Computer Physics Communications 185 (2014) 2609–2621

Contents lists available at ScienceDirect

Computer Physics Communications

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

# A measure of spatial disorder in particle methods

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ARTICLE INFO

*Article history:*
Received 14 November 2013
Received in revised form
21 May 2014
Accepted 9 June 2014
Available online 16 June 2014

*Keywords:*
Particle methods
Meshless methods
Particle disorder
Smoothed particle hydrodynamics

ABSTRACT

In the present work we describe a numerical algorithm which gives a measure of the disorder in particle distributions in two and three dimensions. This applies to particle methods in general, disregarding the fact they use topological connections between particles or not. The proposed measure of particle disorder is tested on specific configurations obtained through the perturbation of a regular lattice. It turns out that the disorder measure may be qualitatively related to the mean absolute value of the perturbation. Finally, some applications of the proposed algorithm are shown by using the Smoothed Particle Hydrodynamics (SPH) method.



## 1. Introduction

In recent years a large amount of studies on particle methods has been developed, concerning several fields of Physics, Engineering and Mathematics. The increasing interest in particle methods has been driven by their powerful applications and by the attractive mathematical background on which they rely. The main advantage of particle schemes is that they do not implement fixed computational grids but use particles as computational nodes and move them in a Lagrangian fashion. This allows the modeling of complex dynamics with large deformations of the computational domain.

Generally, these schemes may be divided in two wide classes: those which use topological connections between particles (i.e. [1]) and meshless methods (like, for example, [2,3]). For all these schemes, the attainment and maintenance of a regular particle distribution is a crucial point, since the particle disorder may strongly affect their accuracy and stability [4,5]. This challenged many researchers to regularize the particle arrangement through remeshing or shifting algorithms (see, for example, [6–8]). Notwithstanding the idea of particle order/disorder is a natural and innate concept, its theoretical definition and quantitative measurement is hard to identify in a clear and unambiguous manner. This is what we try to address in the present work: we propose a measure of the particle disorder and check it on a number of test cases. These have been gathered in two groups: the former one is made by applications of the disorder measure on different particle distributions while the latter one contains dynamical test cases obtained by using a Smoothed Particle Hydrodynamics (SPH) scheme.

The basic idea for the particle disorder measure relies on the definition of two different *local* distances (that is, distances related to each single particle). The first local distance is simply the minimum distance of a particle from its neighbor particles. The definition of the second local distance is more complex, since this must account for any directional anisotropy in the particle distribution. This is computed by searching the nearest neighbor particles in different directions and, then, taking the maximum distance all over them.

By construction, the second distance is greater or equal to the first distance. Hence, we define a *local* disorder measure as the ratio between half the difference between the second and the first distance and their arithmetic mean. A *global* disorder measure is obtained as the arithmetic mean of the local measure all over the particles. If the distribution is regular, the first and second distances coincide all over the computational domain, the local measure is zero everywhere and so does the global measure (see Section 2). Then, intuitively, the global measure represents how far the actual particle distribution is from a regular lattice. In Section 2.1 we heuristically found that it has the same order of magnitude of the mean absolute error of the particle distribution with respect to a hypothetical regular distribution. Finally, in Section 3 the global measure has been applied to study dynamical test cases.

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http://dx.doi.org/10.1016/j.cpc.2014.06.008
0010-4655/

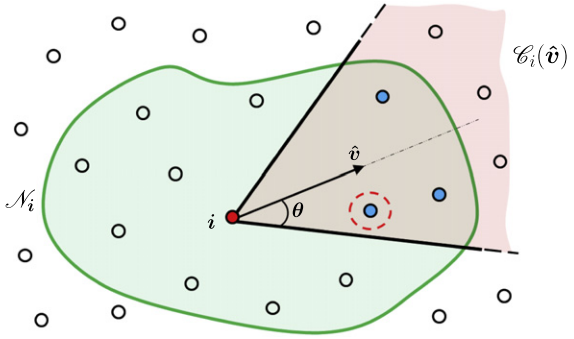


**Fig. 1.** Sketch of a generic set of the neighbor particles, $\mathscr{N}_i$ (green shaded area), and of the cone $\mathscr{C}_i(\hat{\boldsymbol{v}})$ with angle $2\,\theta$ and axis direction $\hat{\boldsymbol{v}}$ (red shaded area). The selected particle is the nearest to the $i$th particle inside the cone. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

## 2. The particle disorder measure

Let us consider a particle $i$ at the position $\boldsymbol{r}_i$. In particle methods, the $i$th particle has its own neighbor particles which may be identified through topological connections (e.g. PFEM) or as particles inside a proper domain (as, for example, the compact support of the kernel function in SPH). We denote the set of the neighbor particles to the particle $i$ as $\mathscr{N}_i$ (note that $\mathscr{N}_i$ does not include the $i$th particle itself). We define the first local distance as follows:

$$d_m^{(i)} = \min_{j\in\mathscr{N}_i} \|\boldsymbol{r}_j - \boldsymbol{r}_i\|, \tag{1}$$

where $\boldsymbol{r}_j$ is the position of the $j$th neighbor particle. If $\mathscr{N}_i$ is empty, $d_m^{(i)}$ is set equal to zero. This is an arbitrary choice and it means that we consider isolated/not-connected particles as a part of disconnected computational domains.

To construct the second local measure, we first define the right circular cone. The vertex of the cone is placed on the $i$th particle and its axis is identified by a unit vector $\hat{\boldsymbol{v}}$. The cone aperture is denoted by $2\theta$. Then, the cone is given by:

$$\mathscr{C}_i(\hat{\boldsymbol{v}}) = \left\{ \boldsymbol{r} \in \mathbb{R}^d \text{ such that } \frac{(\boldsymbol{r}-\boldsymbol{r}_i)}{\|\boldsymbol{r}-\boldsymbol{r}_i\|} \cdot \hat{\boldsymbol{v}} \geq \cos(\theta) \right\}, \tag{2}$$

where $d$ indicates the spatial dimension. A sketch of the cone is displayed in Fig. 1. The definition of the angle $\theta$ is of crucial importance. Specifically, we require that, in the presence of a regular lattice, the cone includes at least one of the nearest neighbor particles (see Fig. 2). In two dimensions only three regular distributions are possible, namely, the Triangular, the Cartesian and the Hexagonal one. Among these, the Hexagonal distribution has the largest angle between two subsequent nearest particles, i.e. $2\pi/3$ radiants. This suggests that $\theta$ has to be larger than $\pi/3$. In three dimensions, the only regular lattice is the Cartesian grid. In this case, we require the cone to be large enough to include an octant. This corresponds to $\cos(\theta) > 1/\sqrt{3}$ which, similar to the two dimensional case, approximately corresponds to choosing $\theta \geq \pi/3$. The influence of $\theta$ on the results is analyzed in Section 2.1. In all the cases, the axis direction $\hat{\boldsymbol{v}}$ is arbitrary.

After the cone has been defined, we select the neighbor particles inside it and compute the minimum distance from the $i$th particle. Then, the cone is rotated (this corresponds to a rotation of the axis or, equivalently, of the vector $\hat{\boldsymbol{v}}$) and the procedure is repeated. In numerical simulations it is not possible to rotate the cone *continuously*. For this reason, we select a finite number of rotations to obtain a cover of the neighborhood of the particle $i$. This strategy influences the value of the measure we are going to define but it does not alter its global properties. This aspect will be examined in-depth in Section 2.1. For the time being, let us assume that there are $k$ rotations of the cone or, equivalently, $k$ cones with axes identified by unit vectors $\hat{\boldsymbol{v}}_k$. When the neighborhood of the $i$th particle has been covered, the second distance is set equal to the supremum of the minimum distances, that is:

$$d_M^{(i)} = \max_k \left\{ \min_{j\in\mathscr{N}_i | \boldsymbol{r}_j \in \mathscr{C}_i(\hat{\boldsymbol{v}}_k)} \|\boldsymbol{r}_j - \boldsymbol{r}_i\| \right\}. \tag{3}$$

A sketch of the procedure is drawn in Fig. 3. By construction, this definition allows detecting any eventual anisotropy in the particle distribution and, in the case of a regular lattice, it coincides with $d_m^{(i)}$. If any of the $k$ cones is empty (that is, no neighbor particles are inside it), the minimum distance inside it is set equal to zero. This is done to be consistent with the case in which the particle $i$ has no neighbor particle at all. In this way, the above definitions imply $d_M^{(i)} = d_m^{(i)} = 0$.

By construction, the second distance is greater or equal to the first distance. Hence, we define a *local* disorder measure as follows:

$$\lambda_i = \begin{cases} \dfrac{d_M^{(i)} - d_m^{(i)}}{d_M^{(i)} + d_m^{(i)}} & \text{if } d_M^{(i)} > 0, \\ 0 & \text{if } d_M^{(i)} = 0. \end{cases} \tag{4}$$

The latter case corresponds to isolated particles. Obviously, we exclude from the present analysis the eventuality that all (or a great part of) the particles are isolated. Finally, the global measure of the particle disorder is defined as follows:

$$\Lambda = \frac{\sum_i \lambda_i}{N}, \tag{5}$$

where the summation is performed over all particles and $N$ is the total number of particles. Since $\lambda_i \leq 1$, it is $\Lambda \leq 1$ as well. If the particle distribution is regular, the second and first local distances

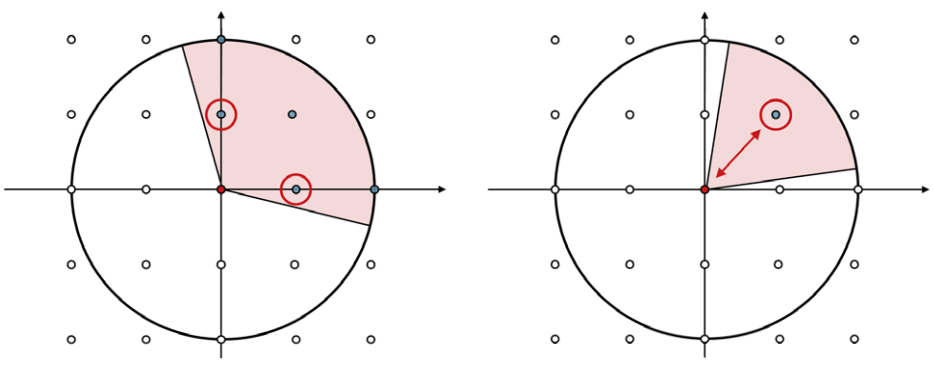

**Fig. 2.** A sketch with the Cartesian tessellation. Left: a cone with large enough value of $\theta$. Right: a cone with a wrong value of $\theta$.