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On the Gauss Runge-Kutta and Method of Lines Transpose for Initial-Boundary Value Parabolic PDEs

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Abstract. It has been shown in existing analysis that the Gauss Runge-Kutta (GRK) (also called Legendre-Gauss collocation) formulation is super-convergent when applied to the initial value problem of ordinary differential equations (ODEs) in that the discretization error is order $2s$ when s Gaussian nodes are used. Additionally, the discretized system can be solved accurately and efficiently using the spectral deferred correction (SDC) or Krylov deferred correction (KDC) method. In this paper, we combine the GRK formulation with the Method of Lines Transpose (MoL^T) to solve time-dependent parabolic partial differential equations (PDEs). For the GRK-MoL^T formulation, we show how the coupled spatial differential equations can be decoupled and efficiently solved using the SDC or KDC method. Preliminary analysis of the GRK-MoL^T algorithm reveals that the super-convergent property of the GRK formulation no longer holds in the PDE case for general boundary conditions, and there exists a new type of "stiffness" in the semi-discrete spatial elliptic differential equations. We present numerical experiments to validate the theoretical findings.

AMS subject classifications: 65F08, 65M12, 65M22, 65M70

Key words: Gauss Runge-Kutta, Method of Lines Transpose, parabolic system, stiffness, order reduction, spectral deferred correction, Krylov deferred correction.

1 Introduction

One approach to numerically discretizing the initial value problem of ordinary differential equations (ODEs) is to use the Gauss Runge-Kutta (GRK) formulation (also called the Gaussian collocation, or Legendre-Gauss collocation, or differential quadrature method)

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[13,21,23]. In such a formulation, to march from $t=0$ to $t=\Delta t$, s Gaussian nodes in $[0,\Delta t]$ are chosen, and a polynomial solution in t is sought such that it satisfies the differential equation at the Gaussian collocation points. It was shown that GRK formulation has excellent accuracy and stability properties for the ODE systems. Particularly, assuming the solution is sufficiently smooth, the formulation is A-stable, B-stable, symplectic, symmetric, and super-convergent (order $2s$ when s Gaussian nodes are used) [23]. For a fixed Δt and a smooth solution, the discretization error decays exponentially when s increases. This is not surprising as the GRK formulation is also the *pseudo-spectral* formulation in the temporal direction.

Despite of such excellent accuracy and stability properties, higher order GRK formulation was rarely used previously to solve the initial value problem of ODEs. As far as we know, the highest order of available GRK solvers based on the Newton's method is 10 using 5 Gaussian nodes [23]. The reasons for this choice can be partially seen by considering the computational complexity when solving a system of N nonlinear ODEs using the GRK formulation. Notice that in order to solve the linearized equations at each Newton's iteration of a nonlinear GRK formulation, a prohibitive $\mathcal{O}(s^3N^3)$ work is required if Gauss elimination is used because the unknowns at different nodes (times) are coupled. In comparison, at the cost of reduced step size for stiff systems, an explicit time-stepping method involves significantly less work at each time step as no equation solve is needed. Also, a backward differentiation formula (BDF) type linear multistep method only requires $\mathcal{O}(N^3)$ work [7], and a diagonally implicit Runge-Kutta (DIRK) method requires $\mathcal{O}(N^3s)$ operations at each time step [22].

Recently, the classical deferred and defect correction strategies [3–5,32,33,40,41] have been revisited to efficiently solve the higher-order (more than 20) orthogonal polynomial-based collocation discretizations of the initial value ODEs, including the GRK formulation. In particular, the spectral deferred correction (SDC) method was studied in [15], in which a low-order method was used to solve an "error" equation iteratively to refine the polynomial approximation on the Gaussian nodes. The computational complexity of the SDC method is $\mathcal{O}(ksN^p)$, where k is the number of corrections (iterations) that is often set to s in existing implementations, $p=3$ when Gauss elimination is applied to the linearized equation in the Newton's method, and $1\leq p<3$ when the special structures in the linearized system are utilized. Later in [24], it was pointed out that if the iterative procedure converges, the solution solves the GRK formulation, and the SDC procedure is a special path to the convergence. In fact, for linear ODE problems, the SDC method is equivalent to a preconditioned Neumann series expansion where the low-order method is used as a preconditioner to the higher-order GRK discretization (see Eq. (33) in [24]). These observations not only clarify the analysis of the SDC method, but also suggest the possibility of introducing the Krylov subspace method to the preconditioned system for further acceleration. We refer interested readers to [25] for the details of the Krylov deferred correction (KDC) method for the efficient solution to the GRK formulation for ODEs. In their numerical experiments, orders up to 80 (40 Gaussian nodes) were tested and the KDC method compared favorably against many existing time-marching tech-