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Multirate Time Integration for ODEs and DAEs Final Report

C. S. Woodward, L. Loffeld, D. J. Gardner

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Project Title: Multirate Time Integration for ODEs and DAEs Final Report

PI and Tracking Number: Carol S. Woodward (17-ERD-035)

Abstract

This project investigated multirate time integration methods. These methods evolve a differential equation system in time by advancing parts of the problem with fast time scales at small time steps and parts of the problem with slow time scales with larger time steps. The project developed new methods and theory as well as a set of prototype software implementations. Multirate methods were tested on combustion and climate applications. A series of five presentations were given on project results and two papers are planned.

Background and Research Objectives

With exascale systems, scientific simulations, such as in climate, combustion, power grid, and hydrological sciences, will include more physics, resulting in a growing number of changing time scales. Starting with (Gear 1984) and continuing with (Savcenco et al., 2007, Guenther et al. 2016, and Sarshar 2019), multirate methods were developed to address these issues. Multirate methods lower computational cost by using small time steps only for fast evolving components and larger steps elsewhere. These methods address two types of problems, ones with multiple processes each with its own time scale (additive processes) and ones with unknowns evolving at differing time scales (variable partitioned processes).

While multirate methods had been in use in some applications, at the start of this project, little work had been done to develop methods that were both efficient and had favorable mathematical properties, including high stability and high order accuracy. In addition, no multirate methods appeared in any general-purpose time integration software. This project explored multirate time integrators that could be amenable to an integrator package. The original 3 objectives were: 1) Establish consistency and stability theory for multirate methods suitable for a time integration package, 2) Develop partitioning and parallelization strategies, and 3) Develop and prototype common software infrastructure for multirate integrators and test the prototypes in applications.

As the project progressed, we observed that the infrastructure required for variable partitioned methods would be fairly substantial both in run time cost and in development time for a general-purpose software library. We thus deemphasized work on variable partitioned methods. As a result of these changes, we replaced Objective 2 with a new Objective: Investigate viability of hybrid exponential-multirate methods and the viability of multirate multistep methods for additive systems. This objective allowed us to evaluate multirate methods outside the traditional multistage, Generalized Additive Runge-Kutta (GARK) and the Recursive Flux-Splitting MultiRate (RFSMR) frameworks that have been examined already in the literature.

Overall, our objectives have been met. We identified a number of multirate methods that could be candidates for a general-purpose software package. We established stability theory for methods for additive problems and developed a set of prototype Matlab and C (parallel) implementations of methods and tested them in combustion and climate applications. We have given five presentations including results of this work and have two papers in progress.

Scientific Approach and Accomplishments

Objective 1: Establish consistency and stability theory for multirate methods suitable for a time integration package

A review of the literature determined that accurate and efficient explicit multirate methods were well handled. Methods with streamlined accuracy had been developed in the multirate GARK (MrGARK) (Guenther et al. 2016) and RFSMR (Schlegel et al. 2009) Runge-Kutta frameworks. At the time, implicit methods were less developed, and we focused our attention in the project on developing implicit methods.

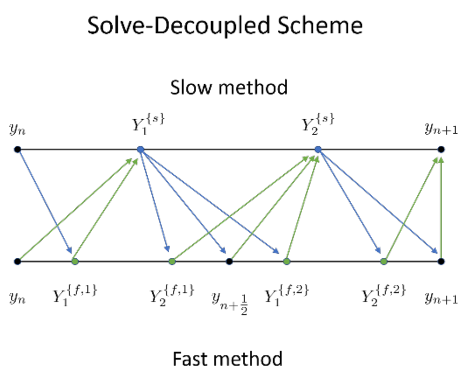

Figure 1: Each fast and slow stage of a solve-decoupled method is only implicit with itself and receives information from the other timeline only from prior computed stages. The stability of such methods is limited.

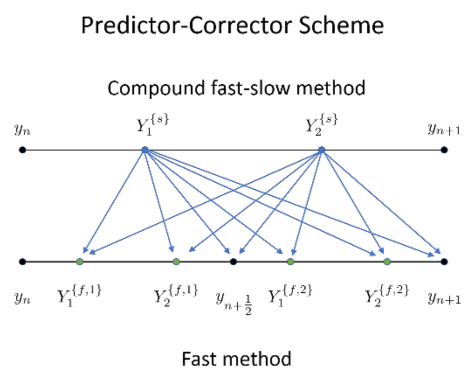

Figure 2: Predictor-Corrector methods first compute the solution in an unpartitioned manner using a coarse step size then recompute the fast stages using a small step size. Such methods are highly stable but more expensive.

We conducted detailed stability analyses of implicit methods using a variety of coupling strategies. A fully implicit multirate method would use an implicit solve over all fast steps together with the slow steps, but the cost of such a method would be far greater than a unirate method rendering the multirate implicit method useless. In order to be cost-effective, implicit multirate methods can afford to use only a minimal amount of joint implicit solves between both the fast and slow partitions. However, decoupling the solves makes the methods less stable.

If a method is wholly solve-decoupled, each fast and slow stage is implicit only with itself and receives information from the other timeline in an explicit manner (Fig. 1). While of low cost, our tests showed that such methods have highly reduced stability compared to unirate methods. We also found that methods that couple a small number of fast and slow steps together (Gunther et al. 2016, Guenther et al. 2001), but leave most of the fast steps decoupled, are more stable than decoupled methods but remain far from the stability of unirate implicit methods.

We did a breakdown of the stability structure of the methods and showed that solves over a fast step with a small δt co-stepped with a slow step with a larger Δt have an algebraic form with compromised stability. Motivated by this result, we used the MrGARK framework (Guenther et al. 2016) to develop a type of implicit method that takes joint coarse steps between the fast and slow partitions but then re-sweeps the fast steps to refine the fast timeline for accuracy (see Fig. 2). The resulting methods have nearly unconditional stability, which is a vast improvement over prior approaches and results in methods with only marginally less stability than unirate implicit methods. Our collaborators at VA Tech then developed refined versions of the initial methods with accuracy-optimized coefficients, which, along with our work, are being written into a joint publication (Roberts et al. 2019).

Objective 2: Investigate viability of hybrid exponential-multirate methods and the viability of multirate multistep methods, both for additive systems.

Hybrid exponential-multirate methods are a hybridization of standard exponential methods that partition a problem into a portion that is advanced with a standard implicit step and a portion using exponential integration. Exponential functions of matrices within exponential integrators can be naturally substepped (Gaudreault et al. 2018) and, in the unpartitioned case, give trivially unconditionally stable methods (Tokman 2006).

In this project, highly stable, third-order hybrid exponential multirate methods were derived. A stability analysis was conducted putting the new methods on par with the most stable implicit GARK methods. A breakdown of the stability structure of the schemes was conducted, and a means for deriving unconditionally stable second-order methods was found. The stability of those methods was analytically proved, and the approach taken for second-order seems extensible to higher order. The order of accuracy of the methods were numerically confirmed, and a paper on these methods is being prepared for submission within the next few months.

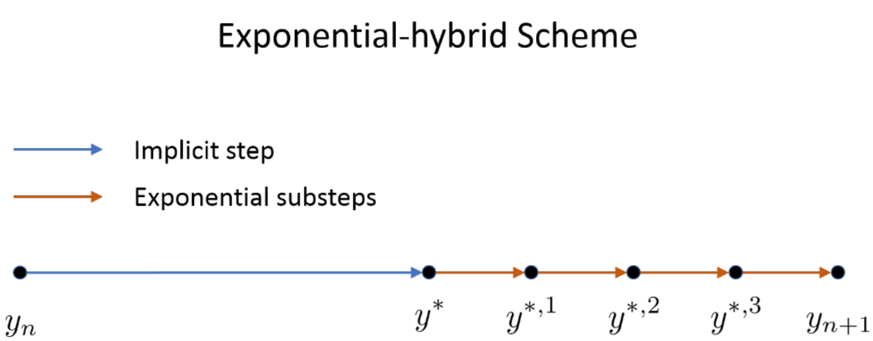

Figure 3: The implicit and exponential portions of the hybrid schemes are coupled in a splitting like manner where partitions are interleaved in time and only the final result of one partition is fed into the other.

Hybrid exponential multirate methods have a structure similar to splitting methods (see Fig. 3) but are able to obtain higher than second order without the need for backward time steps that make higher-order splitting methods untenable for most problems (Blanes et al. 2005). Further, these methods do not result in a fast-to-slow ratio dependent coupling error in the scheme in contrast with GARK and RFSMR methods that have a coupling error that grows with this ratio.

Multirate Backward Differentiation Formula (BDF) Methods. We conducted a review of the multirate multistep integrator literature and identified 7 coupling strategies and their impact on stability of the methods. Stability analysis is considerably more difficult for these methods than for the Runge-Kutta methods, but tentative conclusions about the approaches were drawn from a combination of results from literature and results on test problems. The compound-fast approach which first coarsely solves the problem in an unpartitioned manner then recomputes the fast partition alone using small time steps, is the most stable.

All the coupling strategies except one (which is just a hybridization of two of the others) were implemented in Matlab using BDF multistep methods of orders 1-6 as base methods, and the implementations were tested on several test problems. The methods were implemented with the Nordsieck array approach used in CVODE, making the results directly relevant to the BDF implementations in SUNDIALS. Using that representation, all the multirate BDF methods could share most of their code, so supporting all coupling strategies in CVODE should be very straightforward. The methods were tested on two very simple ODE test problems and a hydrogen combustion problem. Performance of the methods was similar on all problems, but the compound-fast method was deemed the best balance of cost and stability. Since different coupling strategies can be straightforwardly implemented on a common BDF framework (which already exists in CVODE), the best approach is certainly to implement all coupling strategies in SUNDIALS and choose the best strategy on a problem-by-problem basis.

Objective 3: Develop and prototype common software infrastructure for multirate integrators and test in applications.

Development of prototype codes and test problems. We developed prototype codes in both Matlab and C that allowed for assessing the software infrastructure needed to support multirate methods. Both code frameworks implement two types of GARK-based methods. The first was solve-decoupled GARK methods in which the fast and slow operators are always evolved independently of each other, and the second was the predictor-corrector methods, where the first stage can involve a coupled evolution of the fast and slow operators. Both classes of methods were implemented with similar internal structures. The methods take as inputs multirate Generalized Additive Runge-Kutta (MrGARK) tables of coefficients allowing the code to be general to any solve-decoupled or predictor-corrector GARK method. The codes were both frameworks that can have any methods of the discussed forms instantiated underneath them. The predictor-corrector frameworks were tested using the 2nd-order and 3rd-order methods in (Roberts 2019), as well as a 3rd-order predictor-corrector method created as part of the project which uses a Kvaerno-Rentrop style coupling (Guenther et al. 2016). The decoupled method frameworks were tested using all 12 methods described in (Sarshar et al., 2019).

An array of test problems was also implemented in both Matlab and C so that methods could be tested and compared. Test problems included the Gray-Scott pattern formation problem, the inverter chain problem, the FlameSolver application from M. McNenly's LLNL combustion simulation group, and the MG2 climate microphysics originally given to us from P. Caldwell's Kinematic Driver implementation.

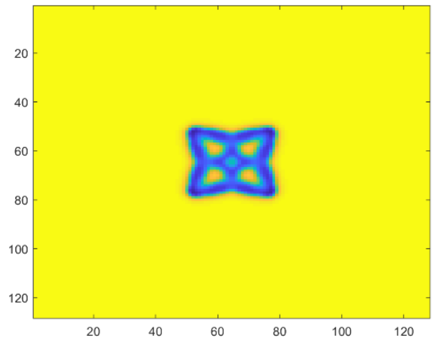

Figure 4: The Gray-Scott pattern formation problem still early at t = 1000. The pattern is growing from the center.

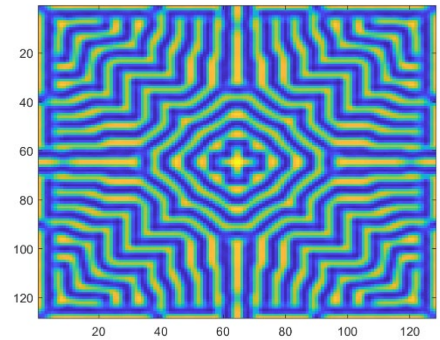

Figure 5: The Gray-Scott pattern formation at time t = 10,000. The pattern has expanded to fill the entire domain.

Multirate Integrators for Climate Microphysics. Climate processes inherently occur at a wide range of time scales, and many models include low accuracy schemes that will soon become insufficient as higher spatial resolutions are adopted. We explored the application of high order explicit-explicit multirate time integration methods in a MATLAB version of the Morrison-Gettleman 2 (MG2) cloud microphysics model (Gettelman and Morrison, 2015). In microphysics models sedimentation (e.g., rain) can occur at rates on the order of 100 times faster than other microphysics processes. Currently MG2 evolves the model state using a sequentially split explicit Euler method with substepped sedimentation. As shown in Figure 7, a third order multirate infinitesimal step method (Schlegel et al. 2009) is more efficient when compared to single rate explicit (Euler) and sub-stepped (Euler-SS) methods as greater accuracy is required. These gains in efficiency are in spite of a loss of order in the method likely due to discontinuities in the model, and we expect larger efficiency gains with model reformulation to remove these.

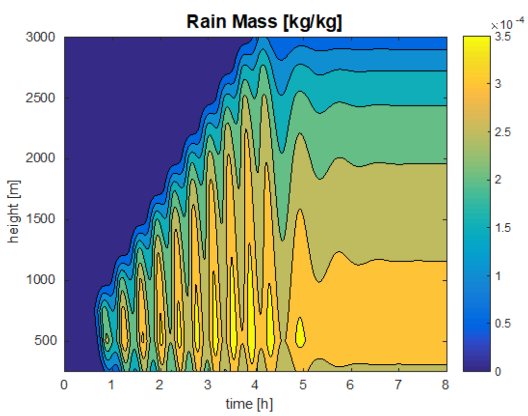

Figure 6: The evolution of rain mass in the Warm0 test case with a height dependent constant moisture source.

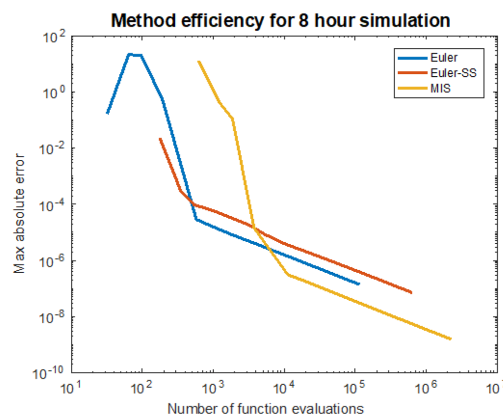

Figure 7: The max absolute error in rain mass after 8 hours versus the total number of function evaluations. For a given accuracy, lines further to the left indicate greater efficiency.

Multirate Integrators for Combustion. The Zero-RK (Zero-order Reaction Kinetics) software framework (McNenly et al., 2015) was utilized to explore the application of multirate Rosenbrock methods to chemical combustion simulations. We focused on variable partitioning of the state and a compound-fast multirating strategy. The partitioning approach divided the state into a limited subset of system variables that produce a local truncation error that is significantly larger than the local truncation error for other system variables. Tests with a second order Rosenbrock method showed improved compound step sizes in the two test cases employed. However, the cost of the refinement steps outweighed any savings from the increased compound step size. Tests with higher order Rosenbrock methods revealed the need for higher order Rosenbrock-W methods to handle approximate Jacobian data (Rang et al., 2005). A higher order Rosenbrock-W method could prove more efficient and offer more opportunities for optimization. However, outperforming an adaptive order and step single-rate linear multistep integrator will still be challenging given the increased number of stage solves required for a multistage method. As such, further development of multirate multistep methods could be beneficial for this problem.

Multirate Integrators for Reacting Flow. Solve-decoupled implicit mulitrate and predictor-corrector implicit multirate methods were tested on a reactive-flow unsteady flame problem using two reaction mechanisms (Lapoint, et al. 2019). The stiff chemical reactions were assigned to the fast partitions and the advection-diffusion transport to the slow partition of each integrator. Previously, linear multistep methods (BDF) were applied. The stability region of the BDF methods corresponds well to the real-axis dominated eigen-spectrum of the problem. The solve-decoupled multirate methods were found to lack sufficient stability to be competitive, requiring the step size to be reduced relative to the unirate methods. The predictor-corrector methods, on the other hand, were found to be more than sufficiently stable. However, the methods' use of a coarse-first step resulted in a large cost. Furthermore, there was strong coupling between the problem components resulting in a lack of regime where the efficiency of the predictor-corrector method was as good as a unirate method. Thus, either the problem is too coupled for multirate methods or the cost of the fast partition must be greatly lowered before the predictor-corrector method will be competitive on a reactive-flow problem of this type.

Impact on Mission

This project was directly relevant to the Laboratory's Core Competency in High-Performance Computing, Simulation, and Data Science. Specifically, it has increased Laboratory expertise in time integration methods and software for multiphysics and multiscale problems, such as are found in climate, combustion, and astrophysics, among many others throughout the DOE, especially among exascale applications. The LLNL SUNDIALS library is at the forefront of time integration libraries for single physics applications. This project provided the necessary research foundation that, along with later implementations, will move SUNDIALS to the forefront of packages for multiphysics applications. In addition, the project allowed the time integration group at LLNL to strengthen ties with three academic researchers through student summer projects. Lastly, the project brought a series of excellent summer students to LLNL which will, hopefully, provide a pool of future job candidates.

Conclusion

This project developed both new multirate time integration methods and accuracy and stability theory. The project also built collaborations between LLNL and academic researchers in the area, and the project team will continue these collaborations through completion of papers and participation on student PhD committees. Follow-on work in the area of software for multirate integration methods has been initiated through a project in the DOE Office of Science Advanced Scientific Computing Research (ASCR) office and further work will be proposed in an upcoming proposal. In addition, the SUNDIALS team has begun working with applications beyond those in this project, including WCI and fusion areas, to apply multirate methods to their problems. Lastly follow-on work in the climate area was approved for funding in a project jointly funded through the ASCR and BER offices of the DOE Office of Science.

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Notes to the Editors

Is there anything you think we should know? Are there any special symbols, super-, or subscripts to watch out for?