Electronic Supplementary Materials

For https://doi.org/10.1631/jzus.A2100158

A novel multi-level model for quasi-brittle cracking analysis with complex microstructure

Xiao-xiao SUN, Xiang-yu CHEN, Xiao-ming GUO

Data S1 Implementation of MLPU

In this section, the implementation of MLPU is detailed. The degrees of freedom and element status of the global problem are to be obtained in each time step, and the responses of RVEs are solved simultaneously.

Denoting ${}^{h}\boldsymbol{d}$, ${}^{h}\boldsymbol{\chi}$ and ${}^{h}\boldsymbol{t}^{\mathrm{m}}$ the degrees of freedom, element status, and RVE reaction forces vector obtained in the *h*th time step, the procedure for solutions of the (*h*+1)th time step is described as follows.

(1) Determine element status

Using element status obtained from previous time step determine initial element status in time step (*h*+1). Here *iters* denotes the number of iterations corresponding to element status and $iters = 1$.

$$ {}^{h+1}_{iters}\boldsymbol{\chi} = {}^{h}\boldsymbol{\chi} \tag{S1}$$

Or using solved element status from previous iteration update current element status if convergence relating to element status has not been reached. Here $iters \geq 2$.

$$ {}^{h+1}_{iters}\boldsymbol{\chi} = {}^{h+1}_{iters-1}\boldsymbol{\chi}_{sol} = \Psi\left({}^{h+1}_{iters-1}\boldsymbol{d}, {}^{h+1}_{iters-1}\boldsymbol{\chi} \right) \tag{S2}$$

(2) Solve degrees of freedom

(i) $iters = 1$

(a) Using degrees of freedom obtained from the previous time step initialize current degrees of freedom if $iter = 1$, and initialize its increment. Here *iter* denotes the number of iterations corresponding to degrees of freedom.

$$ {}^{h+1}_{iter,iters}\boldsymbol{d} = {}^{h}\boldsymbol{d} \tag{S3} $$

$$ {}^{h+1}_{iter,iters}\Delta\boldsymbol{d} = \boldsymbol{0} \tag{S4} $$

Or use Newton's method updating degrees of freedom ${}^{h+1}_{iter,iters}\boldsymbol{d}$ and its increment ${}^{h+1}_{iter,iters}\Delta\boldsymbol{d}$. Here $iter \geq 2$.

(b) If the RVE corresponding to material particle *l* is activated, update the status and reaction forces vector of the RVE using increment ${}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}$ and element status ${}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}$.

$$ {}^{h+1}_{iter,iters}\boldsymbol{t}^{\mathrm{m}}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) = {}^{h}\boldsymbol{t}^{\mathrm{m}} + {}^{h+1}_{iter,iters}\Delta\boldsymbol{t}^{\mathrm{m}}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \tag{S5} $$

(c) Update domain forces using RVE reaction forces

$$ \begin{aligned} {}^{h+1}_{iter,iters}\boldsymbol{F}^{0,[l]}_{fp} = & \sum_{np\in m_{k'_{fp}}} \boldsymbol{N}^{0,\left(k'_{fp}\right)}_{fp}\left(\cdot\right)_{np}\ {}^{h+1}_{iter,iters}\boldsymbol{t}^{\mathrm{m}}_{np}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \\ & + \sum_{np\in m_{k_{fp}}} \boldsymbol{N}^{0,\left(k_{fp}\right)}_{fp}\left(\cdot\right)_{np}\ {}^{h+1}_{iter,iters}\boldsymbol{t}^{\mathrm{m}}_{np}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \quad fp \in DF^{\mathrm{nor}}_{[l]} \end{aligned} \tag{S6} $$

$$ {}^{h+1}_{iter,iters}\tilde{\boldsymbol{F}}^{[l]}_{fp} = \sum_{np\in m_{k_{fp}}} \tilde{\boldsymbol{N}}^{\left(k_{fp}\right)}_{fp}\left(\cdot\right)_{np}\ {}^{h+1}_{iter,iters}\boldsymbol{t}^{\mathrm{m}}_{np}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \quad fp \in DF^{\mathrm{enr}}_{[l]} \tag{S7} $$

Or update domain forces directly using domain stiffness matrix if the material particle is intact or unloaded, and update the domain stiffness matrix ${}^{h+1}_{iter,iters}\boldsymbol{K}^{[l]}$.

(d) Compute internal force vector and tangent stiffness matrix of the global problem.

$$ {}^{h+1}_{iter,iters}\boldsymbol{F}^{\mathrm{int}} = \mathop{\mathsf{A}}_{l=1}^{N_{\mathrm{d}}} {}^{h+1}_{iter,iters}\boldsymbol{F}^{[l]} \tag{S8} $$

$$ {}^{h+1}_{iter,iters}\boldsymbol{K} = \mathop{\mathsf{A}}_{l=1}^{N_{\mathrm{d}}} {}^{h+1}_{iter,iters}\boldsymbol{K}^{[l]} \tag{S9} $$

where A is the assembly operator and ${}^{h+1}_{iter,iters}\boldsymbol{F}^{[l]}$ is the updated domain force vector of material particle *l*.

(ii) $iters \geq 2$

(a) Using degrees of freedom obtained from the previous time step initialize the common part of current degrees of freedom and define the deleted vector. Initialize added degrees of freedom ${}^{h+1}_{iter,iters}\boldsymbol{d}^{\mathrm{add}}$ and the increment of current degrees of freedom vector ${}^{h+1}_{iter,iters}\Delta\boldsymbol{d}$. Here $iter = 1$.

$$ {}^{h+1}_{iter,iters}\boldsymbol{d} = \begin{Bmatrix} {}^{h+1}_{iter,iters}\boldsymbol{d}^{\text{common}} \\ {}^{h+1}_{iter,iters}\boldsymbol{d}^{\text{add}} \end{Bmatrix} \tag{S10} $$

$$ {}^{h}\boldsymbol{d} = \begin{Bmatrix} {}^{h}\boldsymbol{d}^{\text{common}} \\ {}^{h}\boldsymbol{d}^{\text{del}} \end{Bmatrix} \tag{S11} $$

$$ {}^{h+1}_{iter,iters}\boldsymbol{d}^{\text{common}} \overset{\leftarrow}{=} {}^{h}\boldsymbol{d}^{\text{common}} \tag{S12} $$

$$ {}^{h+1}_{iters}\boldsymbol{d}^{\text{del}} \overset{\leftarrow}{=} -\, {}^{h}\boldsymbol{d}^{\text{del}} \tag{S13} $$

$$ {}^{h+1}_{iter,iters}\boldsymbol{d}^{\text{add}} = \boldsymbol{0} \tag{S14} $$

$$ {}^{h+1}_{iter,iters}\Delta\boldsymbol{d} = \boldsymbol{0} \tag{S15} $$

where ${}^{h+1}_{iter,iters}\boldsymbol{d}^{\text{common}}$ and ${}^{h}\boldsymbol{d}^{\text{common}}$ denote the common part of current and previous degrees of freedom. ${}^{h+1}_{iters}\boldsymbol{d}^{\text{del}}$ is the deleted vector associated with deleted degrees of freedom ${}^{h}\boldsymbol{d}^{\text{del}}$ in ${}^{h}\boldsymbol{d}$.

Or use Newton's method updating degrees of freedom ${}^{h+1}_{iter,iters}\boldsymbol{d}$ and its increment ${}^{h+1}_{iter,iters}\Delta\boldsymbol{d}$. Here $iter \geq 2$.

(b) If the RVE corresponding to material particle l is activated, update the status and reaction forces vector of RVE using increment ${}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}$, deleted vector ${}^{h+1}_{iters}\boldsymbol{d}^{\text{del},[l]}$, and element status ${}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}$.

$$ \begin{aligned} {}^{h+1}_{iter,iters}\boldsymbol{t}^{\text{m}}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{d}^{\text{del},[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) &= {}^{h}\boldsymbol{t}^{\text{m}} \\ &+ {}^{h+1}_{iter,iters}\Delta\boldsymbol{t}^{\text{m}}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{d}^{\text{del},[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \end{aligned} \tag{S16} $$

(c) Update domain forces using RVE reaction forces

$$ \begin{aligned} {}^{h+1}_{iter,iters}\boldsymbol{F}^{0,[l]}_{fp} &= \sum_{np\in m_{k'_{fp}}} \boldsymbol{N}^{0,\left(k'_{fp}\right)}_{fp}\left(\cdot\right)_{np}\, {}^{h+1}_{iter,iters}\boldsymbol{t}^{\text{m}}_{np}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{d}^{\text{del},[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \\ &+ \sum_{np\in m_{k_{fp}}} \boldsymbol{N}^{0,\left(k_{fp}\right)}_{fp}\left(\cdot\right)_{np}\, {}^{h+1}_{iter,iters}\boldsymbol{t}^{\text{m}}_{np}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{d}^{\text{del},[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \quad fp\in DF^{\text{nor}}_{[l]} \end{aligned} \tag{S17} $$

$$ {}^{h+1}_{iter,iters}\tilde{\boldsymbol{F}}^{[l]}_{fp} = \sum_{np\in m_{k_{fp}}} \tilde{\boldsymbol{N}}^{\left(k_{fp}\right)}_{fp}\left(\cdot\right)_{np}\, {}^{h+1}_{iter,iters}\boldsymbol{t}^{\text{m}}_{np}\left({}^{h+1}_{iter,iters}\Delta\boldsymbol{d}^{[l]}, {}^{h+1}_{iters}\boldsymbol{d}^{\text{del},[l]}, {}^{h+1}_{iters}\boldsymbol{\chi}^{[l]}\right) \quad fp\in DF^{\text{enr}}_{[l]} \tag{S18} $$

Or update domain forces directly using domain stiffness matrix if the material particle is intact or unloaded, and update the domain stiffness matrix ${}^{h+1}_{iter,iters}\boldsymbol{K}^{[l]}$.

(d) Compute internal force vector and tangent stiffness matrix of the global problem using Eq. (S8) to Eq. (S9).

The flowchart of the process is shown in Fig. S1.

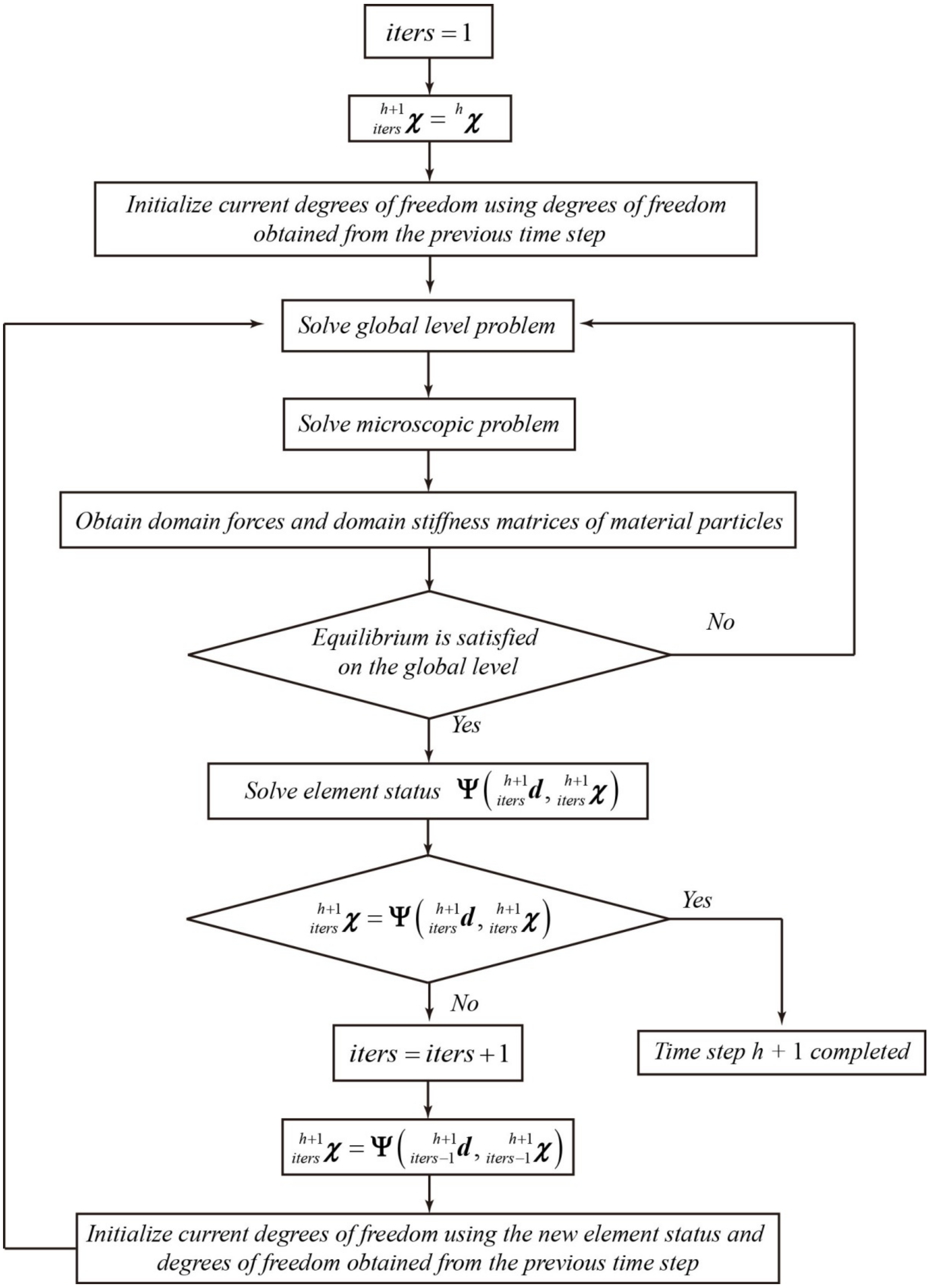

Fig. S1 The implementation of MLPU

As depicted in Fig. S2, deleted vector relates to the elements turning to the normal status from enriched status. It stores enriched degrees of freedom that are to be deleted according to current element status and remains unchanged when solving current degrees of freedom. Given element status ${}^{h+1}_{iters}\boldsymbol{\chi}$, if there are any deleted degrees of freedom, the displacement increment actually depends on both ${}^{h+1}_{iter,iters}\Delta\boldsymbol{d}$ and ${}^{h+1}_{iters}\boldsymbol{d}^{\mathrm{del}}$ for the reason that ${}^{h+1}_{iter,iters}\Delta\boldsymbol{d}$ contains no deleted degrees of freedom and these degrees of freedom have to be eliminated to satisfy the new displacement mode. The deleted degrees of freedom exit computation in the following time steps, which reduces the computational cost. One should note that the numbers of enriched degrees of freedom at the same location may change due to the variation of element status in different time steps. So, the displacement is determined by degrees of freedom vector and element status, not the degrees of freedom vector only.

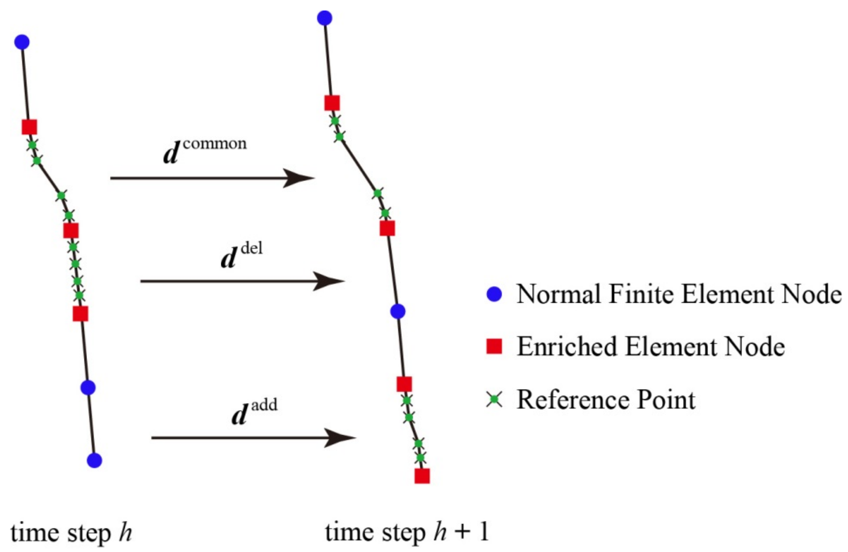

Fig. S2 Variation of element status and degrees of freedom

Usually, the convergence concerning element status is very fast, and the update of element status is not needed to be conducted in most cases for the reason that the status is not changed frequently.