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The Smoothed Particle Hydrodynamics method via residual iteration

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Abstract In this paper we propose for the first time an iterative approach of the Smoothed Particle Hydrodynamics (SPH) method. The method is widespread in many areas of science and engineering and despite its extensive application it suffers from several drawbacks due to inaccurate approximation at boundaries and at irregular interior regions. The presented iterative process improves the accuracy of the standard method by updating the initial estimates iterating on the residuals. It is appealing preserving the matrix-free nature of the method and avoiding to modify the kernel function. Moreover the process refines the SPH estimates and it is not affected by disordered data distribution. We discuss on the numerical scheme and experiments with a bivariate test function and different sets of data validate the adopted approach.

Keywords Kernel based methods · Smoothed Particle Hydrodynamics · Iterated residuals · Accuracy · Convergence

1 Introduction

On the last decades mesh-free methods have become a valid alternative to mesh-based due to various advantages in many different areas providing numerical solutions without using any mesh in the problem domain [8,9,13,14,18]. The Smoothed Particle Hydrodynamics (SPH) is a popular approach for the representation of physical models dealing with nodes located in the problem domain, avoiding the numerical overhead of handling explicit mesh topology. The method was originally developed for solving astrophysical problems [15,24] and nowadays spans many areas of science and engineering due to its capabilities of handling complex evolution problems as well as modeling complicated physics in a relatively simple manner

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[2–4,20,25,27,28,31,32]. However the method suffers from several drawbacks due to inaccurate approximation at boundaries and at irregular interior regions. Many techniques have been devised to alleviate these problems and some of these have been documented in [1,5,6,21–23] and in the references therein. In this paper we discuss for the first time on sources of enhancement in accuracy of the discrete approximation by iterating on the residuals.The iterative refinement provides accurate estimates preserving the matrix-free nature of the method furnishing the values of a function via a sum based directly on the given data. The method was introduced in [10,11] for moving least-square approximation and it is appealing in SPH framework because no changes on the kernel function need [21–23], avoiding to lead unphysical results such as negative density or negative energy that can give rise to breakdown of the entire computation in simulating some problems [20]. Moreover, in convergence it improves the SPH estimates and it is not affected by disordered data distribution. The difficulties associated with the solution of linear systems required in improving the SPH accuracy, as many times occurs [12, 22,23], are also successfully avoided. This occurence is a computational burden expecially for time-evolving simulations often coupled with the ill conditioning of the system matrix for some specific problems.With the aim to address numerical features of the method we propose some numerical simulations conducted on gridded and scattered data sets.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 iterative strategies and in the next Section numerical simulations for function recovery problems are proposed. In Section 4 some discussions on the errors versus the number of data are reported with the standard SPH as initial estimates. In Section 5 the conclusions and the future work are shortly summarized.

2 SPH standard formulation

In this section we briefly discuss on the standard SPH method based on the ideas from distribution theory for approximating a function with a delta distribution representation [19]. The method is founded 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* such that

$$\lim_{h \to 0} \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}; h) = \delta(\mathbf{x}, \boldsymbol{\xi}).$$

with δ the delta Dirac function and h the *smoothing length*, localizing its influence in Ω. The kernel is required to be sufficiently smooth, symmetric and normalized to unity so that the error of the kernel approximation can be estimated as second order of accuracy, or of first order of consistency [19,20]. The Gaussian kernel function is a common choice

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

The kernel clearly decays when $\mathbf{x}$ moves away from $\boldsymbol{\xi}$ and with the dimensional constant $\alpha_d = 1/(h\sqrt{\pi})^d$ it satisfies the unity requirement [19]. Moreover, it is infinitely differentiable, radial and strictly positive definite function on $\mathbb{R}^d$ for any d [10]. This function will be taken into consideration as kernel from now on.

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

where $d\Omega_j$ is the measure of the subdomain Ω_j associated to each data site $\boldsymbol{\xi}_j$. The standard method does not yield to satisfactory results throughout and the particle approximation is not according with the second order of accuracy as claimed in the kernel approximation due to the accuracy of the kernel approximation not always preserved in the discrete particle counterpart.This is evident with data near the boundary of the problem domain or with a scattered data distribution which provide an unbalanced contribution to the summations [19,20]. With the goal to improve the accuracy we introduce an iterative scheme [10,11] in approximating via SPH, which is not affected by data distribution, preserving the matrix-free nature of the standard method and without changes on the kernel function. In the next section we discuss on the notions distinguishing the improved approach.

3 Iterative corrective scheme

The corrective method is based on the idea to iteratively generate approximate solutions $f_h^{(n)}(\mathbf{x})$ making corrections on the SPH approximant defined in (3) with the SPH approximations of the difference between the function and $f_h^{(n-1)}(\mathbf{x})$ on the same data sites

$$f_h^{(n)}(\mathbf{x}) = f_h^{(n-1)}(\mathbf{x}) + R^{(n-1)}(\mathbf{x}) \tag{4}$$

where

$$f_h^{(0)}(\mathbf{x}) = f_h(\mathbf{x}) \quad \text{and} \quad R^{(n-1)}(\mathbf{x}) = \sum_{j=1}^{N} [f(\boldsymbol{\xi}_j) - f_h^{(n-1)}(\boldsymbol{\xi}_j)]\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_j; h)d\Omega_j. \tag{5}$$

A question on the convergence of the approximations $f_h^{(n)}(\mathbf{x})$ arises and a fundamental result is provided assessing the convergence to the interpolant $P_h(\mathbf{x})$ generated as linear combination of the same kernel functions. To this aim we proceed by adopting the algebraic notation for the $f_h^{(n)}(\mathbf{x})$ and $P_h(\mathbf{x})$ and we write

$$f_h^{(n)}(\mathbf{x}) = \mathbf{K}(\mathbf{x})\boldsymbol{\Omega}\mathbf{f} \tag{6}$$

where

$$\mathbf{K}^T(\mathbf{x}) = \begin{pmatrix} \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_1; h) \\ \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_2; h) \\ \vdots \\ \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_N; h) \end{pmatrix}, \boldsymbol{\Omega} = \begin{pmatrix} d\Omega_1 & & & \\ & d\Omega_2 & & \\ & & \ddots & \\ & & & d\Omega_N \end{pmatrix}, \mathbf{f} = \begin{pmatrix} f(\boldsymbol{\xi}_1) \\ f(\boldsymbol{\xi}_2) \\ \vdots \\ f(\boldsymbol{\xi}_N) \end{pmatrix}. \tag{7}$$

The vector $\mathbf{K}(\mathbf{x})$ and the diagonal matrix $\mathbf{\Omega}$ also feature the interpolant

$$P_h(\mathbf{x}) = \mathbf{K}(\mathbf{x})\mathbf{\Omega}\mathbf{c} \tag{8}$$

defined by enforcing the constraints

$$P_h(\boldsymbol{\xi}_i) = f(\boldsymbol{\xi}_i) \qquad i = 1, ..., N. \tag{9}$$

The unknown vector $\mathbf{c}$ is obtained by solving the linear system

$$\mathbf{A}\mathbf{c} = \mathbf{f} \tag{10}$$

with associated matrix

$$\mathbf{A} = \begin{pmatrix} \mathsf{K}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1; h) & \mathsf{K}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2; h) & ... & \mathsf{K}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_N; h) \\ \mathsf{K}(\boldsymbol{\xi}_2, \boldsymbol{\xi}_1; h) & \mathsf{K}(\boldsymbol{\xi}_2, \boldsymbol{\xi}_2; h) & ... & \mathsf{K}(\boldsymbol{\xi}_2, \boldsymbol{\xi}_N; h) \\ \vdots & & & \\ \mathsf{K}(\boldsymbol{\xi}_N, \boldsymbol{\xi}_1; h) & \mathsf{K}(\boldsymbol{\xi}_N, \boldsymbol{\xi}_2; h) & ... & \mathsf{K}(\boldsymbol{\xi}_N, \boldsymbol{\xi}_N; h) \end{pmatrix} \begin{pmatrix} d\Omega_1 & & & \\ & d\Omega_2 & & \\ & & \ddots & \\ & & & d\Omega_N \end{pmatrix}.$$

By assuming $\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_i; h)$ strictly definite positive and $\boldsymbol{\xi}_i \neq \boldsymbol{\xi}_j$, $i \neq j$, we are sure that the data interpolation admits solution without no restriction on the distribution of the data except for being pair-wise distinct [7, 10, 11].
A convergence result is provided by the following theorem which guarantees the convergence of $\{f_h^{(n)}(\mathbf{x})\}$ to $P_h(\mathbf{x})$ without assumptions for the data distribution.

Theorem 1. *The* $\{f_h^{(n)}(\mathbf{x})\}$ *converges to* $P_h(\mathbf{x})$ *for a given set of distinct data sites if and only if* $\|\mathbf{I} - \mathbf{A}\|_2 < 1$.
Proof.
We want to prove that $\{f_h^{(n)}(\mathbf{x})\}$ can be expressed as linear combination of the same kernel functions interested in $f_h(\mathbf{x})$ but with different coefficient factors

$$f_h^{(n)}(\mathbf{x}) = \mathbf{K}(\mathbf{x})\mathbf{\Omega}[\sum_{k=0}^{n}(\mathbf{I} - \mathbf{A})^k]\mathbf{f}. \tag{11}$$

We proceed by induction on n. For $n = 0$ the (11) is verified by taking into account the relation (6).
Now we suppose it holds for $n = n$. Let consider

$$f_h^{(n+1)}(\mathbf{x}) = f_h^{(n)}(\mathbf{x}) + R^{(n)}(\mathbf{x}) = f_h^{(n)}(\mathbf{x}) + \sum_{j=1}^{N}[f(\boldsymbol{\xi}_j) - f_h^{(n)}(\boldsymbol{\xi}_j)]\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_j; h)d\Omega_j =$$

$$= f_h^{(n)}(\mathbf{x}) + \sum_{j=1}^{N} f(\boldsymbol{\xi}_j)\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_j; h)d\Omega_j - \sum_{j=1}^{N} f_h^{(n)}(\boldsymbol{\xi}_j)\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_j; h)d\Omega_j.$$

In algebra notation

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

$$= \mathbf{K}(\mathbf{x})\mathbf{\Omega}[\sum_{k=0}^{n}(\mathbf{I}-\mathbf{A})^k + \mathbf{I} - \mathbf{A}\sum_{k=0}^{n}(\mathbf{I}-\mathbf{A})^k]\mathbf{f} =$$

$$= \mathbf{K}(\mathbf{x})\mathbf{\Omega}[\mathbf{I} + (\mathbf{I}-\mathbf{A})\sum_{k=0}^{n}(\mathbf{I}-\mathbf{A})^k]\mathbf{f} = \mathbf{K}(\mathbf{x})\mathbf{\Omega}[\mathbf{I} + \sum_{k=0}^{n}(\mathbf{I}-\mathbf{A})^{k+1}]\mathbf{f} =$$

$$= \mathbf{K}(\mathbf{x})\mathbf{\Omega}[\sum_{k=0}^{n+1}(\mathbf{I}-\mathbf{A})^k]\mathbf{f}.$$

Therefore, by remembering that [16]

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

$\{f_h^{(n)}(\mathbf{x})\}$ converges to $P_h(\mathbf{x})$ if and only if $\|\mathbf{I}-\mathbf{A}\|_2 <$ □

Thus, the convergence condition is valid for uniform and for scattered data sites too.

In the following the fundamental computational steps are underlined.

Algorithm

Input $\{\boldsymbol{\xi}_j, f(\boldsymbol{\xi}_j)\}_{j=1}^N, \{d\Omega_j\}_{j=1}^N, \mathbf{x}$, tolerance tol, maxlevel

1. Compute the vector $\mathbf{K}(\mathbf{x})$ based on the distance between the evaluation point and the data sites
2. Compute the interpolation matrix $\mathbf{A}$ based on the distance between the data sites
3. $f_h^{(0)}(\mathbf{x}) = \sum_{j=1}^{N} f(\boldsymbol{\xi}_j)\mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_j; h)\, d\Omega_j$
4. $s_j = f(\boldsymbol{\xi}_j)$
5. Repeat for all levels $n >$
   (a) $s_j = s_j - \sum_{i=1}^{N}$

(b) $R^{(n-1)}(\mathbf{x}) = \sum_{j=1}^{N} s_j \mathsf{K}(\mathbf{x}, \boldsymbol{\xi}_j; h) d\Omega_j$

(c) $f_h^{(n)}(\mathbf{x}) = f_h^{(n-1)}(\mathbf{x}) + R^{(n-1)}(\mathbf{x})$

until $||R^{(n-1)}(\mathbf{x})||_2 < tol$ or n=maxlevel

4 Numerical validation

In this section we discuss on the numerical results to assess the iterative approach. Gridded, Halton[17], Sobol[29] and random data sites, denoted as Ξ_G, Ξ_H, Ξ_S and Ξ_R respectively, are considered in the square domain $\Omega = [0,1]^2$. The random data are generated with the function *rand* of MATLAB© and in Fig. 1 we show Ξ_R in our simulations with N=289. Moreover, M=1600 evaluation points are picked up in Ω to validate the proposed approach. The results are collected by increasing

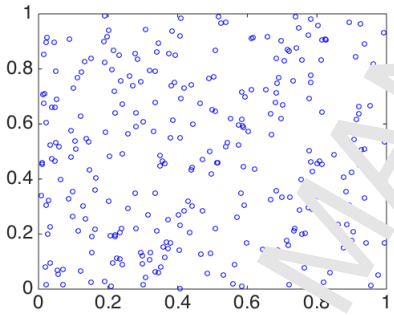

Fig. 1 N=289 random data sites (Ξ_R) generated with the function *rand* of MATLAB©.

the data and the iteration number and the root-mean-square-error (RMSE)

$$RMSE = \sqrt{\frac{\sum_{i=1}^{M} |f_h^{(n)}(\mathbf{x}_i) - f(\mathbf{x}_i)|^2}{M}}. \tag{12}$$

is used in the validation. We discuss here on the results obtained with the following test function taken from the scattered data literature [26,30]

$$f(x^{(1)}, x^{(2)}) = \frac{\sin(2\pi x^{(1)}) \cos(2\pi x^{(2)})}{2}. \tag{13}$$

In the Tables 1, 2, 3 and 4 the RMSEs are reported for a different number of data and iterations. Good improvements in the approximation are observed and depicted in Fig. 2 in loglog plots increasing the iterations from 10 to 1000.

Moreover, in Fig. 3 we report the convergence behavior for the test function (13) compared with the interpolant at N=289 data in Ξ_G, Ξ_H,Ξ_S and Ξ_R respectively by adopting a logarithmic scale for the y-axis. Both the Maximum Absolute Error (MAE)

$$MAE = \max_{1\leq i\leq M} |f_h^{(n)}(\mathbf{x}_i) - f(\mathbf{x}_i)|, \tag{14}$$

and the RMSEs give evidence that the major improvements are reached with few iterations.

Table 1 RMSEs with Ξ_G. Function test (13).

N	SPH	$iteration$		
		10	100	1000
9	0.2478	0.2319	0.1476	0.1601
25	0.2268	0.1207	0.0483	0.0255
81	0.1550	0.0350	0.0154	0.0110
289	0.0823	0.0203	0.0106	0.0083
1089	0.0501	0.0172	0.0097	0.0078
4225	0.0407	0.0168	0.0093	0.0076
16641	0.0392	0.0162	0.0090	0.0072

Table 2 RMSEs with Ξ_H. Function test (13).

N	SPH	$iteration$		
		10	100	1000
9	0.2499	0.2541	0.23[illegible]	0.2[illegible]8
25	0.2360	0.1697	0.0989	0.[illegible]567
81	0.1488	0.0335	0.0160	0.0116
289	0.0850	0.0220	0.[illegible]118	[illegible].0083
1089	0.0494	0.0163	0.008[illegible]	0.0055
4225	0.0421	0.0155	0.0062	0.0034
16641	0.0395	0.01[illegible]	[illegible].0073	0.0045

Table 3 RMSEs with Ξ_S. Function test (13)

N	SPH	$iteration$		
		[illegible]0	100	1000
9	0.2[illegible]27	0.2688	0.2507	0.2570
25	0.2[illegible]51	0.1765	0.0850	0.0396
81	[illegible].1948	0.0590	0.0192	0.0102
289	0.0[illegible]21	0.0214	0.0104	0.0076
10[illegible]9	0.0601	0.0165	0.0070	0.0039
4[illegible]25	0.0[illegible]25	0.0157	0.0080	0.0047
16641	0[illegible].0398	0.0143	0.0056	0.0027

Anyhow, we remark that a better accuracy is reached at the cost of an increased computational effort related to the iterations number on the residuals.

Table 4 RMSEs with Ξ_R. Function test (13).

N	SPH	$iteration$		
		10	100	1000
9	0.2467	0.2366	0.2202	0.2034
25	0.2403	0.2124	0.1796	0.1459
81	0.1300	0.0441	0.0348	0.0317
289	0.1016	0.0287	0.0134	0.0100
1089	0.0757	0.0197	0.0101	0.0063
4225	0.0623	0.0197	0.0090	0.0056
16641	0.0685	0.0247	0.0151	0.0114

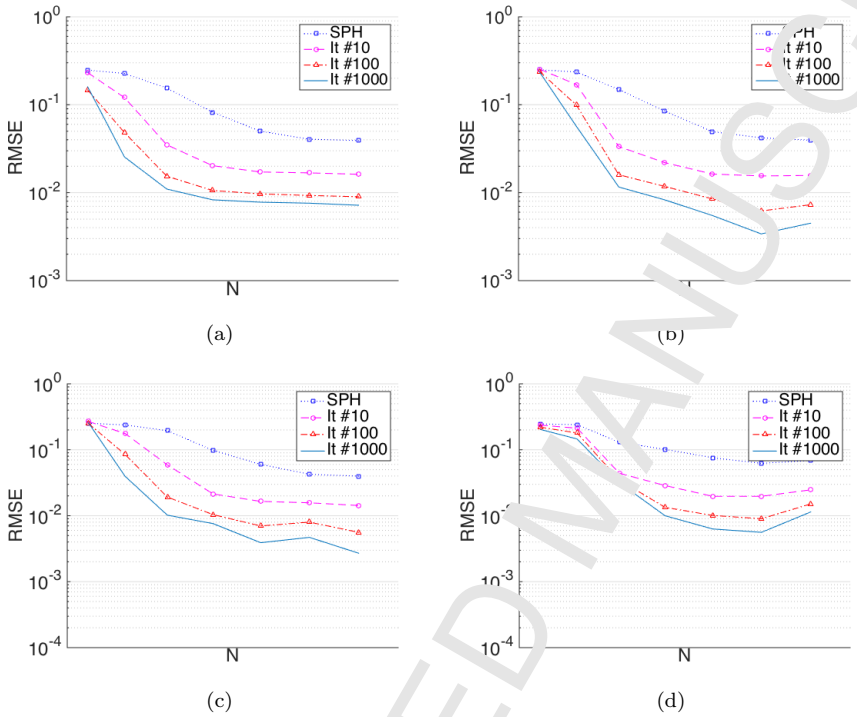

Fig. 2 RMSEs versus number of data sites for the standard SPH and the iterative method with 10,100,1000 iterations. Function test (13) (a) Ξ_G; (b) Ξ_H; (c) Ξ_S; (d) Ξ_R.

In summary the SPH method, widely used in the applications with the advantage to overcome the spatial topological connections of the grid based methods, can be iteratively improved in accuracy. In convergence, the proposed iterative procedure provides more accurate results than those obtained with the standard one, preserving the mesh-free nature of the method and the matrix-free feature of the computational process, without changes on the kernel function and requirements on data locations. The computational demanding is an important point to address, considering that it increases applying the iterative scheme, but the numerical sim-

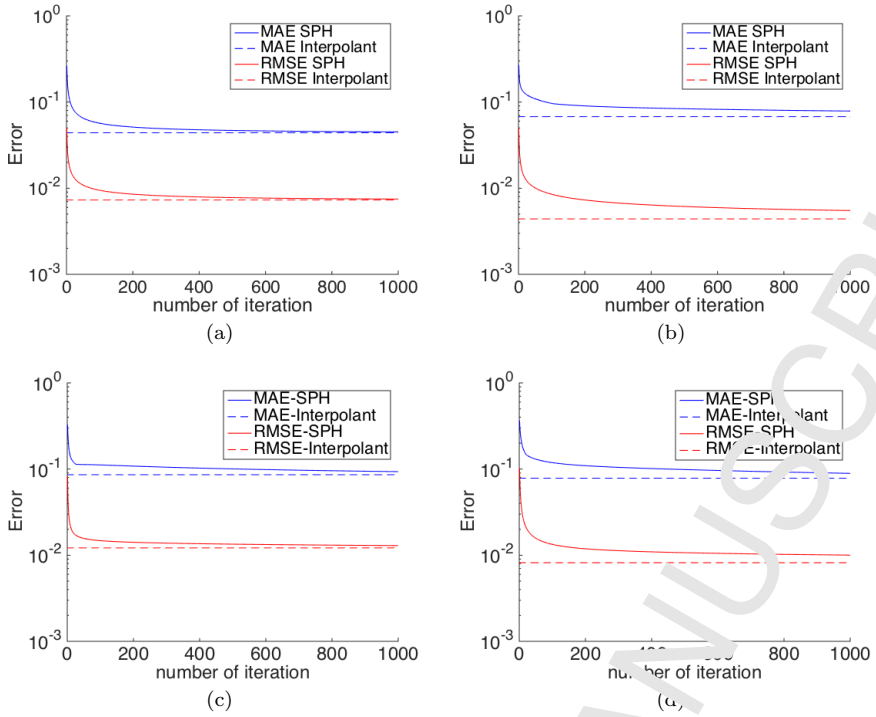

Fig. 3 Convergence for the iterated SPH and RBF interpolant with N=289 for the function test (13) MAEs and RMSEs for (a) Ξ_G; (b) Ξ_H;(c) Ξ_S; (d)

ulations suggest us that a satisfying accuracy is generally reached with not many iterations and further studies need along this direction.

5 Conclusions

In this paper we present a novel SPH method via residual iteration. The method improves the standard one preserving the matrix-free nature of the SPH method and indipendently by the data distribution. We illustrate results on the convergence and on the accuracy giving evidence of better results than SPH ones. Many experiments are conducted with the aim to address the basic features of the method which works with gridded and scattered data sets. The results encourage to proceed in applying the method also in the approximation of derivatives and in applying it for modeling the evolution in time of transient phenomena.

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