

Sensitivity to Numerical Integration Scheme in Calculation of Transport Barriers

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Abstract

Sammendrag

Preface

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Notation

1 Theory

1.1 SOLVING SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

In physics, like other sciences, modeling a system often equates to solving an initial value problem. An initial value problem can be described in terms of a differential equation of the form

$$\dot{x}(t) = f(t, x(t)), \quad x(t_0) = x_0, \quad (1.1)$$

where x is an unknown function (scalar or vector) of time t . The function f is defined on an open subset Ω of $\mathbb{R} \times \mathbb{R}^n$. The initial condition (t_0, x_0) is a point in the domain of f , i.e., $(t_0, x_0) \in \Omega$. In higher dimensions (i.e., $n > 1$) the differential equation (1.1) is replaced by a family of equations

$$\begin{aligned} \dot{x}_i(t) &= f_i(t, x_1(t), x_2(t), \dots, x_n(t)), \quad x_i(t_0) = x_{i,0}, \quad i = 1, \dots, n \\ \mathbf{x}(t) &= (x_1(t), x_2(t), \dots, x_n(t)) \end{aligned} \quad (1.2)$$

The system is nonlinear if the function f in equation (1.1), alternatively, if at least one of the functions f_i in equation (1.2), is nonlinear in one or more of its arguments.

1.1.1 The Runge-Kutta family of numerical methods

For nonlinear systems, analytical solutions frequently do not exist. Thus, such systems are often analyzed by means of numerical methods. In numerical analysis, the Runge-Kutta family of methods are a frequently used collection of implicit and explicit iterative methods, used in temporal discretization in order to obtain numerical approximations of the *true* solutions of systems like (1.1). The German mathematicians C. Runge and M. W. Kutta developed the first of the family's methods at the turn of the twentieth century (Hairer, Nørsett, and Wanner 1993, p.134 in the 2008 printing). The general scheme of what is now known as a Runge-Kutta method is as follows:

Definition 1. Let s be an integer and $a_{1,1}, a_{1,2}, \dots, a_{1,s}, a_{2,1}, a_{2,2}, \dots, a_{2,s}, \dots, a_{s,1}, a_{s,2}, \dots, a_{s,s}, b_1, b_2, \dots, b_s$ and c_1, c_2, \dots, c_s be real coefficients. Let h be the numerical step length used in the temporal discretization. Then, the method

$$\begin{aligned} k_i &= f\left(t_n + c_i h, x_n + h \sum_{j=1}^s a_{i,j} k_j\right), \quad i = 1, \dots, s \\ x_{n+1} &= x_n + h \sum_{i=1}^s b_i k_i \end{aligned} \quad (1.3)$$

is called an *s-stage Runge-Kutta method* for the system (1.1).

The main reason to include multiple stages s in a Runge-Kutta method, cf. definition 1, is to improve the numerical accuracy of the computed solutions. Hairer, Nørsett, and Wanner (1993, p.2 in the 2010 printing) define the *order* of a Runge-Kutta method as follows:

Definition 2. A Runge-Kutta method (1.3) is said to be of *order* p if, for sufficiently smooth systems (1.1),

$$\|x_{n+1} - x(t_{n+1})\| \leq Kh^{p+1} \quad (1.4)$$

i.e., if the Taylor series for the exact solution $x(t_{n+1})$ and the numerical solution x_{n+1} coincide up to (and including) the term h^p .

It is easy to show that if the local error of a Runge-Kutta method is of order p , cf. definition 2, the global error, i.e., the total accumulated error resulting of applying the algorithm a number of times, is expected to scale as h^p . Showing this is left as an exercise for the interested reader.

In definition 1, the matrix $(a_{i,j})$ is commonly called the *Runge-Kutta matrix*, while b_i and c_i are known as the *weights* and *nodes*, respectively. Since the 1960s, it has been customary to represent Runge-Kutta methods (1.3) symbolically, by means of mnemonic devices known as Butcher tableaus (Hairer, Nørsett, and Wanner 1993, p.134 in the 2008 printing). The Butcher tableau for a general s -stage Runge-Kutta method, introduced in definition 1, is presented in table 1.1.

Table 1.1: Butcher tableau representation of a general s -stage Runge-Kutta method.

c_1	$a_{1,1}$	$a_{1,2}$	\dots	$a_{1,s}$
c_2	$a_{2,1}$	$a_{2,2}$	\dots	$a_{2,s}$
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	$a_{s,1}$	$a_{s,2}$	\dots	$a_{s,s}$
	b_1	b_2	\dots	b_s

For explicit Runge-Kutta methods, the Runge-Kutta matrix $(a_{i,j})$ is lower triangular. Similarly, for fully implicit Runge-Kutta methods, the Runge-Kutta matrix is upper triangular. Unlike explicit methods, implicit methods require the solution of a linear system at every time level, making them more computationally demanding than their explicit siblings. The main selling point of implicit methods is that they are more numerically stable than explicit methods. This property means that implicit methods are particularly well-suited for *stiff* systems, i.e., physical systems with highly disparate time scales (Hairer and Wanner 1996, p.2 in the 2010 printing). For such systems, most explicit methods are highly numerically unstable, unless the numerical

step size is made exceptionally small, rendering most explicit methods practically useless. For *nonstiff* systems, however, implicit methods behave similarly to their explicit analogues in terms of numerical accuracy and convergence properties.

During the first half of the twentieth century, a substantial amount of research was conducted in order to develop numerically robust, high-order, explicit Runge-Kutta methods. The idea was that using such methods would mean one could resort to larger time increments h without sacrificing precision in the computational solution. However, the number of stages s grows quicker than linearly as a function of the required order p . It has been proven that, for $p \geq 5$, no explicit Runge-Kutta method of order p with $s = p$ stages exists (Hairer, Nørsett, and Wanner 1993, p.173 in the 2008 printing). This is one of the reasons for the attention shift from the latter half of the 1950s and onwards, towards so-called *embedded* Runge-Kutta methods.

The basic idea of embedded Runge-Kutta methods is that they, aside from the numerical approximation x_{n+1} , yield a second approximation \widehat{x}_{n+1} . The difference between the two approximations then yields an estimate of the local error of the less precise result, which can be used for automatic step size control. The trick is to construct two independent, explicit Runge-Kutta methods which both use the *same* function evaluations. This results in practically obtaining the two solutions for the price of one, in terms of computational complexity. The general structure of an embedded, explicit Runge-Kutta method is illustrated in table 1.2.

Table 1.2: Butcher tableau representation of general, embedded, explicit Runge-Kutta methods.

0					
c_2	$a_{2,1}$				
c_3	$a_{3,1}$	$a_{3,2}$			
\vdots	\vdots	\vdots	\ddots		
c_s	$a_{s,1}$	$a_{s,2}$	\dots	$a_{s,s-1}$	
	b_1	b_2	\dots	b_{s-1}	b_s
	\widehat{b}_1	\widehat{b}_2	\dots	\widehat{b}_{s-1}	\widehat{b}_s

For embedded methods, the coefficients are tuned such that

$$x_{n+1} = x_n + h \sum_{i=1}^s b_i k_i \quad (1.5a)$$

is of order p , and

$$\widehat{x}_{n+1} = x_n + h \sum_{i=1}^s \widehat{b}_i k_i \quad (1.5b)$$

is of order \widehat{p} , typically with $\widehat{p} = p \pm 1$. Which of the two approximations x_{n+1} or \widehat{x}_{n+1} varies

depending on the embedded method in question. Continuing the integration with the higher order result is commonly referred to as *local extrapolation*. The details on how to implement adaptive stepsize control are not immediately relevant for the topic of this project, but can be found in Hairer, Nørsett, and Wanner (1993, pp.167-168 in the 2008 printing).

Table 1.3: Butcher tableau representation of the explicit Euler method.

0	
	1

Table 1.4: Butcher tableau representation of the explicit Heun method.

0		
1	1	
	$\frac{1}{2}$	$\frac{1}{2}$

Table 1.5: Butcher tableau representation of the explicit Kutta method.

0			
$\frac{1}{2}$	$\frac{1}{2}$		
1	-1	2	
	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$

1.2 SETUP

We consider flow in two-dimensional dynamical systems of the form

$$\dot{\mathbf{x}} = \mathbf{v}(t, \mathbf{x}), \quad \mathbf{x} \in \mathcal{U}, \quad t \in [t_0, t_1], \quad (1.6)$$

i.e., systems defined for the finite time interval $[t_0, t_1]$, on an open, bounded subset \mathcal{U} of \mathbb{R}^2 . In addition, the velocity field \mathbf{v} is assumed to be smooth in its arguments. Depending on the exact nature of the velocity field \mathbf{v} , analytical particle trajectories, i.e., solutions of system (??), may or may not be computed.

Table 1.6: Butcher tableau representation of the explicit, classical Runge-Kutta method.

0				
$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{1}{2}$	0	$\frac{1}{2}$		
1	0	0	1	
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

Table 1.7: Butcher tableau representation of the Bogacki- Shampine 3(2) embedded Runge-Kutta method. The b coefficients correspond to a 3rd order accurate solution used to continue the integration. The \hat{b} coefficients correspond to a 2nd order accurate interpolant, which can be used to estimate the error of the numerical approximation, and to dynamically adjust the time step. For reference, see Bogacki and Shampine (1989).

0				
$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{3}{4}$	0	$\frac{3}{4}$		
	$\frac{2}{9}$	$\frac{1}{3}$	$\frac{4}{9}$	
	$\frac{7}{24}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{8}$

Table 1.8: Butcher tableau representation of the Bogacki- Shampine 5(4) embedded Runge-Kutta method. The b coefficients correspond to a 5th order accurate solution used to continue the integration. The two rows of \widehat{b} coefficients correspond to two independent 4th order accurate interpolants. They can be used to estimate the error of the numerical approximation, and to dynamically adjust the time step. The fact that two independent interpolants are included is a part of the reason for which the method nearly behaves like a 6th order method (Hairer, Nørsett, and Wanner 1993, p.194 in the 2008 printing). For reference, see Bogacki and Shampine (1996).

0								
$\frac{1}{6}$	$\frac{1}{6}$							
$\frac{2}{9}$	0	$\frac{2}{27}$	$\frac{4}{27}$					
$\frac{3}{7}$	$\frac{183}{1372}$	$\frac{-162}{343}$	$\frac{1053}{1372}$					
$\frac{2}{3}$	$\frac{68}{297}$	$\frac{-4}{11}$	$\frac{42}{143}$	$\frac{1960}{3861}$				
$\frac{3}{4}$	$\frac{597}{22528}$	$\frac{81}{352}$	$\frac{63099}{585728}$	$\frac{58653}{366080}$	$\frac{4617}{20480}$			
1	$\frac{174197}{959244}$	$\frac{-30942}{79937}$	$\frac{8152137}{19744439}$	$\frac{666106}{1039181}$	$\frac{-29421}{29068}$	$\frac{482048}{414219}$		
1	$\frac{587}{8064}$	0	$\frac{4440339}{15491840}$	$\frac{24353}{124800}$	$\frac{387}{44800}$	$\frac{2152}{5985}$	$\frac{7267}{94080}$	
	$\frac{587}{8064}$	0	$\frac{4440339}{15491840}$	$\frac{24353}{124800}$	$\frac{387}{44800}$	$\frac{2152}{5985}$	$\frac{7267}{94080}$	
	$\frac{6059}{80640}$	0	$\frac{8559189}{30983680}$	$\frac{26411}{124800}$	$\frac{-927}{89600}$	$\frac{443}{1197}$	$\frac{7267}{94080}$	
	$\frac{2479}{34992}$	0	$\frac{123}{416}$	$\frac{612941}{3411720}$	$\frac{43}{1440}$	$\frac{2272}{6561}$	$\frac{79937}{1113912}$	$\frac{3293}{556956}$

Table 1.9: Butcher tableau representation of the Dormand-Prince 5(4) embedded Runge-Kutta method. The b coefficients correspond to a 5th order accurate solution used to continue the integration. The \hat{b} coefficients correspond to a 4th order interpolant, which can be used to estimate the error of the numerical approximation, and to dynamically adjust the time step. For reference, see Hairer, Nørsett, and Wanner (1993, p.178 in the 2008 printing).

0							
$\frac{1}{5}$	$\frac{1}{5}$						
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$					
$\frac{4}{5}$	$\frac{44}{45}$	$-\frac{56}{15}$	$\frac{32}{9}$				
$\frac{8}{9}$	$\frac{19372}{6561}$	$-\frac{25360}{2187}$	$\frac{64448}{6561}$	$-\frac{212}{769}$			
1	$\frac{9017}{3168}$	$-\frac{355}{33}$	$\frac{46732}{5247}$	$\frac{49}{176}$	$-\frac{5103}{18656}$		
1	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	
	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	
	$\frac{5179}{57600}$	0	$\frac{7571}{16695}$	$\frac{393}{640}$	$-\frac{92097}{339200}$	$\frac{187}{2100}$	$\frac{1}{40}$

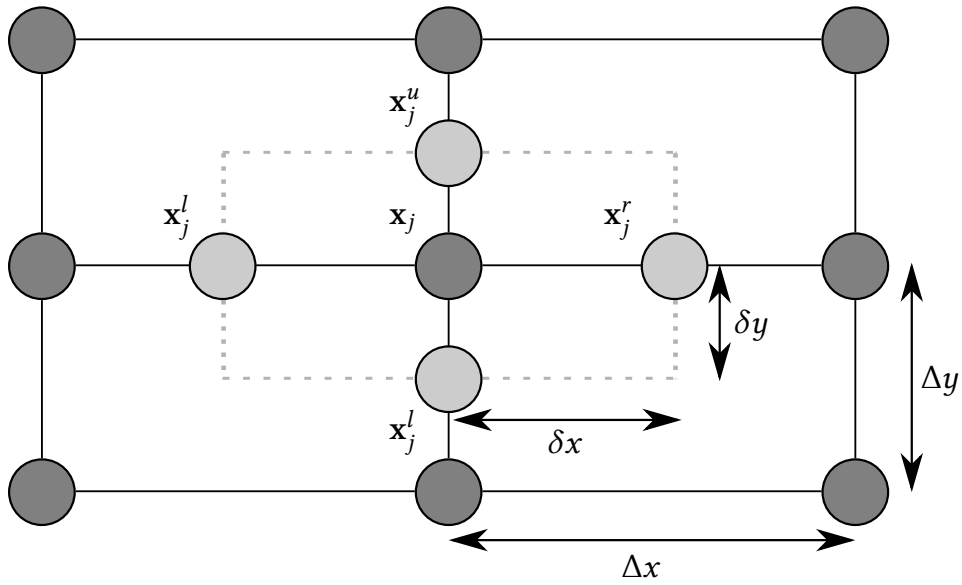


Figure 1.1: Dawg

$$A\mathbf{x} = \mathbf{b} \tag{1.7}$$

2 Introduction

Only interested in hyperbolic LCSs as they are the only ones relevant for transport barriers.

2.1 COMPLEX SYSTEMS → NEED SHORTCUTS

2.2 INTUITIVELY, WHAT IS AN LCS?

2.3 LCS DEFINITION

2.4 DIFFERENT TYPES OF LCSS

2.5 HYPERBOLIC LCSS

→ Connect to application

3 Theory

3.1 SOLVING ODE SYSTEMS

→ General ODE systems → Numerical integrators dump → Interpolation necessary for discrete systems

3.2 FLOWMAPS

→ Introduce system and limitations → Introduce the concept of a flow map

3.3 LCS DEFINITION

→ Different kinds of LCSs (hyperbolic, elliptic and parabolic, cf. LCS tool) → More mathematical definitions? Ask Thör

3.4 FTLE AS LCS PREDICTOR

→ Prone to false positives and negatives → Definition somewhat arbitrary (what is a ridge)?
→ Strogatz' motivation as a simple explanation of why we consider it at all?

3.5 IDENTIFY HYPERBOLIC LCS FROM VARIATIONAL THEORY

→ Mathematically involved.

4 Tool!

4.1 ADVEKSJON

→ Si noe om system, glatte vektorfelt/hastighetsfelt → Integrasjonsteknikker

4.2 CG TENSORS

→ Auxiliary grid → Extended grids i fire retninger → Beregn CG tensors → Centered differencing, consistently for all main particles → Har med gitterpunkter på utsiden av hoveddomenet for å inkludere diskontinuitet i oppførsel i hastighetsfeltet

4.3 EIGENVALUES/EIGENVECTORS

→ Auxiliary grid → Laplacian, extended grid layer 2 for centered differencing

4.4 IDENTIFY AB DOMAIN

→ Klargjør måten vi tolket Laplacian på

4.5 COMPUTE STRAINLINES

→ Define G_0 along vertical and horizontal lin → Avoid redundant computations of trajectories
→ Integrate forwards and backwards → (Notice that strainlines "fall out" of AB domain, likely due to num. error) → Special linear interpolation with local direction correction → Higher order spline interpolations are inappropriate because of orientation → discontinuities (in case of vectors) and great variance (in case of evals) → Linear spline interpolation without orientation fix caused random turns → at discontinuities. → Stop criteria → Alpha scaling introduced by Haller gave unpredictable leaps → After linear interp? → Used just one integrator here, because [...] → Choice of integration step (needs test!) → Note that this step is very sensitive to the flow map details, → components in the strain tensors down to the 10^{-15} level. → LCS results sensitive to continuous failure length, needed to increase → it in order to replicate results from Haller due to different AB domain

4.6 IDENTIFY INTERSECTIONS

→ Which lines and why (maximize intersections with as few lines as possible) → Include all intersections between a strainline and a vert / horz linear

4.7 IDENTIFY NEIGHBORS

→ Neighbor length essential for LCS results

4.8 SELECT LCSS

→ Identify LCS as local maxima of λ_2 which are also long enough → Needs at least one neighbor other than itself → **Cut tail of strainlines which exit AB domain and do not return** → That part is no LCS! → Parts/sections of strainlines may qualify as LCSs

5 Experiments

→ What did we try and why?

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Curabitur consectetur.

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Sed commodo posuere pede. Mauris ut est. Ut quis purus. Sed ac odio. Sed vehicula hendrerit sem. Duis non odio. Morbi ut dui. Sed accumsan risus eget odio. In hac habitasse platea dictumst. Pellentesque non elit. Fusce sed justo eu urna porta tincidunt. Mauris felis odio, sollicitudin sed, volutpat a, ornare ac, erat. Morbi quis dolor. Donec pellentesque, erat ac sagittis semper, nunc dui lobortis purus, quis congue purus metus ultricies tellus. Proin et quam. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos hymenaeos. Praesent sapien turpis, fermentum vel, eleifend faucibus, vehicula eu, lacus.