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DISCONTINUITIES IN ODEs.

-systems with change of state.

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1. abstract

he occurrence of discontinuous right hand sides in ODE-systems often appears in technical applications. Such applications may be characterised by the cases where the system changes between several states. Each state is defined by a system of ODEs and the transition between states is defined by an algebraic condition. The numerical solution that is done in order to simulate the behaviour of the system will be possible by using standard numerical software but this approach is very ineffecient. We present an alternative approach based upon the tracking of state-changes and accurate numerical determination of transition points. Real applications are used to illustrate the approach.

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2. Systems with changes of state.

In many applications of numerical simulation the systems may change state. Such cases are found in the simulation of multibody dynamics and control systems, for example when a thermostat makes some part of the system cut in and off. This means in the mathematical model that the equations for the dynamic system are changing in a discontinuous way across a solution point [1].
The direct application of a numerical method for the solution of such a system will lead to unwanted growth of errors as well as a wasted extra computational effort. All in all this is an unwanted situation.
By applying modern continuous extensions in combination with the solution method we may derive a strategy for passing the discontinuity points without loss of accuracy and at a very minimal extra cost in computational effort.

2.1. Discontinuous right hand sides.

The dynamic system we will consider for illustration can be defined the following way

$$y' = f(t, y)\ ,\ t \in [a, b]\ ,\ y(a) = \eta \tag{1}$$

where the function $f(t, y)$ is given by

$$f(t, y) = \begin{cases} f_1(t, y) & for \quad \phi(t, y) < 0 \\ f_2(t, y) & for \quad \phi(t, y) \geq 0 \end{cases} \tag{2}$$

The functions $f_1(t, y)$ and $f_2(t, y)$ need not have the same value at the point where the solution crosses the curve $\phi(t, y) = 0$. This means that the solution will have a discontinuous derivative across this curve (see [4]) . We illustrate the situation in the figure below.

The existence and continuity of the solution is guaranteed under very modest assumptions for the differential system, we refer to [4] for the details. If we assume that $\phi(t, y)$ is analytic in t and y we will

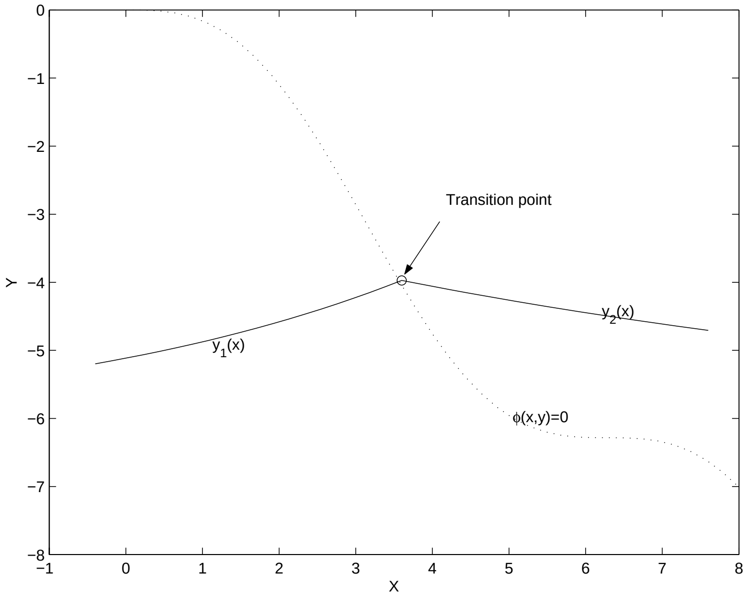

Figure 1: Discontinuity across curve of state change.

obtain that the curve $\phi(t, y)$ is differentiable with respect to both t and y and the solution to

$$y_1'(t) = f_1(t, y_1(t)) \ , \ y_1(a) = \eta \tag{3}$$

will cross the curve $\phi(t, y)$ at some point P defined by the condition

$$\phi(t_1, y_1(t_1)) = 0 \tag{4}$$

The differential equation (1) define a new initial value problem that may be rewritten as

$$y_2'(t) = f_2(t, y_2(t)) \ , \ y_2(t_1) = y_1(t_1). \tag{5}$$

The solution to (1) can now be found as the solution to (3) in combination with the solution to (5). The simple form of a discontinuous problem is found when we have a jump-discontinuity that satisfy the condition

$$| \ f_1(t, y) - f_2(t, y) \ | < C \tag{6}$$

We will consider in this report problems where this condition is assumed to be satisfied everywhere.

2.2. The numerical solution across a jump-discontinuity.

Following the idea from [2] we consider the problem specified in the previous section using either a one-step method like a Runge Kutta method or a multistep method. In the two domains specified by the regions where the function ϕ is either positive or negative the methods are solving IVP's in the usual manner and all we need to consider is the region close to the point where the solution crosses from one region to the other. The point P is called the transition point.

2.2.1. Multistep methods.

When solving the system (1) using a multistep method we consider for simplicity a constant stepsize defined by

$$y_n \approx y(t_n)\ ,\ t_n = a + nh\ ,\ h = t_{n+1} - t_n\ ,\ n = 1, 2, \dots, N. \quad (7)$$

We follow the treatise of multistep methods in [3] where the multistep method is defined as

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = \sum_{j=0}^{k} \beta_j y'_{n+j} \quad (8)$$

The accuracy of the formula is found by looking at the local truncation error given by the linear difference operator

$$\mathbf{L}[y(t_n); h] = \sum_{j=0}^{k} (\alpha_j y(t_n + jh) - h\beta_j y'(t_n + jh)) \quad (9)$$

The assumption that $y(t)$ has continuous derivatives of sufficiently high order leads to the result that for a method of order p we find that

$$\mathbf{L}[y(t_n); h] = C_p h^{p+1} y^{(p+1)} + O(h^{p+2}) \quad (10)$$

This is the traditional result that leads to convergence when $p \geq 1$. Now consider the situation shown in the figure below where the step is across a transition point.
In this case we can derive the result for the truncation error by using Taylor expansions of the sum from (10) and we arrive to the result (after some derivation) using the conditions for order p that

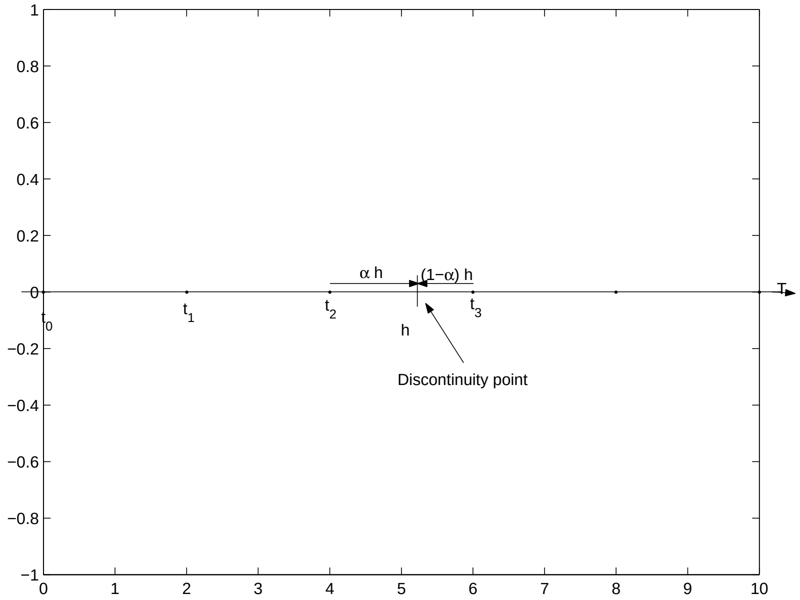

Figure 2: Integrating across a point of state change.

$$\mathbf{L}[y(t_n);h] = h(1-\delta-\beta_k)(y'(\xi^+)-y'(\xi^-)) + O(h^2) \quad (11)$$

According to the normal definition of order we conclude that in this case the order is $p = 0$ and the method is no longer convergent. We may simplify the expression for the local truncation error by using the bound from the jump-condition (6) and we obtain

$$\mid \mathbf{L}[y(t_n);h] \mid \leq h \mid (1-\delta-\beta_k) \mid C \quad (12)$$

Basically we obtain that the local truncation error is proportional to h and to the size of the jump in first derivative across the discontinuity. For discontinuities in higher order derivatives we may use the same type of derivation to obtain the result that if the jump is in the q'th derivative and bounded like (6) we find

$$lteq\mathbf{L}[y(t_n);h] \approx h^q \hat{C} \quad (13)$$

We see that in cases where $q < p+1$ we may expect a decrease in the order observed. This result means that we will be able to predict the local behaviour of a given method across boundaries with discontinuities in derivatives of variable orders.

2.2.2. One-step methods.

The general form of a onestep method is the following

$$y_{n+1} = y_n + h\Phi(t_n, y_n; h) \quad (14)$$

Again assuming smoothness of all derivatives up to the order $p+1$ will lead to a local truncation error of the form

$$T_{n+1} = \psi(t_n, y(t_n))h^{p+1} \quad (15)$$

The result of the analysis in the case with a discontinuity in the derivative will in this case lead to a similar result to the case with multistep methods and we find

$$T_{n+1} \approx \tilde{\psi}(t_n, \xi^+ - \xi^-)h \tag{16}$$

In the onestep case we find that the discontinuity may be in any of the mixed derivatives of the function $f(t, y)$ of orders lower than the order of the method. In principle though the two types of methods behave in a similar way. To get more details we refer to the reference [2] . Example 1. In order to give an example of how the behaviour of a standard solver is reflecting the results we have looked at the problem

$$y' = \begin{cases} y & for \quad 0 \leq t \leq 1 \\ -y & for \quad 1 < t \leq 2 \end{cases} \; y(0) = 1 \;,\; t \in [0, 1] \tag{17}$$

The figure shows that the automatic stepsize control will cut down the stepsize to the smallest allowable value because the error estimator becomes unreliable due to the fact that the error behaves like order zero instead of order p. If we assume the correct order of the method the error will be estimated to the actual stepsize times the size of the jump. For the example this would mean that the step should be of the order of 10^{-4} compared to the value 10^{-6} observed from the result. The driver wastes many unaccepted steps cutting down the stepsize before passing the transition point.

2.3. Continuous extension.

A traditional method for the solution of ODE's is basically finding the approximate solution on a discrete set of points, the discretization is defined by the stepsize control. The transition points wil however not in general be at one of these points. In order to develop a method for passing the transition point we need to be able to find an approximate solution in a continuous way. The tool for doing that is the continuous extension, developed for Runge Kutta methods ([7] and [5]) and the general interpolant for multistep methods ([8]).

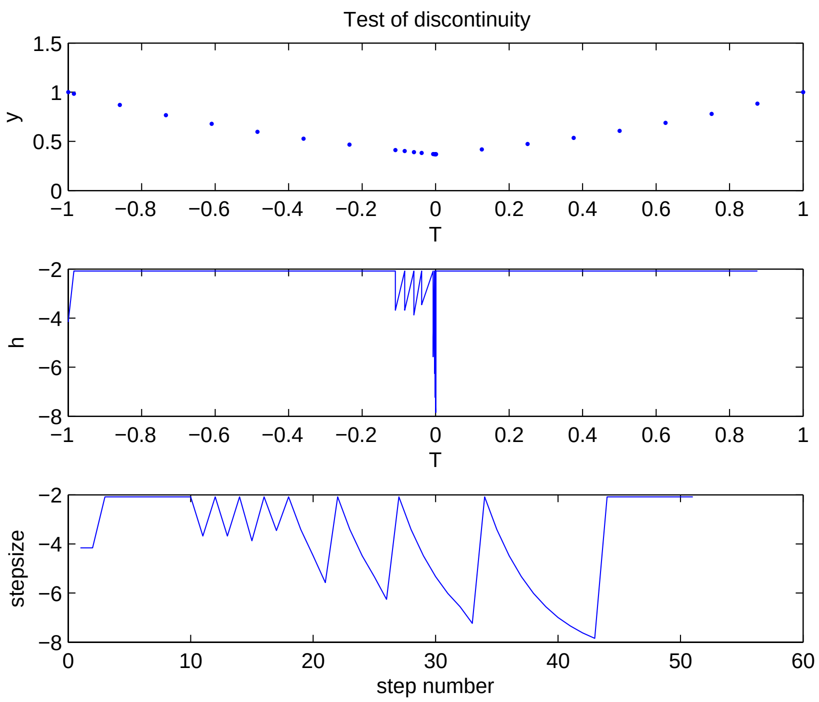

Figure 3: Solution and stepsize history with a discontinuity.

Ex: The Trapezodal method **Trapezoidal method with continuous extension.**

As a simple example of an implicit method we illustrate the ideas by using the Trapezoidal method, in this case we use the GERK-formulation by giving the Butcher tableau of the method.

0	0	
1	$\frac{1}{2}$	$\frac{1}{2}$
y_{n+1}	$\frac{1}{2}$	$\frac{1}{2}$
$\tilde{y}_{n+1}(\theta)$	$\theta(1-\frac{\theta}{2})$	$\frac{\theta^2}{2}$

Coefficients for the trapezoidal-method with continued extension.

It is customary to use θ as the parameter for defining the interpolation point. This point will in connection with the discontinuity be defined by the position of the transition point. We wish to determine this point and the condition for this is the function $\phi(t,y)$ being zero.

$$\phi(t, y(\theta)) = 0\ ,\ 0 \leq \theta \leq 1. \tag{18}$$

This equation is a normal condition for a zero of the function with θ as the variable. Any convenient zero-finding method may be used for determining the solution, if $\phi(t,y)$ is a smooth function the most efficient method will be based on a Newton-Raphson method. This assumes that derivatives of the functions are available. In the following example we treat a system which passes a level, like in an application where a thermostat reaches a set-point. The system is the

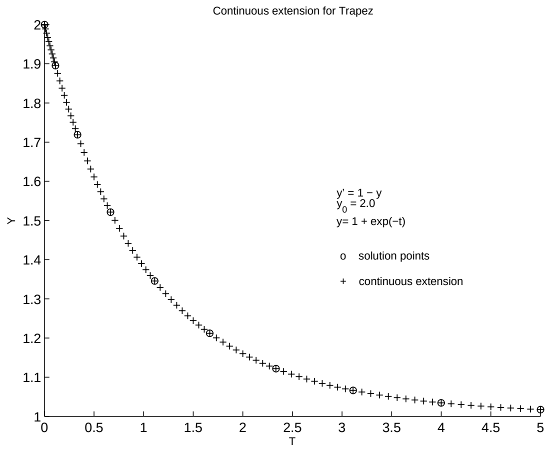

Figure 4: Solution and Continuous Extension.

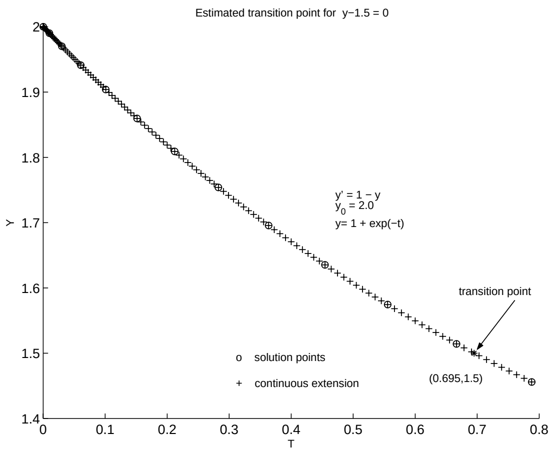

Figure 5: solution and determination of a transition point.

following.

$$y' = 1 - y \ , \ y(0) = 2 \ , \ y(t) = 1 + \exp(-t) \tag{19}$$

The set-point is defined by the condition,

$$\phi(t, y) = y - 1.5 = 0. \tag{20}$$

The solution is shown in the figure and the transition point is marked. We have applied a constant stepsize to get to the setpoint and then the value θ is found from the equation that is derived from (4) leading to the equation.

$$\begin{aligned} y_n - 1.5 - h(\frac{\theta^2}{2}(f_{n+1} - f_n) + \theta f_n) &= 0 \\ \theta = & \ 0.084 \quad t = 0.6931 \end{aligned}$$

The stepsize strategy here is very different from the one leading to the results in figure (2) and no steps are wasted for the approach to the transition point. The solution may be restarted using the transition point as the initial value for a solution in the new state.

2.4. Implementations.

The example in the previous section has shown that a quite general strategy may be applied to change from state to state if we apply the conditions (18) in connection with the continuous extension a discussion is found in [9]. This is straightforward in the scalar case with only one active condition as in the example. In the general case where we may have a system of ODE's and where change of state may happen between several states and guided by a number of conditions, the implementation must be done very carefully to give satisfactory performance.

In the DALI [6] a matrix of conditions are kept , rows representing the active states and columns containing the conditions for passing to another state. Thus $\phi_{i,j}(t, y)$ changing sign will mean that the system in state i will change to state j . Not all states are reachable from all other states and we define a state-transition matrix containing 'ones' where a change is possible and 'zeros' where there is no possible state transition. The next figure shows the situation for a system illustrated by a state diagram and the corresponding state transition matrix . The example is from a simulation of a glider in the starting process over a free flight to landing , the transition is one-way following the numbering of the states assuming that the landing leads back to the original state of start. $\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$

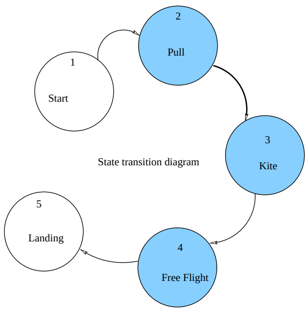

Figure 6: State transition diagram and matrix

Tank-heater example. We consider the simulation of a tank heated to a given temperature and controlled by thermostats to keep its temperature between given bounds. The system is shown in the figure below. The states of the system can be identified quite easily and the

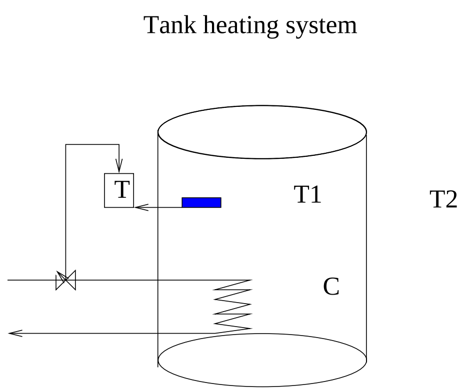

Figure 7: The tank with heater and thermostat.

state diagram is shown in figure (8). When carrying out the simulation the model will change state using the continuous extension for determining the transitions between states and the solution will look like shown here.

In the **Intersim** package for simulations a similar structure is applied but is derived from a language description of the system. The model is defined in a Pseudo-programming language with a syntax that incorporates switch-conditions. From the model description the transition matrix is derived and the system refers to this to indirectly apply the transition functions in a Newton type iterative solution process.

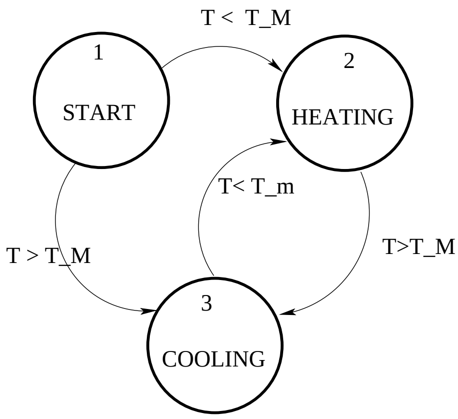

Figure 8: State diagram for the tank-heater

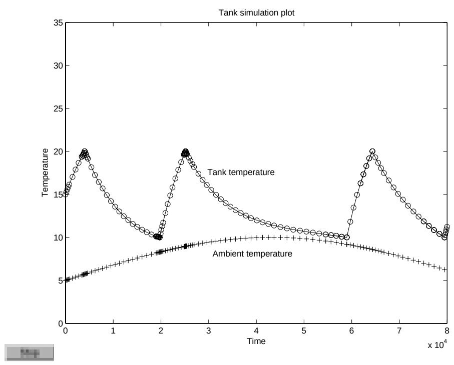

Figure 9: Simulation of the tank-heater

References

1ex8plus2minus44plus2minus

[1] C. Bendtsen and Per G. Thomsen. Numerical solution of differential algebraic equations. 1998.

[2] C.W. Gear and O. Østerby. Solving ordinary differential equations with discontinuities. *ACM Trans. Math. Softw.*, 10(1):23–44, 1984.

[3] J.D. Lambert. *Computational Methods in Ordinary Differential Equations*. J.Wiley & sons, 1972.

[4] R. Mannshardt. One step methods of any order for ode's with discontinuous right hand sides. *Numerische Mathematik*, 31(1), 1978.

[5] B. Owren and M Zennaro. Derivation of Efficient Continuous Explicit Runge-Kutta Methods. *SIAM J. Sci. Stat. Comput.*, 13: 1488–1501, 1992.

[6] K.F.Askjær. Dali , en differential-algebraisk ligningsløser. *Eks.proj. Lab. f. Køleteknik*, F94-02(1):51, 1986.

[7] S.P.Nørsett and P.G.Thomsen. Imbedded sdirk-methods of basic order three. *BIT*, 24:634–646, 1984.

[8] S.P.Nørsett W.A.Enright, K.R.Jackson and P.G.Thomsen. Interpolants for Runge-Kutta formulas. *ACM TOMS*, 12(3):193–218, 1986.

[9] S.P.Nørsett W.A.Enright, K.R.Jackson and P.G.Thomsen. Effective solution of discontinuous ivp's using a runge kutta formula pair with interpolants. *Applied Mathematics and Computation*, 27, 1988.