Possibilities of Finite Calculus in Computational Mechanics

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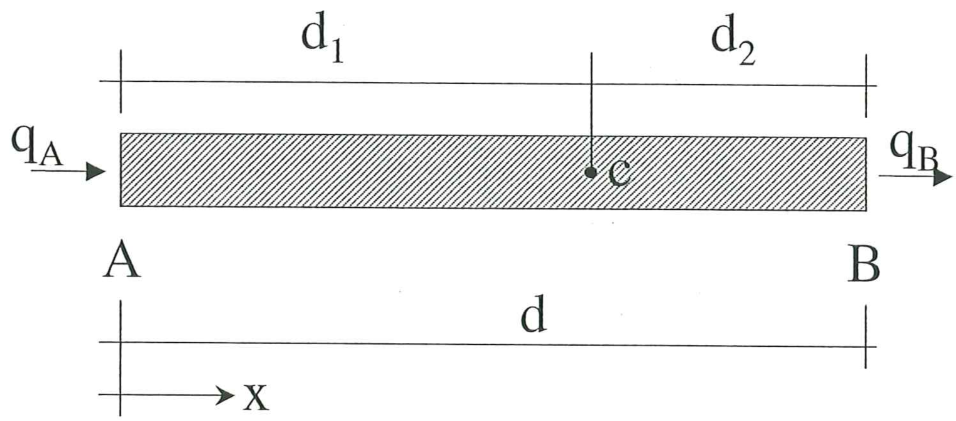

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POSSIBILITIES OF FINITE CALCULUS IN COMPUTATIONAL MECHANICS

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ABSTRACT

The expression "finite calculus" refers to the derivation of the governing differential equations in mechanics by invoking balance of fluxes, forces, etc. in a domain of finite size. The governing equations resulting from this approach are different from those of infinitessimal calculus theory and they incorporate new terms depending on the dimensions of the balance domain. The new modified equations allow to derive naturally stabilized numerical schemes using finite element, finite difference, finite volume or meshless methods. The paper briefly discusses the possibilities of the modified governing equations derived via the finite calculus technique for the numerical solution of convection-diffusion problems, incompressible flow and incompressible solid mechanic problems and strain localization problems.

KEYWORDS

Finite calculus, computational mechanics, finite element method, finite difference method, finite volume method, meshless method.

INTRODUCTION

It is well known that standard numerical methods such as the central finite difference (FD) method, the Galerkin finite element (FE) method and the finite volume (FV) method, among others lead to unstable numerical schemes when applied to problems involving different scales, multiple constraints and/or high gradients. Examples of these situations are typical in the solution of convection-diffusion problems, incompressible problems in fluid and solid mechanics and strain or strain rate localization problems in solids and compressible fluids using the Galerkin finite element method, the central difference scheme or the finite volume method (Zienkiewicz and Taylor (2000), Hirsch (1990)). Similar situations are found in the application of meshless methods to those problems (Oñate, Sacco and Idelsohn (2000)).

The sources of the numerical instabilities in finite element and finite difference methods, for instance, have been sought in the apparent unability of the standard Galerkin FE method and the analogous central difference method in FD, to provide a numerical scheme able to capture the different scales appearing in the numerical solution for all ranges of the physical parameters.

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Typical examples of these difficulties are the spurious numerical oscillations in convection-diffusion problems for high values of the convective terms. The same type of oscillations are found in the vecinity of sharp internal layers appearing in high speed compressible flows (shocks) or in strain localization problems (shear bands) in solids. A similar problem of different nature emerges in the solution of incompressible fluid or solid mechanic problems, where the difficulties in satisfying the incompressibility constraint limit the choices of the approximation for the velocitiy (or displacement) variables and the pressure (Zienkiewicz and Taylor (2000)).

The solution of above problems has been attempted in a number of ways. The underdiffusive character of the central difference scheme has been corrected in and ad-hoc manner by adding the so called "artificial diffusion" terms to the standard convection-diffusion equation. The same idea has been successfully applied to derive stabilized finite volume and finite element methods for convection-diffusion and fluid-flow problems. Other stabilized FD schemes are based on the "upwind" computation of the first derivatives appearing in the convective operator (Hirsch (1990)). The counterpart of upwind techniques in the FEM are the so called Petrov-Galerkin methods (Hughes, Hauke and Jansen (1994)), or the more general perturbed Galerkin methods (Codina (1998)) based on ad-hoc residual-based extensions of the Galerkin variational form so as to achieve a stabilized numerical scheme. Among the many methods of this kind we can name the SUPG method (Brooks and Hughes (1982), Hughes and Mallet (1986a), Hansbo and Szepessy (1990), Cruchaga and Oñate (1999)), the Galerkin Least Square (GLS) method (Hughes, Franca and Hulbert (1989), Tezduyar *et al.* (1992)), the Characteristic Galerkin method (Zienkiewicz and Codina (1995) and the Subgrid Scale (SS) method (Hughes (1995), Brezzi, Franca and Hughes (1995)).

In this paper we propose a different route to derive stabilized numerical methods. The starting point are the modified governing differential equations of the problem derived using a finite calculus (FIC) approach. The FIC method is based in invoking the balance of fluxes (or forces) in a domain of finite size. This introduces naturally additional terms in the classical differential equations of infinitessimal theory which are a function of the balance domain dimensions. The merit of the modified equations via the FIC approach is that they lead to stabilized schemes using *any* numerical method. In addition, the different stabilized FD, FE and FV methods typically used in practice can be *recovered* using the new modified equations. Moreover, the FIC equations are the basis for deriving an iterative procedure for computing the stabilization parameters.

The layout of the paper is the following. In the next section, the main concepts of the FIC method are introduced. Applications of the FIC method to convection-diffusion and fluid flow problems are briefly explained next. Finally the possibilities of the FIC method in solid mechanics are discussed.

THE FINITE CALCULUS METHOD

We will consider a convection-diffusion problem in a 1D domain Ω of length L. The equation of balance of fluxes in a subdomain of size d belonging to Ω (Figure 1) is written as

$$q_A - q_B = 0 \tag{1}$$

where q_A and q_B are the incoming and outgoing fluxes at points A and B, respectively. The flux q includes both convective and diffusive terms; i.e. $q = -v\phi + k\frac{d\phi}{dx}$, where ϕ is the transported variable, v is the velocity and k is the diffusivity of the material.

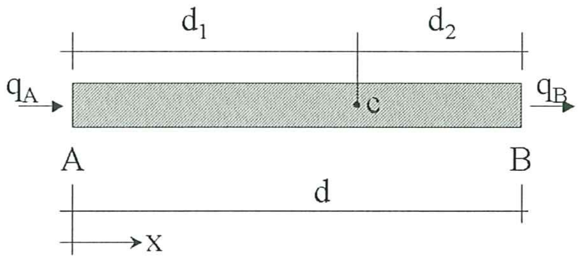

Figure 1. Equilibrium of fluxes in a balance domain of finite size

Let us express now the fluxes q_A and q_B in terms of the flux at an arbitrary point C within the balance domain (Figure 1). Expanding q_A and q_B in Taylor series around point C up to second order terms gives

$$q_A = q_C - d_1 \frac{dq}{dx}|_C + \frac{d_1^2}{2}\frac{d^2q}{dx^2}|_C + O(d_1^3) \quad , \quad q_B = q_C + d_2 \frac{dq}{dx}|_C + \frac{d_2^2}{2}\frac{d^2q}{dx^2}|_C + O(d_2^3) \tag{2}$$

Substituting eq.(2) into eq.(1) gives after simplification

$$\frac{dq}{dx} - \underline{\frac{h}{2}\frac{d^2q}{dx^2}} = 0 \tag{3}$$

where $h = d_1 - d_2$ and all derivatives are computed at point C.

Standard calculus theory assumes that the domain d is of infinitessimal size and the resulting balance equation is simple $\frac{dq}{dx} = 0$. We will relax this assumption and allow the balance domain to have a *finite size*. The new balance equation (3) incorporates now the underlined term which introduces the *characteristic length* h. Obviously, accounting for higher order terms in eq.(2) would lead to new terms in eq.(3) involving higher powers of h.

Distance h in eq.(3) can be interpreted as a free parameter depending, of course, on the location of point C (note that $h = 0$ for $d_1 = d_2$). However, the fact that eq.(3) is the exact balance equation (up to second order terms) for any 1D domain of finite size and that the position of point C is arbitrary, can be used to derive numerical schemes with enhanced properties simply by computing the characteristic length parameter from an adequate "optimality" rule.

Consider, for instance, the modified equation (3) applied to the convection-diffusion problem. Neglecting third order derivatives of ϕ, eq.(3) can be written in an explicit form as

$$-v\frac{d\phi}{dx} + \left(k + \frac{vh}{2}\right)\frac{d^2\phi}{dx^2} = 0 \tag{4}$$

We see clearly that the modified equation via the FIC method introduces *naturally* an additional diffusion term into the standard convection-diffusion equation. This is the basis of the popular "artificial diffusion" procedure (Brooks and Hughes (1982), Hirsh (1990), Zienkiewicz and Taylor (2000)). The characteristic length h is typically expressed as a function of the cell or element dimensions. The optimal or critical value of h for each cell or element can be computed from numerical stability conditions such as obtaining a physically meaningful solution, or even obtaining "exact" nodal values (Zienkiewicz and Taylor (2000)).

GENERAL FIC EQUATION FOR CONVECTIVE-DIFFUSIVE PROBLEMS

Application of the FIC procedure to a general multidimensional convective-diffusive problem leads to the following governing equations (Oñate (1998))

$$r - \underline{\frac{1}{2}\mathbf{h}^T \boldsymbol{\nabla} r} = 0 \qquad \text{in } \Omega \tag{5}$$

with boundary conditions

$$\phi - \bar{\phi} = 0 \qquad \text{on } \Gamma_\phi \tag{6a}$$

$$\mathbf{n}^T \mathbf{D} \boldsymbol{\nabla} \phi + \bar{q}_n - \underline{\frac{1}{2}\mathbf{h}^T \mathbf{n} r} = 0 \qquad \text{on } \Gamma_q \tag{6b}$$

where Γ_ϕ and Γ_q are the Dirichlet and Neumann boundaries where the variable ϕ and the normal flux are prescribed to values $\bar{\phi}$ and $\bar{q}_n$, respectively. In above equations

$$r := -\left[\frac{\partial \phi}{\partial t} + \mathbf{v}^T \boldsymbol{\nabla} \phi\right] + \boldsymbol{\nabla}^T \mathbf{D} \boldsymbol{\nabla} \phi + Q \tag{7}$$

where $\mathbf{v}$ is the velocity vector, $\mathbf{D}$ is the diffusivity matrix, $\boldsymbol{\nabla}$ is the gradient operator and Q is the external source term. Vector $\mathbf{h}$ in eqs.(5) and (6b) is the *characteristic length* vector. For 2D problems $\mathbf{h} = [h_x, h_y]^T$, where h_x and h_y are characteristic distances along the sides of the rectangular domain where balance of fluxes is enforced (Oñate (1998)).

The modified equation (6b) is obtained by invoking balance of fluxes in a finite domain next to the Neumann boundary (Oñate (1998)). The underlined terms in eqs.(5) and (6b) introduce the necessary stabilization in the numerical solution using FD, FE, FV and meshless methods (Oñate and Manzan (2000)).

Equivalence with the SUPG method

A finite element interpolation of the unknown can be written as

$$\phi \simeq \hat{\phi} = \sum N_i \hat{\phi}_i \tag{8}$$

where N_i are the shape functions and $\hat{\phi}_i$ are the nodal values of the approximate function $\hat{\phi}$ (Zienkiewicz and Taylor (2000)).

Application of the Galerkin FE method to eqs.(5)-(6) leads, after integration by parts of the term involving $\boldsymbol{\nabla} r$, to

$$\int_\Omega N_i \hat{r} d\Omega - \int_{\Gamma_q} N_i (\mathbf{n}^T \mathbf{D} \boldsymbol{\nabla} \hat{\phi} + \bar{q}_n) + \sum_e \frac{1}{2} \int_{\Omega^e} \mathbf{h}^T \boldsymbol{\nabla} N_i \hat{r} d\Omega = 0 \tag{9}$$

The last integral in eq.(9) has been expressed as a sum of the element contributions to allow for interelement discontinuities in the term $\boldsymbol{\nabla} \hat{r}$, where $\hat{r} = r(\hat{\phi})$.

We could further assume that the direction of the characteristic vector $\mathbf{h}$ is *parallel* to that of the velocity $\mathbf{v}$, i.e. $\mathbf{h} = h\frac{\mathbf{v}}{|\mathbf{v}|}$ where h is a characteristic length. Further, vector $\mathbf{v}$ and the velocity module can be taken as constants within each element. Under these conditions, eq.(9) reads

$$\int_\Omega N_i \hat{r} d\Omega - \int_{\Gamma_q} N_i (\mathbf{n}^T \mathbf{D} \boldsymbol{\nabla} \hat{\phi} + \bar{q}_n) d\Omega + \sum_e \frac{h^{(e)}}{2|\mathbf{v}|} \int_{\Omega^e} \mathbf{v}^T \boldsymbol{\nabla} N_i \hat{r} d\Omega = 0 \tag{10}$$

Eq.(10) coincides precisely with the so called Streamline-Upwind-Petrov-Galerkin (SUPG) method. The ratio $\frac{h^{(e)}}{2|\mathbf{v}|}$ has dimensions of time and it is usually termed element *intrinsic time* parameter $\tau^{(e)}$. The element characteristic length $h^{(e)}$ is taken in practice as an average element dimension (e.g. $h^{(e)} = [\Omega^{(e)}]^{1/2}$ for 2D problems).

It is important to note that the SUPG expression is a *particular case* of the more general FIC formulation. This explains the limitations of the SUPG method to provide stabilized numerical results in the vecinity of high gradients of the solution transverse to the flow direction (Zienkiewicz and Taylor (2000)). In general, the direction of $\mathbf{h}$ is not coincident with that of $\mathbf{v}$ and the components of $\mathbf{h}$ introduce the necessary stabilization along the streamline and transverse directions to the flow. Therefore, the FIC method reproduces the best-features of the so-called stabilized discontinuity-capturing schemes (Hughes and Mallet (1986b), Codina (1993)).

TIME STABILIZATION USING THE FIC METHOD

Application of the FIC method to a space-time slab domain of finite size leads to the following modified governing equation for the convective-diffusive problem

$$r - \frac{1}{2}\mathbf{h}^T \nabla r - \frac{\delta}{2}\frac{\partial r}{\partial t} = 0 \tag{11}$$

where r is given by eq.(7), $\mathbf{h}$ is the characteristic length vector and δ is a time stabilization parameter.

Eq.(11) can be used to derive a number of stabilized space-time integration schemes. A recent application of the FIC method to the FE analysis of transient convective-diffusive problems can be found in Oñate and Manzan (1999).

THE FIC METHOD IN INCOMPRESSIBLE VISCOUS FLUID MECHANICS

The FIC method can be applied to derive the modified equations of momentum and mass conservation in fluid mechanics. The resulting equations for an incompressible viscous flow are

Momentum

$$r_i - \underline{\frac{h_j}{2}\frac{\partial r_i}{\partial x_j}} - \underline{\frac{\delta}{2}\frac{\partial r_i}{\partial t}} = 0 \tag{12}$$

Mass balance

$$r_d - \underline{\frac{h_j}{2}\frac{\partial r_d}{\partial x_j}} = 0 \tag{13}$$

with

$$r_i := \frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} - b_i \quad , \quad r_d := \frac{\partial v_i}{\partial x_i} \tag{14}$$

In eq.(14) v_i are the velocities, p is the pressure, τ_{ij} the viscous stresses and b_i the body forces with $i, j = 1, 2, 3$ for 3D problems. As usual, h_j and δ are the characteristic lengths and the time stabilization parameters, respectively.

Eqs.(12) and (13) are completed with the adequate boundary conditions. Once more the FIC approach introduces additional stabilization terms in the momentum and mass balance equations and the Neumann boundary conditions similar to that appearing in eqs.(5) and (6b). For details see Oñate (1998).

The underlined stabilization terms in the momentum equations (12) account for the instabilities due to high convection effects. The underlined term in eq.(13) introduces a pseudo-compressibility effect in the mass balance equation. This term is essential to allow for equal order FE interpolations of the velocities and pressure. Application of the FIC method to the FE solution of the incompressible Navier-Stokes equations acounting for free surface waves using linear triangles and tetraedra can be found in Oñate and García (1999a,b) and (2000). Extensions of the FIC method to the compressible flow equations can be found in Oñate (1998).

Similar governing equations to that found using the FIC method have been derived by Ilinca, Hétu and Pelletier (2000) for incompressible advective-diffusive and fluid flow problems by expanding in Taylor series the residuals of the original FE equations. Analogous modified equations for compressible gas flow problems have been obtained by Chetveruskin (2000) using discrete Boltzman schemes. The general modified equations provided by the FIC method, based on simple physical concepts of balance of fluxes and forces over a finite size domain, reproduce the particular forms of the governing differential equations obtained by these authors.

The FIC method has been recently classified by Felippa (2001) as a particular case of "modified equations" methods where the standard differential equations are first augmented using physical concepts and then discretized using any numerical technique.

POSSIBILITIES OF THE FIC METHOD IN SOLID MECHANICS

Application of the FIC method to the force equilibrium equations in solid mechanics leads to the following modified governing equations (for the steady state case)

$$r_i - \underline{\frac{h_j}{2}\frac{\partial r_i}{\partial x_j}} = 0 \qquad i,j = 1,2,3 \text{ for 3D} \tag{15}$$

with

$$r_i := \frac{\partial \sigma_{ij}}{\partial x_j} + b_i \tag{16}$$

where σ_{ij} are the stresses and b_i the body forces. The underlined term in eq.(15) results from the FIC assumptions and, as usual, h_j are the characteristic length parameters. Eq.(15) is completed with the adequate boundary conditions. Note that, for consistency, the Neumann boundary conditions must incorporates an aditional stabilization term similar to that of eq.(6b) (Oñate *et al.* (2001)).

The FIC approach can also be applied to derive a modified equation relating the pressure and the volumetric strain change over a finite size domain as

$$p = K\left[\varepsilon_v - \frac{h_j}{2}\frac{\partial \varepsilon_v}{\partial x_j}\right] \tag{17}$$

where K is the volumetric elastic modulus, $\varepsilon_v = \frac{\partial u_i}{\partial x_i}$ and u_i are the displacements. Note that for an incompressible material $K \to \infty$ and in this case eq.(17) recovers a form analogous to that of the stabilized mass balance equation in fluid mechanics (see eq.(13)).

Eqs.(15) and (17) with the adequate boundary conditions are the basis for deriving stabilized FE formulations for quasi-incompressible and full incompressible solids allowing for equal order interpolations of the displacement and pressure variables. A recent application of the FIC method to the non linear explicit dynamic analysis of solids using linear triangles and tetrahedra can be found in Oñate *et al.* (2001).

It is interesting to note that the FIC method introduces naturally higher order derivative terms of the displacements in the equilibrium equations. These terms resemble those introduced by the Cosserat model (Peric, Yu and Owen (1994)) and the so called "non local" constitutive models (de Borst (1992)). These models are typically used in order to preserve the ellipticity of the solid mechanics equations in the presence of localized high displacement gradient zones such as shear bands and fracture lines. This opens a world of possibilities for the modified governing equations derived via the FIC method to analyze strain localization problems in solid mechanics.

COMPUTATION OF THE STABILIZATION PARAMETERS

Accurate evaluation of the stabilization parameters is one of the crucial issues in stabilized methods. Most of the existing methods use expressions which are direct extensions of the values obtained for the simplest 1D case. As already mentioned, it is also usual to accept the so called SUPG assumption, i.e. to admit that vector $\mathbf{h}$ has the direction of the velocity field (Oñate (1998), Oñate and Manzan (2000)). This unnecessary restriction leads to instabilities when sharp layers transversal to the velocity direction are present. This deficiency of the SUPG assumption is usually corrected in the FEM by adding a shock capturing or crosswind stabilization term (Hughes and Mallet (1986b), Codina (1993)).

The FIC method does not suffer from these restrictions and the components of $\mathbf{h}$ introduce the necessary stabilization along both the streamline and transversal directions to the flow .

Excellent results have been obtained in convective-diffusive problems solved using linear triangle and tetrahedra with the value of the characteristic length vector given by (Oñate and Manzan (2000))

$$\mathbf{h} = h_s \frac{\mathbf{u}}{|\mathbf{u}|} + h_c \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|} \tag{18}$$

where h_s and h_c are the "streamline" and "cross wind" characteristic length given by

$$h_s = \max(\mathbf{l}_j^T \mathbf{u})/|\mathbf{u}| \quad , \quad h_c = \max(\mathbf{l}_j^T \boldsymbol{\nabla}\phi)/|\boldsymbol{\nabla}\phi| \quad , \quad j = 1, n_s \tag{19}$$

where $\mathbf{l}_j$ are the vectors defining the element sides ($n_s = 6$ for tetrahedra).

Note that the cross-wind term in eq.(18) accounts for the effect of the gradient of the solution in the stabilization parameters. This is a standard assumption in most "shock-capturing" stabilization procedures (Hughes and Mallet (1986b), Codina (1993)).

An alternative method for computing vector $\mathbf{h}$ in a more consistent manner using a *diminishing residual* technique is explained below.

Regarding the time stabilization parameters δ in eqs.(11) and (12) the value $\delta = \Delta t$ was taken for solution of the problems presented in Oñate and García (2000). A more consistent evaluation following the diminishing residual technique is described in Oñate and Manzan (1999) and (2000) for transient advective-diffusive problems.

Computation of the characteristic length vector using a diminishing residual technique

The idea of this technique first presented in Oñate (1997) and tested in Oñate (1998), Oñate, García and Idelsohn (1998) and Oñate and Manzan (1999), (2000) for advective-diffusive problems is the following. Let us assume that a finite element solution for a fluid mechanics problem has been found for a given mesh. The point wise residual of the momentum equation corresponding to this particular solution is (assuming $\delta = 0$ in eq.(12))

$$ {}^1r_i = r_i - \frac{1}{2} h_j \frac{\partial r_i}{\partial x_j} \tag{20} $$

The average residual over an element can be defined as

$$ {}^1r_i^{(e)} = \frac{1}{\Omega^{(e)}} \int_{\Omega^{(e)}} {}^1r_i d\Omega \tag{21} $$

Let us assume now that an *enhanced* numerical solution has been found for the same mesh and the same approximation (i.e., neither the number of elements nor the element type have been changed). The enhanced solution could be based, for instance, in a superconvergent recovery of derivatives (Wiberg, Abdulwahab and Li (1997), Zienkiewicz and Taylor (2000)). The element residual for the enhanced solution is denoted by ${}^2r_i^{(e)}$. The element residuals must obviously tend to zero as the solution improves and the following condition must be satisfied

$$ {}^1r_i^{(e)} - {}^2r_i^{(e)} \geq 0 \tag{22} $$

Above diminishing residual condition applies for ${}^1r_i^{(e)} > 0$. Clearly for ${}^1r_i^{(e)} < 0$ the inequality in eq.(22) should be changed to ≤ 0. Substituting eq.(20) into (22) and applying the identity condition in eq.(22) gives the following system of equations for each element which unknowns are the characteristic length parameters for the element

$$ \mathbf{A}\mathbf{h}^{(e)} = \mathbf{f} \tag{23} $$

with

$$ A_{ij} = 2 \left[\frac{{}^2\partial r_i^{(e)}}{\partial x_j} - \frac{{}^1\partial r_i^{(e)}}{\partial x_j} \right] \quad , \quad f_i = {}^2r_i^{(e)} - {}^1r_i^{(e)} \tag{24} $$

The following “adaptive” algorithm can be proposed for obtaining a stabilized solution in fluid mechanics problems:

1. Solve for the numerical values of the nodal velocities and the pressure. This solution is found by choosing an initial value $\mathbf{h}^{(e)} = {}^o\mathbf{h}^{(e)}$.
2. Compute ${}^1r_i^{(e)}$.
3. Evaluate the enhanced velocity and pressure fields. Compute ${}^2r_i^{(e)}$.
4. Compute the updated value of $\mathbf{h}^{(e)}$ solving eq.(23).
5. Repeat steps (1)–(4) until a stable solution is found.

The above strategy can be naturally incorporated into a transient solution scheme by simply updating the value of $\mathbf{h}^{(e)}$ after the solution for each time step has been found (Oñate and Manzan (1999), (2000)). A similar procedure can be followed to compute the characteristic length vector in solid mechanics problems.

CONCLUSIONS

The paper has briefly discussed the possibilities of the finite calculus (FIC) method for obtaining modified governing equations in mechanics with intrinsic advantages for the numerical analysis of convective-diffusive transport, fluid flow and structural problems. Starting with the modified equations many of the well known stabilized FE, FD and FV methods can be reproduced and new stabilized numerical methods can be found. In addition, the FIC equations can be used to derive an iterative scheme for computing the stabilization parameters. In summary, the FIC method opens many possibilities for deriving new numerical methods for the steady state and transient solution of problems in mechanics. Some topics which require further research include the application of the FIC method for capturing strain localization bands in solids or shocks waves in compressible flows, and the advantages of accounting for even higher order terms in the FIC equations in order to model large zones with high gradients of the solution, such as it occurs in turbulent flow situations.

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