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Distributed Computing for Phase-Field Models

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Abstract – ***We summarize here our recent results on the implementation of the Isogeometric Analysis (IGA) code for phase-field modelling, cluster configuration and weak performance studies, focusing on distributed computing aspects. Main examples are given for phase-field models for materials with memory.***

Key words – distributed computing, NURBS basis functions, shape memory alloys, MPI communication time.

I. Introduction

The phase-field (PF) models provide a unified framework that can describe phase transformations in many areas of applications. They are well suited for the description of complex dynamics. Among other applications, these models have been used to study microstructures and mechanical properties of materials across different scales, including materials with memory such as shape memory alloys (SMAs). We highlight here our recent results on the application of the Isogeometric Analysis to such models and our implementation of the code in the distributed computing environment.

II. Mathematical Model

In [1] we applied for the first time the Isogeometric Analysis (IGA) to deal with complex dynamics of materials with memory, focusing on SMAs. IGA employs the complex non-uniform rational B-spline (NURBS) based geometry in a finite element analysis application directly. IGA offers unique advantages in solving problems involving higher-order PDEs such as higher order accuracy, robustness, two- and three- dimensional geometric flexibility, compact support, and higher-order continuity. In many cases, higher dimensional PF models are too complex (e.g., having highly nonlinear hysteretic behavior, strong thermo-mechanical coupling, and fourth-order spatial differential terms for SMA models). Hence, to solve them on a regular workstation is not always possible. We use the distributed computing environment for their numerical solutions. The model we use here, as an example, is based on the following coupled equations derived from the Gizburg-Landau theory

$$\dot{\mathbf{u}} = \mathbf{v},$$

$$\rho\dot{\mathbf{v}} = \nabla \cdot \boldsymbol{\sigma} + \nabla \cdot \boldsymbol{\sigma}' + \boldsymbol{\sigma}_g + \mathbf{f},$$

$$\rho\dot{e} - \boldsymbol{\sigma}^T : (\nabla \mathbf{v}) + \nabla \cdot \mathbf{q} = g,$$

where our notations here are identical to those in [1]. We convert the system of the governing equations into the weak formulation. The domain is discretized where we use NURBS for our basis functions, while the generalized-α method is used for time integration along with an adaptive time stepping scheme.

III. Computational Implementation

The numerical implementation of the 2D and 3D IGA models for SMAs using the distributed computing environment has been first reported in [1]. In this implementation, the IGA codes use a multiple instruction, multiple data (MIMD) architecture. The domain decomposition technique has been employed in the distributed computing. The domain has been decomposed spatially into smaller subdomains using a separate script. We have used the high-performance clusters of the Sharcnet computational facilities in Canada, in particular the simulations have been carried out on the Saw cluster (with each node having two 4-core Intel E5440 Quad Core Processors (2.83GH, 4 GB + 8GB FBD PC2-5300 Memory, and 120GB of local storage) with InfiniBand 4X DDR running Linux CentOS release 6.3). The simulations have been performed utilizing full nodes and the performance data has been collected.

We have also performed the weak scaling test with each MPI (message passing interface) task on a tile of spatial dimension 16 nm × 16 nm for the 2D model. The geometry has been chosen such that it confirms the multiple of $8n$ processors, where node n has been chosen as $n = 1, 2, 3, 4$ and 8 for the MPI studies. A number of examples have been calculated on which it has been shown that the microstructure evolution is in agreement with known results from the literature.

We have observed that there is an opportunity to improve the computational efficiency by changing the code implementation, which is being investigated. The scaling can be improved, e.g. by using the concept of Bezier extraction or PETSc-based implementations.

Conclusion

In this contribution we have highlighted the methodology of solution of the coupled non-linear Ginzburg-Landau type PF models for SMAs reformulated in a variational framework. The numerical solution has been based on the IGA and its implementation in the distributed computing environment.

References

[1] *R. Dhote* et al, "Isogeometric Analysis of Coupled Thermo-Mechanical Phase-Field Models for Shape Memory Alloys Using Distributed Computing", Procedia Computer Science 18 (2013) 1068 – 1076, 2013.

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