Multirate GARK Schemes for Multiphysics Problems

Michael Günther, Christoph Hachtel, and Adrian Sandu

Abstract Multirate GARK schemes define a multirate extension of GARK schemes, generalized additive Runge-Kutta schemes. In contrast to additive schemes, GARK schemes allow for different stage values as arguments of different components of the right hand side. They introduce additional flexibility when compared to traditional partitioned Runge-Kutta methods, and therefore offer additional opportunities for the development of flexible solvers for systems with multiple scales, or driven by multiple physical processes.

Consequently, multirate GARK schemes allow for exploiting multirate behaviour in both the right-hand sides and in the components in a rather general setting, and are thus especially useful for coupled problems in a multiphysics setting. We apply MGARK schemes to a benchmark example from thermal-electrical coupling, characterized by a slow and fast part with a stiff and non-stiff characteristic, resp. We test two MGARK schemes: (a) an IMEX method, which completely utilizes the dynamics and differing stability properties of the coupled subsystem; and (b) a fully implicit schemes, which inherits the stability properties from both underlying schemes without any coupling constraint.

1 Introduction

Multiphysical systems are often characterized by a very different dynamical behavior in the subsystems, with time constants differing by orders of magnitude. To be efficient, numerical time integration schemes have to exploit this multirate behavior,

M. Günther (✉)
Applied Math. & Numerical Analysis, Bergische Universität Wuppertal, Wuppertal, Germany
e-mail: guenther@math.uni-wuppertal.de

C. Hachtel
Bergische Universität Wuppertal, Institute of Mathematical Modelling, Analysis and Computational Mathematics (IMACM), Gaußstraße 20, D-42119 Wuppertal, Germany
e-mail: hachtel@math.uni-wuppertal.de

A. Sandu
Department of Computer Science, Virginia Polytechnic Institute and State University, Computational Science Laboratory, 2202 Kraft Drive, Blacksburg, VA 22060, USA
e-mail: asandu@cs.vt.edu

A. Bartel et al. (eds.), *Scientific Computing in Electrical Engineering*, Mathematics in Industry 23, DOI 10.1007/978-3-319-30399-4_12

which is physically given and allows for a static partitioning of the subsystems into slow and fast parts, resp.

Multirate time integration schemes aim at exploiting this property by applying different time step sizes to the subsystems, according to their different activity level. To get higher order schemes, these schemes have to fulfill additional order conditions, and at the same time preserve the stability properties of the respective subsystems.

This paper discusses the application of a new class of multirate schemes, multirate GARK [1] schemes based on a generalized view on additive Runge-Kutta schemes [3], to a multiphysical problem from electro-thermal coupling.

The paper is organized as follows: Sect. 2 gives a synopsis on multirate GARK schemes and their relation to GARK schemes. Section 3 introduces two multirate GARK schemes, based on an explicit-implicit and implicit-implicit pair of order-2 basis schemes. Section 4 discusses the numerical results obtained for both schemes. The last section concludes with final remarks and an outlook.

2 Multirate GARK Schemes

We consider a two-way partitioned system

$$y' = f(y) = f^{\{\mathfrak{s}\}}(y) + f^{\{\mathfrak{f}\}}, \quad y(t_0) = y_0\,, \tag{1}$$

with a slow component $\{\mathfrak{s}\}$, and an active (fast) component $\{\mathfrak{f}\}$. Note that this setting contains component-wise splitting as a special case:

$$y = \begin{pmatrix} y_{\mathfrak{s}} \\ y_{\mathfrak{f}} \end{pmatrix}, \quad f^{\mathfrak{s}} = \begin{pmatrix} f_{\mathfrak{s}} \\ 0 \end{pmatrix}, \quad f^{\mathfrak{f}} = \begin{pmatrix} 0 \\ f_{\mathfrak{f}} \end{pmatrix}. \tag{2}$$

The slow component is solved with a large step H, and the fast one with small steps $h = H/M$. We will consider the multirate generalization of GARK schemes [3] with M micro steps $h = H/M$, as given in the following

Definition 1 (Multirate GARK Method [1]) One macro-step of a generalized additive multirate Runge-Kutta method with M equal micro-steps reads

$$Y_i^{\{\mathfrak{s}\}} = y_n + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right) + h \sum_{\lambda=1}^{M} \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{f},\lambda\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f},\lambda\}}\right),$$

$$Y_i^{\{\mathfrak{f},\lambda\}} = y_n + h \sum_{l=1}^{\lambda-1} \sum_{j=1}^{s^{\{\mathfrak{f}\}}} b_j^{\{\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f},l\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{s},\lambda\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right) +$$

$$+h \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f},\lambda\}}\right), \quad \lambda = 1,\ldots,M,$$

$$y_{n+1} = y_n + h \sum_{\lambda=1}^{M} \sum_{i=1}^{s^{\{\mathfrak{f}\}}} b_i^{\{\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_i^{\{\mathfrak{f},\lambda\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} b_i^{\{\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_i^{\{\mathfrak{s}\}}\right).$$

The base schemes are Runge-Kutta methods, $(A^{\{\mathfrak{f},\mathfrak{f}\}}, b^{\{\mathfrak{f}\}})$ for the slow component and $(A^{\{\mathfrak{s},\mathfrak{s}\}}, b^{\{\mathfrak{s}\}})$ for the fast component. The coefficients $A^{\{\mathfrak{s},\mathfrak{f},\lambda\}}$ and $A^{\{\mathfrak{f},\mathfrak{s},\lambda\}}$ for $\lambda = 1,\ldots,M$ realize the coupling between the two components.

2.1 Order Conditions

The MGARK scheme can be written as a GARK scheme [3] over the macro-step H with the fast stage vectors $Y^{\{\mathfrak{f}\}} := [\,Y^{\{\mathfrak{f},1\}\,T},\ldots,Y^{\{\mathfrak{f},M\}\,T}]^T$. The corresponding Butcher tableau reads (with the vector $\mathbf{1} := (1,\ldots,1)^T$ of ones)

$$\begin{array}{cccc|c}
\frac{1}{M}A^{\{\mathfrak{f},\mathfrak{f}\}} & 0 & \cdots & 0 & A^{\{\mathfrak{f},\mathfrak{s},1\}} \\
\frac{1}{M}\mathbf{1}b^{\{\mathfrak{f}\}\,T} & \frac{1}{M}A^{\{\mathfrak{f},\mathfrak{f}\}} & \cdots & 0 & A^{\{\mathfrak{f},\mathfrak{s},2\}} \\
\vdots & & \ddots & & \vdots \\
\frac{1}{M}\mathbf{1}b^{\{\mathfrak{f}\}\,T} & \frac{1}{M}\mathbf{1}b^{\{\mathfrak{f}\}\,T} & \ldots & \frac{1}{M}A^{\{\mathfrak{f},\mathfrak{f}\}} & A^{\{\mathfrak{f},\mathfrak{s},M\}} \\
\hline
\frac{1}{M}A^{\{\mathfrak{s},\mathfrak{f},1\}} & \frac{1}{M}A^{\{\mathfrak{s},\mathfrak{f},2\}} & \cdots & \frac{1}{M}A^{\{\mathfrak{s},\mathfrak{f},M\}} & A^{\{\mathfrak{s},\mathfrak{s}\}} \\
\hline
\frac{1}{M}b^{\{\mathfrak{f}\}\,T} & \frac{1}{M}b^{\{\mathfrak{f}\}\,T} & \ldots & \frac{1}{M}b^{\{\mathfrak{f}\}\,T} & b^{\{\mathfrak{s}\}\,T}
\end{array}$$

Therefore the order conditions for MGARK schemes can be derived from the corresponding ones for GARK schemes [3]. Up to order two the order conditions given in Table 1 have to be fulfilled.

Table 1 Order conditions for MGARK schemes

p	Order condition
1	$b^{\{\mathfrak{s}\}\,T}\mathbf{1} = 1$
	$b^{\{\mathfrak{f}\}\,T}\mathbf{1} = 1$
2	$b^{\{\mathfrak{s}\}\,T}A^{\{\mathfrak{s},\mathfrak{s}\}}\mathbf{1} = \frac{1}{2}$
	$b^{\{\mathfrak{s}\}\,T}\left(\sum_{\lambda=1}^{M} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}}\right)\mathbf{1} = \frac{M}{2}$
	$b^{\{\mathfrak{f}\}\,T}A^{\{\mathfrak{f},\mathfrak{f}\}}\mathbf{1} = \frac{1}{2}$
	$b^{\{\mathfrak{f}\}\,T}\left(\sum_{\lambda=1}^{M} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}}\mathbf{1}\right) = \frac{M}{2}$

2.2 Stability

We consider systems (1) where each of the component functions is dispersive (with constants $\nu^{\{\mathfrak{s}\}} < 0$, $\nu^{\{\mathfrak{f}\}} < 0$):

$$\left\langle f^{\{\mathfrak{s}\}}(y) - f^{\{\mathfrak{s}\}}(z)\,,\, y - z \right\rangle \le \nu^{\{\mathfrak{s}\}}\ \|y - z\|^2\,,$$
$$\left\langle f^{\{\mathfrak{f}\}}(y) - f^{\{\mathfrak{f}\}}(z)\,,\, y - z \right\rangle \le \nu^{\{\mathfrak{f}\}}\ \|y - z\|^2\,,$$

with respect to the same scalar product $\langle \cdot, \cdot \rangle$. As for two solutions $y(t)$ and $\tilde{y}(t)$ of (1), each starting from a different initial condition, the norm of the solution difference $\Delta y(t) = \tilde{y}(t) - y(t)$ is non-increasing, we demand a similar property from the numerical approximations: the MGARK scheme is said to be nonlinearly stable, if the inequality

$$\| y_{n+1} - \tilde{y}_{n+1} \| \le \| y_n - \tilde{y}_n \|$$

holds for any two numerical approximations y_{n+1} and $\tilde{y}_{n+1}$ obtained by applying the scheme to the ODE (1) with dispersive functions and with initial values y_n and $\tilde{y}_n$.

As a consequence of stability theory for GARK schemes, an MGARK scheme applied to a component-wise partitioned right-hand side (2) is nonlinearly stable, if both base schemes are algebraically stable [1].

3 Two Basic GARK Schemes for Multiphysics Application

In general, one is interested in a rough approximation of coupled multiphysics problems, which reflect the impact of the couplings of both systems. Hence we restrict to MGARK schemes of order 2. As we are interested in the nonlinear stability properties of MGARK schemes, and how the stability properties of both base schemes influence the stability of the overall scheme, we define two new IMEX and IMIM schemes as basic methods:

- MGARK-IMEX-2: The implicit-explicit version solves the fast, stiff part with an implicit base scheme, and the slow, non-stiff part with an explicit one. The coefficients are given by

$$b^{\{\mathfrak{s}\}} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \quad A^{\{\mathfrak{s},\mathfrak{s}\}} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad A^{\{\mathfrak{s},\mathfrak{f},1\}} = \begin{pmatrix} 0 \\ M \end{pmatrix},$$
$$A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \forall \lambda = 2, \ldots, M,$$

$$b^{\{\mathfrak{f}\}} = 1, \quad A^{\{\mathfrak{f},\mathfrak{f}\}} = \frac{1}{2}, \quad A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} = \left(\tfrac{1}{2}\ 0\right) \quad \forall\lambda = 1,\ldots,M.$$

The slow components are implicitly solved together with the fast components of the first micro step. The fast components of the remaining micro steps can be computed explicitly.

Note that only the fast part is algebraically stable, but neither the slow part nor the joint system.

- MGARK-IMIM-2: To get an overall stable scheme, both parts are solved by an implicit base scheme. The coefficients are given by

$$b^{\{\mathfrak{s}\}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad A^{\{\mathfrak{s},\mathfrak{s}\}} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \quad A^{\{\mathfrak{s},\mathfrak{f},1\}} = \begin{pmatrix} 0 \\ \frac{M}{2} \end{pmatrix},$$

$$A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \forall\lambda = 2,\ldots,M,$$

$$b^{\{\mathfrak{f}\}} = 1, \quad A^{\{\mathfrak{f},\mathfrak{f}\}} = \frac{1}{2}, \quad A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} = \left(\tfrac{1}{2}\ 0\right) \quad \forall\lambda = 1,\ldots,M.$$

Note that again the slow components are implicitly defined together with the fast components after the first micro step. The fast components of the remaining micro steps can be computed one after the other by solving nonlinear systems in the dimension of the active part only.

As both base schemes are algebraically stable, the MGARK method inherits this property for a component-wise partitioning.

4 Numerical Test Results for a Benchmark Example

We will test both MGARK implementations for a thermal–electrical multiphysics system, for specifications see [2]; its circuit diagram is given in Fig. 1 (left). The thermal component defines the slow (and non-stiff) part, the electrical component the fast (and stiff) part of the system.

The distributed temperature T of the resistor (wire) is described by the 1-D heat equation, which is semi-discretised using a finite volume approach, see Fig. 1 (right). Due to the electric current, the resistor is heated and so the resistance of this device changes: $R = R(T)$. The characteristic curve of the diode is also temperature dependent. The voltages are modeled by a nodal analysis using Kirchhoff's laws. Finally we get a partitioned system of ordinary differential equations like in (1). The vector of unknowns $y = (u_3, u_4, e, T)^T$ comprises the voltages u_3 and u_4 at nodes 3 and 4, resp., the dissipated energy e in the thermally dependent resistor and the vector of temperatures T in the semi-discretised resistor. The multirate behaviour of this system is given by the physical properties: the voltages and the dissipated energy change very fast (due to the source of the network), and the temperature in

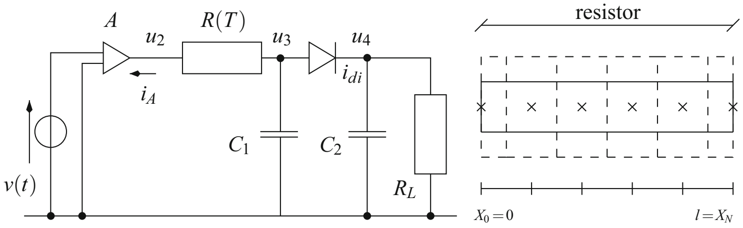

Fig. 1 Circuit and discretised resistor

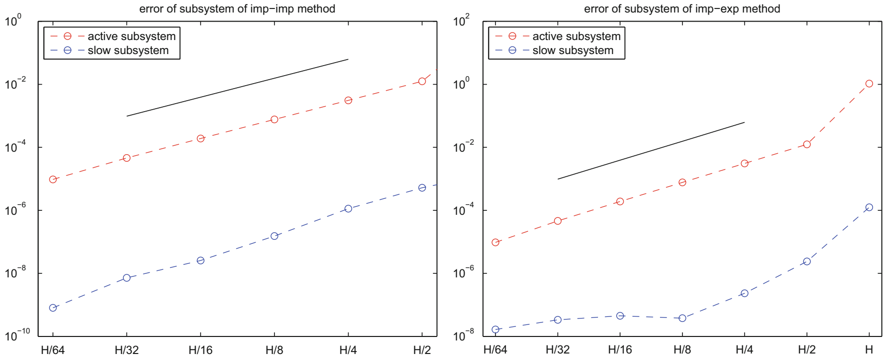

Fig. 2 Numerical results for the fast and slow subsystems (macro step size vs. achieved accuracy, measured in Euclidean norm): MGARK-IMIM-2 (*left*) and MGARK-IMEX-2 (*right*) with parameters $H = 10^{-3}$, $m = 5$. The *solid lines* represent the slope of order 2

the resistor changes much slower. Hence the partitioning according to the dynamical behaviour is quite natural:

$$y^{\{\mathfrak{f}\}} := \begin{pmatrix} u_3 \\ u_4 \\ e \end{pmatrix}, \qquad y^{\{\mathfrak{s}\}} := T.$$

The numerical results for both Multirate GARK schemes are given in Fig. 2. The IMIM scheme nicely shows in both fast and slow subsystems an order-2 behavior for all step sizes. The accuracy of the IMEX scheme in the slow part (which is not algebraically stable and computed explicitly), however, seems to be reduced for small step sizes.

5 Conclusion

By testing Multirate GARK schemes on a multiphysical test example from electro-thermal coupling, we have shown the feasibility of this multirate approach for both implicit-implicit and implicit-explicit pairing of basic schemes. Whereas the IMIM scheme shows an order-2 behavior for both subsystems at all step sizes, the IMEX schemes has a reduced accuracy in the slow system for small step sizes only. This behavior fits to the theoretical properties of both schemes: the IMIM scheme is algebraically stable in both subsystems, whereas the IMEX scheme is only stable in the fast (electric) part.

As next steps, we will follow three directions: (a) we will apply MGARK schemes to a range of multiphysical problems in a more realistic setting; (b) we will further analyze the stability of IMEX-MGARK schemes and its dependence on the coupling structure for both weak and slow coupling; (c) the excellent stability properties of IMIM-MGARK schemes suggest to use these schemes as basic schemes in a Multirate-MOR approach.

Acknowledgements The work of A. Sandu has been supported in part by NSF through awards NSF DMS—1419003, NSF CMMI—1130667, NSF CCF—1218454, AFOSR FA9550-12-1-0293-DEF, AFOSR 12-2640-06, and by the Computational Science Laboratory at Virginia Tech.

The work of M. Günther and C. Hachtel has been supported in part by the German BMBF Program, through grant 05M13PXA (BMBF Verbundprojekt KoSMOS, see http://scwww.math.uni-augsburg.de/projects/kosmos/) and by the EU through grant 619166 (FP7-STREP nanoCOPS, see http://www.fp7-nanoCOPS.eu/).

References

1. Günther, M., Sandu, A.: Multirate generalized additive Runge Kutta methods. Numer. Math. doi:10.1007/s00211-015-0756-z
2. Hachtel, C., Bartel, A., Günther, M.: Efficient simulation for electrical-thermal systems via multirate-MOR. In: Proceedings of SCEE 2014, Wuppertal (2014)
3. Sandu, A., Günther, M.: A generalized-structure approach to additive Runge-Kutta methods. SIAM J. Numer. Anal. **53**(1), 17–42 (2015)