

ACCELERATING MULTI-TIME-STEP METHODS USING MACHINE LEARNING FOR COMPUTATIONAL FLUID AND STRUCTURAL DYNAMICS

Sunbeom Kwon

In semi-discrete methods for solving partial differential equations (PDEs), direct time integration schemes are widely used to obtain fully discrete equations from ordinary differential equations (ODEs). Time integration can be categorized into implicit and explicit schemes. For nonlinear problems, implicit-explicit (IMEX) schemes have been proposed to achieve a lower computational cost than fully implicit schemes, while leading to a larger stability range than fully explicit schemes. In IMEX schemes, linear terms are handled implicitly and nonlinear terms are treated explicitly, eliminating the need for nonlinear iterations at each time step.

In conventional time integration schemes, a uniform time step is used for the entire problem domain. However, for large structures with complex geometries, wave propagation problems in heterogeneous media, and computational fluid dynamics (CFD), the use of a uniform time step leads to a high computational cost and/or yields less accurate numerical solutions. As an alternative, we can use multi-time-step (MTS) methods, where different time steps are used for temporal discretizations for different subdomain.

In this study, novel MTS methods for various types of time integration schemes (e.g. explicit, implicit, and IMEX schemes) in fluid dynamics and transient structural mechanics are developed using a dual-Schur domain decomposition, where constraint conditions are imposed at the subdomain interfaces using Lagrange multipliers. Using these methods, a problem domain can be divided into smaller subdomains which are integrated in time using different time steps and/or different time integration schemes to achieve accurate solutions at low computational cost. Furthermore, the machine learning approach is incorporated into MTS methods to streamline the computationally intensive process of conventional MTS methods to accelerate simulations.

First, we introduce a scalar auxiliary variable (SAV) stabilization of IMEX k th-order backward difference formulas (BDF k) schemes for nonlinear structural dynamics. The proposed IMEX-BDF k -SAV schemes achieve up to k th-order accuracy, while maintaining unconditional energy stability, eliminating the need for nonlinear iterations at each time step. Extending the stable IMEX schemes, we develop a MTS-IMEX-SAV method in conjunction with a non-overlapping domain decomposition for solving incompressible Navier-Stokes equations. The proposed IMEX-IMEX-SAV method is unconditionally stable and involves only linear algebraic systems, reducing computational costs.

Next, to tackle the challenge of simulating stiff-flexible structural systems, we propose, for the first time, a MTS method for composite time integration schemes. We prove its unconditional stability analytically and demonstrate its superior performance compared to existing MTS methods. Furthermore, to overcome a critical limitation of existing MTS methods (i.e. drift in displacements), a unified MTS framework with SAV stabilization is developed to enable simultaneous enforcement of multiple continuity constraints. Using the framework, new MTS methods are designed to eliminate the drift in displacements.

Finally, to streamline the computationally intensive 3-step process of MTS methods, we incorporate the machine learning (ML) approach into MTS methods. In the proposed ML-assisted MTS method, a recurrent neural network predicts the time series of Lagrange multipliers needed to couple the subdomains. The predicted Lagrange multipliers are used to advance the subdomain solutions using conventional time integration schemes, enabling coupling of subdomains in a single pass. The performance of this ML-assisted approach is compared to existing MTS methods in terms of accuracy and computational costs.