Applications of Differential Algebra

François Boulier
University of Lille, CRIStAL, France

CIMPA School: *Algebraic and Tropical Methods for Solving Differential Equations*

June 13, 2023

References

The reference books are

Joseph Fels Ritt. *Differential Algebra*. 1950

Ellis Robert Kolchin. *Differential Algebra and Algebraic Groups*. 1973

Software demos, lecture notes and other documents available at

https://codeberg.org/francois.boulier/DifferentialAlgebra

Definitions 1

Differential rings, fields are rings, fields endowed with finitely many derivation operators $\delta_1, \ldots, \delta_m$

$$\begin{aligned} \delta(a+b) &= \delta(a) + \delta(b)\,, \\ \delta(a\,b) &= \delta(a)\,b + a\,\delta(b)\,, \\ \delta_i \delta_j a &= \delta_j \delta_i a\,. \end{aligned}$$

In the *DifferentialAlgebra* packages, an independent variable x is associated to each derivation operator, which is viewed as $\mathrm{d}/\mathrm{d}x$

$\mathscr{F}$ differential field of characteristic zero

Definitions 2

$\mathscr{F}\{y_1, \ldots, y_n\}$ differential polynomial ring in n differential indeterminates (= n unknown functions of the m independent variables)

$y, \dot{y}, \ddot{y}, \ldots$ are the derivatives (of the differential indeterminates)

$3\,\dot{y}^2\,\ddot{y} + y^3 + 4$ is a differential polynomial of $\mathscr{F}\{y\}$

$3\,\dot{y}^2\,y^{(3)} + 6\,\dot{y}\,\ddot{y}^2 + 3\,y^2\,\dot{y}$ is its derivative

Let Σ be a set of differential polynomials then

$[\Sigma]$ is the differential ideal generated by Σ (= the ideal generated by the infinite set of all the derivatives of the elements of Σ)

$\{\Sigma\} = \sqrt{[\Sigma]}$ is the perfect differential ideal generated by Σ

For many different meanings of "solution", Σ, $[\Sigma]$ and $\{\Sigma\}$ have the same solution set

Academic Example 1

Let $y(x)$ be a polynomial, say

$$y \quad = \quad x^2 \,. \tag{1}$$

Find an ODE for y (answer: $\dot{y}^2 - 4\,y$).

Academic Example 1

Let $y(x)$ be a polynomial, say

$$y = x^2 . \quad (1)$$

Find an ODE for y (answer: $\dot{y}^2 - 4\,y$).

To convert (1) as a differential polynomial, y and x need to be both differential indeterminates. Let us rename the derivation $\mathrm{d}/\mathrm{d}x$ to $\mathrm{d}/\mathrm{d}\xi$ i.e. view $y = y(\xi)$ and $x = x(\xi)$ and encode (1) as

$$\Sigma \begin{cases} y = x^2 , \\ \dot{x} = 1 \end{cases} \quad \text{(derivation w.r.t } \xi\text{)}$$

In the differential polynomial ring $\mathscr{F}\{x, y\}$ differential elimination permits to compute a characteristic set / regular differential chain representation of

$$\{\Sigma\} \cap \mathscr{F}\{y\} .$$

Ranking $x \gg y$

Definitions 3

A ranking is a total ordering on the infinite set of the derivatives of the differential indeterminates. It permits to transform differential polynomials into rewrite rules. W.r.t ranking $x \gg y$

$$\Sigma \left\{ \begin{array}{lcl} y & = & x^2 \,, \\ \dot{x} & = & 1 \end{array} \right.$$

becomes

$$\Sigma \left\{ \begin{array}{ccl} x^2 & \rightarrow & y \,, \\ \dot{x} & \rightarrow & 1 \,. \end{array} \right.$$

The derivatives on the left hand sides are the leading derivatives of the differential polynomials. Differential elimination, applied to Σ and the ranking, produces a regular differential chain

$$A \left\{ \begin{array}{ccl} x & \rightarrow & \frac{1}{2}\,\dot{y} \,, \\ \dot{y}^2 & \rightarrow & 4\,y \,. \end{array} \right.$$

It can be proved that $f \in \{\Sigma\}$ iff it is rewritten to zero by A

Academic Example 2

Let $y(x)$ be a more complicated expression, say

$$y = x^2 + x^{\frac{3}{2}}. \quad (2)$$

Find an ODE for y.

Academic Example 2

Let $y(x)$ be a more complicated expression, say

$$y = x^2 + x^{\frac{3}{2}}\,. \tag{2}$$

Find an ODE for y.

Rename the derivation $\mathrm{d}/\mathrm{d}x$ to $\mathrm{d}/\mathrm{d}\xi$. Introduce some $z = x^{\frac{3}{2}}$ encoded by a differential polynomial. Encode (1) as

$$\Sigma \left\{ \begin{array}{rcl} y & = & x^2 + z\,, \\ z^2 & = & x^3\,, \\ \dot{x} & = & 1 \qquad \text{(derivation w.r.t } \xi) \end{array} \right.$$

In the differential polynomial ring $\mathscr{F}\{x, y, z\}$ compute a regular differential chain which describes

$$\{\Sigma\} \cap \mathscr{F}\{y\}\,.$$

Ranking $(x, z) \gg y$

Definitions 4

If the input system Σ involves an inequation $h \neq 0$ then the differential elimination process systematically simplifies

$$h\,p = 0 \quad \text{to} \quad p = 0\,.$$

In algebraic terms, it computes a representation of the saturation ideal

$$\{\Sigma\} : h^\infty \quad = \quad h^{-1}\,\{\Sigma\} \cap \mathscr{F}\{y_1, \ldots, y_n\}$$

This mechanism allows it to handle differential fractions

$$\frac{g}{h} \quad = \quad 0$$

which are interpreted as $g = 0,\ h \neq 0$

Academic Example 3

F. Lemaire and A. Poteaux. *Decoupling multivariate fractions.* CASC 2021

If $F(x,y) \in \mathbb{Q}(x,y)$ then four exclusive cases may occur
where $G \in \mathbb{Q}(x)$, $H \in \mathbb{Q}(y)$, $c, d \in \mathbb{Q}$:

$$F = G + H\,,\ F = c + G\,H\,,\ F = c + \frac{1}{G+H}\,,\ F = c + \frac{d}{1+G\,H}.$$

Consider case (2). The formula

$$c \quad = \quad F - \frac{F_x\,F_y}{F_{xy}}$$

can be obtained by differential elimination over the partial differential system

$$F = c + G\,H\,,\ G_y = 0\,,\ H_x = 0\,,\ c_x = 0\,,\ c_y = 0\,,\ G_x \neq 0\,,\ H_y \neq 0\,.$$

Ranking $(G, H) \gg c \gg F$

Academic Example 3

F. Lemaire and A. Poteaux. *Decoupling multivariate fractions*. CASC 2021

If $F(x, y) \in \mathbb{Q}(x, y)$ then four exclusive cases may occur
where $G \in \mathbb{Q}(x)$, $H \in \mathbb{Q}(y)$, $c, d \in \mathbb{Q}$:

$$F = G + H\,,\ F = c + G\,H\,,\ F = c + \frac{1}{G + H}\,,\ F = c + \frac{d}{1 + G\,H}.$$

Differential elimination can be used to prove that cases are exclusive
Proving that (1) and (2) are exclusive amounts to proving that the differential ideal defined by the following system contains 1

$$F = c + G\,H\,,\ G_y = 0\,,\ H_x = 0\,,\ c_x = 0\,,\ c_y = 0\,,\ G_x \neq 0\,,\ H_y \neq 0\,,$$

$$F = \bar{G} + \bar{H}\,,\ \bar{G}_y = 0\,,\ \bar{H}_x = 0\,,\ \bar{G}_x \neq 0\,,\ \bar{H}_y \neq 0\,.$$

Any ranking

The Next Example

The example shows that general differential polynomial systems may arise as limit systems when studying fast-slow dynamics

It features a nice encoding trick of flow conservation

The demo shows that sophisticated base fields may be useful

Sophisticated base fields too can be defined through regular differential chains

The Henri-Michaelis-Menten Formula

Differential elimination permits to perform a quasi-equilibrium approximation of a polynomial differential system modeling a chemical reaction system

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} ES \xrightarrow{k_2} E + P$$

The polynomial differential system before the approximation

One differential indeterminate by concentration. Three kinetic coefficients

$$\begin{aligned}
\mathrm{d}/\mathrm{d}t\; E(t) &= k_2\, ES(t) - k_1\, E(t)\, S(t) + k_{-1}\, ES(t)\,,\\
\mathrm{d}/\mathrm{d}t\; ES(t) &= -k_2\, ES(t) + k_1\, E(t)\, S(t) - k_{-1}\, ES(t)\,,\\
\mathrm{d}/\mathrm{d}t\; S(t) &= -k_1\, E(t)\, S(t) + k_{-1}\, ES(t)\,,\\
\mathrm{d}/\mathrm{d}t\; P(t) &= k_2\, ES(t)\,.
\end{aligned}$$

The Formula After Reduction

Main assumption: there are fast reactions $(= k_1,\ k_{-1} \gg k_2)$

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} ES \xrightarrow{k_2} E + P$$

Henri-Michaelis-Menten Formula

$$\frac{\mathrm{d}}{\mathrm{d}t} S(t) = -\frac{V_{\max} S(t)}{K + S(t)} \quad (V_{\max}, K \text{ constants})$$

Victor Henri, 1903
Leonor Michaelis and Maud Menten, 1913

The Henri, Michaelis, Menten reduction, revisited

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_2} E + P$$

Contributions of fast reactions highlighted

$$\begin{aligned}
\mathrm{d}/\mathrm{d}t\ E(t) &= k_2\, ES(t) - k_1\, E(t)\, S(t) + k_{-1}\, ES(t)\,, \\
\mathrm{d}/\mathrm{d}t\ S(t) &= -k_1\, E(t)\, S(t) + k_{-1}\, ES(t)\,, \\
\mathrm{d}/\mathrm{d}t\ ES(t) &= -k_2\, ES(t) + k_1\, E(t)\, S(t) - k_{-1}\, ES(t)\,, \\
\mathrm{d}/\mathrm{d}t\ P(t) &= k_2\, ES(t)\,.
\end{aligned}$$

The Henri, Michaelis, Menten reduction, revisited

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} ES \xrightarrow{k_2} E + P$$

Encode the conservation of the flow by replacing the contribution of the fast reactions by a new symbol $F_1(t)$.

$$\begin{aligned} d/dt\ E(t) &= k_2\, ES(t) - F_1(t)\,, \\ d/dt\ S(t) &= -F_1(t)\,, \\ d/dt\ ES(t) &= -k_2\, ES(t) + F_1(t)\,, \\ d/dt\ P(t) &= k_2\, ES(t)\,. \end{aligned}$$

The Henri, Michaelis, Menten reduction, revisited

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} ES \xrightarrow{k_2} E + P$$

Encode the conservation of the flow by replacing the contribution of the fast reaction by a new symbol $F_1(t)$.

Encode the fast reactions assumption: restrict the dynamics to the variety where fast reactions would be at equilibrium if they were alone

$$\begin{aligned}
\mathrm{d}/\mathrm{d}t\ E(t) &= k_2\, ES(t) - F_1(t)\,,\\
\mathrm{d}/\mathrm{d}t\ S(t) &= -F_1(t)\,,\\
\mathrm{d}/\mathrm{d}t\ ES(t) &= -k_2\, ES(t) + F_1(t)\,,\\
\mathrm{d}/\mathrm{d}t\ P(t) &= k_2\, ES(t)\,,\\
0 &= k_1\, E(t)\, S(t) - k_{-1}\, ES(t)\,.
\end{aligned}$$

The Henri, Michaelis, Menten reduction, revisited

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} ES \xrightarrow{k_2} E + P$$

Encode the conservation of the flow by replacing the contribution of the fast reaction by a new symbol $F_1(t)$.

Encode the fast reactions assumption: restrict the dynamics to the variety where fast reactions would be at equilibrium if they were alone

$$\begin{aligned}
\mathrm{d}/\mathrm{d}t\ E(t) &= k_2\, ES(t) - F_1(t)\,, \\
\mathrm{d}/\mathrm{d}t\ S(t) &= -F_1(t)\,, \\
\mathrm{d}/\mathrm{d}t\ ES(t) &= -k_2\, ES(t) + F_1(t)\,, \\
\mathrm{d}/\mathrm{d}t\ P(t) &= k_2\, ES(t)\,, \\
0 &= k_1\, E(t)\, S(t) - k_{-1}\, ES(t)\,.
\end{aligned}$$

Raw formula by eliminating $F_1(t)$ from Lemaire's DAE

$$\frac{\mathrm{d}}{\mathrm{d}t}\, S(t) = -\frac{ES(t)\, S(t)^2\, k_1\, k_2 + ES(t)\, S(t)\, k_{-1}\, k_2}{k_{-1}\, ES(t) + S(t)^2\, k_1 + S(t)\, k_{-1}}.$$

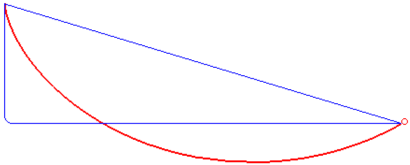
The Next Example

The example shows that general differential polynomial systems may arise by polynomial encoding of non polynomial functions

It shows that case splitting may be important (general and singular solution)

It shows that numerical integration problems are related to non existence of formal power series solutions and can sometimes be overcome by Puiseux series

Assumptions A point with mass m is forced to follow a curve $y(x)$ in the (x, y)-plane between two fixed points $(x, y) = (a, y_a)$ and (b, y_b). Its movement follows the gravitational law. Its initial speed is zero. There is no friction.



Problem Find the curve $y(x)$ which minimizes the time needed to reach the point (b, y_b)

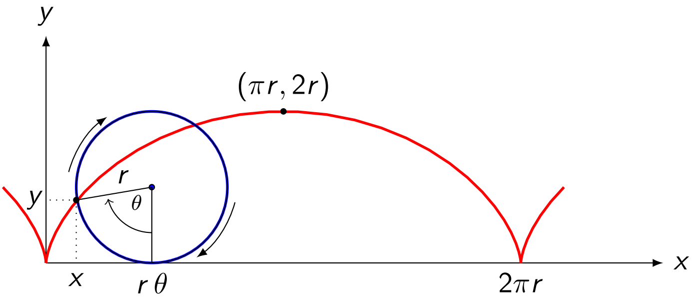
The solution is known as the *brachistochrone* curve

The Brachistochrone Curve is a Cycloid

The classical equation

$$y\,\dot{y}^2 + y \quad = \quad D \quad (D = 2\,r \text{ diameter of the circle})$$

Numerical integration problems at $(x, y) = (0, 0)$ and $(x, y) = (\pi\,r, D)$



Picture from `https://tex.stackexchange.com/questions/196957`

The Brachistochrone is Solution of Euler-Lagrange Equation

Functions $y(x)$ which satisfy the assumptions are solutions of

$$\frac{\mathrm{d}t}{\mathrm{d}x} = \sqrt{\frac{1+\dot{y}^2}{2\,g\,y}}.$$

We are thus looking to the function $y(x)$ which minimizes the functional

$$y \mapsto \int_a^b \sqrt{\frac{1+\dot{y}^2}{2\,g\,y}}\,\mathrm{d}x\,.$$

Introduce the following Lagrangian:

$$\mathscr{L}(y,\dot{y}) = \sqrt{\frac{1+\dot{y}^2}{2\,g\,y}}.$$

By the Beltrami identity, $y(x)$ function satisfies the following equation where c is a constant:

$$\mathscr{L} - \dot{y}\,\frac{\partial \mathscr{L}}{\partial \dot{y}} = c\,.$$

Differential Elimination for Applying Euler-Lagrange

$$\mathscr{L}(y,\dot y) \;=\; \sqrt{\frac{1+\dot y^2}{2\,g\,y}}\,, \qquad \mathscr{L} - \dot y\,\frac{\partial \mathscr{L}}{\partial \dot y} \;=\; c\,.$$

The Lagrangian is not polynomial but the Beltrami identity can be encoded by a differential polynomial system Σ

The separant $\partial \mathscr{L}/\partial \dot y$ is denoted S_L

The last equation aims at renaming a constant

Apply differential elimination over the system

$$(\Sigma) \quad L^2 = \frac{1+\dot y^2}{2\,g\,y}\,, \quad 2\,L\,S_L = \frac{\dot y}{g\,y}\,, \quad L - \dot y\,S_L = c\,, \quad D = \frac{1}{2\,g\,c^2}.$$

Ranking $(L, S_L, g, c) \gg (y, D)$

From a Differential Algebra Point of View

Two regular differential chains are produced

$$(A_1) \quad g = \frac{1}{2\,D\,c^2}\,, \quad \dot{y}^2 = \frac{D-y}{y}\,, \quad S_L = c\,\dot{y}\,, \quad L = \frac{D\,c}{y}\,.$$

$$(A_2) \quad g = \frac{1}{2\,D\,c^2}\,, \quad y = D\,, \quad S_L = 0\,, \quad L = c\,.$$

Regular differential chain A_1 contains the brachistochrone equation

$$y\,\dot{y}^2 + y \;=\; D\,. \tag{3}$$

Regular differential chain A_2 corresponds to a singular solution of Σ

$$y \;=\; D\,. \tag{4}$$

The curve $y(x) = D$ meets the cycloid at $(x, y) = (\pi\,r, D)$
A numerical integration problem there

Puiseux Series Solution

The brachistochrone equation

$$y\,\dot{y}^2 + y \quad = \quad D$$

No formal power series solution and a numerical integration problem at

$$(x, y) \quad = \quad (0, 0)$$

A Puiseux series permits to perform the first numerical integration step

$$y(x) \quad = \quad \frac{3^{\frac{2}{3}}\,\sqrt[3]{2}\,\sqrt[3]{D}}{2}\,x^{\frac{2}{3}} - \frac{2^{\frac{2}{3}}\,3\,\sqrt[3]{3}}{20\,\sqrt[3]{D}}\,x^{\frac{4}{3}} - \frac{27}{700\,D}\,x^2 + \cdots$$

The Next Example

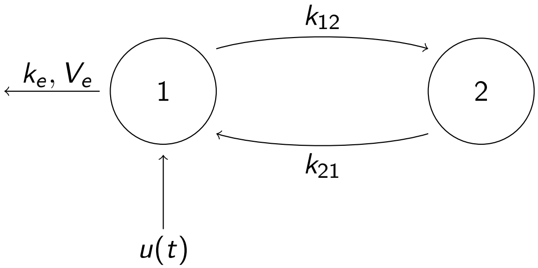
Quite an applied example related to parameter estimation

It features a recent algorithm which applies symbolic integration method to differential fractions

It shows the usefulness of differential fractions

A relationship to be investigated with tropical differential geometry?

[In some cases,] differential elimination permits to transform a nonlinear least squares problem into a linear one by guessing a starting point for a Newton like method.



Statement of the Problem

Given a parametric ODE system (parameters k_e, V_e, k_{12}, k_{21}):

$$\begin{aligned}\dot{x}_1(t) &= -k_{12}\,x_1(t) + k_{21}\,x_2(t) - \frac{V_e\,x_1(t)}{k_e + x_1(t)} + u(t),\\ \dot{x}_2(t) &= k_{12}\,x_1(t) - k_{21}\,x_2(t).\end{aligned}$$

some measures:

$y(t) = x_1(t)$ is observed

$x_2(t)$ is not observed

t	$y(t) = x_1(t)$
0.00000	5.00000
0.11111	4.12917
...	
1.00000	2.96261

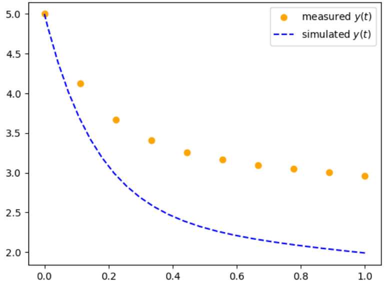
some further data: command $u(t)$, initial values, estimate of k_e ...

Estimate the values of the unknown parameters V_e, k_{12}, k_{21}

Principle of the Method

To any candidate tuple (k_{12}, k_{21}, V_e) associate an error as follows

Integrate numerically the ODE system using the candidate tuple



The error is defined as the sum of the squares of the differences between the ordinates of the measured points and that of the computed ones (here *error* $\simeq 6.38$)

Apply a Newton/gradient method to decrease the error

The Input-Output Equation

Newton/gradient methods require a starting point

The input-output equation provides it

Differential elimination permits to eliminate the non observed variable x_2.
A pretty-printed form of the differential input-output equation is:

$$-\theta_1\, u(t) + \theta_2\, \frac{y(t)}{y(t)+k_e} + \theta_3\, \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{y(t)^2}{y(t)+k_e}\right) - \theta_4\, \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{y(t)+k_e}\right) = \dot{u}(t) - \ddot{y}(t)\,,$$

where the θ_i stand for the following *blocks of parameters*:

$$\theta_1 = k_{21}\,, \quad \theta_2 = k_{21}\, V_e\,, \quad \theta_3 = k_{12} + k_{21}\,, \quad \theta_4 = k_{12} + k_{21} + V_e\,.$$

Overview of the Parameter Estimation Process

1. Compute the starting point

Build an overdetermined linear system $A\,x = b$ by evaluating all terms but the θ, over the measures, at many different t

$$-\theta_1\, u(t) + \theta_2\, \frac{y(t)}{y(t)+k_e} + \theta_3\, \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{y(t)^2}{y(t)+k_e}\right) - \theta_4\, \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{y(t)+k_e}\right) = \dot{u}(t) - \ddot{y}(t)\,,$$

Solve $A\,x = b$ by linear least squares: the θ are estimated

2. Recover the model parameter from the θ

Solve the nonlinear system

$$\theta_1 = k_{21}\,, \quad \theta_2 = k_{21}\,V_e\,, \quad \theta_3 = k_{12} + k_{21}\,, \quad \theta_4 = k_{12} + k_{21} + V_e\,.$$

3. Refine it by a Newton/gradient method

Towards Integro-Differential Equations?

The *DifferentialAlgebra* packages contain an algorithm to transform the input-output differential polynomial produced by the differential elimination process into the following form, which is not the standard form of a polynomial in the derivatives of the differential indeterminates

$$-\theta_1\, u(t) + \theta_2\, \frac{y(t)}{y(t)+k_e} + \theta_3\, \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{y(t)^2}{y(t)+k_e}\right) - \theta_4\, \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{y(t)+k_e}\right) \quad = \quad \dot{u}(t) - \ddot{y}(t)\,,$$

In general, any differential fraction f can be written (with some minimality conditon on the differential fractions f_i)

$$f \quad = \quad f_0 + \frac{\mathrm{d}}{\mathrm{d}t}\, f_1 + \cdots + \frac{\mathrm{d}^k}{\mathrm{d}t^k}\, f_k$$

F. Boulier et *al.* *Additive Normal Forms and Integration of Differential Fractions*. JSC 2016

Towards Integro-Differential Equations?

The particular form of the input-output equation permits to transform it into an integral equation, less sensitive to noisy data at the linear system building stage

$$
\begin{aligned}
& - \theta_1 \int_a^t \int_a^{\tau_1} u(\tau_2)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \\
& + \theta_2 \int_a^t \int_a^{\tau_1} \frac{y(\tau_2)}{y(\tau_2)+1}\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \\
& + \theta_3 \left(\int_a^t \frac{y(\tau)^2}{y(\tau)+1}\, \mathrm{d}\tau - \frac{y(a)^2}{y(a)+1}\,(t-a) \right) \\
& - \theta_4 \left(\int_a^t \frac{1}{y(\tau)+1}\, \mathrm{d}\tau - \frac{1}{y(a)+1}\,(t-a) \right) \\
& - \dot{y}(a)\,(t-a) \\
& = \int_a^t u(\tau)\, \mathrm{d}\tau - u(a)\,(t-a) - y(t) + y(a)\,.
\end{aligned}
$$