Sensitivity to Numerical Integration Scheme in Calculation of Transport Barriers

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Abstract

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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

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

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

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

The system if 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.

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. 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

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

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),

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

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 upper triangular. Similarly, for fully implicit Runge-Kutta methods, the Runge-Kutta matrix is lower 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.

1.2 SETUP

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

$$\dot{\mathbf{x}} = \mathbf{v}(t, \mathbf{x}), \quad \mathbf{x} \in \mathcal{U}, \quad t \in [t_0, t_1], \tag{1.5}$$

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.

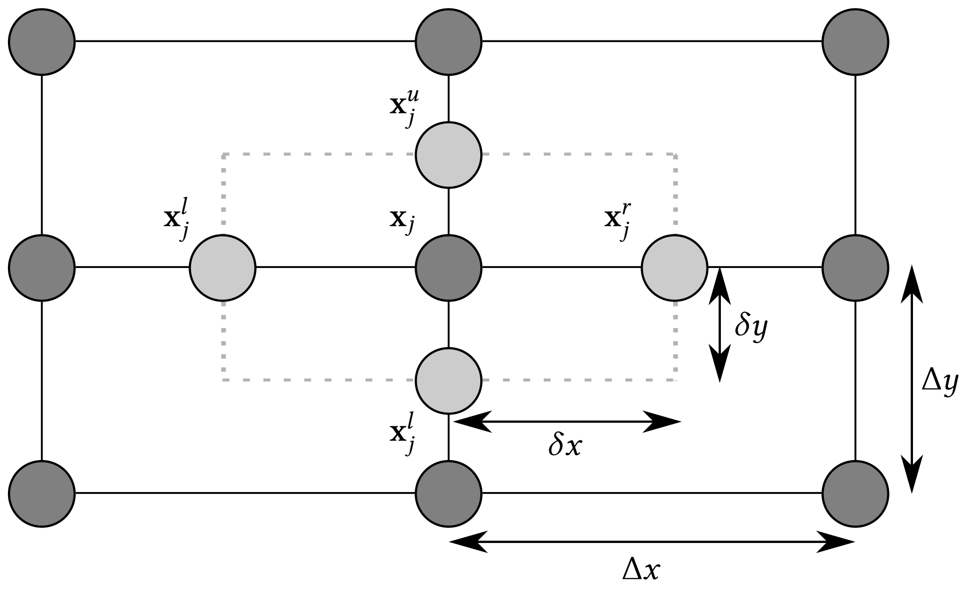

Figure 1.1: Dawg

$$\boldsymbol{A}\mathbf{x} = \mathbf{b} \tag{1.6}$$

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 G0 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 oriental −> 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 continious 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 intersetions 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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