Sensitivity to Numerical Integration Scheme in Calculation of Transport Barriers

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November 20, 2017

Abstract

Sammendrag

Preface

Table of Contents

Lis	et of Figures	v
Lis	et of Tables	vi
No	tation	vii
1	Theory	1
	1.1 Solving systems of ordinary differential equations	. 1
	1.1.1 The Runge-Kutta family of numerical methods	
	1.1.2 The Runge-Kutta methods under consideration	
	1.2 The type of flow systems considered	
2	Introduction	11
	2.1 Complex systems -> Need shortcuts	. 12
	2.2 Intuitively, what is an LCS?	. 12
	2.3 LCS definition	. 12
	2.4 Different types of LCSs	. 12
	2.5 Hyperbolic LCSs	. 12
3	Theory	12
	3.1 Solving ODE systems	. 12
	3.2 Flowmaps	. 12
	3.3 LCS definition	. 12
	3.4 FTLE as LCS predictor	. 12
	3.5 Identify hyperbolic LCS from variational theory	. 12
4	Tool!	12
	4.1 Adveksjon	. 12
	4.2 CG tensors	. 13
	4.3 Eigenvalues/Eigenvectors	. 13
	4.4 Identify AB domain	. 13
	4.5 Compute strainlines	
	4.6 Identify intersections	
	4.7 Identify neighbors	
	4.8 Select LCSs	. 13
5	Experiments	14
Re	ferences	15
ΔT	PFNDIX A Haller er en dust	16

List of Figures

		_	_																
1	.1	1	Jawg	 															11

List of Tables

1.1	Butcher tableau representation of a general s-stage Runge-Kutta method	2
1.2	Butcher tableau representation of general, embedded, explicit Runge-Kutta	
	methods	3
1.3	Butcher tableau representation of the explicit Euler method	4
1.4	Butcher tableau representation of the explicit Heun method	4
1.5	Butcher tableau representation of the explicit Kutta method	5
1.6	Butcher tableau representation of the explicit, classical Runge-Kutta method .	5
1.7	Butcher tableau representation of the Bogacki-Shampine 3(2) embedded Runge-	
	Kutta method	6
1.8	Butcher tableau representation of the Bogacki-Shampine 5(4) embedded Runge-	
	Kutta method	7
1.9	Butcher tableau representation of the Dormand-Prince 5(4) embedded Runge-	
	Kutta method	8
1.10	Butcher tableau representation of the Dormand-Prince 8(7) embedded Runge-	
	Kutta method	9

Notation

Newton's notation is used for differentiation with respect to time, i.e.:

$$\dot{f}(t) \equiv \frac{\mathrm{d}f(t)}{\mathrm{d}t}$$

Vectors are denoted by upright, bold letters, like this:

$$\boldsymbol{\xi} = (\xi_1, \xi_2, \dots, \xi_n)$$

Matrices and matrix representations of rank-2 tensors are denoted by bold, italicized letters, like this:

$$\mathbf{A} = \begin{pmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,n} \\ a_{2,1} & a_{2,2} & \dots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \dots & a_{m,n} \end{pmatrix}$$

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

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

$$\dot{x}_{i}(t) = f_{i}(t, x_{1}(t), x_{2}(t), \dots, x_{n}(t)), \quad x_{i}(t_{0}) = x_{i,0}, \quad i = 1, \dots, n$$

$$\mathbf{x}(t) = (x_{1}(t), x_{2}(t), \dots, x_{n}(t))$$
(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.

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

$$k_{i} = f\left(t_{n} + c_{i}h, x_{n} + h\sum_{j=1}^{s} a_{i,j}k_{j}\right), \quad i = 1, \dots, s$$

$$x_{n+1} = x_{n} + h\sum_{i=1}^{s} b_{i}k_{i}$$
(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),

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

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	$a_{1,1}$	$a_{1,2}$		$a_{1,s}$
c_2	$a_{2,1}$	$a_{2,2}$		$a_{2,s}$
:	:	:	٠.	÷
c_s	$a_{s,1}$	$a_{s,2}$		$a_{s,s}$
	b_1	b_2		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 $p \ge 5$, 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 Butcher tableau of an embedded, general, explicit Runge-Kutta method is illustrated in table 1.2.

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

For embedded methods, the coefficients are tuned such that

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

is of order p, and

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

1.1.2 The Runge-Kutta methods under consideration

Naturally, an abundance of Runge-Kutta methods exist. Many of them are fine-tuned for specific constraints, such as problems of varying degrees of stiffness. It is neither possible nor meaningful to investigate them all in the context of general flow dynamics. For this reason, I consider two classes of explicit Runge-Kutta methods, namely singlestep and adaptive stepsize methods. From both classes, I include four different general-purpose ODE solvers of varying order.

Singlestep methods

The singlestep methods under consideration are the classical, explicit Runge-Kutta methods of orders one through to four, i.e., the *Euler*, *Heun*, *Kutta* and *classical Runge-Kutta* methods. The Euler method is 1st order accurate, and requires a single function evaluation of the right hand side of the ordinary differential equation (1.1) or (1.2) at each time step. Its Butcher tableau representation can be found in table 1.3. It is the simplest explicit method for numerical integration of ordinary differential equations. The Euler method is often used as a basis to construct more complex methods, such as the Heun method, which is also known as the *improved Euler method* or the *explicit trapezoidal rule*. The Heun method is 2nd order accurate, and requires two function evaluations at each time step. Its Butcher tableau representation can be found in table 1.4.

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

0	
	1

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

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

The Kutta method is 3^{rd} order accurate, and requires three function evaluations of the right hand side of the ordinary differential equation (1.1) or (1.2) at each time step. Its Butcher tableau representation can be found in table 1.5. The classical Runge-Kutta method is 4^{th} order accurate,

and perhaps the most well-known and frequently used of the four singlestep schemes discussed in this project. One reason for its popularity is that it is exceptionally stable numerically (i.e., of the aforementioned singlestep methods, the classical Runge-Kutta method has the largest numerical stability domain). Another is that, as mentioned previously, for $p \ge 5$, no explicit Runge-Kutta method of order p with s=p stages exist (Hairer, Nørsett, and Wanner 1993, p.173 in the 2008 printing) – which means that the required number of function evaluations grows at a disproportional rate with the required accuracy order. For systems with right hand sides which are computationally costly to evaluate, this means that one frequently is able to obtain the desired numerical accuracy more effectively e.g. by using the classical Runge-Kutta method with a finer step length. The Butcher tableau representation of the classical Runge-Kutta method can be found in table 1.6.

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

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

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

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

Adaptive stepsize methods

The adaptive stepsize methods under consideration are the Bogacki-Shampine 3(2) and 5(4) methods, and the Dormand-Prince 5(4) and 8(7) methods. The digit outside of the parentheses indicates the order of the solution which is used to continue the integration, while the digit within the parentheses indicates the order of the interpolant solution. Note that the concept

of *order* does not translate directly from singlestep methods, as a direct consequence of the adaptive time step. Generally, lower order methods are more suitable than higher order methods for cases where crude approximations of the solution are sufficient. Bogacki and Shampine argue that their methods outperform other methods of the same order (Bogacki and Shampine 1989; Bogacki and Shampine 1996), a notion which, for the 5(4) method, is supported by Hairer, Nørsett, and Wanner (1993, p.194 in the 2008 printing).

Butcher tableau representations of the aforementioned adaptive stepsize methods can be found in tables 1.7–1.10, the latter of which has been typeset in landscape orientation for the reader's convenience. Three of the methods, namely the Bogacki-Shampine 3(2) and 5(4) methods, in addition to the Dormand-Prince 5(4) method, possess the so-called *First Same As Last* property. This means that the last function evaluation of an accepted step is exactly the same as the first function evaluation of the next step. This is readily apparent from their Butcher tableaus, where the *b* coefficients correspond exactly with the last row the Runge-Kutta matrix. The *First Same As Last* property reduces the computational cost of a successive step.

Table 1.7: Butcher tableau representation of the Bogacki- Shampine 3(2) embedded Runge-Kutta method. The b coefficients correspond to a $3^{\rm rd}$ order accurate solution used to continue the integration. The \hat{b} coefficients correspond to a $2^{\rm nd}$ order accurate interpolant, which can be used to estimate the error of the numerical approximation, and to dynamically adjust the time step. The *First Same As Last* property is apparent from the fact that the b coefficients correspond exactly to the last row of coefficients in the Runge-Kutta matrix. For reference, see Bogacki and Shampine (1989).

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

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 \hat{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). The *First Same As Last* property is apparent from the fact that the b coefficients correspond exactly to the last row of coefficients in the Runge-Kutta matrix. For reference, see Bogacki and Shampine (1996).

0								
U								
1_	$\frac{1}{6}$							
- 6	6							
$\frac{2}{9}$	0	$\frac{2}{27}$	$\frac{4}{27}$					
3	183	-162	1053					
7	1372	343	1372					
$\frac{2}{3}$	68	-4	42	1960				
3	297	11	143	3861				
$\frac{3}{4}$	597	81	63099	58653	4617			
$\overline{4}$	22528	352	585728	366080	$\overline{20480}$			
1	174197	-30942	8152137	666106	-29421	482048		
1	959244	79937	19744439	1039181	29068	414219		
1	587	0	4440339	24353	387	2152	7267	
	8064	<u> </u>	15491840	$\overline{124800}$	44800	5985	94080	
	587	0	4440339	24353	387	2152	7267	
	8064	0	15491840	124800	44800	5985	94080	
	6059	0	8559189	26411	-927	443	7267	
	80640	0	30983680	$\overline{124800}$	89600	1197	94080	
	2479	0	123	612941	43	2272	79937	3293
	34992	U	416	3411720	1440	6561	1113912	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. The *First Same As Last* property is apparent from the fact that the b coefficients correspond exactly to the last row of the Runge-Kutta matrix. 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	$\frac{500}{1113}$	$\frac{125}{192}$	$\frac{-2187}{6784}$	$\frac{11}{84}$	
	5179 57600	0	$\frac{7571}{16695}$	$\frac{393}{640}$	$\frac{-92097}{339200}$	$\frac{187}{2100}$	$\frac{1}{40}$

Table 1.10: Butcher tableau for the Dormand-Prince 8(7) embedded Runge-Kutta method. The b coefficients correspond to an 8^{th} order accurate solution used to continue the integration. The \hat{b} coefficients correspond to a 7^{th} order interpolant, which can be used to estimate the error of the numerical approximation, and to dynamically adjust the time step. Note that the provided coefficients are rational approximations, accurate to about 24 significant decimal digits – sufficiently well-resolved for most numerical applications. For reference, see Prince and Dormand (1981).

									1-4	0
								0	$\frac{-528747749}{2220607170}$	$\frac{2}{45}$
							$\frac{65686358}{487910083}$	$\frac{248638103}{1413531060}$	$\frac{118820643}{751138087}$	$\frac{53011238}{667516719}$
						$\frac{3065993473}{5917172653}$	$\frac{3962137247}{1805957418}$	$\frac{-160528059}{685178525}$	$\frac{760417239}{1151165299}$	465885868 322736535
					$\frac{123872331}{1001029789}$	$\frac{-45442868181}{339846796}$	$\frac{-4093664535}{808688257}$	$\frac{3936647629}{1978049680}$	$\frac{-1041891430}{1371343529}$	$\frac{-3867574721}{1518517206}$
				$\frac{800635310}{3783071287}$	$\frac{393006217}{1396673457}$	$\frac{15336726248}{1032824649}$	5232866602 850066563	$\frac{-13158990841}{6184727034}$	$\frac{56129285}{797845732}$	$\frac{656045339}{265891186}$
			$\frac{-180193667}{1043307555}$	$\frac{790204164}{839813087}$	$\frac{6005943493}{2108947689}$	$\frac{-48777925059}{3047939560}$	$\frac{5731566787}{1027545527}$	$\frac{11173962825}{925320556}$	$\frac{181606767}{758867731}$	$\frac{1757004468}{5645159321}$
		$\frac{23124283}{18000000000}$	$\frac{545815736}{2771057229}$	$\frac{100302831}{723423059}$	$\frac{-12992083}{490766935}$	$\frac{-10304129995}{1701304382}$	$\frac{-703635378}{230739211}$	$\frac{652783627}{914296604}$	$\frac{-59238493}{1068277825}$	$\frac{-808719486}{976000145}$
	20 3 20 3	$\frac{-28693883}{1125000000}$	$\frac{22789713}{633445777}$	$\frac{-421739975}{2616292301}$	$\frac{-309121744}{1061227803}$	$\frac{1311729495}{1432422823}$	$\frac{-477755414}{1098053517}$	$\frac{-411421997}{543043805}$	0	0
	75 64 3 16	$\frac{77736358}{692538347}$	$\frac{61564180}{158732637}$	$\frac{-433636366}{683701615}$	$\frac{-37695042795}{15268766246}$	8478235783 508512851	$\frac{-3185094517}{667107341}$	$\frac{-5068492393}{434740067}$	0	0
33	$\frac{-75}{64}$	0	0	0	0	0	0	0	0	0
$\frac{1}{16}$	0 0	0	0	0	0	0	0	0	0	0
$\frac{1}{18}$ $\frac{1}{48}$ $\frac{1}{32}$	5 16 3 80	$\frac{29443841}{614563906}$	$\frac{16016141}{946692911}$	$\frac{39632708}{573591083}$	$\frac{246121993}{1340847787}$	$\frac{-1028468189}{846180014}$	$\frac{185892177}{718116043}$	$\frac{403863854}{491063109}$	$\frac{1400451}{335480064}$	$\frac{13451932}{455176623}$
0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	3 8 8	59 400	$\frac{93}{200}$	$\frac{5490023248}{9719169821}$	$\frac{13}{20}$	$\frac{1201146811}{1299019798}$	П	1		

1.2 THE TYPE OF FLOW SYSTEMS CONSIDERED

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

$$\dot{\mathbf{x}} = \mathbf{v}(t, \mathbf{x}), \quad \mathbf{x} \in \mathcal{U}, \quad t \in [t_0, t_1],$$
 (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., analytical solutions of system (1.6), may or may not be computed. The flow particles are assumed to be infinitesimall and massless, i.e., non-interacting *tracers* of the overall circulation.

Letting $\mathbf{x}(t; t_0, \mathbf{x}_0)$ denote the trajectory of a tracer in the system defined by (1.6), the flow map is defined as

$$\mathbf{F}_{t_0}^t(\mathbf{x}_0) = \mathbf{x}(t; t_0, \mathbf{x}_0), \tag{1.7}$$

i.e., the flow map describes the mathematical movement of the tracers from one point in time (e.g. the initial condition) to another. Generally, the flow map is as smooth as the velocity field ${\bf v}$ in system (1.6) (Farazmand and Haller 2012). For sufficiently smooth velocity fields, the right Cauchy-Green strain tensor field is defined as

$$\boldsymbol{C}_{t_0}^t(\mathbf{x}_0) = \left(\nabla \mathbf{F}_{t_0}^t(\mathbf{x}_0)\right)^{\mathsf{T}} \nabla \mathbf{F}_{t_0}^t(\mathbf{x}_0), \tag{1.8}$$

where $\nabla \mathbf{F}_{t_0}^t$ denotes the Jacobian matrix of the flow map $\mathbf{F}_{t_0}^t$, and the T refers to matrix transposition. Component-wise, the Jacobian matrix of a general vector-valued function \mathbf{f} is defined as

$$(\nabla \mathbf{f})_{i,j} = \frac{\partial f_i}{\partial x_i} \tag{1.9}$$

which, for our two-dimensional flow, reduces to

$$\nabla \mathbf{f} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{pmatrix}.$$
 (1.10)

By construction, the Cauchy-Green strain tensor $C_{t_0}^t$ is symmetric and positive definite. Thus, it has two real, positive eigenvalues and orthogonal, real eigenvectors. Its eigenvalues λ_i and corresponding unit eigenvectors ξ_i are defined by

$$C_{t_0}^t(\mathbf{x}_0)\xi_i(\mathbf{x}_0) = \lambda_i \xi_i(\mathbf{x}_0), \quad \|\xi_i(\mathbf{x}_0)\| = 1, \quad i = 1, 2,$$

$$0 < \lambda_1(\mathbf{x}_0) \le \lambda_2(\mathbf{x}_0),$$
(1.11)

where, for the sake of notational transparency, the dependence of λ_i and ξ_i on t_0 and t has been suppressed. If the flow is incompressible, the eigenvalues satisfy

$$\lambda_1(\mathbf{x}_0)\lambda_2(\mathbf{x}_0) = 1 \quad \forall \ \mathbf{x}_0 \in \mathcal{U}$$
 (1.12)

where, for our case, incompressibility is equivalent to the velocity field v being divergence-free (i.e., $\nabla \cdot v \equiv 0$), because the tracer particles are massless (Farazmand and Haller 2012).

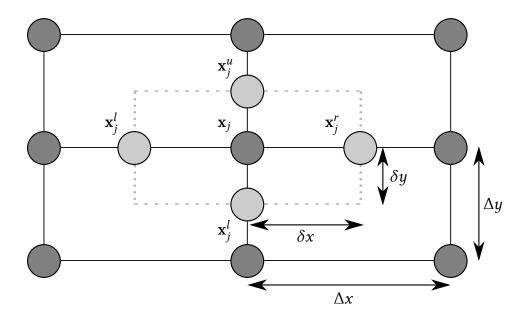


Figure 1.1: Dawg

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{1.13}$$

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 ADVEKSION

-> 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 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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