# Ten good reasons for using polyharmonic spline reconstruction in particle fluid flow simulations

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**Abstract** We develop supporting arguments in favour of kernel-based reconstruction methods in the recovery step of particle simulations. We strongly recommend polyharmonic spline kernels, whose key features and advantages are briefly explained.

## 1 Introduction

Particle methods provide flexible discretizations for the numerical simulation of multiscale phenomena in fluid flows. For time-dependent evolution processes, for instance, particle models are particularly well-suited to cope with rapid variation of domain geometries and anisotropic large-scale deformations. To discuss their governing equation, we remark that fluid flow simulations require the numerical solution of a *hyperbolic conservation law* of the form

$$\frac{\partial u}{\partial t} + \nabla f(u) = 0, \tag{1}$$

on given computational domain $\Omega \subset \mathbb{R}^d$, $d \geq 1$, compact time interval $[0, T]$, $T > 0$, and flux tensor $f(u) = (f_1(u), \dots, f_d(u))^T$, where at time $t = 0$ *initial conditions*

$$u(0, x) = u_0(x) \qquad \text{for } x \in \Omega \tag{2}$$

are assumed. Nonlinear flux tensors $f$ lead to *discontinuous* solutions $u$, *shocks*, which may develop spontaneously, even at smooth initial data $u_0$ in (2). Therefore, nonlinear flow simulation requires flexible computational methods to solve (1), (2). For an introduction to numerical methods for fluid dynamics we refer to [10, 12, 13].

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## 2 The basic reconstruction problem of particle flow simulation

To compute the numerical solution $u : [0,T] \times \Omega \longrightarrow \mathbb{R}$ of (1), (2), particle methods are popular tools, especially for their high flexibility. The Eulerian *finite volume particle method* (FVPM) [4] and the *semi-Lagrangian particle method* (SLPM) [8] are only two prototypes. For a comprehensive discussion on particle-based flow simulation, we refer to [8] and references therein.

Although Eulerian and Lagrangian particle methods, such as FVPM and SLPM, are conceptually different, they rely on the solution of a specific reconstruction problem, which we can describe as follows. To this end, let $\Xi = \{\xi_1, \ldots, \xi_n\} \subset \Omega$ be a *stencil*, i.e., a finite point set of particle positions. For any particle $\xi \in \Xi$, we assume a scalar value $u(\xi) \equiv u(\xi, t) \in \mathbb{R}$, which is used, at time $t$, to compute the numerical solution $u$ of (1), (2). In the Eulerian FVPM, for instance, $u(\xi, t)$ is the *particle average* for the *influence area* of particle $\xi$, cf. [7, 8] for further details.

Now the generic formulation of the basic reconstruction problem is as follows.

**Problem 1** Compute from a given stencil $\Xi = \{\xi_1, \ldots, \xi_n\} \subset \Omega$ of $n \in \mathbb{N}$ pairwise distinct particle positions in the domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, and a data vector

$$u_\Xi = (u(\xi_1), \ldots, u(\xi_n))^T \in \mathbb{R}^n$$

a reconstruction $s : \Omega \longrightarrow \mathbb{R}$ satisfying $s_\Xi = u_\Xi$, i.e.,

$$s(\xi_j) = u(\xi_j) \qquad \text{for all } 1 \leq j \leq n. \tag{3}$$

Although particle-based simulation methods are so popular for their high flexibility, they may have severe drawbacks. Indeed, especially in relevant situations of *anisotropic* stencils $\Xi$, e.g. in WENO schemes [11], the numerical stability is very critical, due to the heterogenous distribution of particles in $\Xi$. In such cases, it is desirable to work with robust reconstruction schemes in order to better capture discontinuities (shocks fronts) and preference directions of the flow. Other problems of particle methods are moving boundaries and highly turbulent flows. Needless to say that high performance particle simulation methods essentially require high performance reconstruction schemes. For the solution of Problem 1, accurate, stable, efficient and flexible reconstruction algorithms are therefore of vital importance.

## 3 Kernel-based reconstruction vs polynomial reconstruction

Most of the particle-based simulation methods rely on *polynomial* reconstruction. However, as documented for WENO methods [1], polynomials may lead to severe numerical instabilities. Especially in situations of *anisotropic* stencils $\Xi$, polynomial reconstructions are often doomed to fail. In this paper, we propose to avoid polynomial reconstruction methods. We rather give a strong recommendation in favour of *kernel-based* reconstructions, where *polyharmonic splines* are our favourite choice.

Before we start our discussion on kernel-based reconstructions, we wish to provide only one argument against using polynomials, which should convince the numerical reader already now: Recalling polynomial interpolation from univariate data, where $d = 1$ and $\Omega \subset \mathbb{R}$, we understand from basic numerical analysis that polynomial interpolation (a) is numerically unstable, especially for large and unevenly distributed data; (b) is highly sensitive with respect to noisy input data; (c) may lead to high oscillations near the boundary of the domain (interval) $\Omega$. On the other hand, we understand from basic numerical analysis that *splines*, e.g. cubic splines, are powerful tools for univariate interpolation. In fact, spline reconstruction schemes avoid the well-known shortcomings (a)-(c) of polynomial interpolation. Thereby, spline reconstruction is far superior to polynomial reconstruction, already in the case of one dimension, $d = 1$, and so the following two leading questions are not undue:

*(Q1) Should we use polynomial reconstruction for the multivariate case?*

*(Q2) Is there a generalization of univariate splines to higher dimensions?*

Our answer to (Q1) is *clearly no*, since polynomial reconstruction does not even work properly for the univariate case. Our answer to (Q2) is *yes*: polyharmonic splines extend univariate splines to higher dimensions $d > 1$, as we explain here.

## 4 Kernel-based reconstruction in particle fluid flow simulations

To introduce basic ingredients of kernel-based reconstruction, let us first recall the conditions $s_\Xi = u_\Xi$ in Problem 1, for whose solution $s : \Omega \longrightarrow \mathbb{R}$ we now assume the form

$$s(x) = \sum_{j=1}^{n} c_j \varphi(x - \xi_j) + p(x) \qquad \text{for } p \in \mathcal{P}_m^d \tag{4}$$

with parameters (coefficients) $c = (c_1, \ldots, c_n)^T \in \mathbb{R}^n$. Moreover, $\varphi : \Omega \longrightarrow \mathbb{R}$ is an even *kernel* function and $\mathcal{P}_m^d$ denotes the linear space of all $d$-variate polynomials of order $m \in \mathbb{N}_0$. The order $m$ in (4) is determined by the choice of $\varphi$ as follows.

For the well-posedness of the reconstruction scheme, we require the kernel $\varphi$ to be *conditionally positive definite* of order $m$ on $\mathbb{R}^d$ (see [14, Chapter 8]), in short: $\varphi \in \text{CPD}(m, \mathbb{R}^d)$. For the following discussion, it is sufficient to say that, for $\varphi \in \text{CPD}(m, \mathbb{R}^d)$, we obtain under the moment conditions

$$\sum_{j=1}^{n} c_j p(\xi_j) = 0 \qquad \text{for all } p \in \mathcal{P}_m^d \tag{5}$$

a reconstruction $s$ of the form (4), where $s$ is unique, if the stencil $\Xi$ is $\mathcal{P}_m^d$*-unisolvent*, i.e., any polynomial $p \in \mathcal{P}_m^d$ can uniquely be reconstructed from its values at $\Xi$, or, in other words, $p_\Xi = 0$ implies $p \equiv 0$.

Therefore, the coefficients $c = (c_j)_{1 \le j \le n} \in \mathbb{R}^n$ and $d = (d_\alpha)_{|\alpha|<m}^T \in \mathbb{R}^q$ for $s$ in (4) are characterized by the solution of the $(n + q) \times (n + q)$ linear system

$$\begin{bmatrix} \Phi & P \\ P^T & 0 \end{bmatrix} \cdot \begin{bmatrix} c \\ d \end{bmatrix} = \begin{bmatrix} u_\Xi \\ 0 \end{bmatrix}, \tag{6}$$

resulting from the reconstruction conditions (3), under constraints (5), where

$$\Phi = \left(\varphi(\xi_k - \xi_j)\right)_{1 \le j,k \le n} \in \mathbb{R}^{n \times n} \quad \text{and} \quad P = \left(\xi_k^\alpha\right)_{1 \le k \le n; |\alpha| < m} \in \mathbb{R}^{n \times q},$$

and where $q = \binom{m-1+d}{d}$ is the dimension of the polynomial space $\mathcal{P}_m^d$.

We can conclude the discussion of this section as follows.

**Proposition 1** *The system (6) has for any $\mathcal{P}_m^d$-unisolvent stencil $\Xi \subset \mathbb{R}^d$ a unique solution, if $\varphi$ is conditionally positive definite of order $m$ on $\mathbb{R}^d$, $\varphi \in \mathrm{CPD}(m, \mathbb{R}^d)$.*

For a more comprehensive account to conditionally positive definite kernels, we refer to [14], where examples for commonly used kernels $\varphi \in \mathrm{CPD}(m, \mathbb{R}^d)$ are given.

## 5 Kernel-based reconstruction by polyharmonic splines

The special case of *polyharmonic splines* is due to Duchon [3]. Polyharmonic splines are radial kernels $\varphi_{d,m}(x) = \phi_{d,m}(r)$, with $r = \|x\|$ (the Euclidean norm), of the form

$$\phi_{d,m}(r) = \left\{ \begin{array}{ll} r^{2m-d} \log(r) & \text{for } d \text{ even} \\ r^{2m-d} & \text{for } d \text{ odd} \end{array} \right\} \qquad \text{for } 2m > d,$$

where $\phi_{d,m} \in \mathrm{CPD}(m, \mathbb{R}^d)$. According to [3], polyharmonic spline reconstruction is *optimal* with respect to the *Beppo Levi space*

$$\mathrm{BL}^m(\mathbb{R}^d) = \left\{ u : D^\alpha u \in L^2(\mathbb{R}^d) \text{ for all } |\alpha| = m \right\} \subset \mathscr{C}(\mathbb{R}^d) \qquad \text{for } 2m > d,$$

which is equipped with the semi-norm

$$|u|_{\mathrm{BL}^m}^2 = \sum_{|\alpha|=m} \binom{m}{\alpha} \|D^\alpha u\|_{L^2(\mathbb{R}^d)}^2 \qquad \text{for } u \in \mathrm{BL}^m(\mathbb{R}^d).$$

In other words, the polyharmonic spline reconstruction $s$ in (4), satisfying $s_\Xi = u_\Xi$, minimizes the energy $|\cdot|_{\mathrm{BL}^m}$ among all recovery functions $u$ in $\mathrm{BL}^m(\mathbb{R}^d)$, i.e.,

$$|s|_{\mathrm{BL}^m} \le |u|_{\mathrm{BL}^m} \qquad \text{for all } u \in \mathrm{BL}^m(\mathbb{R}^d) \text{ with } u_\Xi = s_\Xi, \tag{7}$$

where the semi-norm $|s|_{\mathrm{BL}^m}$ of the polyharmonic spline reconstruction $s$ is given by the quadratic form

$$|s|_{\mathrm{BL}^m}^2 = \sum_{j,k=1}^n c_j c_k \phi_{d,m}(\|\xi_k - \xi_j\|), \tag{8}$$

whose coefficient vector $c = (c_1, \ldots, c_n)^T \in \mathbb{R}^n$ comes with the solution in (6).

## 6 Ten good reasons for using polyharmonic spline reconstruction

We summarize the discussion of this contribution by giving ten good reasons in favour of using polyharmonic spline reconstruction in particle flow simulations.

**Reason 1: Well-posedness.** Polyharmonic splines yield a well-posed reconstruction method, which guarantees the existence and uniqueness for a solution of Problem 1, for arbitrary stencils $\Xi \subset \mathbb{R}^d$ and values $u_\Xi$, and for any dimension $d \geq 1$. Indeed, due to Proposition 1, the system (6) has for $\phi_{d,m} \in \mathrm{CPD}(m, \mathbb{R}^d)$ a unique solution. This is in contrast to polynomial reconstruction. In fact, due to the *Mairhuber-Curtis theorem* [5, Theorem 5.25] from approximation theory, a reconstruction scheme can, for $d > 1$, only be well-posed, if the reconstruction space depends on the stencil $\Xi$.
**Reason 2: Efficient implementation and preconditioning.** The implementation of the polyharmonic spline reconstruction scheme merely requires solving square linear systems of the form (6), which can be set up very easily. To obtain efficient and numerically stable solutions of (6), we recommend our recent preconditioner, relying on hierarchical matrix approximation [6].
**Reason 3: Stable and efficient evaluation.** Polyharmonic splines allow for stable and efficient evaluations of their reconstructions. This is due to the scale-invariance of the reconstruction scheme's Lagrange basis, see [7, Sections 7.4] for more details.
**Reason 4: Stability by orthogonal projection.** The polyharmonic spline reconstruction $s$, satisfying $s_\Xi = u_\Xi$, is characterized by the (unique) orthogonal projection of $u \in \mathrm{BL}^m(\mathbb{R}^d)$ onto the linear subspace of reconstructions of the form (4). This property is covered by approximation theory in Euclidean spaces, cf. [5, Chapter 4], which further implies that $s$ is the *best approximation* to $u \in \mathrm{BL}^m(\mathbb{R}^d)$ w.r.t. $|\cdot|_{\mathrm{BL}^m}$.
**Reason 5: Optimality by energy minimization.** Polyharmonic spline reconstruction by $\phi_{d,m}$ is *optimal* in the Beppo-Levi space $\mathrm{BL}^m(\mathbb{R}^d)$, by the energy minimization in (7). The latter already follows from the best approximation property of the polyharmonic spline reconstruction scheme in $\mathrm{BL}^m(\mathbb{R}^d)$ w.r.t. $|\cdot|_{\mathrm{BL}^m}$ (cf. Reason 3).
**Reason 6: Polynomial reproduction.** If the stencil $\Xi$ is $\mathcal{P}_m^d$-unisolvent and if the input data $u_\Xi$ is sampled from a polynomial $u \in \mathcal{P}_m^d$, then we have $c = 0$ for the major part of the reconstruction $s$ in (4), satisfying $s_\Xi = u_\Xi$. This implies the polynomial reproduction property $s \equiv u$, due the well-posedness of the reconstruction scheme.
**Reason 7: Arbitrary local approximation order.** Polyharmonic spline reconstruction by $\phi_{d,m}$ has *local approximation order* $m$ with respect to $\mathscr{C}^m$ functions, i.e.,

$$|u(hx) - s^h(hx)| = \mathcal{O}(h^m) \quad \text{for } h \searrow 0 \qquad \text{for } u \in \mathscr{C}^m,$$

where $s^h$ is the (unique) polyharmonic spline reconstruction satisfying $s_{h\Xi} = u_{h\Xi}$. This result is due to the reproduction of polynomials from $\mathcal{P}_m^d$, cf. [7, Section 7.5].
**Reason 8: Flexible stencil selection.** According to the kernel-based reconstruction scheme of Section 4, we merely require $n \geq q$ for the number of particles $n = |\Xi|$, which allows us to work with variable stencil sizes. This is contrast to polynomial reconstruction, where the stencil size $|\Xi|$ is fixed a priori by the dimension of the polynomial space. The latter is often viewed as a severe restriction of polynomial WENO reconstructions (see [2]), where flexible stencils (of variable sizes) are desired.

**Reason 9: Natural oscillation indicator.** To avoid oscillations of reconstructions $s$, satisfying $s_\Xi = u_\Xi$, WENO schemes work with *oscillation indicators*. To this end, the polyharmonic spline reconstruction scheme provides a natural choice by the energy functional $|\cdot|_{\mathrm{BL}^m}$. This is further supported by the variational principle, according to which $s$ minimizes $|\cdot|_{\mathrm{BL}^m}$ among all recovery functions in $\mathrm{BL}^m(\mathbb{R}^d)$, see (7). Moreover, the minimum $|s|_{\mathrm{BL}^m}$ is readily available by the quadratic form (8).
**Reason 10: Meshfree reconstruction and high flexibility in adaptive methods.** The reconstruction scheme of polyharmonic splines is meshfree and therefore very flexible, especially when it comes to modifying the set of moving particles adaptively (cf. [9, Chapter 6]), which is particularly important for problems with solutions of rapid variation or singularities, or for problems with free or complicated boundaries.

Finally, meshfree reconstruction does obviously not rely on sophisticated algorithms for the generation and maintenance of a computational mesh, unlike in FD, FV, FE, DG and other mesh-based methods. This gives polyharmonic spline reconstructions (and other meshfree methods) yet another advantage, in particular for high-dimensional problems, where mesh generation is prohibitively expensive.

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