

Technical Report

Advanced Practical in Optimal Control

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18-July-2021

Abstract

The main scope of this practical is to expose the interfaces of **IDAS/CVODES** integrators from the **SUNDIALS suite** [4] into **MATLAB**. To this end, the implementation provides the mean to define a **Dynamical System**, to compute **forward integration** as well as **first and second order sensitivity** in a **parallelized** way. All of these are done by **automatically C++ code generation** of the **integrator** and of the **sensitivity** by using a **high level language** to define a **Dynamical System** on top of **CasADi**, which closely resembles a **symbolical framework** but without having the corresponding disadvantages.

Alongside with this report, a full implementation can be found here: [SUNDIALS2Matlab](#)

1 Introduction

The main task of this practical was to research 2 ways of integrating **SUNDIALS suite** as part of **MLI** project and also to provide the necessary **backend Framework**.

The 2 possible libraries considered for this task were: **CasADi** [2] and **AMICI** [3] both of them providing an automatic way of exposing **SUNDIALS** c/c++ code integrators to dynamical languages like **Python** and **Matlab**.

The final decision of using **CasADi** was taken after multiple testing on each of them and was based on the fact that is a better integrated project with a comprehensive documentation and a wider community.

Besides providing access to **SUNDIALS suite**, **CasADi** offers a way of defining **Dynamical Systems** using a **high level language** as well as doing **C++ code generation** at run time (**JIT**) starting from a **symbolical representation** of the problem and general means to **parallelize** the computation.

2 Structure of the report

In *Section 3* we start by defining the **Optimal Control problem** by spiting it using a **hierarchical layer architecture**. At the end of this section, it will be clear how the **backend Framework** provided can be integrated into a general **OCP** framework.

Section 4 starts by describing the general **backend Framework design** ???. It continues by introducing **CasADi's high level language**. Based on that it describes how a **Dynamical System** can be defined using **CasADi's framework** and how **CVODES integrator**, **first and second order sensitivity Code Generation** is done. Last but not least, it describes the the **API** required by all the functionalities abovementioned.

Section 5 is meant to underline the advantages of using **CVODES integrator** over the default ones offered by **Matlab** by comparing the computation time required in multiple dynamical systems scenarios.

We end this report with a section of conclusions and recommendations **6** and possible feature extensions of the provided **backend Framework**.

3 Problem Definition

The problem that needs to be solved regards the following OCP (Optimal Control problem):

$$\min_{x(\cdot), u(\cdot)} \quad \Phi(x(t_f)) \quad (1a)$$

$$\text{s.t.} \quad \dot{x}(t) = f(x(t), u(t), p), \quad (1b)$$

$$x(t_0) = x_0 \quad (1c)$$

$$x^{lo} \leq x(t) \leq x^{up}, \quad (1d)$$

$$u^{lo} \leq u(t) \leq u^{up} \quad \forall t \in [t_0, t_f] \quad (1e)$$

To solve 1 numerically, we are using a discretized version by introducing the following multiple shooting variables: s_0, \dots, s_N q_0, \dots, q_N

$$\min_{x(\cdot), u(\cdot)} \quad \Phi(S_N) \quad (2a)$$

$$\text{s.t.} \quad s_{i+1} = x(t_{i+1}; t_i, s_i, q_i, p) \quad i = 0, \dots, N-1 \quad (2b)$$

$$s_0 = x_0 \quad (2c)$$

$$x^{lo} \leq s_i \leq x^{up}, \quad i = 0, \dots, N \quad (2d)$$

$$u^{lo} \leq q_i \leq u^{up} \quad i = 0, \dots, N \quad (2e)$$

where $x(t; t_0, s, q, p)$ is the solution of 3

$$\dot{x}(t) = f(x(t), q, p) \quad (3a)$$

$$x(t_0) = s \quad (3b)$$

Next, we define the primal variables as $w = (s, q)$ and we introduce the following functions for equality and inequality constraints:

$$a(w) = \begin{bmatrix} x_0 - s_0 \\ x(t_1; t_0, s_0, q_0, p) - s_1 \\ \vdots \\ x(t_N; t_{N-1}, s_{N-1}, q_{N-1}, p) - s_N \end{bmatrix} \quad (4)$$

$$b(w) = \begin{bmatrix} x^{lo} - s \\ s - x^{up} \\ q^{lo} - q \\ q - q^{up} \end{bmatrix} \quad (5)$$

Based on 4 and 5 one can write the OCP in a more compact form:

$$\min_w \quad \Phi(w) \quad (6a)$$

$$\text{s.t.} \quad a(w) = 0 \quad (6b)$$

$$b(w) \leq 0 \quad (6c)$$

For 6 the Lagrange function and its derivatives at point (w, λ, μ) are defined as follows:

$$\mathcal{L}(w, \lambda, \mu) = \Phi(w) - \lambda^\top a(w) - \mu^\top b(w) \quad (7)$$

$$\nabla \mathcal{L}(w, \lambda, \mu) = \begin{bmatrix} \nabla_w \Phi(w) - \nabla_w a(w) \lambda - \nabla_w b(w) \mu \\ a(w) \\ b(w) \end{bmatrix} \quad (8)$$

$$\nabla^2 \mathcal{L}(w, \lambda, \mu) = \begin{bmatrix} \nabla_w^2 \Phi(w) - \nabla_w^2 a(w) \lambda & \nabla_w a(w) & \nabla_w b(w) \\ \nabla_w a(w)^\top & & \\ \nabla_w b(w)^\top & & \end{bmatrix} \quad (9)$$

We want to be able to solve:

$$\nabla \mathcal{L}(w, \lambda, \mu) = 0. \quad (10)$$

We apply Newton's method and we have to solve for (w_i, λ_i, μ_i) :

$$\nabla^2 \mathcal{L}(w_i, \lambda_i, \mu_i) \Delta w + \nabla \mathcal{L}(w_i, \lambda_i, \mu_i) = 0. \quad (11)$$

Equivalently, the following QP (Quadratic Programming) needs to be solved:

$$\min_{\Delta w} \quad \Delta w^\top \nabla_w^2 \mathcal{L}(w_i, \lambda_i, \mu_i) \Delta w + \nabla \Phi(w_i) \Delta w \quad (12a)$$

$$\text{s.t.} \quad a(w_i) + \nabla a(w_i) \Delta w = 0 \quad (12b)$$

$$b(w_i) + \nabla b(w_i) \Delta w \leq 0 \quad (12c)$$

To solve 12, the following terms, which include the evaluation of the dynamical system, must be evaluated: $a(w_i), \nabla_w a(w_i), \nabla_w^2 a(w) \cdot \lambda$

The process of evaluation of $\mathbf{a}(\mathbf{w}_i), \nabla_{\mathbf{w}} \mathbf{a}(\mathbf{w}_i), \nabla_{\mathbf{w}}^2 \mathbf{a}(\mathbf{w}) \cdot \boldsymbol{\lambda}$ requires the implementation of the following functions, as part of integration of **SUNDIALS**:

S.1 $\mathbf{x}(t; t, \mathbf{s}, \mathbf{q}, \mathbf{p})$ Standard forward integration.

S.2 $\nabla_{\mathbf{w}} \mathbf{x}(t; t, \mathbf{s}, \mathbf{q}, \mathbf{p}) \cdot \mathbf{d}$ This is the directional derivative of $\mathbf{x}(t; t, \mathbf{s}, \mathbf{q}, \mathbf{p})$ in the direction \mathbf{d} . Multiple directions can be evaluated at the same time. The complete Jacobian can be computed by computing directional derivatives in all unit directions.

S.3 $\nabla_{\mathbf{w}}^2 \mathbf{x}(t; t, \mathbf{s}, \mathbf{q}, \mathbf{p}) \cdot \boldsymbol{\lambda}$ Hessian of $\boldsymbol{\lambda}^\top \cdot \mathbf{x}(t; t, \mathbf{s}, \mathbf{q}, \mathbf{p})$ with respect \mathbf{w} .

Where the dimensions are:

$$\mathbf{t} \in \mathbb{R} \quad (13a)$$

$$\mathbf{x} \in \mathbb{R}^{n_x} \quad (13b)$$

$$\mathbf{q} \in \mathbb{R}^{n_q} \quad (13c)$$

$$\mathbf{p} \in \mathbb{R}^{n_p} \quad (13d)$$

$$(13e)$$

A simplified, comprehensive way to visualize this problem can be seen using Figure 1 which introduces a 3 layer architecture where the first 2 (the

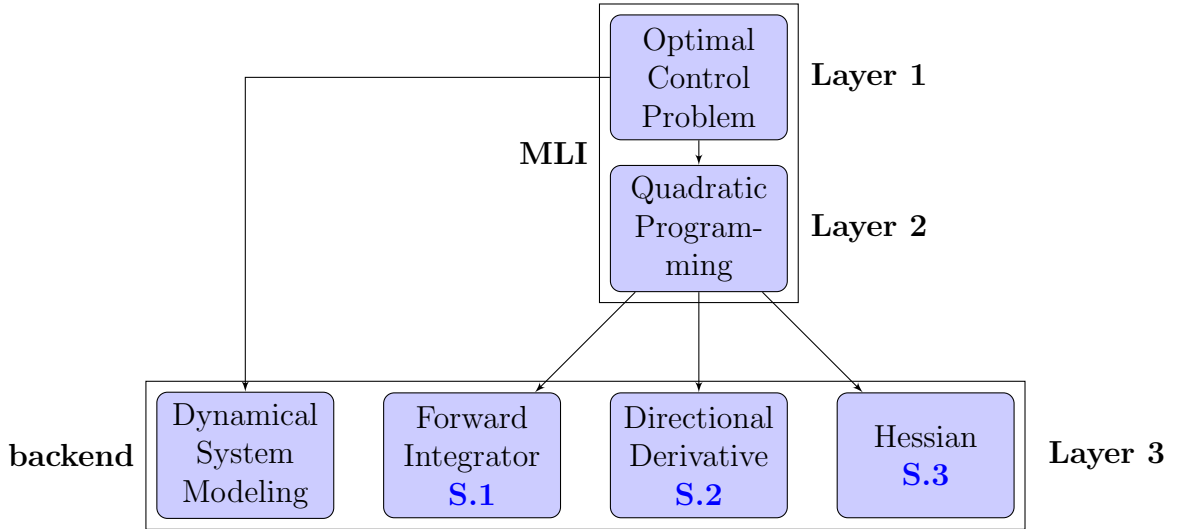


Figure 1: Problem architecture

OCP and **QP**) are provided by **MLI** whereas, the 3rd layer, introduces the **backend Framework** which is build on top of **CasADi** and represents the *main contribution of this practical*.

Long story short, solving the **OCP** (defined by the **Layer 1**) requires multiple **QP** queries (introduced by the **Layer 2**) which in turn, requires a way to define the **Dynamical System** and to compute **S.1**, **S.2** and **S.3** (exposed by **Layer 3**).

4 Framework

4.1 Framework Structure

This project requires the latest version of **CasADi** framework (which can be obtained from [1]) as part of the main structure of the project under a folder called **casadi**.

Alongside, the structure introduced by Figure: 2 defines the the components of the framework where:

- *DynamicalSystems* – Is the folder containing all the **Dynamical Systems** defined as separated files using **CasADi's high level language**.

- *functions* – Is the folder containing the main functionalities of the project: **One time code generation** and the **binding functors** for calling **forward integration** as well as **first** and **second order sensitivity**.
- *MatlabFunc* – Is the folder where the corresponding **Matlab Dynamical Systems** are defined used for performance comparisons with **CVODES**.

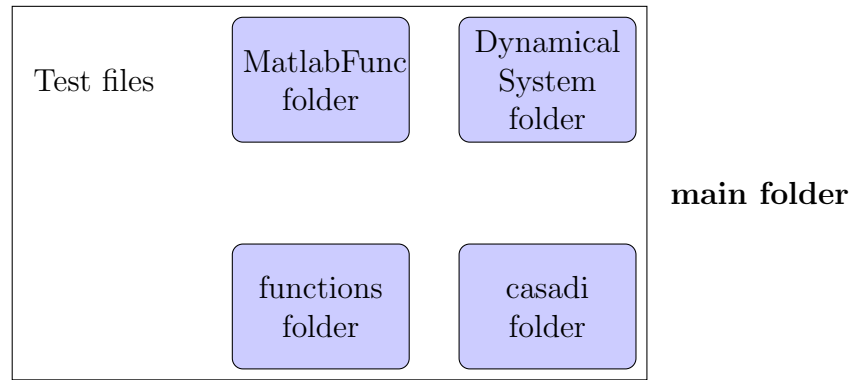


Figure 2: Framework folder structure

4.2 Framework use case workflow

In a nutshell, the **workflow** of the project is determined by 3 steps in the following order:

1. *Dynamical System definition*
2. *One time code generation* by calling one of the following functions:
3. *Multiple function calls of:* **integrate()**, **integrateWSensitivies()** and **integrateWSensitiviesAndHessian()**

The use case **workflow** of the of the project can be summarized by Figure:3.

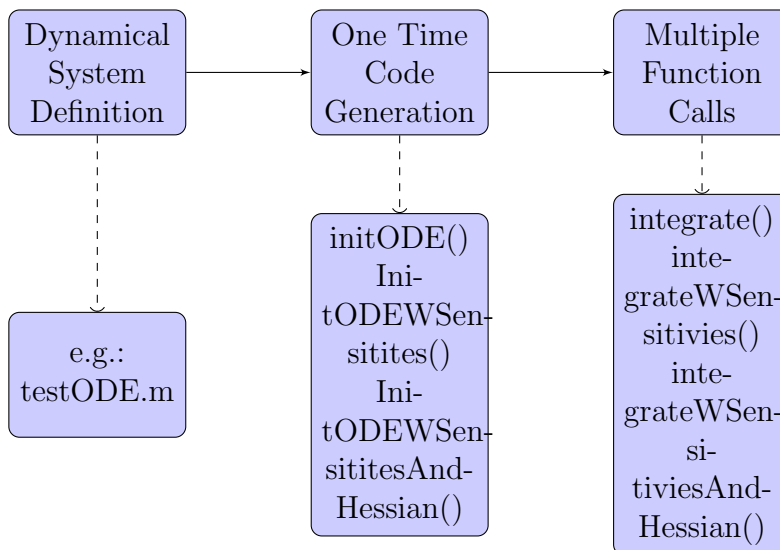


Figure 3: Use case workflow

4.3 CasADi

CasADi is an open-source software tool for **numerical optimization** in general and **optimal control** (i.e. optimization involving differential equations) in particular. [2]

The main scope of **CasADi** is **automatic differentiation**. Besides that, it has also support for **ODE/DAE integration** and **sensitivity analysis**, nonlinear programming and interfaces to other numerical tools (**SUNDIALS suite**)

At the core of **CasADi** is a self-contained **symbolic framework** that allows the user to construct symbolic expressions using a **Matlab** inspired everything-is-a-matrix syntax, i.e. vectors are treated as n-by-1 matrices and scalars as 1-by-1 matrices. Further on, the constructed symbolical expression is used by numerical means.

CasADi symbolical framework defines multiple data types but the most relevant for this project is **SX**. The **SX** data type is used to represent **matrices** whose elements consist of symbolic expressions made up by a sequence of unary and binary operations. Below are some examples of **CasADi's API** for defining **symbolical expressions**.


```

%Defining 2 symbolical variables 'a' and 'b':
a = SX.sym('a');
b = SX.sym('b');

%Computing the Jacobian of 'sin(a)' with respect to 'a'.
J = jacobian(sin(a),a);
%Computing the Hessian
H = hessian([a;b],[a;b]);

% Function with two scalar inputs, one output.
x = a^2+b^2;
f = Function('f',{a,b},{x});
x_res = f(2,3);

% Function with one vector input, one output.
x = a^2+b^2;
f = Function('f',{[a;b]},{x});
x_res = f([2;3]);

% Solving a QP.
y = a^2+b^2;
solver = qpsol('solver','qpoades',struct('x',[a;b],'f',y));
res = solver('x0',[0.1;0.2]);
full(res.x)

% Solving NLP.
y = a^2+b^2;
solver = nlpsol('solver','ipopt',struct('x',[a;b],'f',y));
res = solver('x0',[0.1;0.2]);
full(res.x)

% Defining an ODE
% dot(a) = 1,
% dot(b) = a^2+b^2 = y
y = a^2+b^2;
intg = integrator('intg','cvcodes',struct('x',[a;b],'ode',[1;y]));
res = intg('x0',[0.1;0.2]);
full(res.xf)

```

A comprehensive documentation for CasADi can be accessed here: [CasADi](#).

4.4 Dynamical System definition

Given the **Dynamical System** described by 14, where t is the time, x is the differential states, q is the control (constant) and p is the parameter we are aiming for a way to use **CasADi** to define it.

$$\dot{x}(t) = f(t, x(t), q, p) \quad (14a)$$

$$x(t_0) = x_0 \quad (14b)$$

This is done in a separate file as part of the folder *DynamicalSystems* and it must follow the previously introduced **CasADi's high level language** definition convention for **ODE/DAE**.

A more comprehensive example using **Lotka-Volterra ODE** would be:

```
import casadi.*

%define the states
x = SX.sym('x',2);

%define the parameters
a = SX.sym('a',1);
b = SX.sym('b',1);
c = SX.sym('c',1);
d = SX.sym('d',1);

%define the control
u = SX.sym('u',1);

%building the dynamical system
sys = struct;
%states
sys.x = x;
%parameters
sys.p = [u;a;b;c;d];
%defining the ODE/DAE
```

```
sys.ode = [
    a * x(1) - b * x(1) * x(2) - x(1) * u ;
    c * x(1) * x(2) - d * x(2) - x(2) * u
];
```

4.5 Code Generation

Based on the above definition of the dynamical system, the user needs to call **one time**, a function that **generates, on the fly**, the customized C/C++ code for the corresponding integrator, **compiles** the newly generated code (**JIT compiling**) and returns a **Functor** that provides future access to it.

The corresponding call for *Lotka-Volterra ODE* defined in the file *lotka_volterraCasADi.m* would look like as follows:

```
InitODE( 'lotka_volterraCasADi' , tStart , tEnd );
```

The corresponding call for DAE looks like as follows:

```
InitDAE( 'DinamicalSystem' , tStart , tEnd );
```

The mandatory parameters of **InitODE()/InitDAE()** are as follows:

- *lotka_volterraCasADi* : Name of the file that contain the dynamical system
- *tStart* : The start time (most of the time, it's **0**)
- *tEnd* : The end time of the integration interval. The current **CasADi's code generation** is **limited to initial, fixed time-step** for **SUNDIALS suite**.

If one requires also access to the **first** and **second order sensitivity**, one must call one of the following functions with the same list of parameters as above:

- *InitODEWSensitites*
- *InitODEWSensititesAndHessian*

At this point, all the prerequisites for the future calls of *integrator*, *sensitivity* and *hessian* (*integrate(inp)*, *integrateWSensitivies(inp)* and

integrateWSensitiviesAndHessian(inp)) w.r.t. the ODE are satisfied as they are the result of the automatic generation. These can be access using the **global variable: s2m**. Another important aspect is that one of the optional parameter **nrThreads/threads** can be used to parallelize the process by explicitly defining the **number of threads** used.

Each of the calls must contain, as parameter, an object that contains a subset of the variables defined below:

- *inp.M* : Number of multiple shooting intervals.
- *inp.sd* : Initial value for differential states for each multiple shooting interval.
- *inp.q* : A vector of controls used by each integrator call with size: *inp.M*
- *inp.p* : The values of the parameters in the same order it was defined previously in the dynamical system.
- *inp.nx* : The size of x .
- *inp.nq* : The number of control parameters.
- *inp.np* : The number of parameters.
- *inp.fwd.x0* : The sensitivity directions in form of matrix containing only the components corresponding to x_0
- *inp.fwd.p* : The sensitivity directions in form of matrix containing only the components corresponding to *parameters*
- *inp.nr_sensdirs* : The number of sensitivity directions.
- *inp.lambda* : The adjoint sensitivity direction
- *inp.threads* : The number of threads for the thread pool used by the integrator

For complete examples (*input/output*) please check the following files: *test_integrate.m*, *test_integrateWSensitivies.m* and *test_integrateWSensitiviesAndHessia.m*

5 Integrator comparison

The development of this project is based on the *hypothesis* that a **c native backend integrator** exposed in **Matlab** is faster than the **Matlab native** one. To see how well the **CVODES integrator** works, a set of tests was been developed. For comparison, the comprehensive list can be checked in Figure:4.

| Integration time (s) | Dynamical system | Matlab integrator | Matlab integration steps | Matlab computation time (s) | SUNDIALS integrator | SUNDIALS computation time (s) | Computation time ratio: (Matlab / SUNDIALS) | Test file |
|----------------------|--------------------------|-------------------|--------------------------|-----------------------------|---------------------|-------------------------------|---|--------------|
| 1 | Pendulum | ode45 | 65 | 0.0027 | CVODES | 0.0016 | 1.69 | main_test1.m |
| 5 | Pendulum | ode45 | 137 | 0.0048 | CVODES | 0.0031 | 1.55 | main_test1.m |
| 10 | Pendulum | ode45 | 249 | 0.0055 | CVODES | 0.0018 | 3.06 | main_test1.m |
| 50 | Pendulum | ode45 | 1153 | 0.0244 | CVODES | 0.0046 | 5.30 | main_test1.m |
| 100 | Pendulum | ode45 | 2101 | 0.0492 | CVODES | 0.0078 | 6.31 | main_test1.m |
| 500 | Pendulum | ode45 | 5541 | 0.0971 | CVODES | 0.0157 | 6.18 | main_test1.m |
| 1 | Second order ODE | ode23 | 17 | 0.0029 | CVODES | 0.0015 | 1.93 | main_test2.m |
| 5 | Second order ODE | ode23 | 32 | 0.0049 | CVODES | 0.0016 | 3.06 | main_test2.m |
| 10 | Second order ODE | ode23 | 38 | 0.0032 | CVODES | 0.0014 | 2.29 | main_test2.m |
| 50 | Second order ODE | ode23 | 58 | 0.0042 | CVODES | 0.0015 | 2.80 | main_test2.m |
| 100 | Second order ODE | ode23 | 65 | 0.0052 | CVODES | 0.0017 | 3.06 | main_test2.m |
| 500 | Second order ODE | ode23 | 79 | 0.0057 | CVODES | 0.0016 | 3.56 | main_test2.m |
| 1 | The van der Pol equation | ode15s | 40 | 0.004 | CVODES | 0.0015 | 2.67 | main_test3.m |
| 5 | The van der Pol equation | ode15s | 43 | 0.006 | CVODES | 0.0024 | 2.50 | main_test3.m |
| 10 | The van der Pol equation | ode15s | 43 | 0.0042 | CVODES | 0.0014 | 3.00 | main_test3.m |
| 50 | The van der Pol equation | ode15s | 46 | 0.0042 | CVODES | 0.0015 | 2.80 | main_test3.m |
| 100 | The van der Pol equation | ode15s | 46 | 0.0052 | CVODES | 0.0015 | 3.47 | main_test3.m |
| 500 | The van der Pol equation | ode15s | 49 | 0.0058 | CVODES | 0.0015 | 3.87 | main_test3.m |
| 1 | Lorenz system | ode45 | 65 | 0.0029 | CVODES | 0.0017 | 1.71 | main_test4.m |
| 5 | Lorenz system | ode45 | 309 | 0.006 | CVODES | 0.0023 | 2.61 | main_test4.m |
| 10 | Lorenz system | ode45 | 601 | 0.0105 | CVODES | 0.0033 | 3.18 | main_test4.m |
| 50 | Lorenz system | ode45 | 2989 | 0.0467 | CVODES | 0.0121 | 3.86 | main_test4.m |
| 100 | Lorenz system | ode45 | 5989 | 0.0651 | CVODES | Error 1 | N/A | main_test4.m |
| 500 | Lorenz system | ode45 | 29721 | 0.2691 | CVODES | Error 2 | N/A | main_test4.m |
| 1 | Lotka Volterra | ode23 | 11 | 0.0003 | CVODES | 0.0014 | 0.21 | main_test5.m |
| 5 | Lotka Volterra | ode23 | 15 | 0.0004 | CVODES | 0.0014 | 0.29 | main_test5.m |
| 10 | Lotka Volterra | ode23 | 33 | 0.0011 | CVODES | 0.0016 | 0.69 | main_test5.m |
| 50 | Lotka Volterra | ode23 | 150 | 0.0037 | CVODES | 0.0023 | 1.61 | main_test5.m |
| 100 | Lotka Volterra | ode23 | 303 | 0.005 | CVODES | 0.0026 | 1.92 | main_test5.m |
| 500 | Lotka Volterra | ode23 | 1503 | 0.022 | CVODES | 0.0083 | 2.65 | main_test5.m |

Error 1 : CV_TOO_MUCH_WORK (at t = 75.62)
Error 2 : CV_TOO_MUCH_WORK (at t = 74.7571)

Figure 4: **CVODES integrator** *vs.* **Matlab native integrator**

From Figure:5 one can observe that the **CVODES integrator** tend to be, on average, **2** up to **3** times faster. For longer integration time, an exponential computation improvement can be observed. These comparisons don't take into consideration that, most of the time, multiple integration intervals are computed within a **multiple shooting** problem which can be **parallelized for free** based on the provided **backend Framework** implementation and can also **improve the computation time significantly**.

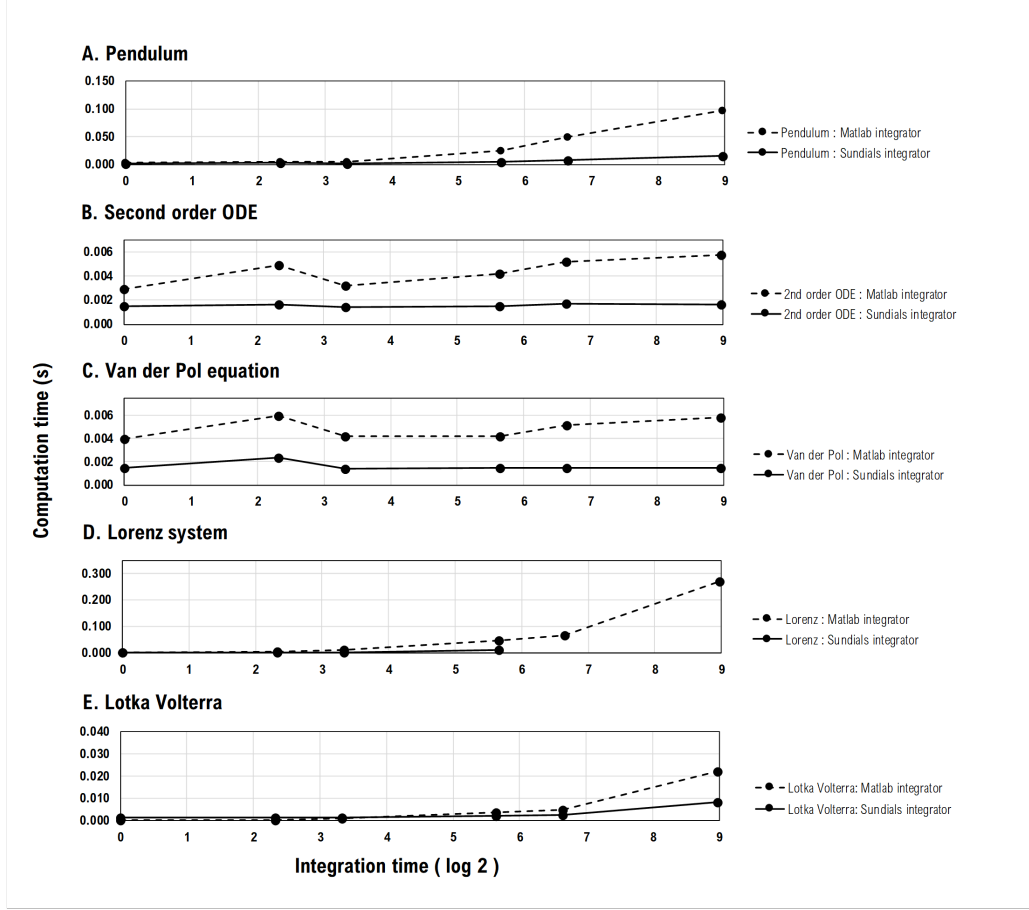


Figure 5: Integration time *vs.* Computation time

6 Conclusions and Recommendations

The next natural step for this project will be to integrate it into **MLI project**. To this end, the current provided *API* should make this process smooth enough. Current implementation contains the complete necessary backend for the initial **ODE** problem definition 3. On top of that, it contains also the necessary implementation for **DAE** and it also partially implements the *API*. The remaining **first** and **second order** sensitivity functionality should be straightforward to implemented based on the counterpart **ODE** implementation. More work should be putted into exposing more optional configuration parameters for the **code generation API**.

References

- [1] Joel A E Andersson, Joris Gillis, Greg Horn, James B Rawlings, and Moritz Diehl. Casadi framework download @ONLINE. <https://web.casadi.org/get/>, 2021.
- [2] Joel A E Andersson, Joris Gillis, Greg Horn, James B Rawlings, and Moritz Diehl. CasADi – A software framework for nonlinear optimization and optimal control. *Mathematical Programming Computation*, In Press, 2018.
- [3] Fabian Fröhlich, Daniel Weindl, Yannik Schälte, Dilan Pathirana, Łukasz Paszkowski, Glenn Terje Lines, Paul Stapor, and Jan Hasenauer. Amici: High-performance sensitivity analysis for large ordinary differential equation models. *Bioinformatics*, 04 2021. btab227.
- [4] Alan C Hindmarsh, Peter N Brown, Keith E Grant, Steven L Lee, Radu Serban, Dan E Shumaker, and Carol S Woodward. SUNDIALS: Suite of nonlinear and differential/algebraic equation solvers. *ACM Transactions on Mathematical Software (TOMS)*, 31(3):363–396, 2005.