Implementation of Finite Element Method with Higher Order Particle Discretization Scheme

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This paper studies the extension of particle discretization scheme (PDS) in order to improve finite element method implemented with this discretization scheme (PDS-FEM). Polynomials are included in the basis functions, while original PDS uses a characteristic function or zero-th order polynomial only. It is shown that including 1st order polynomials in PDS, the rate of the convergence reaches the value of 2 even for the derivative. 1st order polynomials are successfully included in PDS-FEM. A numerical experiment is carried out by applying 1st order PDS-FEM, and the improvement of the accuracy is discussed.

Key Words: *particle discretization scheme, higher order extension, Taylor expansion, FEM*

1. Introduction

Cracking of solid is a common phenomenon which leads to failure. It strongly depends on local material properties, since no identical crack pattern is found for experimental samples of the same configuration subjected to the same loading. Also, surfaces of cracks are complicated, as they kink or branch in a bulk body.

The numerical analysis of cracking must account for the two characteristics, namely, the dependence on local material heterogeneities and the formation of complicated surfaces. Conventional numerical methods may not be capable of studying these characteristics in an efficient manner, since it is not a simple task to determine the configuration of the propagating crack surface, which could kink or branch, by considering local material heterogeneities. A few recent advancements^{1),2),3),4),5)} have increased the capability of the conventional numerical methods to analyse cracking. For instance, a new enhancement is tracking of the crack front, which is supported with automated modification, in simulating the propagating crack. However, objective decision on tracking of the crack front is deceptive. Also, this enhancement is computationally expensive and complex in imple-

mentation.

Particle Discretization Scheme-Finite Element Method (PDS-FEM)^{6),7),8),9)} is a new numerical method of simulating cracking phenomena, which enables us to make simple modelling of the crack surface considering material heterogeneities. In PDS, a function is discretized by using the characteristic functions of each tessellation, so that a function discretized in PDS allows discontinuities across all neighbouring tessellations. It is rigorously proved that PDS-FEM has the identical stiffness matrix with linear element FEM. Hence, cracking is easily treated as discontinuity of the discretized function, and the reduction of the stiffness due to cracking is rigorously computed.

The limitation of the accuracy that is inherent to the linear element FEM is shared by PDS-FEM. Thus, the improvement of the accuracy of PDS-FEM is of primary importance, with the key feature of FEM, the simple determination of the crack surface considering material heterogeneities, being preserved as it is. To this end, this paper considers higher order PDS. The basic idea is to regard PDS as a discretization scheme which assembles a set of Taylor series expansions. A target function is expanded in polynomials in each tessellation, and these polynomials are connected to

form a discretized function.

It should be emphasized that taking the Taylor series expansion is most accurate in representing a smooth function locally. The disadvantage of this expansion is that the expanded polynomials do never decay near the boundary of the domain of expansion. In higher order PDS, we allow the presence of discontinuity in neighbouring Taylor series expansions, so that crack surfaces can be simply modelled as the interface between the neighbouring domains of expansion. The presence of numerous discontinuities is a hinge in computing derivatives of a discretized function. In higher-order PDS, derivatives are discretized by using another tessellation, to overcome this hinge, just as the present PDS employs the conjugate Voronoi and Delaunay tessellations in discretizing a function and its derivative, respectively.

The contents of this paper are as follows: First, we formulate higher order PDS in Section 2, clarifying the discretization of a function and its derivative. As the simplest case, 1st order PDS is implemented in FEM in Section 3. A numerical example is solved by using PDS-FEM, and the improvement of the accuracy of PDS-FEM is discussed in Sections 4. Some remarks are made in the last section.

The Cartesian coordinate system is used, with index notation such as x_i , representing the i -th coordinate; summation convention is employed, and an index following a comma denotes the partial derivative with respect to that coordinate. For simpler expressions, symbolic notation is used as well for a vector or tensor quantity.

2. Higher order PDS

While any pair of conjugate geometries can be used for tessellating an analysis domain, PDS-FEM has utilized the pair of conjugate Voronoi and Delaunay tessellations; a certain error of discretization identically vanishes for this pair. In this paper, we follow the previous works of PDS-FEM and use conjugate Voronoi and Delaunay tessellations.

Let f be a target function in an analysis domain V . We take conjugate Voronoi and Delaunay tessellations, $\{\Phi^\alpha\}$ and $\{\Psi^\beta\}$, for this V , and denote by $\mathbf{y}^\alpha$ or $\mathbf{z}^\beta$ the mother point of Ψ^α and the centre of gravity of Ψ^β , respectively and denote by ϕ^α and ψ^β the characteristic function of Φ^α and Ψ^β , respectively. Here, the characteristics function $\{\Phi^\alpha\}$ satisfies $\Phi^\alpha(x) = 1$ for $x \in \Omega^\alpha$ and $= 0$ for $x \notin \Omega^\alpha$. We define a discretized function and derivative of f , as follows:

$$f^d(x) = \sum_{\alpha=1}^{N^\alpha} \left(\sum_{n=0}^N f^{\alpha n} P_n(\mathbf{x} - \mathbf{y}^\alpha) \phi^\alpha(\mathbf{x}) \right), \quad (1)$$

$$g_i^d(x) = \sum_{\beta=1}^{N^\beta} \left(\sum_{n=0}^N g_i^{\beta n} P_n(\mathbf{x} - \mathbf{z}^\beta) \psi^\beta(\mathbf{x}) \right), \quad (2)$$

where $P_0 = 1$ and $P_n = x_n$ for $n = 1, \dots, N$ of the N dimension setting, N^α is a number of Voronoi tessellations and N^β is a number of Delaunay tessellations. The coefficient $f^{\alpha n}$ is determined by minimizing $E^f = \int (f - f^d)^2 dv$, which results into the following system of equation,

$$\sum I^{\alpha n \alpha m} f^{\alpha m} = \int P_n(\mathbf{x} - \mathbf{y}^\alpha) \phi^\alpha(\mathbf{x}) f(\mathbf{x}) dv. \quad (3)$$

Also, the coefficient $g_i^{\beta n}$ is determined by minimizing $E^g = \int |\mathbf{g}^d(\mathbf{x}) - \nabla f^d(\mathbf{x})|^2 dv$ with $|\cdot|^2$ being the norm of a vector $(\cdot)$, which results into the following system of equation,

$$\sum I^{\beta n \beta m} g_i^{\beta m} = \int P_n(\mathbf{x} - \mathbf{z}^\beta) \psi^\beta(\mathbf{x}) f_{,i}^d(\mathbf{x}) dv. \quad (4)$$

Here, by definition, $f_{,i}^d$ is expressed in terms of $\{f^{\alpha n}\}$ as $\sum f^{\alpha n} (P_n(\mathbf{x} - \mathbf{y}^\alpha) \phi^\alpha(\mathbf{x}))_{,i}$. Here $I^{\alpha n \alpha m} = \int P_n(\mathbf{x} - \mathbf{y}^\alpha) P_m(\mathbf{x} - \mathbf{y}^\alpha) dv$.

As is seen, it is straightforward to include the 1st order polynomials in the original PDS that uses the characteristic functions as the basis functions of discretization. The conversion from the discretized function to the discretized derivative is straightforward as well, since the closed function (that is measured in terms of natural L^2) is chosen by minimizing a naturally defined error. From now on, we call this PDS as 1st order PDS. Further extension of PDS to higher order polynomials is also straightforward. Indeed, Eq.(1) or (2) gives an expression of this higher order PDS, just by including higher order polynomials in $\{P_n\}$. The number of the coefficients, however, increases as the order of the polynomial increases; for instance, the number of the coefficients increase from 4 to 10 if the second order polynomials are included.

In presenting higher order PDS, the authors use the term Taylor expansion in a naive sense. As is seen, the coefficients $f^{\alpha n}$ and $g_i^{\beta n}$ are not exactly the coefficient one would obtain if Taylor series expansion is performed. However, the higher the order of polynomials used in PDS, the closer the coefficients of PDS to that of Taylor expansion. This naive use of Taylor expansion makes it easy to deliver a clear mental image about the higher order PDS.

It is of interest to investigate the rate of convergence in discretizing the derivative, $g_{,i}^d$, which is computed by using the discretized function, f^d ; see Eq. (4). Using the simple one-dimensional setting, we pick up two examples, a smooth function of $\sin x$ and a singular function of $x/\sqrt{10x+x^3}$, for this investigation as shown in Fig. 1. The convergence of the L^2 norm

Fig.1 (a) & (b) Approximation of function and (c) & (d) its derivative with two different tessellation

Fig.2 Convergence of derivative approximation of $\sin(x)$ and $\frac{x}{\sqrt{10x+x^3}}$.

of $f' - g_1^d$ is plotted in Fig. 2 for the both examples. As is seen, the second order convergence rate is obtained for the discretized derivative. This speed is the same as the convergence rate of the function. This is a major advantage of PDS, in which the conjugate tessellations are used to separately discretize a function and its derivative.

While f^d and g_i^d of Eqs. (1) and (2) are computed by minimizing E_f^f and E_g^g , respectively, we can regard them as a union of Taylor series expansions for f and $f_{,i}$, respectively. The summed term,

$$\sum_n f^{\alpha n} P_n(\mathbf{x} - \mathbf{y}^\alpha) \quad \text{or} \quad \sum_n g_i^{\beta n} P_n(\mathbf{x} - \mathbf{z}^\beta),$$

is of the same form as the Taylor series expansion of f or $f_{,i}$ at $\mathbf{y}^\alpha$ or $\mathbf{z}^\beta$, if the expansion domain is chosen as Φ^α or Ψ^β ; see Appendix A for more detailed discussion in regarding higher order PDS as a union of Taylor series expansion.

3. PDS-FEM formulation

As the simplest problem, we consider a linearly elastic body problem at quasi-static state and small deformation, in the absence of a body force. We implement 1st order PDS to FEM, to solve this problem using the following Lagrangian:

$$L[\mathbf{u}, \boldsymbol{\epsilon}, \boldsymbol{\sigma}] = \int_V \frac{1}{2} \boldsymbol{\epsilon} : \mathbf{c} : \boldsymbol{\epsilon} - \boldsymbol{\sigma} : (\nabla \mathbf{u} - \boldsymbol{\epsilon}) \, dv. \quad (5)$$

Here, $\mathbf{u}$, $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ are displacement vector, strain and stress tensors, respectively, and $\mathbf{c}$ is the elasticity tensor; $:$ stands for the second-order contraction, and $\nabla \mathbf{u}$ is the gradient of $\mathbf{u}$. This Lagrangian is equivalent with the standard Lagrangian,

$$L'[\boldsymbol{\epsilon}] = \int_V \frac{1}{2} \boldsymbol{\epsilon} : \mathbf{c} : \boldsymbol{\epsilon} \, dv, \quad (6)$$

with $\boldsymbol{\epsilon}$ being the symmetric part of $\nabla \mathbf{u}$; indeed, $\delta L = 0$ leads to $\nabla \cdot (\mathbf{c} : \nabla \mathbf{u}) = \mathbf{0}$, which is also derived from $\delta L' = 0$.

According to higher order PDS, we discretize the three functions of $\mathbf{u}$, $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ as follows:

$$\mathbf{u}(\mathbf{x}) = \sum_{\alpha, n} \mathbf{u}^{\alpha n} P_n(\mathbf{x} - \mathbf{y}^\alpha) \phi^\alpha(\mathbf{x}), \quad (7)$$

and

$$\boldsymbol{\epsilon}(\mathbf{x}) = \sum_{\beta, n} \boldsymbol{\epsilon}^{\beta n} P_n(\mathbf{x} - \mathbf{z}^\beta) \psi^\beta(\mathbf{x}), \quad (8)$$

$$\boldsymbol{\sigma}(\mathbf{x}) = \sum_{\beta, n} \boldsymbol{\sigma}^{\beta n} P_n(\mathbf{x} - \mathbf{z}^\beta) \psi^\beta(\mathbf{x}). \quad (9)$$

Here, $\{\mathbf{u}^{\alpha n}\}$, $\{\boldsymbol{\epsilon}^{\beta n}\}$ and $\{\boldsymbol{\sigma}^{\beta n}\}$ are a set of unknown coefficients. Substitution of Eqs. (7)~(9) into Eq. (5) and stationalization of the resulting L with respect to $\boldsymbol{\epsilon}^{\beta n}$ and $\boldsymbol{\sigma}^{\beta n}$ leads to

$$\boldsymbol{\epsilon}^{\beta n} = \sum_{\alpha, m} \text{sym}(\mathbf{b}^{\beta n \alpha m} \otimes \mathbf{u}^{\alpha m}),$$

and

$$\boldsymbol{\sigma}^{\beta n} = \mathbf{c} : \boldsymbol{\epsilon}^{\beta n}.$$

Here, sym stands for the symmetric part of the second-order tensor, and $\mathbf{b}^{\beta n \alpha m}$ is a vector defined as

$$\mathbf{b}^{\beta n \alpha m} = \sum_k B_{nk}^\beta \int_V P_k(\mathbf{x} - \mathbf{z}^\beta) \psi^\beta(\mathbf{x}) \nabla (P_m(\mathbf{x} - \mathbf{y}^\alpha) \phi^\alpha(\mathbf{x})) \, dv, \quad (10)$$

and B_{nk}^β is the inverse of the matrix of

$$A_{nk}^\beta = \int_V P_n(\mathbf{x} - \mathbf{z}^\beta) P_k(\mathbf{x} - \mathbf{z}^\beta) \psi^\beta(\mathbf{x}) \, dv; \quad (11)$$

B_{nk}^β is a $N + 1$ -by- $N + 1$ matrix for the N dimension setting. Finally, expressing $\boldsymbol{\epsilon}^{\beta n}$ and $\boldsymbol{\sigma}^{\beta n}$ in terms of $\mathbf{u}^{\alpha n}$, we can derive the following equation from the stationalization of L of Eq. (5):

$$\sum_{\alpha', m'} (\mathbf{b}^{\beta n \alpha m} \cdot \mathbf{c} \cdot \mathbf{b}^{\beta n \alpha' m'}) \cdot \mathbf{u}^{\alpha' m'} = 0, \quad (12)$$

for α and m . This matrix equation is the equation that is solved by higher order PDS-FEM. Indeed,

$$\mathbf{b}^{\beta n \alpha m} \cdot \mathbf{c} \cdot \mathbf{b}^{\beta n \alpha' m'} \quad \text{or} \quad \sum_{i,k} b_i^{\beta n \alpha m} c_{ijkl} b_k^{\beta n \alpha' m'}$$

gives the stiffness matrix of higher order PDS-FEM.

It is possible to derive Eq. (12) using the standard Lagrangian, L' , of Eq. (6). When $\mathbf{u}$ is discretized as Eq. (7), we compute the gradient as

$$\nabla \mathbf{u}(\mathbf{x}) = \sum_{\beta, m} (\mathbf{b}^{\beta n \alpha m} \otimes \mathbf{u}^{\alpha m}) P_n(\mathbf{x} - \mathbf{z}^\beta) \psi^\beta(\mathbf{x}).$$

Note that this discretization of $\nabla \mathbf{u}$ follows the discretization of a function's derivative, which is explained in the preceding section. Substitution of $\nabla \mathbf{u}$ into Eq. (6) and stationalization of the resulting L yields the identical matrix equation as given in Eq. (12).

Although expressions appear simple, the computation of $\mathbf{b}^{\beta n \alpha m}$ defined in Eq. (10) needs careful manipulation. We summarize key equations in computing this vector, together with the matrix A_{nk}^β defined in Eq. (11). There are cases in which special care have to be taken in enforcing boundary conditions for PDS-FEM; Appendix B discusses this issue.

4. Numerical Example

In this section, we present some numerical results to demonstrate the improvements in implementing first order polynomials in PDS-FEM. Some details of the difficulty in setting boundary conditions has been mentioned in the latter part of the this section. Results of first order PDS-FEM is compared with that of zero-th order and analytical solutions. Further, the rate of convergence for displacement and stress are evaluated to ensure the improvements.

(1) Problem Setting

The standard plate of infinite extent with a circular hole subjected to far field tensile loading is considered as the numerical example. Plane stress conditions are assumed and the far field tensile stress in x -direction is assumed to be $\sigma_0 = 10\text{MPa}$. The Young's modulus and the Poisson's ratio of the plate is assumed to be 1GPa and 0.33, respectively. The simulated domain shown in Fig. 3 has the dimension of $6\text{m} \times 3\text{m}$ and the radius of the circular hole is set to 1 meter. The same figure shows a sample of the Delaunay tessellation used for approximating the derivative related

fields (i.e. ϵ , σ , etc.). Symmetric boundary conditions are set for the two straight edges at the bottom, while the displacement boundary conditions are set along the top and two vertical edges according to the analytical solution. Further details on setting of boundary conditions are discussed below.

(2) Setting boundary condition

Setting the correct boundary condition is essential in solving a boundary value problem. This is not a problem with ordinary FEM; it requires only the point values of force or displacement at the boundary nodes. However, it is not straightforward to impose boundary conditions in first-order PDS-FEM. Unlike in ordinary FEM, 1st order PDS-FEM has $N + 1$ unknowns in each of N spatial dimension. For instance, there are six unknown coefficients of displacement in 2D settings; the constants $u_i^{\alpha 0}$ and coefficients of linear terms $u_i^{\alpha n} (n = 1, 2)$, in each coordinate direction. Tied to these, there are six coefficients related to external force, which appear in the global stiffness matrix as follows.

$$[K] \begin{Bmatrix} \vdots \\ u_1^{\alpha 0} \\ u_1^{\alpha 1} \\ u_1^{\alpha 2} \\ \vdots \end{Bmatrix} = \begin{Bmatrix} \vdots \\ f_1^{\alpha 0} \\ f_1^{\alpha 1} \\ f_1^{\alpha 2} \\ \vdots \end{Bmatrix}$$

Approximate values of the constant coefficients $u^{\alpha 0}$ or $f^{\alpha 0}$ can be readily set, just as in ordinary FEM. On the contrary, the evaluation of gradient terms, $u^{\alpha n}$ or $f^{\alpha n}$ for $n = 1, 2$, is not straightforward. If all the $f^{\alpha n}$'s, for $n = 1, 2$, are set to unknown on the boundary, the linear system becomes singular. On the other hand, setting all the $u^{\alpha n}$'s, for $n = 1, 2$, to zero produces a solution which significantly deviates from the analytical solution as shown in Fig. 4(b). As is seen in Fig. 4(a) there is high fluctuations along the boundary, especially at corners.

A proper way to deal with the above mentioned boundary condition problem is discussed in the Appendix B. For the sake of checking the properties like convergence rate of first order PDS-FEM, we make use of the known analytical solution to set all the $u^{\alpha n}$'s, for $n = 1, 2$, along all the straight edges at the boundary. Surely, this is not applicable for general problems and boundary conditions must be set as discussed in Appendix B.

(3) Results with artificially set boundary conditions

The plate with a hole problem is solved using both the zero-th order and first order PDS-FEM, setting the boundary conditions as explained above. As it

Fig.3 Numerical Example

Fig.4 Result from PDS-FEM 1st order without any special treatment to boundary conditions (a) Stress σ_{xx} Distribution (b) Comparison of result with analytical solution along section AB

has been stated in earlier section, the field variables are approximated as unions of local Taylor series expansions. The approximated variables are discontinuous since PDS-FEM does not enforce any conditions to smoothly connect Taylor expansions in neighbouring Voronoi or Delaunay elements. These discontinuities are clearly visible in Fig. 5. A course mesh composed of 738 nodes and 1378 elements is used, so that the discontinuities in the approximated fields are visible. Figure 5(a) shows x component of displacement while 5(c) shows the stress component σ_{xx} , obtained with first order PDS-FEM. While the solution for displacement field consists of local patches of planes which are orderly arranged, there are discontinuities along the Voronoi boundaries. Figure 5(c) shows σ_{xx} estimated with the discontinuous displace-

Fig.6 Comparison of stress in x -direction, σ_{xx} from (a) 0-th order PDS-FEM (b) 1st order PDS-FEM

ment field shown in Fig. 5(a). As is seen, the stress field is also made of orderly arranged local patched of planes, which are discontinuous along Delaunay boundaries. Figure 5(b) and 5(d) shows the surface plot of displacement and stress with a fine mesh respectively. These figures advocate the smoothing of solution, even though no smoothing conditions are enforced along Voronoi or Delaunay boundaries. Deviation from the exact solution along the boundary is eliminated with artificial treatment of boundary condition.

It is of interest to examine the improvement in accuracy and smoothness of solution, which is accomplished by comparing the stress component σ_{xx} along the section A-B in Fig. 3. Figure 7 shows the analytical solutions and numerical solutions, which are calculated using zero-th and first order PDS-FEM, of σ_{xx} . The comparison made in Fig. 7 indicates that the numerical results are in good agreement with analytical solution with artificial boundary condition, and the first order PDS-FEM has relatively smoother than zero-th order, which is clearly visible in the vicinity of the stress concentration in Fig. 6. A quick comparison of Fig. 4(b) and 7 indicates the significant improvement in the results along the boundary.

The increase of the order of polynomials is also

Fig.5 Surface plot of displacement and stress fields obtained with first order PDS-FEM. The color indicates the scale of vertical axis.

expected to deliver an increase in the rate of convergence to the solution. When solving the boundary value problem, first order PDS-FEM uses localized first order Taylor expansions to approximate both functions and derivatives. To examine what rates of convergence are attained for both displacement and stress, the same plate with the hole problem is solved with four different tessellations increasing fineness. According to the Fig. 8 the average of convergence rate for u_x is 2.14 and that for σ_{xx} is 1.87. Both the displacement and stress have nearly second order con-

vergence. A possible reason for convergence rate to be slightly lower than 2, which is the expected, is the assumption made in the setting of boundary conditions. As mentioned all the six displacement components, $u_i^{\alpha n}$ for $i = 1, 2$ and $p = 0, 1, 2$, are set according to the analytical solution. However, along the curved boundary, it is assumed that $f_i^{\alpha 1}$ and $f_i^{\alpha 2}$, for $i = 1, 2$, to be zero. This assumption, which is not strictly valid, is a possible reason for convergence rate to be slightly lower than the expected. The proper treatment of boundary conditions, which is discussed

Fig.7 Comparison of stress, σ_{xx} with analytical solution along the width of plate (AB section)

Fig.8 Convergence rate for displacement (left) and stress (right). dof stands for the degree of freedoms in one direction (i.e. square root of total degree of freedom).

in Appendix B, should improve the convergence rates to the expected value of 2. The second order rate of convergence for both displacement field and stress field confirms the improvement made by first order PDS-FEM.

5. Concluding Remarks

Extension of PDS-FEM, a novel numerical technique has been presented in this paper. Detailed formulation of extended PDS-FEM has been described and verified with conventional numerical example. Improvement in accuracy has been observed. Results show the good agreement with the analytical solution. Higher convergence rate in stress and displacement has been observed with first order polynomial. Higher convergence rate is an advantage of proposed formulation, since it is quantitative measurement of efficiency. In order to ease the implementation of ex-

Fig.9 Explanation of function and derivative approximation

tended numerical method, qualitative and illustrative treatment of boundary condition is needed to be address.

APPENDIX A Taylor Series Expansion for PDS

PDS is a discretization scheme which use discontinuous basis functions so that discontinuity of functions are naturally expressed. In a mathematical view-point, allowing discontinuity in a discretized function could be accepted if Taylor series expansion is considered. A smooth function allows Taylor series expansion, but when the expansion is taken at two neighboring points, the two expanded polynomials are not smoothly connected and discontinuity appears.

A union of Taylor series expansions which are taken at a set of points could be regarded a discretization of a smooth function. The connection of neighboring expansion is a key point for this union. Higher order PDS uses derivatives of the function; polynomials in neighboring Voronoi blocks share derivative in polynomial form in a common Delaunay block. Figure 9 shows illustrated the approximation of function and calculation of derivative using Voronoi and Delaunay tessellation.

Union of Taylor series expansions is a key characteristic of higher order PDS, which differentiates it from other particle methods ^{(10),(11)}, which enforce smoothness to fields produced by particle as well as fields in particles; fields in particle are requested to vanish near the boundary of the particle. Enforcing smoothness is surely attractive in solving a differen-

tial equation. However, it is contradicting to the consequence of the Taylor series expansion, i.e., a smooth function allows Taylor series expansion but the expanded polynomials cannot be smoothly connected to each other.

We are not denying the usefulness of the well-established particle methods. Instead, we are pointing out the consequence of Taylor series expansion, and there could be a room to improve the particle methods. A function discretized by PDS has discontinuity everywhere, which is a draw back in the viewpoint of the particle method. A further study is needed to investigate discontinuities of a discretized function.

When higher order PDS is regarded as a union of local Taylor series expansion, the accuracy could be examined by checking the coefficients of the expansion. For instance, the following errors could be useful:

$$E^{f*} = \sum_{\alpha} ((f(\mathbf{y}^{\alpha}) - f^{\alpha 0})^2 + \sum_n (f_{,n}(\mathbf{y}^{\alpha}) - f^{\alpha n})^2),$$

$$E^{g*} = \sum_{\beta, n} ((f_{,n}(z^{\beta}) - g_n^{\beta 0})^2 + \sum_m (f_{,nm}(\mathbf{z}^{\beta}) - g_m^{\beta n})^2).$$

Note that E^f and E^g should be used to check the convergence rate of PDS discretized function; E^{f*} and E^{g*} are for the Taylor series expansion coefficients.

APPENDIX B Consistency of Boundary Conditions

Consider the following one-dimensional boundary value problem:

$$u''(x) = 0 \quad 0 < x < 1, \quad u(0) = 0, \quad u(1) = 1. \quad (\text{B.1})$$

We decompose the analysis domain into two parts, $\Phi^1 = \{x | 0 < x < \frac{1}{2}\}$ and $\Phi^2 = \{x | \frac{1}{2} < x < 1\}$, and use the entire domain as Ψ^1 . According to 1st order PDS, discretized functions of u and u' are

$$u^d = (u^{10} + u^{11}x)\phi^1 + (u^{20} + u^{21}(x-1))\phi^2,$$

$$g^d = ((-u^{10} + u^{20}) + \frac{1}{8}(u^{11} - u^{21})(x - \frac{1}{2}))\psi^1,$$

where $\{u^{\alpha n}\}$ are unknowns. Lagrangian that corresponds to Eq. (B.1) is $L[\epsilon] = \int_0^1 \frac{1}{2}\epsilon^2 dx$, and substitution of $\epsilon = g^d$ into L leads to

$$L = \frac{1}{2}(u^{20} - u^{10})^2 + \frac{1}{8}(u^{21} - u^{11})^2.$$

Even if the boundary conditions are posed to u^d , (i.e., $u^{10} = 0$ and $u^{20} = 1$), stationalization of L does not determine $\{u^{\alpha 1}\}$ uniquely.

As a sort of consistency, we introduce the following conditions for the derivative:

$$(u^d)'(x) = g^d(x) \quad x = 0, 1. \quad (\text{B.2})$$

These two conditions determine $u^{11} = u^{21} = 1$, which stationalize L , and this the exact solution of Eq. (B.1).

Unlike Voronoi blocks inside the analysis domain, a Voronoi block on the boundary is covered by a unique Delaunay block. Hence, we may request derivatives of a function discretized in this Voronoi block to coincide with those of the unique Delaunay block. It might be more natural to use flux rather than derivative if we use this request as a sort of consistency for boundary conditions. That is,

$$\mathbf{n} \cdot (\nabla f^d(\mathbf{x}) - \mathbf{g}^d(\mathbf{x})) = 0, \quad \mathbf{x} \text{ on } \partial V \quad (\text{B.3})$$

where $\mathbf{n}$ is the outer unit normal on ∂V .

APPENDIX C Computation of $\mathbf{b}^{\beta, n \alpha m}$

In order to compute $\mathbf{b}^{\beta, n \alpha m}$, we make use of the following integrations that are easily carried out:

1. $V^{\beta \alpha} = \int \phi^{\alpha} \psi^{\beta} dv.$
2. $V^{\beta n m} = \int_{\Phi^{\alpha}} (x_n - z_n^{\beta})(x_m - z_m^{\beta}) dv.$
3. $S_j^{\beta 0 \alpha 0} = \int_{\partial \Phi^{\alpha}} n_j(\mathbf{x}) \psi^{\beta}(\mathbf{x}) ds.$
4. $S_j^{\beta n \alpha 0} = \int_{\partial \Phi^{\alpha}} n_j(\mathbf{x})(x_n - z_n^{\beta}) \psi^{\beta}(\mathbf{x}) ds.$
5. $S_j^{\beta 0, \alpha m} = \int_{\partial \Phi^{\alpha}} n_j(\mathbf{x})(x_m - y_m^{\alpha}) \psi^{\beta}(\mathbf{x}) ds.$
6. $S_j^{\beta n \beta m} = \int_{\partial \Phi^{\alpha}} n_j(\mathbf{x}) \psi^{\beta}(\mathbf{x})(x_n - z_n^{\beta})(x_m - y_m^{\alpha}) dv.$
7. $V_j^{\beta 0 \alpha 0} = V_j^{\beta 0 \alpha m} = 0.$
8. $V_j^{\beta n \alpha 0} = \int_{\Phi^{\alpha}} (\psi^{\beta}(\mathbf{x})(x_n - z_n^{\beta}))_{,j} dv$
9. $V_j^{\beta n \alpha m} = \int_{\Phi^{\alpha}} (\psi^{\beta}(\mathbf{x})(x_n - z_n^{\beta}))_{,j}(x_m - y_m^{\alpha}) dv.$

Note that $S_j^{\beta \dots}$ and $V^{\dots}$ are for the surface integration on $\partial \Phi^{\alpha}$ and the volume integration in Φ^{α} .

Using the above defined volume and surface integrations, we can efficiently compute $\mathbf{b}^{\beta, n \alpha m}$ of Eq. (10). Note that

$$\int_V P_n(\mathbf{x} - \mathbf{z}^{\beta}) \psi^{\beta}(\mathbf{x})(P_m(\mathbf{x} - \mathbf{y}^{\alpha}) \phi^{\alpha}(\mathbf{x}))_{,j} dv$$

$$= S_j^{\beta n \alpha m} - V_j^{\beta n \alpha m}.$$

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