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VARIATIONAL FORMULATION OF THE FINITE CALCULUS EQUATIONS IN SOLID MECHANICS AND DIFFUSION-REACTION PROBLEMS

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SUMMARY

We present a variational formulation of the finite calculus (FIC) equations for problems in mechanics governed by differential equations with symmetric operators. Applications considered include solid mechanics, diffusion-transport and diffusion-reaction problems. The key of the variational formulation is the identification of the FIC governing equations with the classical differential equations of mechanics written in terms of modified non-local variables. A total potential energy (TPE) functional is found in terms of the modified variables. The FIC equations in the domain and the boundary are recovered as the Euler-Lagrange equations and the natural boundary condition of the TPE functional, respectively. Symmetric finite element equations are obtained after discretization of the TPE functional, therefore preserving the symmetry of the governing infinitesimal equations. The variational FIC expression is reinterpreted as a Petrov-Galerkin weighted residual form of the original FIC equations with non-local weighting functions. The analogy of the variational FIC-FEM formulation with a discontinuous Galerkin method is recognized. Extensions to multidimensional linear elastostatics and diffusion-reaction problems are presented.

1 INTRODUCTION

Finite calculus (FIC) is a formulation of the governing equations of mechanics based on enforcing conservation laws over a domain of finite size. This procedure leads to a set of governing equations that differ from those of classical infinitesimal calculus. For a one-dimensional (1D) problem governed by a scalar-valued field variable $\phi(x)$, the FIC differential equation that includes up to first-order residual derivatives can be written as [9, 16].

$$r(\phi) - \frac{h}{2} r(\phi)' = 0, \tag{1}$$

where $r(\phi) = 0$ is the residual differential equation of the classical infinitesimal theory. In Eq. (1) a prime denotes differentiation with respect to the space variable x and h is a

characteristic distance or *characteristic length* parameter related to the dimension of the finite domain over which a conservation law (e.g., balance of fluxes, momentum or mass, or equilibrium of forces) is enforced. If $h \to 0$, i.e. as the size of the balance domain tends to zero, the standard residual form of the infinitesimal theory is recovered.

Eq. (1) admits of several interpretations. On its own it may be viewed as a modified *non-local form* of the standard governing equation since it involves a derivative of the original differential equation and a characteristic length scale. For numerical solution it may be discretized with standard methods including finite elements (FEM), finite differences (FDM) or finite volumes (FVM). Upon discretization the underlined non-local term $\frac{h}{2}r'$ brings forth additional contributions to the discrete equations that may be interpreted as *stabilization* terms. Satisfactory numerical results have been obtained by suitably selecting the characteristic length h as a function of mesh size dimension. This is analogous to the purpose of stabilization parameters. Therefore the FIC approach can be placed within the class of *stabilized methods* [9]–[20]. In fact, several well known methods of this kind, such as the streamline-upwind-Petrov-Galerkin (SUPG) method widely used for convective transport problems, can be interpreted as a particular case of the FIC formulation [9]. Successful applications of the FIC approach in conjunction with FEM have been reported for problems in convection-diffusion [9, 10, 16, 19], convection-diffusion-absorption [18, 20], fluid flow [11, 12, 17] and incompressible solid mechanics [14, 15, 16].

Variational principles for FIC equations cannot be constructed within the framework of classical variational calculus (CVC). The reason is that such equations generally contain odd derivatives in the space variables. For example, the FIC equilibrium equation for the 1D linear elasticity example worked out in Section 2 is, for zero body forces and expressed in terms of the displacement $u(x)$:

$$(Eu')' - \frac{h}{2}(Eu')'' = 0, \tag{2}$$

in which E is the elastic modulus. The highest space derivative in Eq. (2) is 3. But Euler-Lagrange (E-L) differential equations are always of *even* order. It follows that (2) cannot be the E-L equation of a functional with primary variable $u(x)$ derived via CVC. Consequently Petrov-Galerkin weighted residual methods have been favoured for the FEM discretization of FIC differential equations.

For problems that are essentially conservative, such as elastic solid mechanics, heat diffusion or diffusion-reaction applications, use of weighted residual methods seems unnecessary and may delay consideration of FIC methods by FEM practitioners already trained in energy formulations [26]. It is thus appealing to place FIC within a variational framework. As noted above, this cannot be the classical one. However, over the last three decades a notable development of what may be called *extended variational calculus* or EVC has taken place. The monograph of Vujanovic and Jones [24] provides a comprehensive exposition of recent developments, superseding the dated book of Finlayson [7]. The powerful array of methods described in [24] essentially places *any* differential system within the reach of EVC. Whether these new formulations can and should replace the Petrov-Galerkin discretization approach remains an open question. The answer is likely to be problem and dimensionality dependent.

For FIC equations in mechanics, an extended variational formulation offers the following advantages:

1. If the characteristic distance h is set to zero, the classical variational forms are recovered along with their FEM approximations. This simplifies verification of FIC programs against existing FEM codes.

2. The standard machinery of FEM based on energy methods such as shape functions, numerical integration, energy-consistent lumping of masses and forces, etc., can be reused.

3. Natural boundary conditions emerge naturally from the varied functional. In Petrov-Galerkin methods such conditions must be established by ad-hoc techniques or physical reasoning, risking inconsistencies.

4. Variational expressions can be shown to be equivalent to a Petrov-Galerkin weighted residual treatment of the original FIC equations. This PG form can be extended to treat non-symmetric problems, such as convection-diffusion or advective flow, where a variational principle is not available.

The first advantage fosters flexibility in modeling complicated systems. Some system components that require numerical stabilization, for example near-incompressible materials or regions undergoing plastic deformations or dislocations, could be treated by FIC-FEM methods, whereas those not requiring special treatment may be modeled by the conventional FEM approach. This simplifies the connection of FIC and conventional models.

The content of the paper is the following. In the next section the FIC equations for 1D linear elastic solids is presented. A set of modified variables is defined which allows to express the FIC equations by the standard infinitesimal expressions. A Total Potential Energy (TPE) functional is defined in terms of the modified variables. It is shown that the E-L equations of the TPE functional coincide with the FIC governing equations. The variational form of the TPE functional is reinterpreted as a weighted residual expression of the original FIC equations with non-local weighting functions. An interesting analogy between the FIC variational form and a discontinuous Galerkin formulation is briefly discussed. The functional derivation process is repeated for the 1D diffusion and diffusion-radiation equations with identical conclusions. Extensions to the multidimensional case of the FIC-TPE functional for elastic solids and diffusion-radiation problems are presented.

2 ONE-DIMENSIONAL ELASTOSTATICS

To illustrate the variational formulation in Section 3 the FIC equations for solid mechanics are specialized first to 1D elasticity as exemplified by a Hookean material fiber of length L aligned with the x axis and subjected to a uniaxial stress state. [The relations that follow may be used to derive equations of a bar or of a Bernoulli-Euler beam by integrating over the cross section.] The multidimensional problem is covered in Section 8.

The problem domain Ω is the segment of length L aligned along $x \in [0, L]$. The boundary points are $\Gamma \equiv \{x = 0, x = L\}$. The axial displacement, axial strain and axial stress are $u = u(x), \varepsilon = \varepsilon(x)$ and $\sigma = \sigma(x)$, respectively. The elastic modulus is E. The boundary set is decomposed into $\Gamma = \Gamma_u \cup \Gamma_t$. On Γ_u the displacement is prescribed and set to a prescribed value u^p. On Γ_t the surface traction is prescribed and set to a prescribed value t^p. The body force per unit length $b = b(x)$ is given.

2.1 FIC Equations

The 1D elasticity equilibrium equation in FIC form is derived in Appendix A. The result can be written as

$$r - \underline{\frac{h}{2} r'} = 0 \quad \text{in } \Omega. \tag{3}$$

Here $r := \sigma' + b$ is the equilibrium residual and h is a characteristic length that is assumed to be a constant property over a finite equilibrium domain. Equivalently $h' = 0$ will be assumed in the discrete problem (see also Remark 1). The other two field equations: kinematic and constitutive, are assumed to hold pointwise

$$\sigma = E\varepsilon \quad , \quad \varepsilon = u'. \tag{4}$$

The natural boundary condition, also derived in Appendix A, is

$$\sigma_n - t^p - \underline{\frac{h}{2} r} = 0 \quad \text{on } \Gamma_t. \tag{5}$$

where σ_n is the normal stress $\sigma_n = \sigma|_{\Gamma_t}$ (see Figure 1 of the Appendix). The essential boundary condition is

$$u - u^p = 0 \quad \text{on } \Gamma_u. \tag{6}$$

Eqs. (3) and (5) are obtained by expressing the equilibrium of axial forces in a domain of finite size and retaining higher order terms in the Taylor series expansion of the equilibrium variables. Details are given in Appendix A. The underlined terms in those equations are typical of the FIC formulation, and vanish if $h \to 0$.

2.2 Variational FIC Formulation

For the derivation of variational forms it is convenient to introduce the following *modified* versions of displacements, strains, stresses, body forces and tractions:

$$\bar{u} = u - \frac{h}{2} u', \quad \bar{\varepsilon} = \varepsilon - \frac{h}{2}\varepsilon' = \bar{u}', \quad \bar{\sigma} = \sigma - \frac{h}{2}\sigma' = E\bar{\varepsilon}, \quad \bar{b} = b - \frac{h}{2} b', \quad \overline{t}^p = t^p + \frac{h}{2} b. \tag{7}$$

These modified variables can be considered *non-local*, because they involve the function, its space derivative and a characteristic distance parameter. Then the FIC equations (3) and (5) can be compactly written

$$\boxed{\bar{\sigma}' + \bar{b} = 0 \quad \text{in } \Omega, \quad \bar{\sigma} - \overline{t}^p = 0 \quad \text{on } \Gamma_t} \tag{8}$$

In terms of the modified displacements:

$$\boxed{(E\bar{u}')' + \bar{b} = 0 \quad \text{in } \Omega, \quad E\bar{u}' - \bar{t}^p = 0 \quad \text{on } \Gamma_t, \quad \bar{u} - u^p = 0 \quad \text{on } \Gamma_u.} \tag{9}$$

A glance at Eqs. (9) shows that the FIC equations coincide with the classical equations of solid mechanics if the standard fields u, ε, σ, b and t^p are substituted by their non-local counterparts $\overline{u}$, $\overline{\varepsilon}$, $\overline{\sigma}$, $\overline{b}$ and $\overline{t}^p$, respectively. Note that we have assumed that $\bar{u}$ satisfies exactly the essential boundary conditions on Γ_u. This can be understood as h vanishing at Γ_u so that $u = u^p$ on that boundary.

The following Total Potential Energy (TPE) functional is introduced

$$\Pi(\bar{u}) = U(\bar{u}) - W(\bar{u}) \tag{10}$$

with

$$U(\bar{u}) = \frac{1}{2}\int_0^L E\bar{\varepsilon}^2 dx = \frac{1}{2}\int_0^L E\left(\bar{u}'\right)^2 dx, \quad W(\bar{w}) = \int_0^L \bar{u}\bar{b}dx + (\bar{u}\bar{t}^p)_{\Gamma_t} \tag{11}$$

Taking the variation of Π with respect to $\bar{u}$ and integrating by parts yields

$$\delta\Pi = -\int_0^L \delta\bar{u}\left(\left(E\bar{u}'\right)' + \bar{b}\right)dx + \left[\left(E\bar{u}' - \bar{t}\right)\delta\bar{u}\right]_{\Gamma_t} \tag{12}$$

Assuming that the $\delta\bar{u}$ are arbitrary gives the E-L equations as

$$\left(E\bar{u}'\right)' + \bar{b} = \left(\sigma' - \frac{h}{2}\sigma''\right) + b - \frac{h}{2}b' = r - \frac{h}{2}r' = 0 \quad \text{in } \Omega : x \in [0, L], \tag{13}$$

and the natural boundary condition as

$$E\bar{u}' - \bar{t} = Eu' - \frac{h}{2}u'' - t^p - \frac{h}{2}b^n = \sigma - t^p - \frac{h}{2}r = 0 \quad \text{on } \Gamma_t. \tag{14}$$

The E-L relation (13) reproduces the FIC residual equation (3) whereas the natural BC (14) reproduces the boundary traction condition (5).

Remark 1. The equivalence of Eqs.(8) with the original FIC forms of Eqs.(3) and (5) requires that $h' = 0$, i.e. the space derivative of the characteristic distance parameter is assumed to be zero. This can be accepted by interpreting h as a parameter that is constant over the finite equilibrium domain surrounding each point. Removal of this constraint has not been investigated.

2.3 Changes From Standard Variational Calculus

We have constructed, within the framework of extended variational calculus, a FIC equivalent of the well known TPE functional. The changes from standard variational calculus can be interpreted in various ways. One is that we have effectively changed the variation rules since

$$\begin{aligned} \delta\bar{u} &= \delta u - \frac{1}{2}h(\delta u)' \Rightarrow \delta u = \delta\bar{u} + \frac{1}{2}h(\delta u)' \\ \delta\bar{u}' &= \delta u' - \frac{1}{2}h(\delta u')' \Rightarrow \delta u' = \delta\bar{u}' + \frac{1}{2}h(\delta u')' \end{aligned} \tag{15}$$

from which $(\delta u)' = (d/dx)\delta u \neq \delta u'$; likewise $(\delta u')' = (d/dx)\delta u' \neq \delta u''$. Thus commutativity of differential and variation has been abandoned. This is in line with the method of "noncommutative variations" discussed in Ch. 6 of [24].

Yet another interpretation can be illustrated by expressing $\Pi(\bar{u})$ back in terms of the actual displacement u. On assuming constant E and h the E-L equation given by standard variational calculus is

$$\begin{aligned} &-\frac{\partial\Pi}{\partial u} + \frac{d}{dx}\frac{\partial\Pi}{\partial u'} - \frac{d^2}{dx^2}\frac{\partial\Pi}{\partial u''} = Eu'' + b - \frac{h}{2}(Eu''' - b') + E\frac{h^2}{4}u^{IV} = \\ &r - \frac{h}{2}r' + E\frac{h^2}{4}u^{IV} = 0 \quad \text{in} \quad \Omega. \end{aligned} \tag{16}$$

This agrees with the FIC residual equation (1) up to $O(h)$. Thus another functional-seeking approach for one dimensional problems would be to augment (1) with appropriate terms in h^2, h^3, etc., to form an exact first variation $\delta\Pi$. This is in line with the method of "vanishing parameters" also covered in [24]. This method, however, becomes unwieldy in multiple dimensions.

2.4 FEM Implementation

The numerical solution based on the functional $\Pi(\bar{u})$ is naturally done with the Finite Element Method. The domain $[0, L]$ is divided into N_e finite elements with nodes $1, 2 \ldots N_e{+}1$. Two procedural choices for choosing the interpolation variable and degrees of freedoms emerge:

(1) Interpolate the modified displacement $\bar{u}$ over elements, and pick $\bar{u}_i$ as nodal values. Actual displacements are recovered from $u = \bar{u} + \frac{h}{2}u'$, and may jump at the nodes.

(2) Interpolate the actual displacement u over elements, and pick u_i as nodal values. The derivative u' is treated as a slave field, and only C^0 continuity is imposed.

Both choices were tried for fixed-free bar problems under uniform body force, using piecewise linear interpolation for $\bar{u}$ and u in (1) and (2), respectively, with h taken to be a fraction of the element size. In choice (1) the only effect of h enters through the essential BC at the fixed end and optimal results are obtained for $h = 0$, as expected. In choice (2) the FEM system is independent of h because $u'' = 0$ over each element and $b' = 0$ over the problem domain, and one recovers the nodally exact solution of standard FEM.

The conclusion from numerical experiments is that for one-dimensional elastostatics the additional flexibility provided by the FIC steplength h is not realized. The added value of the variational formulation is realized in three-dimensional elasticity that obeys internal constraints such as incompressibility or plastic flow.

2.5 Interpretation as Petrov-Galerkin Form

The variational form $\delta\Pi = 0$ of (12) can be reinterpreted as particular case of the general weighted residual form of the original FIC equations with a weighting function w defined by

$$w := \delta\bar{u} = \delta u - \frac{h}{2}(\delta u)' \tag{17}$$

Expression (12) is therefore equivalent to the following Petrov-Galerkin form of the original FIC equations (3) and (5)

$$\int_0^L \left(\delta u - \frac{h}{2}(\delta u)'\right)\left(r - \frac{h}{2}r'\right) dx - \left[\left(\delta u - \frac{h}{2}(\delta u)'\right)\left(\sigma - t^p - \frac{h}{2}r\right)\right]_{\Gamma_t} = 0 \tag{18}$$

Substituting the expression of r into (18) and writing σ in terms of u using the constitutive equation (4) gives

$$\begin{aligned}\int_0^L \left(\delta u - \frac{h}{2}(\delta u)'\right)\left[(Eu')' + b - \frac{h}{2}\left((Eu')'' + b'\right)\right] dx - \\ - \left[\left(\delta u - \frac{h}{2}(\delta u)'\right)\left(\sigma - t^p - \frac{h}{2}\left((Eu')' + b'\right)\right)\right]_{\Gamma_t} = 0\end{aligned} \tag{19}$$

Integrating by parts the terms involving u'', u''' and b' leads to the following weak form

$$\int_0^L \left[-(\delta u)' E u' + \frac{h}{2} \left[(\delta u)'' E u' + (\delta u)' E u'' \right] - \frac{h^2}{4} (\delta u)'' E u'' \right] dx + \int_0^L \left(\delta u - \frac{h^2}{4} (\delta u)'' \right) b dx + \left[\left(\delta u - \frac{h}{2} (\delta u)' \right) t^p \right]_{\Gamma_t} = 0 \tag{20}$$

The first integral of Eq. (20) is *symmetric* with respect to u and δu. This naturally leads to a symmetric form of the discretized equations using the Galerkin FEM method [26] with the same interpolation for u and δu. Note that all terms involving derivatives of order higher than one would vanish for a piecewise linear Galerkin interpolation.

Remark 2. The non-local weighting function $w := \delta u - \frac{h}{2} \delta u'$ chosen in Eq. (17) is consistent with the non-local displacement field $\bar{u} = u - \frac{h}{2} u'$ taken as the prime variable of the FIC equations. The resulting symmetric variational form preserves the symmetry of the differential operators in the governing equations of the infinitesimal theory. This symmetry is lost for other weighting functions (such as $w = \delta u$) applied to the FIC equations [9, 16, 18, 19].

Remark 3. The integration by parts of Eq. (19) assumes C^1 continuity of u and δu, and C^0 continuity of h. The former can be relaxed in the FEM discretization by computing integrals that involve the second derivative of u within each element domain only and discarding contributions from first derivative interelement jumps. The second can be obviated in a similar manner, by assuming h to be uniform over each element and ignoring interelement jump effects.

Remark 4. An alternative for overcoming the C^1 continuity requirement is to impose the continuity of the first derivative of u and δu between elements in a *weak form*. The resulting FIC-FEM formulation is similar to a *discontinuous-Galerkin* (DG) method [1, 2, 3, 4, 5, 8, 23, 25]. The analogy between FIC and DG methods may help to understand better various features of DG techniques and their link to stabilized finite element methods.

3 ONE DIMENSIONAL DIFFUSION

The foregoing formulation extends to other problems in mechanics governed by elliptic operators. Consider next one-dimensional, steady-state heat diffusion by conduction. The primary variable is the temperature $\phi = \phi(x)$. The heat flux q is linked to ϕ by Fourier's law of heat conduction $q = -k\, d\phi/dx = -k\phi'$, where k is the diffusion parameter (also called conductivity coefficient). The heat source per unit length is Q. As usual the problem domain is denoted by Ω. The boundary is split into Γ_ϕ and Γ_q on which temperature ϕ^p and flux q^p, respectively, are prescribed. The governing ordinary differential equation in terms of ϕ is $-q' + Q = (k\phi')' + Q = 0$, whence the residual is defined as

$$r = -q' + Q = (ku')' + Q. \tag{21}$$

The FIC governing equation and boundary conditions are [9, 16].

$$r - \underline{\frac{h}{2} r'} = 0 \quad \text{in } \Omega, \quad -q + q^p - \underline{\frac{h}{2} r} = 0 \quad \text{on } \Gamma_q, \quad \phi - \phi^p = 0 \quad \text{on } \Gamma_\phi. \tag{22}$$

The additional terms brought by the FIC formulation have been underlined.

3.1 Variational Formulation

As before introduce the modified *non-local* fields $\bar{\phi}$, $\bar{q}$, $\bar{Q}$ and $\bar{q}^p$ by the definitions

$$\bar{r} := -\bar{q}' + \bar{Q}, \quad \bar{\phi} := \phi - \frac{h}{2}\phi', \quad \bar{q} := q - \frac{h}{2}q', \quad \bar{q}^p := q^p - \frac{h}{2}Q, \quad \bar{Q} := Q - \frac{h}{2}Q' \tag{23}$$

The modified constitutive (Fourier) law is $q' = -k\bar{\phi}'$. The FIC governing equations rewritten in terms of the modified fields (23) are

$$\bar{r} = 0 \quad \text{in } \Omega, \quad -\bar{q} + \bar{q}^p = 0 \quad \text{on } \Gamma_q, \quad \bar{\phi} - \phi^p = 0 \quad \text{on } \Gamma_\phi. \tag{24}$$

The TPE/FIC functional in terms of the modified temperature $\bar{\phi}$ is

$$\Pi(\bar{\phi}) = U(\bar{\phi}) - W(\bar{\phi}) \tag{25}$$

with

$$U(\bar{\phi}) = \frac{1}{2}\int_0^L k(\bar{\phi}')^2\, dx, \qquad W(\bar{\phi}) = \int_0^L \bar{\phi}\bar{Q}dx - (\bar{\phi}\bar{q}^p)_{\Gamma_q}, \tag{26}$$

Taking the variation of Π with respect to $\bar{\phi}$ and integrating by parts the term involving $k\bar{\phi}'$ gives

$$\delta\Pi = -\int_0^L \delta\bar{\phi}\left[(k\bar{\phi}')' + \bar{Q}\right] dx + \left[(k\bar{\phi}' + \bar{q}^p)\delta\bar{\phi}\right]_{\Gamma_q} \tag{27}$$

In the derivation of Eq. (27) we have used the assumption that $\bar{\phi}$ satisfies exactly the essential boundary conditions, i.e. $\bar{\phi} = \phi^p$ on Γ_ϕ. Assuming that $\delta\bar{\phi}$ is arbitrary gives the Euler-Lagrange equations and the natural boundary conditions

$$(k\bar{\phi}')' + \bar{Q} = \bar{r} = 0 \quad \text{in} \quad \Omega, \qquad k\bar{\phi}' + \bar{q}^p = -\bar{q} + q^p = 0 \quad \text{on} \quad \Gamma_q. \tag{28}$$

These reproduces the FIC governing equation and the boundary condition on Γ_q in (24).

4 ONE DIMENSIONAL DIFFUSION-REACTION

The combination of diffusion with reactive or radiation effects is important in chemical, biological and enviromental engineering. In those applications diffusion denotes the process of intermingling of molecules in gases, liquids or solids as a result of random thermal agitation, whereas reaction is a process by which substances are produced, changed or destroyed as function of the state. Here we consider the one-dimensional steady-state case. The same equation but in hyperbolic form governs linear wave propagation in the frequency domain, as further discussed in Subsection 4.3.

4.1 Variational Formulation

The TPE/FIC functional $\Pi(\bar{\phi})$ of Eqs. (25–26) can be made to account for reactive or radiation effects by augmenting the internal energy U with a reaction term:

$$U(\bar{\phi}) = \frac{1}{2}\int_0^L \left[k(\bar{\phi}')^2 + s(\bar{\phi})^2\right] dx, \quad W(\bar{\phi}) = \int_0^L \bar{\phi}\bar{Q}dx - (\bar{\phi}\bar{q}^p)_{\Gamma_q}, \tag{29}$$

Here s is a reaction or radiation parameter, with $s > 0$ for absorption or destruction and $s < 0$ for production. Note that W does not change. The modified fields in Eq. (23) do not change except for the boundary flux:

$$\bar{q}^p = q^p - \frac{h}{2}(Q - s\phi) \tag{30}$$

Upon integration by parts the first variation of Π with respect to $\bar{\phi}$ leads to

$$\delta\Pi = -\int_0^L \delta\bar{\phi}\left[(k\bar{\phi}')' - s\bar{\phi} + \bar{Q}\right] dx + \left[(k\bar{\phi}' + \bar{q}^p)\,\delta\bar{\phi}\right]_{\Gamma_q} \tag{31}$$

Setting $\delta\Pi = 0$ gives the Euler-Lagrange equation

$$(k\bar{\phi}')' - s\bar{\phi} + \bar{Q} = r - \frac{h}{2}r' = 0 \quad \text{in} \quad \Omega, \qquad \text{with} \qquad r := (k\phi')' - s\phi + Q, \tag{32}$$

and the natural boundary condition

$$k\bar{\phi}' + \bar{q}^p = k\phi' + q^p - \frac{h}{2}r = 0 \quad \text{on} \quad \Gamma_q. \tag{33}$$

Eqs. (32) and (33) reproduce the FIC governing equations for the diffusion-radiation problem. As expected if $h \to 0$ the standard differential forms for the infinitesimal formulation are recovered:

$$(k\phi')' - s\phi + Q = 0 \quad \text{in} \quad \Omega, \qquad k\phi' + q^p = 0 \quad \text{on} \quad \Gamma_q. \tag{34}$$

4.2 Petrov-Galerkin Form

The variational expression $\delta\Pi = 0$ of (31) can be interpreted as the Petrov-Galerkin form

$$\int_0^L \left(\delta\phi - \frac{h}{2}(\delta\phi)'\right)\left(r - \frac{h}{2}r'\right) dx - \left[\left(\delta\phi - \frac{h}{2}(\delta\phi)'\right)\left(k\phi' + q^p - \frac{h}{2}r\right)\right]_{\Gamma_q} = 0, \tag{35}$$

with the residual r as defined in Eq. (32). Substituting r into Eq. (35) and integrating by parts the terms involving $k\phi'$ and $(h/2)(\delta\phi)'$ in the first integral gives

$$\begin{aligned}\int_0^L \left[-(\delta\phi)'\left(k + s\frac{h^2}{4}\right)\phi' - s(\delta\phi)\phi + \frac{h}{2}\left[(\delta\phi)''k\phi' + (\delta\phi)'k\phi''\right] - \frac{h^2}{4}(\delta\phi)''k\phi''\right] + \\ + \left[\int_0^L \delta\phi - \frac{h^2}{4}(\delta\phi)''\right] Q dx - \left[\left(\delta\phi - \frac{h}{2}(\delta\phi)'\right) q^p - s\frac{h^2}{4}(\delta\phi)'\phi\right]_{\Gamma_q} = 0.\end{aligned} \tag{36}$$

The first integral of Eq. (36) is symmetric with respect to $\delta\phi$ and ϕ. This leads to a symmetric stiffness-like matrix after a finite element discretization that uses the same interpolation function for ϕ and $\delta\phi$; that is, the Galerkin method. If piecewise linear finite elements are used, terms involving derivatives of order two will vanish, and Eq. (36) simplifies to

$$-\int_0^L \left[(\delta\phi)'\left(k + s\frac{h^2}{4}\right)\phi' + s(\delta\phi)\phi\right] dx + \int_0^L \delta\phi\, Q dx - \left[\left(\delta\phi - \frac{h}{2}(\delta\phi)'\right) q^p - s\frac{h^2}{4}(\delta\phi)'\phi\right]_{\Gamma_q} = 0. \tag{37}$$

Note that the formulation introduces naturally an additional diffusion term $sh^2/4$. As observed below, this term is essential to stabilize the numerical solution for large positive values of the reaction parameter.

Remark 5. The boundary term $s(h^2/4)(\delta\phi)'\phi$ in the foregoing equations will lead to an unsymmetric matrix in problems where the flux q^p is prescribed at the Neumann boundary Γ_q. Experience shows that the FIC terms are not relevant near boundaries where the flux is prescribed and that terms involving h can be disregarded there without loss of accuracy. On the other hand, at Dirichlet boundaries where sharp boundary layers are found for large values of the production term $s\phi$ (i.e. for $s \gg 0$) the Neumann boundary terms do not play a significant role in the solution process.

4.3 Numerical Results

The TPE functional $\Pi(\bar{\phi}) = U - W$ with U and W as per Eq. (29) has been recently used by Felippa and Oñate [6] for numerically solving 1D diffusion-absorption model problems. In that study ϕ was piecewise linear interpolated over two-node finite elements with ϕ' treated as a slave variable. (The alternative interpolation of the modified field $\bar{\phi}$ was not tried.) The same formulation was tested on the 1D Helmholtz problem of wave mechanics, in which case s is negative with $-s$ proportional to the square of the wavenumber.

The inclusion of the FIC terms was found essential for stabilizating the numerical solution when s is large and positive, which causes sharp exponential boundary layers. Furthermore, for discretizations that obey certain modeling constraints, it was possible to adjust h as a function of the physical parameters so that *nodally exact* values were obtained for both problems.

In addition to the Helmholtz problem we note that the diffusion-reaction equations are equivalent to those of a spring resting on an elastic Winkler foundation with support modulus s per unit length. The present variational formulation also holds in that case.

5 MULTIDIMENSIONAL PROBLEMS

The FIC variational formulations described in the foregoing sections extend naturally to two- and three-dimensional problems. The detailed derivation of the equations falls outside the scope of this paper and only a summary of the relevant expressions will be presented.

5.1 Variational and Weak FIC Forms for Elastostatics

Following the lead of the one-dimensional case, modified non-local fields are introduced for general elastic solids. Roman indices i and j run over the number of space dimensions. The body, referred to a rectangular Cartesian reference system $\{x_i\}$ occupies domain Ω with boundary Γ. The exterior normal to Γ has components n_i. In the following equations u_i, ε_{ij}, σ_{ij}, b_i and t_i^p denote the standard displacements, strains, stresses, body forces and prescribed surface tractions of linear elastostatics, respectively. The summation convention over repeated indices applies unless explicitly suppressed. A subscripted comma as in $(.)_{,i}$ denotes the partial derivative with respect to the coordinate x_i. As usual the boundary is split into $\Gamma = \Gamma_t \cup \Gamma_u$. The generalization of the one-dimensional FIC steplength h for multidimensional problems is the second-order tensor h_{ij} [21].

The modified displacements, strains and stresses are defined as

$$\bar{u}_i = u_i - \frac{1}{2}h_{ij}(u_i)_{,j}, \quad \bar{\varepsilon}_{ij} = \varepsilon_{ij} - \frac{1}{2}h_{ik}(\varepsilon_{ij})_{,k}, \quad \bar{\sigma}_{ij} = \sigma_{ij} - \frac{1}{2}h_{ik}(\sigma_{ij})_{,k}. \tag{38}$$

The modified body forces and surface tractions are

$$\bar{b}_i = b_i - \frac{1}{2}h_{ij}b_{i,j} \text{ (no sum on } i), \quad \bar{t}_i^p = t_i^p + \frac{1}{2}h_{ij}n_j b_i, \text{ (no sum on } i). \tag{39}$$

It will be assumed that the modified stresses and strains are related by the relationship

$$\bar{\sigma}_{ij} = D_{ijkl}\,\bar{\varepsilon}_{kl} \tag{40}$$

in which D_{ijkl} are the constitutive moduli of linear elasticity [26].

The internal equilibrium equations in residual form are

$$r_i = \sigma_{ij,j} + b_i. \tag{41}$$

The FIC equilibrium equations are written compactly as

$$\bar{r}_i := r_i - \underline{\frac{1}{2}h_{ij}r_{i,j}} = 0. \tag{42}$$

The boundary conditions can be stated as

$$\begin{aligned} &\bar{\sigma}_{ij}n_j - \bar{t}_i^p = \sigma_{ij}n_j - t_i^p - \underline{\tfrac{1}{2}h_{ij}n_j r_i} = 0 \quad \text{on } \Gamma_t \quad \text{(no sum on } i), \\ &\bar{u}_i - u_i^p = 0 \quad \text{on } \Gamma_u. \end{aligned} \tag{43}$$

The underlined terms in Eqs. (42) and (43) are introduced by the FIC formulation. As expected if $h_{ij} \to 0$ the standard equations of infinitesimal linear elastostatic are recovered.

The TPE/FIC functional is written as

$$\Pi(\bar{u}_i) = U(\bar{u}_i) - W(\bar{u}_i) \tag{44}$$

with

$$U(\bar{u}_i) = \frac{1}{2}\int_\Omega \bar{\varepsilon}_{ij}\bar{\sigma}_{ij}d\Omega, \qquad W(\bar{u}_i) = \int_\Omega \bar{u}_i\bar{b}_i d\Omega + \int_{\Gamma_t} \bar{u}_i\bar{t}^p d\Gamma. \tag{45}$$

It can be verified that the first variation of $\Pi(\bar{u}_i)$ with respect to the modified displacements yields the FIC governing equations (42) and (43) as E-L equations and natural boundary conditions, respectively.

As in the case of the 1D problem, the first variation of the functional is equivalent to a weighted form of the original FIC equations with the following Petrov-Galerkin weighting functions

$$w_i := \delta\bar{u}_i = \delta u_i - \frac{1}{2}h_{ij}(\delta u_i)_{,j} \tag{46}$$

The resulting weak form expression can be written

$$\begin{aligned} &\int_\Omega \left(\delta u_i - \frac{1}{2}h_{ij}(\delta u_i)_{,j}\right)\left(r_i - \frac{1}{2}h_{ij}r_{i,j}\right)d\Omega - \\ &\int_{\Gamma_t} \left(\delta u_i - \frac{1}{2}h_{ij}(\delta u_i)_{,j}\right)\left(\sigma_{ij}n_j - t_i^p - \frac{1}{2}h_{ij}n_j r_i\right)d\Gamma = 0 \end{aligned} \tag{47}$$

The weak form (47) leads to a symmetric finite element formulation after discretization of the displacements and the virtual displacements with the same interpolating functions in the Galerkin manner.

5.2 Variational FIC Form for Diffusion-Reaction

The indicial convention of the previous subsection is followed. In two and three space dimensions, diffusion-reaction problems are still defined in terms of a primary scalar field $\phi(x_i)$, which may represent for example temperature, substance concentration, etc. The source production per unit volume is also a scalar field Q. The flux becomes a vector q_i, and normal flux across a surface of exterior normal n_i is $q_n = q_i n_i$. The residual balance equation is $r = (k\phi_{,i})_i - s\phi + Q$, where k and s are scalar coefficients that may depend on x_i. (This can be generalized to the anisotropic case by making k a second order tensor k_{ij}, but we consider only the isotropic case here.) The FIC steplength h generalizes to a vector h_i.

As usual we introduce modified non-local fields

$$\bar{\phi} = \phi - \frac{1}{2}h_j\phi_{,j}, \qquad \bar{Q} = Q - \frac{1}{2}h_j Q_{,j}, \qquad \bar{q}^p_n = q^p_n - \frac{1}{2}h_j n_j(Q - s\phi). \tag{48}$$

The modified residual is

$$\bar{r} := (k\bar{\phi}_{,i})_i - s\bar{\phi} + \bar{Q}. \tag{49}$$

With these, the FIC governing equations can be written compactly as

$$\bar{r} = 0 \quad \text{in} \quad \Omega, \qquad k\bar{\phi}_{,j}n_j + \bar{q}^p_n = 0 \quad \text{on} \quad \Gamma_q, \qquad \bar{\phi} - \phi^p = 0 \quad \text{on} \quad \Gamma_\phi. \tag{50}$$

All the terms in these equations have been previously defined except q^p_n, which is the prescribed flux normal to the Neuman boundary Γ_q.

The TPE functional is

$$\Pi(\bar{\phi}) = U(\bar{\phi}) - W(\bar{\phi}) \tag{51}$$

in which

$$U(\bar{\phi}) = \frac{1}{2}\int_\Omega \left[\bar{\phi}_{,i}k\bar{\phi}_{,i} + s\bar{\phi}^2\right] dx, \quad W(\bar{\phi}) = \int_\Omega \bar{\phi}Q d\Omega - \int_{\Gamma_q}\left(\bar{\phi}\bar{q}^p_n + \frac{1}{2}s\bar{\phi}^2\right) d\Gamma. \tag{52}$$

Setting the first variation of Π to zero gives the first two of (49) as the E-L equation and natural boundary condition, respectively. The expanded form of these two equations, as given in [9, 19, 20], are

$$r - \frac{1}{2}h_j r_{,j} = 0 \quad \text{in} \quad \Omega, \qquad k\phi_{,j}n_j + q^p_n - \frac{1}{2}h_j n_j r = 0 \quad \text{on} \quad \Gamma_q. \tag{53}$$

As in the case of multidimensional elasticity, we note that the first variation of Π is equivalent to the following Petrov-Galerkin weighted residual form of the original FIC equations

$$\begin{aligned} &\int_\Omega \left(\delta\phi - \frac{1}{2}h_j(\delta\phi)_{,j}\right)\left(r - \frac{1}{2}h_j r_{,j}\right) d\Omega \\ &- \int_{\Gamma_q}\left(\delta\phi - \frac{1}{2}h_j(\delta\phi)_{,j}\right)\left(k\phi_{,j}n_j + q^p_n - \frac{1}{2}h_j n_j r\right) d\Gamma = 0 \end{aligned} \tag{54}$$

Discretization of Eq. (54) by Galerkin methods leads to symmetric finite element equations.

5.3 Open Research Areas

The appropriate choice of a "FIC steplength tensor" h_{ij} in multidimensional elasticity is still open. Progress in the particular case of near-incompressible isotropic material has been made in [14, 15] using a simplification of the tensor FIC equations via a "FIC step length vector" $\mathbf{h} = [h_1, h_2, h_3]^T$ (for 3D). The selection of the h_i's on this case has been shown to be similar to that of choosing characteristic lengths in subgrid scale methods. Choosing the distances h_i in multidimensional scalar diffusion-reaction problem is simpler, as it can be linked to resolving boundary layers [6, 20]. Successful applications of the tensor form of the multidimensional FIC equations for incompressible fluid flow problems at high Reynolds numbers are reported in [20].

Another open problem is the question broached in Section 2.4: selection of nodal freedoms and interpolated variable when using a FIC variational formulation or a Galerkin weak form for FEM implementation. The choice is between the original primary variable (e.g., displacements in elasticity) and the modified one. The former has advantage of simpler implementation in existing FEM codes (particularly as regards application of essential BCs) whereas the latter opens up possibilities of linkage to discontinuous Galerkin methods as noted in Remark 4.

6 Conclusions

We have presented a variational formulation of the FIC equations for elastic solids, diffusion and diffusion-reaction problems. The total potential energy functional is expressed in terms of modified non-local variables. The variational form recovers the original governing equations of FIC theory, which can also be expressed in terms of the modified variables. The FEM discretization of the variational form leads to a symmetric system of equations. An equivalent weighted residual form of the original FIC equations using non-local weighting functions is identified. The FIC-FEM formulation presented has found to be analogous to a discontinuous Galerkin method.

These formulations are not intended to supersede but to complement the conventional FEM. In self-adjoint problems, stabilization is best reserved to cases when FEM (or conventional Galerkin) yields nonphysical results, as when sharp boundary layers occur at Dirichlet boundaries. For those cases it may useful to be able to inject FIC-based elements in certain regions while retaining ordinary elements elsewhere. Retaining matrix symmetry offers computational advantages when introducing FIC elements into existing codes. The variational and Galerkin formulations presented here may simplify that task.

These conclusions can be taken as the starting point for deriving new FIC-FEM formulations for convective transport, quasi/fully incompressible problems in solid and fluid mechanics and thick/thin beam, plate and shell elements [22] with enhanced stability properties.

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Appendix A. Derivation of 1D FIC Equilibrium Equation

To illustrate the steps of the FIC approach in some detail, we consider an elastostatic problem posed in a 1D domain Ω of length L. The equation of equilibrium of axial stresses in a subdomain of size d in Ω (Figure A.1) may be written as

$$\sigma_B - \sigma_A = 0. \tag{A.1}$$

where σ_A and σ_B are the stresses at end points A and B, respectively.

Next, express stresses σ_A and σ_B in terms of the stress at an arbitrary point C within the equilibrium domain (Figure A.1). This may be viewed as a control point. Expanding in Taylor series about C up to second order terms gives

$$\sigma_A = \sigma_C - d_1\sigma'_C + \frac{d_1^2}{2}\sigma''_C + O(d_1^3) \quad , \quad \sigma_B = \sigma_C + d_2\sigma'_C + \frac{d_2^2}{2} + \sigma''_C + O(d_2^3). \tag{A.2}$$

Substitution of Eqs.(A.2) into Eq.(A.1) gives, after simplification

$$\sigma' - \frac{h}{2}\sigma'' = 0, \tag{A.3}$$

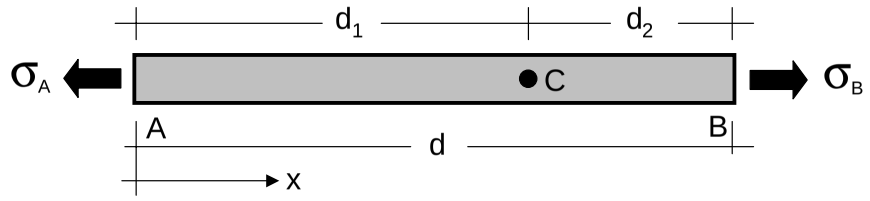

Figure A.1. Arbitrary domain of a bar subjected to axial stresses σ_A and σ_B at the ends

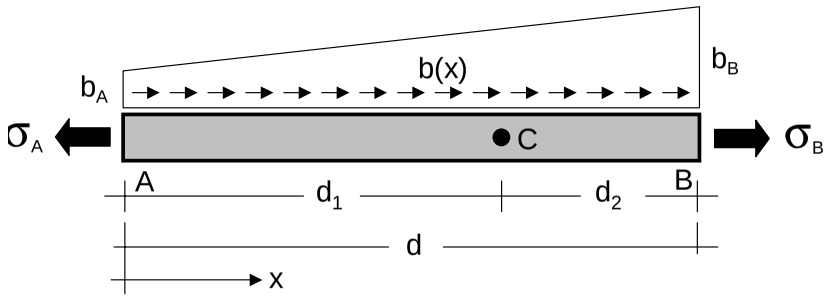

Figure A.2. Equilibrium of forces in a finite domain of a bar loaded with a distributed axial force $b(x)$

in which $h = d_1 - d_2$, and all the derivatives are computed at C.

Standard calculus assumes that the domain d is of infinitesimal size. Hence $h \to 0$ and the resulting infinitesimal equilibrium equation becomes $d\sigma/dx = \sigma' = 0$. We relax this assumption by allowing the equilibrium domain to have a *finite size*. The new equilibrium equation (A.3) incorporates now the underlined term that introduces the *characteristic distance* h. Obviously, accounting for higher order terms in Eq.(A.2) would lead to additional terms in Eq. (A.3) involving higher powers of h.

Eq.(A.3) is the *FIC equilibrium equation* (up to second order terms) for a 1D domain of finite size. The distance h in Eq.(A.3) can be interpreted as a free parameter depending on the dimension of the equilibrium domain and the dimensions of the subdomains d_1 and d_2 chosen about C. Note that $-d \leq h \leq d$ and, hence, h may take a negative value. In a node-based discretization process such as FEM or FVM, domain d should be replaced by a *balance domain* around each node. For a regular 1D discretization $-l^e \leq h \leq l^e$ where l^e is the element or cell dimension.

The method can be extended to account for a distributed axial load $b(x)$ (the source field), which is assumed to vary linearly between the end points of the equilibrium domain (Figure A.2). Note the difference with classical theory, in which case a uniform distribution of $b(x)$ over an infinitesimal domain is typically assumed since any variation disappears in the $h \to 0$ limit.

The equilibrium of axial forces is

$$\sigma_B - \sigma_A + \int_0^d b(x)dx = 0, \tag{A.4}$$

i.e.

$$\sigma_B - \sigma_A + \frac{b_A + b_B}{2} d = 0. \tag{A.5}$$

The end forces b_A and b_B are expressed in terms of their values at the arbitrary internal point C as

$$\begin{aligned} b_A &= b_C - d_1 b'_C + O(d_1^2), \\ b_B &= b_C - d_2 b'_C + O(d_2^2). \end{aligned} \tag{A.6}$$

Substitution of Eqs.(A.6) into (A.5) and use of Eqs.(A.2) gives upon simplifying

$$\sigma' + b - \frac{h}{2}(\sigma'' + b') = 0. \tag{A.7}$$

This is the FIC equilibrium equation for 1D elasticity used in Section 2.1; cf. Eq. (3).

Force equilibrium at a boundary segment (Figure A.3) of length $\frac{h}{2}$ where a prescribed traction t^p is applied requires

$$-\sigma_A + b\frac{h}{2} + t^p = 0. \tag{A.8}$$

Note that h is assumed to be positive in Eq.(A.8). The stress σ_A is expressed in terms of the value at the boundary point B by

$$\sigma_A = \sigma_B - \frac{h}{2}\sigma'_B. \tag{A.9}$$

Substitution of Eq.(A.9) into (A.8) gives, after reordering terms

$$\sigma - t^p - \frac{h}{2}(\sigma' + b) = 0, \tag{A.10}$$

or

$$\sigma - t^p - \frac{h}{2} r = 0, \tag{A.11}$$

This is the FIC equation for a prescribed traction boundary (natural boundary condition) used in Section 2.1; cf. Eq. (5).

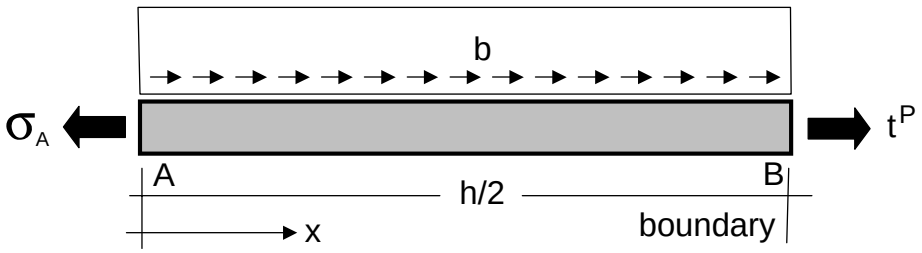

Figure A.3. Equilibrium of forces in a boundary domain of length $h/2$