Time step selection for shock problems

Karl Hörnell and Per Lötstedt*

August 15, 2000

Abstract

The solution to a conservation law is integrated in time by an embedded Runge-Kutta method. The time steps are chosen so that a bound on the local error is satisfied. At discontinuities such as shocks in the solution the time step is too pessimistic. By filtering the error estimate the time steps are determined by the smooth parts of the solution. The technique is justified theoretically and in numerical experiments.

Subject classification: 65M20, 65L06

Keywords: shock problem, time steps, error control

1 Introduction

A solution algorithm for time dependent partial differential equations (PDEs) is improved in at least two respects if the time step is automatically adapted to the solution. Firstly, a control of the error in the solution is introduced by choosing the time step so that the local discretization error in the solution due to the time stepping is less than a given tolerance. Local error control has been used in the solution of ordinary differential equations (ODEs) for a long time [4], [9], and parabolic PDEs, e.g. [11], and gives good results in practice. Secondly, the user is not required to supply the solver with a time step which is then kept constant in the whole time interval of interest. For flow problems this is usually done by introducing a CFL number. The time step is then obtained by multiplying the space step by the CFL number divided by an estimate of the maximum local speed. The choice of CFL number is usually based on the user's experience, the equation and the time stepping method.

In the numerical solution of ODEs, the local error l^n in step n is estimated by comparing the solutions computed by two different time steps $\Delta t^n = t^{n+1} - t^n$ or two different methods [4], [9]. The assumption is that

$$l^n = \Phi(t^n)(\Delta t^n)^{p+1} + \mathcal{O}((\Delta t^n)^{p+2}), \tag{1}$$

*Dept. of Information Technology, Scientific Computing, Uppsala University, SE-75104 Uppsala, Sweden

where Φ is smooth and depends on the solution and the method and p is the order of the discretization. A tentative time step $\Delta\hat{t}^n$ is computed by comparing the error estimate $\hat{l}^n$ with the tolerance ε e.g. as follows

$$\Delta\hat{t}^n = \theta(\varepsilon/r^n)^{1/p+1}\Delta t^n,\ r^n = \|\hat{l}^n\|_\infty, \tag{2}$$

where $\theta < 1$ is a safety factor chosen to be 0.8 here and $\|\cdot\|_\infty$ is the maximum norm. In the simplest form of the algorithm, the next time step at t^{n+1} is taken to be $\Delta t^{n+1} = \max(\Delta t^n, \Delta\hat{t}^n)$ if $r^n \leq \varepsilon$. If $r^n > \varepsilon$, then the step from t^n to t^{n+1} is recomputed with $\Delta t^n = \Delta\hat{t}^n$. This procedure works well for problems with smooth solutions.

Time dependent conservation laws in one (1D) or two (2D) dimensions

$$\mathbf{u}_t + \sum_{i=1}^{N} \mathbf{f}^i_{x_i}(\mathbf{u}) = 0,\ x \in \Omega,\ t > 0,\ \mathbf{u}(x,0) = \mathbf{u}^0(x), \tag{3}$$

with $N = 1, 2$, are integrated for $\mathbf{u}(x,t) \in \mathbf{R}^M$ with an embedded Runge-Kutta method [4] in this note. Derivation with respect to time t and space coordinate x_i is denoted by a subscript in (3). The space derivatives are first discretized and then the equations are integrated by an optimal second order method [2] in time ("method of lines") and compared with a third order method for a local error estimate. The time step is chosen as in (2).

In a first order time-stepping method, Φ in (1) depends on u_{tt}. For Burgers' equation in 1D with an upwind discretization at a shock moving to the right, our system of ODEs is

$$u_{jt} = -0.5h^{-1}(u_j^2 - u_{j-1}^2),$$

where u_j approximates $u(x,t)$ in cell j and h is the cell size. Suppose that the shock is represented in a few cells around j. Then $u_j - u_{j-1}$ is of $\mathcal{O}(1)$ and consequently $u_{jtt} \sim h^{-2}$. For $\hat{l}^n$ in (1) to become small, we must choose $\Delta t^n \ll h$. Neither a correct shock speed nor stability requires such small time steps. In cell j, $\Phi_j(t)$ is not smooth and the local error estimate breaks down at a shock.

The usual error estimates are not relevant and too pessimistic when shocks are present in the solution resulting in too short time steps and loss of efficiency. Time steps should be chosen for an accurate integration of the smooth part of the solution. By not allowing the error estimates in the neighborhood of shocks and contact discontinuities to influence the time step selection, the same accuracy in the solution is obtained with a longer time step. To this end, a filter is applied to $\hat{l}^n$ before it is used in (2). It is motivated theoretically and in numerical experiments that the correct shock speed is obtained in this way.

2 Adapted time steps

We present the time stepping scheme in this section and analyze it for a scalar conservation law in one space dimension. A two dimensional numerical example is found in the next section. The space derivatives are approximated by a conservative finite volume method on an equidistant grid with cell j between x_{j-1} and x_j. The solution is advanced in time by an explicit Runge-Kutta scheme.

Let $\mathbf{u}_j^n$ be the approximation of $\mathbf{u}$ in 1D in cell j at time t^n. Assume that the space derivative for $N = 1$ in (3) is approximated by a total variation diminishing (TVD) scheme in cell j at t^n so that

$$\begin{aligned}\mathbf{f}_x(\mathbf{u}) &\approx h^{-1}(F(\mathbf{u}_{j-k}^n \ldots \mathbf{u}_{j+k+1}^n) - F(\mathbf{u}_{j-k-1}^n \ldots \mathbf{u}_{j+k}^n)) \\ &= h^{-1}(F_{j+1/2}^n - F_{j-1/2}^n),\end{aligned}$$

where F is the numerical flux function [7] and $k \geq 0$. We assume that F is consistent so that $F(\mathbf{u}, \mathbf{u}, \ldots \mathbf{u}) = f(\mathbf{u})$. Let $G_j = F_{j+1/2} - F_{j-1/2}$ and $\lambda^n = \Delta t^n / h$. The optimal Runge-Kutta method of second order with TVD property is [2]

$$\begin{aligned}\mathbf{u}_j^* &= \mathbf{u}_j^n - \lambda^n G_j, \\ \mathbf{u}_j^{n+1} &= \mathbf{u}_j^n - \tfrac{1}{2}\lambda^n (G_j^* + G_j^n),\end{aligned} \tag{4}$$

where G^* is evaluated at $\mathbf{u}^*$. The method is optimal in the sense that it allows the largest CFL number among all second order schemes.

The local error l^n is estimated by comparing two solutions of second and third order in time as in the Runge-Kutta method RKF2(3) [4] of Fehlberg type. In addition to (4) evaluate also

$$\begin{aligned}\mathbf{u}_j' &= \mathbf{u}_j^n - \tfrac{1}{4}\lambda^n (G_j^n + G_j^*), \\ \tilde{\mathbf{u}}_j^{n+1} &= \mathbf{u}_j^n - \lambda^n (\tfrac{1}{6}(G_j^* + G_j^n) + \tfrac{2}{3} G_j'),\end{aligned} \tag{5}$$

where G_j' is computed at $\mathbf{u}_j'$. The second order solution $\mathbf{u}_j^{n+1}$ is chosen and

$$\hat{l}^n = \mathbf{u}^{n+1} - \tilde{\mathbf{u}}^{n+1}. \tag{6}$$

The integration (4) can be rewritten in conservative form as

$$\begin{aligned}\mathbf{u}_j^{n+1} &= \mathbf{u}_j^n - \lambda^n (H_{j+1/2}^n - H_{j-1/2}^n), \\ H_{j+1/2}^n &= 0.5(F_{j+1/2}^n + F_{j+1/2}^*) = 0.5(F(\mathbf{u}_{j-k}^n \ldots \mathbf{u}_{j+k+1}^n) \\ &+ F(\mathbf{u}_{j-k}^n - \lambda^n (F(\mathbf{u}_{j-2k}^n \ldots \mathbf{u}_{j+1}^n) - F(\mathbf{u}_{j-2k-1}^n \ldots \mathbf{u}_j^n)) \ldots \\ &\quad \mathbf{u}_{j+k+1}^n - \lambda^n (F(\mathbf{u}_{j+1}^n \ldots \mathbf{u}_{j+2k+2}^n) - F(\mathbf{u}_j^n \ldots \mathbf{u}_{j+2k+1}^n)))).\end{aligned} \tag{7}$$

Control of the accuracy of the time discretization of smooth solutions follows from the same arguments as in the solution of ODEs. For conservation laws with discontinuities in the solution, properties are usually derived assuming constant time steps. For variable time steps we make the following two observations. The first result is a consequence of the convergence proof by Lax and Wendroff [6]. Let $\varphi(x,t)$ be an arbitrary test function in C_0^∞ with $\varphi(x,0)=\varphi^0(x)$.

Proposition 2.1 *Assume that $\boldsymbol{u}_j^n$ is computed by a consistent approximation in conservative form with variable time steps Δt^n in 1D and that $\boldsymbol{u}_j^n$ converges to $\boldsymbol{u}(x,t)$ boundedly and almost everywhere as $h, \max_n \Delta t^n \to 0$. Then $\boldsymbol{u}(x,t)$ is a weak solution of (3) satisfying*

$$\int_0^\infty \int_{-\infty}^\infty (\varphi_t \boldsymbol{u} + \varphi_x \boldsymbol{f})\, dx\, dt + \int_{-\infty}^\infty \varphi^0 \boldsymbol{u}^0\, dx = 0. \tag{8}$$

Proof Rewrite (7) as

$$(\mathbf{u}_j^{n+1} - \mathbf{u}_j^n)/\Delta t^n + (H_{j+1/2}^n - H_{j-1/2}^n)/h = 0,$$

multiply by $h\Delta t^n$ and φ_j^n and sum over all cells and time steps. Use partial summation and let $h, \Delta t^n \to 0$ to obtain (8).

We find that the numerical solution converges to a weak solution of (3) regardless of the time step sequence as long as $\mathbf{u}^n$ is stable.

For a 1D scalar problem, the shock speed s is given by the Rankine-Hugoniot condition. Let two constant states u_L and u_R be separated by a shock. Furthermore, let x_L and x_R be such that $x_L < x_R$, $u(x_L) = u_L$, and $u(x_R) = u_R$ when $t \in [0,T]$. Then

$$\begin{aligned} s(u_L - u_R) &= \tfrac{d}{dt}\int_{x_L}^{x_R} u(x,t)\, dx \\ &= -\int_{x_L}^{x_R} f(u)_x\, dx = f(u_L) - f(u_R). \end{aligned} \tag{9}$$

Define the shock speed s_h of the discrete problem to be

$$s_h(u_L - u_R) = (\Delta t^n)^{-1}\left(\sum_{j=\ell}^{r} u_j^{n+1} h - \sum_{j=\ell}^{r} u_j^n h\right). \tag{10}$$

with $r = R + 2k + 1$ and $\ell = L - 2k - 1$. Then we have

Proposition 2.2 *Assume that $N = 1$, f in (3) is scalar and that $u_j^n = u_L$ for $j \le L$ and $u_j^n = u_R$ for $j \ge R$ for $t^n \in \mathcal{I} = [0,T]$. Then $s = s_h$ independent of Δt^n in I.*

Proof By the definition of s_h in (10), conservation, the consistency of H in (7), and (9)

$$s_h(u_L - u_R) = -(H_{r+1/2}^n - H_{\ell-1/2}^n) = -(f(u_R) - f(u_L)) = s(u_L - u_R).$$

In the special case when H is independent of Δt^n the propagation at the shock is constant independent of Δt^n. Suppose that u^n_{j-1} and u^n_j are part of the shock representation. Let x' be the point such that the linear approximation

$$u^n(x) = u^n_{j-1} + \frac{x - x_{j-1}}{x_j - x_{j-1}}(u^n_j - u^n_{j-1}) \tag{11}$$

of the profile between x_{j-1} and x_j satisfies $u^n(x') = u^{n+1}_j$. The interpretation of x' is that the shock is propagated from x' to x_j in step n from t^n to t^{n+1}. Thus, by (11) and (7) the local shock speed s_l is

$$s_l = \frac{x_j - x'}{\Delta t^n} = \frac{H^n_{j+1/2} - H^n_{j-1/2}}{u_j - u_{j-1}},$$

which is independent of Δt^n if $H^n_{j\pm 1/2}$ is so.

In [3] and [10], the time step regulation is investigated using control theory. The time steps in (2) are selected with an integrative I-controller. Increased robustness in time step control is achieved by introducing a PI-controller in [3], [10]. The oscillatory behavior of the local error estimates in the vicinity of discontinuities also after filtering in our numerical tests in [5] suggests that a pure I-controller in the best choice here.

We conclude that we obtain the correct shock speed for any Δt^n as long as the time-integration is stable. Thus, we can exclude the local error in cells in the neighborhood of shocks from influencing the time steps. This is achieved by introducing a filter Ψ^n such that $(\Psi^n \hat{l}^n)_j$ is small for a component j in u^n with a discontinuity and $(\Psi^n \hat{l}^n)_j = \hat{l}^n_j$ otherwise. Then take r^n in (2) to be

$$r^n = \|\Psi^n \hat{l}^n\|_\infty. \tag{12}$$

3 Numerical results

The filtering of the local error is tested in two examples in this section. The Euler equations of gas dynamics are solved in a 1D shock tube with standard initial data and the 2D solution to the inviscid Burgers equation is computed with smooth initial data so that a shock eventually develops.

The filter is designed to be sensitive to steep gradients in the solution and to be close to zero there. In the 1D experiment

$$\Psi^n_{jm} = 1/\max(1, |u^n_{xjm}|/\zeta). \tag{13}$$

Here u^n_{xjm} is approximated by $(u^n_{j+1,m} - u^n_{jm})/h$ for each of the M components of $\mathbf{u}^n_j$. In (13), ζ should be greater than the derivative except for the vicinity of a shock or a contact discontinuity. In the experiments below,

$$\zeta = \max(5\,\mathrm{median}(|u^n_{xjm}|), \max_{jm}(|u^n_{xjm}|)/1000). \tag{14}$$

The derivative in a cell is compared to the median multiplied by a weight in the computational domain. The median may be very small if the solution is constant almost everywhere. To avoid numerical difficulties with a vanishing ζ the maximum of the two quantities in (14) is taken. The median is computed in $\mathcal{O}(k \log k)$ operations for a vector of length k and can be updated now and then during the integration.

3.1 A Riemann problem in one dimension

The Euler equations of gas dynamics are solved in a shock tube with initial data consisting of two constant states.

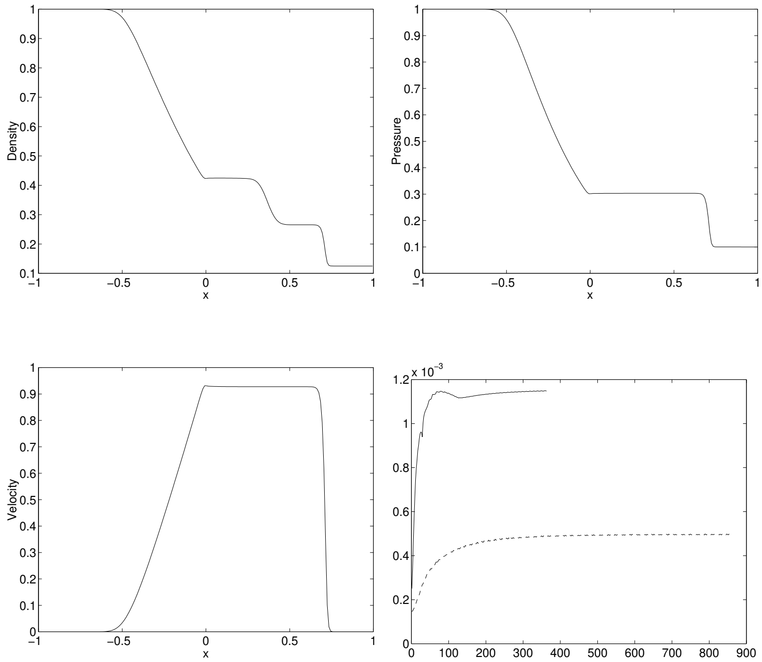


Figure 1: *The Riemann solution (15), (17), and time steps with filtered error (solid) and default control (dashed).*

The equations are

$$\begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (e+p)u \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \tag{15}$$

where ρ is the density, u is the speed, p is the pressure, and e is the total energy. The equations are closed by the relation

$$p = (\gamma - 1)(e - \frac{1}{2}\rho u^2), \tag{16}$$

in which the gas constant $\gamma = 1.4$. We take the initial solution

$$\mathbf{u}^0(x) = \begin{cases} (1,\ 0,\ 2.5)^T & x < 0 \\ (0.125,\ 0,\ 0.25)^T & x \geq 0 \end{cases}, \tag{17}$$

proposed by Sod [9]. This is a Riemann problem and the solution is a rarefaction wave propagating to the left and a shock and a contact discontinuity moving to the right. If we integrate (15) with the P-version of the Osher scheme [8] with $h = 1/200$ until $t = 0.4$, then we arrive at the result in Figure 1. The number of steps needed is significantly reduced and the cost of the filter is negligible in each step. It is found in [5] that the gain with the filter increases when h decreases. Also the number of rejected steps is much lower for a filtered local error estimate.

A comparison between a solution computed with the local error estimate and the filtered estimate is made. The result is that for (17) with $\varepsilon = 10^{-4}$ we have $\|\mathbf{u}(0.4) - \mathbf{u}_f(0.4)\|_\infty \approx 5.3 \cdot 10^{-5}$, where $\mathbf{u}_f$ is the filter solution. The dominant part of the difference is concentrated to the shock. The agreement is much better in the rest of the domain. It does not seem to be necessary for the performance to exclude the discontinuities in the first derivative in the beginning and the end of the rarefaction.

Another similar shock problem is solved in [5] with the same accuracy and the same increase in the length of the time steps.

3.2 Burgers' equation in two dimensions

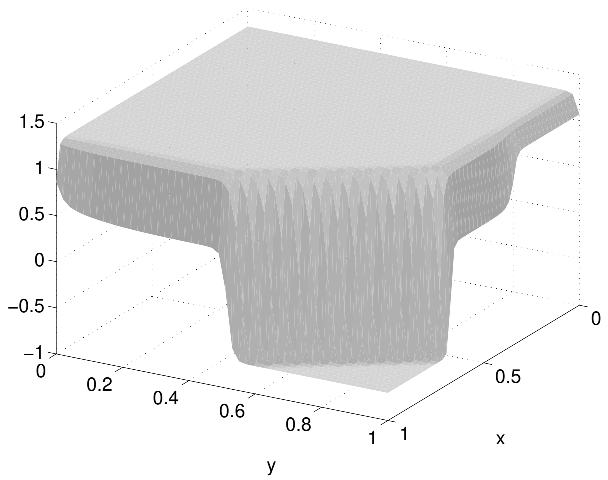


Figure 2: *Solution to Burgers' equation in 2D at $t = 1$.*

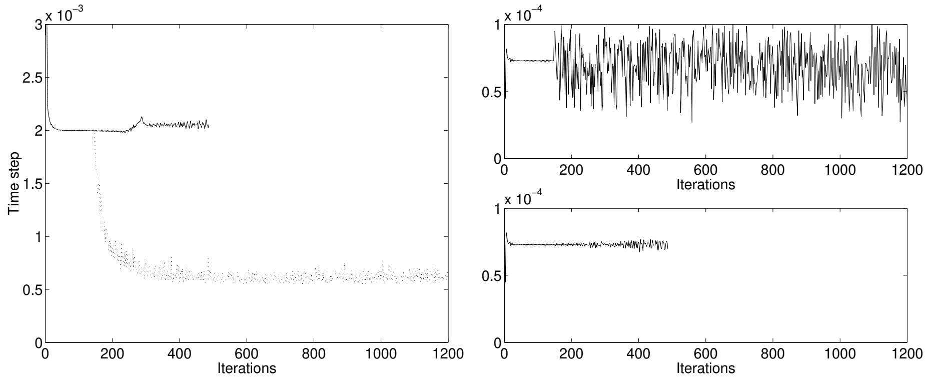
The 2D inviscid Burgers equation

$$u_t + \left(\frac{u^2}{2}\right)_x + \left(\frac{u^2}{2}\right)_y = 0 \tag{18}$$

is solved with the Engquist-Osher scheme [1] applied in each space dimension separately. The computational domain is $[0, 1] \times [0, 1]$ and the initial and boundary data are

$$\begin{cases} u(x, y, 0) = \cos(\pi(0.6x + 0.4y)) + 0.3, \\ u_x(0, y, t) = u_x(1, y, t) = 0, \\ u_y(x, 0, t) = u_y(x, 1, t) = 0. \end{cases} \tag{19}$$

The solution is a shock travelling slightly off-diagonally towards $(1, 1)$ (see Figure 2). The filter is extended to 2D by using the norm of the gradient instead of the absolute value of the slope as the discontinuity sensor in (13).



(a) Time steps, with filter (solid) and without (dotted)

(b) Error estimates, with filter (below) and without (above)

Figure 3: *Solving Burgers' equation in 2D.*

Figure 3 shows the result when integrating from $t = 0$ to $t = 1$ with $\varepsilon = 10^{-4}$ and a space discretization $h = 1/100$ in both directions. When the shock begins to form, the unfiltered error forces the time step down to approximately 1/3 of the previous average value, whereas the filtered error lets the controller proceed with essentially the same time step as before. We can also see that the filtered error itself behaves much more smoothly than its unfiltered counterpart.

References

[1] B. Engquist, S. Osher One-sided difference approximations for nonlinear conservation laws, *Math. Comp.*, 36 (1981), 321–351.

[2] S. Gottlieb, C.-W. Shu, Total variation diminishing Runge-Kutta schemes, *Math. Comp.*, 67 (1998), 73–85.

[3] K. Gustafsson, Control theoretic techniques for stepsize selection in explicit Runge-Kutta methods, *ACM Trans. Math. Software*, 17, (1991), 533–554.

[4] E. Hairer, S. P. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I - Nonstiff Problems*, 2nd ed., Springer-Verlag, Berlin, 1993.

[5] K. Hörnell, *Runge-Kutta time step selection for flow problems*, PhD thesis, Uppsala Dissertations 16, Faculty of Science and Technology, Uppsala University, Uppsala, Sweden, 1999.

[6] P. Lax, B. Wendroff, Systems of conservation laws, *Comm. Pure Appl. Math.*, XIII (1960), p. 217–237.

[7] R. LeVeque, *Numerical Methods for Conservation Laws*, Birkhäuser, Basel, 1992.

[8] S. Osher, F. Solomon, Upwind difference schemes for hyperbolic systems of conservation laws, *Math. Comp.*, 38 (1982), 339–374.

[9] G. Sod, A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws, *J. Comput. Phys.*, 27 (1978), 32–78.

[10] G. Söderlind, The automatic control of numerical integration, *CWI Quarterly*, 11 (1998), 55–74.

[11] B. P. Sommeijer, L. F. Shampine, J. G. Verwer, RKC: An explicit solver for parabolic PDEs, *J. Comput. Appl. Math.*, 88 (1997), 315–326.