

# Recent developments in parametrized variational principles for mechanics

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**Abstract** This paper gives an introduction to the formulation of parametrized variational principles (PVPs) in mechanics. This is complemented by more advanced material describing selected recent developments in hybrid and nonlinear variational principles. A PVP is a variational principle containing free parameters that have no effect on the Euler-Lagrange equations and natural boundary conditions. The theory of single-field PVPs, based on gauge functions, is a subset of the Inverse Problem of Variational Calculus that has limited value. On the other hand, multifield PVPs are more interesting from both theoretical and practical standpoints. The two-dimensional Poisson equation is used to present, in a tutorial fashion, the formulation of parametrized mixed functionals. This treatment is then extended to internal interfaces, which are useful in treatment of discontinuities, subdomain linkage and construction of parametrized hybrid functionals. This is followed by a similar but more compact treatment of three-dimensional classical elasticity, and a parametrization of nonlinear hyperelasticity.

## 1

### Introduction

This paper introduces basic concepts behind the formulation of parametrized variational principles (PVPs) in mechanics. This is complemented by more advanced material describing recent developments made since the publication of a comprehensive survey (Felippa 1994). Most of the introductory exposition is taken from that reference. For reasons of space the present article does not discuss applications to computational mechanics in general and finite element methods in particular. Such applications are summarized in that survey and elaborated in the references given therein.

A PVP derives from a functional with free parameters if the Euler-Lagrange equations and natural boundary conditions turn out to be independent of those parameters. It is useful to emphasize the distinction between single-field PVPs, in which only one primary field is varied, and multifield (mixed or hybrid) PVPs. Single-field PVPs have been extensively studied but lack interest for applications. Multifield PVPs are less understood but are far more interesting from the dual standpoint of theory and applications.

The present study of multifield PVPs was originally motivated by the desire of finding a variational framework for finite elements based on the Free Formulation of Bergan and Nygård (1984), later expanded to the Scaled Free Formulation of Bergan and Felippa (1985). In numerical tests those elements had displayed excellent performance, but a theoretical explanation was lacking. This foundation was provided by parametrized functionals (Felippa 1989). As sometimes happens, this modest goal led to unexpected discoveries, chief among them a general parametrization of the functionals of classical elasticity (Felippa and Militello 1989, 1990). Subsequently more applications to finite elements were revealed.

## 1

### Basic concepts and definitions

#### 2.1

##### Some simple examples

Beginner calculus students are soon taught about the presence of an integration constant when obtaining indefinite integrals of functions of one variable:

$$\frac{dy}{dx} = F(x), \quad y(x) = \int F(x) dx = G(x) + C, \quad (1)$$

where  $G(x)$  is a primitive of  $F(x)$ . Later on, in multivariable calculus they learn about partial integrals:

$$\frac{\partial z}{\partial x} = F(x, y), \quad z(x, y) = \int F(x, y) dx = G(x, y) + C(y). \quad (2)$$

The fact that primitive functions are not unique, because differentiation is a restricting operation, can be viewed as the simplest example of parametrized functionals.

As a next example consider a single-field functional  $\Pi(u)$  that depends on a function  $u(x)$  of a single spatial variable that satisfies appropriate smoothness requirements. The functional

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$\Pi$  also contains a free parameter  $\beta$ :

$$\Pi(u; \beta) = \frac{1}{2} \int_a^b F(u; \beta) dx = \frac{1}{2} \int_a^b [-(u')^2 + 2\beta uu' + u^2] dx, \quad (3)$$

where primes denote derivative with respect to  $x$ . The Euler-Lagrange equation associated with  $\delta\Pi = 0$  is

$$E(u) = u'' + u = 0, \quad (4)$$

which is independent of  $\beta$ . The natural boundary conditions

$$\left. \frac{\partial F}{\partial u'} \right|_{x=a} = \beta u(a) - u'(a) = 0, \quad \left. \frac{\partial F}{\partial u'} \right|_{x=b} = \beta u(b) - u'(b) = 0, \quad (5)$$

are not independent of  $\beta$  unless  $u(a) = u(b) = 0$ . The parameter-independence of the Euler-Lagrange equation and natural boundary conditions characterize parametrized variational principles, which are defined more precisely in Section 2.3.

The example can be generalized with arbitrary functions by replacing  $\beta uu'$  with  $\beta(Pu' + Q)$ , where  $P$  and  $Q$  are functions of  $u$  and  $x$  only, as shown in the next subsection.

## 2.2

### Principal and gauge functionals

The explanation for the behavior of the preceding functionals is straightforward. Consider (3) in which the parametrized term is split as

$$\Pi(u; \beta) = \Pi_p(u) + \beta \Pi_G(u), \quad (6)$$

$$\begin{aligned} \Pi_p(u) &= \frac{1}{2} \int_a^b [-(u')^2 + u^2] dx, & \Pi_G(u) \\ &= \int_a^b uu' dx = \frac{1}{2} [u^2(b) - u^2(a)]. \end{aligned} \quad (7)$$

Here  $\Pi_p$  is labeled as the *principal functional* whereas  $\Pi_G$  is labeled as a *gauge functional*. The latter is also called a *null Lagrangian* in the literature. Because  $\Pi_G$  depends only on boundary values, its contribution to the Euler-Lagrange equation of  $\Pi$  is obviously zero; thus cancelling the effect of  $\beta$ .

The converse statement is also a well known theorem of variational calculus: if the Euler-Lagrange equation of a single-field functional containing up to first-order derivatives vanishes identically, that functional must depend only on boundary values. For a scalar function of one variable the proof is short. The Euler-Lagrange equation of a gauge functional  $F_G(u)$  depending on  $u(x)$  and  $u'(x)$  is

$$\frac{\partial F_G}{\partial u} - \frac{d}{dx} \left( \frac{\partial F_G}{\partial u'} \right) = \frac{\partial F_G}{\partial u} - \frac{\partial^2 F_G}{\partial x \partial u'} - \frac{\partial^2 F_G}{\partial u \partial u'} u' - \frac{\partial^2 F_G}{\partial u' \partial u'} u'' \equiv 0. \quad (8)$$

If (8) is an identity for any  $F_G$ , the function coefficient of  $u''$  must vanish; thus  $F_G$  must be of the form  $Pu' + Q$ , where  $P$  and  $Q$  are functions of  $u$  and  $x$ . Substitution into (8) yields  $\partial Q/\partial u = \partial P/\partial x$ ,

which shows that  $Pdu + Qdx$  must be the exact differential of a function  $G(u, x)$ . Consequently  $\int F_G(u) dx = G(u, x)$  and the value of the integral depends only on its end points. This result is easily generalized to vector functions  $u(x)^T = \{u_1(x), \dots, u_n(x)\}$ . These are particularly relevant to semi-discrete dynamical systems with  $n$  degrees of freedom, in which  $x$  becomes the time  $t$ .

Should the single-field functional depend on several independent variables  $x, y, \dots$ , one can obviously add the divergence or curl of multidimensional functions multiplied by free parameters, because application of Green's or Stokes' theorems reduces such functions to boundary terms. If the functional depends on derivatives of higher order than first, the situation becomes more complicated; that case is studied in Chapter IV of the textbook by Courant and Hilbert (1953).

## 2.3

### Terminology

A functional that contains one or more free parameters, such as  $\Pi$  in the foregoing example, is called a *parametrized functional*. If its Euler-Lagrange equation and natural boundary conditions are independent of the parameters, then the stationarity condition  $\delta\Pi = 0$  is called a *parametrized variational principle* or PVP.

A PVP is most useful from the standpoint of applications if the value of the functional, evaluated at an extremal, is *independent* of the free parameters. This value has often the meaning of energy. Such a principle will be called an *invariant parametrized variational principle* or IPVP. The example functional (3) yields an IPVP if, in addition to  $u(a) = u(b) = 0$ ,  $[u''(b)]^2 = [u''(a)]^2$  or if  $[u'(b)]^2 = [u'(a)]^2$ . (To prove the latter, insert  $u = -u'$  into  $\Pi_G$  and integrate.) The condition for a PVP to be invariant can be generally expressed through Noether's conservation-law theorem of variational calculus; see for instance Sec. 20 of Gelfand and Fomin (1963). But for many cases that kind of invariance can be checked directly.

The most useful invariant PVPs are those in which invariance does not depend on boundary conditions. Such functionals will be encountered in Sections 4 and 6.

## 2.4

### Connections with the inverse problem

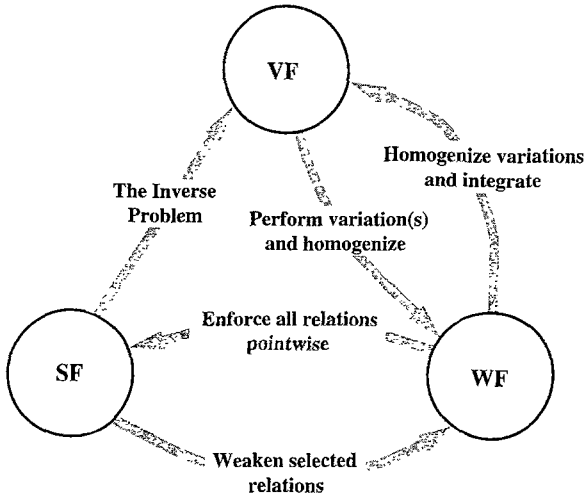
The study of single-field PVPs constitutes a subset of the Inverse Problem of Variational Calculus: given a system of ordinary or partial differential equations – herein called the Strong Form or SF – find the Lagrangians that have system as Euler-Lagrange equations. These Lagrangians, if they exist, collectively embody the Variational Form (VF) of the problem. The Weak Form (WF), which is also known by the alternative names listed in Fig. 1, is an intermediary between SF and VF. Relations between those forms are annotated in that Figure.

The Inverse Problem linking ordinary differential equations to single-field functionals is treated in several monographs (e.g., Santilli 1979; Sewell 1987; Vujanovic and Jones 1989). On the other hand, the multifield case is less developed, particularly in the case of multiple space variables.

## 2.5

### Theoretical and practical advantages

PVPs are interesting from a theoretical standpoint because of their unifying value: a single PVP is equivalent to a family of



**Fig. 1.** Diagram sketching Strong, Weak and Variational Forms, and relationships between form pairs. (Weak Forms are also called weighted-residual equations, variational equations, Galerkin equations and integral statements in the literature.)

functionals. Specific functionals can be obtained by setting parameters to specific values. A theorem proved for a PVP is “economical” in the sense that it need not be redone for specific cases.

Books and articles on the variational formulations of field problems for physics and engineering usually focus on the so-called *canonical* functionals, which are those found to be either of substantial practical value, or historical interest. Examples of these are the Minimum Potential Energy, Hellinger-Reissner and Hu-Washizu functionals of classical elasticity. That kind of presentation has two drawbacks. First, what ought to be shared properties are proved over and over, a feat that can result in voluminous expositions. Second, readers may be left with the impression that only a limited number of functionals for say, elasticity, have been discovered, which encourages the publication of “new” functionals in an nonending stream of articles.

The main interest of PVPs, in the applications, center on *direct methods* that use variational principles as a source of analytical or numerical approximations. Chief among the latter is the Finite Element Method (FEM). The key observation is that *approximations depend on the free parameters*. On the other hand, the converged solution, assuming a convergent discretization method, does not. Thus an obvious question arises: can the free parameters be chosen in such a way that errors are minimized while the number of degrees of freedom remain modest? An implementation of this idea in the FEM arena leads to High Performance Elements and templates (Felippa 1994). Additional information on these research thrusts is given in the Conclusions section.

### 3 A Two-field 1-D example

As our first encounter with a multifield PVP, the following 6-coefficient generalization of (3) to two independently varied

fields;  $u$  and  $p = u'$ , is postulated:

$$\begin{aligned} \Pi(u, p; J) &= \int_a^b F(u, u', p) dx \\ &= \frac{1}{2} \int_a^b \begin{Bmatrix} u \\ u' \\ p \end{Bmatrix}^T \begin{bmatrix} j_{11} & j_{12} & j_{13} \\ j_{12} & j_{22} & j_{23} \\ j_{13} & j_{23} & j_{33} \end{bmatrix} \begin{Bmatrix} u \\ u' \\ p \end{Bmatrix} dx = \frac{1}{2} \int_a^b \mathbf{z}^T \mathbf{J} \mathbf{z} dx, \end{aligned} \quad (9)$$

in which

$$\mathbf{z} = \begin{Bmatrix} u \\ u' \\ p \end{Bmatrix}, \quad \mathbf{J} = \begin{bmatrix} j_{11} & j_{12} & j_{13} \\ j_{12} & j_{22} & j_{23} \\ j_{13} & j_{23} & j_{33} \end{bmatrix}. \quad (10)$$

are the *generalized field vector* and the *functional generating matrix*, respectively. This parameter matrix – the “kernel” of the quadratic form in the  $\mathbf{z}$  vector – may be taken as symmetric because only its symmetric part participates in the first variation. This general notational arrangement is followed in more complicated linear problems of mathematical physics presented later.

The Euler-Lagrange equations supplied by  $\delta_u \Pi = 0$  and  $\delta_p \Pi = 0$  are

$$\begin{aligned} E_u : F_u - \frac{d}{dx} F_{u'} &= j_{11} u + j_{12} u' + j_{13} p \\ &\quad - (j_{12} u' + j_{22} u'' + j_{23} p') = 0, \\ E_p : F_p - \frac{d}{dx} F_p &= j_{13} u + j_{23} u' + j_{33} p = 0. \end{aligned} \quad (11)$$

Consistency of  $E_p$  and  $E_u$  with the field equations  $u' - p = 0$  and  $u + p' = 0$ , respectively, dictates that  $\mathbf{J}$  be of the form

$$\mathbf{J} = \begin{bmatrix} \alpha & \beta & 0 \\ \beta & 0 & -\alpha \\ 0 & -\alpha & \alpha \end{bmatrix}. \quad (12)$$

Thus  $\Pi(u, p)$  is found to depend on two independent free parameters:  $\alpha$  and  $\beta$ . The one-field functional (3) is recovered if the “strong connection”  $p = u'$  is enforced *a priori* and  $\alpha = 1$ . The parametric independence of natural boundary conditions, however, imposes additional constraints on  $\alpha$  and  $\beta$  unless appropriate boundary terms are added to  $\Pi$ . In the next example such terms appear naturally from the beginning.

## 4 A three field example: The 2-D Poisson equation

### 4.1 Problem description

As an example which is more typical of practical applications, we develop an invariant PVP for the 2-D isotropic Poisson equation (the Laplace equation with a source term). This PDE is posed over a finite two-dimensional region  $\Omega$  bounded by

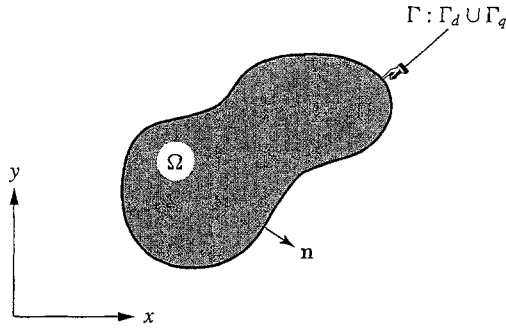


Fig. 2. Two-dimensional region for isotropic Poisson equation (13)

a curve  $\Gamma$ , as illustrated in Fig. 2:

$$k\nabla^2 u = k\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = -f \quad \text{in } \Omega, \quad (13)$$

where  $u = u(x, y)$  is the unknown primary function,  $k(x, y) > 0$ , and  $f(x, y)$  is a given scalar function in  $\Omega$ . The physical meaning of this equation is left unspecified. In technical applications, however,  $u$  may stand for such diverse field quantities as temperature, fluid pressure, Prandtl's torsion stress function, or electrostatic potential. [For non-isotropic problems  $k$  must be replaced by a  $2 \times 2$  constitutive matrix  $S$  and (13) becomes  $\nabla^T S \nabla u = -f$ , but the underlying framework is unchanged.]

The boundary  $\Gamma$  is decomposed into  $\Gamma_d \cup \Gamma_q$ , on which the following Dirichlet and Neumann (flux-type) boundary conditions, respectively, are imposed:

$$u = \hat{d} \quad \text{on } \Gamma_d, \quad k \frac{\partial u}{\partial n} = k(\mathbf{grad} u)^T \mathbf{n} = \hat{q} \quad \text{on } \Gamma_q, \quad (14)$$

where  $\hat{d}$  and  $\hat{q}$  are prescribed on  $\Gamma_d$  and  $\Gamma_q$ , respectively, and  $\mathbf{n}$  is the exterior unit normal on  $\Gamma$ . It should be noted that  $\hat{d}$  is used instead of  $\hat{u}$ , which seems a more logical notation for prescribed values, to link up smoothly with "functional hybridization" in Section 5. For such developments it will be convenient to notationally distinguish the interior field  $u$  from the boundary field  $d$ .

The single-field functional  $\Pi(u)$  associated with (13) and (14) is well known:

$$\Pi = U(u) - P(u) \quad (15)$$

where

$$U(u) = \frac{1}{2} \int_{\Omega} k \left[ \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 \right] d\Omega,$$

$$P(u) = \int_{\Omega} f u d\Omega + \int_{\Gamma_q} \hat{q} u d\Gamma, \quad (16)$$

in which  $u$  satisfies strongly the Dirichlet B.C.  $u = \hat{d}$  on  $\Gamma_d$ . In this functional  $U(u)$  has the meaning of internal energy, whereas  $P(u)$  is an external energy associated with the source and prescribed-normal-flux terms  $f$  and  $\hat{q}$ . As previously noted, functional (15) can be trivially parametrized by adding

multiples of the divergence or curl of gauge functions. But such PVPs have no practical importance.

To allow the construction of a multifield PVP we introduce the two vector fields: gradient  $\mathbf{g}$  and flux vector  $\mathbf{p}$ , as candidates for independent variation:

$$\mathbf{g} = \begin{Bmatrix} g_x \\ g_y \end{Bmatrix} = \mathbf{grad} u = \begin{Bmatrix} \partial u / \partial x \\ \partial u / \partial y \end{Bmatrix},$$

$$\mathbf{p} = \begin{Bmatrix} p_x \\ p_y \end{Bmatrix} = k \mathbf{g} = k \mathbf{grad} u = k \begin{Bmatrix} \partial u / \partial x \\ \partial u / \partial y \end{Bmatrix}. \quad (17)$$

The second order PDE (13) decomposes into the three field equations

$$\mathbf{g} = \nabla u = \mathbf{grad} u, \quad \mathbf{p} = k \mathbf{g}, \quad \nabla^T \mathbf{p} + f = \mathbf{div} \mathbf{p} + f = 0, \quad (18)$$

where  $\mathbf{div} \equiv \nabla^T$  is the divergence operator. In mechanical applications (18) are called the kinematic, constitutive and balance (or equilibrium) equations, respectively.

The projection of the flux  $\mathbf{p}$  on a unit normal  $\mathbf{n}$  to some curve is called the normal flux and denoted by  $p_n = \mathbf{p}^T \mathbf{n}$ . Hence the boundary conditions (14) may be compactly stated as

$$u = \hat{d} \quad \text{on } \Gamma_d, \quad p_n = \hat{q} \quad \text{on } \Gamma_q. \quad (19)$$

The three field equations (8) and two boundary conditions (19) collectively make up the Strong Form (SF) of the isotropic Poisson equation. This SF is graphically represented in Fig. 3 using a modified Tonti diagram. Relations such as  $\mathbf{g} = \mathbf{grad} u$  are called *strong connections* (which means that they are enforced point by point) and depicted as solid lines. The main departure of Figure 2 from Tonti's original diagrams (Tonti 1973; Oden and Reddy 1982) is the explicit separation of field equations and boundary conditions; this has been found useful in teaching variational methods. In addition, a graphical distinction is made between unknown and data fields, as indicated in Fig. 3, also for instructional reasons.

A variational form (VF) substitutes one or more strong connections by weak ones. For example the functional  $\Pi(u)$

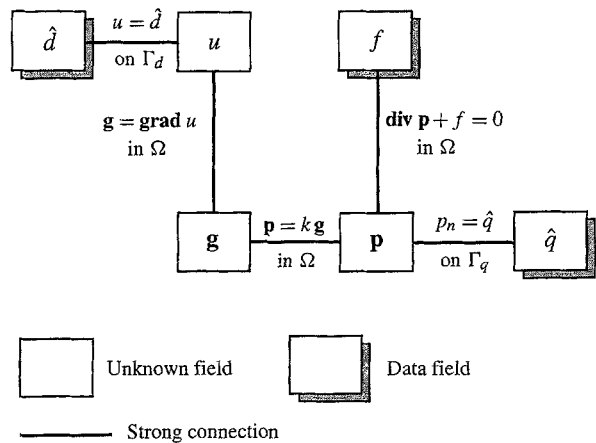


Fig. 3. Graphical representation of the Strong Form (SF) of the isotropic two-dimensional Poisson equation (13) with the B.Cs (14) as a modified Tonti diagram

defined by (15) and (16) weakens the equilibrium equations and Neumann boundary conditions, and may be graphically represented as shown in Fig. 4. More general forms are constructed in the following subsection.

#### 4.2 A three-field PVP for Poisson equation

The configuration of (16) suggests trying to parametrize the internal energy  $U$  as a three-field quadratic form, leading to the arrangement displayed below in full:

$$U(u, \mathbf{p}, \mathbf{g}) = \frac{1}{2} \int_{\Omega} \begin{Bmatrix} p_x \\ p_y \\ k g_x \\ k g_y \\ k \partial u / \partial x \\ k \partial u / \partial y \end{Bmatrix}^T \begin{bmatrix} j_{11} & j_{11} & j_{12} & j_{12} & j_{13} & j_{13} \\ j_{11} & j_{11} & j_{12} & j_{12} & j_{13} & j_{13} \\ j_{12} & j_{12} & j_{22} & j_{22} & j_{23} & j_{23} \\ j_{12} & j_{12} & j_{22} & j_{22} & j_{23} & j_{23} \\ j_{13} & j_{13} & j_{23} & j_{23} & j_{33} & j_{33} \\ j_{13} & j_{13} & j_{23} & j_{23} & j_{33} & j_{33} \end{bmatrix} \begin{Bmatrix} k^{-1} p_x \\ k^{-1} p_y \\ g_x \\ g_y \\ \partial u / \partial x \\ \partial u / \partial y \end{Bmatrix} d\Omega, \quad (20)$$

in which, for simplicity, the explicit dependence of  $U$  on the  $j$  coefficients is dropped from its arguments. The symmetry of the kernel matrix can be justified by inspection, whereas its  $2 \times 2$  block structure is a consequence of avoiding distortions in the vector-component contributions to the internal energy. This functional is fully specified if the  $3 \times 3$  generating matrix  $J$ , which has the same form as in (10), is given.

Now, Eq. (20) looks unduly complicated for such a simple problem. At the same time, what is being varied is not easily seen. We clarify and simplify this form in two steps: passing to matrix-vector notation, and then applying the primary-versus derived-field convention, as explained below:

$$U(\tilde{u}, \tilde{\mathbf{g}}, \tilde{\mathbf{p}}) = \frac{1}{2} \int_{\Omega} \begin{Bmatrix} \tilde{\mathbf{p}} \\ k \tilde{\mathbf{g}} \\ k \mathbf{grad} \tilde{u} \end{Bmatrix}^T \begin{bmatrix} j_{11} \mathbf{I} & j_{12} \mathbf{I} & j_{13} \mathbf{I} \\ j_{12} \mathbf{I} & j_{22} \mathbf{I} & j_{23} \mathbf{I} \\ j_{13} \mathbf{I} & j_{23} \mathbf{I} & j_{33} \mathbf{I} \end{bmatrix} \begin{Bmatrix} k^{-1} \tilde{\mathbf{p}} \\ \tilde{\mathbf{g}} \\ \mathbf{grad} \tilde{u} \end{Bmatrix} d\Omega \\ = \frac{1}{2} \int_{\Omega} \begin{Bmatrix} \tilde{\mathbf{p}} \\ \mathbf{p}^g \\ \mathbf{p}^u \end{Bmatrix}^T \begin{bmatrix} j_{11} \mathbf{I} & j_{12} \mathbf{I} & j_{13} \mathbf{I} \\ j_{12} \mathbf{I} & j_{22} \mathbf{I} & j_{23} \mathbf{I} \\ j_{13} \mathbf{I} & j_{23} \mathbf{I} & j_{33} \mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{g}^p \\ \tilde{\mathbf{g}} \\ \mathbf{g}^u \end{Bmatrix} d\Omega. \quad (21)$$

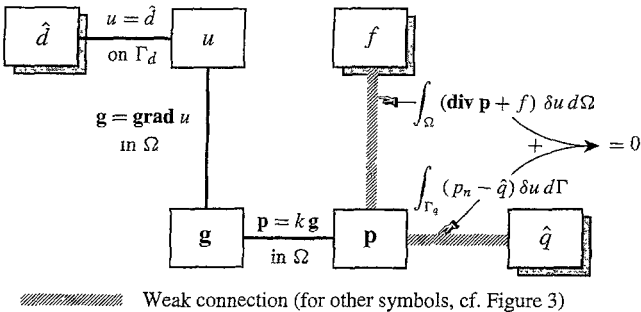


Fig. 4. Graphical representation of the single-field Variational Form (15)–(16) as a modified Tonti diagram

Here  $\mathbf{I}$  denotes the  $2 \times 2$  identity matrix,  $\mathbf{p}^g = k \tilde{\mathbf{g}}$ ,  $\mathbf{p}^u = k \mathbf{g}^u = k \mathbf{grad} \tilde{u}$ ,  $\mathbf{g}^p = k^{-1} \tilde{\mathbf{g}}$ ,  $\mathbf{g}^u = \mathbf{grad} \tilde{u}$ . This notational convention, introduced in (Felippa 1989), is based on two rules:

1. A varied (primary) field is marked with a superposed tilde such as  $\tilde{u}$  or  $\tilde{\mathbf{p}}$ . This allows one to reserve tildeless symbols such as  $u$  or  $\mathbf{p}$  for *generic* or *exact* fields. The tilde may be omitted where variation is evidently implied; for instance  $\delta u$  is obviously the same as  $\delta \tilde{u}$ .
2. A derived (secondary) field is identified by writing its “parent” primary field as superscript; for example  $\mathbf{p}^u = k \mathbf{grad} \tilde{u}$  is the flux associated with the varied field  $\tilde{u}$ .

Of course at the exact solution of (13), all  $\mathbf{p}$ 's and  $\mathbf{g}$ 's coalesce, but the distinction is crucial in variational-based approximation methods.

Note the pleasing appearance of the last term in (21): the notation groups fluxes on the left and gradients on the right. Flux times gradient is internal energy density, so the kernel matrix simply weights, through the  $j$  coefficients, the nine possible combinations  $\tilde{\mathbf{p}}^T \mathbf{g}^p, \tilde{\mathbf{p}}^T \tilde{\mathbf{g}}, \dots$  etc. [It is possible to further streamline (21) into  $U = \frac{1}{2} \int_{\Omega} \mathbf{z}^T \mathbf{W} \mathbf{z} d\Omega$ , as in the last of (9), but this is too compact for most developments.] These notational conventions are especially helpful for the more complicated application problems in elasticity presented later.

To express the first variation of  $U$  compactly, the following weighted combinations are introduced:

$$\overset{\Delta}{\mathbf{g}} = j_{11} \mathbf{g}^p + j_{12} \tilde{\mathbf{g}} + j_{13} \mathbf{g}^u, \quad \overset{\Delta}{\mathbf{p}} = j_{12} \tilde{\mathbf{p}} + j_{22} \mathbf{p}^g + j_{23} \mathbf{p}^u, \\ \overset{\sqcup}{\mathbf{p}} = j_{13} \tilde{\mathbf{p}} + j_{23} \mathbf{p}^g + j_{33} \mathbf{p}^u. \quad (22)$$

Then

$$\delta U = \int_{\Omega} (\overset{\Delta}{\mathbf{g}})^T \delta \mathbf{p} + (\overset{\Delta}{\mathbf{p}})^T \delta \mathbf{g} - (\mathbf{div} \overset{\sqcup}{\mathbf{p}})^T \delta u d\Omega + \int_{\Gamma} (\overset{\sqcup}{\mathbf{p}})^T \mathbf{n} \delta u d\Gamma, \quad (23)$$

in which the boundary integral may be reduced to  $\Gamma_q$  because  $\delta u = 0$  on  $\Gamma_d$ . On linking  $\delta U$  with the variation  $\delta P$  of the parameter-free external-energy term given in (16), we obtain the Euler-Lagrange equations in  $\Omega$ :

$$E_p : \overset{\Delta}{\mathbf{g}} = 0, \quad E_g : \overset{\Delta}{\mathbf{p}} = 0, \quad E_u : \mathbf{div} \overset{\sqcup}{\mathbf{p}} + f = 0, \quad (24)$$

while the Neumann boundary condition on  $\Gamma_q$  is  $\overset{\sqcup}{\mathbf{p}}_n = (\overset{\sqcup}{\mathbf{p}})^T \mathbf{n} = \hat{q}$ . Consistency with the field equations (18) and the boundary condition  $q = \hat{q}$  leads to constraint conditions on the  $j$  coefficients. These can be expeditiously obtained by noting that at the exact solution of the Poisson problem,  $\mathbf{p} = \tilde{\mathbf{p}} = \mathbf{p}^g = \mathbf{p}^u$  and  $\mathbf{g} = \tilde{\mathbf{g}} = \mathbf{g}^g = \mathbf{g}^u$ . Consequently

$$j_{11} + j_{12} + j_{13} = 0, \quad j_{11} + j_{12} + j_{13} = 0, \quad j_{11} + j_{12} + j_{13} = 1. \quad (25)$$

It follows that the functional (21) combined with  $P$  yields a PVP, which is in fact a three-parameter family. Two explicit forms

of  $\mathbf{J}$  that identically satisfy the constraints (25) are

$$\mathbf{J} = \begin{bmatrix} j_{11} & j_{33} - j_{sum} - \frac{1}{2} & j_{22} - j_{sum} + \frac{1}{2} \\ & j_{22} & j_{11} - j_{sum} + \frac{1}{2} \\ \text{symm} & & j_{33} \end{bmatrix}$$

$$= \begin{bmatrix} s_2 + s_3 & -s_3 & -s_2 \\ & s_1 + s_3 & -s_1 \\ \text{symm} & & 1 + s_1 + s_2 \end{bmatrix}, \quad (26)$$

where  $j_{sum} = (j_{11} + j_{22} + j_{33})/2$ . The second form, in which the negated off-diagonal entries  $s_1$ ,  $s_2$  and  $s_3$  are taken as the free parameters, has been generally found to be more convenient than the first one, which uses the diagonal entries  $j_{11}$ ,  $j_{22}$  and  $j_{33}$  for such purpose.

The choice  $s_1 = s_2 = s_3 = 0$  yields the single-field functional (15). Other choices for  $\mathbf{J}$  are discussed in conjunction with the classical elasticity problem, which has a similar parametric structure, in Section 7.

Using the decomposition of  $\mathbf{J}$  as the sum of rank-one matrices

$$\mathbf{J} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} + s_1 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{bmatrix} + s_2 \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

$$+ s_3 \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (27)$$

one can rewrite the three Euler-Lagrange equations (24) in a form that illuminates the weighted-residual connection to the field equations (18):

$$E_p : s_2 (\mathbf{g}^p - \mathbf{g}^u) + s_3 (\mathbf{g}^p - \tilde{\mathbf{g}}) = \mathbf{0},$$

$$E_g : s_3 (\mathbf{p}^g - \tilde{\mathbf{p}}) + s_1 (\mathbf{p}^g - \mathbf{p}^u) = \mathbf{0},$$

$$E_u : \text{div} [\mathbf{p}^u + s_1 (\mathbf{p}^u - \mathbf{p}^g) + s_2 (\mathbf{p}^u - \tilde{\mathbf{p}})] + f = 0. \quad (28)$$

What happens if, say,  $s_2 = s_3 = 0$ ? Then  $E_p$  becomes an identity and  $\tilde{\mathbf{g}}$  drops out as an independently varied field [note that  $j_{11} = 0$  because of (25) and thus the first row and column of  $\mathbf{J}$  vanish.] Similarly if  $s_1 = s_3 = 0$ ,  $E_g$  becomes an identity and  $\tilde{\mathbf{p}}$  drops out as varied field. The case  $s_1 = s_2 = 0$  reduces  $E_u$  to  $\text{div} \mathbf{p}^u + f = 0$  but (uncoupled) three-field principles are still possible because one may select  $j_{11} = j_{22} = -j_{12} = s_3$ , where  $s_3$  is arbitrary; setting  $s_3 = 0$  gives back the functional (15).

The form of Eq. (28) shows that the  $s$ 's, or their reciprocals, can be interpreted as weights on the field equations. No such flexibility is available with single-field functionals because the parameters factor out at the first variation level. This is the key reason behind the importance of multifield PVPs.

Is this PVP invariant? At an extremal the  $\mathbf{p}$ 's and  $\mathbf{g}$ 's coalesce. The internal energy reduces to  $\int_{\Omega} \mathbf{p}^T \mathbf{g} d\Omega$  multiplied by  $j_{11} + j_{12} + \dots + j_{33}$ , which is unity because of (25). Thus we have an IPVP. The same property holds for the elasticity functionals presented in Section 7, and is crucial in the application to finite element error estimation (Felippa 1994).

If  $\mathbf{p}$  is a varied field (that is,  $s_2$  and  $s_3$  are not simultaneously zero) a generalization of the external potential  $P(u)$  that relaxes

the condition  $u = \hat{d}$  on  $\Gamma_d$  is

$$P^c(\tilde{u}, \tilde{\mathbf{p}}) = \int_{\Omega} f \tilde{u} d\Omega + \int_{\Gamma_d} \tilde{p}_n (\tilde{u} - \hat{d}) d\Gamma + \int_{\Gamma_q} \hat{q} \tilde{u} d\Gamma. \quad (29)$$

where  $\tilde{p}_n = \tilde{\mathbf{p}}^T \mathbf{n}$  on  $\Gamma_d$ . This is called the *conventional* potential. Its first variation is

$$\delta P^c = \int_{\Omega} f \delta u d\Omega + \int_{\Gamma_d} (u - \hat{d}) \delta p_n d\Gamma + \int_{\Gamma_q} p_n \delta u d\Gamma$$

$$+ \int_{\Gamma_q} \hat{q} \delta u d\Gamma. \quad (30)$$

Note that  $p_n$  must not be replaced by  $\tilde{p}_n$  in (29), or in general, by any other combination that contains  $\mathbf{p}^g$  or  $\mathbf{p}^u$ , as incorrect natural boundary conditions on  $\Gamma_d$  would otherwise result.

### 4.3

#### Parametrized null space functionals

The parametrized  $U(\tilde{u}, \tilde{\mathbf{g}}, \tilde{\mathbf{p}})$  does not contain all possible quadratic forms for the internal energy of the Poisson equation. This is because  $u$  must be a primary field in  $\Pi$ , although  $\tilde{\mathbf{p}}$  and/or  $\tilde{\mathbf{g}}$  may drop out for certain parameter choices as discussed above. To make  $u$  disappear, the last row and column of  $\mathbf{J}$  must have all zero entries, which contradicts the last of (25).

To accommodate functionals with internal energy of the form  $U(\tilde{\mathbf{p}}, \tilde{\mathbf{g}})$  one starts from the following specialization of the generating matrix:

$$\mathbf{J}^* = \begin{bmatrix} s_0 - 1 & -s_0 & 1 \\ -s_0 & s_0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad (31)$$

in which  $s_0$  is a free parameter. Inserting this into (21) and integrating the  $\tilde{\mathbf{p}} \mathbf{g}^u = \tilde{\mathbf{p}}^T \text{grad } \tilde{u}$  term by parts yields

$$\Pi = \frac{1}{2} \int_{\Omega} \begin{Bmatrix} \tilde{\mathbf{p}} \\ \mathbf{p}^g \end{Bmatrix}^T \begin{bmatrix} (s_0 - 1) \mathbf{I} & -s_0 \mathbf{I} \\ -s_0 \mathbf{I} & s_0 \mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{g}^p \\ \tilde{\mathbf{g}} \end{Bmatrix} d\Omega$$

$$- \int_{\Omega} \tilde{u} (\text{div } \tilde{\mathbf{p}} + f) d\Omega + \int_{\Gamma_d} \tilde{p}_n \hat{d} d\Gamma + \int_{\Gamma_q} \tilde{u} (\tilde{p}_n - \hat{q}) d\Gamma. \quad (32)$$

Next, the flux  $\mathbf{p}$  is restricted to vary on the subset that identically satisfies: (i) the balance equation  $\text{div } \mathbf{p} + f = 0$  in  $\Omega$  and (ii) the Neumann boundary condition  $p_n = \hat{q}$  on  $\Gamma_q$ . This process collapses (32) to

$$\Pi^*(\tilde{\mathbf{p}}, \tilde{\mathbf{g}}) = U^*(\tilde{\mathbf{p}}, \tilde{\mathbf{g}}) - P^{c*}(\tilde{\mathbf{p}})$$

$$= \frac{1}{2} \int_{\Omega} \begin{Bmatrix} \tilde{\mathbf{p}} \\ \mathbf{p}^g \end{Bmatrix}^T \begin{bmatrix} (s_0 - 1) \mathbf{I} & -s_0 \mathbf{I} \\ -s_0 \mathbf{I} & s_0 \mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{g}^p \\ \tilde{\mathbf{g}} \end{Bmatrix} d\Omega$$

$$+ \int_{\Gamma_d} \tilde{p}_n \hat{d} d\Gamma, \quad (32)$$

which is a one-parameter, two-field form called a *null-space functional*. Such functionals will be identified by a superscript asterisk.

Setting the parameter  $s_0 = 0$  eliminates  $\mathbf{g}$  as varied field and reduces (33) to the single-field functional  $\Pi^*(\tilde{\mathbf{p}})$  in which the  $\Omega$  integrand is  $-\frac{1}{2}\tilde{\mathbf{p}}^T \mathbf{g}^p = -\tilde{\mathbf{p}}^T \tilde{\mathbf{p}}/(2k)$ . In mechanical applications  $\Pi^*(\tilde{\mathbf{p}})$  is called a complementary energy functional.

A functional  $\Pi^*(\tilde{\mathbf{g}})$  that contains only the gradient as primary field cannot be obtained as an instance of (33), but may be constructed by another variation-restriction process that eliminates  $\mathbf{p}$  as varied field. That functional is merely a curiosity.

## 5 Internal interfaces and hybrid functionals

### 5.1 Treatment of internal interfaces

The PVPs constructed in the preceding Section are of *mixed* type. As first step in the construction of parametrized hybrid functionals for Poisson equation, a smooth internal interface  $\Gamma^i$ , such as the one depicted on the left of Fig. 5, is introduced. This allows the consideration of certain solution discontinuities. Those discontinuities may be of physical or computational nature, as discussed later.

This interface  $\Gamma^i$ , also called an interior boundary, divides  $\Omega$  into two subdomains:  $\Omega^+$  and  $\Omega^-$  so that  $\Gamma^i: \Omega^+ \cap \Omega^-$ . The outward normals to  $\Gamma^i$  that emanate from these subdomains are denoted by  $\mathbf{n}^+$  and  $\mathbf{n}^-$ , respectively. The external boundary is relabeled  $\Gamma^x$ ; thus the complete boundary is  $\Gamma: \Gamma^x \cup \Gamma^i$ . For many derivations it is convenient to view  $\Omega^+$  and  $\Omega^-$  as disconnected subdomains with matching boundaries  $\Gamma^{i+}$  and  $\Gamma^{i-}$ , as illustrated on the right of Fig. 5. Values of the primary variable, flux vector and normal flux on both sides of  $\Gamma^i$  are denoted by

$$u^+ = u|_{\Gamma^{i+}}, \quad u^- = u|_{\Gamma^{i-}}, \quad \mathbf{p}^+ = \mathbf{p}|_{\Gamma^{i+}}, \quad \mathbf{p}^- = \mathbf{p}|_{\Gamma^{i-}},$$

$$p_n^+ = (\mathbf{p}^+)^T \mathbf{n}^+, \quad p_n^- = (\mathbf{p}^-)^T \mathbf{n}^-. \quad (34)$$

At each point of  $\Gamma^i$ , jumps of  $u$  and  $p_n$  may be specified:

$$[[d]] = u^+ - u^-, \quad [[q]] = p_n^+ + p_n^- \quad \text{on } \Gamma^i. \quad (35)$$

Note that unlike the external boundary  $\Gamma^x$ , both jumps can be prescribed at the same point because there are two faces to an interface. In this and following equations, “plus/minus combinations” of  $u$  and  $p_n$  are replaced by  $d$  and  $q$ , respectively, to distinguish them as interface fields. That notation simplifies the transition to weak connections.

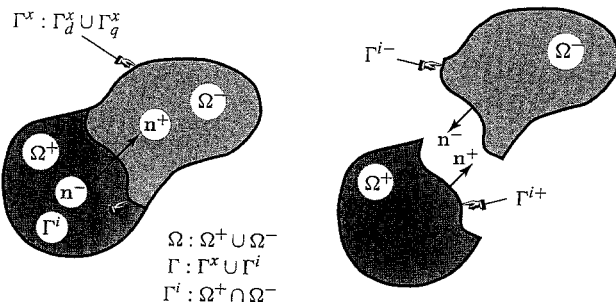


Fig. 5. The domain of Figure 2 with an internal interface  $\Gamma^i$

If the jumps (35) vanish one recovers the standard data coherency conditions of continuity of  $u$  and strong diffusivity of  $p_n$ ; the latter being one of the transversality conditions of variational calculus. Following Fraeijns de Veubeke (1974), prescribed nonzero jumps may be conveniently resolved by setting

$$u^+ = d + \frac{1}{2}[[d]], \quad u^- = d - \frac{1}{2}[[d]], \quad p_n^+ = q + \frac{1}{2}[[q]],$$

$$p_n^- = -q + \frac{1}{2}[[q]], \quad (36)$$

where

$$d = \frac{1}{2}(u^+ + u^-), \quad q = \frac{1}{2}(p_n^+ - p_n^-), \quad (37)$$

can be treated as unknown interface variables. That is, both  $d$  and  $q$  may be varied independently from  $u$ ,  $\mathbf{g}$  and  $\mathbf{p}$  on  $\Gamma^i$ .

### 5.2 A four-field parametrized interface integral

The presence of the internal interface can be accounted for by adding a dislocation potential to the parametrized internal energy (21) and external potential (29):

$$\Pi(\tilde{u}, \tilde{\mathbf{g}}, \tilde{\mathbf{p}}, \tilde{d}, \tilde{q}) = U(\tilde{u}, \tilde{\mathbf{g}}, \tilde{\mathbf{p}}) - P^c(\tilde{u}, \tilde{\mathbf{p}}) - P^i(\tilde{u}, \tilde{\mathbf{p}}, \tilde{d}, \tilde{q}). \quad (38)$$

The potential  $P^i$  will be considered to depend on four varied fields:  $u$ ,  $\mathbf{p}$ ,  $d$  and  $q$ , with the last two defined only on the interface. Consequently  $\Pi$  may contain up to five varied fields.

The following 8-parameter form of  $P^i$  assumes that both  $u$  and  $\mathbf{p}$  are varied fields in  $\Omega$ . It generalizes a non-parametric potential discussed by Fraeijns de Veubeke (1974) for problems in linear elasticity. This potential accounts for possible discontinuities on both  $u$  and  $p_n$ :

$$P^i(\tilde{u}, \tilde{\mathbf{p}}, \tilde{d}, \tilde{q}) = \int_{\Gamma^i} [(\beta_1 \tilde{q} + \alpha_2(\tilde{p}_n^+ - \tilde{p}_n^-))(\tilde{u}^+ - \tilde{u}^- - [[d]] + \beta_2 \tilde{d})$$

$$+ (\beta_3(\tilde{p}_n^+ + \tilde{p}_n^-) + [[q]] + \beta_4 \tilde{q})(\alpha_1(\tilde{u}^+ - \tilde{u}^-)$$

$$+ \beta_5 \tilde{d}) + \beta_6(p_n^+(u^+ - \tilde{d} - \frac{1}{2}[[d]])$$

$$+ \tilde{p}_n^-(\tilde{u}^- - \tilde{d} + \frac{1}{2}[[d]])] d\Gamma. \quad (39)$$

Here  $\alpha_1, \alpha_2, \beta_1, \dots, \beta_6$  are numerical coefficients. This expression is not the most general one because the following restrictions are enforced:

- Isotropy of interface side (face) values. For example, the side values of  $u$  are allowed to appear only in combinations such as  $u^+ + u^-$  or  $u^+ - u^-$ . Lack of isotropy can seriously distort interface energy contributions in numerical approximations.
- Least-square terms are not considered as, for example, a term such as  $\gamma_1(u^+ - u^- + \gamma_2[[d]]) (u^+ - u^- + \gamma_3[[d]])$ . Including least-square terms is inconvenient in that their physical dimensions have to be adjusted, through dimensional coefficients or weighting matrices, to conform to those of energy density ( $pg$  or  $qd$ ). Furthermore, those terms generally destroy the

connector locality desirable in the construction of hybrid elements.

- (c) The jumps  $\llbracket q \rrbracket$  and  $\llbracket d \rrbracket$  are not independently varied. This extension will be considered in future studies.

Enforcing consistency of the first variation of (39) on  $\Gamma'$  so that (36) and (37) emerge as natural boundary conditions provides six relations among the coefficients:  $\beta_1 = 2(\alpha_1 - \alpha_2)$ ,  $\beta_2 = \beta_3 = \beta_4 = 0$  and  $\beta_5 = \beta_6 = 1 - 2\alpha_1$ . This leaves two free parameters:  $\alpha_1$  and  $\alpha_2$ , reducing (39) to

$$P'(\tilde{u}, \tilde{\mathbf{p}}, \tilde{d}, \tilde{q}) = \int_{\Gamma'} [(2(\alpha_1 - \alpha_2)\tilde{q} + \alpha_2(\tilde{p}_n^+ - \tilde{p}_n^-)) \cdot (\tilde{u}^+ - \tilde{u}^- - \llbracket d \rrbracket) + \alpha_1 \llbracket q \rrbracket (\tilde{u}^+ + \tilde{u}^-) + (1 - 2\alpha_1)(\tilde{p}_n^+(u^+ - \tilde{d} - \frac{1}{2}\llbracket d \rrbracket) + \tilde{p}_n^-(\tilde{u}^- - \tilde{d}) + \frac{1}{2}\llbracket d \rrbracket) + \tilde{d}\llbracket q \rrbracket)] d\Gamma. \quad (40)$$

This expression can be specialized to various kinds of potentials that differ on the presence or absence of certain terms or interface fields.

**Functionals with uncoupled interior fields** If  $\alpha_2 = 0$  all cross terms of the form  $p_n^+ u^-$  and  $p_n^- u^+$  drop out reducing (40) to

$$P'(\tilde{u}, \tilde{\mathbf{p}}, \tilde{d}, \tilde{q}) = \int_{\Gamma'} [2\alpha_1 \tilde{q}(\tilde{u}^+ - \tilde{u}^- - \llbracket d \rrbracket) + \alpha_1 \llbracket q \rrbracket (\tilde{u}^+ + \tilde{u}^-) + (1 - 2\alpha_1)(\tilde{p}_n^+(\tilde{u}^+ - \tilde{d} - \frac{1}{2}\llbracket d \rrbracket) + \tilde{p}_n^-(\tilde{u}^- - \tilde{d} + \frac{1}{2}\llbracket d \rrbracket) + \tilde{d}\llbracket q \rrbracket)] d\Gamma. \quad (41)$$

Those dropped terms would couple the interior fields  $u$  and  $\mathbf{p}$  on both sides of the interface. As noted in Section 5.6, that coupling is undesirable in the construction of hybrid finite elements because it destroys the locality of interface connectors.

**Functionals without  $q$**  If  $\alpha_1 = \alpha_2$ ,  $q$  drops as an independently varied field and  $P'$  reduces to a one-parameter, three-field potential:

$$P'(\tilde{u}, \tilde{\mathbf{p}}, \tilde{d}) = \int_{\Gamma'} [\alpha_1(\tilde{p}_n^+ - \tilde{p}_n^-)(\tilde{u}^+ - \tilde{u}^- - \llbracket d \rrbracket) + \alpha_1 \llbracket q \rrbracket (\tilde{u}^+ + \tilde{u}^-) + (1 - 2\alpha_1)(\tilde{p}_n^+(\tilde{u}^+ - \tilde{d} - \frac{1}{2}\llbracket d \rrbracket) + \tilde{p}_n^-(\tilde{u}^- - \tilde{d} + \frac{1}{2}\llbracket d \rrbracket) - \tilde{d}\llbracket q \rrbracket)] d\Gamma. \quad (42)$$

These potentials are called  $d$ -generalized. The simplest instance, called *canonical*, is obtained if  $\alpha_1 = 0$ :

$$P'(\tilde{u}, \tilde{\mathbf{p}}, \tilde{d}) = \int_{\Gamma'} [(\tilde{p}_n^+(\tilde{u}^+ - \tilde{d} - \frac{1}{2}\llbracket d \rrbracket) + \tilde{p}_n^-(\tilde{u}^- - \tilde{d} + \frac{1}{2}\llbracket d \rrbracket) + \tilde{d}\llbracket q \rrbracket)] d\Gamma. \quad (43)$$

**Functionals without  $d$**  If  $\alpha_1 = 1/2$ ,  $d$  drops as an independently varied field and  $P'$  reduces to a one-parameter,

three-field potential:

$$P'(\tilde{u}, \tilde{\mathbf{p}}, \tilde{q}) = \int_{\Gamma'} [(1 - 2\alpha_2)\tilde{q} + \alpha_2(\tilde{p}_n^+ - \tilde{p}_n^-) \cdot (\tilde{u}^+ - \tilde{u}^- - \llbracket d \rrbracket) + \alpha_2 \llbracket q \rrbracket (\tilde{u}^+ + \tilde{u}^-)] d\Gamma. \quad (44)$$

These potentials are called  $q$ -generalized. The simplest instance, called *canonical*, is also obtained if  $\alpha_2 = 0$ :

$$P'(\tilde{u}, \tilde{q}) = \int_{\Gamma'} \tilde{q}(\tilde{u}^+ - \tilde{u}^- - \llbracket d \rrbracket) d\Gamma. \quad (45)$$

Note that this canonical form, unlike (43), cannot cope with a flux jump  $\llbracket q \rrbracket$ .

**Functional without  $d$  and  $q$**  If  $\alpha_1 = \alpha_2 = 1/2$ , both  $d$  and  $q$  drop as independently varied fields and  $P'$  reduces to a two-field potential:

$$P'(\tilde{u}, \tilde{\mathbf{p}}) = \int_{\Gamma'} [\frac{1}{2}(\tilde{p}_n^+ - \tilde{p}_n^-)(\tilde{u}^+ - \tilde{u}^- - \llbracket d \rrbracket) + \frac{1}{2}\llbracket q \rrbracket (\tilde{u}^+ + \tilde{u}^-)] d\Gamma. \quad (46)$$

This functional involves only the interior field variables  $u$  and  $\mathbf{p}$ , and can handle jumps in both  $u$  and  $p_n$ , but contains the cross terms  $p_n^+ u^-$  and  $p_n^- u^+$ .

The preceding parameter choices are graphically summarized in Fig. 6.

### 5.3 Interior functionals lacking $p$

If the internal energy functional lacks  $\mathbf{p}$ , as in (15), it is still possible to use the interface potential (45), because that canonical  $q$ -generalized form does not contain the flux.

On the other hand, it is not possible to construct a potential  $P'(u, d)$  that yields the correct first variation according to the rules of variational calculus. One can formally replace  $\tilde{p}_n$  in (41) by  $p_n^{u+} = k \partial u / \partial n^+$  and  $p_n^{u-} = k \partial u / \partial n^-$ ; or, more generally,

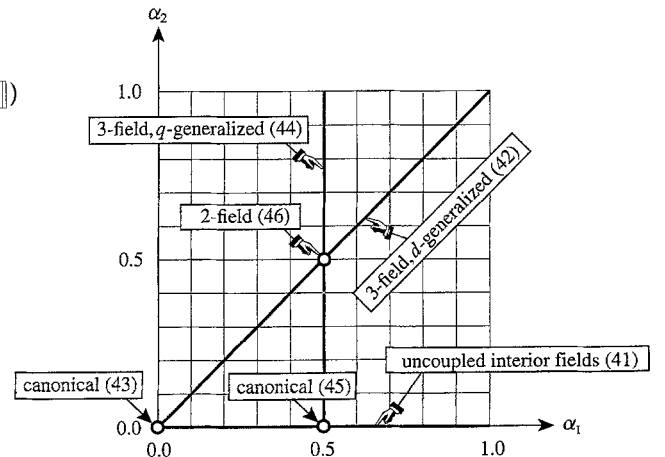


Fig. 6. Effect of parameter selection on the dislocation functional (40), assuming that both  $u$  and  $\mathbf{p}$  are varied in the internal energy functional



by a weighted combination of  $p_n^u$  and  $p_n^s$  if  $\mathbf{g}$  is a primary field. This only provides, however, a *restricted variational principle* because  $\tilde{p}_n \equiv p_n^u$  only at an extremal. For a discussion of that kind of variational statements, which are more in the spirit of Galerkin methods, Chapter 10 of Finlayson (1972) may be consulted.

#### 5.4 Null-space interior functionals

If the interior energy is expressed by a null-space functional such as (32), field  $u$  is missing. Then one may set  $u^+ = u^- = d$  and  $[[d]] = 0$  in (43) to get the two-field interface potential:

$$P^i(\tilde{\mathbf{p}}, \tilde{d}) = \int_{\Gamma^i} \tilde{d} [[q]] d\Gamma = \int_{\Gamma^i} \tilde{d} (\tilde{p}_n^+ + \tilde{p}_n^-) d\Gamma. \quad (47)$$

In this case a potential  $P^i(\tilde{\mathbf{p}}, \tilde{q})$  cannot be obtained, even formally, because it is generally impossible to reconstruct  $u$  pointwise from  $\mathbf{p}$ .

#### 5.5 Physical and computational interfaces

The foregoing dislocation potentials are useful for the treatment of actual solution discontinuities caused by interface-concentrated source data. For example in the steady thermal conduction problem a heat source  $f$  concentrated on  $\Gamma^i$  will cause a jump  $[[q]]$  in the normal heat flux, whereas a doublet heat source on  $\Gamma^i$  will induce a jump  $[[u]]$  in the temperature. For these applications the choice of an interface potential can be simply based on the proper variational representation of the physical model.

Another important application is that of *subdomain linkage*. In this case  $\Omega^+$  and  $\Omega^-$  are solution subdomains discretized by different techniques such as the FEM and BEM, or two FEM-discretized domains with generally non-coincident node locations. The domains are tied up by enforcing interface conditions weakly through a three-field dislocation potential

$P^i$  that includes either  $q$  or  $d$ . This interface field mathematically functions as a Lagrange multiplier field. Because of its linking role, the field is also called (in the FEM literature) a *connector field* or simply *connector*. In this case the jumps  $[[d]]$  and  $[[q]]$  are set to zero, and computed solution discontinuities are a byproduct of the numerical approximation. A good review of the use of the canonical interface functionals for this situation is given by Zienkiewicz and Taylor (1989).

If the subdomains reduce to individual finite elements, interface potentials are the basis for the construction of *hybrid* elements. For such applications the complete functional (38) receives the name of *hybrid functional*. A brief historical account of the development of those functionals for elasticity is provided in Section 6.5.

#### 5.6 Constructing Hybrid Elements

Key conceptual steps in the construction of hybrid elements are illustrated in Fig 7. To show how such elements are linked, a two element patch (b) is extracted from a finite element mesh (a). As illustrated in (c), element interior fields do not interact directly (as in non-hybrid elements) but do so indirectly through "boundary frames" The frame is implemented by using the interface field on each side as the connector device depicted in (d) and (e). The device consists of the nodal degrees of freedom and the connector field interpolated from those freedoms. It is seen that a hybrid element consists of two ingredients:

- (1) The choice of internal fields, which is defined by those appearing in the internal energy functional  $U$  or  $U^*$ , and the interpolation of such fields.
- (2) The choice of interface connector field, which is defined by that kept in  $P^i$ . This field is interpolated along  $\Gamma^i$  from the nodal degrees of freedom located on the element side.

It should be noted that for these applications the one-pass expression of the interface integral used here is usually replaced

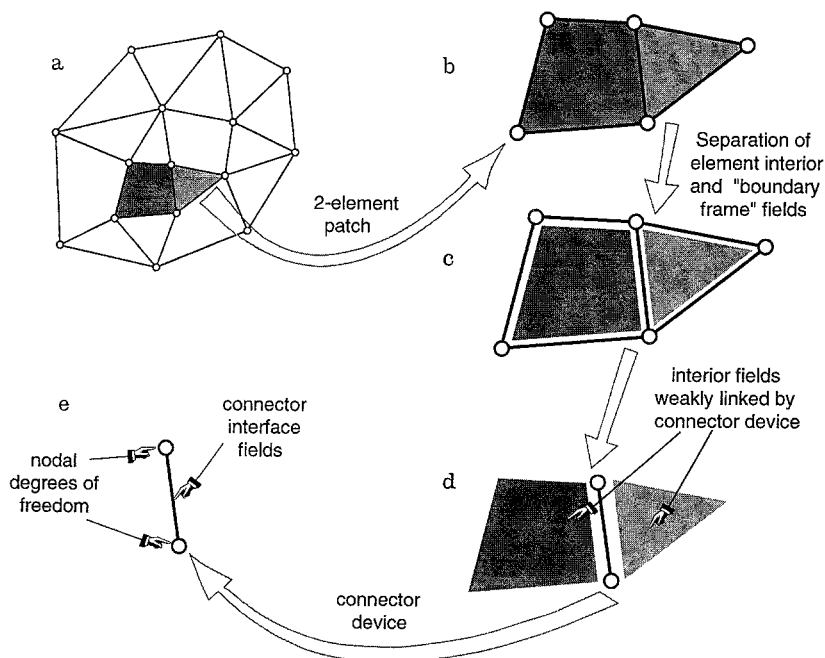


Fig. 7a-e. Key conceptual steps in the construction of hybrid finite elements. Note that the nodal arrangement of the mesh depicted here would be appropriate for  $d$  connectors. For  $q$  connectors, nodes would be likely be placed on element sides

Table 1. Classification of Hybrid Functionals for the Poisson Equation

Connector field	Nodal DOFs	Internal energy	Appropriate $p^i$	Comments
$d$	$u$	$U(u, p)$ or $U(u, p, g)$	(42)	restricted variational principle historically important, also the basis of Trefftz elements
$d$	$u$	$U(u)$ or $U(u, g)$	(42), $p_n^u \rightarrow p_n$	
$d$	$u$	$U^*(p)$ or $U^*(p, g)$	(47)	
$q$	$p_n$	$U(u, p)$ or $U(u, p, g)$	(44)	historically important may be sensitive to limitation principles
$q$	$p_n$	$U(u)$ or $U(u, g)$	(45)	
$q, d$	$u, p_n$	$U(u, p)$ or $U(u, p, g)$	(40)	

by a two-pass version (that is, each interelement boundary is traversed twice) to simplify the formulation of individual elements.

Viewed in the light of PVPs the range of possibilities for construction of hybrid elements, as well as subdomain linking, appears large. However, it should be emphasized that the potential (39) can be generalized further. Table 1 attempts to organize “reasonable” combinations that comply with the restrictions enforced in the construction of that potential.

6  
Classical elasticity

The words “classical elasticity” are used here as shorthand for the more precise “compressible linear hyperelastostatics.” This is the application area in which the multifield PVPs discussed here originated in response to needs from finite element technology. As a result, it is still the best developed one in terms of FEM applications. The ensuing discussion emphasizes three-dimensional elasticity. Section 6.1 through 6.4 outline material presented more fully in other articles. Section 6.5 gives an interpretation of hybrid functionals suggested by the parametrization developed in Section 5 for the Poisson problem.

6.1  
Governing equations

Consider a body of volume  $V$  referred to a rectangular Cartesian coordinate system  $x_i, i = 1, 2, 3$  as depicted in Fig. 8. The body is bounded by surface  $S$  of external unit normal  $\mathbf{n} \equiv n_i$ . The surface is decomposed into  $S: S_d \cup S_r$ . Displacements  $\hat{\mathbf{d}} \equiv \hat{d}_i$  are prescribed on  $S_d$  whereas surface tractions  $\hat{\mathbf{t}} \equiv \hat{t}_i$  are prescribed on  $S_r$ . Body forces  $\mathbf{f} \equiv f_i$  are prescribed in volume  $V$ .

The three unknown internal fields are: displacements  $\mathbf{u} \equiv u_i$ , strains  $\mathbf{e} \equiv e_{ij}$  and stresses  $\boldsymbol{\sigma} \equiv \sigma_{ij}$ . The traction vector on  $S$  is  $\boldsymbol{\sigma}_n \equiv \sigma_{ni} = \sigma_{ij}n_j$  (summation convention implied). To facilitate

the construction of elasticity functionals in a matrix form, stresses and strains are arranged in the usual 6-component vector forms

$$\boldsymbol{\sigma}^T = [\sigma_{11} \quad \sigma_{22} \quad \sigma_{33} \quad \sigma_{12} \quad \sigma_{23} \quad \sigma_{31}],$$

$$\mathbf{e}^T = [e_{11} \quad e_{22} \quad e_{33} \quad 2e_{12} \quad 2e_{23} \quad 2e_{31}], \tag{48}$$

These fields are connected by the kinematic, constitutive and balance equations

$$\mathbf{e} = \mathbf{D}\mathbf{u}, \quad \boldsymbol{\sigma} = \mathbf{E}\mathbf{e}, \quad \mathbf{D}^T\boldsymbol{\sigma} + \mathbf{f} = \mathbf{0}, \tag{49}$$

where  $\mathbf{E}$  is the  $6 \times 6$  stress-strain matrix of elastic moduli arranged in the usual manner,  $\mathbf{D}$  is the  $6 \times 3$  symmetric-gradient operator and its transpose the  $3 \times 6$  tensor-divergence operator:

$$\mathbf{D}^T = \begin{bmatrix} \partial/\partial x_1 & 0 & 0 & \partial/\partial x_2 & 0 & \partial/\partial x_3 \\ 0 & \partial/\partial x_2 & 0 & \partial/\partial x_1 & \partial/\partial x_3 & 0 \\ 0 & 0 & \partial/\partial x_3 & 0 & \partial/\partial x_2 & \partial/\partial x_1 \end{bmatrix}. \tag{50}$$

The boundary conditions are

$$\mathbf{u} = \hat{\mathbf{d}} \text{ on } S_d, \quad \boldsymbol{\sigma}_n = \hat{\mathbf{t}} \text{ on } S_r. \tag{51}$$

The field equations (49) and boundary conditions (51) make up the Strong Form (SF) of the classical-elasticity problem. The SF is graphically represented in Fig 9, using a Tonti diagram of the primal (displacement-based) formulation.

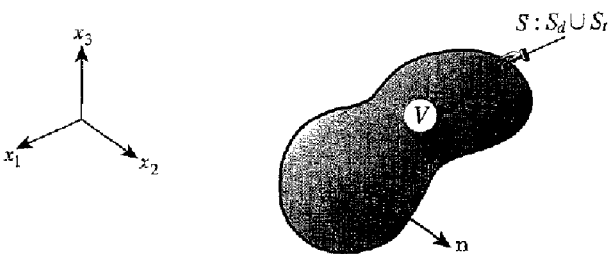


Fig. 8. Linear elastic body in 3D space

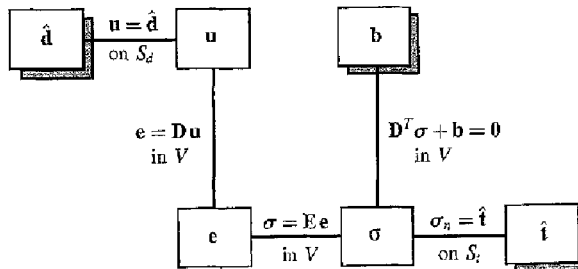


Fig. 9. Graphical representation on the Strong Form (SF) of the primal (displacement-based) formulation of classical elasticity. Refer to Figure 3 display conventions

## 6.2

### Parametrization

The structural similarity of classical elasticity with the Poisson equation is evident on comparing the configuration of Figs 3 and 9. It may be therefore expected that PVPs appear in one-to-one correspondence if  $u, \mathbf{g}, \mathbf{p}, p_n, f, q$  and  $d$  are replaced by  $\mathbf{u}, \mathbf{e}, \boldsymbol{\sigma}, \sigma_n, \mathbf{b}, \mathbf{t}$  and  $\mathbf{d}$ , respectively. And indeed this is the case. The formal counterparts of (21) and (29) for classical elasticity are

$$U(\mathbf{u}, \boldsymbol{\sigma}, \mathbf{e}) = \frac{1}{2} \int_V \left\{ \begin{matrix} \tilde{\boldsymbol{\sigma}} \\ \boldsymbol{\sigma}^e \\ \boldsymbol{\sigma}^u \end{matrix} \right\}^T \begin{bmatrix} j_{11} \mathbf{I} & j_{12} \mathbf{I} & j_{13} \mathbf{I} \\ j_{12} \mathbf{I} & j_{22} \mathbf{I} & j_{23} \mathbf{I} \\ j_{13} \mathbf{I} & j_{23} \mathbf{I} & j_{33} \mathbf{I} \end{bmatrix} \left\{ \begin{matrix} \mathbf{e}^\sigma \\ \tilde{\mathbf{e}} \\ \mathbf{e}^u \end{matrix} \right\} dV. \quad (52)$$

$$P^c(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\sigma}}) = \int_V \mathbf{b}^T \mathbf{u} dV + \int_{S_d} \tilde{\boldsymbol{\sigma}}_n (\tilde{\mathbf{u}} - \hat{\mathbf{d}}) dS + \int_{S_r} \hat{\mathbf{t}} \tilde{\mathbf{u}} dS. \quad (53)$$

Here  $\mathbf{I}$  denotes the  $6 \times 6$  identity matrix, the  $\boldsymbol{\sigma}$  and  $\mathbf{e}$  vectors have 6 components, and the kernel matrix in (52) is  $18 \times 18$ . The derived quantities that appear in  $U$  are  $\mathbf{e}^\sigma = \mathbf{E}^{-1} \tilde{\boldsymbol{\sigma}}$ ,  $\mathbf{e}^u = \mathbf{D} \tilde{\mathbf{u}}$ ,  $\boldsymbol{\sigma}^e = \mathbf{E} \tilde{\mathbf{e}}$ , and  $\boldsymbol{\sigma}^u = \mathbf{E} \mathbf{D} \tilde{\mathbf{u}}$ . To justify again the symmetric arrangement of the  $j$  coefficients note that, because of linearity,  $(\boldsymbol{\sigma}^u)^T \mathbf{e}^\sigma = \tilde{\boldsymbol{\sigma}}^T \mathbf{e}^u$ ,  $(\boldsymbol{\sigma}^e)^T \mathbf{e}^u = \tilde{\boldsymbol{\sigma}}^T \tilde{\mathbf{e}}$ , etc.

The first variation of  $U$  can be compactly written

$$\delta U = \int_V [(\hat{\tilde{\mathbf{e}}})^T \delta \boldsymbol{\sigma} + (\hat{\tilde{\boldsymbol{\sigma}}})^T \delta \mathbf{e} - (\text{div } \hat{\tilde{\boldsymbol{\sigma}}})^T \delta \mathbf{u}] dV + \int_S (\hat{\tilde{\boldsymbol{\sigma}}}_n)^T \delta \mathbf{u} dS, \quad (54)$$

in which  $\hat{\tilde{\mathbf{e}}}$ ,  $\hat{\tilde{\boldsymbol{\sigma}}}$  and  $\hat{\tilde{\boldsymbol{\sigma}}}$  denote the weighted combinations of strains and stresses

$$\begin{aligned} \hat{\tilde{\mathbf{e}}} &= j_{11} \mathbf{e}^\sigma + j_{12} \tilde{\mathbf{e}} + j_{13} \mathbf{e}^u, & \hat{\tilde{\boldsymbol{\sigma}}} &= j_{12} \tilde{\boldsymbol{\sigma}} + j_{22} \boldsymbol{\sigma}^e + j_{23} \boldsymbol{\sigma}^u, \\ \hat{\tilde{\boldsymbol{\sigma}}} &= j_{13} \tilde{\boldsymbol{\sigma}} + j_{23} \boldsymbol{\sigma}^e + j_{33} \boldsymbol{\sigma}^u, \end{aligned} \quad (55)$$

Hence the total variation is

$$\begin{aligned} \delta \Pi &= \delta U + \delta P^c = \int_V [(\hat{\tilde{\mathbf{e}}})^T \delta \boldsymbol{\sigma} + (\hat{\tilde{\boldsymbol{\sigma}}})^T \delta \mathbf{e} - \mathbf{r}^T \delta \mathbf{u}] dV \\ &+ \int_{S_r} (\hat{\tilde{\boldsymbol{\sigma}}}_n - \hat{\mathbf{t}})^T \delta \mathbf{u} dS + \int_{S_d} (\tilde{\mathbf{u}} - \hat{\mathbf{d}})^T \delta \tilde{\boldsymbol{\sigma}}_n dS \\ &+ \int_{S_d} (\hat{\tilde{\boldsymbol{\sigma}}}_n - \tilde{\boldsymbol{\sigma}}_n)^T \delta \mathbf{u} dS, \end{aligned} \quad (56)$$

in which  $\mathbf{r} = \text{div } \hat{\tilde{\boldsymbol{\sigma}}} + \mathbf{b}$  are the internal equilibrium violations.

Consistency arguments again show that the coefficients must satisfy the constraints

$$j_{11} + j_{12} + j_{13} = 0, \quad j_{12} + j_{22} + j_{23} = 0, \quad j_{13} + j_{23} + j_{33} = 1. \quad (57)$$

This leaves  $6 - 3 = 3$  free parameters. If the negated off-diagonal entries of  $\mathbf{J}$  are taken as the free parameters, the functional generating matrix takes the form

$$\mathbf{J} = \begin{bmatrix} s_2 + s_3 & -s_3 & -s_2 \\ & s_1 + s_3 & -s_1 \\ \text{symm} & & 1 + s_1 + s_2 \end{bmatrix}. \quad (58)$$

Four of the canonical functionals listed in Oden and Reddy (1982) are instances of  $\Pi$  obtained by setting the free parameters as indicated in Table 2. Two more can be obtained from the one-parameter null-space form (60) derived below. Figure 10 depicts interesting elasticity functionals in  $(s_1, s_2, s_3)$  space along with their generating matrices.

## 6.3

### Stress-strain duals

Switching the free parameters  $s_1$  and  $s_2$  has the effect of exchanging the role of stresses and strains in  $U$ . Those functionals will be called *stress-strain duals*. For example, the

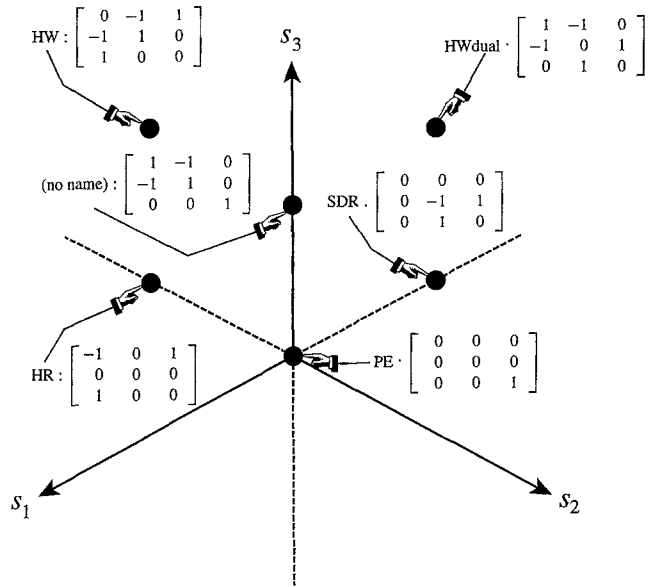


Fig. 10. Representation of the three-parameter PVP for classical elasticity in  $(s_1, s_2, s_3)$  space. Generating matrices for some interesting functionals are shown. (For acronym keys see Table 2.)

Varied fields	Acronym	Functional name	Parameters in $U$ or $U^*$
$\tilde{\mathbf{u}}$	PE	Potential energy	$s_1 = s_2 = s_3 = 0$
$\tilde{\boldsymbol{\sigma}}$	CE	Complementary energy	$s_0 = 0$
$\tilde{\mathbf{e}}$		No name	
$\tilde{\mathbf{u}}, \tilde{\boldsymbol{\sigma}}$	HR	Hellinger-Reissner	$s_1 = s_3 = 0, s_2 = -1$
$\tilde{\mathbf{u}}, \tilde{\mathbf{e}}$	SDR	Strain-displacement Reissner	$s_1 = s_2 = 0, s_3 = -1$
$\tilde{\boldsymbol{\sigma}}, \tilde{\mathbf{e}}$		No name	$s_0 = 1$
$\tilde{\mathbf{u}}, \tilde{\boldsymbol{\sigma}}, \tilde{\mathbf{e}}$	HW	Hu-Washizu	$s_3 = -s_2 = 1, s_1 = 0$

Table 2. Canonical Functionals of Classical Linear Elastostatics after Oden and Reddy (1982)

dual of the Hu-Washizu functional is obtained if  $s_2 = 0$ ,  $s_1 = -1$  and  $s_3 = 1$ , which yields

$$U_{HW}^{dual}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\varepsilon}}) = \int_V [\mathcal{U}^*(\tilde{\boldsymbol{\sigma}}) + (\boldsymbol{\sigma}^j - \tilde{\boldsymbol{\sigma}})^T \tilde{\boldsymbol{\varepsilon}}] dV, \quad (59)$$

where  $\mathcal{U}^*(\boldsymbol{\sigma}) = \frac{1}{2} \boldsymbol{\sigma}^T \mathbf{e}^\sigma$  is the complementary energy density. The HR and SDR functionals are stress-strain duals, and the PE functional is its own dual. In the graphical representation of Figure 10, stress-strain duals are obtained by reflection about the  $s_1 + s_2 = 0$  plane.

#### 6.4 Null space functionals

Elasticity functionals without independently varied displacements can be constructed following essentially the same procedure described in Section 4.3. This gives the one-parameter null-space functional

$$II^*(\tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\varepsilon}}) = U^* - P^{c*} = \frac{1}{2} \int_V \begin{Bmatrix} \tilde{\boldsymbol{\sigma}} \\ \boldsymbol{\sigma}^e \end{Bmatrix}^T \begin{bmatrix} (s_0 - 1)\mathbf{I} & -s_0\mathbf{I} \\ -s_0\mathbf{I} & s_0\mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{e}^\sigma \\ \tilde{\boldsymbol{\varepsilon}} \end{Bmatrix} dV + \int_{S_d} \tilde{\boldsymbol{\sigma}}_n^+ \tilde{\mathbf{d}} dS, \quad (60)$$

which reduces to the complementary energy functional  $II^*(\boldsymbol{\sigma})$  if  $s_0 = 0$ .

#### 6.5 Hybrid functionals

The construction of parametrized hybrid functionals for elastic bodies can be based on the same arguments presented in Section 5. Consider an internal interface  $S^i$  as a two-sided surface that divides the body into two parts  $V^+$  and  $V^-$ , as illustrated in Fig 11. On  $S^i$  the following side values of displacements and stresses are defined:

$$\mathbf{u}^+ = \mathbf{u}|_{\Gamma^+}, \quad \mathbf{u}^- = \mathbf{u}|_{\Gamma^-}, \quad \boldsymbol{\sigma}^+ = \boldsymbol{\sigma}|_{\Gamma^{++}}, \quad \boldsymbol{\sigma}^- = \boldsymbol{\sigma}|_{\Gamma^{--}},$$

$$\boldsymbol{\sigma}_n^+ = (\boldsymbol{\sigma}^+)^T \mathbf{n}^+, \quad \boldsymbol{\sigma}_n^- = (\boldsymbol{\sigma}^-)^T \mathbf{n}^-. \quad (61)$$

At each point of  $S^i$ , jumps of the displacement  $\mathbf{u}$  and tractions  $\boldsymbol{\sigma}_n$  may be specified:

$$[\![\mathbf{d}]\!] = \mathbf{u}^+ - \mathbf{u}^-, \quad [\![\mathbf{t}]\!] = \boldsymbol{\sigma}_n^+ + \boldsymbol{\sigma}_n^- \quad \text{on } S^i. \quad (62)$$

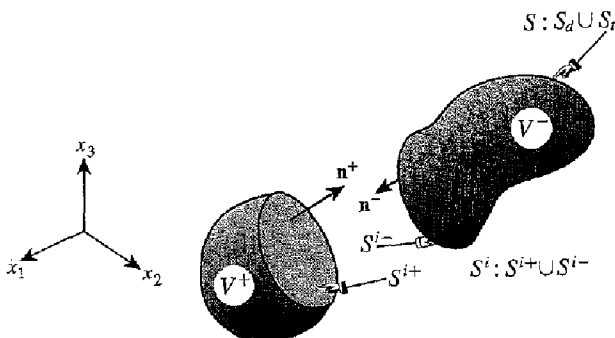


Fig. 11. Internal interface in 3D elastic body

Prescribed jumps are resolved by setting

$$\mathbf{u}^+ = \mathbf{d} + \frac{1}{2} [\![\mathbf{d}]\!], \quad \mathbf{u}^- = \mathbf{d} - \frac{1}{2} [\![\mathbf{d}]\!], \quad \boldsymbol{\sigma}_n^+ = \mathbf{t} + \frac{1}{2} [\![\mathbf{t}]\!],$$

$$\boldsymbol{\sigma}_n^- = -\mathbf{t} + \frac{1}{2} [\![\mathbf{t}]\!], \quad (63)$$

where  $\mathbf{d} = (\mathbf{u}^+ + \mathbf{u}^-)/2$  and  $\mathbf{t} = (\boldsymbol{\sigma}_n^+ - \boldsymbol{\sigma}_n^-)/2$  can be treated as independently varied interface variables. One difference with respect to the Poisson equation is that in elasticity one deals with vector quantities, and it is possible to envision component-by-component specification. For example, in contact problems with friction some combinations of that nature may be encountered. Proceeding as in Section 5 one can derive the following two-parameter interface potential:

$$P^i(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\sigma}}, \tilde{\mathbf{d}}, \tilde{\mathbf{t}}) = \int_V [(2\alpha_1 - \alpha_2)\tilde{\mathbf{t}} + \alpha_2(\tilde{\boldsymbol{\sigma}}_n^+ - \tilde{\boldsymbol{\sigma}}_n^-)]$$

$$(\tilde{\mathbf{u}}^- - \tilde{\mathbf{u}}^+ - [\![\mathbf{d}]\!]) + \alpha_1 [\![\mathbf{t}]\!] (\tilde{\mathbf{u}}^+ + \tilde{\mathbf{u}}^-)$$

$$+ (1 - 2\alpha_1)(\boldsymbol{\sigma}_n^+ (\mathbf{u}^- - \tilde{\mathbf{d}} - \frac{1}{2} [\![\mathbf{d}]\!])$$

$$+ \tilde{\boldsymbol{\sigma}}_n^- (\tilde{\mathbf{u}}^- - \tilde{\mathbf{d}} + \frac{1}{2} [\![\mathbf{d}]\!]) - \tilde{\mathbf{d}} [\![\mathbf{t}]\!]) dS. \quad (64)$$

Again,  $\alpha_2 = 0$  gives local-connector potentials,  $\alpha_1 = \alpha_2$  gives  $d$ -generalized 3-field potentials,  $\alpha_1 = 1/2$  gives  $t$ -generalized 3-field potentials and  $\alpha_1 = \alpha_2 = 1/2$  gives a 2-field potential.

The hybrid element classification of Table 1 holds if appropriate replacements of field variables are made. But the presence of vector interface fields may result in mixed-connector situations. For example, one could have a traction connector in one direction and displacement connectors along the others. That situation could be handled by selecting different  $\alpha_1$  and  $\alpha_2$  for different components.

Hybrid functionals for linear elasticity were developed during the 1960s by Pian and Tong (Pian 1964; Pian and Tong 1969; Tong 1970). An up-to-date review has recently appeared (Pian 1995). The early forms relied on interior single-field functionals. Hybrid functionals with multifield  $U$  (also called "mixed-hybrids" in the literature) were proposed by Fraeijns de Veubeke (1974) and Atluri (1975).

Atluri's 1975 paper gives an extensive classification using modified Hu-Washizu (HWM) functionals as departure points. For example, the functional labeled as  $II_{HWM1}$  therein results if one sets  $s_1 = 0$ ,  $s_3 = -s_2 = 1$ ,  $\alpha_1 = 1/2$ ,  $\alpha_2 = 0$ ,  $[\![\mathbf{d}]\!] = \mathbf{0}$  and  $[\![\mathbf{t}]\!] = \mathbf{0}$ . An interesting second version, labeled  $II_{HWM2}$ , is obtained by setting those values except for the last one, and then allowing  $[\![\mathbf{t}]\!]$  to be independently varied so that  $\mathbf{t}^+$  and  $\mathbf{t}^-$  are weakly connected on  $S^i$  as well as to the interior fields. Generalizations to incompressibility and nonlinear elasticity have been constructed by Atluri and Murakawa (1977), and Atluri, Tong and Murakawa (1983).

#### 6.6 Extensions: Incompressibility and stress tensor unsymmetry

The parametrized functionals of linear elastostatics presented so far fail if the material is incompressible. Appropriate stress and strain splittings made to encompass incompressibility are discussed by Felippa (1991a) where it is shown that functionals with 4 to 15 free parameters in the internal energy  $U$  result.

If the symmetry of the stress tensor in compressible elasticity is relaxed into a weak condition, functionals with 6 to 9 parameters in  $U$  are obtained (Felippa 1991b). These functionals are useful for micropolar models with or without couple stresses, as well as for the derivation of finite elements with independently varied rotation fields.

## 7 Nonlinear hyperelasticity

In the present section a parametrization of a class of three-field *mixed* functionals of nonlinear hyperelasticity is derived. The generalization to hybrid functionals is not considered. This study represents the first application to nonlinear problems of the techniques discussed in the previous sections. Nonlinear functionals are more difficult to handle because the range of “trial scenarios” is wider, and techniques tend to be more problem dependent.

A PVP for Lagrangian nonlinear hyperelasticity is obtained here by using a weighted decomposition of contributions to the internal energy functional. This family has the advantage of including all important published functionals as instances. Two differences with respect to the derivation techniques presented for linear problems should be noted:

1. Matrix notation is awkward because the quadratic-form configuration of the internal energy, used in (21) and (52), is not applicable. Consequently the more flexible indicial notation is used instead. Matrix forms would reappear naturally when nonlinear functionals are rate-linearized for incremental analysis.
2. Parameter symmetries cannot be assumed *ab initio*. Because the number of possible parametrization schemes is greatly increased for nonlinear functionals, less definite claims as to “including all existing functionals as instances” can be expected.

### 7.1 Governing equations

A Lagrangian kinematic description with respect to a fixed Cartesian coordinate system ( $X_1 \equiv x_1, X_2 \equiv x_2, X_3 \equiv x_3$ ) is followed. In the sequel Roman indices such as  $i, j, k, \ell$  range from 1 through 3 and the summation convention applies.

The kinematics of finite deflections is summarized in Fig. 12. The body occupies an *undeformed* reference configuration of volume  $V$  at  $t = 0$ , where  $t$  is a timelike parameter. This

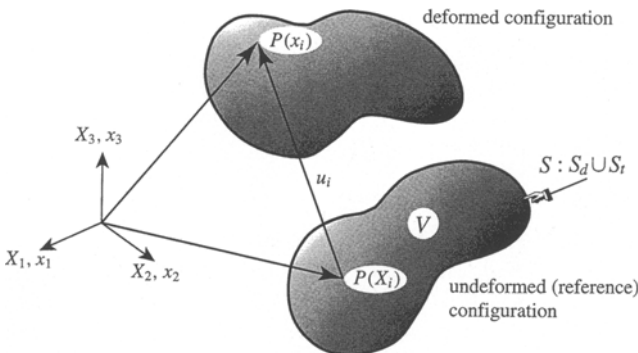


Fig. 12. Nonlinear hyperelastic body in 3D space

configuration is bounded by a surface  $S$  separated into two portions  $S : S_a \cup S_b$ , where boundary conditions of displacement and traction type, respectively, are prescribed. A generic material  $P(X_1, X_2, X_3)$  is located by its position vector  $X_i$ .

At another value of  $t$  the body occupies a *deformed* configuration. The generic particle moves to  $P(x_1, x_2, x_3)$ , where the spatial coordinates  $x_i(t)$  are measured with respect to the same Lagrangian coordinate system. The displacement components are  $u_i = x_i - X_i$ . The displacement gradient, deformation gradient and Green strain tensors are defined by

$$g_{ij} = \frac{\partial u_i}{\partial X_j}, \quad F_{ij} = \frac{\partial x_i}{\partial X_j} = \delta_{ij} + g_{ij}, \quad (64)$$

$$e_{ij} = \frac{1}{2}(g_{ij} + g_{ji} + g_{ik}g_{jk}) \quad \text{in } V, \quad (65)$$

respectively, where  $\delta_{ij}$  is the Kronecker delta. Both  $g_{ij}$  and  $F_{ij}$  are unsymmetric while  $e_{ij}$  is symmetric.

The stress measure conjugate to  $e_{ij}$  is the second (symmetric) Piola-Kirchhoff tensor, which will be denoted by  $s_{ij}$ . The equilibrium equations in terms of this measure are

$$\frac{\partial (s_{ik} F_{jk})}{\partial X_i} + b_j = 0 \quad \text{in } V, \quad (66)$$

where  $b_j$  are components of the prescribed body force field in the deformed configuration but specified per unit volume of the undeformed configuration.

The preceding properties hold for any deformable continuum. A hyperelastic solid is characterized by the existence of a strain energy density function  $\mathcal{U}$ , expressed in terms of the reference configuration volume, which links the conjugate deformation and stress measures:

$$s_{ij} = \frac{\partial \mathcal{U}(e_{ij})}{\partial e_{ij}} \quad \text{in } V. \quad (67)$$

Function  $\mathcal{U}$  must satisfy smoothness, symmetry and invariance conditions discussed in the continuum mechanics literature. The stress-strain relation (67) will be assumed invertible so that  $e_{ij}$  can be expressed as a function of  $s_{ij}$ . Its possible multi-valuedness, due to possible non-convexity of  $\mathcal{U}$ , is discussed by Ogden (1984) and Sewell (1987). Under those invertibility conditions the complementary energy density function  $\mathcal{U}^*$  is defined through the contact (Legendre) transformation

$$\mathcal{U}^* = e_{ij} \frac{\partial \mathcal{U}(e_{ij})}{\partial e_{ij}} - \mathcal{U}(e_{ij}). \quad (68)$$

Following the replacement of  $s_{ij}$  in terms of  $e_{ij}$  as independent variables, this function generates the inverse relations

$$e_{ij} = \frac{\partial \mathcal{U}^*(s_{ij})}{\partial s_{ij}} \quad \text{in } V. \quad (69)$$

The problem is closed by the specification of boundary conditions

$$u_j = \hat{d}_j \quad \text{on } S_a, \quad s_{ij} F_{jk} n_i = \hat{t}_j \quad \text{on } S_b \quad (70)$$

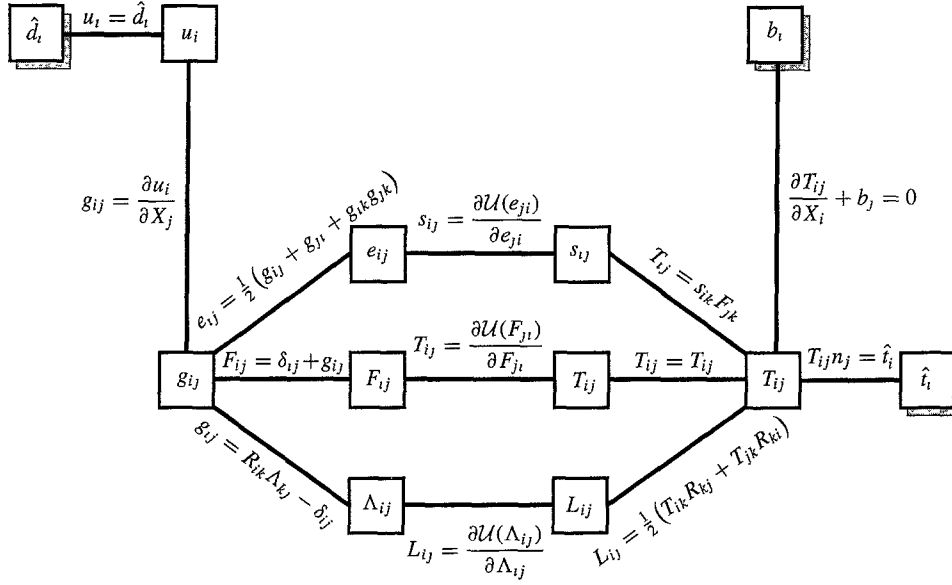


Fig. 13. Representation of the Strong Form of nonlinear hyperelasticity in a Lagrangian kinematic description. In addition to  $s_{ij}$  and  $e_{ij}$ , the figure also shows two other stress-deformation measure pairs: the deformation gradient  $F_{ij}$  paired with the first Piola-Kirchhoff stress  $T_{ij}$ , and the right stretch deformation tensor  $\Lambda_{ij}$  paired with the Biot-Jaumann-Lure stress  $L_{ij}$ . Symbol  $R_{ij}$  is the finite rotation tensor, extractable from  $F_{ij}$  through the polar decomposition

where prescribed displacements  $\hat{d}_i$  and tractions  $\hat{t}_i$  in the deformed body are referred back to the reference configuration. In a typical nonlinear analysis  $\hat{d}_i$  and  $\hat{t}_i$  (as well as  $b_i$ ) are functions of pseudo time  $t$ , and a sequence of problems is solved.

The foregoing field equations and boundary conditions are illustrated in the Strong Form diagram of Fig. 13. As noted in the legend, for completeness the diagram includes, besides  $s_{ij}$  and  $e_{ij}$ , two other commonly used conjugate measure pairs for stresses and deformations.

## 7.2

### Parametrized strain energy functional

The parametrized mixed functionals of nonlinear hyperelasticity presented here benefit the primal form

$$\Pi(\tilde{u}_i, \tilde{s}_{ij}, \tilde{e}_{ij}) = U(\tilde{u}_i, \tilde{s}_{ij}, \tilde{e}_{ij}) - P^c(\tilde{u}_i, \tilde{s}_{ij}). \quad (71)$$

Here  $U$  and  $P^c$  denote again the internal energy and the conventional load-potential functionals, respectively. Three interior fields are varied: the displacements  $\tilde{u}_i$ , the second Piola-Kirchhoff stresses  $\tilde{s}_{ij}$  and the Green strains  $\tilde{e}_{ij}$ . The varied displacement field  $\tilde{u}_i$  is always present. The displacement gradients  $g_{ij} = \partial u_i / \partial X_j$  and the deformation gradients  $F_{ij} = \delta_{ij} + g_{ij}$  are kept *strongly connected* to the displacements and consequently are not subject to independent variation. The derived fields are

$$e_{ij}^u = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial X_j} + \frac{\partial \tilde{u}_j}{\partial X_i} + \frac{\partial \tilde{u}_i}{\partial X_k} \frac{\partial \tilde{u}_j}{\partial X_k} \right), \quad e_{ij}^s = \frac{\partial \mathcal{U}^*(\tilde{s}_{ij})}{\partial \tilde{s}_{ij}}, \quad s_{ij}^e = \frac{\partial \mathcal{U}(\tilde{e}_{ij})}{\partial \tilde{e}_{ij}}, \quad (72)$$

$$s_{ij}^u = \frac{\partial \mathcal{U}(\tilde{e}_{ij}^u)}{\partial \tilde{e}_{ij}^u}.$$

Also appearing in the first-variation expressions are the instantaneous compliances and moduli:

$$A_{ijkl} = \frac{\partial^2 \mathcal{U}^*(s_{ij})}{\partial s_{ij} \partial s_{kl}}, \quad E_{ijkl} = \frac{\partial^2 \mathcal{U}(e_{ij})}{\partial e_{ij} \partial e_{kl}}, \quad E_{ijkl}^u = \frac{\partial^2 \mathcal{U}(e_{ij}^u)}{\partial e_{ij}^u \partial e_{kl}^u}. \quad (73)$$

The assumed form of the parametrized internal energy is  $U = U_1 + U_2$ , with

$$U_1 = \int_V [\bar{J}_{11} \mathcal{U}^*(\tilde{s}_{ij}) + \bar{J}_{22} \mathcal{U}(\tilde{e}_{ij}) + \bar{J}_{33} \mathcal{U}(e_{ij}^u)] dV,$$

$$U_2 = \int_V [\bar{J}_{12} \tilde{s}_{ij} \tilde{e}_{ij} + \bar{J}_{13} \tilde{s}_{ij} e_{ij}^u + \bar{J}_{21} s_{ij}^e e_{ij}^s + \bar{J}_{23} s_{ij}^e e_{ij}^u + \bar{J}_{31} s_{ij}^u e_{ij}^s + \bar{J}_{32} s_{ij}^u e_{ij}^u] dV. \quad (74)$$

Here the coefficients  $\bar{J}_{kl}$  serve as weights of the nine possible internal energy combinations. Barred symbols are used to facilitate later specialization to the  $j$  coefficients of classical elasticity. The expression for the conventional load potential is non parametric:

$$P^c(\tilde{u}_i, \tilde{s}_{ij}) = \int_V b_j u_j dV + \int_{S_d} s_{ij} F_{jk} n_i (u_j - \hat{d}_j) dS + \int_{S_t} u_i \hat{t}_i dS. \quad (75)$$

The appropriate integration by parts formula, as given for instance on page 453 of Fung (1965), is

$$\int_V s_{ij} e_{ij}^u dV = - \int_V \frac{\partial (s_{jk} F_{ik})}{\partial X_j} u_i dV + \int_S s_{jk} F_{ik} n_j u_i dS, \quad (76)$$

where  $s_{ij}$  is any symmetric stress tensor such as  $\tilde{s}_{ij}$  or  $s_{ij}^u$ . The resulting first variation is

$$\delta \Pi = \int_V \left[ \hat{e}_{ij} \delta s_{ij} + \hat{s}_{ij} \delta e_{ij} - \left( \frac{\partial \hat{s}_{ij} F_{jk}}{\partial X_j} + b_i \right) \delta u_i \right] dV + \int_{S_t} (\hat{s}_{jk} F_{ik} n_j - \hat{t}_i) \delta u_i dS + \int_{S_d} (u_i - \hat{d}_i) \delta \hat{s}_{jk} F_{jk} n_j dS + \int_{S_d} (\hat{s}_{jk} - s_{jk}) F_{ik} n_j \delta u_i dS, \quad (77)$$

in which

$$\begin{aligned}\bar{e}_{ij}^{\Delta} &= \bar{J}_{11} e_{ij}^s + \bar{J}_{12} \bar{e}_{ij} + \bar{J}_{13} e_{ij}^u + A_{ijk'} (\bar{J}_{21} s_{k'l}^e + \bar{J}_{31} s_{k'l}^u), \\ \bar{s}_{ij}^{\Delta} &= \bar{J}_{12} \bar{s}_{ij} + \bar{J}_{22} s_{ij}^e + \bar{J}_{32} s_{ij}^u + E_{ijk'} (\bar{J}_{21} e_{k'l}^s + \bar{J}_{23} e_{k'l}^u), \\ \bar{s}_{ij}^{\sqcup} &= \bar{J}_{13} \bar{s}_{ij} + \bar{J}_{23} s_{ij}^e + \bar{J}_{33} s_{ij}^u + E_{ijk'} (\bar{J}_{31} e_{k'l}^s + \bar{J}_{32} e_{k'l}^u).\end{aligned}\quad (78)$$

Because the material functions (73) are arbitrary, field consistency requires

$$\begin{aligned}\bar{J}_{11} + \bar{J}_{12} + \bar{J}_{13} &= 0, & \bar{J}_{12} + \bar{J}_{22} + \bar{J}_{32} &= 0, & \bar{J}_{13} + \bar{J}_{23} + \bar{J}_{33} &= 1, \\ \bar{J}_{21} + \bar{J}_{31} &= 0, & \bar{J}_{21} + \bar{J}_{23} &= 0, & \bar{J}_{31} + \bar{J}_{32} &= 0.\end{aligned}\quad (79)$$

If  $\bar{s}_1 = \bar{J}_{23}$ ,  $\bar{s}_2 = -\bar{J}_{13}$  and  $\bar{s}_3 = -\bar{J}_{12}$  are taken as the three free parameters, a generating matrix that meets the six conditions (79) is

$$\bar{J} = \begin{bmatrix} \bar{J}_{11} & \bar{J}_{12} & \bar{J}_{13} \\ \bar{J}_{21} & \bar{J}_{22} & \bar{J}_{23} \\ \bar{J}_{31} & \bar{J}_{32} & \bar{J}_{33} \end{bmatrix} = \begin{bmatrix} \bar{s}_2 + \bar{s}_3 & -\bar{s}_3 & -\bar{s}_2 \\ \bar{s}_1 & -\bar{s}_1 + \bar{s}_3 & -\bar{s}_1 \\ -\bar{s}_1 & \bar{s}_1 & 1 + \bar{s}_1 + \bar{s}_2 \end{bmatrix}.\quad (80)$$

As can be seen this generating matrix is not symmetric.

### 7.3 Some instances

By assigning numerical values in (80) one can obtain well known functionals for nonlinear elasticity (e.g. Washizu 1972; Oden and Reddy 1982; Sewell 1987), as well as others that are comparatively unknown or even unpublished. In the four examples given below only the  $U$  functional is listed.

Potential Energy (PE);  $\bar{s}_1 = \bar{s}_2 = \bar{s}_3 = 0$ :

$$U(\bar{u}) = \int_V \mathcal{U}(e_{ij}^u) dV.\quad (81)$$

Analog of HR, due to Reissner (1953);  $\bar{s}_3 = \bar{s}_1 = 0$ ,  $\bar{s}_2 = -1$ :

$$U(\bar{u}, \bar{s}_{ij}) = \int_V [-\mathcal{U}^*(s_{ij}) + \bar{s}_{ij} e_{ij}^u] dV.\quad (82)$$

Analog of Hu-Washizu (HW);  $\bar{s}_1 = 0$ ,  $\bar{s}_2 = -1$ ,  $\bar{s}_3 = 1$ :

$$U(\bar{u}, \bar{s}_{ij}, \bar{e}_{ij}) = \int_V [\mathcal{U}(\bar{e}_{ij}) + s_{ij}(e_{ij}^u - \bar{e}_{ij})] dV.\quad (83)$$

Rough analog of SDR;  $\bar{s}_1 = -1$ ,  $\bar{s}_2 = \bar{s}_3 = 0$ :

$$U(\bar{u}, \bar{s}_{ij}, \bar{e}_{ij}) = \int_V [\mathcal{U}(\bar{e}_{ij}) + s_{ij}^e (e_{ij}^u - e_{ij}^s) + s_{ij}^u (e_{ij}^s - \bar{e}_{ij})] dV.\quad (84)$$

Note that the ‘‘SDR analog’’ (84) contains the stresses as varied field. Indeed there are no strain-displacement functionals  $\mathcal{H}(\bar{u}, \bar{e}_{ij})$ . This is evident from the expression (80), because to get rid of the stresses one must set  $\bar{s}_1 = \bar{s}_2 = \bar{s}_3 = 0$ , which eliminates the deformations as well.

## 7.4

### Reduction to classical elasticity

The specialization to classical elasticity requires some care. In that case the compliances and moduli (73) are solution independent, although they may depend on  $X_p$  and

$$e_{ij}^s = A_{ijk'} s_{k'l}^e, \quad e_{ij}^u = A_{ijk'} s_{k'l}^u, \quad s_{ij}^e = E_{ijk'} e_{k'l}^s, \quad \text{etc.}\quad (85)$$

The six conditions (79) fold into three:

$$\begin{aligned}\bar{J}_{11} + \bar{J}_{12} + \bar{J}_{13} + \bar{J}_{21} + \bar{J}_{31} &= 0, & \bar{J}_{12} + \bar{J}_{22} + \bar{J}_{32} + \bar{J}_{21} + \bar{J}_{23} &= 0, \\ \bar{J}_{13} + \bar{J}_{23} + \bar{J}_{33} + \bar{J}_{31} + \bar{J}_{32} &= 1,\end{aligned}\quad (86)$$

which on symmetrizing the off-diagonal coefficients reduce to

$$\begin{aligned}\bar{J}_{11} + 2\bar{J}_{12} + 2\bar{J}_{13} &= 0, & 2\bar{J}_{12} + \bar{J}_{22} + 2\bar{J}_{32} &= 0, \\ 2\bar{J}_{13} + 2\bar{J}_{23} + \bar{J}_{33} &= 1,\end{aligned}\quad (87)$$

Renaming  $j_{11} = \bar{J}_{11}$ ,  $j_{22} = \bar{J}_{22}$ ,  $j_{33} = \bar{J}_{33}$ ,  $j_{12} = \frac{1}{2}\bar{J}_{12}$ ,  $j_{13} = \frac{1}{2}\bar{J}_{13}$ ,  $j_{23} = \frac{1}{2}\bar{J}_{23}$  recovers (57) and (58). The divisions by 2 may be avoided if  $U_j$  in (74) is scaled by  $\frac{1}{2}$ , but that would complicate (80).

## 7.5

### Generalizations

The use of  $e_{ij}$  and  $s_{ij}$  as deformation and stress measures, respectively, is traditional in Total Lagrangian formulations of computational mechanics. Other two conjugate measures: the deformation gradient  $F_{ij}$  paired with the first Piola-Kirchhoff stress  $T_{ij}$ , and the right stretch  $\Lambda_{ij}$  paired with the Biot-Jaumann-Lure stress  $L_{ij}$  have also been extensively studied.

The  $(F, T)$  pair, popularized through the monograph of Truesdell and Toupin (1961), leads to linear kinematic and equilibrium equations. However, it suffers from unsymmetries and most especially from controversy as to the existence of inverse stress-strain relations; see Koiter (1976) and references therein. The  $(\Lambda, L)$  pair has attracted attention from researchers because it provides a natural vehicle to extract finite-rotation effects for solids undergoing large deformations but small strains (e.g. Biot 1965; Hill 1978).

Reworking of the PVP (74) to fit other stress-deformation measures is formally straightforward. Additional complications arise, however, if the displacement gradients or the deformation gradients are weakly connected to the displacements. Alternatively, the finite rotation tensor, extracted through the polar decomposition, may be allowed to vary independently while weakening the symmetry of the stress tensor, or using multiple stress measures. The number of possible extensions is large. A recent review of nonlinear variational principles with emphasis on the handling of finite rotations has been given by Atluri and Cazzani (1995).

The question of whether the energy-splitting technique can be used to construct nonlinear PVPs with additional varied interior fields, as well as generalizations to include hybrid functionals, is presently open.

## 8

### Conclusions

This paper has discussed the basic concepts underlying Parametrized Variational Principles and presented selective new

developments. The latter material covers (i) a parametrized expression of interface functionals on which families of hybrid elements can be based, and (ii) a parametrization of a class of functionals for Lagrangian nonlinear hyperelasticity.

For reasons of space other theoretical developments, which are still largely in progress, have been omitted. These include: the parametrization of linear dynamics, the construction of PVPs for transient heat conduction using the method of vanishing parameters, and the parametrization of the potential-based equations of compressible inviscid fluids. Similarly, applications to computational mechanics in general and finite elements in particular, which are the primal motivators for these developments, have been left out. As previously noted, a summary of those applications are listed in a recent survey article (Felippa 1994). An application of parametrization techniques to the unification of matrix structural analysis has recently appeared (Felippa 1995).

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