm{BC}((\mathrm{E}[\mathrm{Pi}]\,.\,\mathrm{A}\,.\,(\sin(x)),\ (\mathrm{E}[\mathrm{Pi}])\,.\,\mathrm{A}\,.\,(\cos(x)))$$

```
> CompatibilityConditions(BpA);
```

$$\mathrm{BC}((\mathrm{E}[\mathrm{Pi}]\,.\,\mathrm{A}\,.\,(\sin(x)),\ (\mathrm{E}[\mathrm{Pi}])\,.\,\mathrm{A}\,.\,(\cos(x)))$$

Now we enter a generalized boundary problem and check that our choice $[1,\ x]$ as exceptional space is a complement of $T(\mathcal{B}^{\perp})$. Then we compute the projector Q onto $T(\mathcal{B}^{\perp})$ and the Green's operator for the generalized boundary problem $(T, [\mathrm{b}[1], \mathrm{b}[2], \mathrm{b}[3], \mathrm{b}[4], \mathrm{b}[5], \mathrm{b}[6]], [1, x])$,

```
> gBp := GBP(T, BC(b[1],b[2],b[3],b[4],b[5],b[6]), ES(1,x)):
> IsComplement(gBp);
```

$$true$$

```
> Q := Projector(gBp):
```

$$Q := 1 - \frac{1}{2}((\mathrm{E}[\mathrm{Pi}])\,.\,A\,.\,(\sin(x))) + \left(\left(-\frac{\mathrm{Pi}}{4} + \frac{x}{2}\right)\,.\,(\mathrm{E}[\mathrm{Pi}])\,.\,A\,.\,(\cos(x)\right)$$

```
> G := GreensOperator(gBp):
```

Finally we verify that the Green's operator G fulfills the equation $TG = Q$ and the six boundary conditions.

```
> simplify(SubtractOperator(MultiplyOperator(T, G), Q))
```

$$0$$

```
> seq(simplify(MultiplyOperator(b[i], G)), i=1..6);
```

$$0,\ 0,\ 0,\ 0,\ 0,\ 0$$