Applied Mathematics and Computation 339 (2018) 899–915

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Highlighting numerical insights of an efficient SPH method

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ARTICLE INFO

Dedicated to Maryam Mirzakhani

Keywords:
Kernel based methods
Smoothed Particle Hydrodynamics
Accuracy
Convergence
Improved fast Gaussian transform

ABSTRACT

In this paper we focus on two sources of enhancement in accuracy and computational demanding in approximating a function and its derivatives by means of the Smoothed Particle Hydrodynamics method. The approximating power of the standard method is perceived to be poor and improvements can be gained making use of the Taylor series expansion of the kernel approximation of the function and its derivatives. The modified formulation is appealing providing more accurate results of the function and its derivatives simultaneously without changing the kernel function adopted in the computation. The request for greater accuracy needs kernel function derivatives with order up to the desidered accuracy order in approximating the function or higher for the derivatives. In this paper we discuss on the scheme dealing with the infinitely differentiable Gaussian kernel function. Studies on the accuracy, convergency and computational efforts with various sets of data sites are provided. Moreover, to make large scale problems tractable the improved fast Gaussian transform is considered picking up the computational cost at an acceptable level preserving the accuracy of the computation.

1. Introduction

In recent years, meshless methods have gained growing interest in many different areas of science [2,4,8,9,21,39]. The basic idea of these methods is to provide numerical solutions without using any mesh in the problem domain. Methods without a predefinite connections are easily adapted to domains with complex and/or time evolving geometries without the difficulties that would be required to handle those features with topological data structures. They can be useful in non-linear problems involving viscous fluids, heat and mass transfer, linear and non-linear elastic or plastic deformations, etc. In the Lagrangian approach the points, describing the problem domain, move with the medium, and points may be added or deleted in order to maintain a prescribed sampling density. In the Eulerian approach the points are fixed in space, but new points may be added where there is need for increased accuracy. So, in both approaches the nearest neighbors of a point are not set. Numerical simulations usually need the values of a function and its derivatives at certain point and in this paper we focus on their approximation by means of the Smoothed Particle Hydrodynamics (SPH) method. This method was originally developed for solving astrophysical problems [16,17,29–33] and subsequently it has been also used in other areas of science and engineering [1,3,5,12–14,22–24,26,33,36,37,41]. The method results very attractive but it suffers from several drawbacks due to inaccurate approximation at boundaries and at irregular interior regions. This often confines its utility to limited scenarios. Many techniques have been devised to alleviate these problems and some of these have been documented

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https://doi.org/10.1016/j.amc.2018.07.060
0096-3003/

in [6,25,27,28] and in the references therein. In this paper we discuss on sources of enhancement in accuracy of the standard SPH method via Taylor expansion of the kernel approximation of a function and its derivatives [27]. In this way, accurate estimates of the function and its derivatives are simultaneously provided and no lower order derivatives are inherent in approximating the higher order derivatives. Therefore, the possible numerical errors in a lower order derivative will not be brought to the higher order ones. Moreover, high order of accuracy can be obtained without changes on the kernel function avoiding to lead unphysical results such as negative density or negative energy that can lead to breakdown of the entire computation in simulating some problems [23]. Accuracy can be increased in approximating a function or its derivatives by employing kernel function derivatives with order up to the desidered accuracy order in approximating the function or higher when more accurate results for the derivatives of the function are requested.So the Gaussian kernel function, infinitely differentiable and adequately smooth even for higher order derivatives is a suitable choice. In our study we propose numerical investigations on the standard and improved method dealing with the Gaussian kernel. Many experiments are conducted with the aim to address numerical features of the method accomplished with various data sets locations, gridded and scattered in a unit square domain, referring to bivariate test functions [35,40]. The modified approach is very interesting for the applications, but the computational demanding is a bottleneck as data locations get finer and for an high number of evaluation points. The computational effort is mainly due to the summations of kernel and its derivatives in assembling the matrix of the solving system for each evaluation point. Motivated to speed up the computation and to make large scale problems tractable we focus on efficient processing of this task. Working with Gaussian kernel, the derivatives involve sums of products of the polynomials and Gaussian one. This allows us to take advantage in the computation and to make use of fast algorithms [19] for all the summations set out for the proposed strategy. Namely, we consider the improved fast Gaussian transform [34] picking up the computational cost at an acceptable level preserving the accuracy of the computation. Furthermore, the matrix and the known vector assembly is generated by taking into account the Gaussian function as common element in the fundamental tasks. The overall computational work performs to linear for a fixed level of accuracy. We present the computations with the direct and the improved fast summation algorithm showing satisfactory results referring to a bivariate case study. The remainder of the paper is as follows. In Section 2 we present a review of the standard formulation. In Section 3 we describe the improved method supported by numerical simulations for some test functions in a unit square domain. In this section some discussions on the errors versus the number of data are reported referring to different orders of accuracy and with different data sets. The Section 4 is devoted to computational topics presenting the direct and the fast sum computation via Improved Fast Transform Gaussian adapted for our purposes. In Section 5 the results presented in the paper are shortly summarized.

2. Ab initio formulation

To make the paper self-contained we briefly review the SPH standard formalism from first principles. The method makes use of a *kernel approximation* using ideas from distribution theory for approximating a function with a delta distribution representation [15].

Definition 1. Let $f : \Omega \subset \mathbb{R}^d \to \mathbb{R}$, $d \geq 1$, the *kernel approximation* is defined as

$$< f_h(\mathbf{x}) > := \int_\Omega f(\boldsymbol{\xi}) \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h) d\Omega \tag{1}$$

with $\mathbf{x} = (x^{(1)}, \ldots, x^{(d)}), \boldsymbol{\xi} = (\xi^{(1)}, \ldots, \xi^{(d)}) \in \Omega$.

The function $\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h)$ is named *kernel function* and h is the *smoothing length*. The parameter h localizes the influence of the kernel function which approximates a Dirac δ-function in the limit $h \to 0$. The kernel is usually normalized to unity and it is required to be symmetric and sufficiently smooth. Under these assumptions the error of the kernel approximation can be estimated as second order of accuracy, or of first order of consistency [16,17,23]. Any function $\mathsf{K}(\mathbf{x}, \xi; h)$ with the above properties can be employed as smoothing kernel function. A common choice is the Gaussian function

$$\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h) = \frac{1}{h^d \sqrt{\pi^d}} e^{-\frac{\|\boldsymbol{\xi} - \mathbf{x}\|_2^2}{h^2}}. \tag{2}$$

The kernel (2) clearly decays when $\mathbf{x}$ moves away from $\boldsymbol{\xi}$ and the dimensional constant $\alpha_d = 1/h^d \sqrt{\pi^d}$ is to satisfy the unity condition requirement [23]. Moreover, it is infinitely differentiable, radial and strictly positive definite function on $\mathbb{R}^d$ for any d [7,10,11,42]. This function will be taken into consideration as kernel from now on.

When the entire domain is represented by a finite number of data sites we proceed in the approximation as follows

Definition 2. Given a set of data sites $\Xi = \left\{\boldsymbol{\xi}_j\right\}_{j=1}^N \subset \Omega$ and the corresponding measurements $\left\{y_j = f(\boldsymbol{\xi}_j)\right\}_{j=1}^N \in \mathbb{R}$ the *particle approximation* of the function is defined as

$$f_h(\mathbf{x}) := \sum_{j=1}^{N} f(\boldsymbol{\xi}_j) \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_j; h) d\Omega_j, \tag{3}$$

where $d\Omega_j$ is the measure of the subdomain Ω_j associated to each data site.

The triple (K, Ξ, h) essentially characterizes the approximation.