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Computational aspects of the weak micro-periodicity saddle point problem

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The finite element implementation of the weak micro-periodicity problem in computational homogenisation requires special preconditioning techniques owing to the saddle point formulation. The saddle point nature arises from enforcing periodicity constraints using Lagrange multipliers. This manuscript addresses the solution techniques and preconditioning options for the aforementioned problem in a monolithic setting. Furthermore, an alternative technique is proposed, based on a linear multi-point constraints strategy. The latter approach eliminates the Lagrange multiplier Degrees of Freedom (DOFs), thereby preventing the break-down of conventional incomplete LU (ILU) variants and multi-grid method based preconditioners.

1 Euler-Lagrange form of the weak micro-periodicity problem

The Euler-Lagrange equations for the weak micro-periodicity RVE[1] problem [1] is given as follows:

$$\frac{1}{|\Omega_\square|}\int_{\Omega_\square} \boldsymbol{\sigma} : \boldsymbol{\epsilon}[\delta \mathbf{u}] \, \mathrm{d}\Omega \; - \; \frac{1}{|\Omega_\square|}\int_{\Gamma^+_\square} \mathbf{t} \cdot [\![\delta \mathbf{u}]\!] \, \mathrm{d}\Gamma = 0 \quad \forall\, \delta \mathbf{u} \in \mathbb{U}_\square, \tag{1a}$$

$$- \frac{1}{|\Omega_\square|}\int_{\Gamma^+_\square} \delta \mathbf{t} \cdot [\![\mathbf{u}]\!] \, \mathrm{d}\Gamma = - \frac{1}{|\Omega_\square|}\int_{\Gamma^+_\square} \delta \mathbf{t} \cdot \boldsymbol{\epsilon}[\bar{\mathbf{u}}] \cdot [\![\mathbf{x}]\!] \, \mathrm{d}\Gamma \quad \forall\, \delta \mathbf{t} \in \mathbb{T}_\square, \tag{1b}$$

using the test and trial spaces, $\mathbb{U}_\square := \left\{ \mathbf{u} \in [H^1(\Omega)]^{\mathrm{dim}} \;\middle|\; \int_{\Omega_\square} \mathbf{u} \, \mathrm{d}\Omega = 0 \text{ in } \Omega_\square \right\}$, $\mathbb{T}_\square := \left\{ \mathbf{t} \in [L_2(\Gamma^+_\square)]^{\mathrm{dim}} \right\}$.
Here, the solution fields $\mathbf{u} \in \mathbb{U}_\square$ and $\mathbf{t} \in \mathbb{T}_\square$ represent the displacements and Lagrange multipliers (surface tractions), respectively, $\boldsymbol{\sigma}$ is the Cauchy stress, and $[\![\bullet]\!]$ is the jump operator defined as $\bullet^+ - \bullet^-$. Note that the superscripts $+$ and $-$ indicate RVE boundaries with positive and negative outward normal respectively.

The discrete form of the linear problem (1a,1b) attains the form

$$\begin{bmatrix} \mathbf{K} & \mathbf{P} \\ \mathbf{P}^{\mathrm{T}} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \tilde{\mathbf{u}} \\ \tilde{\mathbf{t}} \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \tilde{\mathbf{g}} \end{Bmatrix}, \tag{2}$$

where $\tilde{\bullet}$ indicates nodal values. Explicit expressions for $\mathbf{K}$, $\mathbf{P}$ and $\tilde{\mathbf{g}}$ are avoided for brevity. They can be derived upon linearisation of (1a,1b).

2 A note on solution and preconditioning techniques

A fully monolithic technique solves (2), for both displacement and Lagrange multiplier fields simultaneously. However, the presence of zero on the matrix diagonal leads to break-down in ILU and Cholesky factorisations and in the computation of multi-grid preconditoners. This manuscript uses symmetric incomplete LDL [2] and signed incomplete Cholesky factorisations [3]. Furthermore, a block diagonal preconditioning technique is also adopted with $\mathbf{P}^{\mathrm{T}}\mathrm{diag}(\mathbf{K})^{-1}\mathbf{P}$ for the Lagrange multiplier block and an ILU threshold pivoting factorisation for the displacement block.

Alternatively, the second block of equations in (2), i.e., $\mathbf{P}^{\mathrm{T}}\tilde{\mathbf{u}} = \tilde{\mathbf{g}}$ is re-arranged into a linear multi-point constraints formulation (see [4] for details). This approach eliminates the Lagrange multiplier DOFs, thereby allowing the use of ILU factorisation and multi-grid preconditioning techniques.

3 Numerical Study

The numerical study is carried out on a 2D plane strain linear elastic RVE of dimension 1 mm^2, with Young's Modulus 100 GPa and Poisson's Ratio 0.3. The displacement and Lagrange multiplier fields are discretised with constant strain triangular and piece-wise constant elements respectively. Weak micro-periodicity constraints allows independent discretisations for the

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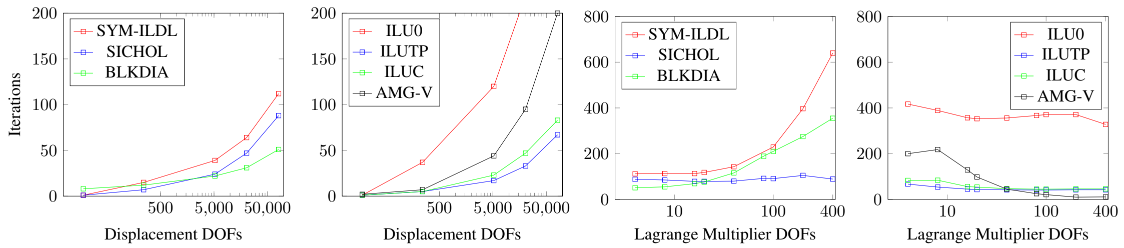
[1] RVE: Representative Volume Element

displacement and Lagrange multiplier fields. In this regard, the use of one Lagrange multiplier element per RVE edge $\in \Gamma_\square^+$ results in strain-controlled Neumann Boundary Condition (NBC), whereas using the same discretisation for both displacement and Lagrange multiplier results in Strong Periodic Boundary Conditions (SPBC). However, one could also choose a Lagrange multiplier discretisation that yields a constraint between NBC and SPBC [1].

Figure 1a and 1b presents the iterations required by the GMRES method to reach an absolute residual less than $1e-10$, for the fully monolithic and the linear multi-point constraints condensed method respectively. For both methods, irrespective of the preconditioning techniques, iterations required for convergence increases with system size (depicted with increase in displacement DOFs). For the fully monolithic method, the block diagonal preconditioner (BLKDIA) performs the best in terms of iterations required for convergence. The symmetric incomplete LDL (SYM-ILDL) and signed incomplete Cholesky (SICHOL) factorisation requires comparatively higher number of iterations. The linear multi-point constraint condensed method allows the use of ILU variants (no fill (ILU0), Threshold Pivoting (ILUTP) and Crout (ILUC) versions) and Algebraic Multi-Grid V-cycle (AMG-V) preconditoner [5]. The ILU0 preconditioning performs poorly whereas ILUTP and ILUC results in convergence with fewer iterations.



(a) (b) (c) (d)

Fig. 1: Iterations required the GMRES method to achieve convergence for (a) fully monolithic - NBC, (b) linear multi-point constraints condensed method - NBC, (c) fully monolithic - varying $\mathbf{t}$ discretisation, and (d) multi-point constraints condensed method - varying $\mathbf{t}$ discretisation.

Figure 1c and 1d presents the case where the displacement mesh is fixed (80802 DOFs) while the Lagrange multipliers DOFs are increased gradually starting for one element per RVE edge $\in \Gamma_\square^+$ (NBC case) towards SPBC. For the fully monolithic method, the SICHOL preconditioning is the best as the number of iterations does not change with an increase in the number of Lagrange multiplier DOFs. The use of the linear multi-point constraints condensed method results in decreasing number of iterations with increase in the Lagrange multiplier DOFs for ILUTP, ILUC and AMG-V preconditioners. In this context, the AMG-V preconditioner is found to be optimal for the 'nearly' periodic constraint (400 Lagrange Multiplier DOFs).

4 Conclusion

This manuscript addressed the solution techniques and preconditioning options for the weak micro-periodicity problem in computational homogenisation. For the strain-controlled NBC (one Lagrange multiplier element per RVE edge $\in \Gamma_\square^+$), the block-diagonal preconditioner, based on inverse diagonal of the $\mathbf{K}$ matrix led to faster convergence of the GMRES method. However, on adopting the linear multi-point constraints condensed method, ILUTP and ILUC also resulted in similar number of iterations. Moreover, on increasing the number of Lagrange multiplier elements (DOFs), the linear multi-point constraints condensed method augmented with the AMG preconditioner out-performs all other preconditioning techniques. In the view of future research, the solution and preconditioning techniques explored in this manuscript could be incorporated in studies involving computational homogenisation of complex heterogeneous RVEs, for instance, with micro-cracks [6], voids or inclusions.

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