Implicit time integration schemes in electromagnetic-micromagnetic and quantum problems

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Efficient numerical time integration schemes are of great importance in solving time domain problems in electromagnetics, micromagnetics, and quantum mechanics. Problems addressing magnetic materials are often non-linear and the electromagnetic-magnetization dynamics is solved by coupled time domain Maxwell-Landau-Lifshitz-Gilbert (LLG) equations. Such formulations allow modeling materials and devices used in various applications, such as integrated inductors, soft materials used in power applications, and magnetic write heads. In quantum mechanics, time domain density functional theory (TD-DFT) is widely used to model non-stationary excitations of complex atomistic and molecular systems and it can also be coupled with time domain Maxwell equations to account for electromagnetic time retardation effects. In these examples, there is a need to numerically integrate the solutions in time, which is challenging because the non-linear problems can be numerically stiff and unstable.

Here, we present efficient time integration schemes for significantly increasing the numerical time step and increasing the computational speed in time integrating non-linear time domain Maxwell-Landau-Lifshitz-Gilbert (LLG) equations and TD-DFT. In solving micromagnetic problems, the time integration difficulties arise from instability and numerical stiffness caused by the exchange field, which becomes very strong when the basis functions of unknown spatial locations are closely spaced. Related to the exchange field, numerical instabilities arise when using explicit time integration schemes and they require using very small time steps. Addressing these difficulties requires using implicit time integration schemes. Specifically, we use an implicit midpoint rule specifically designed to exactly preserve the magnetization vector length as well as the backward differentiation formulas (BDF) with an automatic variable step variable order implementation to allow handling drastic differences in the time step required for highly non-linear switching processes. These schemes are based on Newton iterations assisted with a linear solver. For stiff problems the linear solver has a slow converge. We introduced and implemented efficient preconditioning techniques, referred to as block inverse preconditioner (BIP), which are based on directly inverting critical matrix blocks. Such preconditioners lead to a major reduction of the number of linear iterations, thus leading to the reduction of the time step and increase of the computational speed. Similar techniques are used in time domain integration of TD-DFT. Here, we also use the mid-point rule and BDF with Newton iterations assisted with a linear solver. We identify that the source of a slow convergence is the presence of the Laplacian operator and use its approximate inversion as a preconditioner for the linear solver. This approach reduces the number of linear iterations at a low computational cost as omits doing computationally heavy operations of computing superpositions.

We, then, demonstrate how such time integration techniques are used for applications in solving the magnetization dynamics and complex magnetic devices, such as magnetic random access memories and magnetic hard drive heads, as well as wave function dynamics in quantum systems.