Title: Development of Higher Order Particle Discretization Scheme for analysis of cracking phenomena Name: Mahendra Kumar Pal (亀裂解析のための高次粒子離散化手法の開発)

マヘント・ラ クマール パール

Abstract

In this thesis, higher order extension of Particle Discretization Scheme (PDS) and its implementation in FEM framework are considered, with the aim of simulating cracking phenomena in brittle elastic solids. The main advantages of PDS-FEM, proposed by Hori *et at.*, are its numerically efficient failure treatment, ability to reproduce crack branching without any special treatments and modelling the effects of material heterogeneities. On the contrary, most of existing FEM approaches involves complex treatments for modelling these phenomena. The present implementation of PDS-FEM has first order accuracy. The main objectives of this thesis are to increase the order of accuracy, implement a suitable failure treatment and application to simulate cracking phenomena in brittle solids.

A unique property of PDS is the uses of conjugate tessellations to approximate functions and their derivatives, respectively. In the original formulation, characteristic functions of Voronoi and Delaunay tessellations,  $\{\phi^{\alpha}(x)\}$  and  $\{\psi^{\beta}(x)\}$ , are used for approximating functions and derivatives, respectively, leading to constant variation of the approximated fields within each tessellation element. In the higher order extension of PDS, the fields within each tessellation element is approximated as local polynomial expansion about the mother point of the respective tessellation element, and the field over the whole domain is approximated as the union of these local polynomial expansions. As an example, a function f(x) and its derivative g(x) are approximated as  $f^{d}(x) \cong \sum_{\alpha,n} f^{\alpha_n} P^{\alpha_n}$  and  $g^{d}(x) \cong \sum_{\beta,m} g^{\beta_m} P^{\beta_m}$ , where  $\{P^{\alpha_n}\} = \{1, x - x^{\alpha}, ...\} \varphi^{\alpha}(x)$  and  $\{P^{\beta_m}\} = \{1, x - x^{\beta}, ...\} \psi^{\beta}(x)$  are the local polynomial bases with the respective tessellation element, to approximate a function gives rise to the particle nature of this discretization scheme and produces numerous discontinuities in  $f^{d}(x)$ . It is to smoothly connect those discontinuous local polynomial expansions and define a bounded approximation for the derivatives, the conjugate tessellation:  $\{\Psi^{\beta}\}$ , is used for approximating the derivatives. The numerous discontinuities in  $f^{d}(x)$  is utilized by PDS-FEM to numerically efficiently model discontinuities or cracks in solving boundary value problems.

The above mentioned formulation (hereafter, refereed as *formulation-A*) doesn't guarantee that approximation scheme will necessarily satisfy the fundamental requirement;  $\nabla \times g^d = 0$ , which is called the curl free condition, hereafter. Another formulation, based on the curl free constraint is also proposed and referred as *formulation-B*. In formulation-B, functions are approximated just as in formulation-A, while the derivative approximations are redefined such that the curl-free condition is always satisfied. Formulation-B performs better in function approximation, but same is not translated while solving BVP.

The higher order PDS is implemented in FEM framework and codes for simulating cracks in brittle elastic solids are developed. The developed codes are designed such that arbitrary sets of polynomials can be used in approximating functions and derivatives. Further, the codes are enhanced with distributed parallel computing extensions so that large scale models can be simulated. The developed codes for higher order PDS-FEM are validated and verified with different benchmark problems, and the patch tests are conducted. It is demonstrated that compatible higher order convergence rate can be obtained; second order accuracy in the displacement field is attained with the polynomial bases up to the first order both in 2D and 3D. Furthermore, problem associated with imposing essential boundary conditions is discussed and demonstrated that the choice polynomial order for approximating derivatives to be one order higher than

that of function mitigates the need of specifying derivatives as essential boundary conditions. Both the formulation-A and B are validated using benchmark tests and demonstrated that both formulation-A and B have p + 1-order convergence rate for function and derivatives, when using  $p^{th}$  and  $(p + 1)^{th}$  order polynomial bases for approximating functions and derivatives, respectively. Further, both the formulation-A and B exhibit nearly the same accuracy. Formulation-B doesn't offer the expected results in analysing the BVPs.

In order to validate the modelling of brittle cracks, standard benchmark problems are considered; mode-I crack in 2D and penny shaped crack in 3D subjected to far-field tensile loading. It is shown that the both the displacement and stress fields are in good agreement with analytic solution except the near neighbourhood of the crack tips. Point of inflection is an important factor, which decides the nature of approximated function. Hence, sensible selection of inflection point is suggested and investigated with several numerical example. Selection of mid point of broken edge of Delaunay triangle encapsulating crack-tip as inflection point in place of center of gravity rectifies the above mentioned problem. Obtained results are in good agreements with analytic solution but a slight shift in stress singularity is observed. Seeking the improvement in results, problem is re-analysed with curl free formulation. But, curl free formulation doesn't enhance result anymore. Even, it doesn't offer traction free surface. Further, J-integral calculation is done. It is shown that error in J-integral calculation disappears at the rate of 1.7, which is 1.0 in case of  $0^{th}$ -order PDS-FEM.

It is shown that even the proposed higher order extensions of PDS-FEM can also offer a simple and numerically efficient crack treatment, just as the original  $0^{th}$  -order PDS-FEM. The proposed crack treatment, which involves judicious selection of point of inflection, the verification tests conducted with standard mode-I crack problem indicate it produces higher accuracy and convergence rate of J-integral, compared to those of  $0^{th}$  -order PDS-FEM. Further, the formulation-A is superior in modeling cracks; formulation-A has higher and sustained convergence rate of J-integral compared to formulation-B. Further, crack surfaces produced by formulation-A are nearly traction free, while those with both formulation-B and  $0^{th}$  -order PDS-FEM have notable surface traction. Because of the superior performance in modeling cracks, the formulation-A is adopted as the higher order PDS-FEM. When it comes to crack modeling, improved accuracy in crack tip stress field and surface traction are the main improvement in higher order PDS-FEM compared to  $0^{th}$  -order. Irrespective of the crack configuration, higher order PDS-FEM reproduces a nearly traction free crack surface. Such salient feature of proposed numerical scheme, categorized it into the list of numerically efficient methods.