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A stabilization approach for mesh-free simulations of systems developing shocks or extreme strain localizations

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ABSTRACT

A new stabilization scheme, based on a stochastic representation of the discretized field variables, is proposed with a view to reduce or even eliminate unphysical oscillations in the mesh-free numerical simulations of systems developing shocks or exhibiting localized bands of extreme deformation in the response. The origin of the stabilization scheme may be traced to nonlinear stochastic filtering and, consistent with a class of such filters, gain-based additive correction terms are applied to the simulated solution of the system, herein achieved through the element-free Galerkin method, in order to impose a set of constraints that help arresting the spurious oscillations. The method is numerically illustrated through its applications to inviscid Burgers' equations, wherein shocks may develop as a result of intersections of the characteristics, and to a gradient plasticity model whose response is often characterized by a developing shear band as the external load is gradually increased. The potential of the method in stabilized yet accurate numerical simulations of such systems involving extreme gradient variations in the response is thus brought forth.

1. Introduction

Robust stabilization approaches are often needed in the numerical simulations of systems whose response may contain sharp layers of extreme gradient variations, as evidenced, for instance, in cases that involve propagating an evolving shock. Yet another case, of considerable significance in computational solid mechanics, is that of gradient plasticity models whose numerical solutions may contain such sharp layers that correspond to highly localized deformation zones (e.g. shear bands). The need for stabilization in all these cases is mainly owing to spurious oscillations in the computed response profiles within or around such layers that mainly occur due to an inadequate numerical resolution of the fine-scaled response variations. In the context of a gradient plasticity model, for instance, the spuriously wiggly nature of the computed stress profiles is often ascribed to the weak formulation (i.e. the discretized weighted residual) that fails to enforce the rate form of the yield condition in a point-wise manner. A possible way to obtain a relatively more locally monotone (i.e. less oscillatory) solution could be diffuse or 'smear out' the steep gradients enabling the numerical method to avoid over- and undershoots. Indeed, except for the extreme cases of shocks with strict discontinuities, many of such apparent jumps in the response may be locally approximated through higher order polynomials or Taylor series expansions whilst retaining many terms. An implication of the above observation is that mesh-free methods [1], using higher order globally smooth shape functions, should be the preferred choice vis-à-vis their mesh-based counterparts, e.g. the finite element method (FEM), enabling substantively lower order smoothness (typically C^0 continuity) in the approximation. Many such mesh-free or smooth discretization methods have of late been developed and numerically explored; see [2–7]. Unfortunately, higher smoothness in mesh-free methods, beyond a certain order, is often achieved at the cost of deteriorating quality of the functional approximation, thereby still necessitating additional stabilization schemes for most such problems of practical interest.

In fluid dynamics, the appearance of an advection term (non self-adjoint operator) is common in the governing partial differential equation (PDE). Here, a Bubnov–Galerkin weak formulation where the test and shape functions are chosen from the same approximation space leads to spurious oscillations in the solution [8]. Large Peclet and Reynolds numbers that indicate the strength of the convection terms further worsen the situation. Adding an artificial diffusive term in the original PDE, as in the case of upwind differencing in the finite difference method (FDM), leads to results that are non-oscillatory but also inaccurate; a problem

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that can be solved by a correct choice of the artificial diffusion [8]. Similar strategies, adapted to the FEM, have led to streamline upwind schemes where the addition of the artificial diffusion term in the streamline direction gives nodally exact solution for the 1-D case, but leads to inconsistency issues [9]. In the non-symmetric Petrov–Galerkin (PG) FEM, the test function is chosen different from the shape function and has been used to weigh disproportionately the upwind and downstream nodes [10,11]. Even though nodally exact solutions result in the FEM formulations described above, their generalization to multidimensional systems is fraught with troubles. Satisfaction of consistency with the weak form vis-à-vis the exact solution and extension to multi-dimensional cases of convection-dominated problems have been introduced in [8,12] as the streamline-upwind Petrov–Galerkin (SUPG) method. Further progresses with the SUPG may be traced in [13–17]. The Galerkin least squares (GLS) method, developed subsequently, has provided further improvements in the stabilized solutions [18]. Despite being widely used, the SUPG and GLS schemes both employ stabilization parameters that are often chosen in a problem- and discretization-specific, if not entirely ad-hoc, manner. Given that numerical pollution is typically restricted within or about the sharp gradient layers, which are localized in the domain of interest, a measure of the solution gradient is exploited in these cases to get a monotone response. The Godunov theorem [19] has prompted explorations of gradient limiting non-linear schemes as the theorem puts restrictions on linear schemes for achieving monotone solutions. The total variation diminishing (TVD) methodology used in the finite volume method (FVM) and the FDM represents such a class of methods [19]. If the weight function is made dependent on the solution gradient then the non-linearity thus introduced results in a monotone PG FEM scheme [20]. The discontinuous Galerkin FEM [21] has also been prominently used in the simulation of response profiles with sharp gradients.

Another source of unphysical oscillations in computational solid mechanics is due to the phenomenon of locking, wherein numerical disturbances in the computed solution arises when a particular system or model parameter approaches its limiting value (e.g. thickness to zero, Poisson's ratio to 0.5 etc.) [22]. Given the impracticability of very fine discretization levels to tackle this degeneracy, various robust methods, including a family of mixed formulations, are available in the literature [23–26]. In the context of mixed FEM, primary stability considerations include K-ellipticity and the Babŭska–Brezzi (BB) conditions [27,28]. The former is concerned with the coercivity of the bilinear form and the latter with the interpolation order of the different variables in the mixed formulation. Apart from utilizing the BB condition, the bilinear form can be stabilized by modifying it with suitable perturbation terms whilst maintaining consistency [29–31]. The pressure stabilizing Petrov–Galerkin (PSPG) method is one such scheme used for the incompressible Navier–Stokes equation [32]. An excellent review of the various stabilization techniques mentioned above along with an in-depth discussion on various aspects of stabilization can be found in [33].

The stabilization scheme proposed in this work is somewhat unconventional in that it draws motivation from the concept of nonlinear stochastic filtering, wherein the aim is typically to arrive at (estimate) the system states such that, modulo the measurement noise, the computed states 'match' with the available measurements on a subset of such states. A generalization of this idea, which herein leads to a stabilization approach for deterministically posed problems, is based on the observation that the noisy measurements in stochastic filtering may be thought of as constraints on the computed system states. Thus, as a first step in treating a more general class of constraints appearing in problems of interest here, a stochastic framework is established wherein the discretized system variables (e.g. the nodal unknowns in a mesh-free method) appear as Markov stochastic processes following an artificial introduction of Brownian noise vectors that may be interpreted as a set of regularizers. Considering a deterministically posed equality constraint in the next step (assuming, without a loss of generality, that the right hand side of the equality evaluates to zero), it is treated as a stochastic process referred to as the 'innovation' process in the current setting, wherein the constraint is deemed to have been imposed when it is driven to a zero-mean Brownian motion process. Thus, in the limit of the variance of the last Brownian motion going to zero, the constraint may be considered to have been enforced deterministically. By way of driving the innovation process to a zero-mean Brownian motion, a gain-based additive correction term is iteratively applied to the deterministic (and possibly numerically polluted) solution of the system, computed via a mesh-free method in this work. The constraint, on the other hand, may be chosen in a problem-specific yet non-unique manner so as to realize the end objective of reduced numerical pollution especially in the sharp gradient layers. The numerical work, reported on simulations of evolving shocks in a 1-D and 2-D Burgers' equation and those of shear band formations in a gradient plasticity model, helps characterize the robustness and efficacy of the proposed method as a powerful stabilization tool.

The rest of the paper is organized as follows. Section 2 describes the proposed stochastic stabilization scheme in the general context of mesh-free discretization of a given system model and provides a step-by-step implementation of the methodology using a pseudo-code. Stabilized simulations of shocks in the solutions of 1D and 2D Burgers' equations are considered in Section 3. Section 4 implements the same strategy, albeit with modifications in the constraint function, for stress stabilization in the simulation of a strain gradient plasticity model. Finally, the concluding remarks are furnished in Section 5.

2. Mesh-free discretization and stabilization based on a pseudo-stochastic approach

Mesh-free methods are superior to FE techniques in several respects. For instance, mesh-free shape functions may be constructed with arbitrary global continuity, thereby bypassing the need for mixed formulations. As the name suggests, the domain discretization or costly meshing is replaced with comparatively simpler scattering of particles in the domain. Thus the problem of remeshing or mesh refinement does not arise and the density of particles can be modified or varied in a relatively straightforward manner. Further, convergence characteristics of mesh-free methods are superior compared to mesh-based implementations for the same order of consistency. The disadvantages vis-à-vis the FEM include failure to satisfy the Kronecker-delta property with the attendant difficulty in enforcing Dirichlet boundary conditions [34]. Moreover, derivations of mesh-free shape functions are not as straightforward as their mesh-based counterparts, each mesh-free variant having its own technique. Finally, the computational effort expended in deriving the shape functions and inverting the post-discretized system matrices, which have relatively higher bandwidth vis-à-vis those in the FEM, is higher with mesh-free methods. Further details on such issues and other aspects of mesh-free methods are available in [1,35–39].

2.1. Element-free Galerkin (EFG) method

In the present work, EFG shape functions are consistently used for functional discretization. It may be stressed as this point that the EFG method forms part of a deterministic approach in constructing the numerical solutions of PDEs. A brief account of