Sub-ODEs Simplify Taylor Series Algorithms for Ordinary Differential Equations

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Outline

Reference: NN & JP, *Sub-ODEs Simplify Taylor Series Algorithms for Ordinary Differential Equations*, Submitted to SISC, December 2024. https://arxiv.org/abs/2503.21078

Introduction

We are concerned with Taylor series solution of an initial-value problem (IVP) for an ordinary differential equation (ODE) system:

$$\dot{x} = f(t, x), \quad x(t_0) = x_0.$$

- We assume $f(t, x)$ consists of basic arithmetic operations $(+, -, \times, /)$ and standard functions such as $\exp, \sin$, etc.
- Non-differentiable functions like $|\cdot|$, $\min$, $\max$, and conditional structures (e.g. "if" statements) are excluded.

Taylor method

A Taylor method (TM) for $\dot{x} = f(t, x),\ x(t_0) = x_0$

- computes the Taylor series (TS), to some order, of the solution at the current t, and
- sums the TS with a suitable step size to move to the next point.

▷ A TM requires $f(t, x)$ to be provided as code, which is executed in the form of recurrences that compute Taylor coefficients.

▷ Recurrences are needed for:
  - ▷ basic arithmetic operations (BAOs)
  - ▷ standard functions: $\exp$, $\sin$, etc.

▷ Most TM implementations use individual recurrences for each standard function.

▷ Our approach eliminates the need for individual recurrences.

Taylor coefficients (TCs)

Automatic (or algorithmic) differentiation, AD, gives a practical scheme for computing coefficients.

Example: Consider $\dot{x} = x^2$, $x(t_0) = x_0$.

- Assume a series $x(t_0 + s) = x_0 + x_1 s + x_2 s^2 + \cdots$.
  Then

$$\dot{x} = x_1 + 2x_2 s + 3x_3 s^2 + \cdots$$
$$x^2 = x_0^2 + (2x_0 x_1)s + (2x_0 x_2 + x_1^2)s^2 + \cdots .$$

- Starting with x_0, and equating these term by term:

$$x_1 = x_0^2$$
$$x_2 = \tfrac{1}{2}(2x_0 x_1)$$
$$x_3 = \tfrac{1}{3}(2x_0 x_2 + x_1^2)$$
$$\vdots$$

ODE's code-list

- Consider an ODE of size n, i.e., $x = (x_1, \ldots, x_n)$.
- The code for f is implemented as a code-list (CL), a sequence of assignments

$$\begin{cases} \dot{x}_j = \widehat{x}_j, & j = 1{:}n, \\ x_{n+1} = t, & j = n{+}1, \\ x_j = \phi_j(x_{\prec j}), & j = n{+}2 : N. \end{cases}$$

- Input values are $x_1, \ldots, x_n, t$; x_{n+1} is an alias for t. The CL sets intermediate variables $x_{n+2}, \ldots, x_N$.
- $x_{\prec j}$ means the x_i's on which x_j depends; they must all have $i < j$, i.e. have already been computed.
- ϕ_j are given functions.
- CL specifies indices $\mathit{out}(1), \ldots, \mathit{out}(n)$ in $1{:}N$ such that $\widehat{x}_j = x_{\mathit{out}(j)}$ form the output vector $\widehat{x} = f(t, x)$.

Example

- Consider the simple ODE $\dot{x} = e^{-x}$.
- Its code-list is

$$\dot{x} = \widehat{x}$$
$$u = -x$$
$$\widehat{x} = \exp(u)$$

Sub-ODE idea

Take $\widehat{x} = \exp(u)$ in the above CL.

- A Taylor solver needs to compute

$$\widehat{x}(t) = \exp(u(t)), \quad \text{where } u(t) \text{ is a TS}$$

(both input and output are truncated to some order).

- We use that

$$\widehat{x} = \exp(u) \quad \text{obeys the ODE } \mathrm{d}\widehat{x}/\mathrm{d}u = \widehat{x}, \text{ whence}$$
$$\dot{\widehat{x}} = \widehat{x}\dot{u}, \qquad \text{since } u, \widehat{x} \text{ are both functions of } t.$$

- The sub-ODE method replaces in the CL

$$\widehat{x} = \exp(u) \quad \text{by its sub-ODE} \quad \dot{\widehat{x}} = \widehat{x}\dot{u}$$

Sub-ODEs make a DAE

- CL of $\dot{x} = e^{-x}$:

$$\dot{x} = \widehat{x}, \qquad u = -x, \qquad \widehat{x} = \exp(u) \tag{1}$$

- Replace $\widehat{x} = \exp(u)$ by its sub-ODE $\dot{\widehat{x}} = \widehat{x}\dot{u}$:

$$\dot{x} = \widehat{x}, \qquad u = -x, \qquad \dot{\widehat{x}} = \widehat{x}\dot{u} \tag{2}$$

- The CL (2) represents a differential-algebraic equation (DAE), so ODE theory no longer applies.
- Namely, to cast (2) as an ODE, one must differentiate $u = -x$:

$$\dot{x} = \widehat{x}, \qquad \dot{u} = -\dot{x}, \qquad \dot{\widehat{x}} = \widehat{x}\dot{u}$$

- How to get the TCs for x?

- Write $x(t) = x(t_0 + s) = x_0 + x_1 s + x_2 s^2 + \cdots$; similarly for $u, \widehat{x}$. Inserting in (2) gives

$$\underbrace{1x_1 + 2x_2 s + 3x_3 s^2 + \cdots}_{\dot{x}} = (\underbrace{\widehat{x}_0 + \widehat{x}_1 s + \widehat{x}_2 s^2 + \cdots}_{\widehat{x}}),$$

$$\underbrace{u_0 + u_1 s + u_2 s^2 + \cdots}_{u} = -(\underbrace{x_0 + x_1 s + x_2 s^2 + \cdots}_{x}),$$

$$\underbrace{1\widehat{x}_1 + 2\widehat{x}_2 s + 3\widehat{x}_3 s^2 + \cdots}_{\dot{\widehat{x}}} = (\underbrace{\widehat{x}_0 + \widehat{x}_1 s + \widehat{x}_2 s^2 + \cdots}_{\widehat{x}})(\underbrace{1u_1 + 2u_2 s + 3u_3 s^2 + \cdots}_{\dot{u}}).$$

- Expanding and equating terms on either side gives

$k = 0$	$k = 1$	$k = 2$	$\cdots$
$x_0 =$ user's IV	$x_1 = \frac{1}{1}\widehat{x}_0$	$x_2 = \frac{1}{2}\widehat{x}_1$	
$u_0 = -x_0$	$u_1 = -x_1$	$u_2 = -x_2$	
$\widehat{x}_0 = \exp(u_0)$	$\widehat{x}_1 = \frac{1}{1}(\widehat{x}_0 u_1)$	$\widehat{x}_2 = \frac{1}{2}(\widehat{x}_1 u_1 + \widehat{x}_0 2u_2)$	

IV: initial value

$k=0$	$k=1$	$k=2$	$\cdots$
$x_0 =$ user's IV	$x_1 = \frac{1}{1}\widehat{x}_0$	$x_2 = \frac{1}{2}\widehat{x}_1$	
$u_0 = -x_0$	$u_1 = -x_1$	$u_2 = -x_2$	
$\widehat{x}_0 = \exp(u_0)$	$\widehat{x}_1 = \frac{1}{1}(\widehat{x}_0 u_1)$	$\widehat{x}_2 = \frac{1}{2}(\widehat{x}_1 u_1 + \widehat{x}_0 2u_2)$	

$k = 0$:

- Set $x_0 =$ the user's IV to start the recursion.
- When u_0 is available, set $\widehat{x}_0 = \exp(u_0)$, the built-in IV of the sub-ODE.

In general:

- A standard function is called at $k = 0$.
- For $k > 0$, only BAOs are used.

Despite the sub-ODE making a DAE, the recurrences work!

The sub-ODE concept

Suppose:

- $v = g(u)$ is an m-vector function of scalar u,
- u, v are variables in the CL of the ODE,
- we can express $\frac{\mathrm{d}v}{\mathrm{d}u}$ as $h(u, v)$, i.e.

$$g'(u) = h(u, g(u)). \tag{3}$$

Then

- u, v denote $u(t), v(t)$, and $v = g(u)$ means $v(t) = g(u(t))$.
- (3) implies

$$\dot{v} = h(u, v)\dot{u} \quad \text{for short, termed a sub-ODE.}$$

- The sub-ODE method replaces in ODE's CL each assignment $v = g(u)$ by $\dot{v} = h(u, v)\dot{u}$.

Examples of sub-ODEs produced by standard functions:

(i) $v = \exp(u)$ has $\dot{v} = v\dot{u}$, $h(u, v) = v$

(ii) $v = u^c$, (c constant) has $\dot{v} = (cv/u)\dot{u}$, $h(u, v) = cv/u$

and, defining $\mathrm{cs}(u) = \left[\begin{smallmatrix} \cos(u) \\ \sin(u) \end{smallmatrix}\right]$,

(iii) $v = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \mathrm{cs}(u)$ has $\dot{v} = \begin{bmatrix} -v_2 \\ v_1 \end{bmatrix} \dot{u}$, $h(u, v) = \begin{bmatrix} -v_2 \\ v_1 \end{bmatrix}$

Computational kernel

Consists of five operations: $+,\ -,\ \times,\ \div,\ \odot$.

- BAOs Given TCs of u and v to order k:

$$(u \pm v)_k = u_k \pm v_k,$$

$$(u \times v)_k = \sum_{r=0}^{k} u_r v_{k-r},$$

$$(u/v)_k = \frac{1}{v_0}\Big(u_k - \sum_{r=0}^{k-1} v_{k-r}(u/v)_r\Big), \quad (v_0 \neq 0).$$

- $\odot$ (sub-ODE) $v = g(u)$ with sub-ODE $\dot{v} = h(u,v)\dot{u}$.

  Given TCs of u to order k:

$$v_k = (h \odot_g u)_k = \begin{cases} g(u_0) & k = 0 \\ \frac{1}{k}\sum_{i=1}^{k} i u_i h_{k-i} & k > 0 \end{cases}$$

Sub-ODEs from a DAE viewpoint

- Inserting sub-ODEs unavoidably turns the ODE into a DAE.
- E.g. in previous $\dot{x} = e^{-x}$ example:

ODE

$$\begin{cases} \dot{x} = \widehat{x} \\ u = -x \\ \widehat{x} = \exp(u) \end{cases}$$

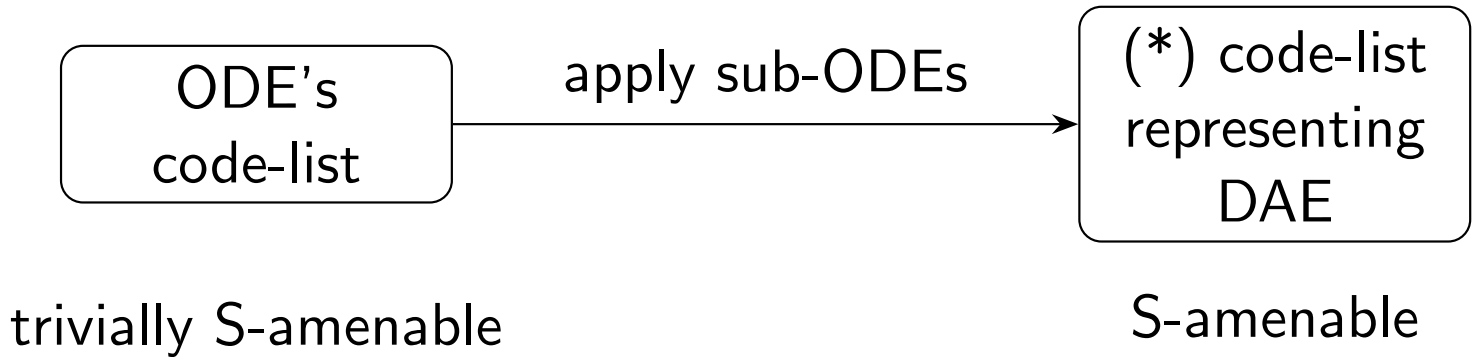
$\longrightarrow$

DAE

$$\begin{cases} \dot{x} = \widehat{x} \\ u = -x \\ \dot{\widehat{x}} = \widehat{x}\dot{u} \end{cases}$$

- ODE existence & uniqueness theory no longer applies.
- If we insert many, how do we know they don't interfere with each other and make nonsense?
- We resolved this using DAE S-amenability theory.

- A DAE is S-amenable if analyzing its sparsity tells you a scheme to solve it numerically.
- S-amenability test: a certain Jacobian must be non-singular.
- Most modeling software (e.g. Modelica) that creates DAEs implicitly assumes they are S-amenable.
- Every S-amenable DAE has a solution scheme by TS.



- An ODE is trivially an S-amenable DAE.
- We have shown that an S-amenable DAE remains so after inserting a single sub-ODE anywhere in it.
- By induction, it remains S-amenable after inserting any number of sub-ODEs.
- DAE's standard solution scheme by TS coincides with the recurrences defined by code-list (*).

ODETS solver

- We have implemented the sub-ODE method in a MATLAB solver **odets**, ODE by Taylor Series.
- The CL generation is done through operator overloading.
- **odets** evaluates the CL on each integration step to compute TCs.
- This is a variable-stepsize integrator, of fixed order determined at the start purely as a function of the accuracy tolerances.

ODETS performance

We compare the performance of **odets** against MATLAB 's built-in ODE solvers on the following problems:

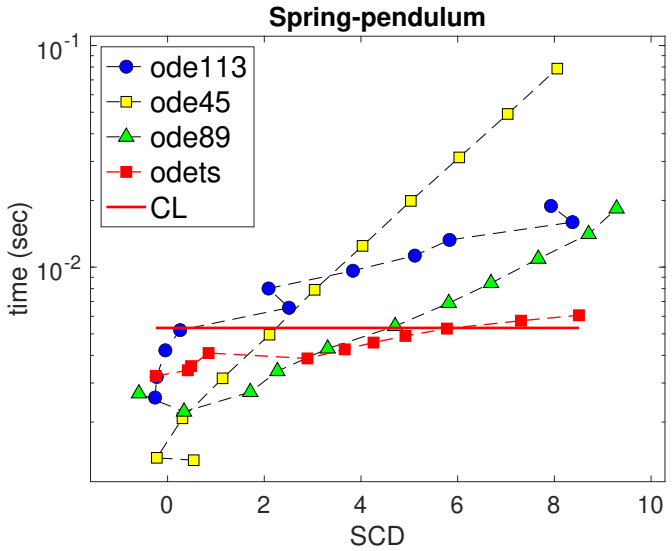
- Nonlinear Spring-Pendulum: A 2D mechanical system modeled by two second-order ODEs, reduced to four first-order equations.
- Pleiades Problem: A problem from the Test Set for IVP Solvers; describes the motion of 7 stars, with a size of 28 when reduced to first-order.
- Brusselator System: Models diffusion in a chemical reaction, becoming increasingly stiff and sparse as the problem size increases.

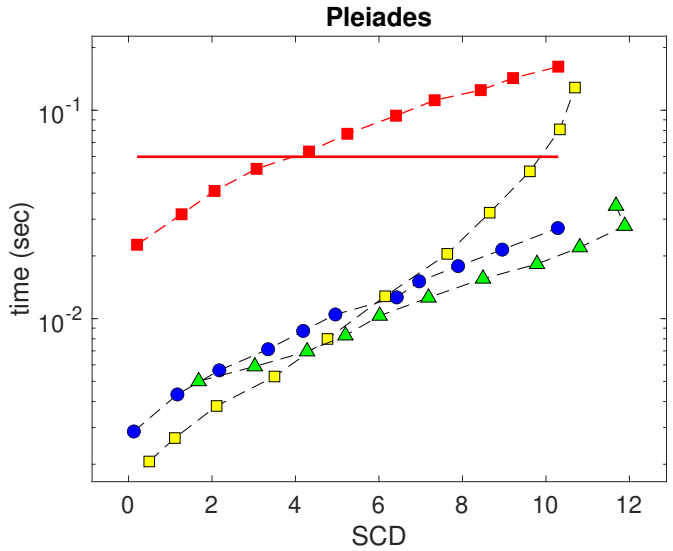
Work-precision diagrams

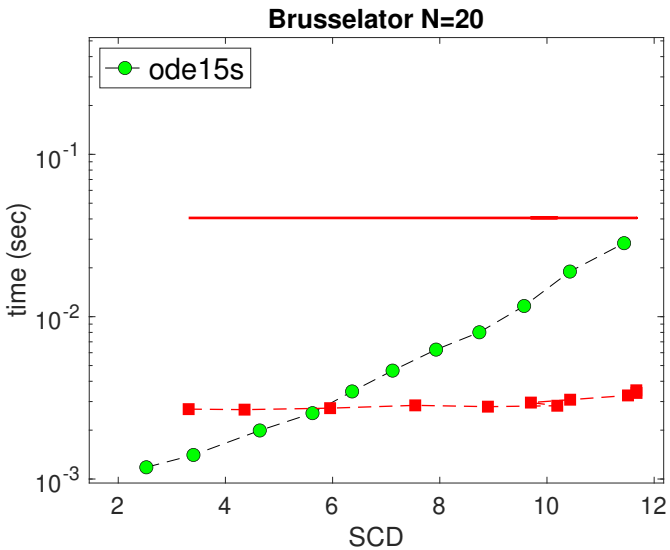
- We plot work-precision diagrams: CPU time versus significant correct digits (SCD), defined as

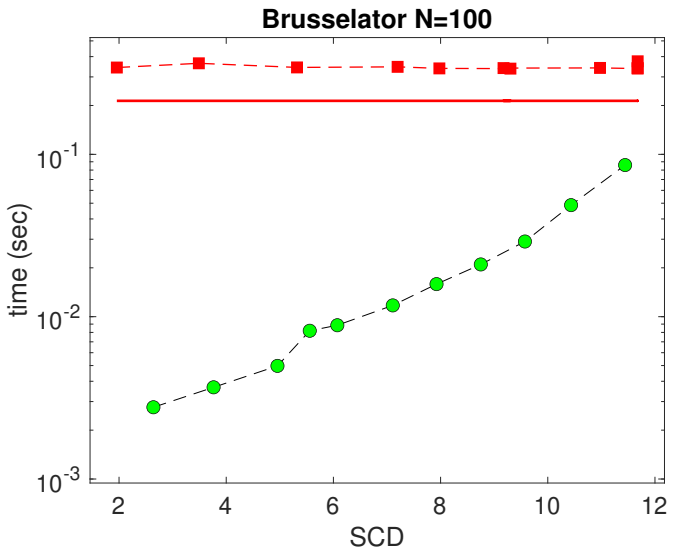
$$\text{SCD} = -\log_{10}\left(\|\text{relative error at } t_{\text{end}}\|_\infty\right).$$

- Work-precision diagrams are a standard way to compare the performance of different solvers.
- CPU times are measured on an Apple M3 MacBook Air 2024.
- Spring-pendulum, Pleiades: Comparison between nonstiff solvers `ode113`, `ode45`, `ode89`, and `odets`.
- Brusselator: Results for problem sizes $N = 20$ and $N = 100$, comparing the stiff solver `ode15s` and `odets`.









CL: time for CL generation, **odets**: time for integration only.

Back story

- Automatic solution of IVPs for ODEs by TS goes back (at least) to Moore (1966).
- So does the idea of converting an ODE to an equivalent rational ODE; he gives an example where $\cos$, $\exp$, and $\log$ occur and are eliminated.
- To our knowledge, Neidinger (2013) is the first person to give an embedding *method* that can, in principle, be automated—an operator he calls `ddot`, nearly equivalent to our $\odot$.
- M&N focus on recurrence relations for calculating TCs without considering the differential system these might represent.
- Corless and Ilie (2008) note that one can convert a DAE to an equivalent one using only BAOs.
  They treat the differential system but do not consider recurrence relations.

ADTAYL

ADTAYL, Automatic Differentiation Taylor Series is a MATLAB package with two parts:

- **adtayl** class for manipulating functions represented as TS, and
- **odets**.
- An **adtayl** object is an array with each element a polynomial, representing a function $x(t)$ expanded about t_0 up to order p:

$$x(t_0 + s) = x_0 + x_1 s + \cdots + x_p s^p + \cdots, \quad x_k = \frac{x^{(k)}(t_0)}{k!}$$

- Each element stores coefficients to order p, e.g. $x_0, x_1, \ldots, x_p$.

- **adtayl** objects behave like MATLAB arrays:
  - Indexing: `x(i,j)`, `x(:,2:end)`, ...
  - Elementwise arithmetic: `x + y`, `x .* y`, `x .^ 2`, ...
  - Standard functions: `sin(x)`, `exp(x)`, ...
  - Linear algebra, `x*y`, `x\y`, inverse `inv(x)`, ...
  - ...
- Coefficients can be real or complex:
  - `double` (default)
  - `vpa` (for variable precision arithmetic)
- **adtayl** implements power series algebra numerically, where all terms of order higher than p are dropped.

Application: Computing Lie derivatives

Let $f : \mathbb{R}^n \to \mathbb{R}^n$ be a smooth vector field, and let $h : \mathbb{R}^n \to \mathbb{R}$ be a smooth output function.

- The Lie derivative (LD) of h along f is defined as

$$L_f h(x) = \frac{\partial h}{\partial x}(x) \cdot f(x).$$

- Higher-order LD are defined recursively:

$$L_f^0 h(x) = h(x), \quad L_f^k h(x) = \frac{\partial}{\partial x}\left(L_f^{k-1} h(x)\right) \cdot f(x), \quad k \geq 1.$$

- Higher-order LD arise in control engineering, e. g. in the design of high-gain observers and differentiators.

- Given

$$\dot{x} = f(x), \quad y(t) = h(x), \quad x(0) = x_0,$$

we wish to compute $y^{(k)}(0)$ for $k \geq 1$.

- From the definition of Lie derivatives:

$$y(0) = L_f^0 h(x_0) = h(x_0), \qquad y^{(k)}(0) = L_f^k h(x_0), \quad k \geq 1.$$

- Then

$$y(t) = \sum_{k=0}^{\infty} \frac{y^{(k)}(0)}{k!} t^k = \sum_{k=0}^{\infty} y_k t^k = \sum_{k=0}^{\infty} \frac{L_f^k h(x_0)}{k!} t^k.$$

- Given TCs of $x(t)$ up to order p, and since $y = h(x)$, compute the TCs of y to order p:

$$h(x_0 + x_1 t + \cdots + x_p t^p) \quad \rightarrow \quad y_0 + y_1 t + \cdots + y_p t^p.$$

Computation with ADTAYL

Given f, h, x_0, and desired order p:

- Compute the TCs $x_0, x_1, \ldots, x_p$ of the solution $x(t)$ to $\dot{x} = f(x), \quad x(0) = x_0$.
- Store them in an **adtayl** object `x`.
- Evaluate

```
y = h(x)
```

- The k-th Lie derivative at x_0 is:

$$L_f^k h(x_0) = k! \cdot y_k = \texttt{factorial(k) * y.gettc(k)}$$

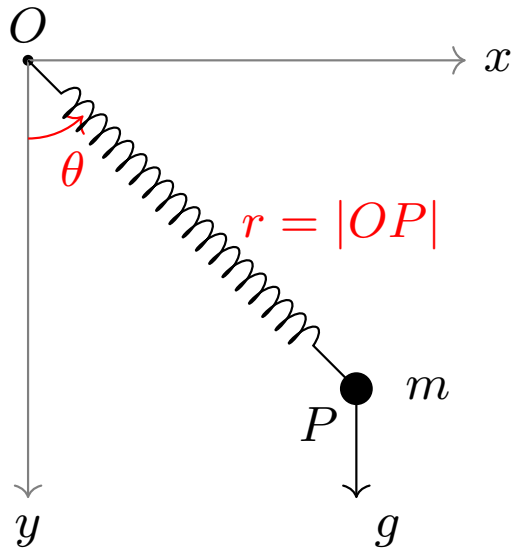
`gettc(k)` extracts the k-th Taylor coefficient of `y`.

Conclusion

- Sub-ODEs are a way to formulate recurrences for TCs.
- Proving they are theoretically sound was non-trivial: in general, they unavoidably transform an ODE to a DAE.
- A broad class of standard functions is expressible in terms of five operations $+$, $-$, $\times$, $\div$, $\odot$.
- **odets**'s performance is comparable to that of MATLAB's built-in nonstiff solvers.
- **odets** can reliably integrate with small tolerances (e.g. 10^{-100}) using MATLAB's variable precision arithmetic (vpa).
- Lie derivatives of arbitrary order can be computed efficiently using **odets** and **adtayl**.
- We are completing a user guide and implementing features such as event location and the computation of high-order Lie derivatives.

Code-list example: a nonlinear spring-pendulum

- Massless spring with a point mass m
- a natural length, k constant
- Nonlinear potential energy



With coordinates (r, θ), the Euler-Lagrange equations are

$$\begin{aligned}
\dot{r} &= s, \\
\dot{s} &= r\omega^2 + g\cos\theta - \tfrac{k}{m}\left((r-a) + 1 - e^{-(r-a)}\right) \\
\dot{\theta} &= \omega, \\
\dot{\omega} &= (-g\sin\theta - 2s\omega)/r
\end{aligned} \quad .$$

Line	Kind	Op	Mode	R1	R2	Imm	Expression
1	ODE		R	2			$\dot{x}_1 = x_2$
2	ODE		R	18			$\dot{x}_2 = x_{18}$
3	ODE		R	4			$\dot{x}_3 = x_4$
4	ODE		R	23			$\dot{x}_4 = x_{23}$
5	ALG	sub	RI	1		1	$x_5 = x_1 - 1$
6	ALG	mul	RR	1	4		$x_6 = x_1 \cdot x_4$
7	ALG	mul	RR	6	4		$x_7 = x_6 \cdot x_4$
8	SUB	cs	RR	10	3		$\begin{bmatrix} x_8 \\ x_9 \end{bmatrix} = \begin{bmatrix} x_{10} \\ x_8 \end{bmatrix} \odot_{\text{cs}} x_3$
9	SUB		RR	8	3		
10	ALG	sub	IR		9	0	$x_{10} = 0 - x_9$
11	ALG	mul	IR		8	9.81	$x_{11} = 9.81 \cdot x_8$
12	ALG	add	RR	7	11		$x_{12} = x_7 + x_{11}$
13	ALG	add	RI	5		1	$x_{13} = x_5 + 1$
14	ALG	sub	IR		5	0	$x_{14} = 0 - x_5$
15	SUB	exp	RR	15	14		$x_{15} = x_{15} \odot_{\text{exp}} x_{14}$
16	ALG	sub	RR	13	15		$x_{16} = x_{13} - x_{15}$
17	ALG	mul	IR		16	40	$x_{17} = 40 \cdot x_{16}$
18	ALG	sub	RR	12	17		$x_{18} = x_{12} - x_{17}$
19	ALG	mul	IR		2	-2	$x_{19} = -2 \cdot x_2$
20	ALG	mul	RR	19	4		$x_{20} = x_{19} \cdot x_4$
21	ALG	mul	IR		9	9.81	$x_{21} = 9.81 \cdot x_9$
22	ALG	sub	RR	20	21		$x_{22} = x_{20} - x_{21}$
23	ALG	div	RR	22	1		$x_{23} = x_{22}/x_1$