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MACRO-MICRO SCALE DYNAMIC ANALYSIS OF 2D POLYCRYSTALLINE MATERIALS USING THE BOUNDARY ELEMENT METHOD

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Abstract. *The relevance of a multiscale analysis in polycrystalline materials is due to the change of physical properties of the modeled scale. This work presents a 2D dynamic analysis by bridging macro-micro scales, considering both isotropic and anisotropic properties for the material in different length scales. The Boundary Element Method (BEM) is formulated at macroscale to evaluate the nodal displacement as a consequence of transient loads applied to the surface. Subsequently, a partial region of the largest domain is modeled with internal points to evaluate the microscale analysis. At the smallest size, the Voronoi tessellation algorithm is included to generate random crystalline orientations, while the BEM multi-region methodology is applied by taking into account an anisotropic formulation. Finally, in order to validate the bridging methodology, a numerical example is presented.*

Keywords: *Polycrystalline Materials, Transient Analysis, Boundary Element Method, Anisotropic and Isotropic formulations.*

INTRODUCTION

The multiscale methodology has been proposed to analyze materials like metals, composites, bones, etc. The reason is the great influence that micro defects have in a macroscopic size. Usually, this methodology is developed by introducing computational methods to evaluate how a material responds to both operational and environmental conditions. However, there are fences to overcome when the information has been transferred between scales. The first one is the continuum and classical model used to approximate the geometric problem, and secondly the computational cost (Liu et al., 2017; Nguyen et al., 2017; Fu et al., 2016; Sun and Sundararaghavan., 2016; Sfantos and Aliabadi., 2007)

This research presents a dynamic analysis of a polycrystalline material from a macro to a micro scale by using the BEM. In order to consider the relevance of material properties at different scales, both isotropic and anisotropic fundamental solutions are included. Moreover, internal points are used as a new approach to share information between scales. A parallelization on a shared memory architecture, based on Fortran-OpenMP, is employed for the calculation for BEM matrices and to solve the sparse system of equations. A numerical example is presented showing the feasibility of the multiscale proposed framework.

BEM formulation for linear elasticity

The BEM is a computational tool used to solve linear elastic problems and particularly suitable in a dynamic approach with rapidly varying stress gradients. The boundary integral equation contains the displacement and traction fields. It is given by:

$$C_{ki}u_i + \int_\Gamma T_{ki}u_i d\Gamma = \int_\Gamma U_{ki}t_i d\Gamma + \int_\Omega U_{ki}b_i d\Omega \tag{1}$$

Equation (1) is an integral equation that rules the behavior of a solid body (domain Ω, boundary Γ), under tractions t_i, body forces b_i, and displacements u_i. U_{ki} and T_{ki} represent displacement and traction fundamental solutions, respectively; the term C_{ki} defines the free term coefficient.

Consequently, the domain integral presented in Equation (1) is modified by using the displacement $\hat{u}_{in}$ and traction $\hat{t}_{in}$ particular solutions (Partridge et al., 2012). It is rewritten as:

$$C_{ki}u_i + \int_\Gamma T_{ki}u_i d\Gamma = \int_\Gamma U_{ki}t_i d\Gamma + \sum_{j=1}^{N+L} \alpha_n \left(C_{ki}\hat{u}_{in} - \int_\Gamma U_{ki}\hat{t}_{in} d\Gamma + \int_\Gamma T_{ki}\hat{u}_{in} d\Gamma \right) \tag{2}$$

where α_n are a set of initially unknown coefficients. After introducing the interpolation functions to approximate the boundary and integrating over each element, Equation (2) can be expressed in terms of influence matrices H and G.

$$u_k + \sum_{j=1}^{N} H_{ki}u_i = \sum_{j=1}^{N} G_{ki}t_i + \sum_{m=1}^{N+L} \alpha_n \left(\hat{u}_{in} - \sum_{j=1}^{N} G_{ki}\hat{t}_{in} \sum_{j=1}^{N} H_{ki}\hat{u}_{in} \right) \tag{3}$$

Finally, Equation (3) can be extended to a transient domain (Dominguez., 1993), and it can be solved by the Houbolt integration approach (Houbolt., 1950). Equation (4) represents the boundary response at instant $\tau + \Delta\tau$ by using the information of the last three time-steps:

$$\left[\frac{2}{\Delta\tau^2}\mathbf{M} + \mathbf{H} \right] \mathbf{u}_{\tau+\Delta\tau} = \mathbf{G}\mathbf{t}_{\tau+\Delta\tau} + \frac{1}{\Delta\tau^2}\mathbf{M}(5\mathbf{u}_\tau - 4\mathbf{u}_{\tau-\Delta\tau} + \mathbf{u}_{\tau-2\Delta\tau}) \tag{4}$$

where $\mathbf{M}$ is the mass matrix defined like: $\mathbf{M} = \rho\mathbf{V} = \rho[\mathbf{H}\hat{\mathbf{u}} - \mathbf{G}\hat{\mathbf{t}}]\mathbf{E}$; the term $\mathbf{E}$ represents the inverse of approximating functions.

Multiscale implementation

The dynamic transition is carried out by using internal points at the macroscale and boundary prescribed conditions are evaluated in the microscale. Firstly, a rectangular isotropic domain is selected with aspect ratio 1:4. The BEM is applied and transient displacements are evaluated. Secondly, the internal response defines the boundary conditions at a micro area, which is characterized with random crystalline orientations by using the Voronoi tessellation algorithm (Okabe et al., 2000). In the microscale, a BEM multi-region technique is applied and anisotropic properties are evaluated. Figure 1 shows a flowchart of this multiscale framework.

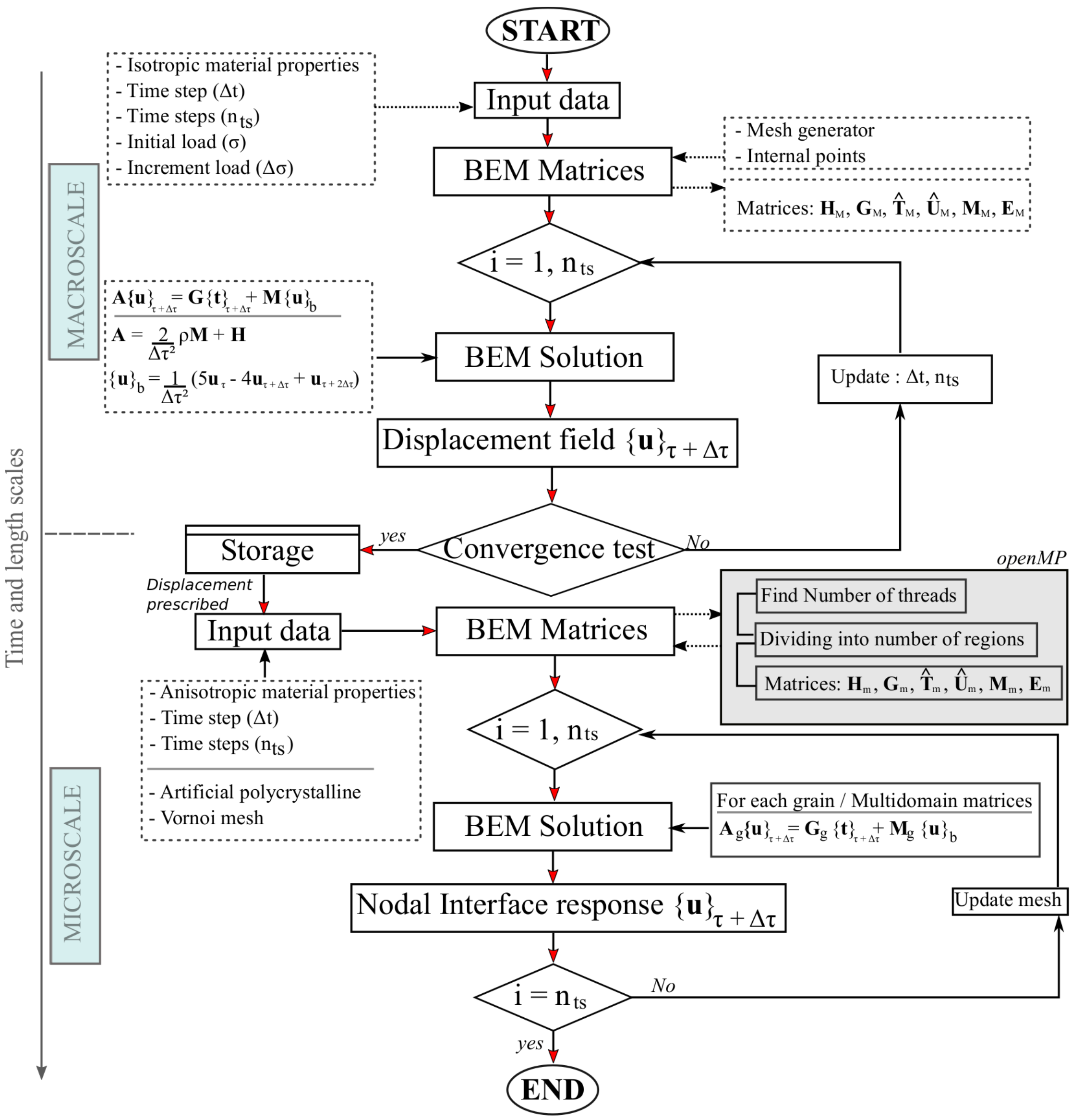

Figure 1: Flowchart of the multiscale framework

The validation of macro transient analysis is made with the exact solution proposed by Clough and Penzien (2002). Even though the effect of the Poisson's ratio is not included by the authors, it can be evaluated in order to compare to the results. The Iron properties are selected: $E = 210.4$ GPa, $\nu = 0.29$, $\rho = 7874.0$ kg/m^3. The 2D domain is defined with dimensions: W $= 50.0$ mm, H $= 200.0$ mm. The upper surface is loaded with a step $\sigma(t) = 100$ MPa, $\Delta t = 1.0$ μs. Figure 2 illustrates the results.

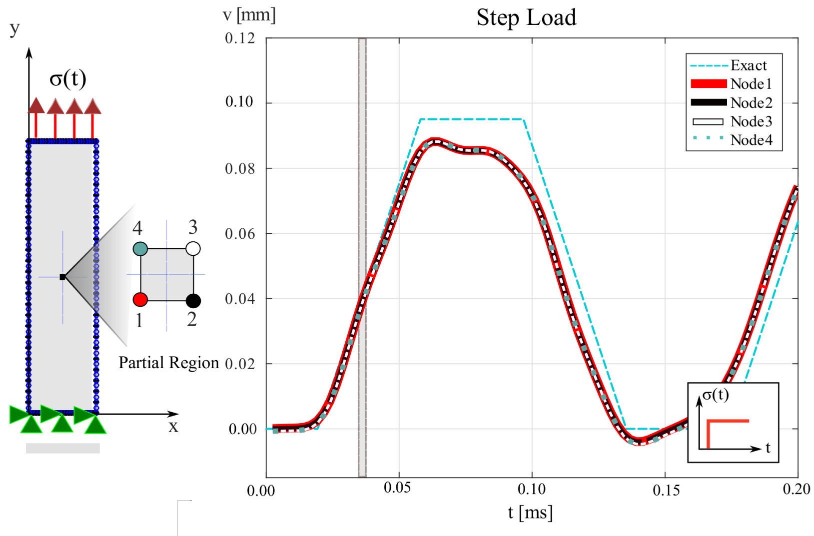

Figure 2: Nodal displacement at the macroscale

The partial region observed in Figure (2), is a granular area of 1 mm^2, and it is characterized with a BCC lattice. The constants registered by Kiewel (1996) are used: $C_{11} = 230.0$ GPa, $C_{44} = 117.0$ GPa, $C_{12} = 135.0$ GPa. In this case, transient displacements from the macroscale are defined like boundary prescribed conditions at the microscale. Furthermore, this polycrystalline contains 200 grains, and it is evaluated between 36.00 ns and 38.40 ns.

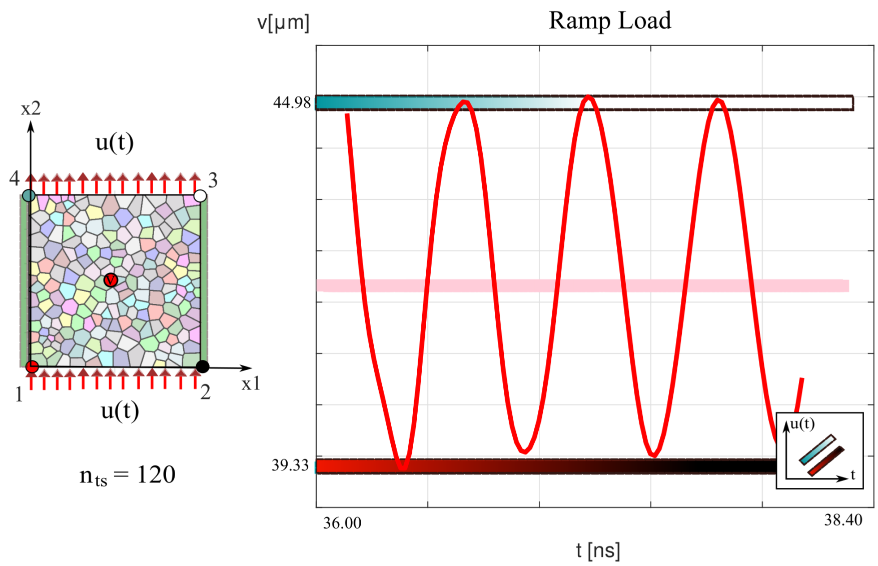

Figure 3: Nodal displacement at the microscale

CONCLUSIONS

This multiscale study intends to show the dynamic behavior of a microscopic area from a macro domain. As a result, a new methodology to transfer transient information is developed. Internal points and boundary prescribed conditions characterized the bridging approach, and an exact solution validated the present work. In order to approximate effectively the geometries of the problem, and to decrease the computational cost, the BEM was a valuable tool.

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