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Title: A Partitioned - Task Parallel Implementation of the NASA Multiscale Analysis Tool for High Performance Computing

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ABSTRACT

The NASA Multiscale Analysis Tool (NASMAT) is a platform for multiscale modeling of composites which can perform analysis of materials with any arbitrary number of length scales. The platform supports modularity, scalability, and interoperability using recursive procedures and data structures. A macro solver driven parallelization scheme often limits the capability of NASMAT to scale as it has access to limited memory and number of cores (often one core/thread) and often forces the user to implement macro solver specific changes to the platform. In this work, a partitioned-task-parallel approach is adopted, where the parallelization strategy adopted for NASMAT is independent of the macro solver and the computational resources are managed independently. The programming architecture takes into account the hierarchy of multiple scales (task-dependence) and the heterogeneous nature (dynamic load balancing) of computation through implementation of a hierarchy-informed task parallel model. The partitioned nature of the framework further extends the “plug and play” capability of NASMAT. preCICE, an open-source library for coupling multi-physics solver in a partitioned manner, is adopted to integrate NASMAT with an external macro solver by implementing a NASMAT adapter for preCICE. Speedup and scalability of the framework is studied for micromechanical models of varying size.

INTRODUCTION

For hierarchical material systems such as composites, accurate simulation relies on understanding the fundamental mechanisms at underlying scales. The multiscale modeling technique enables simulating response of such material systems over multiple length and time scales. The technique aims to accurately capture the entire design envelope for such fit-for-purpose material system and has the potential to reduce the costly material development, testing and certification phases by augmenting and assisting the material development. Liu et al. encapsulated the vision and the broader perspective on multiscale modeling in NASA 2040 Vision [1].

In traditional constitutive modeling approach, a material point is assumed to be homogeneous and heterogeneity such as voids or fiber waviness is accounted through implicit mathematical formulations. In a multiscale setting, response of a given material point is obtained by interfacing with a lower scale with explicit heterogeneous definitions for morphology and constitutive responses. Various mathematical models are developed to solve the micromechanical boundary value problem of varying fidelity and accuracy. Analytical models such as Mori-Tanaka are often utilized to compute the effective response at lower scales [2,3]. Even though such models are computationally cheap, they often fail to provide spatially resolved fields. The Method of Cells (MOC) and its extensions including the Generalized Method of Cells (GMC) and High-Fidelity Generalized Method of Cells (HFGMC) are a set of powerful semi-analytical tools to undertake effective behavior of hierarchical materials and structures at microscale [3]. The coupling scheme employed to capture the interaction between scales is also of key interest, and it is broadly classified as hierarchical, concurrent, and synergistic [3]. The classification is based on the way information is passed between scales, either as boundary conditions or as effective properties.

Even though the adoption of multiscale modeling approaches is on the rise, two aspects that hinder its widespread adoption include:

1. Complexity of implementation associated with coupling (spatial and temporal) of the scales.
2. Computational costs associated with massively multiscale models for real engineering problems and the scalability in large High-Performance Computing (HPC) systems.

The NASA Multiscale Analysis Tool (NASMAT) is a state-of-the-art, “plug and play” software package that provides a multiscale, recursive, micromechanics framework for conducting massively multiscale modeling of hierarchical, nonlinear materials subjected to multi-physical loading conditions[4-6]. NASMAT can be integrated at micro- and macro-level to third-party codes at different scales through application program interfaces (APIs). Pineda et al. have successfully demonstrated the integration of NASMAT with ABAQUS in undertaking multiscale modeling for variety of engineering problems [4,5]. NASMAT has been developed to efficiently operate on HPC platforms to enable solution of industrial sized [>10 million macroscale degrees of freedom (DOF)] multiscale problems [5-6]. Recently, machine-learning based enhancements have been utilized within NASMAT to improve speed-up and scalability [8-9].

The current work aims to enhance the scalability and further expand the HPC-friendly capabilities of NASMAT through a partitioned task-parallel approach. Third-party macro solver integration of NASMAT is achieved in a partitioned manner, a common approach adopted in fluid-structure interaction modeling, through an open-source coupling library preCICE [7]. Macro solver driven parallelization scheme often limits the NASMAT’s capability to scale as it has access to limited memory and number of cores (often one core/thread) and often forces the user to implement macro solver specific changes to the platform. Viability of such schemes also limits the maximum number of scales or numerical size associated with an individual scale within a

multiscale analysis. In this work, the programming architecture takes into account hierarchy of multiple scales (task-dependence) and heterogeneous nature (dynamic load balancing) of the computation through the implementation of a hierarchy-informed task parallel model. Dynamic load balancing remains pivotal as inclusion of non-linearity at multiple scales can further skew the heterogeneity of tasks at runtime. Enhancement of APIs through preCICE allows for easy integration of NASMAT to other macro solvers and dissociates the parallelization strategy adopted within NASMAT from the macro solver. This also allows for quick and easy integration of NASMAT with pre-existing macro solver adapters available from preCICE (such as Calculix, OpenFOAM, FeniCS etc.) with minimal additional implementation [7].

The paper is organized as follows: the architecture of partitioned task-parallel approach is presented in detail in the first section. The scaling of the adopted approach is demonstrated by undertaking a three-scale analysis of RUC models of varying fidelity in the following section. Conclusion and future course of work are also further discussed.

NASA MULTISCALE ANALYSIS TOOL

Method

Four micromechanics theories of varying fidelity and accuracy are available within the NASMAT, including the Mori-Tanaka Method [2], and two from the method-of-cells family of theories [4], namely, double and triply periodic versions of Generalized Method of Cells (GMC) and High-Fidelity Generalized Method of Cells (HFGMC).

A unique feature within the NASMAT is the multiscale recursive micromechanics (MsRM) framework. As depicted in Fig. 1, a given repeating unit cell (RUC) at each scale (level) can be synergistically linked to RUC on the next lower scale. The scales are linked by equilibrating the homogenized average stress, strain and stiffness tensors at level i to the local stress, strain, and stiffness tensors of a given subvolumes at level $i-1$.

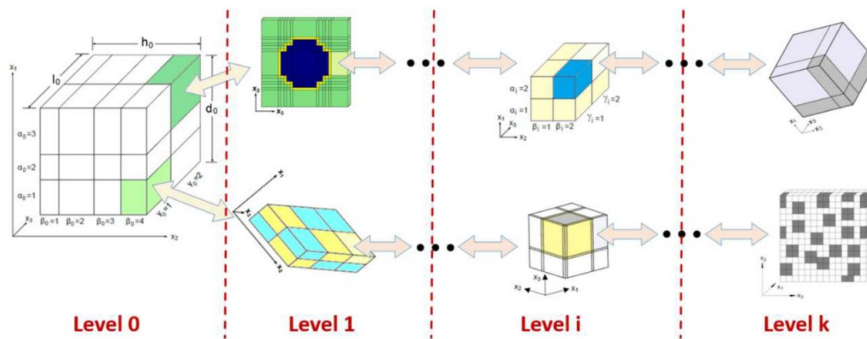


Figure 1: Schematic of the multiscale recursive micromechanics (MsRM) approach in NASMAT wherein micromechanics models are embedded within each other to model microstructure at any number of length scales

The effective stiffness tensor of all RUCs at the lowest scale k can be calculated using any standard micromechanics theory as all of its subvolumes contain only monolithic materials. This computed material stiffness tensor represents the constitutive material stiffness occupying one of the subvolumes within the RUC at the next higher-level $k-1$. Once the material stiffness is computed for all the subvolumes within the level $k-1$, the effective material stiffness tensor of the RUC at this level can be computed after accounting for any required subvolume coordinate transformations. The process is repeated until the highest level 0 is reached. Localization is performed by mapping stress and strain at level 0 (in the form of global applied field components) down through the scales to the lower level k using RUC strain concentration tensors, constitutive relationships, and coordinate transformations. Thus, the MsRM approach necessitates implementation of recursive architecture that allows for definition of any arbitrary number of scales and seamless passing of data across the scales.

Architecture

The design and architecture of NASMAT focuses on modularity, upgradability and maintainability, interoperability, utility and scalability. Modularity is achieved through compartmentalization of the code into 11 major procedure modules: Pre-processing, Driver, Engine, Solution, Homogenization, Material Model, Localization, State Change, Output, Post-processing, and Utilities. Detailed description on each set of procedure can be found in [4,6]. These modules are independently compiled into libraries and employed based on the type of multiscale problem and theory of micromechanics, thereby achieving the target of upgradability and maintainability. Interoperability with external software and libraries is attained through development of Application Program Interface (APIs) [4,5]. The NASMAT MacroAPI has already been successfully integrated with the commercially available ABAQUS finite element software [5]. Scaling NASMAT to support massively multiscale modeling to enable solutions of industrial size is achieved through HPC-friendly parallel implementations.

Partitioned Task-Parallel Approach

Previous versions of NASMAT relied on the parallelization capabilities of the macro solver in order to support massively multiscale modeling on HPC systems. Even though this supports the plug-and-play concept of NASMAT as intended, it severely restricts the available parallelization opportunities within NASMAT for scaling. For instance, maximum memory usage and CPU core/thread availability at runtime are dictated by the macro solver. Moreover, such monolithic external integration may also introduce macro-solver specific changes to the code, which goes against the design principles set forward for NASMAT.

In order to mitigate constraints as well as to expand wide-spread integration of NASMAT, a two-pronged approach is adopted in this work:

1. Extending NASMAT MacroAPI for partitioned approach using preCICE, an open-source library for coupling multi-physics solver [8]
2. Parallelization of NASMAT through task-parallel approach

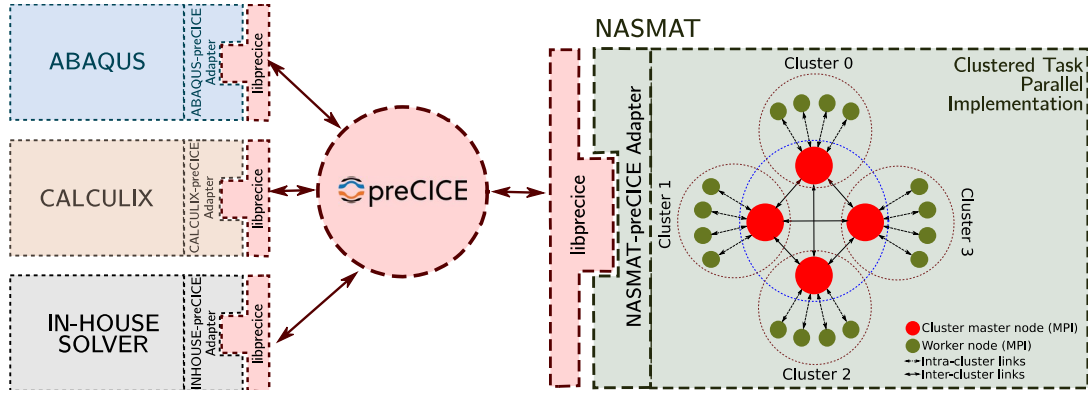


Figure 2: Partitioned task-parallel approach for NASMAT

In the adopted approach, NASMAT and the macro solver runs separately with each of them managing their computational resources independently. preCICE facilitates the synchronous communication between the individually managed processes at runtime. In this work, the NASMAT adapter for preCICE is implemented into the NASMAT MacroAPI. The approach dissociates NASMAT from macro-solver specific limitations for parallelization and allows for independent resource management. In addition, preCICE allows for quick and easy integration of NASMAT with pre-existing preCICE macro solver adapters (such as Calculix, OpenFOAM, FEniCS etc.) with minimal additional implementation.

Task-parallel Architecture

The inherent dependency between RUCs across scales is achieved through building a tree-like structure that accounts for inter-dependency across RUCs. Each tree consists of multiple nodes that correspond to each unique RUC type. A two-level tree with three unique RUC nodes is depicted in Fig. 3 along with material tags associated with each subvolume in each RUC. The parent-child relationship across the nodes is established using material tags associated with each subvolume. Negative material tags indicate that a subvolume contains a lower level RUC while positive values are individual defined constituents. For instance, in Level 0, there are two negative material tags that represent two unique RUC types and 9 total RUCs at Level 1 to allow for differences in subvolume location and field states.

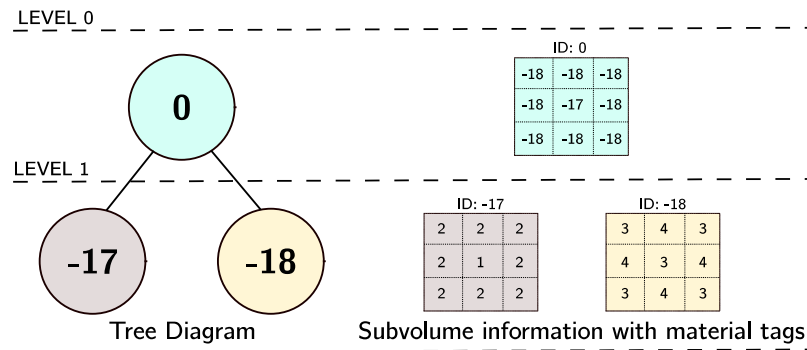


Figure 3: Example of two-level tree with 3 unique RUC nodes

Each homogenization/localization subroutine call is termed as a *Task*. The flowchart depicted in Fig. 4 illustrates the task-parallel architecture adopted in this work. The architecture is based on a Master-Work Parallelization paradigm, where the *Master* CPU orchestrates and manages the task that needs to be parallelized and the *Worker* CPU does the computation for homogenization/localization *Task*. Each RUC node is sent to a worker when all its children are homogenized. Conversely, the localization *Task* is carried out when all the parents are localized. In a clustered system, the current approach designates one *Master* CPU and multiple *Worker* CPUs in each compute node within the HPC. A queue-based data structure is widely adopted to achieve efficient task parallelization.

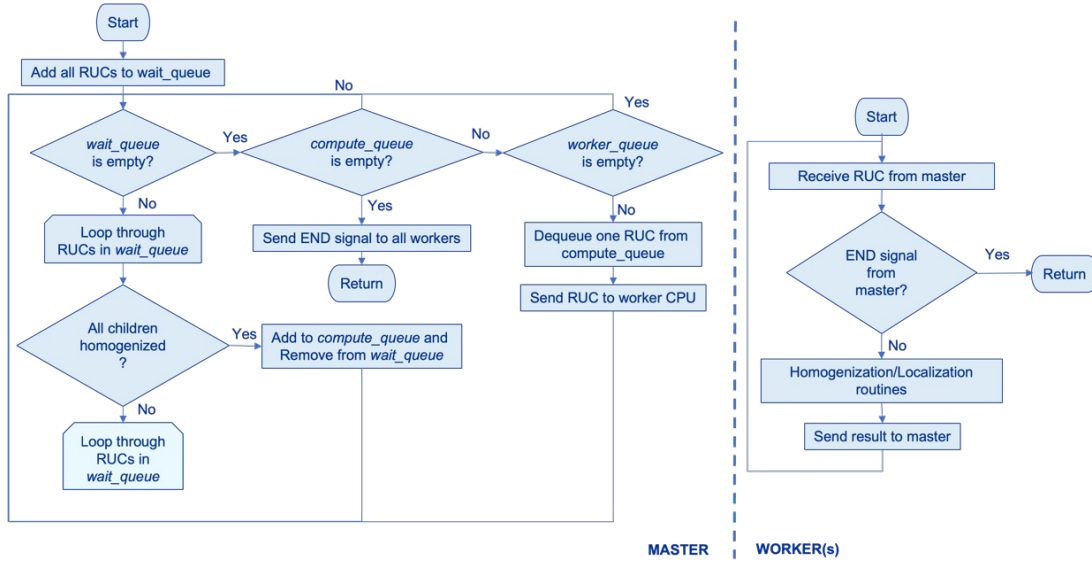


Figure 4: Flowchart for task-parallel architecture in NASMAT for homogenization/localization task

RESULTS AND DISCUSSIONS

The scalability of the partitioned task-parallel version of NASMAT is demonstrated through homogenization of three-scale models with four RUC nodes as depicted in Fig. 5 and *a,b,c* and *d* represents the number of subvolumes in each direction of RUC 0,-17,-18 and -19 respectively. Material tags associated with each RUC of an example subvolume size of 3 is also depicted in Fig. 5. GMC 2D is used as the local micromechanics models at each scale. The effect of problem size on the scalability is studied by varying the subvolume at each scale.

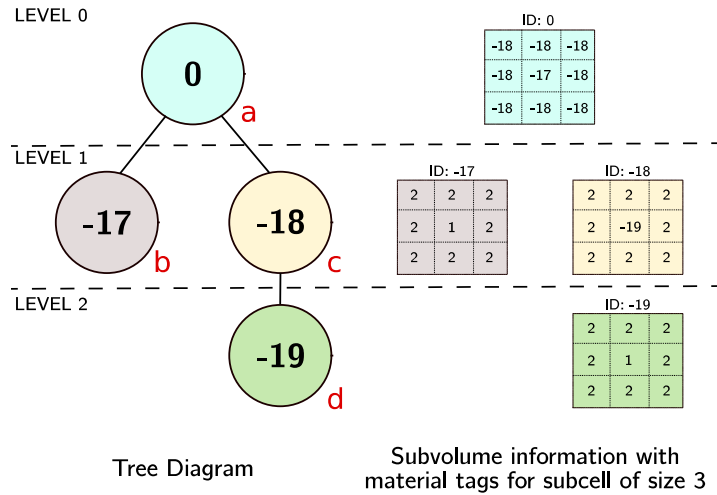


Figure 5: Tree diagram for three-scale homogenization problem

Three models are considered by varying the total number of subvolumes for the lowermost RUC. The number of subvolumes in each direction of the RUC nodes 0, -17 and -18 are kept constant at 5 and the number of subvolumes in each direction of RUC node -19 is varied from 100-500 leading to three configurations: 5-5-5-100, 5-5-5-300- 5-5-5-500. The total number of subvolumes in each RUC in a given configuration is equal to the square of the size. The analysis is run on a workstation consisting of 8 Intel Xeon CPU E5-2630 at 2.4 GHz with 24Gb of memory.

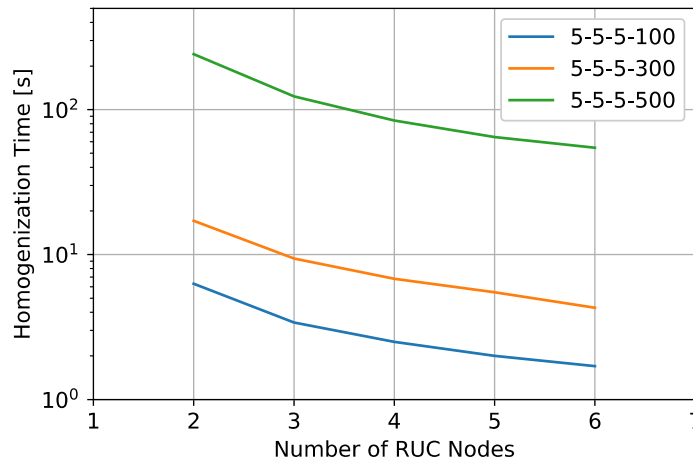


Figure 6: Homogenization time for different configuration of the three-scale problem

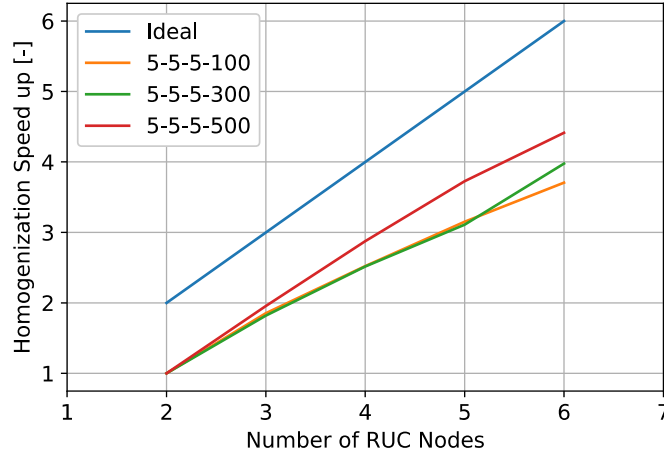


Figure 7: Speedup for different configuration of the three-scale problem

Figure 6 and 7 depicts the time taken and speedup for homogenization task for different configuration. All configurations exhibit reduced runtimes for homogenization as the number of CPUs are increased. It can be observed that the bottom heavy configuration (5-5-5-500) exhibits better speedup which can be attributed to the fact that dip in the speedup is observed when the time taken for inter CPU communication is in the same order as the computation. Since GMC 2D models are semi-analytical in nature, the computational intensity of a GMC 2D homogenization task is limited.

Future scope of work includes studying the scalability for computationally intensive micromechanical models such as HFGMC and finite element models within NASMAT. Most realistic multiscale model can have a combination of micromechanical RUC nodes of varying fidelity. The authors believe that the framework will exhibit stronger scaling for computationally intensive micromechanical models. Studying the scalability in tandem with macro-solver integration will also be investigated.

CONCLUSION

The NASA Multiscale Analysis Tool (NASMAT) is a powerful platform that can undertake multiscale analysis of composite materials and structure of arbitrary number of scales. The platform provides a family of micromechanics theories with varying fidelity and can be easily integrated with third-party macro solvers. The scalability of NASMAT is enhanced through a partitioned task-parallel architecture. The parallel architecture accounts for the hierarchy of multiple scales and their inherent dependence by building task-parallel trees. The integration of NASMAT with macro solver is achieved through an open-source coupling library preCICE, which allows for easy integration and dissociates the parallelization strategy adopted within NASMAT from the macro solver. The scalability is studied by varying the type of

micromechanical model and computational cost associated with each of them. Future scope of work includes the study of dependence of scaling on the size and type of micromechanics models and effect of macro solver integration.

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