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Conserving Galerkin weak formulations for computational fracture mechanics

Shaofan Li*,†,‡ and Daniel C. Simkins Jr.

Department of Civil and Environmental Engineering, University of California, Berkeley, CA 94720, U.S.A.

SUMMARY

In this paper, a notion of invariant Galerkin-variational weak forms is proposed. Two specific invariant variational weak forms, the J-invariant and the L-invariant, are constructed based on the corresponding conservation laws in elasticity, one of which is the conservation of Eshelby's energy-momentum (Eshelby, *Philos. Trans. Roy. Soc.* 1951; **87**:12; In *Solid State Physics*, Setitz F, Turnbull D (eds). Academic Press: New York, 1956; 331; Rice, *J. Appl. Mech.* 1968; **35**:379).

It is shown that the finite element solution obtained from the invariant Galerkin weak formulations proposed here can conserve the value of J-integral, or L-integral exactly. In other words, the J and L integrals of the Galerkin finite element solutions are path independent in the discrete sense. It is argued that by using the J-invariant Galerkin weak form to compute near crack-tip field in an elastic solid, one may accurately calculate the crack extension energy release rate and subsequently the stress intensity factors in numerical computations, because the flux of the energy-momentum is conserved in discrete computations. This may provide an alternative means to accurately simulate crack growth and propagation. Copyright © 2002 John Wiley & Sons, Ltd.

KEY WORDS: discrete conservation laws; Galerkin methods; crack growth; finite element methods; fracture mechanics; energy-momentum tensor

1. INTRODUCTION

For most finite element (FE) analyses in solid mechanics, the equilibrium equation

$$\sigma_{ji,j} + f_i = 0, \quad \forall \mathbf{x} \in \Omega \tag{1}$$

is often chosen as the departure point, where σ_{ji} is the Cauchy stress, f_i is the body force, and Ω is the problem domain.

*Correspondence to: Shaofan Li, Department of Civil and Environmental Engineering, University of California, Berkeley, CA 94720, U.S.A.
†E-mail: li@ce.berkeley.edu
‡Assistant Professor of Applied Mechanics.

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Consider the following boundary conditions:

$$\sigma_{ij} n_j = \hat{T}_i \quad \forall \mathbf{x} \in \Gamma_t \tag{2}$$

$$u_i = \hat{u}_i \quad \forall \mathbf{x} \in \Gamma_u \tag{3}$$

where $\Gamma_t \cup \Gamma_u = \partial\Omega$.

Define function spaces

$$\mathscr{V} := \{\delta\mathbf{u} \mid \delta\mathbf{u} = 0,\ \forall \mathbf{x} \in \Gamma_u;\ \delta\mathbf{u} \in H^1(\Omega)\} \tag{4}$$

$$\mathscr{S} := \{\mathbf{u} \mid \mathbf{u} = \hat{\mathbf{u}},\ \forall \mathbf{x} \in \Gamma_u;\ \mathbf{u} \in H^1(\Omega)\} \tag{5}$$

and consider finite-dimensional function spaces $\mathscr{S}^h \subset \mathscr{S}$ and $\mathscr{V}^h \subset \mathscr{V}$ generated by a mesh. A Galerkin weak form may be derived via the weighted residual method (e.g. Reference [1]),

$$\int_\Omega \sigma_{ij} \delta u_{i,j} \, \mathrm{d}\Omega - \int_{\Gamma_t} \hat{T}_i \delta u_i \, \mathrm{d}S - \int_\Omega f_i \delta u_i \, \mathrm{d}\Omega = 0 \quad \forall \delta u_i \in \mathscr{V} \tag{6}$$

Its discrete counterpart reads as

$$\int_\Omega \sigma_{ij}^h \delta u_{i,j}^h \, \mathrm{d}\Omega - \int_{\Gamma_t} \hat{T}_i \delta u_i^h \, \mathrm{d}S - \int_\Omega f_i \delta u_i^h \, \mathrm{d}\Omega = 0 \quad \forall \delta u_i^h \in \mathscr{V}^h \tag{7}$$

Equation (7) is a discrete weak form of the equilibrium equation Equation (1), and consequently it preserves the force flux after the discretization. This property is apparent in discontinuous Galerkin formulations. Neglect the body force and consider a single element Ω_e in the interior of Ω. The element weak form reads as

$$\int_{\Omega_e} \sigma_{ik}^h \delta u_{i,k}^h \, \mathrm{d}\Omega - \int_{\partial\Omega_e} \sigma_{ik}^h n_k \delta u_i^h \, \mathrm{d}S = 0 \tag{8}$$

Choosing $\delta u_i^h = 1$ (hence $\delta u_{i,k}^h = 0$), one may find the following discrete conservation law:

$$\oint_{\partial\Omega_s} T_i^h \, \mathrm{d}S = 0 \tag{9}$$

where $T_i^h = \sigma_{ik}^h n_k$ is the traction on the element boundary. The global conservation of force flux can then be obtained by integrating the weak form in all the elements in the domain. It has been pointed out in a recent paper by Hughes *et al.* [2] that this local conservative property may hold for continuous Galerkin formulations as well.

In passing, we note that a finite element solution based on the weak form (7) is an approximate solution, and it may not be the exact solution. As mesh size approaches zero, it may approach the exact solution. Even though the stress distributions derived from the solution of (7) are not the exact stress distributions, but the discrete solution of (7) retains an important property of the exact solution: *the conservation of force flux*, that is the force flux is conserved, or balanced in discrete sense, which provides users with certain assurance as well as confidence on stress distributions of the numerical solution.

Nevertheless, the numerical solution of (7) will not conserve *other* invariant quantities, which the original continuous system does. After discretization, most other invariant properties of the Navier equation will be lost, consequently their numerical values may be less accurate than the numerical values of stresses. In this sense, the conventional finite element method in solid mechanics is biased; it is in favour of a particular conservation law, the balance of force or linear momentum. It relies on the Galerkin weak formulation derived from a strong form of most obvious conservation law, the equilibrium equation. In contrast, other conservation laws in elasticity will no longer hold after discretization, and the quantities associated with those conservation laws are no longer invariant in discrete sense.

In fact, the governing equation of linear elasticity has infinitely many conservation laws (see References [3–5]). Among them, a very useful conservation law is the so-called J-integral proposed by Rice [6], which is the conservation of Eshelby's celebrated energy-momentum tensor [7, 8]. Shown by Rice [6], the value of J-integral in a contour surrounding a crack tip is exactly the energy release rate, G, due to the crack extension; moreover, J-integral is also closely related to the stress intensity factors of the crack.

The primary goal of computational fracture mechanics is simulating the near crack-tip field, and evaluating material strength that are relevant to fracture process, such as stress intensity factors, $K_{\rm I}$, $K_{\rm II}$, and $K_{\rm III}$. In computations, stress intensity factors are often evaluated through calculating J-integral; the accuracy of the J-integral computation is therefore of great importance. From this standpoint, a Galerkin weak formulation that can preserve the energy-momentum flux will be very desirable in computational fracture mechanics, because with such formulation one may be able to predict crack growth with more accuracy. Indeed, the loss of accuracy in evaluation of contour J-integral has already caused much concern. As reported by Li *et al.* [9], the range of numerical errors in evaluating J-integral by using the virtual crack extension technique were found to be 5%, 18%, and 7% for elastic, elastoplastic, and fully plastic regimes, respectively. In some cases, the numerical error can reach as high as 30%. To improve the accuracy on numerical computation of J-integral, much effort has been made in the past few decades. The state-of-the-art technique is the so-called *domain integral method*. After numerical solutions are obtained from computations, a post-processing is adopted to evaluate the J-integral by using a domain integral technique proposed by Li *et al.* [9], and Nikishkov and Atluri [10], which was later generalized and perfected by Moran and Shih [11, 12]. Since the discrete solution of weak form (7) does not conserve J-integral to begin with, the domain integral procedure is limited by the accuracy of numerical data that it receives.

The objective of this paper is two-fold: (1) First, we seek an energy-momentum conserving algorithm, a J-invariant Galerkin weak formulation, which can preserve energy-momentum flux in discrete computations, and therefore, provides a better computational algorithm that improves the accuracy in evaluating the J-integral and hence stress intensity factors for crack growth simulations. (2) Second, from a much more broad perspective, the proposed notion of invariant Galerkin weak formulation suggests a theoretical underpinning to form alternative Galerkin weak forms for continuum mechanics problems, or any other problems involved solving partial differential equations.

It is the contribution of this paper to show that by employing the proposed J-invariant Galerkin weak form, the discrete numerical solution will automatically and generically conserve the energy-momentum flux in discrete computations. In other words, the J-integral of the finite element solution is path-independent as the exact solution in the continuum theory, which furnishes the theoretical justifications for the proposed Galerkin weak formulations.

2. A J-INVARIANT GALERKIN WEAK FORMULATION

Consider the equilibrium equation without body force

$$\sigma_{ji,j} = 0, \quad \mathbf{x} \in \Omega \tag{10}$$

where Ω is an elastic solid admitting a potential function W such that

$$\sigma_{ij} = \frac{\partial W}{\partial \varepsilon_{ij}} \tag{11}$$

in which

$$\varepsilon_{ij} := \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{12}$$

are infinitesimal strains.

To introduce the notion of invariant Galerkin variational weak form, we first outline a few properties of Eshelby's energy-momentum tensor. Define the energy-momentum tensor as

$$E_{jk} := W\delta_{jk} - \sigma_{ij}\frac{\partial u_i}{\partial x_k} \tag{13}$$

First of all, the energy-momentum tensor is divergence free, or it obeys an 'equilibrium' equation for '*energy-momentum flux*',

$$\frac{\partial E_{jk}}{\partial x_j} = 0 \quad \text{or} \quad \nabla \cdot \mathbf{E} = 0 \tag{14}$$

By virtue of Equation (10), it can be shown that

$$\begin{aligned} \frac{\partial E_{jk}}{\partial x_j} &= \frac{\partial W}{\partial \varepsilon_{\ell m}}\frac{\partial \varepsilon_{\ell m}}{\partial x_j}\delta_{jk} - \frac{\partial \sigma_{ij}}{\partial x_j}\frac{\partial u_i}{\partial x_k} - \sigma_{ij}\frac{\partial^2 u_i}{\partial x_k \partial x_j} \\ &= \sigma_{\ell m}\frac{\partial \varepsilon_{\ell m}}{\partial x_k} - \sigma_{ij}\frac{\partial^2 u_i}{\partial x_j \partial x_k} = 0 \end{aligned} \tag{15}$$

In general, there is an analogue between Cauchy stress tensor and Eshelby's energy-momentum tensor (see References [13, 14]). By Gauss's theorem, the following invariant integral can be found:

$$J_k = \oint_{\partial\Omega} E_{jk} n_j \, \mathrm{d}S = \oint_{\partial\Omega} (W n_k - T_i u_{i,k}) \, \mathrm{d}S = 0 \tag{16}$$

where $T_i = \sigma_{ij} n_j$. This fact has been thoroughly examined in the context of elasticity by many authors, e.g. References [3, 4, 6, 8, 15–20] among others. In fact, the invariant property of energy-momentum tensor is rooted in Noether's celebrated theorem on invariant variational principles [21]. The contemporary development has been documented in the literature (e.g. Reference [5]).

The objective in this work is, however, different; we do not claim any new contribution in conservation laws of continuum mechanics, but rather we are interested in developing computational algorithms that preserve the discrete counterpart of the conservation laws in continuum mechanics, such as J-integral, which, to the best of the authors' knowledge, has not been studied before, even though it is of practical importance.

Instead of choosing Equation (1) or (10) as the departure point, we choose Equation (14) as the departure point to construct a Galerkin weighted-residual form

$$\int_\Omega (\nabla \cdot \mathbf{E}^h) \cdot \delta \mathbf{u}^h \, \mathrm{d}\Omega = \int_\Omega E^h_{jk,j} \delta u^h_k \, \mathrm{d}\Omega = \int_\Omega \left(W^h \delta_{jk} - \sigma^h_{ij} \frac{\partial u^h_i}{\partial x_k} \right)_{,j} \delta u^h_k \, \mathrm{d}\Omega = 0, \quad \forall u^h_k \in \mathscr{V}^h \tag{17}$$

Integration by parts yields

$$\text{Algorithm I}: \begin{cases} \displaystyle\int_\Omega \mathbf{E}^h : \nabla \delta \mathbf{u}^h \, \mathrm{d}\Omega - \int_{\partial\Omega} (\mathbf{E}^h \cdot \mathbf{n}) \cdot \delta \mathbf{u}^h \, \mathrm{d}S \\ \displaystyle\quad = \int_\Omega E^h_{jk} \delta u^h_{k,j} \, \mathrm{d}\Omega - \int_{\Gamma_t} \left(W^h n_k - \hat{T}_i \frac{\partial u^h_i}{\partial x_k} \right) \delta u^h_k \, \mathrm{d}S = 0, \quad \forall \delta u^h_k \in \mathscr{V}^h \end{cases} \tag{18}$$

On the other hand, define stress spaces

$$\mathscr{P} := \{ \delta\boldsymbol{\sigma} \mid \delta\boldsymbol{\sigma} = 0, \forall \mathbf{x} \in \Gamma_t; \text{ and } \delta\boldsymbol{\sigma} \in H^1(\Omega) \} \tag{19}$$

$$\mathscr{Q} := \{ \boldsymbol{\sigma} \mid \mathbf{n} \cdot \boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}, \ \forall \mathbf{x} \in \Gamma_t, \boldsymbol{\sigma} \in H^1(\Omega) \} \tag{20}$$

Consider finite-dimensional function spaces $\mathscr{P}^h \subset \mathscr{P}$ and $\mathscr{Q}^h \subset \mathscr{Q}$ due to a mesh. One may form the following the Galerkin weighted-residual form:

$$\int_\Omega (\nabla \cdot \mathbf{E}^h) \cdot \delta \boldsymbol{\sigma}^h \, \mathrm{d}\Omega = \int_\Omega E^h_{jk,j} \delta \sigma^h_{k\ell} \, \mathrm{d}\Omega = \int_\Omega \left(W^h \delta_{jk} - \sigma^h_{ij} \frac{\partial u^h_i}{\partial x_k} \right)_{,j} \delta \sigma^h_{k\ell} \, \mathrm{d}\Omega = 0 \quad \forall \delta \sigma^h_{k\ell} \in \mathscr{P}^h \tag{21}$$

Integration by part yields

$$\text{Algorithm II}: \begin{cases} \displaystyle\int_\Omega \mathbf{E}^h \cdot (\nabla \cdot \delta \boldsymbol{\sigma}^h) \, \mathrm{d}\Omega - \int_{\partial\Omega} (\mathbf{E}^h \cdot \mathbf{n}) \cdot \delta \boldsymbol{\sigma}^h \, \mathrm{d}S \\ \displaystyle\quad = \int_\Omega E^h_{jk} \delta \sigma^h_{k\ell,\ell} \, \mathrm{d}\Omega - \int_{\Gamma_u} \left(W^h n_k - \hat{T}_i \frac{\partial u^h_i}{\partial x_k} \right) \delta \sigma^h_{kj} \, \mathrm{d}S = 0 \quad \forall \delta \sigma^h_{kj} \in \mathscr{P}^h \end{cases} \tag{22}$$

It may be noted that the difference between the two algorithms is that Algorithm I takes into account the energy-momentum flux through traction boundary, whereas Algorithm II only consider the energy-momentum flux through the displacement boundary.

Before stating the main results, a few definitions are in order[§]

Definition 2.1 (*Partition*(*Subdivision*))
A partition $T_M = \{\mathscr{T}_1, \mathscr{T}_2, \ldots, \mathscr{T}_M\}$ of Ω is called *admissible* if

1. $\mathscr{T}_i \cap \mathscr{T}_j = \emptyset$, $(i \neq j)$;

[§]These definitions are standard, e.g. References [22–25].

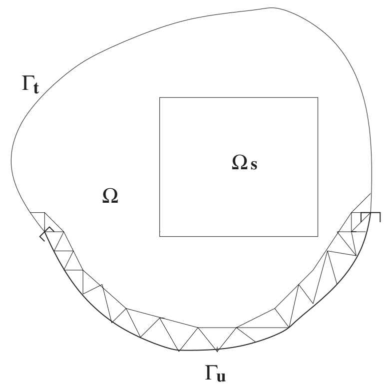

Figure 1. The support and domain of basis functions associated with essential boundary.

2. $\mathscr{T}_M$ is an open cover of Ω, i.e. $\bigcup_{i=1}^{M} \mathscr{T}_i = \bar{\Omega}$;
3. if $\bar{\mathscr{T}_i} \cap \bar{\mathscr{T}_j}$ $(i \neq j)$ consists of exactly one point, then it is the common vertex of $\mathscr{T}_i$ and $\mathscr{T}_j$;
4. if $\bar{\mathscr{T}_i} \cap \bar{\mathscr{T}_j}$ $(i \neq j)$ consists of more than one point, then $\bar{\mathscr{T}_i} \cap \bar{\mathscr{T}_j}$ is the common surface, or common edge between $\mathscr{T}_i$ and $\mathscr{T}_j$.

For convenience, Λ_Ω is denoted as the index set of the partition T_M, i.e. $\Lambda_\Omega = \{i \mid x_i \in \bar{\Omega},\ i = 1, 2, \ldots, M\}$.

Definition 2.2 (*Partition of unity*)
For a given partition T_M, there exists a class of functions, $\{\Phi_I\}_{I=1}^{N} \in C^0(\mathbb{R}^n)$, such that

1. $0 \leqslant \Phi_I(\mathbf{x}) \leqslant 1,\ \forall I$;
2. each Φ_I has its support in some $\mathscr{T}_i$, and
3. $\sum_{I=1}^{N} \Phi_I(\mathbf{x}) = 1,\ \forall \mathbf{x} \in \bar{\Omega}$.

$\{\Phi_I(\mathbf{x})\}_{I=1}^{N}$ is called a partition of unity.

Denote $\Pi_N := \{I \mid I = 1, 2, \ldots, N\}$ as the index set of $\{\Phi_I(\mathbf{x})\}_{I=1}^{N}$; and the mapping between Λ_Ω and Π_N is then the so-called connectivity array in finite element methods (see References [25, 26]).

It is noted that, in general, one may construct a partition of unity such that

$$\mathscr{S}^h = \text{span}\{\Phi_I(\mathbf{x})\}_{I \in \Pi_N} \tag{23}$$

but

$$\mathscr{V}^h \neq \text{span}\{\Phi_I(\mathbf{x})\}_{I \in \Pi_N} \tag{24}$$

due to the essential boundary condition (see Figure 1). To prove general global conservation properties, one has to augment the space $\mathscr{V}^h$ to include the nodes on the essential boundary. The procedure is elaborated by Hughes *et al.* [2].

To get to the point quickly, it is assumed that $\Gamma_u = \emptyset$, $\Omega_s \subset \Omega$ is a singly connected subdomain, and $\Omega_s \cap \Gamma_u = \emptyset$, so that $\{\Phi_I\}_{I \in \Pi_N}, \forall \mathbf{x} \in \Omega_s$ is always a partition of unity.

Let

$$\Phi_I^{\dagger} := \begin{cases} \Phi_I(\mathbf{x}), & \mathbf{x} \in \Omega_s \\ 0, & \mathbf{x} \notin \Omega \end{cases} \tag{25}$$

Definition 2.3 (*Admissible sub-domain*)
For a given subdivision $T_M := \{\mathscr{T}_i\}_{i \in \Lambda_\Omega}$ and a partition of unity $\mathscr{P} := \{\Phi_I\}_{I \in \Pi_N}$ in Ω, the special domain, $\Omega_s \subset \Omega$, is defined as a class of sub-domains, and $\Omega_s \cap \Gamma_t = \emptyset$, such that there exists a sub-partition of unity, $\mathscr{P}^{\dagger} = \{\Phi_I^{\dagger}(\mathbf{x})\}_{I \in \Pi_s}$, a sub index set $\Lambda_{\Omega_s} \subset \Lambda_\Omega$, and $\Pi_s \subset \Pi_N$ that render the following conditions:

$$\Omega_s = \bigcup_{e \in \Lambda_{\Omega_s}} \mathscr{T}_e \tag{26}$$

$$\sum_{I \in \Pi_s} \Phi_I^{\dagger}(\mathbf{x}) = 1, \quad \mathbf{x} \in \bar{\Omega}_s \tag{27}$$

The merit of the invariant weak form (17) is enunciated in the following theorem:

Theorem 2.1
For test function $\delta u_k^h \in \mathscr{V}^h$, the numerical solution, $u_k^h \in \mathscr{S}^h$, of the following weak formulation:

$$\int_\Omega E_{jk}^h \delta u_{k,j}^h \, d\Omega - \int_{\Gamma_t} \left(W^h n_k - \hat{T}_i \frac{\partial u_i^h}{\partial x_k} \right) \delta u_k^h \, dS = 0 \tag{28}$$

satisfies the following discrete conservation law:

$$\oint_{\partial\Omega_s} \left(W^h n_k - T_i^h \frac{\partial u_i^h}{\partial x_k} \right) dS = 0 \tag{29}$$

where $T_i^h = \sigma_{ij}^h n_j$ and $\Omega_s \subset \Omega$ is an admissible sub-domain of Ω.

Note that it is not difficult to deduce that $\partial\Omega_s \subset \bigcup_{i \in \Lambda_{\Omega_s}} \partial\mathscr{T}_i$. The point is that all the admissible sub-domains Ω_s of Ω are surrounded by finite element boundary. An admissible domain has to be surrounded by finite element edges. The concept of the admissible sub-domain Ω_s is illustrated in Figure 2(a) and 2(b).

Proof
Let

$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \Pi_N} \Phi_I(\mathbf{x}) \mathbf{u}_I \quad \forall \mathbf{x} \in \Omega \tag{30}$$

$$\delta\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \Pi_N} \Phi_I(\mathbf{x}) \delta\mathbf{u}_I \quad \forall \mathbf{x} \in \Omega \tag{31}$$

If Λ_{Ω_s} is a special subset of Ω, there exists a subset Π_s of Π_N such that

$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \Pi_s} \Phi_I^{\dagger}(\mathbf{x}) \mathbf{u}_I \quad \forall \mathbf{x} \in \Omega_s \tag{32}$$

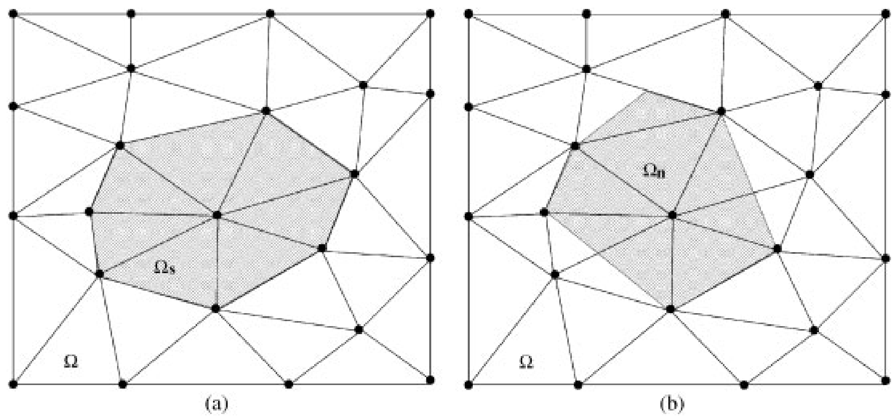

Figure 2. Schematic illustration: (a) admissible sub-domain Ω_s, (b) in-admissible sub-domain Ω_s.

$$\delta\mathbf{u}^h(\mathbf{x}) = \sum_{I\in\Pi_s} \Phi_I^{\dagger}(\mathbf{x})\delta\mathbf{u}_I \quad \forall \mathbf{x}\in\Omega_s \tag{33}$$

For fixed $I\in\Pi_s$, the J-invariant weak form (17) holds $\forall e\in\Lambda_s$,

$$\int_{\mathscr{T}_e} E_{jk}^h \Phi_{I,j}^{\dagger}\,\mathrm{d}\Omega - \oint_{\partial\mathscr{T}_e} \left(W^h n_k - \sigma_{ij}^h n_i \frac{\partial u_i^h}{\partial x_k} \right) \Phi_I^{\dagger}\,\mathrm{d}S = 0 \tag{34}$$

Use the element assembly notation [26] and assume the displacements and the energy-momentum tensor are continuous across the element boundary. One may find that

$$\mathop{\mathbf{A}}_{e\in\Lambda_{\Omega_s}} \oint_{\partial\mathscr{T}_e} \left(W^h n_k - \sigma_{ij}^h n_i \frac{\partial u_i^h}{\partial x_k} \right) \Phi_I^{\dagger}\,\mathrm{d}S = \oint_{\partial\Omega_s} \left(W^h n_k - \sigma_{ij}^h n_i \frac{\partial u_i^h}{\partial x_k} \right) \Phi_I^{\dagger}\,\mathrm{d}S \tag{35}$$

Consequently,

$$\begin{aligned} &\mathop{\mathbf{A}}_{e\in\Lambda_{\Omega_s}} \left\{ \int_{\mathscr{T}_e} E_{jk}^h \Phi_{I,j}^{\dagger}\,\mathrm{d}\Omega - \oint_{\partial\mathscr{T}_e} \left(W^h n_k - \sigma_{ij}^h n_i \frac{\partial u_i^h}{\partial x_k} \right) \Phi_I^{\dagger}\,\mathrm{d}S \right\} \\ &\quad = \int_{\Omega_s} E_{jk}^h \Phi_{I,j}^{\dagger}\,\mathrm{d}\Omega - \oint_{\partial\Omega_s} \left(W^h n_k - \sigma_{ij}^h n_i \frac{\partial u_i^h}{\partial x_k} \right) \Phi_I^{\dagger}\,\mathrm{d}S = 0 \end{aligned} \tag{36}$$

Sum $I\in\Pi_s$ and replace the volume (area) integral in (36) by the Gauss quadrature

$$\begin{aligned} &\sum_{I\in\Pi_s} \left\{ \int_{\Omega_s} E_{jk}^h \Phi_{I,j}^{\dagger}\,\mathrm{d}\Omega - \oint_{\partial\Omega_s} \left(W^h n_k - \sigma_{ij}^h n_i \frac{\partial u_i^h}{\partial x_k} \right) \Phi_I^{\dagger}\,\mathrm{d}S \right\} \\ &\quad = \sum_{I\in\Pi_s} \sum_{k=1}^{\mathrm{GK}} E_{jk}^h(\mathbf{x}_k)\Phi_{I,j}^{\dagger}(\mathbf{x}_k) w_k - \sum_{I\in\Pi_s} \oint_{\partial\Omega_s} \left(W^h n_k - \sigma_{ij}^h n_i \frac{\partial u_i^h}{\partial x_k} \right) \Phi_I^{\dagger}\,\mathrm{d}S \end{aligned}$$

$$= \sum_{k=1}^{\mathrm{GK}} \sum_{I\in\Pi_s} E^h_{jk}(\mathbf{x}_k)\Phi^\dagger_{I,j}(\mathbf{x}_k)w_k - \oint_{\partial\Omega_s} \left(W^h n_k - \sigma^h_{ij} n_i \frac{\partial u^h_i}{\partial x_k}\right)\left(\sum_{I\in\Pi_s}\Phi^\dagger_I(\mathbf{x})\right)\mathrm{d}S$$

$$= 0 \tag{37}$$

where w_k is the Gauss quadrature weight and GK is total number of Gauss points inside Ω. Using the property of partition of unity

$$\sum_{I\in\Pi_s}\Phi^\dagger_I(\mathbf{x}) = 1 \quad \forall \mathbf{x}\in\Omega_s \tag{38}$$

$$\sum_{I\in\Pi_s}\Phi^\dagger_{I,j}(\mathbf{x}) = 0 \quad \forall \mathbf{x}\in\Omega_s \tag{39}$$

We arrive at the conclusion

$$\oint_{\partial\Omega_s}\left(W^h n_k - \sigma^h_{ij} n_i \frac{\partial u^h_i}{\partial x_k}\right)\mathrm{d}S = 0 \tag{40}$$

□

Following a similar procedure, one can easily show that Algorithm II (22) is also conserving the energy-momentum flux.

Remark 2.1
In a finite element discretization, one can find a region, Ω_s, such that $\Omega_s = \bigcup_{e\in\Lambda_{\Omega_s}} \mathscr{T}_e$ and $\Omega_\imath \cap \Omega_\jmath = \emptyset \ \forall \imath, \jmath \in \Lambda_{\Omega_s}$, and all the shape functions, $\Phi^\dagger_I$, associated with nodal points inside Ω_s form a partition of unity, i.e. $\sum_{I\in\Pi_s}\Phi^\dagger_I(\mathbf{x}) = 1$. This is, however, not true for non-interpolate discretization, for instance the moving least-square interpolant [27], and the related mesh-free interpolants, such as those used in element-free Galerkin method (EFG) [28], or the reproducing kernel particle method (RKPM) [29].

3. PRACTICAL ISSUES

3.1. Discrete J-integral

In computational fracture mechanics, the main concern is to calculate the stress intensity factors, which can be accomplished by evaluating the J-integral. To illustrate the invariant property of the new algorithm, we consider the problem shown in Figure 3. In this case,

$$J := J_1 = \int_\Gamma \left(W^h n_1 - \sigma^h_{ij} n_j \frac{\partial u^h_i}{\partial x_1}\right)\mathrm{d}S \tag{41}$$

is relevant to the stress intensity factor calculation. Note that Γ is a special contour through element boundary.

Choose a finite element discretization consisting of quadrilateral elements. In Figure 3, the shaped area, $\Omega_s \subset \Omega$, satisfies the admissible condition. In this particular configuration, the

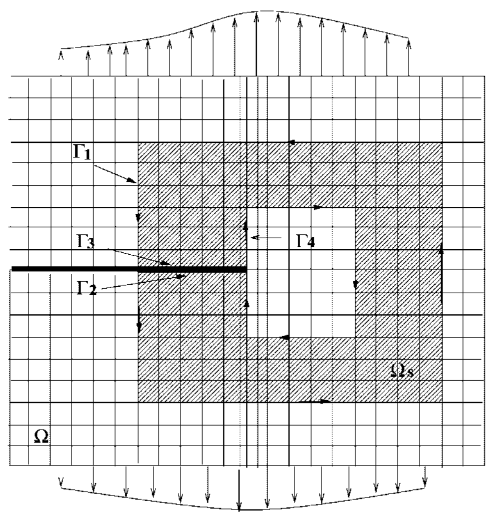

Figure 3. Contour integrals around a crack.

J-invariance implies that

$$\int_{\Gamma_1}\left(W^h n_1-\sigma_{ij}^h n_j\,\frac{\partial u_i^h}{\partial x_1}\right)\mathrm{d}S=\int_{\Gamma_{4-}}\left(W^h n_1-\sigma_{ij}^h n_j\,\frac{\partial u_i^h}{\partial x_1}\right)\mathrm{d}S \qquad (42)$$

There exist index subsets $\Lambda_{\mathrm{s}}\subset\Lambda_M$, and $\Pi_{\mathrm{s}}\subset\Pi_N$, such that $\{\Phi_I\}_{\Pi_{\mathrm{s}}}$ is a partition of unity inside Ω_{s}, and $\forall I\in\Pi_{\mathrm{s}}$

$$\begin{aligned}\mathop{\mathbf{A}}_{e\in\Lambda_{\mathrm{s}}}\left\{\int_{\mathcal{T}_e}E_{j1}^h\Phi_{I,j}\,\mathrm{d}\Omega-\oint_{\mathcal{T}_e}E_{j1}n_j\Phi_I\,\mathrm{d}S\right\}&=\int_{\Omega_{\mathrm{s}}}E_{j1}^h\Phi_{I,j}\,\mathrm{d}\Omega-\oint_{\partial\Omega_{\mathrm{s}}}E_{j1}^h n_j\Phi_I\,\mathrm{d}S\\&=\int_{\Omega_{\mathrm{s}}}E_{j1}^h\Phi_{I,j}\,\mathrm{d}\Omega-\int_{\Gamma_1}E_{j1}^h n_1\Phi_I\,\mathrm{d}S-\int_{\Gamma_2}E_{j1}^h n_j\Phi_I\,\mathrm{d}S\\&\quad-\int_{\Gamma_3}E_{j1}^h n_j\Phi_I\,\mathrm{d}S-\int_{\Gamma_4}E_{j1}^h n_j\Phi_I\,\mathrm{d}S=0\end{aligned} \qquad (43)$$

if the displacement field and stress/strain field are assumed to be continuous across the each element boundary.

Since along Γ_2,Γ_3, $n_1=0$ and $\hat{T}_j=\sigma_{ij}n_i=0$ the above expression can also be expressed as

$$\int_{\Omega_{\mathrm{s}}}E_{j1}^h\Phi_{I,j}\,\mathrm{d}\Omega-\int_{\Gamma_1}E_{j1}^h n_j\Phi_I\,\mathrm{d}S-\int_{\Gamma_4}E_{j1}^h n_j\Phi_I\,\mathrm{d}S=0 \qquad (44)$$

Replace the volume (area) integral in (44) by a chosen quadrature

$$\sum_{k=1}^{\mathrm{GK}}E_{j1}^h(\mathbf{x}_k)\Phi_{I,j}(\mathbf{x}_k)w_k-\int_{\Gamma_1}E_{j1}^h n_j\Phi_I\,\mathrm{d}S-\int_{\Gamma_4}E_{j1}^h n_j\Phi_I\,\mathrm{d}S=0 \qquad (45)$$

where w_k is the quadrature weight and GK is the total number of Gauss quadrature points inside Ω_s.

Sum Equation (45) $\forall I \in \Pi_s$

$$\begin{aligned}
&\sum_{I\in\Pi_s}\sum_{k=1}^{GK} E_{j1}^h(\mathbf{x}_k)\Phi_{I,j}(\mathbf{x}_k)w_{ik} - \sum_{I\in\Pi_s}\int_{\Gamma_1} E_{j1}^h n_j \Phi_I \,\mathrm{d}S - \sum_{I\in\Pi_s}\int_{\Gamma_4} E_{j1}^h n_j \Phi_I \,\mathrm{d}S \\
&= \sum_{k=1}^{GK}\sum_{I\in\Pi_s} E_{j1}^h(x_k)\Phi_{I,j}(x_k)w_k - \int_{\Gamma_1}\sum_{I\in\Pi_s} E_{j1}^h n_j \Phi_I \,\mathrm{d}S - \int_{\Gamma_4}\sum_{I\in\Pi_s} E_{j1}^h n_j \Phi_I \,\mathrm{d}S \\
&= 0
\end{aligned} \tag{46}$$

Using the properties of the partition of unity (38) and (39), one has

$$\sum_{k=1}^{GK}\sum_{I\in\Pi_s} E_j^h(\mathbf{x}_k)\Phi_{I,j}(\mathbf{x}_k)w_k = \sum_{k=1}^{GK} E_j^h(\mathbf{x}_k)w_k\left(\sum_{I\in\Pi_s}\Phi_{I,j}(\mathbf{x}_k)w_k\right) = 0$$

and

$$\int_{\Gamma_1}\sum_{I\in\Pi_s} E_{j1}^h(x)n_j\Phi_I(x)\,\mathrm{d}S = \int_{\Gamma_1} E_{j1}^h(x)n_j\sum_{I\in\Pi_s}\Phi_I(x)\,\mathrm{d}S = \int_{\Gamma_1}\sum_{I\in\Pi_s} E_{j1}^h(x)n_j\,\mathrm{d}S$$

$$\int_{\Gamma_4}\sum_{I\in\Pi_s} E_{j1}^h(x)n_j\Phi_I(x)\,\mathrm{d}S = \int_{\Gamma_4} E_{j1}^h(x)n_j\sum_{I\in\Pi_s}\Phi_I(x)\,\mathrm{d}S = \int_{\Gamma_4}\sum_{I\in\Pi_s} E_{j1}^h(x)n_j\,\mathrm{d}S$$

They lead to the desired result

$$\int_{\Gamma_1} E_{j1}^h n_j \,\mathrm{d}S = \int_{\Gamma_{4-}} E_{j1}^h n_j \,\mathrm{d}S \tag{47}$$

where the path Γ_{4-} is the contour Γ_4 turning in clockwise direction (see Figure 3).

4. CONSISTENT LINEARIZATION

Denote $\mathbf{d} := \{\mathbf{u}_1, \mathbf{u}_2, \ldots, \ldots, \mathbf{u}_N\}$. The discrete balance of energy-momentum equation become

$$(\mathbf{f}^{\text{int}} - \mathbf{f}^{\text{ext}}) \cdot \delta\mathbf{d} = 0 \tag{48}$$

where

$$f_{kI}^{\text{int}} := \int_{\Omega} E_{jk}^h(\mathbf{u})\Phi_{I,j}\,\mathrm{d}\Omega \tag{49}$$

$$f_{kI}^{\text{ext}} := \int_{\Gamma_t}\left(W^h(\mathbf{u})n_k - \hat{T}_i\frac{\partial u_i}{\partial x_k}\right)\Phi_I\,\mathrm{d}S \tag{50}$$

Unlike the conventional Galerkin weak form based on the equilibrium equation, the J-invariant Galerkin weak form (48) leads to a set of non-linear algebraic equations. To find the solution, iterative methods, such as Newton–Raphson scheme, may be needed in the solution procedure, which requires consistent linearization

$$(\mathbf{f}^{\rm int}-\mathbf{f}^{\rm ext})(\hat{\mathbf{u}}+\boldsymbol{\eta})=(\mathbf{f}^{\rm int}-\mathbf{f}^{\rm ext})(\hat{\mathbf{u}})+\Delta(\mathbf{f}^{\rm int}-\mathbf{f}^{\rm ext})(\hat{\mathbf{u}}+\boldsymbol{\eta})+\mathscr{R}(\hat{\mathbf{u}}+\boldsymbol{\eta}) \tag{51}$$

where the remainder $\mathscr{R}(\hat{\mathbf{u}}+\boldsymbol{\eta})$ has the property

$$\lim_{\|\boldsymbol{\eta}\|\to 0}\frac{\mathscr{R}}{\|\boldsymbol{\eta}\|}\to 0 \tag{52}$$

Taking Gateaux derivative, one may have

$$\begin{aligned}\Delta f_{kI}^{\rm int}&:=\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left\{\int_\Omega E_{jk}^h(\mathbf{u}+\varepsilon\Delta\mathbf{u})\Phi_{I,j}\,{\rm d}\Omega-\int_\Omega E_{jk}^h(\mathbf{u})\Phi_{I,j}\,{\rm d}\Omega\right\}\\&=\int_\Omega\left(\sigma_{\ell m}^h\Delta\varepsilon_{\ell m}^h\delta_{jk}-\Delta\sigma_{ij}^h\frac{\partial u_i^h}{\partial x_k}-\sigma_{ij}^h\frac{\partial\Delta u_i^h}{\partial x_k}\right)\Phi_{I,j}\,{\rm d}\Omega\end{aligned} \tag{53}$$

and

$$\begin{aligned}\Delta f_{kI}^{\rm ext}:=\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}&\left\{\int_{\Gamma_t}\left(W^h(\mathbf{u}+\varepsilon\Delta\mathbf{u})n_k-\hat{T}_i\frac{\partial(u_i^h+\varepsilon\Delta u_i^h)}{\partial x_k}\right)\Phi_I\,{\rm d}S\right.\\&\left.-\int_{\Gamma_t}\left(W^h(\mathbf{u})n_k-\hat{T}_j\frac{\partial u_i^h}{\partial x_k}\right)\Phi_I\,{\rm d}S\right\}\end{aligned} \tag{54}$$

$$=\int_{\Gamma_t}\left(\sigma_{\ell m}^h\Delta\varepsilon_{\ell m}^h n_k-\hat{T}_i\frac{\partial\Delta u_i^h}{\partial x_k}\right)\Phi_I\,{\rm d}S \tag{55}$$

Denote $\Delta\mathbf{d}:=\{\Delta\mathbf{u}_1,\Delta\mathbf{u}_2,\ldots,\Delta\mathbf{u}_N\}$. One may write

$$\Delta f_{iI}^{\rm int}=\sum_J K_{ijIJ}^{\rm int}\Delta u_{jJ} \tag{56}$$

$$\Delta f_{iI}^{\rm ext}=\sum_J K_{ijIJ}^{\rm ext}\Delta u_{jJ} \tag{57}$$

and the components of the tangent stiffness matrix can be expressed as

$$K_{ijIJ}^{\rm int}=\int_\Omega\left(\frac{1}{2}\,\sigma_{\ell m}^h\Phi_{I,i}(\Phi_{J,\ell}\delta_{mj}+\Phi_{J,m}^\dagger\delta_{\ell j})-\frac{1}{2}\,C_{\ell mpq}\frac{\partial u_\ell^h}{\partial x_i}\Phi_{I,m}(\Phi_{J,p}\delta_{jq}+\Phi_{J,q}^\dagger\delta_{jp})-\sigma_{jm}^h\Phi_{I,m}\Phi_{J,i}\right){\rm d}\Omega \tag{58}$$

and

$$K_{ijIJ}^{\rm ext}=\int_{\Gamma_t}(\tfrac{1}{2}\,\sigma_{\ell m}^h\Phi_I(\Phi_{J,\ell}\delta_{mj}+\Phi_{J,m}\delta_{\ell j})n_i-\hat{T}_j\Phi_I\Phi_{J,i}){\rm d}S \tag{59}$$

5. OTHER INVARIANT WEAK FORMULATIONS IN ELASTICITY

The following questions may rise:

- Can every conservation law furnish a useful Galerkin weak formulation?
- How many invariant Galerkin weak formulations can we construct for an elastostatic problem?

As shown by Olver [3, 4], there could be infinitely many conservation laws in elastostatics. In principle, an invariant Galerkin formulation may be constructed based on any specific conservation law that a user thinks is most pertinent to the specific aspect of a mechanics problem considered. It will in turn preserve a particular physical quantity in discrete sense. In other words, a given invariant Galerkin variational formulation is equivalent to a specific discrete conservation law. Nevertheless, not all conservation laws can furnish a useful invariant variational weak form. In some cases, a conservation law may fail to establish an invariant Galerkin variational weak form. To illustrate this point, two additional invariant Galerkin weak forms are constructed in the following.

In the first example, the following L-invariant variational formulations is constructed based on the conservation of angular energy-momentum. Following Budiansky and Rice [30], we define the angular energy-momentum tensor

$$Q_{ik} := \varepsilon_{ikm} x_m W + \varepsilon_{imj}(\sigma_{mk} u_j - \sigma_{\ell k} u_{\ell,m} x_j) \tag{60}$$

It is elementary to verify that $\mathbf{Q}$ is divergence free for linear elastic solids:

$$\begin{aligned}\frac{\partial Q_{ik}}{\partial x_k} &= \varepsilon_{ikm}\delta_{mk} W + \varepsilon_{imk} x_m W_{,k} + \varepsilon_{imj}(\sigma_{mk} u_{j,k} - \sigma_{\ell k} u_{\ell,mk} x_j - \sigma_{\ell k} u_{\ell,m}\delta_{jk}) \\ &= \varepsilon_{imj}(\sigma_{m\ell} u_{j,\ell} - \sigma_{\ell j} u_{\ell,m}) = 0\end{aligned} \tag{61}$$

In fact, Knowles and Sternberg [18] showed that the above expression holds for more general elastic constitutive relations.

Since

$$\int_\Omega \frac{\partial Q_{ik}}{\partial x_k}\,\delta u_i \,\mathrm{d}\Omega = \int_\Omega Q_{ik}\delta u_{i,k}\,\mathrm{d}\Omega - \int_{\Gamma_t} Q_{i,k} n_k \delta u_i \,\mathrm{d}S = 0 \tag{62}$$

the following discrete L-invariant weak form may be constructed.

Theorem 5.1

For $\delta u_i^h \in \mathscr{S}^h$, the numerical solution, $u_i^h \in \mathscr{V}^h$, of the following Galerkin weak formulation,

$$\int_\Omega Q_{ik}^h\,\delta u_{i,k}^h\,\mathrm{d}\Omega - \int_{\Gamma_t} \varepsilon_{ikm}\left(x_m n_k W^h + \hat{T}_k u_m^h - \hat{T}_\ell u_{\ell,k}^h x_m\right)\delta u_i^h\,\mathrm{d}S = 0 \tag{63}$$

will satisfy the following discrete conservation law:

$$\oint_{\partial\Omega_s} \varepsilon_{ikm}(x_m n_k W^h + T_k^h u_m^h - T_\ell^h u_{\ell,k}^h x_m)\,\mathrm{d}S = 0 \tag{64}$$

where $\Omega_s \subset \Omega$ is an admissible sub-domain.

The proof is omitted here.

In the second example, let

$$R_k = Wx_k - \sigma_{jk}(u_{j,i}x_i + \tfrac{1}{2}u_j) \tag{65}$$

It is straightforward that

$$\begin{aligned}\frac{\partial R_k}{\partial x_k} &= W\delta_{kk} + x_k W_{,k} - \sigma_{jk}(u_{j,ik}x_i + u_{j,i}\delta_{ik} + \tfrac{1}{2}\,u_{j,k}) \\ &= x_k \sigma_{\ell m}\varepsilon_{\ell m,k} - x_k \sigma_{\ell m} u_{\ell,mk} = 0\end{aligned} \tag{66}$$

Consequently, the following M-invariant integral holds in continuum level [30],

$$\oint_{\partial\Omega_s} \left(Wx_k n_k - T_j u_{j,i} x_i + \tfrac{1}{2}\,T_i u_i\right)\,\mathrm{d}S = 0, \quad \Omega_s \subset \Omega \tag{67}$$

But this conservation law fails to produce a Galerkin weak formulation since $\mathbf{R}$ is only a vector.

6. CLOSURE

The notion of invariant Galerkin variational formulation is a generalization of the conventional Galerkin variational method. The conventional Galerkin variational method establishes its weighted residual form based on the original strong form of a partial differential equation (PDE) that is under consideration, whereas the invariant Galerkin variational method establishes its weighted residual form based on the strong form of a suitable conservation law that the PDE possesses. Most PDEs have many different conservation laws, which may be infinitely many. In fact, the original strong form of the PDE itself is also a particular conservation law. Therefore, from a computational standpoint, one could construct many different invariant Galerkin weak formulations for a PDE. It should be noted that all these invariant variational weak forms are not equivalent in discrete sense; each may conserve one special physical quantity in computation, and hence the accuracy of different quantities obtained in different weak formulations will vary. In engineering applications, one may prefer to conserve one physical quantity over another, if one cannot preserve all of them at the same time. The significance of this contribution is that it extends the options and choices on how to construct Galerkin variational weak forms. Based on the notion of invariant weak formulation proposed here, one may have many different choices to form a Galerkin weak form while solving a specific engineering problem. In the area of computational fracture mechanics, the energy-momentum tensor is obviously a more important quantity than the Cauchy stress tensor. Therefore, preserving energy-momentum flux is more important than preserving traction flux.

It may be pointed out that the energy-momentum conserving algorithms proposed in this paper are different from so-called energy-momentum conserving algorithms in time integration schemes, such as the work done by late Prof. J. C. Simo and his co-worker [31, 32]. Nonetheless, Simo and Honein [33] did intend to construct a variational formulation to preserve discrete conservation laws. We believe that at least part of that goal has been achieved in this work. In the end, we would like to pose the following question:

> Can one construct an invariant Galerkin-variational weak form that preserves discrete force flux as well as energy-momentum flux?

which, we believe, is a challenging one.

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