Techniques for Locally Adaptive Time Stepping Developed over the Last Two Decades

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Adaptive mesh refinement techniques are well established and widely used for space 7 discretizations. In contrast, local time stepping is much less used, and the corre- 8 sponding techniques are less mature, needing delicate synchronization steps, which 9 involve interpolation, extrapolation or projection. These operations can have adverse 10 effects on the stability, and can also destroy important geometric properties of the 11 scheme, like for example the conservation of invariants. We give here a survey on 12 the intensive research performed in this direction over the last two decades. 13

1 Methods from the ODE Community

Local time stepping started in the ODE community with the development of split 15 Runge-Kutta methods with Rice [34]. Nowadays called multirate Runge-Kutta meth- 16 ods, these methods were first developed for naturally split systems of ordinary dif- 17 ferential equations y' = b(y, z, t) and z' = c(y, z, t), in which the z components need 18 to be integrated on a finer time mesh than the y components. One then uses a Runge- 19 Kutta method for the fast, so called active components with a small time step, and 20 another one for the slow, so called latent components, with a large time step, and uses 21 either interpolation or extrapolation for the missing values, depending on which of 22 the components are computed first, see [27]. 23

Multirate time integration methods were also proposed for linear multistep meth- 24 ods in [22], with two main approaches: fastest-first and slowest-first. Suppose an 25 implicit linear multistep method is used. In the fastest-first approach, one advances 26 the z components with small time steps h, and whenever one needs a component of 27the slow part y, one uses a predictor step for it. Once the fine stepping scheme arrives 28 at a coarse step H, the slow solution component y is also computed. The major disad- 29 vantage of this approach is that it is very difficult to do adaptive time stepping. This 30 is easier in the slowest-first approach, where first the slow component is doing an 31 adaptive integration step, until one is accepted with step size H. Then the adaptive 32 fine integration is tried with small steps h, until one reaches with several accepted 33 small steps the coarse level H. For the slow adaptive step H however, one needs also $_{34}$

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an approximation of the fast component for coupled components, and the authors in 35 [22] say: "There are several possible ways to control the fast extrapolation error, none 36 of which is entirely satisfactory". The stability properties of such multirate schemes 37 were analyzed in [35] for Backward Euler multirate schemes; see also [23]. 38

In contrast to the multirate methods, multirate extrapolation methods aim at 39 integrating systems of ODEs without a priori knowledge of which components need 40 finer time integration steps than others. A method based on Richardson extrapolation 41 was proposed in [13]: one computes approximations for all components for a time 42 step sequence $\{h_1, h_2, h_3, \ldots\}$, e.g. $h_2 = \frac{h_1}{2}$, $h_3 = \frac{h_1}{3}$, ..., and then builds the Richard- 43 son extrapolation table. As soon as a component has reached the desired accuracy 44 at step h_k (an error estimate is available automatically in the Richardson table), 45 extrapolation for this component is marked inactive, and only components needing 46 further accuracy continue the extrapolation. Inactive components must then however 47 be approximated in order for the extrapolation to continue. Using interpolation from 48 the continuous approximation obtained from the Richardson extrapolation can com- 49 pletely destroy the extrapolation process, which is based on the same error expansion 50 for all the components. The authors in [13] propose instead an elegant approximation 51 from the asymptotic expansion assumption itself, and also introduce a defect control 52 to avoid that inactivation fails in certain situations. 53

2 Methods from the PDE Community

Local time stepping schemes in the PDE community started with experimental work, 55 see for example [28]. Such ad hoc solutions were quite different for parabolic and 56 hyperbolic PDEs. 57

Hyperbolic Problems: a first complete mathematical analysis of two space-time 58 adaptive schemes for the wave equation $u_t = u_x$, an interpolation based variant, and 59 the so called coarse mesh approximation method were given by Berger [2] (see also 60 [3], and an early analysis for a different technique based on finite volumes in [31]). 61 Using for example a three point explicit scheme, the interpolation based approach 62 starts with a coarse step at the interface, shown in red in Fig. 1 on the left, followed 63 by an interpolation for the fine grid values, shown in blue. In the coarse mesh approximation, one uses the coarse spatial mesh to compute small time steps Δt , $2\Delta t$, 65 $3\Delta t$,... at the interface, instead of interpolating these values, as indicated in Fig. 1 on 66 the right for the second step $2\Delta t$ in red, where the blue value at Δt has already been 67



Fig. 1. Interpolation based approach on the *left*, and the coarse mesh method on the *right*

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Fig. 2. First energy-preserving local time stepping for the wave equation on the *left*, and symplectic scheme for Maxwell's equation on the *right*

computed. The author proves for the hyperbolic model problem $u_t = u_x$ that both 68 approaches are stable for the Lax-Wendroff scheme, but stability for the Leapfrog 69 scheme can only be achieved with overlap. Elegant recursive versions of such algo-70 rithms are in [33].

A key new ingredient to obtain stability for a Leapfrog type scheme for the 72 locally adaptive solution of the wave equation can be found in the seminal papers 73 by Collino et al. in [7, 8]: the introduction of a discrete energy conservation. In pre-74 sentations, this approach was always introduced with an impressive movie, where a 75 wave passes a locally refined patch, and everything looks fine for quite a long time 76 after the wave has passed, until suddenly an instability forms at the boundary of the 77 patch, and the numerical solution explodes, if a simple interpolation based scheme 78 is used. The method was first described for the 1d Maxwell system $u_t + v_x = 0$, 79 $v_t + u_x = 0$, which is equivalent to the 1d second order wave equation $u_{tt} = u_{xx}$, and 80 can best be described with the original picture from [7] shown in Fig. 2 on the left. 81 Thinking just about the second order wave equation, discretized with a centered finite difference scheme both in space and time, we get the five point star, well visible 83 with the black squares in Fig. 2 (the triangles would be for the unknowns v we do not 84 consider here). Now all points can be computed with this star at time levels t^{2n+1} and 85 t^{2n+2} , given the values at earlier time levels, except for the values in the dashed box. 86 The key idea of the energy preserving scheme is now to permit two different values 87 at x = 0 at even time levels t^{2n} , and to introduce as additional equation the discrete 88 energy, which needs to be preserved. This leads naturally to a stable scheme, but it 89 requires the solution of a small linear system at the interface. Energy conservation 90 turned out to be a key tool for stability analysis, and is used now for other space-91 time adaptive methods, see for example [11], where the authors introduce an unusual 92 energy, in order to analyze the stability of their space-time locally adaptive scheme. 93

A very elegant way of generalizing a symplectic integrator (which naturally pre- $_{94}$ serves a nearby energy) for variable step size integration was presented in [26], and $_{95}$ adapted to Maxwell's system in [32]. The Störmer-Verlet scheme is symplectic for $_{96}$ these equations, and is shown in Fig. 2 on the right. Without refinement, the scheme $_{97}$ is visible in the right part under H_2, E_2 : we see that first a half step denoted by 4 $_{98}$ is performed for the magnetic field H, followed by a full step denoted by 5 for the $_{99}$ electric field E, and concluded by a second half step for H denoted by 6. In each of $_{100}$ these steps, the Störmer-Verlet scheme uses for H the newest values available from $_{101}$

the other field E, and vice versa. It turns out that doing the same over the locally ¹⁰² refined region shown in Fig. 2 on the right, and performing the steps in the given ¹⁰³ order, starting with 1 and ending with 9, and using each time the newest information ¹⁰⁴ available, is still symplectic! Since symplectic schemes preserve a nearby energy, ¹⁰⁵ this scheme has all the good stability properties needed. ¹⁰⁶

In a finite volume or discontinuous Galerkin in the time domain setting (DGTD), 107 on unstructured meshes in space, the scheme in each subdomain with given time step 108 can be advanced until the new time value reaches that of its neighbor, according to 109 the stability constraint, see [12] for elastodynamics computations in the context of 110 ADER methods (Arbitrary high order, using high order DERivatives of polynomials). 111

Parabolic Problems are often integrated using implicit methods, which require 112 the solution of large systems of equations. These systems are obtained using the 113 same time step over the entire domain, and it is thus a priori not possible to use a 114 local time step. The first ideas to change this are based on domain decomposition 115 methods, where then interface values have to be predicted in some way, before the 116 subdomain problems are advanced in time by an implicit method. 117

A first interesting way to explicitly predict the interface values appeared in [9], 118 where a third spatial discretization size H is introduced, in addition to h_l and h_r , see 119 Fig. 3 on the left. The method then first does an explicit prediction step over the big 120 Δt , stable because the corresponding spatial step H is big, as indicated in red. This 121 is followed by interpolation (in blue) to obtain all needed values at the interface, and 122 then on each side one can do implicit solves to advance the method. It is proved in 123 [9] that this scheme is stable for the heat equation with a centered finite difference 124 discretization in space, and forward/backward Euler in time, if $\Delta t \leq \frac{1}{2}H^2$, and the 125 error satisfies the estimate max $|err| \leq C(h_l^2 + h_r^2 + H^3 + \Delta t_l + \Delta t_r + H\Delta t)$, which 126 shows impressively that the big prediction step Δt , H only affects the accuracy in 127 higher order terms!

A different approach was proposed by Blum et al. [4], as shown in Fig. 3 on the 129 right. The authors do not consider local refinement in time and space, their main 130 interest is to break up a large linear system from the implicit time integration into 131 smaller ones, but their idea can also be used for local adaptation in time and space. 132 The key idea is to use overlap, predict all values needed at the interfaces using a 133 higher order extrapolation method, and then solve implicitly on the corresponding 134 subdomains to advance the method. The authors prove for the heat equation without 135



Fig. 3. Explicit prediction of the interface values on an intermediate spatial grid on the *left*, and by extrapolation with overlap on the *right*



Fig. 4. A completely general space time mesh on the *left*, and the one-way and two way approaches on the *right*

local refinement, $h_l = h_r = h$ and $\Delta t_l = \Delta t_r = \Delta t$, that the Crank-Nicolson scheme 136 is stable, provided that $\Delta t \leq C \left(\frac{L}{\log L}\right)^2 h^2$, where *Lh* is the overlap, and an error esti-137 mate of the form $O(\Delta t^2 + h^2)$. So here increasing the overlap can lessen the stability 138 constraint on the time step. 139

If one wants to avoid any time step constraints, one can perform the coupling 140 fully implicitly, as proposed in [16]. Here, one simply writes the implicit scheme on 141 the fine and coarse subdomain, and the interpolation conditions into one big system 142 of linear equations, which is then solved. The authors show for a linear advection 143 reaction diffusion equation that a standard centered scheme with backward Euler in 144 time is unconditionally stable, and satisfies for $\Delta t = O(h)$ the error estimate $O(\Delta t + 145 h^2)$ in 1d, but in 2d there is a loss of $|\log h|^{\frac{1}{2}}$, and in 3d a loss of $\frac{1}{\sqrt{h}}$ in accuracy.

A more general approach based on domain decomposition can be found in [17]. 147 For the heat equation $u_t = u_{xx}$, and the decomposition of the domain $\Omega = (-1, 1)$ 148 into two subdomains $\Omega_1 = (-1, 0)$ and $\Omega_2 = (0, 1)$, the authors propose to discretize 149 the coupling conditions $u_1(0) = u_2(0)$, $\partial_x u_1(0) = \partial_x u_2(0)$ using a conservative finite 150 volume discretization over non-matching time grids. They also obtain, for each vari-151 ant of the method, a very large system of equations to solve, but propose to solve it using one or several steps of an iterative Dirichlet-Neumann algorithm. They show 153 that these schemes are conservative, provided one stops the iteration after a Neumann 154 step, and satisfy an error estimate $O(\Delta t + h)$ under certain conditions. One can show 155 that one of their methods corresponds to the approach in [16].

Space-Time Finite Element Methods consider the time direction like one of the 157 spatial directions, and discretize the problem directly in space-time by a finite element method, which leads to a large discrete problem in space-time. These methods 159 have their roots in the work of C. Johnson and co-authors, see for instance [15] for 160 a review. Discontinuous Galerkin methods were used, and the adaptation was done 161 through a posteriori estimates. In the first versions of the method, the space-time 162 finite elements were still special, since they always had boundaries in time aligned 163 with the time direction, for example prisms. Completely general triangular meshes 164 in space time require special meshing techniques, since they need to satisfy certain 165 angle constraints, in order to avoid total global coupling in space-time, see [36] for 166 applications to Burger's equation and elastodynamics. An impressive example of 167 such a mesh from [14] is reproduced in Fig. 4 on the left. A very recent contribution 168 using discontinuous Galerkin methods can be found in these proceedings, see [30]. 169

One-Way and Two-Way Methods are in principle very different from all the 170 methods we considered earlier, since they have both a coarse *and* a fine mesh in parts 171 of the domain. They have their roots in weather and climate simulations, which of-172 ten use a global model over a large region, for example the entire planet, and then 173 refined models over a small region, for example a country. The question is then how 174 to compute a refined solution based on the solution of the global coarse problem. In 175 [10] and [6], the so called one-way (or "offline") and two-way (or "online") methods are proposed. In the one-way method, the coarse model is first solved once and 177 for all, and stored. Then boundary data is extracted to be imposed on the boundary 178 of the smaller refined region. The simplest approach is to use Dirichlet conditions, 179 which can however lead to large errors. A more refined approach is to use so called 180 open boundary conditions, which are related to absorbing boundary conditions, but 181 different, see [6, 29]. Open boundary conditions lead in general to substantially more 182 accurate fine models. In the two way approach, one only performs one or a few time 183 steps of the coarse model, then solves the fine model in the refined region as before, 184 but updates the coarse result whenever a more accurate fine result is available, before 185 continuing the next coarse time step, see Fig. 4 on the right. If one simulates only one 186 time step of the coarse model before solving the fine model and uses Dirichlet condi-187 tions, this approach is very much related to the first approach for hyperbolic problems 188 described earlier. 189

Schwarz waveform relaxation methods are the most flexible methods for solv- 190 ing evolution problems locally adaptively in space time, since they permit not only 191 refined time steps, but even different numerical methods, or different models in dif- 192 ferent regions. They were first described in [20] and are based on a decomposition 193 in space of the domain over which the evolution problem is posed and a subdomain 194 iteration in space-time: starting with an initial guess on each space-time interface 195 between subdomains, on each subdomain the evolution problem is solved over an 196 entire so called time window. Then information is exchanged between subdomains 197 using transmission conditions, and the subdomain problems are solved again and 198 again until a suitable matching is reached. So the price to pay for this flexibility and 199 generality is the iteration. The method from [17] we have seen earlier is in this class 200 of methods, but much faster convergence can be obtained when optimized transmis- 201 sion conditions are used, see [1, 18, 21, 24, 25], and references therein. Very general 202 non-matching space-time grids can be coupled like this using a projection algorithm 203 with optimal linear complexity from [19]. For recent realistic applications in a com- 204 plex setting, see [5]. 205

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