



Bergische Universität Wuppertal

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Mathematics (IMACM)

Preprint BUW-IMACM 19/12

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Multirate Schemes

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April 9, 2019

<http://www.math.uni-wuppertal.de>

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An Answer of Numerical Analysis to a Demand from Applications

Andreas Bartel and Michael Günther

Abstract In science and engineering, simulation tasks often involve numerical time integration of differential equations. Usually, these systems contain different time constants of the involved components and/or right-hand side. This multirate behavior may be caused by coupling subsystems in multiphysics problems acting on different time scales. Such a behavior does already occur if one deals with just single-physics problems: for example, in mechanical systems the equations of motion may depend on weak and strong forces, which demand to sample these forces with different frequencies to gain the same rate of approximation; another example is given by electrical network equations, where the activity level of components may strongly vary depending on the signal structure within the network.

To be efficient, or even enable the simulation in many fields of application, numerical integration schemes have to be adapted to exploit this multirate behavior. One idea proposed by Rice in 1960 are multirate schemes, which use different step sizes adapted to the various activity levels. In the last 50 years, the methodology of numerical time integration schemes has been advanced in a constant interplay between the demands defined by the need of exploiting multirate behavior in different fields of applications and the development of tailored multirate schemes to answer these demands.

1 Introduction

In many technical applications, ranging from electric circuits to multibody systems and in particular for multiphysics simulation, the governing set of differential equations is characterized by a multirate behavior in time domain: that is to say, some parts of the right-hand side follow a fast dynamics, whereas the other parts are char-

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acterized by a respectively slow dynamics. To be efficient, a numerical (time) integration scheme needs to exploit this multirate potential.

For the moment, let us consider the case of an initial-value problem of ordinary differential equations

$$\dot{w} = h(t, w), \quad w(t_0) = w_0 \quad (1)$$

with $h : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ assumed to be Lipschitz continuous in w . We denote the unique solution of (1) at time point t by $w(t; w_0)$. Furthermore, we assume that in h we have some multirate potential, i.e., some coordinates or a summands of h are slower than some remaining ones.

On the one hand, the interpretation of fast and slow coordinates in h leads to a partitioning of the unknowns $w^\top = (y_S^\top, y_F^\top)$ in slow $y_S(t) \in \mathbb{R}^m$ and fast components $y_F(t) \in \mathbb{R}^{n-m}$. In this way, the ODE (1) is transferred to a partitioned system:

$$\begin{aligned} \dot{y}_S &= f_S(t, y_S, y_F), & y_S(t_0) &= y_{S,0}, \\ \dot{y}_F &= f_F(t, y_S, y_F), & y_F(t_0) &= y_{F,0}, \end{aligned} \quad (2)$$

with corresponding slow right-hand side $f_S : \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^{n-m} \rightarrow \mathbb{R}^m$ and fast right-hand side $f_F : \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^{n-m} \rightarrow \mathbb{R}^{n-m}$. This is termed as *component-wise partitioning*. On the other hand, one can split the right-hand side:

$$\dot{w} = h_s(t, w) + h_f(t, w), \quad w(t_0) = y_0 \quad (3)$$

into slow and fast terms. This induces an additive splitting of the unknown $w = w_s + w_f$ into slow and fast varying parts w_s and w_f . This is referred to as *right-hand side partitioning*. Note that both formulations are equivalent in the sense that each component-wise partitioned system can be rewritten as a right-hand side partitioned system and vice versa.

Multiorde r as multirate. There are many ways to exploit multirate behavior in such systems. One idea is to use multi-order methods. Here a single method with a single step size is employed for the whole system. To adapt to the activity level, the order of the method is modified accordingly. This class comprises, for example, the schemes MURX [16] and MUR8 [15] by Engstler and Lubich. The first method (MURX) is based on Richardson extrapolation of the explicit Euler scheme. Thereby the computation of extrapolation tableau is stopped if a component is accurate enough. The latter MUR8 uses low-order methods embedded in high-order method, where the update of the slow components is deactivated after a first few function evaluations.

Multiple step sizes as multirate. To our knowledge, the first method based on exploiting multirate behavior by adapting step sizes to the activity level of components was derived by Rice [31] in 1960 for missile simulations. This method is based on Runge-Kutta schemes and employs a so-called compound step. Later, Gear and Wells [20] proposed an alternative approach based on linear multistep methods as well as extrapolation and interpolation.

The work at hand focuses on the multiple step size approaches. In Section 2, we discuss the ideas of Rice and Gear/Wells. The class of extra- and interpolation coupling

is strongly linked to waveform relaxation or dynamic iteration schemes, which we treat in Section 3. In fact, dynamic iteration enables the application the general application to multiphysics systems. Subsequently, we treat some applications. Section 4 covers electric circuits simulation, where the compound-step approach has been successfully applied to develop multirate strategies for single-physics problems. Then molecular dynamics is discussed in Section 5, in which multirate potential has to be exploited, but at the same time geometric structures have to be preserved, operator splitting has turned out to be the right framework for developing application-tailored multirate schemes.

2 Strategies for Multirate and Convergence

Before discussing in details the methods by Rice [31] as well as by Gear and Wells [20], we first focus on the common idea behind these approaches: the combination of basic numerical integration schemes with extra- and interpolation techniques to solve (2) with a small step size h for the fast variable z and large step size $H = M \cdot h$ for the slow y . Here, the multirate factor is a fixed number $M \in \mathbb{N}$.

2.1 Combining extra- and interpolation for multirate properly

We have the following main result:

Theorem 1. *We consider (2) with both right-hand sides f and g Lipschitz continuous in both variables y_S and y_F . Furthermore, we consider an arbitrary macro step from $\bar{t} \rightarrow \bar{t} + Mh$ and respective initial values $y_S(\bar{t}) = y_{S,\bar{t}}, y_F(\bar{t}) = y_{F,\bar{t}}$. Let be a fixed multirate factor $M \in \mathbb{N}$ be given and two integration schemes of order p be applied: a first scheme for one macro step of size $H = M \cdot h$ for the slow y_S and a second scheme is applied for M steps of size h for fast y_F . If we use an integration scheme of order p and combine this with an extra- and interpolation procedure of order $p - 1$, the overall scheme has order p .*

Proof. For the coupled system (2) with initial data $y_S(\bar{t}) = y_{S,\bar{t}}, y_F(\bar{t}) = y_{F,\bar{t}}$, we refer to the unique solution by $(y_S(t; y_{S,\bar{t}}, y_{F,\bar{t}})^\top, y_F(t; y_{S,\bar{t}}, y_{F,\bar{t}})^\top)$. Now, we replace the coupled system (2) by a modified system which decouples both parts:

$$\begin{aligned} \dot{y}_S &= f_S(t, y_S, \tilde{y}_F) =: \tilde{f}_S(t, y_S), & y_S(\bar{t}) &= y_{S,\bar{t}}, \\ \dot{y}_F &= f_F(t, \tilde{y}_S, y_F) =: \tilde{f}_F(t, y_F), & y_F(\bar{t}) &= y_{F,\bar{t}}, \end{aligned} \quad (4)$$

where \tilde{y}_S and \tilde{y}_F are extra-/interpolations of order $p - 1$, i.e.,

$$y_S(t) - \tilde{y}_S(t) = \mathcal{O}(H^p) \quad \text{and} \quad y_F(t) - \tilde{y}_F(t) = \mathcal{O}(h^p) \quad \text{for any } t \in [\bar{t}, \bar{t} + Mh]. \quad (5)$$

We denote the unique solution of (4) by $(\hat{y}_S(t; y_{S,\bar{t}}, y_{F,\bar{t}})^\top, \hat{y}_F(t; y_{S,\bar{t}}, y_{F,\bar{t}})^\top)$.

Next, we solve the decoupled system (4) with two numerical integration schemes of order p , with M step sizes h applied to z and one step size $H = M \cdot h$ applied to y . The numerical solution obtained at $t^* = \bar{t} + Mh$ is denoted by $(y_{S,H}(t^*), y_{F,H}(t^*))^\top$. For the difference between the numerical multirate approximation and the exact solution at t^* , the triangle inequality yields

$$\begin{pmatrix} \|y_{S,H}(t^*) - y_S(t^*)\| \\ \|y_{F,H}(t^*) - y_F(t^*)\| \end{pmatrix} \leq \begin{pmatrix} \|y_{S,H}(t^*) - \widehat{y}_S(t^*)\| \\ \|y_{F,H}(t^*) - \widehat{y}_F(t^*)\| \end{pmatrix} + \begin{pmatrix} \|\widehat{y}_S(t^*) - y_S(t^*)\| \\ \|\widehat{y}_F(t^*) - y_F(t^*)\| \end{pmatrix}. \quad (6)$$

The first term on the right-hand side represents the error of the applied integration schemes. Employing for both coordinates an integration scheme of order p , with one macro step of size $H = M \cdot h$ for the slow y_S and M steps of size h for fast y_F , we have

$$\begin{pmatrix} \|y_{S,H}(t^*) - \widehat{y}_S(t^*)\| \\ \|y_{F,H}(t^*) - \widehat{y}_F(t^*)\| \end{pmatrix} \leq \begin{pmatrix} c_S \\ c_F \\ M^{p+1} \end{pmatrix} H^{p+1} \quad (7)$$

with leading error coefficients respective leading error coefficients c_S and c_F .

For the second term on the right-hand side (6), we get from the Lipschitz continuity of f_S, f_F with corresponding constants ($L_{i,j}$ for f_i w.r.t. y_j)

$$\begin{aligned} \begin{pmatrix} \|\widehat{y}_S(t^*) - y_S(t^*)\| \\ \|\widehat{y}_F(t^*) - y_F(t^*)\| \end{pmatrix} &\leq \int_{\bar{t}}^{t^*} \begin{pmatrix} \|f_S(\tau, \widehat{y}_S(\tau), \widetilde{y}_F(\tau)) - f_S(\tau, y_S(\tau), y_F(\tau))\| \\ \|f_F(\tau, \widetilde{y}_S(\tau), \widehat{y}_F(\tau)) - f_F(\tau, y_S(\tau), y_F(\tau))\| \end{pmatrix} d\tau \\ &\leq \int_{\bar{t}}^{t^*} \begin{pmatrix} L_{S,S} \|\widehat{y}_S(\tau) - y_S(\tau)\| + L_{S,F} \|\widetilde{y}_F(\tau) - y_F(\tau)\| \\ L_{F,S} \|\widetilde{y}_S(\tau) - y_S(\tau)\| + L_{F,F} \|\widehat{y}_F(\tau) - y_F(\tau)\| \end{pmatrix} d\tau \end{aligned}$$

actually a decoupled estimate. Using that \widetilde{y}_S and \widetilde{y}_F are approximation of order $p-1$ (5) and respective Lipschitz constants L_S, L_F of the corresponding extra-/interpolation operators, we find

$$\begin{pmatrix} \|\widehat{y}_S(t^*) - y_S(t^*)\| \\ \|\widehat{y}_F(t^*) - y_F(t^*)\| \end{pmatrix} \leq \begin{pmatrix} \frac{L_{S,F} L_F}{M^p} H^{p+1} + L_{S,S} \int_{\bar{t}}^{t^*} \|\widehat{y}_S(\tau) - y_S(\tau)\| d\tau \\ L_{F,S} \cdot L_S \cdot H^{p+1} + L_{F,F} \int_{\bar{t}}^{t^*} \|\widehat{y}_F(\tau) - y_F(\tau)\| d\tau \end{pmatrix}$$

Applying Gronwall's lemma, it follows:

$$\begin{pmatrix} \|\widehat{y}_S(t^*) - y_S(t^*)\| \\ \|\widehat{y}_F(t^*) - y_F(t^*)\| \end{pmatrix} \leq \begin{pmatrix} \frac{L_{S,F} L_F}{M^p} e^{L_{S,S}(t^* - \bar{t})} H^{p+1} \\ L_{F,S} L_S e^{L_{F,F}(t^* - \bar{t})} H^{p+1} \end{pmatrix}.$$

Finally combining this with the integration error (7) into the split error (6), we obtain that the multirate scheme has consistency order p for the compound step from \bar{t} to $\bar{t} + Mh$ (on the macro step level). \square

Remark 1. a) The method implicitly defined in Theorem 1 is referred to as *extrapolation/interpolation-based multirate scheme*.

b) Notice for a working multirate scheme, we still have to define the extrapolation/interpolation routines. Furthermore, arbitrary high orders of the extra-/interpolation are not possible in the one-step-method context.

Corollary 1. *Under the assumptions of Thm. 1, we have an overall multirate scheme of convergence order p if*

- a) *we use one-step integration schemes.*
- b) *we use multistep schemes, where both schemes are 0-stable.*

Summing up, the art of defining multirate (multistep) schemes lies in implicitly defining the extrapolation and interpolation procedures used within the scheme to be of high enough order.

Corollary 2. *We consider the following initial values problem (IVP)*

$$\begin{aligned} \dot{y}_S &= f_S(t, y_S, y_F, z_S, z_F), & y_S(t_0) &= y_{S,0}, & \dot{y}_F &= f_F(t, y_S, y_F, z_S, z_F), & y_F(t_0) &= y_{F,0}, \\ 0 &= g_S(t, y_S, y_F, z_S, z_F) & & & 0 &= g_F(t, y_S, y_F, z_S, z_F) \end{aligned}$$

of coupled semi-explicit DAEs with slow subsystem (y_S, z_S) and fast subsystem (y_F, z_F) . Provided that the overall system is index-1 and both subsystems are index-1 with Lipschitz continuous f_λ, g_λ ($\lambda \in \{S, F\}$) with uniform Lipschitz constants on any macro step $[\bar{t}, \bar{t} + Mh]$ in $[t_0, T]$. Applying a multirate method, which is for coupled ODEs of order p (Thm. 1) and the algebraic variables z_S, z_F are always consistently computed (i.e., implicit), then the method has still order p .

Proof. The proof is a direct consequence of the recursion estimate Lemma 3.1 in [2] for dynamic iteration schemes of coupled index-1 DAE systems, if only one iteration is considered and the initial iteration error is given by the extrapolation/interpolation error. \square

2.2 Linear multistep methods

How to define the extrapolated and interpolated approximations? Linear multistep schemes are based on polynomial interpolation using information of possibly several previous steps. Here, these methods are advantageous over one-step schemes. This can be seen as follows: let us assume, we use a linear K -step scheme for the slow part, and a k -step scheme for the fast variables. Accordingly, the extrapolation can be based on K macro step approximations for the slow variable and k micro step values for and fast variables. This yields a global error of order $\min\{K, k\}$ (Thm. 1) if the respective schemes are at least of order K and k .

Based on preliminary work by Gear [19], Orailoglu [29] and Wells [47], the first comprehensive study and still fundamental work on multirate linear multistep methods was published in 1984 by Gear and Wells [20]. It covers efficiency considerations, convergence and error analysis, absolute stability and numerical test results

for an Adams-type based algorithm. In addition, there were the following concepts first introduced and discussed:

- Slowest-first method: first, one solves the slow part, using extrapolated information of the fast variables; then, the fast part is solved with interpolated information of the slow variables.
- Fastest-first method: here, one solves first the fast part, using extrapolated information of the slow variables; then, the slow part is solved with interpolated information of the fast variables.

At a first glance, the fastest first strategy seems to be advantageous. The extrapolation error in the computation of the fast part is acceptable, as one is extrapolating over an interval of size H , which is tailored to the activity level of the slow part. In the slowest first strategy, we are extrapolating the fast variables over many micro step h to compute the slow variables, which may only be tolerable if the coupling of the fast into the slow part, measured by $\|\partial f_S / \partial y_F\|$, is small. As a rule of thumb, this quantity will be usually small, as otherwise a high level of activity would be transferred from the fast into the slow part, and the slow part would not be slow anymore. Certainly, this is only a rule of thumb, since there exist — although academic — counterexamples [20].

However, considering an adaptive step sizes selection based on error control, the slowest first strategy can become advantageous. For instance, if a secondly performed macro step $[t, t + H]$ (slow variables) fails, the macro step size H has to be decreased and the computation has to be repeated. If the approximations of the micro steps (fast variable) are not stored (for instance, due to memory reasons) or if the computation of the fast variables is based on extrapolated values on the failed macro step size H_{old} , these values have to be recomputed. In contrast, the slowest first strategy does not introduce any problems: if an integration of the fast part fails, one only has to repeat it with a smaller step size. The necessary information to interpolate the slow part does not change. See [19, 20] for further details.

Remark 2. Some systems do not allow for a static partitioning into fast and slow subsystems (e.g. the inverter chain benchmark [22]). In these settings, slow components can become fast (wake up) and vice versa. This causes a rather large step size modification, which is more problematic for multistep methods, see e.g. [25], than for one-step schemes.

Remark 3. Other linear-multistep approaches have been discussed, for instance, by Verhouvern et al. [46] and [30] (both BDF-based), or by Sandu and Constantinecu (Adams-based) [32]. Stability issues have been addressed first by Skelboe [38] and by Skelboe and Andersen [39].

2.3 Runge-Kutta schemes

In one-step schemes, only information of the last step is available. This limits the approximation order to 1, as only constant or linear interpolation is available in the

multirate scheme with extra- or interpolation (cf. Thm. 1). Of course, the use of approximations at previous steps (in the extra- and interpolation) would turn the one-step scheme into a multistep scheme.

About twenty years before Gear's paper on multirate multistep schemes, Rice proposed a solution to overcome this problem for one-step schemes [31]: split Runge-Kutta schemes first make one large Runge-Kutta compound step with macro step size H for the joint system, but use only the result for the slow variables as approximates. To get the approximations for the fast part in all micro steps of the macro step, the slow part is then integrated using interpolated information of the slow variables based on the Runge-Kutta increments of the macro step. In 2008, this approach has been applied by Verhouvern to BDF schemes [46], see also Section 4.

We give some details for the split Runge-Kutta schemes [31] on system (2). The numerical approximation $y_{S,H}(t^*)$ is given by one explicit Runge-Kutta step from \bar{t} to $t^* = \bar{t} + H$:

$$\begin{aligned} y_{S,H}(t^*) &= y_{S,\bar{t}} + \sum_{i=1}^s b_i k_i, \\ k_i &= H f_S \left(\bar{t} + \sum_{j=1}^{i-1} a_{i,j} H, y_{S,\bar{t}} + \sum_{j=1}^{i-1} a_{i,j} k_j, y_{F,\bar{t}} + \sum_{j=1}^{i-1} a_{i,j} l_j \right), \quad (i = 1, \dots, s), \\ l_i &= H f_F \left(\bar{t} + \sum_{j=1}^{i-1} a_{i,j} H, y_{S,\bar{t}} + \sum_{j=1}^{i-1} a_{i,j} k_j, y_{F,\bar{t}} + \sum_{j=1}^{i-1} a_{i,j} l_j \right), \quad (i = 1, \dots, s), \end{aligned}$$

using internal stages l_i for the active part, which will not be used later on. This is referred to as compound step and it employs the coefficients $b_i, a_{i,j}$ with s stages.

Secondly, for the M micro-steps, another Runge-Kutta scheme with coefficients $\tilde{b}_i, \tilde{a}_{i,j}$ and \tilde{s} stages is used to compute $y_{F,H}(\bar{t}_i + lh)$ for y_F at micro grid points $\bar{t} + \lambda h$ for $\lambda = 1, \dots, M$:

$$\begin{aligned} y_{F,H}(\bar{t} + (\lambda + 1)h) &= y_{F,H}(\bar{t} + \lambda h) + \sum_{i=1}^{\tilde{s}} \tilde{b}_i k_i^\lambda, \quad (\lambda = 1, \dots, M - 1) \\ k_i^\lambda &= h f_F \left(\bar{t} + \lambda h + \sum_{j=1}^{i-1} \tilde{a}_{i,j} h, \hat{y}_S \left(\bar{t} + \lambda h + \sum_{j=1}^{i-1} \tilde{a}_{i,j} h \right), y_{F,H}(\bar{t} + \lambda h) + \sum_{j=1}^{i-1} \tilde{a}_{i,j} k_j^\lambda \right), \end{aligned}$$

($i = 1, \dots, \tilde{s}$). Hereby, the values $\hat{y}_S(\bar{t} + \lambda h + \sum_{j=1}^{i-1} \tilde{a}_{i,j} h)$ of the slow components at grid points $\bar{t} + \lambda h + \sum_{j=1}^{i-1} \tilde{a}_{i,j} h$ are approximated by a dense output of the Runge-Kutta approximation of the compound step, i.e.,

$$\hat{y}_S(\bar{t} + \theta H) := y_{S,\bar{t}} + \sum_{i=1}^s b_i(\theta) k_i,$$

such that it holds

$$\max_{0 \leq \theta \leq 1} \|\hat{y}(\bar{t} + \theta H) - y(\bar{t} + \theta H)\| \leq c_S H^{p-1}.$$

for all $0 \leq \theta \leq 1$ and some constant $c_S > 0$.

Remark 4. Note that the increments l_i according to y_F are only used within the computation of k_i . Consequently, for an explicit Runge-Kutta scheme, l_s does not have to be computed.

Remark 5. Other multirate one-step schemes have been developed and analyzed, for example, by Savcenco et al. [33] and by Günther and Rentrop [22], both based on Rosenbrock-Wanner methods (ROW), by Sandu and Günther [24] based on GARK methods, and by Striebel et al [40] based on ROW methods for index-1 DAE systems, and others.

2.4 Overview on multirate strategies

To conclude this section, we state two main multirate strategies exist for component-wise splitting:

- *Extra-/Interpolation based multirate schemes:* here, one computes the split variables one after the other. We have *slowest-first* and *fastest-first*, where the coupling variables are extrapolated or interpolated based on previously computed approximations. One may use any numerical integration scheme as basis scheme of such multirate schemes; the order of the scheme p is preserved provided that the extra-/interpolation is at least of order $p - 1$.
- *Compound-step based multirate methods:* here, slow and fast variables are jointly computed using one macro step (compound step); then, the fast approximation is disregarded and replaced by M micro steps using the fast dynamics and dense output of the slow variables (*compound-fast approach*).

As the dense output for the coupling term $y_S(t)$ is available on the whole macro step, one may discard the idea of using M micro steps of the same step size h and use the different step sizes according to the step size prediction of the numerical integration scheme. The latter approach, combined with the compound step, is called *mixed multirate* [4].

The *time stepping approach* introduced by Savcenco, Hundsdorfer and Verwer [33] is a generalization of the compound-step approach. First, an approximation for all components after one macro step is computed. For those components not accurate enough the computation is redone with smaller steps. The refinement is recursively continued until the error estimator is below a given tolerance for all components.

One criticism of this compound step approach is the use of the macro step size H also for the fast component y_F inside the computation of the new approximate for the slow variables y_S . One may overcome this problem by combining the macro step for the slow part with the first micro step of the active part (*generalized compound-step approach*). As micro and macro step are interwoven in this case, additional coupling conditions have to be fulfilled for the coefficients of one-step methods to preserve the order of the method for the slow components. This approach has been introduced

by Kværnø and Rentrop in [27] for Runge-Kutta schemes. Corresponding further methods are based on the W-method [9] or on generalized additive Runge-Kutta schemes [24].

If right-hand side splitting is concerned, operator splitting might be the method of choice. For the split system (3), the idea reads as follows: suppose that the slow dynamics h_s is characterized by an expensive evaluation, whereas the fast dynamics h_f can be cheaply evaluated. In this case, one may develop an operator splitting approach where the slow dynamics is solved only once on a macro step, and the fast systems M -times during one macro step. See Section 5 for some more details, in particular, in the context of geometric integration.

3 Dynamic Iteration and Multiphysics

Due to downscaling in electric devices and due to higher accuracy requests to numerical simulation, more and more coupled problems need to be studied and thus simulated for industrial applications. This gives naturally rise to multiphysics problems.

In modular time integration of such multiphysics problems, different subsystems are modeled and simulated by different simulation packages, see e.g. [11, 48, 3]. This allows to exploit the multirate potential, which is caused by different time scales of the subsystems, efficiently within a waveform relaxation approach. We describe this in the following.

To start with, we consider again the component-wise partitioned ODE (2), which comprises a slow subsystems in y_S and fast subsystem in y_F . Furthermore, we assume that the solution or an approximation $y_{S,H}, y_{F,H}$ is available on $[t_0, \bar{t}]$. The coupled initial value problem (2) can be solved iteratively on a time window $[\bar{t}, \bar{t} + H]$ employing old iterates ($i - 1$) and current iterates (i) and respective splitting functions F_S, F_F to encode usage of old and current iterates inside the coupled system. This reads:

$$\begin{aligned} \dot{y}_S^{(i+1)} &= F_S(t, y_S^{(i+1)}, y_S^{(i)}, y_F^{(i+1)}, y_F^{(i)}), & y_S^{(i+1)}(\bar{t}) &= y_S^{(0)}(\bar{t}), \\ \dot{y}_F^{(i+1)} &= F_F(t, y_S^{(i+1)}, y_S^{(i)}, y_F^{(i+1)}, y_F^{(i)}), & y_F^{(i+1)}(\bar{t}) &= y_F^{(0)}(\bar{t}), \end{aligned} \quad (8)$$

where the initial waveform $y^{(0)}, z^{(0)}$ are given by extrapolating from the previous time window:

$$\begin{pmatrix} y_{S,H} \\ y_{F,H} \end{pmatrix} \Big|_{[\bar{t}-H, \bar{t}]} \rightarrow \begin{pmatrix} y_S^{(0)} \\ y_F^{(0)} \end{pmatrix} \Big|_{[\bar{t}, \bar{t}+H]} := \Phi \left(\begin{pmatrix} y_{S,H} \\ y_{F,H} \end{pmatrix} \Big|_{[\bar{t}-H, \bar{t}]} \right).$$

Here, Φ denotes an extrapolation operator and let L_Φ be the respective Lipschitz constant. Furthermore the splitting functions shall fulfill Lipschitz conditions with respect to all components and are consistent, and the consistency with IVP (2):

$$F_S(t, y_S, y_S, y_F, y_F) = f_S(t, y_S, y_F) \quad \text{and} \quad F_F(t, y_S, y_S, y_F, y_F) = f_F(t, y_S, y_F).$$

Depending on the choice of the splitting functions, one may define different instants of waveform relaxation schemes: $Y = (t, y_S^{(i+1)}, y_S^{(i)}, y_F^{(i+1)}, y_F^{(i)})$

- Picard iteration:

$$F_S(Y) = f_S(t, y_S^{(i)}, y_F^{(i)}), \quad F_F(Y) = f_F(t, y_S^{(i)}, y_F^{(i)}).$$

- Jacobi-type iteration:

$$F_S(Y) = f_S(t, y_S^{(i+1)}, y_F^{(i)}), \quad F_F(Y) = f_F(t, y_S^{(i)}, y_F^{(i+1)}). \quad (9)$$

- Gauß-Seidel type iteration (slowest-first):

$$F_S(Y) = f_S(t, y_S^{(i+1)}, y_F^{(i)}), \quad F_F(Y) = f_F(t, y_S^{(i+1)}, y_F^{(i+1)}). \quad (10)$$

- Gauß-Seidel type iteration (fastest-first):

$$F_S(Y) = f_S(t, y_S^{(i+1)}, y_F^{(i+1)}), \quad F_F(Y) = f_F(t, y_S^{(i)}, y_F^{(i+1)}). \quad (11)$$

The iterates converge monotonically to the exact solution provided that the macro step size H is small enough.

If (9) is used, then both new iterates $y_S^{(i+1)}$ and $y_F^{(i+1)}$ in (8) can be computed in parallel, with extrapolation. If the exact integration of (10) or (11) is replaced by a numerical integration, the computation of the new iterates $y_S^{(i+1)}, y_F^{(i+1)}$ is equivalent to applying an extra-/interpolation based multirate scheme (to slow y_S and fast y_F component): (10) represents slowest-first and (11) fastest-first setting. And vice versa, extra-/interpolation based multirate is equivalent to stopping the iteration of the waveform-relaxation after the first step. See also Section 4 for further discussion. IVPs of coupled DAE systems (cf. Cor. 2)

$$\begin{aligned} \dot{y}_S &= f_S(t, y_S, y_F, z_S, z_F), & y_S(t_0) &= y_{S,0}, & \dot{y}_F &= f_F(t, y_S, y_F, z_S, z_F), & y_F(t_0) &= y_{F,0}, \\ 0 &= g_S(t, y_S, y_F, z_S, z_F) & & & 0 &= g_F(t, y_S, y_F, z_S, z_F) & & \end{aligned} \quad (12)$$

arise, for example, in circuit simulation or in electro-thermal coupling (see Section 4). A corresponding dynamic iteration scheme needs splitting functions F_L, G_L, F_A and G_A , which fulfill Lipschitz conditions with respect to all arguments and are consistent, i.e.,

$$\begin{aligned} F_\star(t, y_S, y_S, y_F, y_F, z_S, z_S, z_F, z_F) &= f_\star(t, y_S, y_F, z_S, z_F), \\ G_\star(t, y_S, y_S, y_F, y_F, z_S, z_S, z_F, z_F) &= g_\star(t, y_S, y_F, z_S, z_F) \quad \text{with } \star \in \{S, F\}. \end{aligned}$$

Then, the dynamic iteration scheme reads: for $\star \in \{S, F\}$

$$\begin{aligned}
y_*^{(i+1)} &= F_*(t, y_S^{(i+1)}, y_S^{(i)}, y_F^{(i+1)}, y_F^{(i)}, z_S^{(i+1)}, z_S^{(i)}, z_F^{(i+1)}, z_F^{(i)}), \\
0 &= G_*(t, y_S^{(i+1)}, y_S^{(i)}, y_F^{(i+1)}, y_F^{(i)}, z_S^{(i+1)}, z_S^{(i)}, z_F^{(i+1)}, z_F^{(i)}).
\end{aligned} \tag{13}$$

Again for the actual time window $[\bar{t}, \bar{t} + H]$, initial waveforms $y_L^{(0)}, y_A^{(0)}, z_L^{(0)}, z_A^{(0)}$ are given by extrapolation of the waveform approximates of the last window $[\bar{t} - H, \bar{t}]$. In contrast to coupled ODE systems, monotone convergence can no longer be guaranteed by choosing the window step size H small enough. In addition, one has to fulfill two additional contractivity conditions, see e.g. [3]). For the Gauss-Seidel type approaches, this reads:

- *Convergence within one window:*

$$\alpha < 1, \tag{14}$$

whereas the contractivity constant α is given by the sum of the Schur complement-like quantity

$$\max_{\tau, \text{ with } \bar{t} \leq \tau + \tau H \leq \bar{t} + H} \left\| \left(\begin{array}{cc} \frac{\partial G_S}{z_S^{(i+1)}} & \frac{\partial G_S}{z_F^{(i+1)}} \\ \frac{\partial G_F}{z_S^{(i+1)}} & \frac{\partial G_F}{z_F^{(i+1)}} \end{array} \right)^{-1} \cdot \left(\begin{array}{cc} \frac{\partial G_S}{z_S^{(i)}} & \frac{\partial G_S}{z_F^{(i)}} \\ \frac{\partial G_F}{z_S^{(i)}} & \frac{\partial G_F}{z_F^{(i)}} \end{array} \right) \right\|$$

and a term of order $\mathcal{O}(H)$, which tends to zero for the limit $H \rightarrow 0$.

- *Stable error propagation from window to window:*

$$L_\Phi \alpha^k < 1 \tag{15}$$

with k iterations in the current window and Lipschitz constant L_Φ of the extrapolation operator. Hence, depending on the L_Φ , more than one iteration may be necessary, though convergence within one window is given.

If we replace the exact solution of (13) by a numerical integration and stop after the first iteration, again an extra-/interpolation based multirate scheme is defined, now for coupled DAE systems (12). Note that stability can only be guaranteed if (15) holds; here, additional iterations of the multirate scheme can be necessary to obtain a convergent scheme.

Remark 6. Note that in the case of DAE-ODE coupling, i.e., when the second subsystem to be solved in a Gauss-Seidel type approach is defined by an ODE, then $\alpha = 0$ (14), since both splitting functions G_S and G_F do not depend on old iterates of the algebraic variables. In this case, one can show that the dynamic iteration is convergent of first order in the macro step size H (cf. [5]). In Section 4.3, a electro-thermal problems, which yields a DAE-ODE coupling is discussed. Depending on the fine structure of the coupling, up to second order convergence is possible, see [5].

Multirate schemes on basis of dynamic iteration schemes have been successfully applied to multiphysics problems. See, for example, field-circuit coupling [34, 35], electro-thermal coupling refined network modelling [6].

4 Applications in Circuit Simulation

Large integrated electrical networks are usually modeled via differential algebraic equations (e.g., see [21]): for a charge-flux oriented formulation, we have compactly

$$\mathcal{F}(t, x, \frac{d}{dt}w(x)) = 0, \quad (16)$$

in terms of node potential and currents (through voltage defining elements) x , charges and fluxes $w = q(x)$ as well as time t . Generally, in (16) for $\frac{d}{dw}\mathcal{F} \cdot \frac{d}{dx}w$ is not regular (DAE). In fact, these networks are built up by numerous coupled subcircuits of different functionality. As the subcircuits constitute different functional units, the overall system often shows multirate behaviour. To exploit this multirate potential, such a subcircuit partitioning has to be taken into account.

4.1 Partitioned network modeling

The subcircuits are modeled independently and composed to one macro system by connecting respective terminals, i.e., each pair of connected (terminal) nodes merge to a one node of the coupled system. This can be modeled by inserting virtual voltage sources for each pair of connected (terminal) nodes, where virtual means zero applied voltage. This approach preserves the macro circuit's block structure and produces additional variables: the branch currents u through the coupling voltage sources. These currents are implicitly determined by the property, that the node potentials of each pair of connected boundary nodes have to coincide. Now, we assume given a macro circuit composed of $\lambda = 1, \dots, r$ subcircuits each of type (16) and coupled via the algebraic constraints of virtual voltages sources. This reads:

$$\mathcal{F}_\lambda(t, x, \frac{d}{dt}w_\lambda(x_\lambda), u) = 0, \quad (\lambda = 0, \dots, r) \quad (17a)$$

$$\mathcal{G}(x_1, \dots, x_r) = 0, \quad (17b)$$

with x_λ internal node potentials and voltages, internal fluxes and charges $w_\lambda = q_\lambda(x_\lambda)$ of subsystem λ . Several index-1 conditions can be formulated for system (17) and its subsystems: [10]:

- (C1) The overall system (17) has index 1 (with respect to x_1, \dots, x_r, u).
- (C2) All systems (17a) define index-1 systems with respect to x (and u given as input).
- (C3) For any $\lambda \in \{1, \dots, r\}$, the λ -th system (17a) with coupling condition (17b) has index-1 with respect to x_λ and u given all other x_i (i.e., $i \neq \lambda$) as input).

In analogy to the procedure described in [17], topological conditions to guarantee the index conditions (C1)-(C3) can be derived. Given the above index-1 conditions, the overall model (17) can be transformed into algebraically coupled semi-explicit

systems

$$\left. \begin{aligned} \dot{y}_\lambda(t) &= f_\lambda(t, z_\lambda, u) \\ 0 &= h_\lambda(t, y_\lambda, z_\lambda, u) \\ 0 &= g(z_1, \dots, z_r) \end{aligned} \right\} \lambda = 1, \dots, r \quad (18)$$

with algebraic variables z_λ as node potentials and inner currents of system λ as well as differential variables y_λ defining the charges and fluxes (of system λ). In particular, setting (18) is the basis for developing more efficient schemes.

Remark 7. Notice we have two sets of coupled DAEs: one abstractly coupled DAEs (12), one with dedicated coupling equation (18), which represents networks, which are coupled via virtual voltage sources. In fact, for the latter case, the coupling condition (18-3) is linear in all arguments.

4.2 Multirate schemes

To get a mixed multirate scheme for coupled index-1 DAEs of type (18) (semi-explicit), we first regard the case $r = 2$ with F (fast) and S (slow) scale. It is natural to assume the coupling variable u (defined by $0 = g$) behaves slowly like y_S and z_S . This amounts to the following structure:

$$\begin{aligned} \dot{y}_S &= f_S(t, z_S, u), & \dot{y}_F &= f_F(t, z_F, u), \\ 0 &= h_S(t, y_S, z_S, u), & 0 &= h_F(t, y_F, z_F, u), \\ 0 &= g(z_S, z_F). \end{aligned} \quad (19)$$

With the index assumption (C3), the slow subsystem $[\dot{y}_S = f_S, 0 = h_S, 0 = g]$ is index-1 for algebraic variables z_S and u ; in addition, the fast subsystem $[\dot{y}_A = f_A, 0 = h_A]$ is of index-1 with respect to z_F if (C2) holds.

Now, we can apply multirate schemes to solve system (19). We present two options:

- *Compound-step approach:* Verhoeven et al. have developed a series of multirate schemes [43] for coupled network equations: slowest-first [44] and compound-step approach [46], equipped with step size prediction for both macro and micro step size and error control [46]. His approach does not demand a given subcircuit partitioning, but allows for automatic partitioning of the overall network equations [45].
- *Mixed multirate:* Striebel et al. [40] have developed a mixed multirate scheme on the basis of Rosenbrock-Wanner methods, which uses a generalized compound step to (jointly) compute macro step for the slow part and the first micro step of the fast part. The remaining micro steps of the active part are done by mixed multirate. The scheme allows for more than two time scales in a hierarchical setting by nesting compound steps and later micro-steps in a way that at each time merely a two-level multirate scheme is engaged [41].

Remark 8. In circuit simulation, the slow variable is usually referred to as latent and the fast variable is referred to as active.

4.3 Thermal-Electric Coupling — Silicon on Insulator

The transistor technology, silicon on insulator (SOI), introduces a thin insulator layer within the device. This layer can be made of an oxide, which has the purpose to electrically decouple the substrate and the channel area, see Fig. 1 for a sketch of such a device. Furthermore, it confines the channel to a rather small area and thus lowers parasitic (electrical) capacitance. In the end, the power consumption can be reduced and frequencies enhanced. However, since the electric insulator is often also a thermal insulator, the thermal coupling gains importance and needs to be investigated, see, e.g., [42]. Thus the SOI technology also drives the development of thermal-electric simulation.

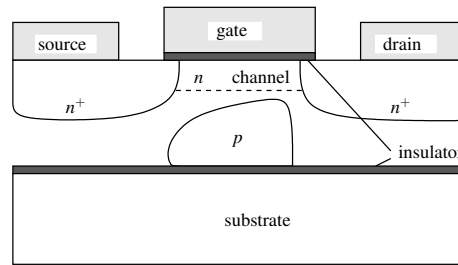


Fig. 1 Sketch of an SOI device.

Such a thermal-electric system is a multiphysics problem. On larger spatial units, one often obtains a multirate system: On the one hand, the electric subsystem switches on a very fast scale (e.g. on GHz scale). On the other hand, the temperature is dissipated and conducted slowly; e.g. the heat diffusivity in silicon is at 300K about $87 \cdot 10^{-6} \text{m}^2/\text{s}$. This yields a multirate setting and demands for an according simulation strategy.

In [7, 8], an according modeling and a simulation strategy was addressed. To this end, an accompanying (thermal) network (AN) for an electric network was proposed. The AN allows the connection of simple, thermal elements. These elements are spatially one dimensional and thus enable heat conduction along dedicated 1d structures.

Coupled thermal-electric model. The standard electric network model is a DAE of type (16), see e.g. [23] for details. To enable a thermal-electric coupling, we introduce a set of parameters p (which are going to be temperature dependent). This slightly generalizes the network equations (16) to the following initial value problem (for given p):

$$\overline{\mathcal{F}}(t, x, \frac{d}{dt} w(x); p) = 0, \quad \text{with consistent initial value } x(t_0) = x_0. \quad (20)$$

Thermally, the AN model comprises a set of heat conduction equations for distributed temperatures: $T : [t_0, t_e] \times [0, 1] \rightarrow \mathbb{R}^k$; all 1d elements shall have a normalized spatial dimension $[0, 1]$. Furthermore, we have lumped temperatures $\theta : [t_0, t_e] \rightarrow \mathbb{R}^m$, which denote the temperatures at the coupling nodes of the AN. This can be cast into the following type of equations (cf. [8])

$$\begin{aligned}\partial_t T &= \partial_{rr} T - (T - T_{\text{env}}) + P_1, \\ \partial_t \theta &= g(\partial_r T(0, t), \partial_r T(1, t)) - (\theta - T_{\text{env}}) + P_2\end{aligned}\quad (21)$$

with source terms P_1, P_2 (for the power dissipation) and material coefficients normalized to one, for simplicity of notation. In addition, we have boundary conditions (or coupling conditions) for the AN:

$$T(0, t) = M_0 \theta, \quad T(1, t) = M_1 \theta$$

with suitable matrices M_0, M_1 identifying coupling of the 1d-elements. Finally, we need to supply suitable initial conditions: $\theta(t_0) = \theta_0 \geq T_{\text{env}}, T(t_0, x) = T_0(x) \geq T_{\text{env}}$, where T_{env} is a given ambient temperature.

Now, the coupling conditions are as follows. On the one hand, the source terms P_i indicate the dissipated powers, which are a function of the network variables x :

$$P_i = P_i(x) \geq 0 \quad (\text{for } i = 1, 2).$$

On the other hand, the electric network does depend on the temperatures T, θ , via the network parameters:

$$p = p(T, \theta).$$

Later on, the accompanying thermal network was generalized to patches, where two spatial dimensional are involved, see [1, 13].

Dedicated multirate strategy for simulation. First, we consider a method of lines approach, where we apply a suitable spatial discretization to the thermal part. Due to the structure of the AN equation (21), we can obtain an ODE model for the thermal part, and thus, a coupled DAE-ODE system.

For the time integration, we apply a dynamic iteration, cf. Section 3, with windowing. Due to the DAE-ODE coupling, the contraction factor $\alpha = 0$ (14) and thus we have linear convergence of the dynamic iteration scheme [6].

Practically, we first solve the electric subsystem. To exploit the multirate setting with fast electric signals and slow thermal adjustments, we pursue an energy coupling, which is based on averaging, cf. [14, 6]. That is, instead of coupling via the fast changing instantaneous power dissipation, one can compute the total dissipated power E^H of electric subsystem during a certain time interval $[\bar{t}, \bar{t} + H]$. This is an energy, and may be computed by simply adding according energy variables E to the network variables and appending the network equations (20) with corresponding differential equations

$$\dot{E} = P(x).$$

Then, the total amount of the dissipated power is added to the thermal network as averaged quantity: $P_t = E^H/H$. This way, the total amount of the dissipated (electric) energy is added to the thermal system. The addition of the actual power as source term to the heat conduction might happen with a little time shift on the scale of the fast system. Of course, this is for a slow heat system of minor importance. The reverse coupling needs to adjust the temperature dependent network parameters, i.e., an updated device temperature needs to be assigned. To this end, the heat equation is solved. Since we expect on the H -scale only minor temperature changes, we can even skip any iterations of the dynamic scheme and compute the preceding communication step (e.g. $[\bar{t}+h, \bar{t}+2H]$), i.e., solve again first the electric subsystem with the new temperatures. This is referred to as multirate co-simulation, since both subsystems may be solved on their time scale and no overhead of iterations occurs. This multirate co-simulation strategy was successfully applied to solve a ring oscillator circuit, see [7]. In fact, it is reasonable to exchange data after one step of the slow subsystem, i.e., the communication step size can be chosen as the inherent step size of the solve subsystem. As a further enhancement, one can apply a dedicated midpoint rule to solve the slow (heat) subsystem and gain formally a second order method, see [6].

5 Molecular Dynamics

In molecular dynamics, one has to solve initial-value problems of the type

$$\dot{w} = h(w), \quad w(t_0) = w_0 \quad (22a)$$

with

$$w := \begin{pmatrix} q \\ p \end{pmatrix}, \quad h(w) := J^{-1} \nabla H(q, p), \quad J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad w_0 := \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \quad (22b)$$

with positions $q : [t_0, T] \rightarrow \mathbb{R}^n$, momenta $p : [t_0, T] \rightarrow \mathbb{R}^n$ and Hamiltonian $H : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$. The separable Hamiltonian $H(q, p) = T(p) + V(q)$ is composed of a kinetic energy T and a potential energy V .

The standard numerical integration scheme applied to Hamiltonian system is the Störmer-Verlet (or leap-frog) scheme, which we refer to as $\psi_{h_0}^H$ for step size h_0 . In fact, we can describe $\psi_{h_0}^H$ for (22a-22b) via operator splitting based on explicit Euler steps ϕ_h for the components q and p :

$$\psi_{h_0}^H(q_0, p_0) := \phi_{h_0/2}^V \circ \phi_{h_0}^T \circ \phi_{h_0/2}^V(q_0, p_0). \quad (23)$$

Here, ϕ_h^T advances the kinetic energy $H = T$ with an explicit Euler step of size h and ϕ_h^V analogously the potential energy $H = V$. In fact, this numerical approximation (23) solves exactly the shadow Hamiltonian \hat{H} , which differs from the original Hamiltonian H by the following expression:

$$\hat{H} - H = -\frac{h_0^2}{24} ([V, [V, T]] + 2[T, [V, T]]) + \mathcal{O}(h_0^4).$$

If the forces derived from the Hamiltonian are hierarchical and the larger forces turn out to be cheap to compute, the integration of molecular dynamics can be accelerated by the means of multirate schemes. For example in lattice quantum chromodynamics [26] holds: the gauge force is cheap to evaluated and largest in size the fermionic force is expensive but smaller in size. Thus, let us assume that the potential energy consists of two parts V_1 and V_2 , which differ as follows:

- V_1 : the contribution

$$f_1(q) := J^{-1} \nabla V_1(q),$$

to the force is strong and with a fast dynamics, but its evaluation is cheap;

- V_2 : the contribution

$$f_2(q) := J^{-1} \nabla V_2(q),$$

to the force is weak with a slow dynamics, but its evaluation is expensive.

Consequently, one may split the ODE (22) with respect to the right-hand side:

$$h_s(w, t) := f_2(q), \quad h_f(w, t) := f_1(q) + J^{-1} \nabla T(p),$$

where we have assumed that the dynamics related to the kinetic energy is fast, but cheap to be evaluated. Thus, we have the structure of (3).

Naturally, one idea to exploit this multirate behavior is an according evaluation: within one macro step H evaluate the slow, expensive part h_s (only) once; the fast, cheap part h_f several times. However, the multirate approach has to preserve the symplectic and time-reversible structure of the Hamiltonian flow. Hence, an operator splitting approach appears to be favorable, as the composition of symplectic and time reversible schemes is again symplectic and time reversible.

For the right-hand side split ODE (3), a multirate method $\tilde{\psi}_{h_0}^H(q_0, p_0)$ [36] with macro step size h_0 and m_1 mirco steps of step size $h_1 = h_0/m_1$ is obtained from

$$\tilde{\psi}_{h_0}^H(q_0, p_0) := \phi_{h_0/2}^{V_2} \circ \left(\psi_{h_1}^{T+V_1} \right)^{m_1} \circ \phi_{h_0/2}^{V_2}(q_0, p_0),$$

where we used the Störmer-Verlet scheme ψ_h^H of the single-rate case with $H := T + V_1$ and step size h_1 . This multirate scheme conserves now the following shadow Hamiltonian \hat{H} , which differs from the original Hamiltonian H by

$$\begin{aligned} \hat{H} - H = & -\frac{h_0^2}{24} ([V_2, [V_2, T]] - 2[V_1, [V_2, T]] - 2[T, [V_2, T]] \\ & \frac{1}{m_1^2} ([V_1, [V_1, T]] - 2[T, [V_1, T]])) + \mathcal{O}(h_0^4). \end{aligned}$$

Remark 9. Let us assume that the dynamics level of V_1 over V_2 is proportional to m_1 , then all commutators involving one or two instances of V_1 are properly scaled with $1/m_1^2$ besides the commutator $[V_1, [V_2, T]]$. However, if the Störmer-Verlet scheme

for m_1 inner micro-steps is replaced by a force-gradient scheme [28], the commutator $[V_1, [V_2, T]]$ is eliminated, and the shadow Hamiltonian for this multirate version [37] is given by

$$H + \left(\frac{h_0}{m_1}\right)^2 \left(\frac{1}{96} [V_1, [T, V_1]] + \frac{1}{48} [T, [T, V_1]] \right) + \mathcal{O}(h_0^4).$$

This multirate approach can be applied to Hamiltonians with a further splitting of the potential energy in a hierarchical manner as follows: let us assume that the Hamiltonian is given by

$$H(q, p) = T(p) + \sum_{l=1}^N V_l(q).$$

If the energies are ordered such that the computational cost are increasing, while at the same time the strength of the associated forces is decreasing, a multirate integration based on the Störmer-Verlet scheme can be defined [36]: using macro step size h_0 and micro step size $h_1 = h_0/M$ proceeds as follows:

$$\varphi_{h_0}^{H_0}(q_0, p_0) = \varphi_{h_0/2}^{H_2} \left(\varphi_{h_1}^{H_1} \right)^{m_1} \varphi_{h_0/2}^{H_2},$$

with $H_1(q, p) = T(p) + \sum_{l=1}^{N-1} V_l(q)$ and $H_2(q, p) = V_N(q)$. This scheme can be nested, by introducing a next finer step size $h_2 = h_1/m_2$ and further splitting H_1 into

$$H_1(q, p) = H_{11}(q, p) + H_{12}(q, p)$$

with $H_{11}(q, p) = T(p) + \sum_{l=1}^{N-2} V_l(q)$ and $H_{12}(q, p) = V_{N-1}(q)$ in order to replace $\varphi_{h_1}^{H_1}$ above by

$$\varphi_{h_1}^{H_1} = \varphi_{h_1/2}^{H_{12}} \left(\varphi_{h_2}^{H_{11}} \right)^{m_2} \varphi_{h_1/2}^{H_{12}}.$$

This procedure can be applied recursively to obtain N different step size ratios at the end, corresponding to the activity levels of the N potential energies $V_l(q)$.

6 Conclusion & Outlook

In many applications, the governing differential equation are characterized by strongly varying time scales. Numerical time integration of these type of models demands integration schemes able to exploit this behavior, not only for efficiency reason, but quite often to enable numerical simulation at all.

In this paper, we have discussed two basic classes of multirate schemes based on extra-/interpolation and compound-step approaches: the pioneering work by Rice for missile applications (compound step approach for one-step methods) and the seminal work by Gear and Wells driven by electrical circuit application (extra-/interpolation for multi-step methods). For the latter, we characterized the overall convergence properties for coupled ODE systems.

Another trend in applications — refined modeling yielding coupled systems consisting of multiphysical subsystems — initialized further development in dynamic iteration approaches. They deliver another class of (full) multirate schemes by stopping the iteration after the first sweep. We discussed the basics of this approach and verified the efficiency of such multirate schemes by inspecting the coupled thermal-electric problem, where we gave a tailored numerical algorithm.

If the multirate behavior is not given by varying solution components, but by different characteristics of the right-hand side, an operator splitting approach is the method of choice to derive multirate schemes, especially if preservation of properties such as in geometric integration is mandatory. Here, molecular dynamics serves as an example of applications in this field.

The increasing interest in parallel-in-time schemes in the last years offers a new way to speed up simulation time by the help of multirate schemes. Here the combination of parallel-in-time schemes with dynamic iteration and multirate schemes seems to be promising, see e.g. [18]. This will be an interesting topic for research on multirate schemes in the coming years.

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