Accelerated multi-temporal scale approach to fatigue failure prediction

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Abstract

In this work, we present a computational approach to high cycle fatigue life prediction with an efficient solver employing time-discontinuous Galerkin (TDG) based space-time finite element method and its enriched version (XTFEM) [1, 2] in three dimensions. While the robustness of TDG based space-time FEM has been extensively demonstrated, a critical barrier for the extensive application is the large computational effort due to the additional temporal dimension and enrichment that are introduced. By formulating a new preconditioner and utilizing the properties of Kronecker product, we developed a generic iterative algorithm for solving the fully-coupled block-structured matrix equations formulated by space-time FEM. This approach reduces the computational cost to the same order of solving the corresponding static FE problems. The established numerical framework is further integrated with a multiscale damage model for the purpose of capturing failure initiation and propagation. The efficiency and robustness of the proposed method are illustrated in numerical examples, in which we show much better performance over direct solution of the original TDG matrix equations using either sparse direct or iterative solvers

Keywords: Space-Time FEM, XTFEM, Parallel Computing, GPU, Fatigue

Introduction

Past studies have shown that space-time finite element based on the time-discontinuous Galerkin (TDG) formulation leads to A-stable, higher-order accurate ODE solvers [3-5]. The TDG-based method has been extended to second-order hyperbolic systems such as elastodynamics [6-9]. It significantly reduces the artificial oscillations that are commonly associated with semi-discrete time integration schemes in capturing sharp gradients. Recently, it has been shown that its predicative capabilities in the temporal domain can be further improved by enriching the standard shape functions with a function that represents the problem physics, such as multi-temporal scale fatigue life prediction problems [2, 10] or coupled atomistic/continuum multiscale problems [1, 11, 12]. The enriched method is termed the extended space-time FEM (XTFEM). However, due to the additional temporal dimension and enrichment that are introduced, space-time FEM and XTFEM lead to systems of coupled equation larger than those emanating from regular semi-discrete methods, which becomes a critical barrier for practical applications in terms of computational cost.

By casting the coupled equations to partly decoupled forms, iterative predictor/multi-corrector algorithms have been developed in past decades [9, 13, 14]. These methods have been proved to be unconditionally stable and widely employed for TDG-based two-field formulation, as the resulting matrix equations are only weakly coupled. However, the single-field formulation employed in current implementation leads to fully coupled matrix systems, thus the algorithms developed for the two-field formulation are not directly applicable. Previously, we proposed a generalized iterative solution approach for both space-time FEM

and XTFEM in two dimensions [10], which significantly reduced the computational effort. In current work, we further extend this approach to three dimensions by developing a new preconditioning technique. Unlike the iterative predictor/multi-corrector algorithms, the new approach reduces the computational cost to the same order of solving the corresponding static finite element equations without explicitly recasting the original block-structured matrix systems. Furthermore, parallel algorithms based on multi-core graphics processing unit (GPU) are established in order to accelerate the solution of nonlinear constitutive model employed in fatigue damage problems. Finally, numerical examples are given to demonstrate the efficiency and robustness of the proposed method.

Space-Time Finite Element Method

Regular Space-Time FEM

The regular space-time FEM in current work follows largely the single-field formulation of TDG for elastodynamics [7]. In TDG formulation, the space-time domain $\Omega \times]0, T[$ is first divided into multiple segments called space-time slabs and the n-th slab given as $Q_n = \Omega \times]t_{n-1}, t_n[$, then Q_n is further discretized into $(n_{el})_n$ space-time elements. We further introduce the jump operators

$$[[\mathbf{u}(t_n)]] = \mathbf{u}(t_n^+) - \mathbf{u}(t_n^-) \tag{1}$$

where $\mathbf{u}(t_n^\pm) = \lim_{\varepsilon \to 0^\pm} \mathbf{u}(t_n \pm \varepsilon)$. By introducing the trial functions $\mathbf{u}^h(\mathbf{x}, t)$ and test functions $\delta\mathbf{u}^h(\mathbf{x}, t)$ to be C^0 continuous within each slab, the weak form of TDG formulation can be expressed as,

$$\begin{aligned} 0 = &\int_{Q_n} \delta\dot{\mathbf{u}}^h \cdot (\rho\ddot{\mathbf{u}} - \mathbf{f})\,\mathrm{d}Q + \int_{Q_n} \delta(\nabla\dot{\mathbf{u}}^h) \cdot \boldsymbol{\sigma}(\nabla\mathbf{u}^h)\,\mathrm{d}Q + \int_{\Gamma_t} \delta\dot{\mathbf{u}}^h \cdot \mathbf{t}\,\mathrm{d}\Gamma \\ &+ \int_{\Omega} \delta\dot{\mathbf{u}}^h(t_{n-1}^+) \cdot \rho[[\dot{\mathbf{u}}(t_{n-1})]]\,\mathrm{d}\Omega + \int_{\Omega} \delta(\nabla\mathbf{u}^h(t_{n-1}^+)) : [[\boldsymbol{\sigma}(\nabla\mathbf{u}^h(t_{n-1}))]]\,\mathrm{d}\Omega \end{aligned} \tag{2}$$

for $n = 1, 2, \ldots, N$, where ρ is the mass density, $\boldsymbol{\sigma}$ is the stress, $\mathbf{f}$ is the body force and $\mathbf{t}$ is the prescribed traction on boundary Γ_t. Note that the first line of Eq. (2) represents the regular weak form of linear elastodynamics in Galerkin formulation, while the second line enforces the velocity and displacement continuity in time.

In current work, a multiplicative form of the space-time shape function is adopted as

$$\mathbf{N}(\mathbf{x}, t) = \begin{bmatrix} N_{t_1}\mathbf{N}_\mathbf{x} & \cdots & N_{t_i}\mathbf{N}_\mathbf{x} & \cdots & N_{t_k}\mathbf{N}_\mathbf{x} \end{bmatrix} \tag{3}$$

where $\mathbf{N}_\mathbf{x}$ and N_t are the spatial and temporal shape functions respectively. This form allows us to discretize the spatial and temporal domain independently. Shape functions from the regular finite element can be employed for $\mathbf{N}_\mathbf{x}$. For temporal shape function, a simple 3-node quadratic interpolation scheme has been employed. Three nodes at t_{n-1}, $t_{n-1/2}$ and t_n are equally spaced along the time axis for each space-time slab and

$$\mathbf{N}_t = \frac{1}{\Delta t^2}\begin{bmatrix} 2(t_n - t)(t_{n-1/2} - t) & -4(t_n - t)(t_{n-1} - t) & 2(t_{n-1} - t)(t_{n-1/2} - t) \end{bmatrix} \tag{4}$$

in which Δt is the time step.

After substituting the space-time approximation into the weak form, we arrive at the space-time stiffness equation in the form of $\mathcal{K}\mathbf{d} = \mathcal{F}$, in which the fully-coupled, block-structured linear system matrix is given as

$$\mathcal{K} = \begin{bmatrix} \frac{5\mathbf{M}}{\Delta t^2} + \frac{\mathbf{K}}{2} & -\frac{4\mathbf{M}}{\Delta t^2} - \frac{2\mathbf{K}}{3} & -\frac{\mathbf{M}}{\Delta t^2} + \frac{\mathbf{K}}{6} \\ -\frac{12\mathbf{M}}{\Delta t^2} + \frac{2\mathbf{K}}{3} & \frac{16\mathbf{M}}{\Delta t^2} & -\frac{4\mathbf{M}}{\Delta t^2} - \frac{2\mathbf{K}}{3} \\ \frac{7\mathbf{M}}{\Delta t^2} - \frac{\mathbf{K}}{6} & -\frac{12\mathbf{M}}{\Delta t^2} + \frac{2\mathbf{K}}{3} & \frac{5\mathbf{M}}{\Delta t^2} + \frac{\mathbf{K}}{2} \end{bmatrix} \tag{5}$$

where **K** and **M** are regular spatial stiffness and mass matrix respectively.

Extended Space-Time FEM

The predicative capability of the space-time FEM can be further improved by introducing an enrichment function $\Phi(\mathbf{x}, t)$ into regular space-time shape function. Choice of such an enrichment function depends on the problem physics. The enriched space-time approximation is given as

$$\mathbf{u}(\mathbf{x},t) = \sum_{I=1}^{n_s} \mathbf{N}_I(\mathbf{x},t)\mathbf{d}_I + \sum_{J=1}^{n_e} \tilde{\mathbf{N}}_J(\mathbf{x},t)\mathbf{a}_J \tag{6}$$

where **a** represents the enriched degrees of freedom (DOFs), n_s and n_e are the numbers of standard and enriched DOFs respectively. There resulting formulation is then termed as XTFEM. For the *J*-th node the enriched shape function is

$$\tilde{\mathbf{N}}_J(\mathbf{x},t) = \mathbf{N}_J(\mathbf{x},t)\Phi_J(\mathbf{x},t) \tag{7}$$

in which $\Phi_J(\mathbf{x},t) = \Phi(\mathbf{x},t) - \Phi(\mathbf{x}_J, t_J)$.

Enrichment function adopted in current work has been proposed for high cycle fatigue problems [2, 10] and coupled atomistic/continuum simulations [1, 11, 12]. By employing a time dependent harmonic function, the enrichment function is given as

$$\Phi_J(t) = \Phi(t) - \Phi(t_J) = \sin(\omega t) - \sin(\omega t_J) \tag{8}$$

Similarly, the linear system matrix of XTFEM is obtained as

$$\mathcal{K}_e = \begin{bmatrix} \mathcal{K} & \mathcal{K}_{ea} \\ \mathcal{K}_{eb} & \mathcal{K}_{ee} \end{bmatrix} \tag{9}$$

where $\mathcal{K}$ is the regular space-time system matrix, $\mathcal{K}_{ea}$ and $\mathcal{K}_{eb}$ reflect the coupling between enriched and regular DOFs, $\mathcal{K}_{ee}$ reflects the coupling between enriched DOFs.

An Efficient Iterative Solver

Mathematical Formulation

As shown in Eqs. (5) and (9), linear system matrices formulated by either regular space-time FEM or XTFEM are block-structured and coupled with both conventional FE stiffness matrix **K** and mass matrix **M**, which can be expressed as

$$\mathcal{K}_{rs\times rs} = \mathbf{A}_{r\times r} \otimes \mathbf{K}_{s\times s} + \mathbf{B}_{r\times r} \otimes \mathbf{M}_{s\times s} \tag{10}$$

where **A** and **B** are non-symmetric coefficient matrices obtained by temporal integration, symbol $\otimes$ denotes the Kronecker product. The size of matrices **A** (or **B**) and **K** (or **M**) are denoted by r and s respectively. The value of r is determined by both the order of temporal shape function and the number of enriched DOFs that are introduced to each node, it could be neglected when compared with the value of s for practical problems. For example, the temporal coefficient matrices formulated by regular space-time FEM in Eq. (5) are given as

$$\mathbf{A}_{r\times r}=\frac{1}{6}\begin{bmatrix}3&-4&1\\4&0&-4\\-1&4&3\end{bmatrix}_{3\times 3},\ \mathbf{B}_{r\times r}=\frac{1}{\Delta t^2}\begin{bmatrix}5&-4&-1\\-12&16&-4\\7&-12&5\end{bmatrix}_{3\times 3} \tag{11}$$

where $r = 3$ in this case.

The proposed linear system solver is based on preconditioned iterative methods. By employing the preconditioning techniques, the original linear equation of $\mathcal{K}\mathbf{d} = \mathcal{F}$ is converted to

$$(\mathcal{P}^{-1}\mathcal{K})\mathbf{d}=\mathcal{P}^{-1}\mathcal{F} \tag{12}$$

in which $\mathcal{P}$ is the preconditioner, **d** and $\mathcal{F}$ are unknown and force vectors respectively.

It is well known that the efficiency and robustness of these methods largely depends on the quality of the preconditioners. A good preconditioner $\mathcal{P}$ should be close to $\mathcal{K}$, and makes the resulting system easier to solve. In order to improve the numerical efficiency of the iterative solver, we further exploit and utilize the unique block-structure of the $\mathcal{K}$ matrix as shown in Eq. (10) to propose a new preconditioner. The new preconditioner is obtained as $\mathcal{P}=\mathbf{A}\otimes\mathbf{P}$, where $\mathbf{P}\approx\mathbf{K}$ is a preconditioning matrix obtained by approximating the spatial stiffness matrix **K**. The resulting computational effort is then reduced to the same order of solving the corresponding static finite element stiffness equations.

Numerical implementation

In current work, the Generalized Minimum Residual method (GMRES) [15] is employed as the iterative solver since the system matrix $\mathcal{K}$ is nonsymmetric. Preconditioning matrix **P** = **LU** in which **L** and **U** matrices are obtained by incomplete lower and upper factorization of the spatial **K** matrix with threshold strategy for dropping small terms and column pivoting (ILUTP) [15]. In order to reduce the number of fill-in entries that are introduced to the factor matrices during the factorization, which could lead to very expensive computation, a permutation of the **K** matrix is performed first by employing the Reversed Cuthill-McKee (RCM) reordering algorithm [16]. To overcome the demanding storage efforts, **K** and **M** matrices are stored in Compressed Sparse Row (CSR) format. Note that explicit formulation of the block-structured matrix $\mathcal{K}$ is no longer required in current implementation.

Numerical Example

Prismatic rod subject to cyclic fatigue loading

We consider a prismatic rod as sketched in Figure 1. The rod is fixed at left end and subject to a fully-reversed cyclic fatigue loading $p(t) = P_0\sin(2\pi ft)H(t)$ Pa at right end, where $H(t)$ is the Heaviside function. The amplitude and frequency of the cyclic loading are 10^6 Pa and 10 Hz respectively. The material properties are given as Young's modulus E = 211 GPa, Poisson's ratio ν = 0.3 and mass density ρ = 7850 kg/m^3.

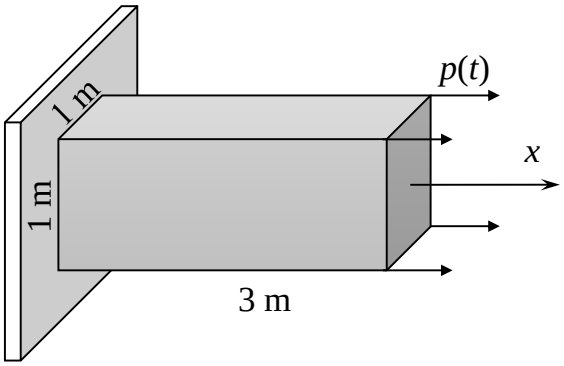

Figure 1. Illustration of the prismatic rod problem

This problem is simulated by XTFEM with a time step $\Delta t = 5T$ where T = 0.1 s is the period of loading cycle. The spatial domain is discretized by 8-node linear cubic elements. The computing environment is a desktop workstation with Intel Xeon CPU E5-2623v3, 16 Gigabytes RAM and NVIDIA TESLA GPU K20c. Displacement response is illustrated in Figure 1 and compared with solutions obtained from both explicit and implicit FEM using ABAQUS. The result obtained by XTFEM agrees well with those from traditional semi-discrete methods which require much smaller time steps. It shows that XTFEM is stable and accurate for the large time steps employed. This advantage of XTFEM would allow fast simulations on high-cycle fatigue loading histories.

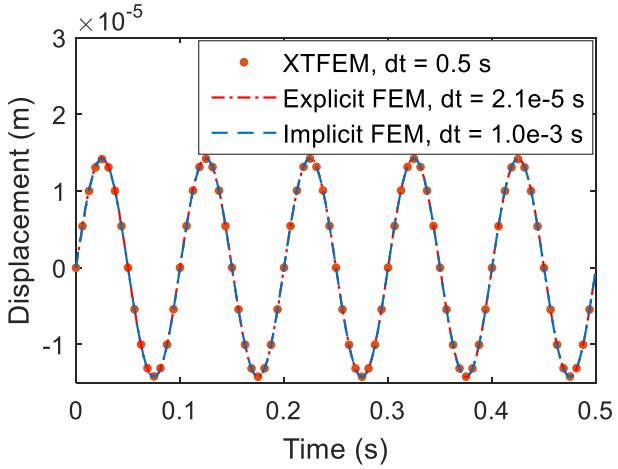

Figure 2. Displacement response at the free end of the rod subject to cyclic fatigue loading

In order to demonstrate the performance of the proposed iterative solver, a comparison study with regarding to both a sparse direct solver (SuiteSparse/UMFPACK) and a regular preconditioned iterative solver is conducted here. Note that the regular preconditioned iterative solver employed here is almost the same with the one developed in current work, except that the preconditioner is obtained directly from the large, block-structured space-time stiffness matrix. For these two iterative solvers, the dropping and pivoting tolerances of ILUTP preconditioner are set to 1.0e-3 and 1.0e-1 respectively, while the GMRES convergence tolerance is 1.0e-8.

By varying the size of spatial elements, N, the number of unknowns in the resulting linear systems formulated by XTFEM, ranges from 5,850 to 3,661,218. The computational performances of different solvers on those linear systems are summarized in Table 1. The memory usage is obtained from the storage of the **L U** factors due to their major contribution,

while time cost is measured by the CPU time for solving the first time step as the LU factorization is only performed at this step. In addition, the number of iterations to converge of the two iterative solvers also provided in Table 1. Symbol "/" indicates no results due to insufficient memory.

Table 1. Performance of different solvers in XTFEM simulations

DOFs	Sparse direct solver		Regular iterative solver			Current solver		
	Mem (MB)	Time (s)	Mem (MB)	Time (s)	Iters	Mem (MB)	Time (s)	Iters
5,850	224	12.5	21.7	4.4	76	1.6	0.04	13
36,450	7,764	3,254	300.5	160	290	20	1.0	47
484,218	/	/	4,865	8,432	1,332	333	41	151
3,661,218	/	/	/	/	/	2,722	680	309

Table 1 clearly demonstrates the advantages of the current solver over the other two and remarkable computational savings are achieved. In terms of computational complexity, the sparse direct solver showed an $O(N^{3.0})$ time cost and $O(N^{1.9})$ memory cost; The regular iterative solver achieved an better performance of $O(N^{1.7})$ and $O(N^{1.2})$ for time and memory costs respectively; Finally, the current solver further reduced the time cost to $O(N^{1.5})$ and memory cost to $O(N)$. In addition, the proposed solver also significantly reduced the number of iterations to converge. Thus, we conclude here that the proposed iterative solver efficiently and robustly accelerated the solution of linear systems formulated by XTFEM.

Conclusion

In summary, an accelerated multi-temporal scale approach is developed in current work for fatigue failure prediction in three dimensions. An efficient iterative solver with a new preconditioning technique is established for the fully-coupled, block-structured matrix equations that are formulated by TDG-based space-time FEM and XTFEM. This solver successfully reduces the computational cost from solving the large space-time matrix equations to the same order of solving the smaller corresponding static finite element equations without explicit matrix recasting. GPU-based parallel algorithms for the nonlinear constitutive fatigue damage model is coupled with XTFEM to predict fatigue failure. Numerical examples with unknowns up to ~3.7 million have been efficiently accelerated by the proposed method using single CPU process on a desktop workstation. The robustness of the solver is also extensively demonstrated. It shows that the computing time and memory of the accelerated implementation scale with the number of DOFs N through $O(N^{1.5})$ and $O(N)$ respectively.

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