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TACO — A Toolkit for AMPL Control Optimization

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Abstract We describe a set of extensions to the AMPL modeling language to conveniently model mixed-integer optimal control problems for ODE or DAE dynamic processes. These extensions are realized as AMPL user functions and suffixes and do not require intrusive changes to the AMPL language standard or implementation itself. We describe and provide TACO, a Toolkit for AMPL Control Optimization that reads AMPL *stub.nl* files and detects the structure of the optimal control problem. This toolkit is designed to facilitate the coupling of existing optimal control software packages to AMPL. We discuss requirements, capabilities, and the current implementation. Using the example of the multiple shooting code for optimal control MUSCOD-II, a direct and simultaneous method for DAE-constrained optimal control, we demonstrate how the problem information provided by the TACO toolkit is interfaced to the solver. In addition, we show how the MS-MINTOC algorithm for mixed-integer optimal control can be used to efficiently solve mixed-integer optimal control problems modeled in AMPL. We use the AMPL extensions to model three exemplary control problems and we discuss how those extensions affect the representation of optimal control problems. Solutions to these problems are obtained by using MUSCOD-II and MS-MINTOC inside the AMPL environment. A collection of further AMPL control models is provided on the web site `mintoc.de`. MUSCOD-II and MS-MINTOC are made available on the NEOS Server for Optimization, using the TACO toolkit to enable input of AMPL models.

Keywords Mixed-Integer Optimal Control, Differential-Algebraic Equations, Domain Specific Languages, Mathematical Modeling

1 Introduction

This paper describes a set of extensions to the AMPL modeling language that extends AMPL's applicability to mathematical optimization problems including dynamic processes. We describe and implement AMPL syntax elements for convenient modeling of ordinary differential equation (ODE) and differential algebraic equation (DAE) constrained optimal control problems.

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We consider the class (1) of mixed-integer optimal control problems on the time horizon $[0,T]$. Our goal is to minimize an objective function that includes an integral Lagrange term L on $[0,T]$, a Mayer term E at the end point T of the time horizon, and a point least-squares term with N_{lsq} possibly nonlinear residuals l_i on a grid $\{t_i\}_{1 \le i \le N_{\text{lsq}}}$ of time points. All objective terms depend on the trajectory $(x(\cdot), z(\cdot)) : [0,T] \to \mathbb{R}^{n_x} \times \mathbb{R}^{n_z}$ of a dynamic process described in terms of a system of ODEs (1b) or DAEs (1b, 1c). This system is affected by continuous controls $u(\cdot) : [0,T] \to \mathbb{R}^{n_u}$ and integer-valued controls $w(\cdot) : [0,T] \to \Omega_{\text{w}}$ from a finite discrete set $\Omega_{\text{w}} := \{w^1, \ldots, w^{n_{\Omega_{\text{w}}}}\} \subset \mathbb{R}^{n_w}$, $|\Omega_{\text{w}}| = n_{\Omega_{\text{w}}} < \infty$ (1h). Both control profiles are subject to optimization. Moreover, we allow the end time T (1g), the continuous model parameters $p \in \mathbb{R}^{n_p}$, and the discrete–valued model parameters $\rho \in \Omega_\rho := \{\rho^1, \ldots, \rho^{n_{\Omega_\rho}}\} \subset \mathbb{R}^{n_p}$, $|\Omega_\rho| = n_\rho < \infty$ (1i) to be subject to optimization as well. Control, parameters, and process trajectory may be constrained by inequality path constraints $c(\cdot)$ (1d), equality constraints $r_{\text{c}}^{\text{eq}}(\cdot)$ and inequality constraints $r_{\text{c}}^{\text{in}}(\cdot)$ coupled in time (1e), and decoupled equality and inequality constraints $r_i^{\text{eq}}(\cdot)$, $r_i^{\text{in}}(\cdot)$, $1 \le i \le n_{\text{r}}$ (1f), imposed on a grid $\{t_i\}_{1 \le i \le N_{\text{r}}}$ of time points on time horizon $[0,T]$. This constraint grid need not coincide with the point least-squares grid. Constraints (1d)–(1f) include initial values and boundary values; mixed state-control constraints; periodicity constraints; and simple bounds on states, controls, and parameters. The optimal control problem is conveniently expressed as follows:

$$
\underset{\substack{x(\cdot),u(\cdot),w(\cdot),\\p,\rho,T}}{\text{minimize}} \quad \int_{t=0}^{T} L(t,x(t),z(t),u(t),w(t),p,\rho)\, \mathrm{d}t + E(T,x(T),z(T),p,\rho) \tag{1a}
$$
$$
+ \sum_{i=1}^{N_{\text{lsq}}} ||l_i(t_i,x(t_i),z(t_i),u(t_i),w(t_i),p,\rho)||_2^2, \quad t_i \in [0,T],
$$

$$
\text{subject to} \quad \dot{x}(t) = f(t,x(t),z(t),u(t),w(t),p,\rho), \qquad t \in [0,T], \tag{1b}
$$

$$
0 = g(t,x(t),z(t),u(t),w(t),p,\rho), \qquad t \in [0,T], \tag{1c}
$$

$$
0 \le c(t,x(t),z(t),u(t),w(t),p,\rho), \qquad t \in [0,T], \tag{1d}
$$

$$
0 = r_{\text{c}}^{\text{eq}}(x(0),z(0),x(T),z(T),p,\rho), \tag{1e}
$$

$$
0 \le r_{\text{c}}^{\text{in}}(x(0),z(0),x(T),z(T),p,\rho),
$$

$$
0 = r_i^{\text{eq}}(x(t_i),z(t_i),p,\rho), \qquad t_i \in [0,T],\ 1 \le i \le N_{\text{r}}, \tag{1f}
$$

$$
0 \le r_i^{\text{in}}(x(t_i),z(t_i),p,\rho),
$$

$$
T_{\min} \le T \le T_{\max}, \tag{1g}
$$

$$
w(t) \in \Omega_{\text{w}}, \qquad t \in [0,T], \tag{1h}
$$

$$
\rho \in \Omega_\rho. \tag{1i}
$$

Direct and simultaneous methods for tackling the class of optimization problems (1) posed in function spaces are based on the first-discretize-then-optimize approach. A discretization scheme is chosen and applied to objective (1a), dynamics (1b, 1c), and path constraints (1d) of the optimization problem in order to obtain a finite-dimensional counterpart problem accessible to mathematical programming algorithms. This counterpart problem will usually be a high-dimensional and highly structured nonlinear problem (NLP) or mixed-integer nonlinear problem (MINLP). Thus, it readily falls into the domain of applicability of many mathematical optimization software packages already interfaced with AMPL, such as ALGENCAN [5, 6], filterSQP [26], IPOPT [63], KNITRO [15, 16, 17], LANCELOT [19], LOQO [62], MINOS [50], NPSOL [32], PENNON [38], or SNOPT [33] for nonlinear programming and Bonmin [12], Couenne [9], MINLPBB [44], or FilMINT [1] for mixed-integer nonlinear programming.

1.1 The AMPL Modeling Language

AMPL is described by Fourer et al [29] and was designed as a mathematical modeling language for linear programming problems. It has been extended to integer and mixed-integer linear problems, to mixed-integer nonlinear problems, to complementarity problems [28], and to semidefinite problems [39]. AMPL's syntax closely resembles the symbolic and algebraic notation used to present mathematical optimization problems and allows for fully automatic processing of optimization problems by a computer system. The availability of a symbolic problem representation enabled by AMPL's approach to modeling mathematical optimization problems has a number of significant advantages. These include the possibility for automatic differentiation, extended error checking facilities, automated analysis of model parts for certain structural properties such as linearity or convexity, and the opportunity for automatically generating model code for lower-level languages [30, 31]. The long–standing popularity and success of AMPL are underlined by the wealth of mathematical optimization software packages available on the NEOS Server for Optimization [34] that provide interfaces to read and solve problems modeled using the AMPL language.

1.2 Benefits of AMPL Extensions

We extend the AMPL modeling language by a facility that conveys the notion of ODE and DAE constraints (1b, 1c) to a nonlinear or mixed-integer nonlinear problem solver. If given a generic description of a selected discretization method, the solver applies this discretization to obtain an (MI)NLP with discretized objective and constraints to work on. Our approach removes the need for tedious explicit encoding of fixed discretization schemes in the AMPL model, as is done, for example, for collocation schemes in [24]. Adaptive choice and iterative refinement of the discretization, see e.g. [36], become possible. At the same time, this idea opens up the possibility of using other and more involved discretization schemes that cannot be expressed directly in AMPL. One example is direct multiple–shooting methods [11] that enable the use of state-of-the-art ODE and DAE solvers (see e.g. [4, 52]) with increased opportunities for exploiting structure and adaptivity. Our approach provides a generic way of tackling challenging mixed-integer dynamic optimization problems with the most recent and up-to-date methods developed in the MINLP community.

1.3 Related Efforts

The idea of a high-level modeling language for dynamic simulation and optimization problems is not new. Driven by demands of the industrial and engineering communities, several efforts have led to the creation of commercial development environments for simulation and partly also for optimization of dynamic processes, some examples being gPROMS [7], Tomlab's PROPT [56], Dymola [25], Modelica [47], and recently the open-source initiative JModelica/Optimica [3]. In contrast to our approach, however, these development environments focus on the end-user's convenience of interaction with the development environment, and are often closely tied to one or a few selected discretization schemes and solvers only.

1.4 Contributions and Structure

In this paper we describe a set of extensions to the AMPL modeling language that extends AMPL's applicability to mathematical optimization problems constrained by ODE and DAE dynamics, in other words optimal control problems. All extensions are realized as either *AMPL user functions* or *AMPL suffixes*. Both user functions and suffixes

are an integral parts of the existing AMPL language standard. Hence, no intrusive changes to the AMPL language standard or implementation itself are required to realize the extensions.

We describe an open-source implementation of our extensions called TACO, a Toolkit for AMPL for Control Optimization. TACO is designed to facilitate the coupling of existing optimal control software packages to AMPL. It allows us to read AMPL *stub.nl* files and detect the optimal control problem's structure. We use TACO to interface the two codes MUSCOD-II and MS-MINTOC with AMPL. MUSCOD-II, the multiple shooting code for optimal control described by [42, 43] and [11, 22], is a direct and simultaneous method for DAE-constrained optimal control. MS-MINTOC extends this software package by multiple-shooting mixed-integer optimal control algorithms [57, 59].

The applicability of our extensions is shown using three examples of ODE-constrained control problems. A larger collection of AMPL models for ODE and DAE-constrained mixed-integer optimal control is made available on the web site `mintoc.de` [59]. In addition, using the TACO interface, the solver MUSCOD-II and its MS-MINTOC extension are made available on the NEOS Server for Optimization [34] at `http://neos-server.org/neos/`. The TACO source code may be obtained from `http://www.iwr.uni-heidelberg.de/groups/agbock/FILES/taco_source.tar.gz`.

The remainder of this paper is structured as follows. In §2 we propose several extensions to the AMPL modeling language and realize them through AMPL user functions and suffixes. Three exemplary AMPL models are discussed in §3, and a collection of further AMPL models available from the web site `mintoc.de` is described. Consistency and smoothness checks performed by TACO and possible errors that may be encountered in this phase are described in §4. We also discuss the communication of optimal solutions of time-dependent variables to AMPL. In §5 we show how to use the information provided by TACO to realize an interface coupling the optimal control software package MUSCOD-II and the mixed-integer optimal control algorithm MS-MINTOC to AMPL. The use of AMPL's automatic derivatives within an ODE/DAE solver is discussed. In §6, limitations and possible future extensions of the considered problem class are addressed. We conclude in §7 with a brief summary.

Three appendix sections hold technical information about the TACO implementation that may be of interest to developers of optimal control codes who wish to interface their codes with AMPL.

2 AMPL Extensions for Optimal Control

The modeling language AMPL has been designed for finite-dimensional optimization problems. When attempting to model optimal control problems for DAE dynamic processes in AMPL without encoding a discretization of the dynamics in the model itself, one is confronted with several challenges. First, variables representing trajectories on a time horizon $[0, T]$ require a notion of time dependency. Second, certain constraints model ODE or DAE dynamics, and this knowledge must be conveyed to the solvers. Third, objectives and constraints containing trajectory-representing variables may refer either to the entire trajectory, or to an evaluation of that trajectory in a certain point in time.

In this section we describe extensions to the AMPL syntax that address these issues and allow for a convenient formulation of the optimal control problem (1). All extensions are realized either as user functions or via AMPL suffixes and do not require modifications of the AMPL system itself. Hence, they are readily applicable in any development or research environment that provides access to AMPL. An example of the new AMPL extensions is shown in Fig. 1 for a nonlinear toy problem found in [21].

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```
var t;
var x >= -1, <= 1, := -0.05;
var u >= -1, <= 1, := 0 suffix type "u0";
param p := 1.0;
```

$$\underset{x(\cdot),u(\cdot),p}{\text{minimize}} \int_0^3 x(t)^2 + u(t)^2 \, dt$$

```
minimize Lagrange: integral (x^2 + u^2, 3);
subject to
```

$$\text{subject to} \quad \dot{x}(t) = (x(t) + p)x(t) - u(t),$$

```
ODE: diff (x, t) = (x + p) * x - u;
```

$$x(0) = -0.05,$$

```
IC: eval (x, 0) = -0.05;
```

$$-1 \leq x(t) \leq 1,$$

$$-1 \leq u(t) \leq 1.$$

Fig. 1 Exemplary use of the new AMPL extensions `integral`, `diff`, and `eval` in the AMPL model (right) for an ODE-constrained optimal control problem (left). Initial guesses for p and for $x(t)$ and $u(t)$ on $[0, T]$ found in the AMPL model are not given in the mathematical problem formulation.

2.1 Modeling Optimal Control Problem Variables

A major task in detecting the optimal control problem's structure is to automatically infer the role AMPL variables should play in problem (1). We introduce the AMPL suffix `type` to describe the rules of inference.

Independent Time. In the following we expect any optimal control problem to declare a variable representing independent time t in (1). For consistency, we assume this variable to always be named `t` in this paper. There is, however, no restriction to the naming or physical interpretation of this variable in an actual AMPL model. The independent time variable is detected by its appearance in a call to the user-function `diff`. The use of the same variable in all calls to `diff` is enforced for well-posedness.

For the end point T of the time horizon $[0, T]$, occasionally named `T` in AMPL models in this paper, the user is free to introduce either a variable, for example, if T is free and subject to optimization, or to use a numerical constant (as in Fig. 1) or a defined variable if T is fixed.

Differential State Variables. States are denoted by $x(\cdot)$ or $x_i(\cdot)$ in this paper. They are detected by their appearance in a call to the user-function `diff` (see Fig. 1), which defines the differential right-hand side for this state. Every differential state variable must appear in exactly one call to `diff`.

Algebraic State Variables. Algebraic state variables are denoted by $z(\cdot)$ or $z_i(\cdot)$ in this paper. Since any DAE constraint may involve more than one algebraic state variable, there is, unlike in the ODE case, no one–one correspondence between DAE constraints and DAE variables. Hence, we detect DAE variables by flagging them as such using an AMPL suffix named `type`, which is set to the symbolic value `"dae"`.

Continuous and Integer Control Variables Control variables, denoted by $u_i(\cdot)$ and $w_i(\cdot)$, are detected by flagging them as such using the new AMPL suffix `type`, which is set to one of several symbolic values representing choices for the control discretization (see Fig. 1). The current implementation offers the following types: piecewise constant (`type` assumes the value `"u0"`), piecewise linear (`"u1"`), piecewise linear continuous (`"u1c"`), piecewise cubic (`"u3"`), and piecewise cubic continuous (`"u3c"`) discretizations. Integer controls may simply be declared by making use of existing AMPL syntax elements such as the keywords `integer` and `binary`.

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Continuous and Integer Parameters Any AMPL variable not inferred to be independent or final time, differential or algebraic state, or control according to the rules described above is considered a model parameter p_i or ρ_i that is constant in time but may be subject to optimization, for example, in parameter estimation problems. Again, integer parameters may be declared by making use of the existing AMPL syntax elements `integer` and `binary`.

2.2 Modeling Optimal Control Problem Constraints

In this section we show how to extend AMPL to model the various types of constraints found in problem (1).

Dynamics: ODE Constraints. We introduce a user-function `diff(var,t)` that is used in equality constraints to denote the left–hand side of an ODE (1b). The first argument `var` denotes the differential state variable for which a right–hand side is to be defined. The second argument `t` is expected to denote the independent time variable. Currently, only explicit ODEs are supported, in other words, the `diff` expression in ODE constraints must appear isolated on one side of the constraint.

The point of interest here is the mere appearance of a call to `diff` in an AMPL constraint expression that allows us to distinguish an ODE constraint from other constraint types. The actual implementation of `diff` is bare of any functionality and may simply return the value zero.

Dynamics: DAE Constraints. An *equality* constraint involving state or control variables that calls neither `eval` nor `diff` is understood as a DAE constraint (1c).

Most DAE solvers will expect the DAE system to be of index 1. This means that the number of DAE constraints (1c) must match the number n_z of algebraic states declared by suffixes, and the common Jacobian of all DAE constraints w.r.t. the algebraic states must be regular in a neighborhood of the DAE trajectory $t \in [0,T] \mapsto (x(t),z(t))$. The first requirement can be readily checked. The burden of ensuring regularity is put on the modeler creating the AMPL model but can be verified locally by a DAE solver at runtime.

Path Constraints. An *inequality* constraint that calls neither `eval` nor `diff` is understood as an inequality path constraint (1d).

Point Constraints. Point constraints impose restrictions on the values of trajectories at discrete points $t_i \in [0,T]$. We introduce a user function `eval(expr,time)` that denotes the evaluation of a state or control trajectory, or more generally an analytic expression `expr` referring to such trajectories, at a given fixed point `time` in $[0,T]$. This function allows us to model point constraints (1e, 1f) in a straightforward way. Figure 1 shows an initial-value constraint.

Note on Evaluation Time Points. For problems with fixed end-time T, time points `time` in calls to `eval` are absolute values in the range $[0,T]$. Negative values and values exceeding T are forbidden.

For problems with free final time T, namely for problems using an AMPL variable `T` representing the final time T properly introduced and free to vary between its lower and upper bound, all time points need to be understood as *relative* times on the normalized time horizon $[0,1]$. For such problems it is neither possible nor desirable to specify absolute time points other than the boundaries $t = 0$ and $t = T$.

2.3 Modeling Optimal Control Problem Objectives

Problem (1) uses an objective function that consists of a Lagrange-type integral term L and a Mayer-type end-point term E. In addition, it is advantageous to detect least-squares structure of the integral Lagrange-term that can be exploited after discretization. We also support a point least-squares term in the objective, arising, for example, in parameter estimation problems.

Lagrange-Type and Integral Least-Squares-Type Objective Terms. We introduce a user function `integral(expr,T)` to denote an integral–type objective function. The first argument `expr` is the integrand, and the second one, `T`, is expected to denote the final time variable or value T; see Fig. 1. We always assume integration with respect to the independent time t, starting in $t = 0$. If `expr` is a sum of squares, the Lagrange-type objective is treated as an integral least-squares one.

Mayer-Type and Point Least-Squares-Type Objective Terms. The function `eval(expr,time)` can be used to model both Mayer-type (`time` is T) and point least-squares–type objective terms (`expr` is a sum of squares, and `time` is an arbitrary point $t_i \in [0,T]$ or $t_i \in [0,1]$). Note that for well-posedness, the Mayer-type objective function must not depend on control variables, a restriction that can be enforced.

2.4 Universal Header File for Optimal Control Problems

For convenience the AMPL declarations of the new functions `diff`, `eval`, and `integral`, as well as of the suffix `type` and its possible symbolic values, are collected in a header file named `OptimalControl.mod` that may be included in the first line of an AMPL optimal control model. Its contents are shown in Fig. 2.

```
suffix type symbolic IN;

option type_table '\
1  u0        piecewise constant control\
2  u1        piecewise linear control\
3  u1c       piecewise linear continuous control\
4  u3        piecewise cubic control\
5  u3c       piecewise cubic continuous control\
6  dae       DAE algebraic state variable\
7  Lagrange  Prevent least-squares detection in an objective\
';

function diff;      # differential operator: usage diff(var,t)
function eval;      # evaluation operator: usage eval(expr,ti)
function integral;  # integral operator: usage integral(expr,T)
```

Fig. 2 Declaration of user functions and suffixes in the header file `OptimalControl.mod`.

3 Examples of Optimal Control Models in AMPL

In this section we give two examples of using the new AMPL extensions to model dynamic optimization problems. The first problem is an ODE boundary value problem from the COPS library [24], and the second one is an ODE-constrained mixed-integer control problem from [57].

3.1 Example from the COPS Library of Optimal Control Problems

One first example involves analyzing the flow of a fluid during injection into a long vertical channel, assuming that the flow is modeled by the boundary value problem

$$u^{(4)}(t) = R\left(u^{(1)}(t)u^{(2)}(t) - u(t)u^{(3)}(t)\right), \tag{2a}$$

$$u(0) = 0, \qquad u(1) = 1, \tag{2b}$$

$$u^{(1)}(0) = 0, \qquad u^{(1)}(1) = 0, \tag{2c}$$

where u is the potential function, $u^{(1)}$ is the tangential velocity of the fluid, and $R > 0$ is the Reynolds number. This problem, from [24], is a feasibility problem for the boundary constraints. Fig. 3 shows the AMPL model of this problem using our extensions. For comparison, the original COPS model is shown in Fig. 4.

```
include OptimalControl.mod

var t;                  # independent time
param tf;               # ODEs defined in [0,tf]
var u{1..4} := 0;       # differential states
param R >= 0;           # Reynolds number


subject to

d1: diff(u[1],t) = u[2];
d2: diff(u[2],t) = u[3];
d3: diff(u[3],t) = u[4];
d4: diff(u[4],t) = R*(u[2]*u[3] - u[1]*u[4]);

u1s: eval(u[1],0)  = bc[1,1];
u2s: eval(u[2],0)  = bc[2,1];
u1e: eval(u[1],tf) = bc[1,2];
u2e: eval(u[2],tf) = bc[2,2];
```

Fig. 3 Fluid flow in a channel problem of the COPS library, using our AMPL extensions.

We believe that the new more compact model is more readable, because in standard AMPL models, the discretization scheme cannot easily be isolated from the remainder of the model. In addition, our extension allows us to pass more structural information to the solver, such as the nature of the differential equation, which is lost in the COPS model, which is just interpreted as a large NLP. Fig. 5 shows the optimal solution obtained with MUSCOD-II for $R = 10^4$.

```
param nc > 0, integer;          # number of collocation points
param nd > 0, integer;          # order of the differential equation
param nh > 0, integer;          # number of partition intervals

param rho {1..nc};              # roots of k-th degree Legendre polynomial
param bc {1..2,1..2};           # boundary conditions
param tf;                       # ODEs defined in [0,tf]
param h := tf/nh;               # uniform interval length
param t {i in 1..nh+1} := (i-1)*h;   # partition

param fact {j in 0..nc+nd} := if j = 0 then 1 else (prod{i in 1..j} i);

param R >= 0;                   # Reynolds number

# The collocation approximation u is defined by the parameters v and w.
# uc[i,j] is u evaluated at the collocation points.
# Duc[i,j,s] is the (s-1)-th derivative of u at the collocation points.

var v {i in 1..nh,j in 1..nd};
var w {1..nh,1..nc};

var uc {i in 1..nh, j in 1..nc, s in 1..nd} =
  v[i,s] + h*sum {k in 1..nc} w[i,k]*(rho[j]^k/fact[k]);

var Duc {i in 1..nh, j in 1..nc, s in 1..nd} =
  sum {k in s..nd} v[i,k]*((rho[j]*h)^(k-s)/fact[k-s]) + h^(nd-s+1)*
  sum {k in 1..nc} w[i,k]*(rho[j]^(k+nd-s)/fact[k+nd-s]);

minimize constant_objective: 1.0;

subject to bc_1: v[1,1] = bc[1,1];
subject to bc_2: v[1,2] = bc[2,1];
subject to bc_3:
  sum {k in 1..nd} v[nh,k]*(h^(k-1)/fact[k-1]) + h^nd*
  sum {k in 1..nc} w[nh,k]/fact[k+nd-1] = bc[1,2];
subject to bc_4:
  sum {k in 2..nd} v[nh,k]*(h^(k-2)/fact[k-2]) + h^(nd-1)*
  sum {k in 1..nc} w[nh,k]/fact[k+nd-2] = bc[2,2];

subject to continuity {i in 1..nh-1, s in 1..nd}:
  sum {k in s..nd} v[i,k]*(h^(k-s)/fact[k-s]) + h^(nd-s+1)*
  sum {k in 1..nc} w[i,k]/fact[k+nd-s] = v[i+1,s];

subject to collocation {i in 1..nh, j in 1..nc}:
  sum {k in 1..nc} w[i,k]*(rho[j]^(k-1)/fact[k-1]) =
  R*(Duc[i,j,2]*Duc[i,j,3] - Duc[i,j,1]*Duc[i,j,4]);
```

Fig. 4 Fluid flow in a channel problem as found in the COPS library.

3.2 Mixed-Integer ODE-Constrained Example

The Lotka-Volterra-type fishing problem with binary restriction on the fishing activity is from [57]. The goal is to minimize the deviation x_2 of predator and prey amounts from desired target values $\bar{x}_0$, $\bar{x}_1$ over a horizon of $T = 12$ time units by repeated decisions of whether to fish off proportional amounts of both predators and prey at every instant
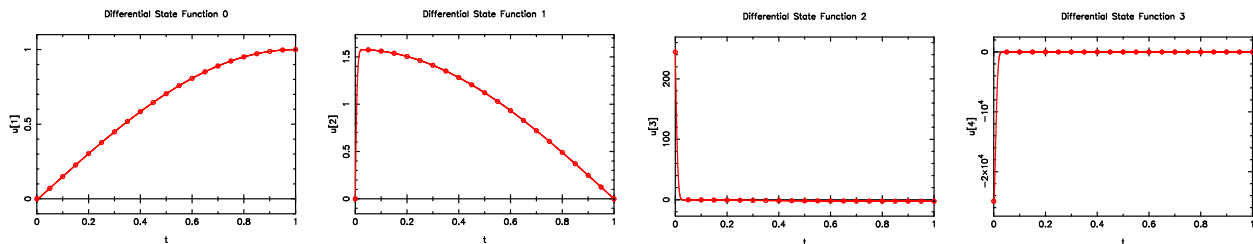
Fig. 5 Optimal solution of the flow in a channel problem for $R = 10^4$, computed with MUSCOD-II interfaced to AMPL using the TACO toolkit. `nshoot=20`.

in time. The problem is formulated as

$$
\begin{align}
\underset{x(\cdot),w(\cdot)}{\text{minimize}} \quad & x_2(T) \tag{3a} \\
\text{subject to} \quad & \dot{x}_0(t) = x_0(t) - x_0(t)x_1(t) - p_0 w(t)x_0(t), & t \in [0,T], \tag{3b} \\
& \dot{x}_1(t) = -x_1(t) + x_0(t)x_1(t) - p_1 w(t)x_1(t), & t \in [0,T], \tag{3c} \\
& \dot{x}_2(t) = (x_0(t) - \bar{x}_0)^2 + (x_1(t) - \bar{x}_1)^2, & t \in [0,T], \tag{3d} \\
& x(0) = (0.5, 0, 7, 0), \tag{3e} \\
& 0 \le x_0(t), \qquad 0 \le x_2(t), & t \in [0,T], \tag{3f} \\
& w(t) \in \{0,1\}, & t \in [0,T], \tag{3g}
\end{align}
$$

where $p_0 := 0.4$, $p_1 := 0.2$, $\bar{x}_0 = 1$, and $\bar{x}_1 = 1$. The AMPL model using our extensions is given in Fig. 6. MS-MINTOC obtains the optimal solution shown in Fig. 7 by applying partial outer convexification and solving the convexified and relaxed optimal control problem. A rounding strategy with an ε-optimality certificate is applied to find the switching structure, which is refined by switching time optimization afterwards. For details, we refer to [57, 59].

3.3 AMPL Models of Optimal Control Problems in the `mintoc.de` Collection

An extensible online library of mixed-integer optimal control problems has been described in [58] and is available from the web site `http://mintoc.de`. This site holds a wiki-based, publicly accessible library and is actively encouraging the optimal control community to contribute interesting problems modeled in various languages. So far, models in C, C++, JModelica, and AMPL (using encoded collocation schemes) can be found together with best known optimal solutions and optimal control and state profiles.

We have added 18 optimal control and parameter estimation problems to this library. The problems are modeled by using the new AMPL extensions, as shown in Table 1. These include ODE-constrained problems and a DAE-constrained control problem as well as continuous problems and a mixed-integer control problem. Among them are 10 dynamic control and parameter estimation problems found in the COPS library [24].

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```
include OptimalControl.mod;


var t;
var xd0 := 0.5, >= 0, <= 20;
var xd1 := 0.7, >= 0, <= 20;
var dev := 0.0, >= 0, <= 20;


var u := 1, >= 0, <= 1 integer suffix type "u0";


param p0 := 0.4;
param p1 := 0.2;
param ref0 := 1.0;
param ref1 := 1.0;


# Minimize accumulated deviation from reference after 12 time units
minimize Mayer: eval(dev,12);


subject to


# ODE system
ODE_0: diff(xd0,t) = xd0 - xd0*xd1 - p0*u*xd0;       # prey
ODE_1: diff(xd1,t) = -xd1 + xd0*xd1 - p1*u*xd1;      # predator
ODE_2: diff(dev,t) = (xd0-ref0)^2 + (xd1-ref1)^2;    # deviation from reference


# initial value constraints
IVC_0: eval(xd0,0) = 0.5;
IVC_1: eval(xd1,0) = 0.7;
IVC_2: eval(dev,0) = 0.0;
```

Fig. 6 Predator-prey mixed-integer problem modeled in AMPL, using our extensions.
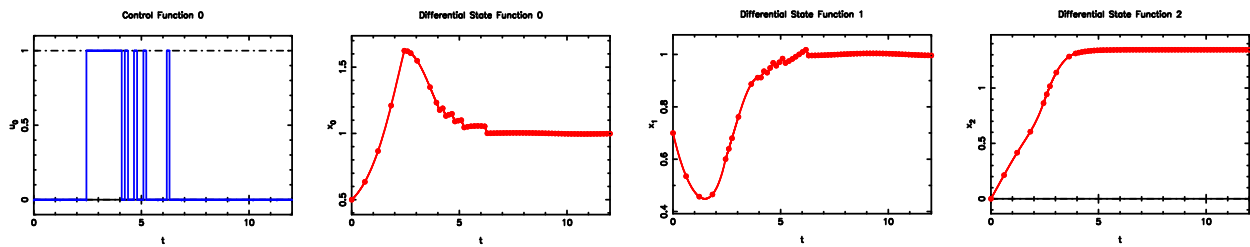
Fig. 7 Optimal integer control (blue) and optimal differential state trajectories (red) of the mixed-integer predator-prey problem, computed with MUSCOD-II and MS-MINTOC running inside the AMPL environment.

4 TACO Toolkit for AMPL Control Optimization

This section describes the design and usage of the TACO toolkit for AMPL control optimization. Its purpose is describe how a solver can infer the role AMPL variables, objectives, and constraints play in problem (1), to verify that the AMPL model conforms to this problem class, and to build a database of its findings for later use by optimal control problem solvers.

Details about data structures and function calls found in the C implementation of TACO, which may be of interest to developers of optimal control codes who wish to interface their code with AMPL, can be found in the appendix

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Table 1 List of AMPL optimal control problems modeled using the new AMPL extensions and contributed to the mixed-integer optimal control problem library at `http://mintoc.de`.

[1] OCP: optimal control, BVP: boundary value, PE: parameter estimation, MIOCP: mixed-integer OCP.

[2] batchdist is a 1-dimensional PDE and n_x can be increased by choosing a finer spatial discretization.

Name	n_x	n_z	$n_u + n_w$	n_{pf}	Type[1]	References
batchdist	$11^{(2)}$	–	1	–	OCP	[23]
brac	3	–	1	–	OCP	[10]
catmix	2	–	1	–	OCP	[24], [60]
cstr	4	–	2	2	OCP	[21]
fluidflow	4	–	–	–	BVP	[24]
gasoil	2	–	–	3	PE	[24], [61]
goddart	3	–	–	1	OCP	[24]
hangchain	3	–	1	–	OCP	[24], [18]
lotka	3	–	1	–	MIOCP	[57]
marine	8	–	–	15	PE	[24], [55]
methanol	3	–	–	5	PE	[24], [27], [46]
nmpc1	1	–	1	–	OCP	[21]
particle	4	–	1	1	OCP	[24], [14]
pinene	5	–	–	5	PE	[24], [13]
reentry	3	–	1	1	OCP	[53], [41], [54]
robotarm	6	–	3	1	OCP	[24], [49]
semibatch	5	1	4	–	OCP	[40], [48]
tocar1	2	–	1	1	OCP	[20], [45]
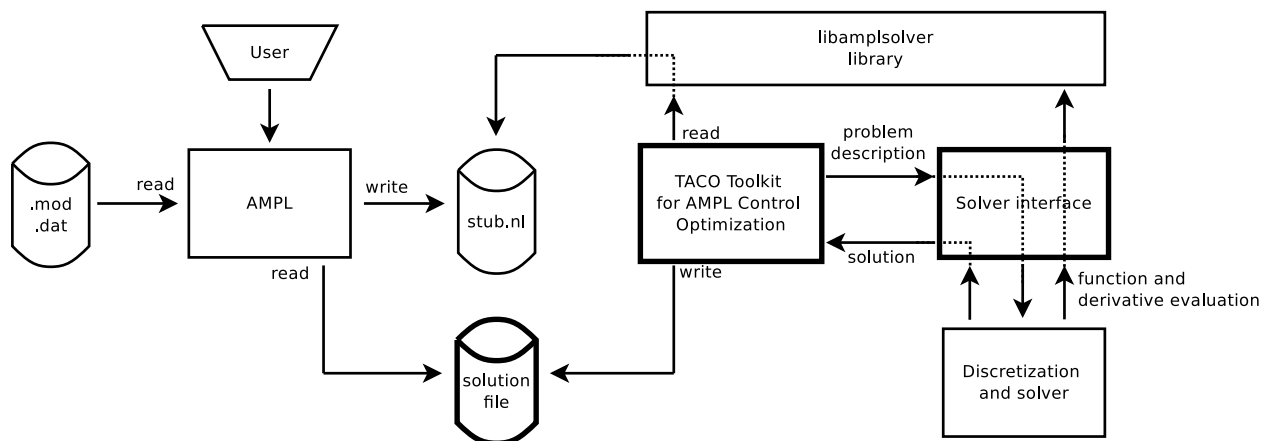
Fig. 8 Data flow between AMPL, the TACO toolkit, and an optimal control problem solver.

to this paper. The source code of TACO is available at `http://www.iwr.uni-heidelberg.de/groups/agbock/FILES/taco_source.tar.gz`.

4.1 Implementations of the New User Functions

For the three new user functions `diff`, `eval`, and `integral`, two sets of implementations need to be provided. The first set is used during parsing of AMPL model files and writing the *stub.nl* file. It indicates the names of the user functions and the number and type of their respective arguments. AMPL expects these implementations to be provided in a

shared object (.so) or dynamic link library (.dll) named `amplfunc.dll` on all systems. Hence, these implementations are readily provided along with the optimal control frontend.

The second set of implementations is used during evaluation of AMPL objectives and constraints by the optimal control problem solver. Here, `diff` returns the value zero as ODE constraints are explicit; `eval` accesses the solver's current iterate to return the expression's current value at the specified point in time; and `integral` return the integrand's value in the same way. Consequentially, the second set of user function implementations is solver dependent and must be carried out separately for each solver to be interfaced with the optimal control frontend. We provide implementations for MUSCOD-II and MS-MINTOC.

4.2 Consistency Checks

In this section we address automated checks for consistency and smoothness of an AMPL optimal control problem formulation, performed by the TACO toolkit before passing the model on to a solver.

Checks for Sufficient Smoothness. Most numerical algorithms for optimal control as well as in mixed-integer nonlinear programming assume all functions to be sufficiently smooth. In particular, this means that the objective terms L, E, r_i, $1 \le i \le n_{\mathrm{lsq}}$, and the constraints c, r_{c}, r_{s}, r_{e} must be twice continuously differentiable with respect to the continuous variables t, $x(t)$, $z(t)$, $u(t)$, and p. This guarantees a continuous Hessian of the Lagrangian of the discretized optimization problems; see, for example, [51]. Depending on the numerical methods applied to solve the DAE system, a higher order of continuous differentiability may be required for the ODE dynamics f (1b), though this is not enforced. The algebraic constraint function g (1c) may need to be invertible w.r.t. $z(t)$ in the neighborhood of trajectories $(t, x(t), z(t))$, $t \in [0, T]$, a property that can be checked by a DAE solver only during runtime.

Consistency Checks for AMPL Extensions. For each objective and constraint the optimal control frontend accesses the directed acyclic graph (DAG) representing the AMPL expression of the objective or constraint's body. This checking allows us to detect which variables are part of the expression, to detect calls to one of the three new user functions, and to check for sufficient smoothness of the expression. The following structural properties of the optimal control problem are currently verified automatically by the optimal control frontend during examination of the DAGs:

Dynamic constraints
  - There is exactly one call to `diff` present per differential state variable.
  - All ODE constraints are explicit; i.e., `diff` appears isolated on either the left-hand or right-hand side.
  - The time variable in calls to `diff` is the same for all such calls.
  - The state variables in calls to `diff` have not already been declared to be control or algebraic variables by means of the suffix `type`.
  - All ODE and DAE constraints are equality constraints.
  - The number of DAE constraints matches the number of algebraic variables.
  - Calls to `eval` do not appear in ODE or DAE constraints.
Objective functions
  - Calls to `diff` do not appear in objectives.
  - All objective functions conform to one of the four types Lagrange, Mayer, integral- or point-least-squares.
  - Expressions evaluated in calls to `integral` are time-dependent and not constants.
  - The end-time in calls to `integral` agrees with the end-time variable or value T.

- – The Mayer-type objective must not depend on control variables.

Path and point constraints

- – Calls to `integral` do not appear in constraints.
- – Expressions evaluated in calls to `eval` are time-dependent and not constants.
- – Evaluation time points in calls to `eval` are in $[0, T]$ if T is fixed, and in $[0, 1]$ if T is free.

Miscellaneous

- – There are no logical, relational, or other nonsmooth operators in the bodies of functions that are assumed to be twice continuously differentiable.
- – The `integer` and `binary` attributes are applied to control and parameter variables only.
- – Calls to `diff`, `eval`, or `integral` are not nested into one another.

Violations are detected before the optimal control problem solver itself is invoked. They terminate the solution process and are reported back to the user in a human-readable way, quoting the name of the offending variable, objective, or constraint.

4.3 User Diagnosis of the Detected Optimal Control Problem Structure

In addition to automated consistency checks, TACO provides the AMPL solver option `verbose` that may be invoked (e.g., `option muscod_solver "verbose=1";`) to obtain diagnostic output of the types, names, and further properties of all variables, constraints, and objectives that are part of the optimal control problem; see Fig. 9. This has proved helpful for narrowing down the source of modeling errors.

```
#    name      svar    lbnd    init     ubnd    scale
t    t          2       -       -        -       -
tf   tf         6      12      12       12       1
Differential States
#    name      svar    lbnd    init     ubnd    scale fix
0    xd0        3       0      0.5       20        1 IVC_0      4
1    xd1        4       0      0.7       20        1 IVC_1      5
2    dev        1       0       0        25        1 IVC_2      6
Controls
#    name      svar    lbnd    init     ubnd    scale discr int
0    u          5       0       1        1        1    u0 yes
ODE Constraints
#    name      scon    factor   scale
0    ODE_0      1       1        1
1    ODE_1      2       1        1
2    ODE_2      3       1        1
Objectives
#    name      sobj     type   dpnd     scale parts
0    -          1      Mayer  .x...       1      -
```

Fig. 9 Exemplary diagnostic output for the predator-prey example of §3.2 invoked by the solver option `verbose`. The output allows one to learn about the automatically detected associations of the different types of optimal control problem variables, constraints, and objectives in problem (1) with their AMPL counterparts.

4.4 Output of Time–Dependent Solution Variables

Following the solution of an optimal control problem using our extensions to AMPL, we must also provide a way to return this solution to the user. Currently, every AMPL variable can assume a single scalar value only, possibly augmented by scalar-valued suffixes. Hence, communication of the values of discretized trajectories is not possible in a straightforward way. For the AMPL optimal control frontend, we opted in favor of writing a separate plain-text solution file holding newline-separated values with the following layout:

- Optimal objective function value
- Remaining infeasibility (exact meaning depends on solver)
- Optimal final time T
- Number N of trajectory output points
- Output grid times (N values)
- Optimal values of free model parameters p (n_p values)
- Optimal differential state trajectories ($n_x \times N$ values, rowwise)
- Optimal algebraic state trajectories ($n_z \times N$ values, rowwise)
- Optimal control trajectories ($n_u \times N$ values, rowwise)

Future solvers may expand this file format. The data format is designed to be read back into the AMPL environment easily by using existing AMPL language elements such as `data` and `read`. An example AMPL code that does so is given in Fig. 10. This functionality is vital because it allows one to solve multiple related optimal control problems in a loop, each one based on the solution of the previous ones.

```
model;
param obj;
param infeas;
param tf;
param ndis integer;
var t_sol{1..ndis}
var p_sol{1..np};
var x_sol{1..nx, 1..ndis};
var z_sol{1..nz, 1..ndis};
var u_sol{1..nu, 1..ndis};

data;
read obj < filename.sol;
read inf < filename.sol;
read tf < filename.sol;
read ndis < filename.sol;
read{j in 1..ndis} (t_sol[j]) < filename.sol;
read{j in 1..np} (p_sol[j]) < filename.sol;
read{i in 1..nx, j in 1..ndis} (x_sol[i,j]) < filename.sol;
read{i in 1..nz, j in 1..ndis} (z_sol[i,j]) < filename.sol;
read{i in 1..nu, j in 1..ndis} (u_sol[i,j]) < filename.sol;
```

Fig. 10 Universal AMPL script for reading a discretized optimal control problem's solution from a file `filename.sol` back to AMPL. Variables `nx`, `nz`, `nu`, and `np` denote dimensions of the differential and algebraic state vectors, the control vector, and the vector of model parameters, respectively, and are assumed to be known from the original AMPL model.

5 Using TACO to Interface AMPL to MUSCOD-II and MS-MINTOC

In this section, we describe the use of TACO to interface the multiple shooting code for optimal control MUSCOD-II [42, 43] with AMPL. MUSCOD-II is based on a multiple shooting discretization in time [11], and implements a direct and all-at-once approach to solving DAE-constrained optimal control problems. MUSCOD-II has been extended by the MS-MINTOC algorithm for DAE-constrained mixed-integer optimal control; see [57, 59]. For more details on these solvers, we refer to the user manual [22].

5.1 Direct Multiple Shooting Method for Optimal Control

This section briefly sketches the direct multiple shooting method, first described by [11] and extended in a series of subsequent works (see, e.g., [43, 57]). An efficient implementation of this method is available in the optimal control software package MUSCOD-II [22].

The purpose of this method is to transform the infinite-dimensional problem (1) into a finite-dimensional (mixed-integer) nonlinear program by discretization of the control functions on a time grid $t_0 < t_1 < \ldots < t_{N_{\text{shoot}}} = T$. To do so, let $b_{ij} : [0,T] \to \mathbb{R}^{n_u}$, $1 \leq j \leq n_{q_i}$, be a set of sufficiently smooth basis functions of the control discretization for the shooting interval $[t_i, t_{i+1}] \subset [0,T]$. Further, let $q_i \in \mathbb{R}^{n_{q_i}}$ be the corresponding set of control parameters, and define

$$\hat{u}_i(t, q_i^{\text{u}}) := \sum_{j=1}^{n_{q_i^{\text{u}}}} q_{ij}^{\text{u}} \, b_{ij}(t) \qquad\qquad t \in [t_i, t_{i+1}], \, 0 \leq i < N_{\text{shoot}}. \tag{4}$$

The control space is hence reduced to functions that can be written as in (4), depending on finitely many parameters q_i. For integer controls $w(\cdot)$ we choose a piecewise constant discretization; that is, we have $n_{q_i^{\text{w}}} = 1$ and $b_{i1}(t) = q_{i1}^{\text{w}}$, leading to $\hat{w}_i(t, q_i^{\text{w}}) = q_{i1}^{\text{w}}$. For continuous controls $u(\cdot)$, more elaborate discretizations based on, for example, linear or cubic base functions $b_{ij}(\cdot)$ are easily implemented.

The right-hand side functions f, g, and the constraint functions c, r_c^{eq}, r_c^{in}, r_i^{eq}, and r_i^{in} are assumed to be adapted accordingly. Multiple shooting variables s_i are introduced on the time grid to parameterize the differential states. The node values serve as initial values for an ODE or DAE solver computing the state trajectories independently on the shooting intervals.

$$\dot{x}_i(t) = f(t, x_i(t), \hat{u}_i(t, q_i), \hat{w}_i(t, q_i), p, \rho), \qquad\qquad t \in [t_i, t_{i+1}], \, 0 \leq i < N_{\text{shoot}}, \tag{5a}$$

$$0 = g(t, x_i(t), z_i(t), \hat{u}_i(t, q_i), \hat{w}_i(t, q_i), p, \rho), \tag{5b}$$

$$x_i(t_i) = s_i, \qquad\qquad 0 \leq i \leq N_{\text{shoot}}. \tag{5c}$$

One advantage of the multiple shooting approach is the ability to use state-of-the-art adaptive integrator methods. In MUSCOD-II, the ODE and DAE initial-value problems are solved using DAESOL [8]. From these IVPs we obtain N_{shoot} trajectories, which in general will not combine to a single continuous trajectory; see Fig. 11. Thus, continuity across shooting intervals needs to be ensured by additional matching conditions entering the NLP as equality constraints,

$$s_{i+1} = x_i(t_{i+1}; \, t_i, s_i, z_i, q_i^{\text{u}}, q_i^{\text{w}}, p, \rho) \qquad\qquad 0 \leq i < N_{\text{shoot}}. \tag{6}$$

Here we denote by $x_i(t_{i+1}; \, t_i, s_i, z_i, q_i^{\text{u}}, q_i^{\text{w}}, p, \rho)$ the solution of the IVP on shooting interval i, evaluated in t_{i+1}, and depending on the initial values s_i, z_i, control parameters $q_i^{\text{u}}, q_i^{\text{w}}$, and model parameters p, ρ. Path constraints $c(\cdot)$ then are discretized on an appropriately chosen grid. To ease the notation, we assume in the following that all constraint grids match the shooting grid.
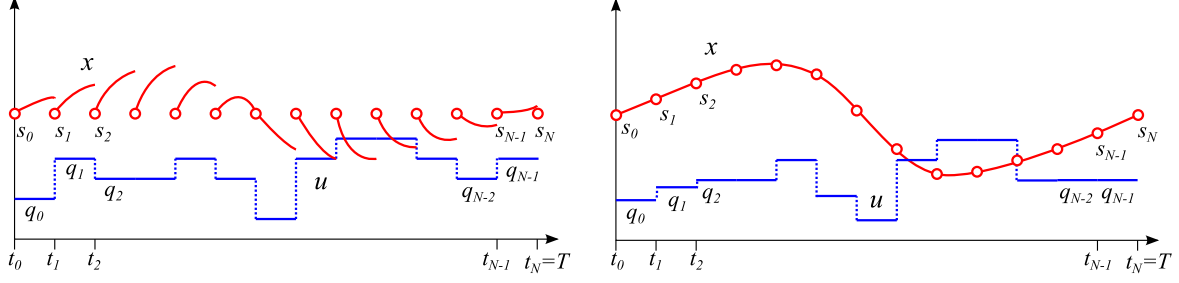
Fig. 11 Multiple shooting discretization in time. A constant initialization of state nodes s_i, $0 \leq i \leq N$ is shown on the left, and a continuous solution after convergence on the right. Continuity is required in the optimal solution only, ensured by matching conditions.

Structured Nonlinear Programming. From this discretization and parameterization, a highly structured (MI)NLP of the form

$$\min_{\xi_C, \xi_I} \sum_{i=0}^{N_{\text{shoot}}} \Phi_i\big(s_i, z_i, \hat{u}_i(t_i, q_i^{\text{u}}), \hat{w}_i(t_i, q_i^{\text{w}}), p, \rho\big) \tag{7a}$$

$$\text{s.t.} \quad 0 = x_i(t_{i+1}; s_i, z_i, q_i^{\text{u}}, q_i^{\text{w}}, p, \rho) - s_{i+1}, \qquad 0 \leq i < N_{\text{shoot}}, \tag{7b}$$

$$0 = g\big(t_i, s_i, z_i, \hat{u}_i(t_i, q_i^{\text{u}}), \hat{w}_i(t_i, q_i^{\text{w}}), p, \rho\big), \qquad 0 \leq i \leq N_{\text{shoot}}, \tag{7c}$$

$$0 \leq c\big(t_i, s_i, z_i, \hat{u}_i(t_i, q_i^{\text{u}}), \hat{w}_i(t_i, q_i^{\text{w}}), p, \rho\big), \qquad 0 \leq i \leq N_{\text{shoot}}, \tag{7d}$$

$$0 = r_{\text{c}}^{\text{eq}}\big(s_0, s_{N_{\text{shoot}}}, p, \rho\big), \tag{7e}$$

$$0 \leq r_{\text{c}}^{\text{in}}\big(s_0, s_{N_{\text{shoot}}}, p, \rho\big),$$

$$0 = r_i^{\text{eq}}\big(s_i, z_i, \hat{u}_i(t_i, q_i^{\text{u}}), \hat{w}_i(t_i, q_i^{\text{w}}), p, \rho\big), \qquad 0 \leq i \leq N_{\text{shoot}}, \tag{7f}$$

$$0 \leq r_i^{\text{in}}\big(s_i, z_i, \hat{u}_i(t_i, q_i^{\text{u}}), \hat{w}_i(t_i, q_i^{\text{w}}), p, \rho\big), \qquad 0 \leq i \leq N_{\text{shoot}},$$

$$q_i^{\text{w}} \in \Omega_{\text{w}}, \quad \rho \in \Omega_\rho, \tag{7g}$$

is obtained. Let the vectors ξ_C, ξ_I contain all unknowns of the problem

$$\xi_C = \big(s_0, \ldots, s_{N_{\text{shoot}}}, q_0^{\text{u}}, \ldots, q_{N_{\text{shoot}}-1}^{\text{u}}, p\big), \quad \xi_I = \big(q_0^{\text{w}}, \ldots, q_{N_{\text{shoot}}-1}^{\text{w}}, \rho\big). \tag{8}$$

For ease of notation in (7d, 7f) we write

$$\hat{u}_{N_{\text{shoot}}}\big(t_{N_{\text{shoot}}}, q_{N_{\text{shoot}}}\big) := \hat{u}_{N_{\text{shoot}}-1}\big(t_{N_{\text{shoot}}}, q_{N_{\text{shoot}}-1}\big)$$

and analogously for $\hat{w}$. We may then continue to solve this large-scale, structured (MI)NLP using one of the solvers mentioned in the introduction. For efficiency, this usually requires extensive exploitation of the arising NLP structures. Possible approaches include SQP methods with blockwise, high-rank updates of Hessian approximations; partial reduction using the algebraic constraints to eliminate the z_i from the problem; and condensing algorithms for a reduction of the size of the arising quadratic subproblems. For details, we refer to [11, 42, 43].

5.2 Sensitivity Computation and Automatic Derivatives

From the structured NLP (7) it is clear that AMPL objectives and most AMPL constraints can be evaluated as usual, and this also holds true for gradients or Jacobians. The exceptions are ODE and DAE constraint functions, since they do not directly enter (7). Evaluation of these functions occurs during solution and sensitivity computation for

the multiple shooting IVPs, carried out by an ODE/DAE solver called to evaluate the residual or a derivative of the matching constraint (7b).

We consider the ODE case and examine the computation of a directional derivative $X \cdot d$ of differential state trajectory with respect to the problem unknowns, where

$$X = \frac{\mathrm{d}x(t_{i+1}; t_i, s_i, z_i, q_i, p, \boldsymbol{\rho})}{\mathrm{d}(s_i, q_i, p)} \in \mathbb{R}^{n_x \times (n_x + n_q + n_p)} \tag{9}$$

is the Jacobian of the solution of the IVP on $[t_i, t_{i+1}]$ with respect to the unknowns (s_i, q_i, p_i) of the problem in the shooting node at t_i. For a direction $d = (d_s, d_{q,p}) \in \mathbb{R}^{n_x + n_q + n_p}$ this may, for example, be done by solving the system (10) of so-called variational differential equations,

$$\dot{x}_\mathrm{d}(t) = f_x(t) \cdot x_\mathrm{d}(t) + f_{q,p}(t) \cdot d_{q,p}, \quad t \in [t_i, t_{i+1}], \tag{10a}$$

$$x_\mathrm{d}(t_i) = d_s, \tag{10b}$$

simultaneously and using the same scheme (e.g., choice of method, step sizes, orders) of the original IVP. Basic calculus then shows that $x_\mathrm{d}(t_{i+1}) = X \cdot d$. In (10), the time-dependent Jacobians of the ODE constraint are denoted by

$$f_x(t) = \frac{\partial f}{\partial x}(t, x(t), \hat{u}(t), w(t), p, \boldsymbol{\rho}), \quad f_{q,p}(t) = \frac{\partial f}{\partial (q, p)}(t, x(t), \hat{u}(t), w(t), p, \boldsymbol{\rho}).$$

Similarly, directional derivatives of $z(t)$ and derivatives into directions containing the shooting node algebraic unknowns z_i can be computed for partial reduction of DAE systems; see [42].

For direct multiple shooting NLPs, typically a significant amount of the total runtime, easily in excess of 80%, is spent on computing sensitivities of IVP solutions. Hence, it is important to exploit the availability of automatic sparse derivatives of the ODE and DAE constraints in AMPL when computing f_x and $f_{q,p}$. Here, our approach of modeling dynamic constraints in AMPL has the additional advantage of not requiring a separate automatic differentiation tool, while at the same time being faster and more precise than finite difference approximations. In the MUSCOD-II interface to AMPL, we provide both dense and sparse Jacobians as well as directional derivatives formed from sparse matrix-vector products to the DAE solver DAESOL.

5.3 Additional Information on Derivatives

This section addresses the implementation of exact derivative interfaces between AMPL and the DAE solver DAESOL for the differential and algebraic right hand side functions f and g. DAESOL comes in a sparse and a dense variant, and requires forward directional derivatives as well as sparse or dense Jacobians of the right hand side functions.

Sparse Jacobians. Sparse Jacobians with respect to a subset of the vectors (t, x, z, u, p) of unknowns, are easily computed from sparse adjoint information stored in `Cgrad` structures [31] by AMPL after calls to `congrd`, and are stored in triplets format for DAESOL.

```
for (all right hand side constraints ii) {
  congrd(ii, ...);
  for (gr = Cgrad[ii]; gr != 0; gr = gr->next) {
    if (jacobian w.r.t. AMPL variable gr->varno desired) {
      jac[ne] = adjoints[gr->varno];
      irn[ne] = 1 + ii;
```

```
      jcn[ne] = 1 + (DAESOL index of AMPL variable gr->varno);
      ++ne;
    }
  }
}
```

Dense Jacobians. Dense Jacobians with respect to a subset of the vectors (t,x,z,u,p) of unknowns, are computed from sparse adjoint information as before; empty matrix entries are filled with zeros.

Forward Directions. Forward directional derivatives of f or g into a direction $d = (d_t, d_x, d_z, d_u, d_p)$ are computed by implicitly carrying out a sparse matrix-vector multiplication with the sparse Jacobian discussed above.

```
for (all right hand side constraints ii) {
  congrd(ii, ...);
  rhs[ii] = 0.0;
  for (gr = Cgrad[ii]; gr != 0; gr = gr->next) {
    if (AMPL variable gr->varno is part of direction) {
        rhs[ii] += adjoints[gr->varno] * dir[(DAESOL index of AMPL variable gr->varno)];
    }
  }
}
```

5.4 MUSCOD-II Solver Options and AMPL Suffixes

This section addresses the specification of shooting discretizations, of interpolated initial guesses, of scaling factors, and of slope constraints in AMPL models solved by MUSCOD-II.

Specifying a Discretization. MUSCOD-II applies a multiple shooting discretization in time to control trajectories, differential and algebraic state trajectories, path constraints, and Lagrange- and integral least-squares-type objectives; see [42]. The number of multiple shooting intervals can be chosen by using the solver option `nshoot`. For point least-squares objectives as well as for point constraints, the MUSCOD-II backend ensures the introduction of shooting nodes in the respective time points. Hence, the solver option `nshoot` specifies a minimum number of shooting intervals only. Moreover, adaptive refinement of the shooting discretization may be triggered by several mixed-integer strategies of the MS-MINTOC algorithms; see [57]. The final number of shooting intervals used for computation of the optimal solution is available from the solution file written by the frontend, see §4.4.

Initial Guesses, Scaling, and Slope Constraints. For MUSCOD-II we provide several additional suffixes that allow us to model more elaborate initializations; to apply scale factors to variables, objective terms, and constraints; and to impose constraints on the slope of linear or cubic spline controls.

`interp_to` Specifies a second initializer for a differential state at the end of the time horizon. Let α be the initial guess and β be the value of suffix `interp_to`. The initialization of the state trajectory is a linear interpolation between the first and the second initializer,

$$x(t) = \frac{T-t}{T}\alpha + \frac{t}{T}\beta, \quad t \in [0,T]. \tag{11}$$

Since AMPL does not provide a means of telling whether a suffix is uninitialized, and since interpreting $\beta = 0$ as uninitialized is not a viable option, the dedicated solver option `s_spec` has to be set in order to enable the `interp_to`. In this case, suffix `interp_to` has to be set for *all* differential state variables.

`scale` Specifies scale factors for variables, constraints, and objective terms. The default value 0 means to infer the scale factor from the initial guess. If none is provided, a default scale factor of 1 is assumed.

`slope_max` and `slope_min` Specify upper and lower bounds on the slopes of piecewise linear or cubic controls. Since AMPL does not allow for nonzero default values of suffices, this suffix *must* be set for *all* controls that are not of piecewise constant type.

Solver Options. Solver options recognized by the MUSCOD-II backend comprise the following keywords:

`nshoot` The minimum number of multiple shooting intervals to use. As described above, constraint grids, point least-squares objective grids, and MS-MINTOC strategies may increase this number.

`itmax` The maximum number of SQP iterations allowed.

`atol` The acceptable KKT tolerance for termination of the SQP solver.

`levmar` Levenberg-Marquardt regularization for the Hessian of the Lagrangian.

`bflag` The MS-MINTOC strategy code; see [57].

`stiff` Set to use the BDF-type solver DAESOL [8], which can cope with stiff DAE systems. Unset to use a faster Runge-Kutta-Fehlberg–type method for nonstiff ODEs.

`deriv` Set to `sparse` to use sparse Jacobians of the ODE/DAE provided by AMPL. Set to `dense` to use dense Jacobians of the ODE/DAE provided by AMPL. Set to `finitediff` to approximate derivatives by finite differences, ignoring AMPL derivatives.

`solve` Selects the globalization method for the SQP solver. Available methods include `solve_fullstep` (no globalization), `solve_slse` (a line search method), and `solve_tbox` (a box-shaped trust region method).

`hess` Selects the Hessian approximation method to use. Available options include `hess_const` (constant Hessian), `hess_update` (a BFGS Hessian approximation), `hess_limitedmemoryupdate` (a limited memory BFGS Hessian approximation), `hess_gaussnewton` (Gauß–Newton approximation of the Hessian), and `hess_finitediff` (finite difference exact Hessian).

Usage in AMPL. Figure 12 shows two lines of exemplary AMPL code that demonstrate how to load the MUSCOD-II solver and pass algorithmic options from an AMPL model file.

```
option solver muscod;
option muscod_options "nshoot=20 atol=1e-8 itmax=200 hess=hess_gaussnewton";
option muscod_auxfiles "rc";
```

Fig. 12 Example of AMPL code to load the MUSCOD-II solver and pass solver options, row, and column names.

6 Limitations and Possible Further Extensions

The extensions to the AMPL modeling language presented so far suffice to treat the class (1) of mixed-integer DAE-constrained optimal control problems. However, a number of possible extensions of this problem class are discussed next.

The first extension concerns the modeling of fully implicit ODE and DAE systems of the form

$$0 = f(t, x(t), \dot{x}(t), z(t), u(t), w(t), p, \rho) \quad t \in [0, T],$$
$$0 = g(t, x(t), z(t), u(t), w(t), p, \rho),$$

or alternatively of a semi-implicit form that is preferred by many DAE solver implementations,

$$A(t, x(t), z(t), u(t), w(t), p, \rho)\dot{x}(t) = f(t, x(t), z(t), u(t), w(t), p, \rho) \quad t \in [0, T],$$
$$0 = g(t, x(t), z(t), u(t), w(t), p, \rho).$$

These extensions can be realized by using a more sophisticated `diff` user function. Unfortunately, the current implementation of the AMPL solver library does not provide sufficient information to associate $\dot{x}(t)$ arguments with $x(t)$ arguments, which would require manipulation of AMPL expression DAGs for all ODE constraints.

For convenience, the functionality of `diff()` could also be extended to allow higher-order ODEs to be formulated by passing the differential's order as a third argument, for example write `diff(x,t,2)` for $\ddot{x}(t)$. This would further reduce the number of lines required for the presented COPS fluid flow problem of §3.1 and is readily implemented. However, because the ODE/DAE solver would typically convert a second-order ODE into a system of first-order ODEs, we prefer to require the user to make this transformation.

For some DAE problems, in order to promote sparsity, automatic introduction of defined variables as additional algebraic states might be preferred over the in-place evaluation of defined variables that is currently carried out.

The use of nonsmooth operators such as max, min, $|\cdot|$, or conditional statements could be allowed inside ODE constraints. This would open the possibility for modeling hybrid and implicitly switched systems in a quick and convenient way, given an ODE and DAE capable of computing derivatives of switching ODEs' solutions. The use of certain logical and nonsmooth operators could also be allowed in path and point constraints, leading, for example, to optimal control problems with complementarity constraints [35] or vanishing constraints [2, 37].

Certain optimal control problems of practical relevance require a multistage setup. Here, the number of differential and/or algebraic states and the number of controls may change at a certain, possibly implicitly determined point in time. Modeling multistage optimal control problems currently appears difficult with the extensions described in this paper. Here AMPL's syntax provides insufficient contextual information about the stage a certain variable or constraint should be assigned to.

7 Conclusions and Outlook

We have described an approach for the AMPL modeling language that extends the applicability of the AMPL modeling language beyond the domain of MINLPs by allowing one to conveniently model mixed-integer DAE-constrained optimal control problems in AMPL. Contrary to prior approaches at modeling such problems in AMPL by explicitly encoding a discretization scheme for the dynamic parts of the model, our approach separates model equations and the discretization scheme.

We have shown that our extensions do not require intrusive changes to the AMPL language standard or implementation itself, as they consist of a set of three AMPL user functions and an AMPL suffix. The TACO toolkit for AMPL control optimization was presented and serves as an interface between AMPL *stub.nl* files and an optimal control code. TACO is open-source and designed to facilitate the coupling of existing optimal control software packages to AMPL.

To demonstrate the applicability of TACO, we have used this new toolkit to implement an AMPL interface for the optimal control software packages MUSCOD-II and its mixed-integer optimal control extension MS-MINTOC.

The modeling and solution of two exemplary control problems in AMPL using the extensions show the benefits of the new approach, namely, shorter model code, improved readability, flexibility in the choice of a discretization scheme, and the possibility to adaptively modify and refine such a scheme.

In the future, it would be desirable to implement of a number of other schemes for evaluating ODE and DAE constraints, such as collocation schemes. These would enable the immediate use of NLP and MINLP solvers.

Appendix

The following sections contain supplementary material intended to guide software developers interested in using the presented TACO toolkit to interface their optimal control codes with AMPL. Section A explains the most important data structures that hold information about the mapping from the optimal control point of view to the AMPL view. Section B lists functions available to optimal control codes for evaluating AMPL functions. Section C explains error codes emitted by the TACO toolkit, and mentions possible remedies.

A TACO Data Structures Exposed to Optimal Control Problem Solvers

This sections lists TACO data structures exposed to developers of codes for solving optimal control problems. We discuss several snippets taken from the header file `ocp_frontend.h`, which should be consulted for additional details.

A.1 Data Structures Mapping from AMPL to Optimal Control

The optimal control frontend provides a collection of fields that hold the optimal control problem interpretation of every AMPL variable passed to the solver. They are laid out as follows:

```
enum vartype_t {
    vartype_AMPL_defined = -2,  // AMPL "defined" variable
    vartype_unknown = -1,       // type not yet known
    vartype_t       = 0,        // independent variable ("time")
    vartype_x       = 1,        // differential state of an ODE/DAE
    vartype_z       = 2,        // algebraic state of a DAE
    vartype_u       = 3,        // control function to be discretized
    vartype_p       = 4,        // global model parameter
    vartype_tend    = 5         // end time variable
};


enum vartype_t *vartypes;      // OCP types assigned to AMPL variables
int            *varindex;      // OCP vector indices assigned to AMPL variables
```

The field `vartypes` gives the OCP variable type of an AMPL variable, that is, whether the variable is t, T, a component of vector p, or a component of one of the vector trajectories x, z, or u and w. For the case of it being a vector component, the field `varindex` holds the index into the OCP variable or trajectory vector. For AMPL constraints and objectives, no mapping information from AMPL to the OCP perspective is provided.

A.2 Data Structures Mapping from Optimal Control to AMPL

The AMPL optimal control frontend provides a collection of structures holding the AMPL perspective for every component of an optimal control problem according to problem class (1). Starting with information about problem dimensions, the following variables are provided and should be self-explanatory.

```
int nx;      // number of differential states
int nz;      // number of algebraic states
int nu;      // number of control functions
int np;      // number of model parameters
int npc;     // number of inequality path constraints
int ncc_eq;  // number of coupled equality constraints
int ncc_in;  // number of coupled inequality constraints
```

Information about both the independent time variable and the end-time variable is held in a structured variable named `endtime` of the following layout.

```
struct ocp_time_t {
    int        index;  // AMPL index of the final time variable, or -1
    const char *name;  // AMPL name of the final time variable
    int        fixed;  // flag indicating whether tf is fixed, index may be -1 then
    real       init;   // initial or fixed end time, even if idx_tf=-1
    real       scale;  // scale factor for tf
    real       lbnd;   // lower bound for tf
    real       ubnd;   // upper bound for tf

    int        idx_t;  // AMPL index of the free time variable t
    const char *name_t; // AMPL name of the free time variable
};

struct ocp_time_t endtime; // time horizon information
```

For a fixed-endtime scenario, `endtime.index` is -1, the field `endtime.init` holds the fixed end time. For a variable end-time scenario, `endtime.index` is nonnegative and the field `endtime.init` holds the initial guess for the free end time if available, and is set to 1.0 otherwise.

The following structured variable `xstates` holds information about differential state trajectory variables, and associated right-hand side functions.

```
struct ocp_xstate_t {
    int        index;      // AMPL index of differential state trajectory variable
    const char *name;      // AMPL name of the differential state trajectory variable
    int        fixed;      // AMPL index of initial value constraint, -1 if none
    real       init[2];    // initializers at t=0 and t=tf
    real       scale;      // scale factor
    real       lbnd;       // lower bound
    real       ubnd;       // upper bound

    int        ffcn_index; // AMPL index of ODE constraint
    const char *ffcn_name;  // AMPL name of ODE constraint
    real       ffcn_scale; // scale factor
    real       rhs_factor; // constant factor in front of diff()
};

struct ocp_xstate_t *xstates; // differential state trajectories information
```

Here, the field `fixed` holds the AMPL index of the initial value constraint for this ODE state. It is -1 if the ODE state's initial value is free. The initializer `init` provides two values for linear interpolation (see suffix `.interp_to`).

The field `ffcn_index` holds the AMPL constraint index of the right-hand side function associated with a differential state. Even though we currently support explicit ODEs only, AMPL-internal rearrangement of constraint expressions may cause a negative sign on the `diff()` call. Hence the field `rhs_factor` is introduced to compensate for AMPL-internal representations of the form $-\dot{x}(t) = f(t, x(t), \dots)$.

Similar to differential states, the structured variable `zstates` holds information about algebraic state trajectories.

```
struct ocp_zstate_t {
    int        index;  // AMPL index of algebraic state trajectory variable
    const char *name;  // AMPL name of algebraic state trajectory variable
    real       init;   // constant initial guess for algebraic state trajectory
    real       scale;  // scale factor
    real       lbnd;   // lower bound
    real       ubnd;   // upper bound

    // we keep gfcn() information here as well, but keep in mind that the relation-
    // ship between z[] and gfcn() is fully implicit, i.e. no 1-1 correspondence!

    int        gfcn_index;  // AMPL index of DAE constraint
    const char *gfcn_name;  // AMPL name of DAE constraint
    real       gfcn_scale;  // scale factor for DAE constraint
};

struct ocp_zstate_t *zstates; // algebraic state trajectories information
```

It is important to keep in mind that DAE constraints are not associated with algebraic state trajectory variables by a one–one mapping. We merely keep both in the same array for simplicity, since their numbers must match.

Information about integer and continuous control trajectories is kept in a structured variable named `controls` with the following layout.

```
struct ocp_control_t {
    int        index;      // AMPL indices of control trajectory variable
    const char *name;      // AMPL name of control trajectory variable
    int        type;       // control discretization type
    int        integer;    // flag indicating integer controls
    real       init;       // initial guess for all control parameters on the horizon
    real       scale;      // scale factor for control
    real       lbnd;       // lower bound for control
    real       ubnd;       // upper bound for control

    // slope information for linear or cubic elements
    real       slope_init;  // initial guess for control slope
    real       slope_scale; // scale factor for control slope
    real       slope_lbnd;  // lower bound for control slope
    real       slope_ubnd;  // upper bound for control slope
};

struct ocp_control_t *controls; // control trajectories information
```

The field `type` denotes the (solver-dependent) discretization type to be applied to this control trajectory The field `integer` is set to 1 if the control is a binary or integer control and to 0 if it is a continuous control. For piecewise linear and piecewise cubic discretization types, additional information about slope limits and initial guesses is provided.

In addition, model parameters information is provided in a structured variable named `params`, with layout as follows. This concludes AMPL variables information.

```
struct ocp_param_t {
    int        index;  // AMPL indices of free model parameters
    const char *name;  // AMPL name of free model parameters
```

```
    real        init;    // initial value for free parameter
    real        scale;   // scale factors for free parameter
    real        lbnd;    // lower bound for free parameter
    real        ubnd;    // upper bound for free parameter
    int         integer; // 1 if integer, 0 if real
};

struct ocp_param_t *params; // free parameters information
```

Information about Mayer-type, Lagrange-type, and integral least-squares-type objective functions (1a) is found in structured variables named `mayer`, `lagrange`, and `clsq`. Their layout is presented below.

```
struct ocp_objective_t {
    int         index;    // AMPL index of objective function
    const char *name;     // AMPL name of objective function
    int         dpnd;     // dependency flags from enum vartype_t
    int         maximize; // 1 for maximization, 0 for minimization
    real        scale;    // scale factor

    // additional information for least-squares type objectives
    int         nparts;   // number of residuals
    expr      **parts;    // residual AMPL expressions
};

struct ocp_objective_t mayer;    // Mayer type objective function information
struct ocp_objective_t lagrange; // Lagrange type objective function information
struct ocp_objective_t clsq;     // Integral least-squares type objective information
```

`dpnd` is a bit field with bit k ($k \geq 0$) set if and only if the objective function's AMPL expression depends on an AMPL variable with `vartypes` entry set to value k (see enum `vartype_t`). This allows for quick dependency checks that may save runtime, for example, in derivative approximation. The field `maximize` is set to 1 if the objective function is to be maximized and to 0 if it is to be minimized. Note that least-squares functions are recognized only if they are to be minimized. The fields `nparts` and `parts` hold information about the AMPL expression DAGs associated with the individual least-squares residual expressions of a least-squares objective.

Path constraints (1d) and coupled constraints (1e) information is held in structured variables named `pathcon`, `cpcon_eq`, and `cpcon_in` with the following layout.

```
struct ocp_constraint_t {
    int         index; // AMPL index of constraint
    const char *name;  // AMPL name of constraint
    int         side;  // side of inequality constraint (0=lower, 1=upper)
    int         dpnd;  // dependency flags from enum vartype_t
    real        scale; // scale factor
};

struct ocp_constraint_t  *pathcon; // inequality path constraints
struct ocp_constraint_t  *cpcon_eq; // coupled equality constraints
struct ocp_constraint_t  *cpcon_in; // coupled inequality constraints
```

Path constraints (1d) always are inequality constraints. For coupled constraints (1e), equality and inequality constraints are stored in separate arrays. For two-sided inequality constraints $l \leq c(x) \leq u$, the field `side` indicates which side of the constraint should be evaluated.

Information about decoupled point constraints (1f) and point least-squares objectives (1a) is stored in a structured variable named `grid`. For each objective or constraint evaluation time, a grid node is introduced and holds information about the associated objective or constraint. Grid nodes are guaranteed to be unique, in other words, no two nodes share

the same time point, and they are sorted in ascending order. The grid is guaranteed to contain at least two nodes: the first grid node will always be at time 0, and the last grid node will always be at time t_f.

```
struct ocp_grid_node_t {
    int                     n_eq;       // number of equality point constraints
    struct ocp_constraint_t *con_eq;    // equality point constraint information
    int                     n_in;       // number of inequality point constraints
    struct ocp_constraint_t *con_in;    // inequality point constraint information
    int                     ncc_eq;     // number of equality coupled constraints
    int                     *ccidx_eq;  // indices of equality coupled constraints
    int                     ncc_in;     // number of inequality coupled constraints
    int                     *ccidx_in;  // indices of inequality coupled constraints
    struct ocp_objective_t  lsq;        // node least-squares objective information
};

struct ocp_grid_t {
    int                     n_nodes;    // number of grid nodes
    real                    *times;     // it's more practical to have the times here
    struct ocp_grid_node_t *nodes;      // information about what is on a grid node
};

struct ocp_grid_t grid;     // constraint and node-least-squares grid information
```

For equality and inequality point constraints (1f) on a grid node, the fields `n_eq` and `n_in` hold the dimensions and the fields `con_eq` and `con_in` the constraint information, respectively. For coupled constraints (1e), we do not store pointers to constraint information structures, but rather indices into the global lists `cpcon_eq` and `cpcon_in`. For solvers requiring linear separability of coupled constraints, this layout eases the setup of the coupled constraints' block structure. The field `lsq` holds information about the point least-squares objective contribution in a node; again index -1 indicates that no point least-squares objective is present.

B TACO Functions Exposed to Optimal Control Problem Solvers

This sections lists TACO functions exposed to developers of codes for solving optimal control problems.

Reading of the AMPL Model. For reading and verifying the AMPL mode as well as creation of management of the database, the optimal control frontend provides the following functions:

`allocate_mappings` allocates memory for the database to be created, prior to reading the *stub.nl* file provided by AMPL.

`read_mappings` calls the AMPL solver library to read the *stub.nl* file. Afterwards, the DAGs of all AMPL objectives and constraints are examined for appearance of variables, calls to user functions, and nonsmooth operators. The role of AMPL variables, constraints, and objectives in (1) is determined, and the database is filled with appropriate information.

`free_mappings` frees memory allocated for the database after the optimal control problem has been solved.

A developer wishing to interface an optimal control problem solver with AMPL is provided with a number of functions that infer the optimal control problem's structure from a *stub.nl* file. The following listing shows a framework that could serve as a starting point for development of a solver interface.

```
// allocate memory for the "fg" reader of AMPL stub files
ASL_alloc (ASL_read_fg);
asl->i.want_xpi0_    = 1; // indicate that we want the initial guesses
```

```
asl->p.need_funcadd_ = 1; // indicate that we need to add user functions

// get AMPL stub file name and allocate memory for AMPL data structures
nl_name = getstub (&argv, &Oinfo);
nl = jac0dim (nl_name, (fint) strlen (nl_name));
if (nl == NULL)
    error_out (error_readfile, nl_name);

// declare AMPL OCP frontend suffixes
declare_suffixes ();

// read AMPL stub file
if (fg_read(nl, ASL_return_read_err|ASL_findgroups) != 0)
    error_out (error_readfile, nl_name);

Oinfo.option_echo &= ~ASL_OI_echo;       // don't echo options
Oinfo.option_echo |= ASL_OI_badvalue;    // but report bad option values

// read solver options
if (getopts(&xargv[3], &Oinfo))
    error_out (error_solverOptions);

allocate_mappings ();       // allocate memory of AMPL OCP frontend data
read_mappings ();           // infer OCP structure from AMPL stub file

// call optimal control problem solver here
// use frontend information to set up problem and evaluate problem functions

free_mappings ();           // free memory of AMPL OCP frontend data
```

Evaluating Problem Functions. Once the database has been successfully filled with the optimal control problem representation of the AMPL model, an appropriate optimal control problem solver can be called. This solver will have to evaluate problem functions. For conveniently doing so, the optimal control frontend provides a set of functions that wrap around the `conival` and `objival` functions provided by AMPL's solver library:

`evaluate_ode_rhs(i,y)` evaluates the ODE right-hand side $\dot{x}_i(t) = f_i(\cdot)$ for a differential state $x_i(t)$, $0 \leq i < n_x$. The vector y here is the plain vector of current AMPL variable values.

`evaluate_dae_rhs(i,y)` evaluates the residual of DAE constraint $g_i(\cdot)$, $0 \leq i < n_z$.

`evaluate_scaled_mayer(y)` evaluates and scales the value of the Mayer objective term, if a Mayer term exists.

`evaluate_scaled_lagrange(y)` evaluates and scales the value of the Lagrange objective term's integrand, if a Lagrange objective exists.

`evaluate_scaled_clsq(y,res)` evaluates and scales the value of the Lagrange objective term's integrand, if the integrand has least-squares structure and if a Lagrange objective exists. Upon return the vector res holds the least-squares residuals, that is, the individual values of each squared summand.

`evaluate_scaled_node_lsq(n,y,res)` evaluates one summand of a point least-squares objective term, if one exists. The integer n specified the number $0 < n < N_{lsq}$ of the measurement point to be evaluated.

`evaluate_path_con(i,y)` evaluates and scales the residual of an inequality path constraint.

`evaluate_coupled_eq_con(i,y)` evaluates and scales the residual of a coupled equality constraint.

`evaluate_coupled_ineq_con(i,y)` evaluates and scales the residual of a coupled inequality constraint.

`evaluate_point_eq_con(n,i,y)` evaluates and scales the residual of an equality point constraint.

`evaluate_point_ineq_con(n,i,y)` evaluates and scales the residual of an inequality point constraint.

Writing Solutions from a Solver. To write a solution file of the proposed format, the optimal control frontend provides three function calls to be used by a backend interfacing an optimal control problem solver with AMPL:

`alloc_solution` allocates a solution structure given a discretization grid length.

`write_solution` writes a solution file according to the new format and fills it with the solution data found in the solution structure. The solver backend should have queried the solver itself for this solution and copied it over to this solution structure.

`free_solution` free a previously allocated solution structure after it has been written to a solution file.

C TACO Toolkit Error Messages

This section lists the error messages emitted by the TACO toolkit during analysis and verification of the optimal control problem structure. If option *solvername*_`auxfiles` is set to contain the characters "r" and "c", error messages will show the name of the offending variable, objective, or constraint. Codes 1 to 5 are reserved for internal errors.

6. "`AMPL error reading stub.nl file` *filename*" AMPL could not read the *stub.nl* file.

7. "`AMPL error getting solver options`" AMPL could not read the solver options. Make sure your solver options string contains known keywords and valid values only.

8. "`I/O error writing solution file` *filename*" AMPL could not write the solution file. Make sure that the current working directory is writeable and that the volume is not full.

9. "`AMPL network variables are not supported`" The AMPL model contains network variables. Network modeling is currently not supported.

10. "`AMPL piecewise linear terms are not supported`" The AMPL model contains piecewise linear terms. Nonsmooth models are currently not supported.

11. "`diff() must be called exactly once for each differential state variable`"
You called `diff()` more than once for the same variable. Every differential state variable is associated with exactly one right hand side function. Most likely, this is a typo in your model.

12. "`Logical operator` *operator* `not permitted`" The shown constraint or objective make use of a logical operator. Nonsmooth models are currently not supported.

13. "`Relational operator` *operator* `not permitted`" The shown constraint or objective make use of a relational operator. Nonsmooth models are currently not supported.

14. "`Nonsmooth operator` *operator* `not permitted`" The shown constraint or objective make use of a nonsmooth operator. Nonsmooth models are currently not supported.

15. "`ODE constraints must be equality constraints`" You called `diff()` in an inequality constraint. All ODE constraints must be equality constraints, though.

16. "`Cannot determine type of objective functions`" The shown objective cannot be determined to be of Mayer, Lagrange, integral least-squares, or point least-squares type. Please refer to Section 2.3 to learn about the structure of supported objective functions.

17. "`Mayer objective function must not depend on controls`" The indicated objective is of Mayer type, and hence must not depend on control trajectory variables.

18. "`The number of DAE constraints does not match the apparent number of algebraic variables`" The number of DAE constraints found in your model does not match the

number of algebraic variables you have declared by letting suffix `.type` to value `"dae"`. Make sure you've set the suffix of all algebraic state variables, and make sure all your DAE constraints are equality constraints.

19. "`Invalid value for suffix .type`" A variable, constraint, or objective has suffix `.type` set to an unrecognized value. This should not happen unless you're using an incompatible `OptimalControl.mod` file.

20. "`Missing independent time variable or end time variable`" TACO could not determine which AMPL variables represent independent time or end time. Make sure that the independent time variable appears as second argument to all `diff()` calls, and that the end-time variable appears as second argument to `integral()` in Lagrange-type objectives, or to `eval()` in Mayer-type objectives or end-point constraints. If your AMPL model uses a time horizon of fixed length, make sure the end-time value shows up consistently in these places.

21. "`Nesting a call to function` *name* `inside another is not allowed`" You nested two calls to functions `diff()`, `eval()`, or `integral()`. This should never be necessary.

22. "`As of now, diff() must be explicit. Try to write your ODE as diff(var, t) = ...;`" The AMPL optimal control frontend currently supported explicit ODEs only, i.e. the permitted formulation is $\dot{x}(t) = f(t,x(t),\ldots)$ instead of the more general $0 = f(t,x(t),\dot{x}(t),\ldots)$. Try to rewrite your model to use explicit ODEs only.

23. "`First argument to eval() must not be a constant`" The shown constraint or objective calls `eval()` with two constant arguments. This is not sensible. Either remove the calls to `eval()`, or make sure the expression to be evaluated references independent time or at least one state or control trajectory variable.

24. "`Second argument to eval() must be >= 0.0, or the final time variable`" The shown constraint or objective calls `eval()` with a time point that a) evaluates to a negative value, or b) is not a simple constant and not the end-time variable.

25. "`First argument to integral() must not be a constant`" An objective calls `integral()` with two constant arguments. This is not sensible. Either remove the call to `integral()`, or make sure the expression to be integrated references independent time or at least one state or control trajectory variable.

26. "`Second argument to integral() must be the final time variable`" The second argument of a call to `integral()` must be the final time variable, or the final time itself.

27. "`Second argument to diff() must be the independent time variable`" The second argument of a call to `diff()` must be the independent time variable.

28. "`Function diff() expects differential state variable and independent time variable as arguments`" The first argument to `diff` must be a differential state trajectory variable, and the second argument of a call to `diff()` must be the independent time variable.

29. "`Calls to integral() not allowed in constraints`" The function `integral()` was called inside a constraint expression. Calls to `integral()` are only allowed in a Lagrange-type or integral least-squares-type objective.

30. "`Function call to` *name* `must enclose entire expression`" Calls to `eval()` and `integral()` must enclose the entire expression to be evaluated or integrated.

31. "`Only controls or parameters can be binary/integer variables`" AMPL's `binary` or `integer` restriction may be applied to control trajectory variables and model parameter variables only. Time as well as differential and algebraic state trajectory variables must be continuous.

32. "`Invalid grid node position, must be within [0,1] (tf free) or [0,tf] (tf fixed)`" A call to `eval()` used an invalid evaluation time. Allowed times are constants 0 to 1,

being relative times on the time horizon $[0, t_\mathrm{f}]$ if t_f is free, absolute times 0 to t_f if t_f is fixed, or the end-time variable t_f itself.

33. "`Duplicate objective of` *name*`-type`" At most one objective of Mayer-, Lagrange-, and least-squares type is allowed per problem.

34. "`Calls to eval() not allowed in ODE constraints`" The function `eval()` was called inside an ODE constraint expression. This is not allowed.

35. "`Calls to diff() not allowed in objective functions`" The function `diff()` was called inside an objective function expression. This is not allowed.

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