# A new transition technique for the combination of meshfree methods with other numerical methods from macro- to nano-scales

Y. T. Gu*, D. Hargreaves

*School of Engineering Systems, Queensland University of Technology, GPO Box 2434, Brisbane, QLD, 4001, Australia*
e-mail: yuantong.gu@qut.edu.au, d.hargreaves@qut.edu.au

**Abstract** Coupling the meshfree methods with othe numerical methods has good potential in computational mechanics. In this paper, to ensure the compatibility conditions for not only displacements but also its gradients, a new transition technique is proposed based on the penalty method and the transition particles. The bridge regions are used to connect the domains of different methods. The high-order compatibility conditions are satisfied through some regularly distributed transition particles. The new transition technique has several advantages: 1) through the use of the transition particles, the nodes (or atoms) in the transition region are totally independent, which will reduce significantly the cost for the node generation in the transition region; 2) the compatibility conditions in the transition region can be conveniently controlled through the adjustment of the number and distribution of the transition particles; 3) the compatibility of higher order derivatives can be easily satisfied. Several problems of fracture mechanics and multiscale analyses for solids are simulated by the newly developed coupled methods. Some key parameters used in the transition technique have been thoroughly studied and recommended. It has been demonstrated that the new transition technique is very accurate and stable, and it has very good potential to become a practical modeling and simulation tool for engineering.

**Key words:** Coupled method, meshfree method, finite element method, molecular dynamics, bridge transition

## INTRODUCTION

Recently, the meshfree (meshless) method (MM) [1,2] and the computational multiscale technique are two hottest topics in computational mechanics. Firstly, it has been reported that the meshfree method has many advantages [1] including: a) high accuracy, b) effectiveness for adaptive analysis, and c) applicability for some special problems etc. However, the meshfree method usually has poorer computational efficiency than FEM [2], because the numerical interpolation and integration in MM require more computational cost. How to improve its computational efficiency is still an open problem in the development of MM. Coupling the meshfree methods with FEM (the coupled MM/FEM) is a possible solution. In MM/FEM, we only use MM in the necessary region, and FEM is used in other parts to save much computational cost. Secondly, the development of multiscale manufacturing and characterization techniques require analyzing multiscale systems resulting in vast new challenges. In these analyses, physically relevant length scales range from macroscopic to molecular dimensions. It is necessary to create an integrated multiscale modeling and characterization technique to capture the true mechanisms across the length scales. Hence, the concurrent multiscale simulation techniques based on the combination of meshfree methods and the molecular dynamics (MM/MD) has been developed [3][4][5].

In short, the coupled methods become more and more important in computational mechanics because they can fully exploit advantages while evading disadvantages of sole numerical techniques. However, the major difficulty for these coupled techniques (the coupled MM/FEM in macro-scale and the coupled MM/MD in multiscale) is how to satisfy the compatibility conditions on the interface between the computational domains of different methods [6]. Two techniques: using the hybrid displacement shape function algorithm [7] and using the modified variational form algorithm [8], have been developed. In

addition, a bridge transition algorithm was newly developed[3] to ensure compatibility between the macro- and the nano-regions in the coupled technique of FEM/MD. However, to develop more effective transition technique is still a major problem in the development of these coupled methods.

In this paper, a new transition technique is developed to ensure the compatibility conditions for not only displacements but also its gradients. The bridge regions are used to connect the domains of different methods. The high-order compatibility conditions are satisfied through some regularly distributed transition particles. Several problems of fracture mechanics and multiscale analyses of solids are simulated by the newly developed coupled techniques. It has been demonstrated that the new transition technique is very accurate and stable, and it has very good potential to become a practical modeling and simulation tool for engineering.

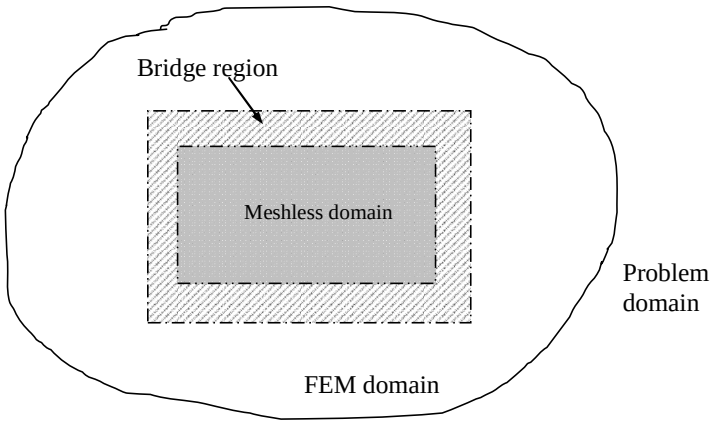
## THE COMBINATION CONDITION

In the following discussions, we will start from the coupled MM/FEM method. The formulations for the coupled MM/MD method can be similarly obtained.

As shown in Figure 1, consider a two-dimensional (2-D) problem domain. A sub-domain, $\Omega_{(MM)}$, is represented by the meshfree nodes and the other sub-domain, $\Omega_{(FE)}$, uses FEM. These two domains are joined together by a transition domain $\Omega_{(T)}$ that possesses displacement compatibility and force equilibrium in coupling $\Omega_{(MM)}$ and $\Omega_{(FEM)}$, i.e.,

$$\mathbf{u}_{(MM)k} = \mathbf{u}_{(FE)k}, \quad \mathbf{f}_{(MM)k} + \mathbf{f}_{(FE)k} = 0 \tag{1}$$

where $\mathbf{u}_{(MM)k}$, $\mathbf{u}_{(FE)k}$, $\mathbf{f}_{(MM)k}$ and $\mathbf{f}_{(FE)k}$ are displacements and forces at a transition particle $k$ obtained by the meshfree method in $\Omega_{(MM)}$ and FEM in $\Omega_{(FE)}$, respectively.




*Figu.1 the coupled model*

It will be ideal to satisfy both the displacement compatibility and the force equilibrium conditions, in which the displacement compatibility Equation (1) is the most important and must be satisfied. In addition, because many types of the meshfree shape functions (e.g. the moving least squares) lack the delta function properties, it is difficult to directly connect these two domains.

To satisfy the displacement compatibility condition, two combination techniques: a) using the hybrid displacement shape function algorithm [7], and b) using the modified variational form algorithm [8] have been developed. In these two techniques, the transition domain is usually reduced to a common boundary (e.g., a curve for a 2-D problem), called the interface, $\Gamma_I$. These two techniques have been used in the development of some coupled methods including the EFG/FEM/BEM and MLPG/FEM/BEM. However, in these two techniques, a common interface boundary is used between FEM domain, $\Omega_{(FE)}$, and the meshfree domain, $\Omega_{(MM)}$. The meshfree nodes and the FEM nodes along this interface boundary coincide

with each other, and are dependent on each other. It is difficult to ensure the high-order compatibility through this interface boundary. In addition, it will increase the effort in "meshing" work, especially for some problems with complex interface boundaries.

## THE BRIDGE TRANSITION TECHNIQUE FOR MM/FEM

A new bridge transition technique is developed based on the idea of the bridge technique proposed by Xiao and Belytschko [3]. As shown in Figure 1, there is transition (bridge) domain $\Omega_{(T)}$ between FEM and meshfree domains. The generalized displacement of a point in the transition domain at **x** can be defined as

$$\mathbf{g} = \mathbf{u}_{(\mathrm{MM})}(\mathbf{x}) - \mathbf{u}_{(\mathrm{FE})}(\mathbf{x}) \tag{2}$$

where $\mathbf{u}_{(\mathrm{MM})}(\mathbf{x})$ and $\mathbf{u}_{(\mathrm{FE})}(\mathbf{x})$ are the displacements of the point at **x**, obtained by the interpolations using the meshfree nodes and the FEM element, respectively, i.e.,

$$\mathbf{u}_{(\mathrm{MM})}(\mathbf{x}) = \sum_I \mathbf{\Phi}_I(\mathbf{x})\mathbf{u}_{(\mathrm{MM})I} \qquad \mathbf{u}_{(\mathrm{FE})}(\mathbf{x}) = \sum_J \mathbf{N}_J(\mathbf{x})\mathbf{u}_{(\mathrm{FE})J} \tag{3}$$

A discretized sub-functional is introduced to enforce the displacement compatibility condition given in Equation (1) by means of Lagrange multiplier $\lambda$ in the transition domain

$$\Pi_{(\mathrm{T})} = \int_{\Omega_{(\mathrm{T})}} \boldsymbol{\lambda} \cdot \mathbf{g} \mathrm{d}\Omega = \Pi_{(\mathrm{T})}^{(\mathrm{MM})} - \Pi_{(\mathrm{T})}^{(\mathrm{FE})} \tag{4}$$

In which, $\Pi_{(\mathrm{T})}^{(\mathrm{MM})}$ and $\Pi_{(\mathrm{T})}^{(\mathrm{FE})}$ are the sub-functional for the meshfree part and the FEM part.

To satisfy the force equilibrium condition, the generalized derivative at a point in the transition domain, **x,** can be written as

$$\mathbf{g}_{(x)} = \frac{\partial \mathbf{u}_{(\mathrm{MM})}(\mathbf{x})}{\partial \mathbf{x}} - \frac{\partial \mathbf{u}_{(\mathrm{FE})}(\mathbf{x})}{\partial \mathbf{x}} \tag{5}$$

and using Lagrange multiplier $\gamma$, we can obtain the sub-functional

$$\Pi_{(\mathrm{T})(\mathbf{x})} = \int_{\Omega_{(\mathrm{T})k}} \boldsymbol{\gamma} \cdot \mathbf{g}_{(\mathbf{x})} \mathrm{d}\Omega = \Pi_{(\mathrm{T})(\mathbf{x})}^{(\mathrm{MM})} - \Pi_{(\mathrm{T})(\mathbf{x})}^{(\mathrm{FE})} \tag{6}$$

In the practical computation, to simplify the integration and reduce the "meshing" cost, several layers of transition particles, which are regularly distributed, can be inserted into the transition domain $\Omega_{(T)}$. The displacement compatibility between FEM and meshfree nodes is achieved through these transition particles. Therefore, we can obtain the coupling equations to satisfy the high-order compatability

$$\begin{bmatrix} \mathbf{K}_{(\mathrm{MM})} & \mathbf{0} & \mathbf{B}_{(\mathrm{MM})} & \mathbf{A}_{(\mathrm{MM})} \\ \mathbf{0} & \mathbf{K}_{(\mathrm{FE})} & -\mathbf{B}_{(\mathrm{FE})} & -\mathbf{A}_{(\mathrm{FE})} \\ \mathbf{B}_{(\mathrm{MM})}^T & -\mathbf{B}_{(\mathrm{FE})}^T & \mathbf{0} & \mathbf{0} \\ \mathbf{A}_{(\mathrm{MM})}^T & -\mathbf{A}_{(\mathrm{FE})}^T & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{U}_{(\mathrm{MM})} \\ \mathbf{U}_{(\mathbf{FE})} \\ \boldsymbol{\lambda} \\ \boldsymbol{\gamma} \end{Bmatrix} = \begin{Bmatrix} \mathbf{F}_{(\mathrm{MM})} \\ \mathbf{F}_{(\mathrm{FE})} \\ \mathbf{0} \\ \mathbf{0} \end{Bmatrix} \tag{7}$$

where

$$\mathbf{B}_{(\mathrm{FE})} = \sum_{k=1}^{m} \mathbf{\Lambda}\mathbf{N}^{\mathrm{T}}, \ \mathbf{B}_{(\mathrm{MM})} = \sum_{k=1}^{m} \mathbf{\Lambda}\mathbf{\Phi}^{\mathrm{T}} \tag{8}$$

$$\mathbf{A}_{(\mathrm{MM})} = \sum_{k=1}^{m} \Psi \frac{\partial \mathbf{\Phi}^{\mathrm{T}}}{\partial \mathbf{x}}, \ \ \mathbf{A}_{(\mathrm{FE})} = \sum_{k=1}^{m} \Psi \frac{\partial \mathbf{N}^{\mathrm{T}}}{\partial \mathbf{x}} \tag{9}$$

## THE COUPLED MM/MD METHOD FOR MULTISCALE ANALYSIS

Similarly, in multiscale simulation based on the combination of MM/MD, the generalized displacement and its derivative of a transition particle at $\mathbf{x}_l$ can also be defined as

$$\begin{cases} \mathbf{g}_l = \mathbf{u}^c(\mathbf{x}_l) - \mathbf{u}^a(\mathbf{x}_l) = \sum_I \mathbf{\Phi}_I(\mathbf{x}_l)\mathbf{u}_I^c - \sum_i \mathbf{\Phi}_i(\mathbf{x}_l)\mathbf{u}_i^a \\ \mathbf{g}_{l(\mathbf{x})} = \dfrac{\partial \mathbf{u}^c(\mathbf{x}_l)}{\partial \mathbf{x}^c} - \dfrac{\partial \mathbf{u}^a(\mathbf{x}_l)}{\partial \mathbf{x}^a} = \sum_I \dfrac{\partial \mathbf{\Phi}_I(\mathbf{x}_l)}{\partial \mathbf{x}^c}\mathbf{u}_I^c - \sum_i \dfrac{\partial \mathbf{\Phi}_i(\mathbf{x}_l)}{\partial \mathbf{x}^a}\mathbf{u}_i^a \end{cases} \tag{10}$$

where $\mathbf{u}^c(\mathbf{x}_l)$ and $\mathbf{u}^a(\mathbf{x}_l)$ are the displacements of the transition particle at $\mathbf{x}_l$ obtained by the interpolations using continuum nodes and atoms, respectively, and $\mathbf{\Phi}$ is the meshfree shape function.

To ensure the conservation of mass and energy, using the method developed by Xiao and Belytschko [3], the total energy and mass are taken to be linear distributions using a scaling parameter $\alpha$ in the transition domain. The Hamiltonian for the total problem domain is the linear combination of the atomic, continuum and the constrain terms of transition particles, i.e.,

$$H = (1-\alpha)H^a + \alpha H^c + \sum_l \beta_l^{(1)}\mathbf{g}_l + \sum_l \beta_l^{(2)}\mathbf{g}_l^{\mathrm{T}}\mathbf{g}_l + \sum_l \beta_l^{(3)}\mathbf{g}_{l(x)}^{\mathrm{T}}\mathbf{g}_{l(x)} \tag{11}$$

where $\beta_l^{(1)}$, $\beta_l^{(2)}$, and $\beta_l^{(3)}$ are penalty coefficients for the transition point *l*.

Hence, the equations of motions for continuum and atomic domains can be re-written as

$$m_{I(c)}\ddot{\mathbf{u}}_{I(c)} = \mathbf{f}_{I(c)} = \mathbf{f}_{I(c)}^{\mathrm{ext}} - \left( \mathbf{f}_{I(c)}^{\mathrm{int}} + \frac{\mathbf{f}_{I(c)}^{\mathrm{tran}} + \mathbf{f}_{I(c)}^{\mathrm{tran}(\mathbf{x})}}{\alpha(\mathbf{X}_I)} \right) \tag{12}$$

$$m_{i(a)}\ddot{\mathbf{u}}_{i(a)} = \mathbf{f}_{i(a)} = \mathbf{f}_{i(a)}^{\mathrm{ext}} - \left( \mathbf{f}_{i(a)}^{\mathrm{int}} + \frac{\mathbf{f}_{i(a)}^{\mathrm{tran}} + \mathbf{f}_{i(a)}^{\mathrm{tran}(\mathbf{x})}}{1-\alpha(\mathbf{X}_i)} \right) \tag{13}$$

where $\mathbf{f}_{I(c)}^{\mathrm{tran}}$, $\mathbf{f}_{I(c)}^{\mathrm{tran}(\mathbf{x})}$, $\mathbf{f}_{i(a)}^{\mathrm{tran}}$ and $\mathbf{f}_{i(a)}^{\mathrm{tran}(\mathbf{x})}$ are constraint forces due to the penalty terms to enforce the displacement and its derivative compatibility conditions for the continuum and atomic domain, respectively, i.e.

$$\mathbf{f}_{I(c)}^{\mathrm{tran}} = \sum_l \beta_l^{(1)}\Phi_{Il}\mathbf{I} + \sum_l \beta_l^{(2)}\left[ \sum_I \Phi_I(\mathbf{x}_l)\mathbf{u}_I^c - \sum_i \Phi_i(\mathbf{x}_l)\mathbf{u}_i^a \right][\Phi_{Il}\mathbf{I}]; \quad \mathbf{f}_{I(c)}^{\mathrm{tran}(\mathbf{x})} = \sum_l \beta_l^{(3)}\Phi_{Il,\mathbf{x}}\mathbf{I} \tag{14}$$

$$\mathbf{f}_{i(a)}^{\mathrm{tran}} = -\sum_l \beta_l^{(1)}\Phi_{il}\mathbf{I} - \sum_l \beta_l^{(2)}\left[ \sum_I \Phi_I(\mathbf{x}_l)\mathbf{u}_I^c - \sum_i \Phi_i(\mathbf{x}_l)\mathbf{u}_i^a \right][\Phi_{il}\mathbf{I}]; \ \mathbf{f}_{i(a)}^{\mathrm{tran}(\mathbf{x})} = -\sum_l \beta_l^{(3)}\Phi_{il,\mathbf{x}}\mathbf{I} \tag{15}$$

From above discussions, we can find that the advantages of using the above presented bridge transition technique include: 1) it allows the meshfree nodes in $\Omega_{(\mathrm{MM})}$ to have an arbitrary distribution and become independent of the distributions of the FEM nodes in $\Omega_{(\mathrm{FE})}$. Hence, the mesh- and node-generation become easy and cheap; 2) the compatibility conditions in the transition domain can be conveniently controlled through the adjustment of the number and distribution of the transition particles. For some sub-transition domains with higher compatibility requirement, a finer transition particle distribution can be used; 3) The compatibility of higher order derivatives can be easily satisfied. It will be very benefit to improve the accuracy for stress field. Hence, the bridge transition technique is more effective than the old transition techniques.

## NUMERICAL RESULTS AND DISCUSSIONS

**1. A muiltscale analysis for wave propagation in a graphite sheet** Here we examine MM/MD in a two-dimensional graphite sheet whose thickness is a single atom layer, and Lennard-Jones (L-J) 6-12 inter-atomic potential is used. The initial displacement is taken as a quarter of sinusoid, and applied on the right portion of the atomic domain. The periodic boundary condition is applied along the vertical direction.

The coupling model of this 2-D sheet is shown in Figure 2. The length of the transition region is 1.95 nm, which is represented by regularly distributed transition particles. The time step for the atomic domain is $\Delta t_{(a)}$=0.005ps.

The displacement fields have been obtained by MM and they are almost identical with the results obtained by the pure MD. The average errors for different numbers of transition particles are obtained, and we have found that the computational results are stable when the number of the transition particles is large enough (the particle number in one direction larger than 25 for this problem). Too few transition particles cannot ensure the compatibility accuracy, and hence lead to a large computational error. On the other hand, if the transition particles are too many, it will significantly increase the computational time without noticeable accuracy improvement. Hence, the number of transition particles should be considered to maximise the computation efficiency with acceptable accuracy. For the present example, *N*=225~600 are a good selection.

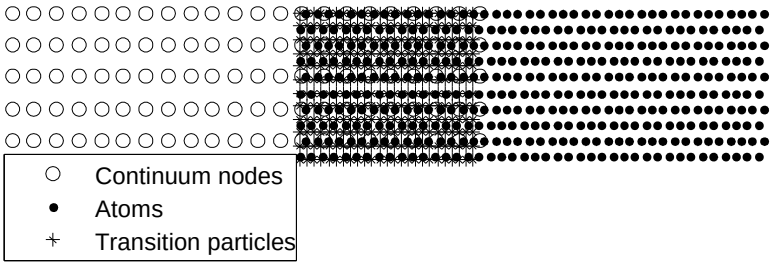



*Fig. 2 Multiscale computational model for 2-D graphite sheet*

To investigate the influence of the size of the transition region, we define $l_t = \alpha \cdot d_{(a)}$, where $d_{(a)}$ is the space between two atoms. From the computational errors, we can find that the transition region should be large enough to ensure the compatibility. However, a larger transition region requires more transition particles and, hence, increases the computational cost. For this study, $\alpha = 5 \sim 20$ is a reasonable choice.

Using the parameters obtained from above studies, Figure 3 shows the energy transfer between the continuum and atomic sub-domains. It demonstrates that all the energy in atomic sub-domain has been transferred into the continuum sub-domain through our transition technique.

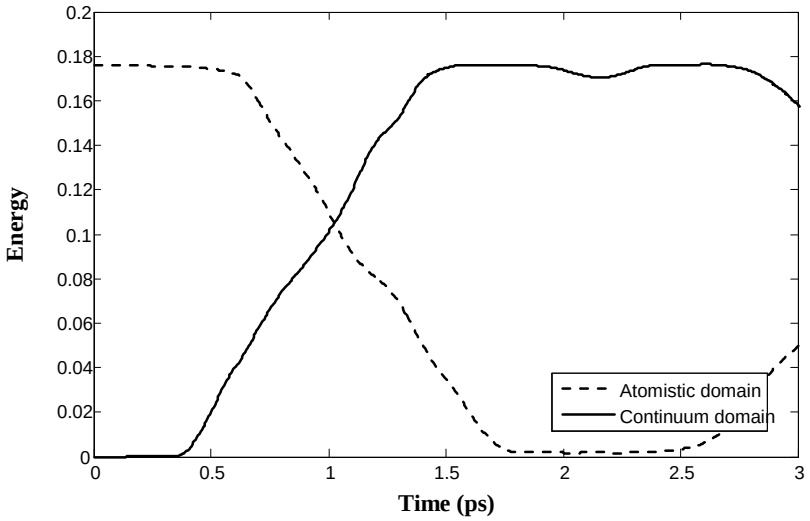



*Fig. 3 Energy transfer between the continuum and atomic domains*

**2. A cracked plate** A well-known near-tip field, which is subjected to mode-I displacement field[9]at its edges, is analyzed by MM/FEM. As shown in Figure 4, an edge-cracked square plate is subjected to the following displacement field for a model-I crack.

$$\begin{Bmatrix} u \\ v \end{Bmatrix} = \frac{K_I}{2\mu}\sqrt{\frac{r}{2\pi}} \begin{Bmatrix} \cos\frac{\theta}{2}\left[\kappa - 1 + 2\sin^2\frac{\theta}{2}\right] \\ \sin\frac{\theta}{2}\left[\kappa + 1 - 2\cos^2\frac{\theta}{2}\right] \end{Bmatrix} \tag{16}$$

where $K_I$ is the stress intensity factors for mode-I dependent upon the crack length, the specimen geometry and the applied loading, and ($r$, $\theta$) are the cylindrical coordinates of a point with the origin located at the crack-tip and the positive angle measured counterclockwise from the axis of the crack. Hence, the analytical solution for the stress field is given

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{Bmatrix} = \frac{K_I}{\sqrt{2\pi r}}\cos\frac{\theta}{2} \begin{Bmatrix} 1 - \sin\frac{\theta}{2}\sin\frac{3\theta}{2} \\ 1 + \sin\frac{\theta}{2}\sin\frac{3\theta}{2} \\ \sin\frac{\theta}{2}\sin\frac{3\theta}{2} \end{Bmatrix} \tag{17}$$

The plate is divided into two parts: the meshfree method is used for the central part, in which the crack embedded, and FEM is used for other parts. The computational model is plotted in Figure 5. Figure 6 shows the stress distributions along the crack axis (when $\theta$=0°). Clearly, the prediction of the new developed coupled method matches the analytical solution very well.

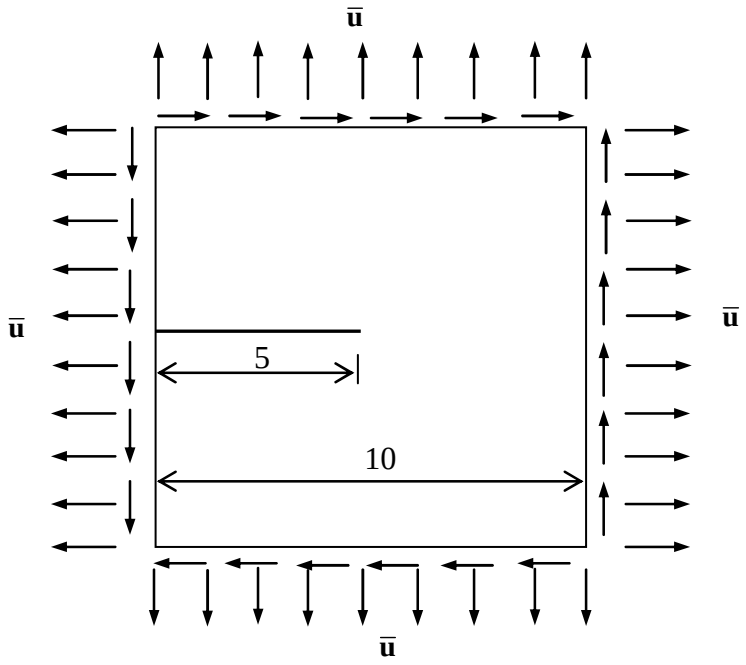



*Fig. 4 A cracked square plate subjected to Mode-I displacement boundary conditions*

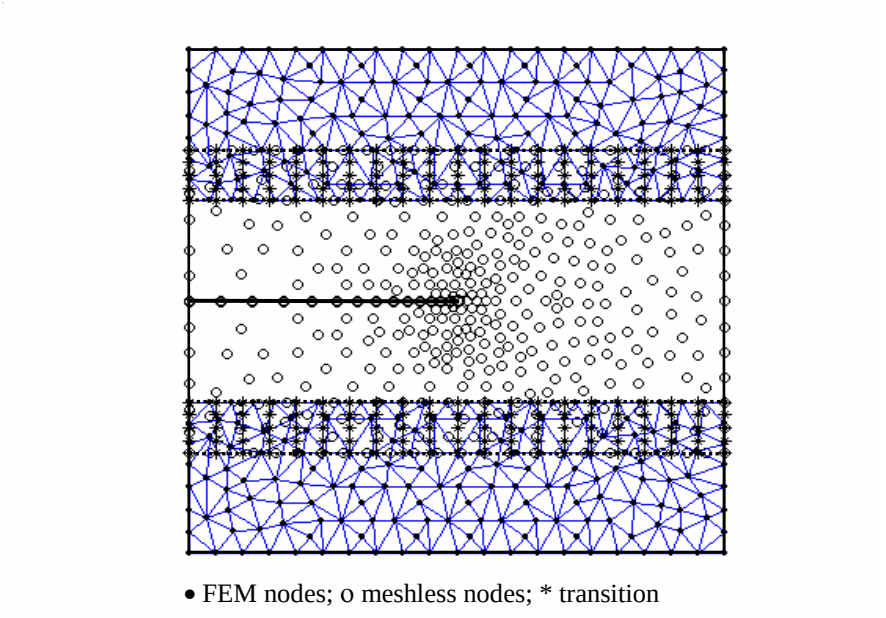



*Fig. 5 The computational model for the cracked square plate*

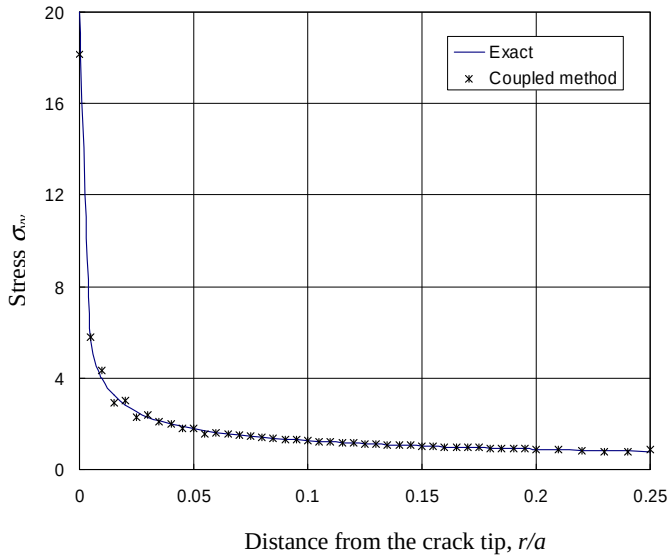



*Fig. 6 The distribution of $\sigma_{yy}$ along the axis of the crack*

## CONCLUSION

A new transition technique is developed based on the penalty method, bridge technique and the transition particles. The bridge regions are used to connect the domains of different methods. The high-order compatibility conditions are satisfied through some regularly distributed transition particles. The formulations of the coupled MM/FEM for the macro-scale and the coupled MM/MD for the multiscales have been obtained based on the new transition technique. Some key paramters, which influence the performance of the coupled methods, have been studied. It has been found that the choice of the number of transition particles and the size of the bridge region has a relative wide range, although it is usually problem dependent.

Several problems of fracture mechanics and multiscale analyses for solids are simulated by the newly developed coupled methods. It has been demonstrated that the new transition technique is very accurate

and stable, and it has very good potential to become a practical modeling and simulation tool for engineering.

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