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The point collocation method with a local maximum entropy approach

Lei Fan *, William M. Coombs, Charles E. Augarde

Department of Engineering, Durham University, Lower Mountjoy, South Road, Durham DH1 3LE, UK

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ABSTRACT

Meshless methods have long been a topic of interest in computational modelling in solid mechanics and are broadly divided into weak and strong form-based approaches. The need for numerical integration in the former remains a challenge often met by using a background mesh or complex stabilised nodal approaches. It is only strong form-based point collocation methods (PCMs) which dispense with meshing and integration entirely, and for this reason PCMs remain of interest. In this paper, a new point collocation method is developed which is based on maximum entropy basis functions which bring benefits in terms of accuracy and efficiency. These basis functions possess non-negativity and a weak Kronecker delta property which decreases the errors on boundaries to improve overall accuracy of solutions. After a discussion of implementation issues in the new method, numerical examples are presented, including 1D and 2D problems with linear elasticity and Poisson PDEs, on both convex and non-convex domains to show the performance. Comparisons of convergence properties with respect to accuracy and computational cost (both CPU time and floating point operations) are made with an existing method, the reproducing kernel collocation method (RKCM), to show the effectiveness of the proposed method. In all examples, higher order convergence rates are obtained using the developed method with increasingly reduced computational effort for higher levels of accuracy due to the fundamental advantages.

1. Introduction

Computational solid mechanics has been dominated by methods based on weak forms for decades, the prime examples being the finite element method (FEM) and the boundary element method (BEM). Many of the difficulties met in using these weak form methods relate to the need for the problem domain to be discretized into a mesh; the generation of the mesh may itself be a major computational problem in 3D, while the performance of a mesh during a non-linear analysis can deteriorate due to distortion. Meshless weak form-based methods, developed since the 1990s, have been seen as a potential solution to this problem (for a comprehensive review, refer to [1]) and include the element-free Galerkin method (EFGM) [2,3], the Meshless Local Petrov-Galerkin method [4] and reproducing kernel particle methods (RKPMs) [5]. These weak-form based meshless methods have been successfully used to model problems involving large deformations [6], crack propagation [7–10] and non-linear materials [11,12]. Despite many positive aspects such as improved accuracy, weak-form based meshless methods have yet to rival finite elements in commercial codes largely due to their computational cost. In addition, some meshless methods have been criticised for not actually being truly meshless as a background grid is needed for integration. To counter this criticism, direct nodal integration has been developed (e.g. [13]) and some initial issues with instability and low accuracy have been addressed, such as in the stabilized conforming approach in [14].

Strong form-based meshless methods based on point collocation offer the possibility of mesh-free methods with low computational cost and have in the past been labelled as "truly meshless" [15–19]. They are straightforward to implement and remove entirely the complexities associated with domain integration [20,21]. These methods discretize a problem domain into collocation (or "data") points at which the PDE is approximated using basis functions associated with a different set of points (the source points or "centres"). Boundary conditions are imposed directly on boundary points and a linear system is derived in which the field variable values at source points are the initial solution. An early example of this type of method is due to Kansa [15,16] who employed radial basis functions (multiquadrics) and in later work, a radial basis collocation method was used to solve singularity [22], and higher order problems [23]. More recently, other meshless collocation methods have been proposed such as schemes with the moving least squares basis for solutions to the incompressible Navier-Stokes (NS) equations in the velocity-pressure formulation

* Corresponding author.
E-mail address: lei.fan@durham.ac.uk (L. Fan).

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[24]. This standard collocation meshless solver has been improved to address laminar flow problems and multiple complex-geometry problems in 2D [25]. However, the condition number of the discrete system formed using radial basis function-based collocation was found to be large and additional approaches [26] have been developed to address this ill-conditioning problem. Alternative strong form collocation frameworks have been used to solve problems defined by PDEs using basis functions obtained by the reproducing kernel approximation [27], where the method is generally referred to as the reproducing kernel collocation method (RKCM). RK-based methods automatically satisfy consistency requirements (similar to completeness in finite elements) assuring algebraic convergence rates [28,29]. While isogeometric methods are usually associated with finite elements, they have made an appearance in collocation methods, first in [30], the aim being to exploit the smoothness properties of NURBS-based basis functions. Different methods are proposed for the generation of optimal locations for collocation points in these methods in [31] and the computational efficiency of these methods is compared with Galerkin methods in [32].

It is important to note that in strong form point collocation methods (PCMs), higher derivatives of the basis functions are required than would typically be the case, for the same problem, in a weak form-based method such as the EFGM. Although approximation schemes such as moving least squares (MLS) and reproducing kernels are smooth, the analytical determination of higher derivatives required for PDEs such as elasticity are complex, and their step-by-step calculation is time-consuming. Basis functions derived using the standard RKPM require the inversion of moment matrices (as do equivalent MLS-based functions). This inversion feature complicates matters when calculating basis function derivatives to first and second order especially in multidimensional problems, increasing the computational cost. Evidence of this can be found in [33,34] and to address it, some novel formulations have been devised such as a gradient RKPM [35] where the calculations of the basis function derivatives are simplified, differential reproducing kernel interpolation (DRK) [36,37] and a fast MLS approach [38] in which novel efficient algorithms are used to enhance the efficiency of the derivative calculations. Another source of computational cost comes from the observation that for optimal convergence more collocation points than source points are required, forming an overdetermined system [35,21] which must be solved in, say, a least squares sense rather than directly. Despite these shortcomings, the RKCM is straightforward to implement and has been an important tool for the analysis of engineering problems [39,40]. However, numerical results sometimes suffer from instability and accuracy issues. A key contributor to these errors is in the imposition of essential boundary conditions [41], as is the case with MLS and RK-based meshless methods of all types.

In this paper, we tackle the latter source of error by making use of maximum-entropy (max-ent) basis functions. These are derived from classical information theory [42] and the max-ent principle [43]. Two key characteristics of max-ent basis functions are non-negativity and the satisfaction of the weak Kronecker-delta property on the boundaries. The former property makes the approximation schemes non-negative (convex) [44] and the max-ent basis functions smoother in contrast with other basis functions with negative values. The latter facilitates the imposition of essential boundary conditions accurately because the Kronecker-delta property on the boundary points makes the essential boundary fully satisfied. In this case "weak" means that the max-ent basis functions for points inside the domain do not possess the Kronecker-delta property [45]. Max-ent basis functions with compact support are derived using weight functions [46] in which the first and second order reproducing conditions are viewed as constraints. The resulting approximations retain the same order of reproducing conditions, namely the first and second order max-ent basis functions [44,47]. Reviews of weak form-based meshless methods using max-ent basis functions can be found in [48–51]. Max-ent basis functions are also used to couple the FEM and the EFGM in [52]. With the satisfaction of a weak Kronecker-delta property in max-ent basis functions, the imposition of essential boundary conditions can be carried out directly. There remain some issues with the imposition of Neumann boundary conditions, however, because the Lagrange multipliers in the expression of the first max-ent basis function derivatives blow up for points on the Neumann boundary which makes the first derivative values indeterminate [53]. This is an open problem beyond the scope of this paper. As indicated above, max-ent approximation has only been used to date for weak form-based meshless methods and in this work, local max-ent basis functions are used in a simple PCM. Considerable computational efficiency is demonstrated for the presented method as compared to a PCM based on RK basis functions.

The structure of this paper is as follows. Section 2 provides a brief review of the basic theory of PCMs, the expressions for local max-ent basis functions and their derivatives. Implementation issues associated with the max-ent PCMs are presented in Section 3. In Section 4, the proposed method is applied to some numerical examples to validate the approach. Final remarks are collected in Section 5.

2. Background

2.1. Review of point collocation methods

The theoretical background now presented is based on two-dimensional spatial domains but it is straightforward to modify for other dimensionalities. Consider a two-dimensional problem domain Ω bounded by boundary Γ ($\Gamma = \Gamma_u \cap \Gamma_t$) as shown in Fig. 1. The collocation points and source points (numbering N_c and N_s respectively) are distributed in the domain Ω and on the boundary Γ. The collocation points are distributed to enforce the governing PDE and corresponding boundary conditions which are satisfied at each collocation point. The surrounding source points, which fall in the local support domain of each collocation point, are used for the construction of the basis functions and determine the approximation of the solution over the domain. The governing PDE and the two types of boundary conditions are described as

$$\mathscr{L}\mathbf{u} = \mathbf{f_b} \quad \text{in } \Omega, \tag{1a}$$

$$\mathscr{L}_u\mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_u \text{ and } \mathscr{L}_t\mathbf{u} = \mathbf{h} \quad \text{on } \Gamma_t, \tag{1b}$$

where $\mathscr{L}$ is the differential operator in Ω, $\mathscr{L}_u$ and $\mathscr{L}_t$ are the differential operators for the Dirichlet and Neumann boundary

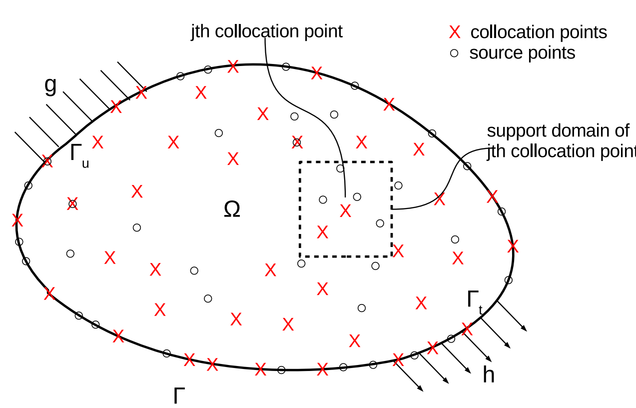

Fig. 1. A problem domain with boundary conditions in PCMs.