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A normalized iterative Smoothed Particle Hydrodynamics method

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Abstract In this paper we investigate on a normalized iterative approach to improve the Smoothed Particle Hydrodynamics (SPH) estimate of a function. The method iterates on the residuals of an initial SPH approximation to obtain a more accurate solution. The iterative strategy preserves the matrix-free nature of the method, does not require changes on the kernel function and it is not affected by disordered data distribution. The iterative refinement is further improved by ensuring a linear approximation order to the starting iterative values. We analyze the accuracy and the convergence of the method with the standard and normalized formulation giving evidence of the improvements obtained with both uniform and non-uniform data density. Numerical experiments in 2D domain with different data sets are presented to validate the iterative approach.

Keywords Iterated residuals · Normalized Smoothed Particle Hydrodynamics · Accuracy · Convergence

1 Introduction

Grid based methods are consolidated numerical techniques applied to a wide range of scientific area requiring the costly mesh generation task. In recent years meshfree methods have been introduced as an interesting computational alternative strategy based only on displacement among the points of the discretized problem domain [8,10,12,16,18,23,25]. When adopting a set of points without topological connections, also the treatment of large deformation problems is relatively easier. Furthermore, algorithms for problems involving interacting objects may be formulated and handled with minimal difficulty. The Smoothed Particle Hydrodynamics

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is one of the most commonly used mesh-free method firstly developed for simulating astrophysical problems [20,21,32–35] and it is being increasingly used [1–3, 19,27,29,36,37,39,40,44]. The idea of SPH is very simple and it can reconstruct a continuous field with summation on a cloud of discrete points and on the kernel function. However, despite its popularity there are many problems related to its accuracy and as a consequence over the past years different corrective strategies have been developed to cope with these difficulties [4–7,28–31,41,47].The improved accuracy is frequently obtained at the price of modifying the kernel function: a typical example is the reproduced kernel particle method (RKPM) proposed by Liu et al. [31]. Sometimes, the accuracy is improved by solving linear systems for each evaluation point giving rise to ill-conditioning of the system matrix for some problems and to high computational effort for time-evolving simulations. This is the case of the corrective smoothed particle method (CSPM) by Chen et al. [11] and the finite particle method (FPM) by Liu et al.[29,30] and improvements developed in [46]. With the aim to guarantee more accurate results while preserving the matrix-free feature of the method and avoiding to modify the kernel function, we propose an iterative approach based on the refinement of the residuals. Starting from an initial SPH estimate we generate some approximation values at any point of the problem domain that, under a suitable condition, convergence to the interpolant. The envelope of strictly definite positive kernel functions is considered and the method, in convergence, can be successfully applied without any restriction on pair-wise distinct data sites. Moreover, ensuring the linear approximation order [13,17,30], the iterative procedure provides more accurate results than those obtained with the standard SPH as initial values for both evenly and irregularly data distribution [19]. The paper is organized as follows. In Section 2 we briefly present the standard and the normalized version of the SPH method and some behaviors, referring to a 2D case study, are discussed. In Section 3 we describe the iterative process. In Section 4 the method is validated for different data sets providing more accurate results when the normalized SPH formulation is considered as starting iteration estimate. Finally, some remarks and ideas on future work are outlined in Section 5.

2 Basic concept of SPH

The method is based on the *kernel approximation* of a function $f\colon \Omega \subset \mathbb{R}^d \to \mathbb{R}$, for $d \geq 1$, defined as

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

at $\mathbf{x} = (x^{(1)}, ..., x^{(d)}), \boldsymbol{\xi} = (\xi^{(1)}, ..., \xi^{(d)}) \in \Omega$ and $\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h)$ is the *kernel function* with *smoothing length* h localizing its influence in Ω. The kernel is required to satisfy the normalization condition

$$\int_\Omega \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h) d\Omega = 1. \tag{2}$$

Moreover symmetry, monotonically decreasing and convergence to the Dirac function is required so that the error of the kernel approximation can be estimated as

second order of accuracy (or of first order of consistency) [26,27].

Given a set of data sites $\Xi = (\boldsymbol{\xi}_j)_{j=1}^N$ and the corresponding measurements $(f(\boldsymbol{\xi}_j))_{j=1}^N$, the discrete counterpart of the kernel approximation, usually named as *particle approximation*, 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 at each data site $\boldsymbol{\xi}_j$. The discrepancy between the kernel and particle approximation, especially on the boundary and with non uniform data locations, makes this computation often not accurate [27,28,30]. In Fig. 1 we show the maximum absolute error (MAE)

$$MAE = \max_{1\leq i\leq M} |f_h(\mathbf{x}_i) - f(\mathbf{x}_i)|, \tag{4}$$

for the bivariate function

$$\begin{aligned} f(x^{(1)}, x^{(2)}) = \quad & 0.75\exp\big[-\frac{(9x^{(1)}-2)^2 + (9x^{(2)}-2)^2}{4}\big] + \\ & + 0.75\exp\big[-\frac{(9x^{(1)}+1)^2}{49} + \frac{(9x^{(2)}+1)^2}{10}\big] + \\ & + 0.5\exp\big[-\frac{(9x^{(1)}-7)^2 + (9x^{(2)}-3)^2}{4}\big] + \\ & - 0.2\exp\big[-((9x^{(1)}-4)^2 + (9x^{(2)}-7)^2))\big]. \end{aligned} \tag{5}$$

In the simulations we consider M=1600 evaluation points, N=4225 gridded (Ξ_G) and random (Ξ_R) data sites in $\Omega = [0,1]^2$. The Ξ_R are generated by the *rand* function of MATLAB©. The infinitely differentiable, radial and strictly definite Gaussian function is the kernel used in the experiments

$$\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h) = \alpha_d e^{-\frac{\|\boldsymbol{\xi}-\mathbf{x}\|_2^2}{h^2}} \tag{6}$$

with the dimensional constant $\alpha_d = 1/h^d\sqrt{\pi^d}$ to satisfy the unity requirement [26].
Improvements can be gained making use of the Taylor series expansion as detailed in the next sub-section.

2.1 Linear approximation order

The first order of accuracy(p=1) can be ensured by considering the Taylor expansion of $f(\boldsymbol{\xi})$ retaining only the first term, multiplying for the kernel function and integrating over Ω

$$\int_\Omega f(\boldsymbol{\xi})\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h)d\Omega = \int_\Omega f(\mathbf{x})\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h)d\Omega + \int_\Omega \mathcal{O}(h)\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h)d\Omega, \tag{7}$$

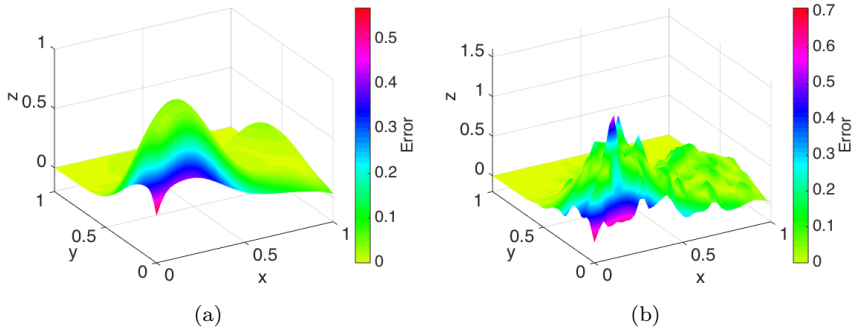


Fig. 1 Maximum Absolute Error (MAE) false-colored by magnitude with N=4225 (a) gridded Ξ_G and (b) random Ξ_R data sites for the test function (5).

$$f(\mathbf{x}) = \frac{\int_\Omega f(\boldsymbol{\xi})\mathsf{K}(\mathbf{x},\boldsymbol{\xi};h)d\Omega}{\int_\Omega \mathsf{K}(\mathbf{x},\boldsymbol{\xi};h)d\Omega} + \mathcal{O}(h). \tag{8}$$

The corresponding discrete formulation is

$$f(\mathbf{x}) = \frac{\sum_{j=1}^{N} f(\boldsymbol{\xi}_j)\mathsf{K}(\mathbf{x},\boldsymbol{\xi}_j;h)d\Omega_j}{\sum_{j=1}^{N} \mathsf{K}(\mathbf{x},\boldsymbol{\xi}_j;h)d\Omega_j} + \mathcal{O}(h). \tag{9}$$

By requiring the SPH particle approximation to satisfy the 1-st order of accuracy (9), we take here a closer look at some results obtained dealing with the function (5). In the Table 1 and 2 the Root Mean Square Errors (RMSEs)

$$RMSE = \sqrt{\frac{\sum_{i=1}^{M} |f_h(\mathbf{x}_i) - f(\mathbf{x}_i)|^2}{M}}, \tag{10}$$

give evidence of the improvements in the approximation when the discrete normalized formulation is considered for both equally and random data distribution. In the Fig. 2 the RMSEs are depicted for the two data sets. Higher order of accuracy could be reached via Taylor expansion, but at the cost of solving linear systems for each evaluation point or modifying the kernel function. In the following we introduce an iterative scheme preserving the kernel function and the matrix-free nature of the standard method. The iterative algorithm refines an initial estimate of SPH and the normalized formulation (9) will be shown as a valid starting choice.

Table 1 RMSEs for equally spaced data sites Ξ_G with the standard SPH and p=1 order of accuracy. Test function (5).

N	SPH	p=1
9	0.3487	0.2656
25	0.3136	0.1234
81	0.2456	0.1617
289	0.1540	0.0880
1089	0.0867	0.0403
4225	0.0621	0.0149
16641	0.0545	0.0054
66049	0.0537	0.0023

Table 2 RMSEs for random data sites Ξ_R with the standard SPH and p=1 order of accuracy. Test function (5).

N	SPH	p=1
9	0.2197	0.1896
25	0.2215	0.1343
81	0.1132	0.0706
289	0.1246	0.0304
1089	0.0781	0.0196
4225	0.0995	0.0082
16641	0.1062	0.0031
66049	0.0974	0.0016

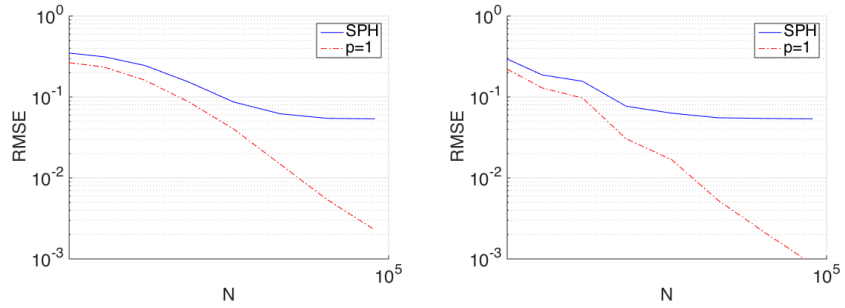


Fig. 2 RMSEs versus the number of data sites (a) equally spaced Ξ_G and (b) random Ξ_R for the test function (5). The blue full line depicts the error of the standard SPH estimates while the red dotted line is for the error of the 1-st order of accuracy.

3 Iterative SPH approximation

The SPH approximant (3) can be defined in matrix-vector notation as

$$f_h(\mathbf{x}) = \mathbf{K}(\mathbf{x})\mathbf{\Omega}\mathbf{f} \tag{11}$$

where

$$\mathbf{K}(\mathbf{x}) = \left[\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_1; h)\ \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_2; h)\ \ldots\ \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_N; h) \right],$$

$$\mathbf{\Omega} = diag\left[\, d\Omega_1 \; d\Omega_2 \; ... \; d\Omega_N \,\right]$$

and $\mathbf{f}$ collects the function values at the data sites. By considering (11) as initial estimate $f_h^{(0)}(\mathbf{x})$ and by iterating on residuals we generate a sequence of approximants $\{f_h^{(n)}(\mathbf{x})\}$. The residual function is itself approximated via SPH. In the following the process is detailed. By considering the matrix $\mathbf{A}$

$$\mathbf{A} = \left[\mathsf{K}(\boldsymbol{\xi}_i, \boldsymbol{\xi}_j; h) d\Omega_j\right]_{i,j=1}^{N}$$

and

$$\mathbf{s}^{(0)} = \mathbf{f} - \mathbf{A}\mathbf{f}$$

we iteratively compute for $n > 0$

$$\mathbf{R}^{(n-1)}(\mathbf{x}) = \mathbf{K}(\mathbf{x})\mathbf{\Omega}\mathbf{s}^{(n-1)}$$

$$f_h^{(n)}(\mathbf{x}) = f_h^{(n-1)}(\mathbf{x}) + \mathbf{R}^{(n-1)}(\mathbf{x}) = \mathbf{K}(\mathbf{x})\mathbf{\Omega}\sum_{k=0}^{n}(\mathbf{I} - \mathbf{A})^k\mathbf{f} \tag{12}$$

$$\mathbf{s}^{(n)} = \mathbf{s}^{(n-1)} - \mathbf{A}\mathbf{s}^{(\mathbf{n-1})}.$$

It is well known that [22]

$$\lim_{n\to\infty}\sum_{k=0}^{n}(\mathbf{I} - \mathbf{A})^k = \mathbf{A}^{-1}$$

if and only if $\|\mathbf{I} - \mathbf{A}\|_2 < 1$, therefore under this condition

$$\lim_{n\to\infty} f_h^{(n)}(\mathbf{x}) = P_h(\mathbf{x}) \tag{13}$$

where

$$P_h(\mathbf{x}) = \mathbf{K}(\mathbf{x})\mathbf{\Omega}\mathbf{A}^{-1}\mathbf{f} \tag{14}$$

is the interpolant.
The solution for $P_h(\mathbf{x})$ is admitted with strictly definite positive kernel functions on pair-wise distinct data sites and this is the only limit on the data location [9,14,15,45]. Hence, with strictly definite positive kernel functions the $\{f_h^{(n)}(\mathbf{x})\}$ converges to the interpolant $P_h(\mathbf{x})$ without assumption on the pair-wise distinct data distribution.

4 Numerical validation

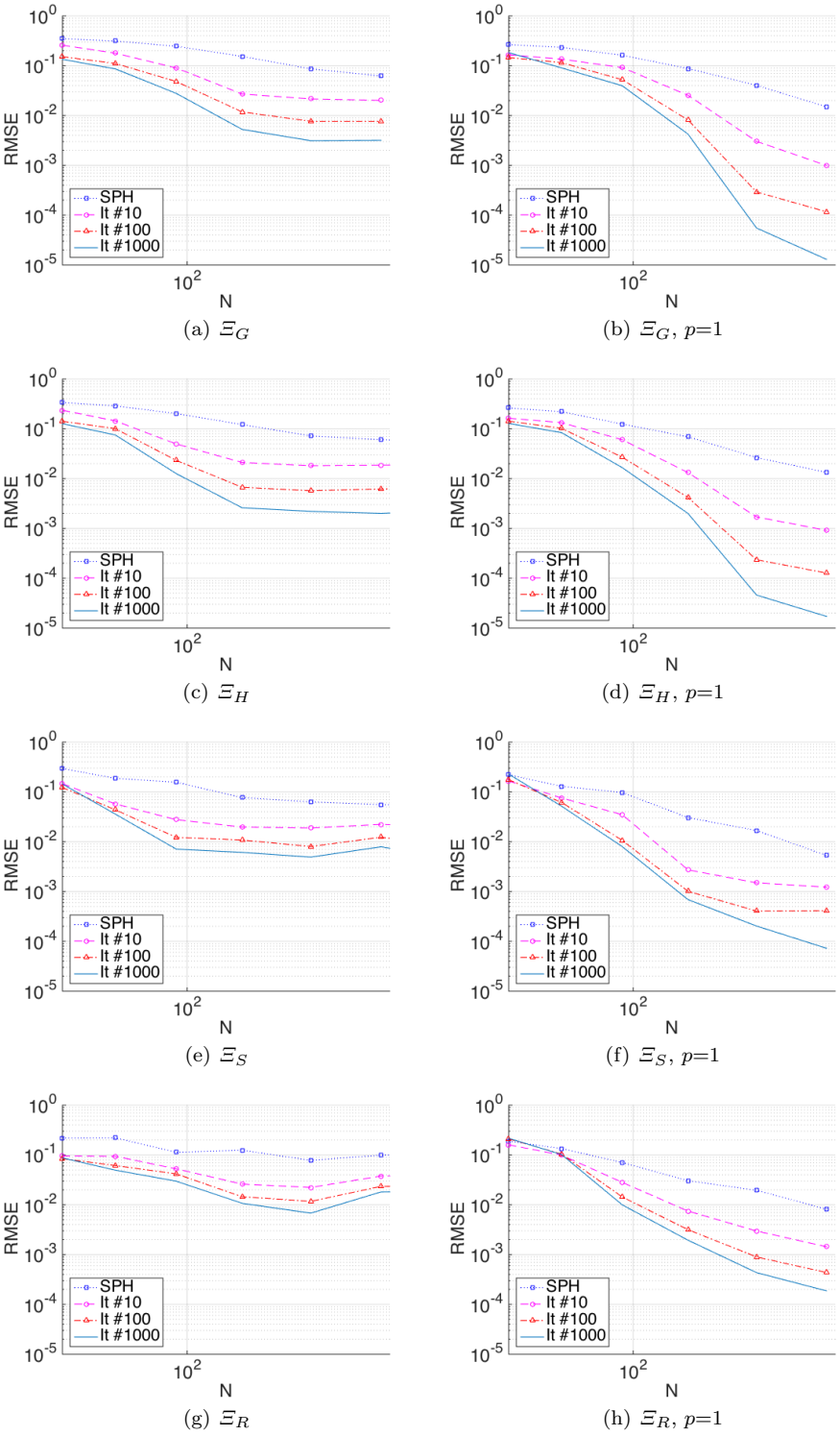
In this section we discuss on the numerical results referring to the test function (5) and proceed in the approximation for the gridded Ξ_G, Halton Ξ_H [24], Sobol′ Ξ_S [42] and random data sites Ξ_R. The *haltonset* and the *sobolset* functions of MATLAB© are adopted to construct the quasi-random data distribution from the Halton and Sobol′ sequence respectively. The *rand* function of MATLAB©is considered for the random distribution. We consider data sets by increasing the density of the data in the unit square domain and the root mean square error measures the accuracy of the estimates. M=1600 points are the number of the evaluation points and the function (6) is adopted as kernel function. We illustrate results on the accuracy and on the convergence. In all the tables the RMSEs are reported with $N = (2^t + 1)^2$, t=1,2,...,6. In the first column the error is related to the standard or normalized SPH formulation, while in the other columns the errors of the iterated method with 10,100,1000 iterations are shown. In the Tables 3,4,5 and 6 the RMSEs for the standard formulation is generated with the eq. (3). We observe improvements in the function approximation by means of $f_h^{(n)}(\mathbf{x})$ by increasing the number of iterations n and of data N. In the Tables 7,8,9 and 10 the RMSEs are reported working with the same data sets but with the normalized formulation as initial values giving evidence of better results obtained with linear accurate approximations as starting estimates. The improvements of the linear approximation are evident in the Fig. 3 where the convergence behavior is depicted in loglog plots. In analogy to the discussed simulations many other experiments have been performed giving evidence of the improvements in the accuracy with the standard and normalized iterative approach. In the Fig. 4 we report some results obtained working with the Wendland's compactly supported kernel function [45]

$$\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h) = (1 - \|\boldsymbol{\xi} - \mathbf{x}\|_2^2)_+^6 (35\|\boldsymbol{\xi} - \mathbf{x}\|_2^2 + 18\|\boldsymbol{\xi} - \mathbf{x}\|_2 + 3). \tag{15}$$

It is a radial strictly positive definite function with degree of smoothness equal to four [14,45]. We use this function for increasingly denser sets of data with the Franke's test function (5) and in the Fig. 4 the RMSEs are depicted with the data sequence in Ξ_G,Ξ_H,Ξ_S,Ξ_R with the standard SPH and the iterative approach compared to the normalized formulations. We experimentally observe that generally a good accuracy is with a reasonable number of iterations, but more efforts need for a theoretical understanding of the convergence behavior. This should be also useful for providing an estimate of the overall computational demanding that also depends on the flatness of the kernel function.

Table 3 RMSEs with Ξ_G.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.3487	0.2579	0.1515	0.1344
25	0.3136	0.1786	0.1112	0.0864
81	0.2456	0.0901	0.0481	0.0214
289	0.1540	0.0270	0.0118	0.0052
1089	0.0867	0.0215	0.0076	0.0031
4225	0.0621	0.0201	0.0075	0.0030



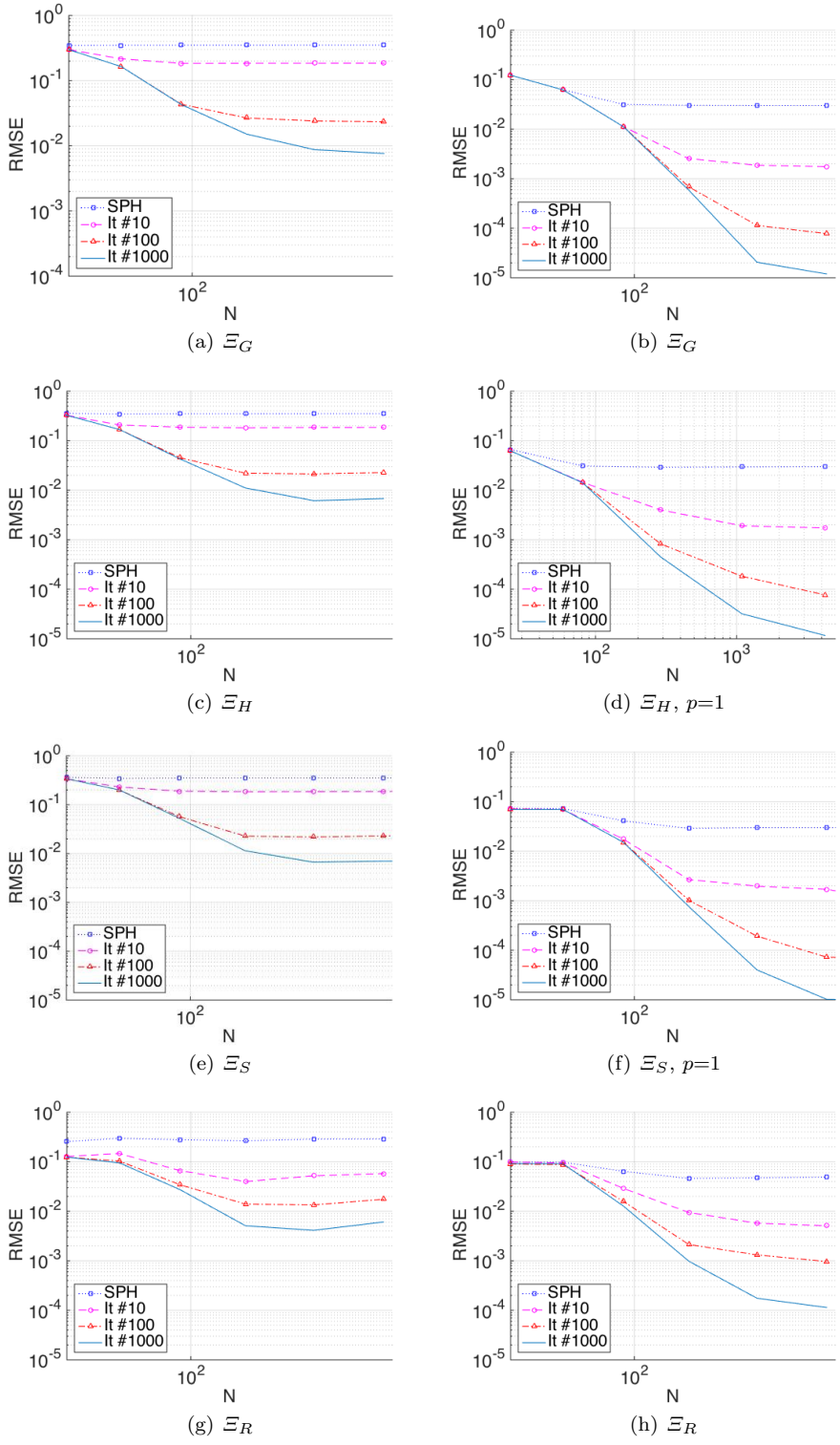
(a) Ξ_G (b) Ξ_G, p=1

(c) Ξ_H (d) Ξ_H, p=1

(e) Ξ_S (f) Ξ_S, p=1

(g) Ξ_R (h) Ξ_R, p=1

Fig. 3 RMSEs versus number of data sites.The function (6) is adopted as kernel function. In the left panels the standard SPH is compared with the iterative method. In the right panels the SPH, with p=1, is compared with the iterative method. 10, 100, 1000 iterations are considered.



(a) Ξ_G (b) Ξ_G

(c) Ξ_H (d) Ξ_H, p=1

(e) Ξ_S (f) Ξ_S, p=1

(g) Ξ_R (h) Ξ_R

Fig. 4 RMSEs versus number of data sites. The function (15) is adopted as kernel function. In the left panels the standard SPH is compared with the iterative method. In the right panels the SPH, with p=1, is compared with the iterative method. 10, 100, 1000 iterations are considered.

Table 4 RMSEs with Ξ_H.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.3376	0.2355	0.1418	0.1265
25	0.2885	0.1441	0.1007	0.0752
81	0.2024	0.0496	0.0232	0.0126
289	0.1215	0.0211	0.0067	0.0026
1089	0.0720	0.0181	0.0057	0.0022
4225	0.0605	0.0186	0.0062	0.0020

Table 5 RMSEs with Ξ_S.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.2945	0.1465	0.1226	0.1437
25	0.1873	0.0571	0.0436	0.0358
81	0.1564	0.0277	0.0122	0.0072
289	0.0769	0.0197	0.0108	0.0102
1089	0.0631	0.0188	0.0080	0.0049
4225	0.0554	0.0223	0.0123	0.0079

Table 6 RMSEs with Ξ_R.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.2197	0.0962	0.0845	0.0874
25	0.2215	0.0942	0.0613	0.0495
81	0.1132	0.0526	0.0417	0.0298
289	0.1246	0.0260	0.0145	0.0107
1089	0.0781	0.0223	0.0117	0.0068
4225	0.0995	0.0377	0.0234	0.0181

Table 7 RMSEs with Ξ_G and p=1.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.2656	0.1657	0.1455	0.1834
25	0.1234	0.1355	0.1156	0.0905
81	0.1617	0.0919	0.0525	0.0396
289	0.0880	0.0255	0.0081	0.0042
1089	0.0403	0.0030	2.91e-4	5.51e-5
4225	0.0149	9.94e-4	1.16e-4	1.29e-5

Table 8 RMSEs with Ξ_H and p=1.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.2624	0.1626	0.1427	0.1280
25	0.2206	0.1331	0.1023	0.0839
81	0.1244	0.0603	0.0269	0.0167
289	0.0693	0.0133	0.0042	0.0021
1089	0.0266	0.0017	2.35e-4	4.60e-5
4225	0.0137	9.15e-4	1.27e-4	1.71e-5

5 Conclusions

In this paper we discuss on an iterative SPH method. The method preserves the matrix-free nature of the standard approach without changes on the kernel func-

Table 9 RMSEs with Ξ_S and p=1.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.2206	0.1654	0.1756	0.2267
25	0.1293	0.0756	0.0616	0.0517
81	0.0972	0.0348	0.0106	0.0079
289	0.0305	0.0027	0.0010	6.82e-4
1089	0.0168	0.0015	4.05e-4	2.01e-4
4225	0.0053	0.0012	4.12e-4	7.24e-5

Table 10 RMSEs with Ξ_R and p=1.

N	f_h	$f_h^{(10)}$	$f_h^{(100)}$	$f_h^{(1000)}$
9	0.1896	0.1598	0.2103	0.2163
25	0.1343	0.0995	0.1044	0.1022
81	0.0706	0.0282	0.0143	0.0100
289	0.0304	0.0075	0.0032	0.0019
1089	0.0196	0.0030	8.98e-4	4.34e-4
4225	0.0082	0.0014	4.35e-4	1.86e-4

tion. We illustrate results on the convergence and on the accuracy giving evidence of better results obtained with the normalized formulation than the standard one. Many experiments are conducted with the aim to highlighting the basic results of the approach dealing with gridded and scattered data sets. Future work will be in investigating more on the convergence behavior and moving forward to extend the iterative method to approximate function derivatives.

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