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Efficient Mapping of High Order Basis Sets for Unbounded Domains

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Abstract. Many physical problems involve unbounded domains where the physical quantities vanish at infinities. Numerically, this has been handled using different techniques such as domain truncation, approximations using infinitely extended and vanishing basis sets, and mapping bounded basis sets using some coordinate transformations. Each technique has its own advantages and disadvantages. Yet, approximating simultaneously and efficiently a wide range of decaying rates has persisted as major challenge. Also, coordinate transformation, if not carefully implemented, can result in non-orthogonal mapped basis sets. In this work, we revisited this issue with an emphasize on designing appropriate transformations using sine series as basis set. The transformations maintain both the orthogonality and the efficiency. Furthermore, using simple basis set (sine function) help avoid the expensive numerical integrations. In the calculations, four types of physically recurring decaying behaviors are considered, which are: non-oscillating and oscillating exponential decays, and non-oscillating and oscillating algebraic decays. The results and the analyses show that properly designed high-order mapped basis sets can be efficient tools to handle challenging physical problems on unbounded domains. Decay rate ranges as large of 6 orders of magnitudes can be approximated efficiently and concurrently.

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1 Introduction

As known, physical phenomena are modeled and represented mathematically by sets of differential equations with appropriate conditions (initial and/or boundary conditions).

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A small number of these differential equations can be solved analytically and hence numerical methods are routinely used to solve such problems. Therefore, numerous methods have been developed accordingly. They can be categorized into two general classes, namely, mesh-based and mesh-free methods [1–8]. In mesh-based methods, the computational window is spatially discretized (meshed) in *a priori*. The resulted predefined mesh is then utilized using low-order and localized basis sets to solve the considered differential equations in different ways [8]. The most commonly used mesh-based numerical methods are finite different methods (FDM) and finite element methods (FEM). Obviously, these methods scale up exponentially with the space dimension (D); i.e. $\mathcal{O}(N^D)$. So, they become computationally very expensive for $D>2$ [5,9,10]. However, for highly sparse matrices, better scaling can be achieved by further exploitation of the sparsity and by imposing locality to reduce the number of required operations. For example, in the sparse grid method, a computational cost of $\mathcal{O}(N(\log N)^{D-1})$ can be achieved [9,11,12]. The second class is meshfree methods, where the unknown quantities are approximated by high order basis sets without the need for the mesh [1,7]. The most known techniques of this family are the various spectral and pseudospectral methods [2,7,13] including Galerkin methods.

Recently, spectral methods (SM) have gained more attention and implementation primarily because of its high-order nature, which would result in high level of accuracy with less required computational resources (i.e. time and memory). This is because a considerable portion of the formulation is handled analytically [6,7,14]. In these methods, the real-space solution of a differential equation is presented in terms of a sum of certain basis or trial functions [15]. The basis functions are chosen to satisfy the constraints and needed conditions [2,6,16–20]. The methods then follow the general steps of weighted residual methods (WRM) where various weight (test) functions can be used. For more details about spectral methods and their applications, we refer the reader to more dedicated sources [1,2,7,13,15,21].

The spectral methods have been implemented successfully for many challenging problems in bounded domains [2,7,11,22]. Basically, this is due to the finite computational domain and the abundance of convenient orthogonal basis sets for such bounded domains. More development is needed to match that for unbounded domains [12,14,16,17,21]. Actually, some numerical techniques have been used to apply SM for unbounded domains; but, with some persistent challenges. Among the commonly used techniques are the domain truncation, implementation of basis functions that are intrinsically unbounded, and coordinate transformation (mapping) [12,14,16,17,21,23].

Domain truncation is one of the most commonly used techniques in FDM and FEM, where the infinite physical domain is represented by a finite computational window. Consequently, it will be inevitable to have a truncation error, which is reduced by increasing the size of the computation window. However, the larger computational window requires an accordingly larger number of mesh points. This can be mitigated by adopting nonuniform meshing and boundary layers. The second approach is to use functions like sinc and Hermite polynomials as basis sets. The computational domain