An interface-fitted subspace projection method for finite element simulations of particulate flows

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Abstract

A novel finite element method for the direct numerical simulation of particles in a Newtonian carrier fluid is presented. The proposed method is based on a fictitious or one-domain formulation and a subspace projection method to account for the rigid body motion of the particles. Underlying equations are posed in an ALE (arbitrary Lagrangian–Eulerian) formulation, allowing for moving computational meshes. The mesh is adapted to the particles by a novel mesh smoothing approach, guaranteeing both mesh optimality and a sharp representation of the particles’ boundaries.

We show that by using quadratic Taylor–Hood finite elements for the discretization of the Navier–Stokes equations and isoparametric elements to represent the geometry, second order convergence can be achieved (as opposed to a sharp $h^{1/2}$ result which holds if no mesh adaptation is performed).

We present numerical examples confirming the theoretical convergence result and show the potential of the method by simulating a lid–driven cavity flow with 100 particles.

Keywords: particulate flow, Navier–Stokes equation, finite element method, fictitious domain method, mesh optimization, arbitrary Lagrangian–Eulerian formulation

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1. Introduction

Highly accurate and efficient direct numerical simulation (DNS) of particulate flows is of great interest in many technical applications and processes [8]. Let us just briefly mention a few scenarios.

DNS of particulate flows may serve as the main building block in multiscale models [18, 26] or give essential insight into problems exhibiting complex behavior due to the presence of particles, for instance in gas flows loaded with particles [25]. Further application scenarios include complex interaction problems such as fluids containing ionized particles [17] or heat transfer processes [5, 12].

In view of various application scenarios and the many numerical methods available, there is still potential to improve upon existing methods in terms of accuracy and efficiency. This article is mainly concerned with addressing the first topic and presents a highly accurate, yet efficient finite element approach.

Over the years, many different methods have been proposed for the simulation of particulate flows. In terms of particle representation, these methods can be divided in two categories: The first category consists of methods based on unstructured computational grids aiming at resolving the particle geometry by the mesh. This can be done either by concentrating the mesh around the particle [28] or by explicitly representing the particle by the mesh [11, 16, 10]. The latter approach is usually facing the need for remeshing if severe mesh deformation occurs. The second category consists of methods which do not rely on an explicit representation of the geometry and are commonly defined on structured grids. Let us mention fictitious domain methods (FDM) based on Lagrange multipliers [13, 4, 3] and immersed boundary methods [19, 27]. Due to their efficiency, these methods are often used for the simulation of large scale particulate flow problems.

As far as the error analysis is concerned, many questions are still open. For most of the mentioned methods, sharp error bounds for the spatial discretization are not available.

This article aims at combining the advantages of both categories (accurate representation of the particle and efficient solution techniques) by making use of two methods presented in [22] and [2]. The first method, the subspace projection method (SPM), is an efficient technique used to enforce rigid body motion inside the discretized particles. The second method addresses the discretization of the particles by aligning a given mesh to the particles’ boundaries in an arbitrary Lagrangian–Eulerian (ALE) framework. The proposed alignment strategy guarantees mesh optimality while maintaining mesh connectivity. We give an error estimate for numerical solutions obtained on the particle aligned meshes. By formulating the equations in a moving coordinate system, both methods can be combined to yield an efficient and (provably) accurate algorithm which can be easily implemented in an existing Navier–Stokes solver due to its modularity.
2. Mathematical Model

In this section we introduce a model for particulate flows and hereby follow [21]. For the ease of presentation we restrict ourselves to the 2d–case with one particle. The extension to 3d and/or more particles is straightforward, and a detailed description can be found in [22]. We denote by $\Omega(t) \subset \mathbb{R}^2$ the area occupied by a Newtonian fluid with homogeneous Dirichlet boundary condition on its outer boundary $\Gamma_D$. $P(t) \subset \mathbb{R}^2$ is the particle of constant density $\rho_P$ and its center of mass is denoted by $X = \frac{1}{|P(t)|} \int_{P(t)} x \, dx$, while $r = x - X$ is its relative coordinate. It should be emphasized that the fluid area and the particle area do not intersect, $\Omega(t) \cap P(t) = \emptyset$. We denote by $\Omega_c(t) = \Omega(t) \cup P(t) \cup \partial P(t)$ the combined fluid/particle domain. The unknowns in the fluid area are the velocity $u$ and the pressure $p$, which are described by the Navier–Stokes–equations. The motion of the particle, being a rigid body, is described by Newton’s law. The describing values are the translatorial and angular velocities $U$, $\omega$, respectively, the position $X$ and the orientation in space given by the angle $\Theta$. In order to follow the motion of the particle explicitly, we consider the governing equations in a moving coordinate system (ALE, arbitrary Lagrangian–Eulerian formulation [15, 7]). We therefore assume that the combined fluid/particle domain can be expressed in terms of a reference domain $\Omega_c$ and a time depending mapping

\[
\chi : \mathbb{R} \times \mathbb{R}^2 \to \mathbb{R}^2 \\
\chi(t, \Omega_c) = \Omega_c(t).
\]  

We assume $\chi$ to be smooth and a homeomorphism for each time instant $t$. By defining the mesh velocity $y$ for each $t$,

\[
y(t, \cdot) : \Omega(t) \to \mathbb{R}^2 \\
y(t, \cdot) = \partial_t \chi(t, \chi(t, \cdot)^{-1}),
\]

Figure 1: Fluid domain $\Omega(t)$ and arbitrarily shaped particle $P(t)$. 

[125x706]
the system in nondimensional form and ALE formulation reads

\[ \partial_t u + (u - y) \cdot \nabla u + \nabla \cdot \left( \sigma \left( \frac{pI - \frac{1}{\text{Re}} D[u]}{\rho} \right) \right) = f \quad \text{in } \Omega(t), \quad (3) \]
\[ \nabla \cdot u = 0 \quad \text{in } \Omega(t), \quad (4) \]
\[ u = 0 \quad \text{on } \Gamma_D, \quad (5) \]
\[ u = U + \omega \times r \quad \text{on } \partial P(t), \quad (6) \]
\[ M \dot{U} = F + \int_{\partial P(t)} \sigma \cdot n \, ds, \quad (7) \]
\[ \dot{X} = U, \quad (8) \]
\[ I \dot{\omega} = \int_{\partial P(t)} r \times \sigma \cdot n \, ds, \quad (9) \]
\[ \dot{\Theta} = \omega. \quad (10) \]

see for example [11, 13, 28]. The two integrals on the right hand side represent the force and the torque, respectively, exerted by the fluid on the particle. Here, \( \sigma \) is the stress tensor, \( M \) denotes the mass of the particle and \( I \) its inertia. \( F \) is an external force acting on the particle (such as gravity or a force due to particle-particle interaction), \( \text{Re} \) denotes the Reynolds number and the deformation tensor is defined by \( D[u]_{i,j} = \partial_j u_i + \partial_i u_j \).

Following an idea of [13], we derive a weak formulation of the problem in the form of the fictitious domain or one-domain approach. To this end, the space of combined velocities is defined by

\[ H_c(\Omega_c) = \left\{ (v, V, \xi) \mid v \in (H^1(\Omega_c))^2, \ V \in \mathbb{R}^2, \ \xi \in \mathbb{R}, \ v = 0 \quad \text{on } \Gamma_D, \ v = V + \xi \times r \quad \text{in } P(t) \right\}, \quad (11) \]

where \( \xi \times r := (-r_2 \xi, r_1 \xi) \). The space \( H_c(\Omega_c) \) is called the space of combined velocities, since it contains all velocities posed in this problem, the fluid velocity, the translational particle velocity and the angular velocity represented by \( v, V \) and \( \xi \) respectively. We emphasize that the fluid velocity is defined on the whole domain \( \Omega_c \) and is restricted to the particle velocity inside the particle by the above definition. With test functions \( (v, V, \xi) \in H_c(\Omega_c) \) and \( q \in L^2(\Omega_c) \) we can state the weak formulation of our problem (3)–(10) as

\[ \int_{\Omega_c} \partial_t u \cdot v + (u - y) \cdot \nabla u \cdot v - p \nabla \cdot v - \frac{1}{2\text{Re}} D[u] : D[v] \, dx \]
\[ + (1 - \alpha) M \dot{U} \cdot V + (1 - \alpha) I \dot{\omega} \cdot \xi = \int_{\Omega_c} f \cdot v \, dx + F \cdot V, \quad (12) \]
\[ \int_{\Omega_c} \nabla \cdot u q \, dx = 0, \quad (13) \]
\[ \dot{X} = U, \quad (14) \]
\[ \dot{\Theta} = \omega. \quad (15) \]
Hereby $\alpha$ is the density fraction defined by $\alpha = \rho/\rho_p$. As we want to focus on the numerical method in the next chapter, we refer the reader to [13, 22] for a detailed derivation of the weak formulation on the combined domain $\Omega_c$.

For a shorter notation we define the linear forms

$$m(u, v) = \int_{\Omega_c} u \cdot v \, dx,$$

$$s(u, v) = \frac{1}{2\text{Re}} \int_{\Omega_c} D[u] : D[v] \, dx,$$

$$k(w; u, v) = \int_{\Omega_c} (w \cdot \nabla)u \cdot v \, dx,$$

$$b(p, v) = \int_{\Omega_c} p \nabla \cdot v \, dx,$$

$$L(U, V) = (1 - \alpha) M U \cdot V,$$

$$S(\omega, \xi) = (1 - \alpha) (I \omega) \cdot \xi,$$

leading to the following compact formulation of the problem

$$m(\partial_t u, v) + k(u - y; u, v) + s(u, v) - b(p, v) + L(\dot{U}, V) + S(\dot{\omega}, \xi)$$

$$= m(f, v) + F \cdot V,$$

$$b(q, u) = 0,$$

$$\dot{X} = U,$$

$$\dot{\Theta} = \omega.$$
3. Numerical method: Overview and time discretization

Our numerical scheme to solve the problem (22)–(25) is based on the following four main building blocks, which will be described in detail in the subsequent sections:

- Splitting: in order to reduce the complexity of the problem we separate the calculation of the particle’s time dependent location from the calculation of the flow field.
- Adaptivity and domain update: a novel mesh deformation method is used to align the mesh to the particle geometry while maintaining mesh connectivity.
- Time discretization: a BDF2 projection scheme is used for the efficient solution of the Navier–Stokes equations on the particle adapted mesh.
- Subspace projection: a novel method to take into account the restriction of the function space $H_c(\Omega_c)$.

3.1. Splitting

For an efficient numerical treatment we initially split the position of the particle from the remaining variables. To this end the time interval $(0, T)$ is subdivided by discrete time instants: $0 = t_0 < t_1 < \cdots < t_N = T$.

For $k = 1, \ldots, N - 1$

1. Predictor: Find solutions $X, U, \Theta$ and $\omega$ for $t \in (t_k, t_{k+1})$ according to equations (24), (25), $M \ddot{U} = F$ and $I \ddot{\omega} = 0$.
2. Velocities: For $t \in (t_k, t_{k+1})$ solve

$$m(\dot{p}, v) + k(u - y; u, v) + s(u, v) - b(p, v) +$$
$$+ L(\dot{\Omega}, V) + S(\dot{\omega}, \xi) = m(f, v),$$
$$b(q, u) = 0.$$  

In the first step the positions $(X, \Theta)$ and velocities $(U, \omega)$ of the particle are calculated, while in the second step the velocities of the particle are corrected and the fluid velocity and pressure is computed. The effect of the external force $F$ is only taken into account in the predictor step. The force the fluid causes on the particle is created implicitly by the terms $L(\dot{\Omega}, V)$, $S(\dot{\omega}, \xi)$ and the usage of the space of combined velocities $H_c(\Omega_c)$.

3.2. Time discretization

For the time discretization of the predictor a velocity verlet method with $a = \frac{F}{M}$ for the variables $X$ and $U$ is used:

$$X^{k+1} = X^k + \tau U^k + \frac{\tau^2}{2} a^k,$$
$$U^{k+\frac{1}{2}} = U^k + \frac{\tau}{2} a^k,$$
$$a^{k+1} = \text{evaluate forces at new positions } X^{k+1},$$
$$U^{k+1} = U^{k+\frac{1}{2}} + \frac{\tau}{2} a^{k+1}.$$
For a more detailed description of the algorithm see for example [20]. The variables $\Theta$ and $\omega$ are discretized by the implicit midpoint rule. Once the new particle position $X^{k+1}$ is obtained, the mesh is adapted to the particle using a novel approach presented in subsection 4.2. This procedure results in a modified triangulation $T_{k+1}$ of $\Omega_{c}^{k+1}$. The mesh velocity is updated using the old and new nodal coordinates of the triangulation, i.e.

$$y^{k+1}_{i} = (x^{k+1}_{i} - x^{k}_{i})/\tau$$

for all nodes $x^{k+1}_{i} \in T^{k+1}$, \hfill (31)

where $\tau = t^{k+1} - t^{k}$ denotes the time step size.

The flow field governed by the Navier–Stokes equations is solved by a BDF2 based projection method in rotational form, see [14]. Introducing $\gamma = \frac{2}{3}\tau$, this scheme is based on three steps to solve the system of equations (26):

1. Burgers problem

$$m(u^{k+1}, v) + \gamma k(u^{k+1} - y^{k+1}; u^{k+1}, v) + \gamma s(u^{k+1}, v)$$

$$+ \frac{2}{3}L(U^{k+1}, V) + \frac{2}{3}S(\omega^{k+1}, \xi)$$

$$= \gamma b(p^{k}, v) + \gamma m(f(t^{k+1}), v)$$

$$+ m\left(\frac{4}{3}u^{k} - \frac{1}{3}u^{k-1}, v\right) + \gamma b\left(\frac{4}{3}k - \frac{1}{3}k^{k-1}, v\right)$$

$$+ \frac{2}{3}L(U^{k}, V) + \frac{2}{3}S(\omega^{k}, \xi)$$ \hfill (32)

2. Poisson problem

$$m(\nabla \chi^{k+1}, \nabla \Psi) = \frac{1}{\gamma}b(\Psi, u^{k+1})$$ \hfill (33)

3. Update

$$m(p^{k+1}, q) = m(p^{k} + \chi^{k+1}, q) - b(q, \frac{2}{\text{Re}}u^{k+1})$$ \hfill (34)

In the practical realization presented later, the form $k$ is linearized by extrapolation: $k(u^{*} - y^{k+1}; u^{k+1}, v)$ with $u^{*} := 2u^{k} - u^{k-1}$.

While problems (33), (34) can be solved in a standard way, the condition $v = V + \xi \times r$ in $P(t)$ used in definition of the space $H_{c}(\Omega_{c})$ (11) has to be taken into account for Burgers problem (32). An efficient realization of this condition by means of the *subspace projection method* will be presented in the following section.
4. Numerical method: Space discretization

The crucial point in the spatial discretization is to define a discrete counterpart $X_c$ of $H_c(\Omega_c)$ and, moreover, the concrete realization of this non–standard finite element space.

4.1. Finite element discretization using the subspace projection method

In this subsection, the definition of $X_c$ and its concrete realization are briefly introduced. A more detailed presentation of the realization can be found in [22].

In the following we will make use of quadratic isoparametric simplicial elements, i.e. elements $T$ which can be written in terms of the standard reference simplex $\hat{T}$ and a quadratic mapping $G_T : \hat{T} \rightarrow T$,

\[
\hat{T} = \{ \hat{x} = (\hat{x}_1, \hat{x}_2) \in \mathbb{R}^2 : \hat{x}_1 + \hat{x}_2 \leq 1, \hat{x}_i \geq 0 \} \quad \text{and} \quad T = G_T(\hat{T}) \quad \text{where} \quad G_T(\hat{x}) := \sum_{i=1}^{6} x_i \varphi_i(\hat{x}) \quad \text{for} \quad \hat{x} \in \hat{T}.
\]

(35)

Here $\{x_i\}$ denotes the positions of the vertices associated with the quadratic Lagrange basis functions $\varphi_i$.

In the following, we assume $T = T^{k+1}$ to be an arbitrary triangulation of $\Omega^{k+1}_c$ consisting of isoparametric elements (35), i.e. we do not (yet) assume the triangulation to be aligned to the particle. We denote by $P_h = P_h(t^{k+1})$ the discrete particle which consists of elements completely enclosed in the continuous particle $P(t^{k+1})$ at time instant $t^{k+1}$, i.e.

\[
P_h = \bigcup \{ T | T \in T^{k+1} \text{ and } T \subset P \}.
\]

Using these notations, we introduce the following finite element spaces

\[
\tilde{X} := \left\{ v \in (C^0(\Omega_c))^2 | v \circ G_T \in \left( P^2(\hat{T}) \right)^2 \forall T \in T, v = 0 \text{ on } \Gamma_D \right\},
\]

\[
X := \left\{ v = (v, V, \xi) | v \in \tilde{X}, V \in \mathbb{R}^2, \xi \in \mathbb{R} \right\},
\]

(36)

\[
X_c := \left\{ v \in X | v|_T = V + \xi \times \mathbf{r} \text{ for all } T \in P_h \right\},
\]

(37)

\[
Y := \left\{ p \in C^0(\Omega_c) | p \circ G_T \in P^1(\hat{T}) \text{ for all } T \in T \right\}.
\]

(38)

\[
\tilde{X} \text{ is the standard Lagrange finite element space consisting of globally continuous, piecewise quadratic functions with homogeneous Dirichlet boundary conditions on } \Gamma_D. \text{ The space } X \text{ augments functions in } \tilde{X} \text{ by three additional degrees of freedom – two for the particle velocity } V \text{ and one for the angular velocity } \xi. \text{ If more than one particle is considered, } X \text{ has to be extended by three degrees of freedom for each additional particle. The pair } \tilde{X} \times Y \text{ is the usual LBB-stable } \textit{Taylor–Hood} \text{ finite element space which is commonly used for the discretization of the Navier–Stokes equations. Note that problems (33) and}
\]
are solved with Y as test– and trialspace. For an arbitrary time step \( k \) the linearized Burgers problem (32) may be rewritten with a bilinear form \( a \), corresponding operator \( A \), and a cumulative right hand side \( g \): find \( u \in X_c \) such that for all \( v \in X_c \)

\[
a(u, v) := (Au, v) = l(v). \tag{39}
\]

holds. The bilinear form \( a \) is defined as

\[
a(u, v) = a((u, U, \omega), (v, V, \xi)) := m(u, v) + \gamma k(u^* - y^{k+1}; u, v) + \gamma s(u, v) + \frac{2}{3} L(U, V) + \frac{2}{3} S(\omega, \xi) \tag{40}
\]

and the cumulative right hand side as \( l(v) \) corresponding to the right hand side in equation (32).

To circumvent the explicit representation of \( H_c(\Omega_c) \), a subspace projection \( \mathcal{P} : X \to X_c \) is used. With this operator (39) may be formulated in terms of the standard finite element space \( X \): find \( \tilde{u} \in X \) such that for all \( v \in X \)

\[
(\mathcal{P}\tilde{u}, \mathcal{P}v) = (g, \mathcal{P}v). \tag{41}
\]

holds. Note that the solution \( u \) is now easily found by taking \( u = \mathcal{P}\tilde{u} \), where \( \tilde{u} \) is a solution of equation (41). The above system leads to a linear system of equations for the nodal finite element vector \( \tilde{U} \) of the form

\[
\mathcal{P}^T A \mathcal{P} \tilde{U} = \mathcal{P}^T G, \tag{42}
\]

where \( A \) is the system matrix corresponding to operator \( A \) and \( \mathcal{P} \) is a matrix representation of \( \mathcal{P} \). Note that when using iterative solvers, one can bypass the explicit computation of the modified system matrix \( \mathcal{P}^T A \mathcal{P} \) by just slightly modifying the matrix vector product since only the action of \( \mathcal{P}^T A \mathcal{P} \) on a vector has to be considered. We call this method the subspace projection method. Because the matrix \( \mathcal{P} \) is quite simple, explicit storage is not necessary. Instead, a short routine can perform the multiplication of \( \mathcal{P} \) and \( \mathcal{P}^T \) with a vector \( v \). Details on the numerical realization of the projection, implementation and preconditioning of the system (42) can be found in [22, 23].

\subsection*{4.2. Mesh adaptation using a novel mesh smoothing approach}

For the method introduced in the previous section, no assumptions were made regarding the representation of the particle’s geometry in terms of the triangulation \( \mathcal{T} \).

However, as was shown in [22], a method which does not explicitly take into account the particle’s geometry is inherently plagued by a low convergence order of \( h^{1/2} \) in the energy norm of the velocity. The authors proposed local mesh adaptivity at the particle’s boundary to deal with the local nature of this behavior.

On the other hand, and as will be shown in subsection 4.3, representing the particle’s boundary using linear or quadratic edges of the triangulation will lead to convergence orders of \( h \) and \( h^2 \), respectively (the later being optimal if the velocity is represented by piecewise quadratics).
In what follows we will introduce a novel moving mesh approach for particulate flows which is able to follow the geometry of the particle explicitly without the need for remeshing. Furthermore, the proposed approach maintains mesh connectivity while guaranteeing optimality of the mesh’s quality. The approach is based on a method presented in [2] where it was used for the simulation of a (simplified) fluid–structure interaction problem and a two–phase flow benchmark problem. In what follows we briefly revisit this approach.

4.2.1. Optimal meshes

The main building block of the mesh smoothing method is a variational mesh optimization technique for simplicial triangulations based on a family of functionals proposed by M. Rumpf [24]. Given an initial triangulation $T$, the idea is to find an “optimal” triangulation $T^* = \varphi^*(T)$ resulting from an optimal mesh deformation $\varphi^*$ which is determined from minimizing a functional $F$ over a set of certain admissible deformations $\{\varphi : T \to \mathbb{R}^2\}$ of the triangulation, i.e.

$$F(\varphi^*) = \min_{\varphi} F(\varphi).$$

(43)

Under some assumptions (we refer to [24] for a detailed discussion), the functionals in (43) can be represented by the sum of weighted, element-wise functionals,

$$F = \sum_{T \in T} \mu_T F_T(\varphi)$$

(44)

where $\mu_T > 0, \sum_T \mu_T = 1$ denotes a positive weight and $F_T$ the contribution of the deformation $\varphi$ restricted to $T$. Assuming translational invariance, isotropy and frame indifference, $F_T$ may expressed in terms of the invariants of the linear reference mapping $R_T : h(T)T^* \to T$, where $T^*$ denotes the normalized equilateral simplex and $h(T)$ denotes the desired edge length for $T$. In two dimensions, $F_T$ takes the form

$$F_T = F(\|\nabla R_T(\varphi)\|^2, \det(\nabla R_T(\varphi))) =: F(a, d).$$

(45)

The optimally deformed simplex $h(T)T^*$ is obtained if $\varphi^*_T = \|$, i.e. if

$$F_T(\varphi^*) = \min_{\varphi} F_T(\varphi) = F_T(\|) = F(\|\|^2, \det(\|)) = F(2, 1).$$

In order to rule out deformations with vanishing determinant, we also assume that

$$\lim_{\det(\nabla R_T(\varphi)) \to 0} F_T(\varphi) = \infty.$$ A typical example of a local function $F_T$ which is also used in the computations presented in this work is given by

$$F(a, d) = (a - 2)^2 + d + \frac{1}{d}.$$}

(46)

Let us close this section by briefly summarizing the properties and benefits of the variational mesh smoothing approach (see also [24], [2]):

- By minimizing (44), one obtains a triangulation $T^*$ which is optimal in the sense of the local measure (46).
• Triangulations obtained from the minimizers of (44) are non–degenerate (no self–intersection of elements occurs).

• The element–wise representation of $F$ allows for local mesh quality control.

• $r$–adaptivity can be easily achieved by prescribing desired edge lengths for each mesh element.

• However, the functional is highly non–linear and global minimizers may be non–unique.

4.2.2. Particle aligned optimal meshes

Let us now extend this method in such a way that resulting triangulations, despite being of optimal quality, are aligned to the particle’s boundary. To this end, we assume that the particle domain $P$ and the fluid domain $Ω$ may be written in terms of a continuous level set function $ϕ$, i.e.

$$P(t) = \{x \in \mathbb{R}^2 : ϕ(t, x) < 0\}$$

$$Ω(t) = \{x \in \mathbb{R}^2 : ϕ(t, x) > 0\}.$$  

(47)  

(48)

The particle’s boundary $∂P$ corresponds to the zero level set of $ϕ$,

$$∂P(t) = \{x \in \mathbb{R}^2 : ϕ(t, x) = 0\}.$$  

(49)

We furthermore assume that the size of the particle is (much) bigger than the mesh size $h$.

Let us start with a fundamental observation on the alignment of edges of the triangulation $T$ and the particle’s boundary $∂P$. Consider the situation depicted in Figure 2 (left) and let $e$ be an arbitrary edge of $T$. Denote by $x_{e,1}$ and $x_{e,2}$ the nodes adjacent to $e$. Due to continuity of $ϕ$ and assumption (49), we observe that

$$ϕ(x_{e,1})ϕ(x_{e,2}) < 0$$  

(50)

if and only if $e$ is intersected by $∂P$.

We thus define the triangulation $T$ to be **linearly aligned** to the particle’s boundary if

$$ϕ(x_{e,1})ϕ(x_{e,2}) ≥ 0$$  

(51)

for all edges $e \in T$, i.e. no edge $e$ of $T$ is intersected by the particle’s boundary. The idea is to introduce an additional constraint for minimization problem (43) which rules out deformations violating condition (51):

$$c(ϕ) = \sum_{e \in ϕ(T)} H(ϕ(x_{e,1})ϕ(x_{e,2}))$$  

where

$$H(z) = \begin{cases} 
> 0 & \text{for } z < 0, \\
= 0 & \text{otherwise.}
\end{cases}$$  

(52)  

(53)

Restricting the set of deformations to deformations for which the particle boundary is aligned to the edges of $ϕ(T)$, i.e. $c(ϕ) = 0$ while maintaining optimality...
of the deformation, we end up with a non–linear optimization problem with a non–linear constraint:

$$\min_{\varphi} F(\varphi) \quad \text{such that} \quad c(\varphi) = 0. \quad (54)$$

Optimization problem (54) may be solved, for instance, using a quadratic penalty method. Details on the realization of such a method in this context can be found in [2].

Recalling that $P_h$ denotes the union of all mesh elements which are located completely inside the particle $P$ (see also Figure 2), we may denote by $\partial P_h$ the discrete particle boundary,

$$\partial P_h = \{ e \in T : e = T_i \cap T_j \quad \text{for} \quad T_i \in P_h, T_j \in T \setminus P_h \}. \quad (55)$$

In order to increase the approximation quality of the discrete interface $\partial P_h$, isoparametric elements are used. For each edge $e \in \partial P_h$, the quadratic degree of freedom $x_m$ located at the midpoint of $e$ is moved onto the zero level set of $\phi$, i.e. the particle’s boundary (see Figure 3). If all edges $e \in \partial P_h$ are aligned to the particle’s boundary, we call the mesh quadratically aligned. The influence of linear and quadratic mesh alignment on the approximation quality of the discrete solution will be subject of the next subsection.

**Remark 1.** Note that applying the proposed mesh adaptation method will result in triangulations which are aligned to the particle’s boundary. However, if time dependent problems are considered, nodes located at $\partial P_h$ for some time instant $t^k$ may not be part of the discrete particle’s boundary at $t^{k+1}$, i.e. nodes and consequently elements are free to change their belonging to $P$ or $\Omega$. It is this aspect which provides the proposed method with enhanced geometrical flexibility (as compared to classical moving mesh schemes), making remeshing unnecessary. We will visualize this behavior in numerical subsection 5.2.

### 4.3. Error estimate

In [22] an error estimate was presented for a slightly simplified version of core problem (56) and the case of no mesh alignment. In the following we closely
follow the presented situation and proof and show that linear and quadratic mesh alignment leads to a significant increase of the order of convergence.

For simplicity set \( u^* = y = 0 \) in the bilinear form (40), i.e. we assume a (quasi–) stationary situation with no mesh movement. We define the corresponding energy norm

\[
\|v\|_c^2 := a(v, v),
\]

and assume \( u \in H_c(\Omega_c) \) to be the continuous solution of

\[
a(u, v) = l(v) \quad \text{for all } v \in H_c(\Omega_c).
\]

(56)

Let \( u_h \in X_c \) be the corresponding finite element solution fulfilling

\[
a(u_h, v_h) = l(v_h) \quad \text{for all } v_h \in X_c.
\]

(57)

The error estimate is complicated by two difficulties: the velocity \( u \) is, in general, not smooth across \( \partial P \) and since \( X_c \not\subset H_c(\Omega_c) \) in general, the proposed approach is a non–conforming method. In what follows we assume that \( \Omega_c \) is discretized by a family of conforming, shape regular quasi–uniform triangulations \((T_h)_{h>0}\) (aligned or non-aligned to the particle’s boundary) while \( h \) denotes the mesh size. We make use of Strang’s Second Lemma to bound the error:

**Theorem 2** (Strang’s Second Lemma). Assume the following:

- The bilinear form \( a(\cdot, \cdot) \) is bounded in \( X_c \times X_c \).
- There exists \( \eta > 0 \) such that

\[
\inf_{0 \neq u_h \in X_c} \sup_{0 \neq v_h \in X_c} \frac{a(u_h, v_h)}{\|u_h\|_c \|v_h\|_c} \geq \eta
\]
Then the following error estimate holds:

\[ \|u - u_h\|_c \leq \left(1 + \frac{\|a\|_{X_e \times X_e}}{\eta}\right) \inf_{v_h \in X_e} \|u - v_h\|_c + \frac{1}{\eta} \sup_{v_h \in X_e} \frac{|(v_h) - a(u, v_h)|}{\|v_h\|_c} \]  

(58)

**Proof.** See for instance [9]. \[ \square \]

**Theorem 3** (Convergence). Let \( u = (u, U, \omega) \) be the continuous solution of problem (56). Denote by \( u_h \) the discrete solution of problem (57). Additionally assuming \( u \in H^3(\Omega) \), \( u \in H^3(P) \), \( u \in H^{1,\infty}(\Omega_c) \) and that \( P \) is a sphere, the error \( \|u - u_h\|_c \) is bounded by

\[ \|u - u_h\|_c \leq C(u) \begin{cases} h^{1/2} & \text{no mesh alignment} \\ h & \text{linear mesh alignment} \\ h^2 & \text{quadratic mesh alignment} \end{cases} \]  

(59)

**Remark 4.** As we will see for a numerical example presented in subsection 5.1, these estimates are sharp. Numerical experiments in [22] suggest that the main source of error is concentrated in the region \( P \setminus P_h \). As a consequence, one expects that reducing the size of this region will lead to better convergence behavior. However, it is worth emphasizing that only quadratic mesh alignment leads to optimal second order convergence for a given family of triangulations \( (T_h) \) (assuming that no additional local mesh refinement is performed).

**Proof.** The proof for the case of no mesh alignment can be found in [22] and we therefore restrict the presentation to the mesh alignment cases. Denote by \( \sigma(P) = \{ T \in T : P \cap T \neq \emptyset, T \not\subset P \} \) elements which are intersected by the particle’s boundary. We also consider a tube region \( P_\delta \subset \Omega \) of width \( \delta \) (\( \delta \) not depending on \( h \)) whose inner boundary coincides with the particle’s boundary \( \partial P \). Let \( A = K \cap P \) for \( K \in \sigma(P) \) be the thin region sketched in Figure 4. Note that in the case of a spherical particle, \( A \) has a width proportional to \( h^2 \) (linearly aligned case) or \( h^4 \) (quadratically aligned case), respectively. Therefore, for the measure of \( A \) we have

\[ \text{meas}(A) \leq C \begin{cases} h^3 & \text{linear mesh alignment} \\ h^5 & \text{quadratic mesh alignment} \end{cases} \]  

(60)

To prove estimate (59), we first observe that the assumptions of Strang’s Second Lemma (58) are fulfilled with \( \eta = 1 \). We start by bounding the approximation error \( \inf_{v_h \in X_e} \|u - v_h\| \) and set \( v_h = (I_h u, U, \omega) \) where \( I_h \) denotes the standard Lagrange interpolation operator. For all elements \( K \in T \setminus \sigma(P) \) (i.e. elements not intersected by the particle boundary) one has the standard interpolation error estimate [6]

\[ \|\nabla (u - I_h u)\|_K^2 \leq C h^4(|u|_{2,K} + |u|_{3,K})^2. \]  

(61)

Note that for elements \( K \subset P \) inside the particle, \( u = I_h u \) holds. It remains to bound the error for \( K \in \sigma(P) \). Denote by \( \tilde{u} \) a \( H^3(\mathbb{R}^2) \) extension of \( u|_{P_h} \in H^3(P_h) \), i.e. \( \tilde{u} \in H^3(\mathbb{R}^2) \) fulfilling

\[ \|\tilde{u}\|_{3,\mathbb{R}^2} \leq C \|u\|_{3,P_h} \]  

(62)

14
Figure 4: Fluid domain $\Omega$, particle $P$, tube region $P_5$ and a linearly aligned triangle $K$ with corresponding quadratic Lagrange nodes. The region $A$ is represented by the striped area within $K$.

where $C$ only depends on $P_5$ (see for instance [1]). Using the extension, we now write

$$
\| \nabla (u - I_h u) \|^2_K \leq \| \nabla (u - \tilde{u}) \|^2_K + \| \nabla (\tilde{u} - I_h u) \|^2_K
$$

and bound the first term:

$$(I) \quad = \quad \| \nabla (u - \tilde{u}) \|^2_A \leq \| u - \tilde{u} \|^2_{1,\infty, A} \text{ meas}(A) \quad (63)$$

For the second term $(II)$, we add and subtract $I_h \tilde{u}$

$$(II) \quad \leq \quad \| \nabla (\tilde{u} - I_h \tilde{u}) \|^2_K + \| \nabla (I_h u - I_h \tilde{u}) \|^2_K \quad (64)$$

$$\leq \quad C h^4 \| \tilde{u} \|^2_{3, K} + \| \nabla (I_h u - I_h \tilde{u}) \|^2_K \quad (65)$$

where we have used the standard estimate (61) for the first term. It remains to bound the second term. Note that in the case of isoparametric elements all Lagrange nodes are located in $K \setminus A$ and due to $I_h u = I_h \tilde{u}$ the second term vanishes. In the case of linear mesh alignment all values of $u, \tilde{u}$ at the Lagrange nodes coincide except for one degree of freedom which we denote by $x_m$ (see Figure 4). Using the notation $\varphi_m$ for the basis function located at node $x_m$, we compute

$$
\| \nabla (I_h u - I_h \tilde{u}) \|^2_K = |u(x_m) - \tilde{u}(x_m)|^2 \| \nabla \varphi_m \|^2_K \leq C \| u - \tilde{u} \|^2_{0,\infty, A}.
$$

Now $u = \tilde{u}$ on $\partial A \setminus \partial K$ and due to a Poincaré-like estimate we obtain

$$
\| u - \tilde{u} \|^2_{0,\infty, A} \leq C h^4 \| u - \tilde{u} \|^2_{1,\infty, A}. \quad (66)
$$
as an additional term in the linear mesh alignment case. Adding (I) and (II) yields the element-wise estimate

\[
\|\nabla (u - I_h u)\|_K^2 \leq \|u - \tilde{u}\|_{2,\infty,A}^2 \text{meas}(A) + C h^4 \|\tilde{u}\|_{3,K}^2 + C h^2 \|u - \tilde{u}\|_{1,\infty,A}^2 \\
+ \begin{cases} 
C h^4 \|u - \tilde{u}\|_{1,\infty,A}^2 & \text{linear mesh alignment} \\
0 & \text{quadratic mesh alignment}
\end{cases}
\]  

(67)

Let \(UA\) be the union of all regions \(A\) and \(\text{meas}(UA)\) be the measure of region \(UA\), i.e.

\[
UA = \bigcup_{K \in \sigma(P)} A \subset P \quad \text{and} \quad \text{meas}(UA) = \sum_{A \in UA} \text{meas}(A).
\]

and

\[
\text{meas}(UA) \leq C \begin{cases} 
h^2 & \text{linear mesh alignment} \\
h^4 & \text{quadratic mesh alignment}
\end{cases}
\]  

(68)

holds. By noting that the cardinality \(#\sigma(P)\) \(\leq Ch^{-1}\) summing estimate (67) over all elements \(K \in \sigma(P)\) we have

\[
\sum_{K \in \sigma(P)} \|\nabla (u - I_h u)\|_K^2 \leq C \text{meas}(UA) \|u - \tilde{u}\|_{2,\infty,U_A}^2 + C h^4 \|\tilde{u}\|_{3,\sigma(P)}^2 + C h^2 \|u - \tilde{u}\|_{1,\infty,U_A}^2 + C h^4 \|u - \tilde{u}\|_{3,\sigma(P)}^2
\]

(69)

Using the embedding \(H^3(P) \hookrightarrow H^{1,\infty}(P)\) and the continuity of the extension operator (62), one obtains

\[
\sum_{K \in \sigma(P)} \|\nabla (u - I_h u)\|_K^2 \leq C \text{meas}(UA) \|u\|_{3,P}^2 + \|u\|_{3,P_h}^2 + C h^4 \|u\|_{3,P}^2 + C h^2 \|u\|_{3,P_h}^2
\]

(69)

Adding error estimates (69) to the sum of (61) for \(K \in \mathcal{T} \smallsetminus \sigma(P)\) and taking the square root yields

\[
\|u - u_h\|_c \leq C(u) \begin{cases} 
h & \text{linear mesh alignment} \\
h^2 & \text{quadratic mesh alignment}
\end{cases}
\]

We now bound the consistency error (i.e. the second term on the right hand side of equation (58)). For an arbitrary \(v_h = (v_h, V, \xi) \in X_c\) a direct computation yields

\[
a(u, v_h) - l(v_h) = \int_P (u - rhs_1) \cdot (v_h - V - \xi \times r) + \frac{\gamma}{Re} \int_{\partial P} \text{D}[u] \cdot (v_h - V - \xi \times r), \quad (70)
\]
where \( \text{rhs}_1 \) denotes the terms on the right hand side of equation (56).

Note that since \( v_h \in X_C \),

\[
v_h - V - \xi \times r = 0 \quad \text{in} \quad P \setminus UA
\]

and furthermore \( v_h - V - \xi \times r = 0 \) on \( \partial(P \setminus UA) \). We thus bound the first term in equation (70) by taking into account the width of \( UA \) and using Poincaré’s inequality

\[
\int_P (u - \text{rhs}_1) \cdot (v_h - V - \xi \times r) = \int_{UA} (u - \text{rhs}_1) \cdot (v_h - V - \xi \times r) \\
\leq C \text{meas}(UA)(\|u\|_{UA} + \|\text{rhs}_1\|_{UA})\|\nabla(v_h - V - \xi \times r)\|_{UA}
\]

(72)

The boundary term in (70) is bounded by using the embeddings \( H^1(UA) \hookrightarrow L^2(\partial P) \) and \( H^1(\Omega) \hookrightarrow L^2(\partial P) \):

\[
\int_{\partial P} D[u] \cdot (v_h - V - \xi \times r) \leq \|D[u]\|_{\partial P}\|v_h - V - \xi \times r\|_{\partial P} \\
\leq C\|u\|_{2,\Omega} \text{meas}(UA)^{1/2}\|\nabla(v_h - V - \xi \times r)\|_{UA}.
\]

(73)

Adding (72) and (73) together with Korn’s inequality for \( \|\nabla(v_h - V - \xi \times r)\| \) finally yields

\[
a(u,v_h) - l(v_h) \leq C \text{meas}(UA)^{1/2} \left( \frac{\gamma}{Re} \|u\|_{2,UA} + \|u\|_{UA} + \|\text{rhs}_1\|_{UA} \right) \|v_h\|_c.
\]
5. Numerical results

In [22] the subspace projection method for particulate flows was validated quantitatively by simulating a sedimentation process and a particle laden fluid in a viscometer. The numerical results were compared to both theoretical predictions and values from literature obtaining good agreement. In this section we present numerical results obtained by the proposed method which extends the subspace projection method for particulate flows by a sharp discretization of the particles’ boundaries. In order to validate the error estimate from subsection 4.3, the first example considers a quasi–stationary situation with an analytical solution.

A second example shows the potential of the method by simulating a lid–driven cavity flow with 100 particles and comparing the results obtained on a fixed mesh simulation with the results obtained by the proposed approach.

5.1. Quasi–stationary model problem

Consider the square \( \Omega_c = [-1,1]^2 \subset \mathbb{R}^2 \) and a spherical particle \( P = B_{1/2}(0) \subset \Omega_c \) of radius 0.5 located at the origin. For an arbitrary \( a > 0 \) and parameters \( \text{Re} = 1, \alpha = 3/4 \) an analytical quasi–stationary solution of problem (56) is given by the velocity field

\[
U = [0,0]^T \quad \text{and} \quad \omega = 1.
\]

Note that \( u \) is not smooth across \( \partial P \).

We obtain numerical solutions \( u_h \) of (56) on three different types of triangulations of \( \Omega_c \):

- a uniform triangulation of \( \Omega_c \) not aligned to the particle (see Figure 5(c)),
- a triangulation obtained from the uniform triangulation and additionally linearly aligned to the particle using the proposed mesh smoothing approach and
- a triangulation quadratically aligned to the particle using the proposed approach (see Figure 5(d)).

The corresponding magnitude of the velocity field on \( \Omega_c \) is plotted in Figure 5 for the first and third case on the coarsest refinement level. On the uniform triangulation we observe oscillations in the velocity magnitude close to the particle’s boundary resulting from its very crude representation. On the aligned triangulation, nodes are located directly on the exact boundary \( \partial P \), allowing for a much finer resolution of \( \partial P_h \).

For five refinement levels and each type of triangulation, we measure the combined error \( ||u - u_h||_c \) and summarize the results in Table 1. As expected from the a priori estimate of Theorem 3 the order of convergence is 1/2 if no mesh alignment is performed. Linear mesh alignment increases the order of convergence to 1 and quadratic alignment yields a convergence order of 2, which is optimal for second order Taylor–Hood finite elements.
Figure 5: Warp of the velocity norm of the numerical solution obtained on the non aligned and aligned triangulation. Figure 5(c)–5(d) show the corresponding triangulations together with elements of the discrete particle \( P_h \) marked red and the boundary of the particle \( P \) (white). The triangulation corresponds to the coarsest mesh (refinement level 3).

<table>
<thead>
<tr>
<th>Level</th>
<th>( |u - u_h|_c )</th>
<th>EOC</th>
<th>( |u - u_h|_c )</th>
<th>EOC</th>
<th>( |u - u_h|_c )</th>
<th>EOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.53136e + 00</td>
<td>–</td>
<td>0.29000e + 00</td>
<td>–</td>
<td>0.39910e - 01</td>
<td>–</td>
</tr>
<tr>
<td>4</td>
<td>0.35533e + 00</td>
<td>0.58</td>
<td>0.14603e + 00</td>
<td>0.99</td>
<td>0.10622e - 01</td>
<td>1.91</td>
</tr>
<tr>
<td>5</td>
<td>0.27877e + 00</td>
<td>0.35</td>
<td>0.73734e - 01</td>
<td>0.99</td>
<td>0.27702e - 02</td>
<td>1.94</td>
</tr>
<tr>
<td>6</td>
<td>0.19231e + 00</td>
<td>0.54</td>
<td>0.36833e - 01</td>
<td>1.00</td>
<td>0.71143e - 03</td>
<td>1.96</td>
</tr>
<tr>
<td>7</td>
<td>0.13067e + 00</td>
<td>0.56</td>
<td>0.18738e - 01</td>
<td>0.98</td>
<td>0.18239e - 03</td>
<td>1.96</td>
</tr>
</tbody>
</table>

Table 1: Combined error norm and experimental order of convergence for different global refinement levels and types of mesh alignment.

5.2. Lid–driven cavity flow with 100 particles

In this second example, we are interested in the dynamic behavior of 100 spherical particles located in a lid–driven cavity flow and a (qualitative) comparison between the results obtained by the standard subspace projection method on a fixed mesh and the proposed higher order method on particle aligned...
Consider the square domain \( \Omega_c = [-1, 1]^2 \subset \mathbb{R}^2 \). We add 100 spherical particles of radius \( r = 0.05 \) (see Figure 7(a)). The Newtonian fluid occupying the liquid domain \( \Omega \) is defined by a Reynolds number of \( \text{Re} = 5 \), and the density ratio between fluid and particle is \( \alpha = 0.5 \). We prescribe a parabolic boundary condition for the velocity at the top of the domain and no slip boundary condition at the remaining boundary. Initially, the fluid and the particles are assumed to be at rest. In order to model particle collisions, we use simple short range forcing terms \( F_{ij} \propto (X_i - X_j)/\|X_i - X_j\| \) for particle–particle and \( F_i \propto (X_i - W)/\|X_i - W\| \) (\( W \) denoting the closest point of the domain’s boundary) for particle–wall interaction if the corresponding distances are small.

We discretize \( \Omega_c \) by a uniform triangulation consisting of 65,536 elements. The time step size used was \( \tau = 0.01 \). The first simulation uses the fixed initial triangulation without any adaptation over time while the second simulation aligns the mesh quadratically to the particles in each time step. Since the particles move over time, the discretization of the particles in terms of the corresponding elements changes as was already stated in Remark 1. This is illustrated in Figure 6 which shows a close-up of one particle and its surrounding triangulation at \( t = 10 \): Initially, a particle is discretized by \( P_h \) consisting of the elements marked red. As the particle moves over time, nodes (and elements) initially belonging to \( P_h \) may move to \( \Omega \), or vice versa in subsequent time steps.

![Figure 6: Close-up of a particle \( P \) (white boundary) and its surrounding triangulation. Mesh elements belonging to the discretized particle \( P_h \) at \( t = 10.0 \) are marked red. In subsequent time steps \( P \) is discretized by different elements.](image)

In Figure 7, the evolution of the velocity field and the position of the particles are depicted for three time instants. From a qualitative point of view, both simulations agree very well regarding the position of the particles. After a certain period of time, slight differences in the velocity fields lead to differences in the particle positions.

Figure 8 shows the graph (warp) of the velocity magnitude close to the top boundary. Also, the triangulation of the discretized particles \( P_h \) is shown. One can observe that the much crisper resolution of the particles’ boundaries in the case of the mesh alignment simulation leads to a much smoother flow field, as was already seen for the quasi-stationary model problem.
Figure 7: Velocity norm and particle positions for the mesh aligned (a)–(c) and non aligned (fixed mesh) (d)–(f) simulations at three different time instants.

Figure 8: Warp of the velocity norm for the mesh aligned (a) and non aligned (fixed mesh) (b) simulation at $t = 6$ and triangulations of the discrete particles $P_h$. 
6. Conclusion

A novel finite element method for the simulation of particulate flows was presented. The main building blocks are

- the formulation of the underlying equations using a fictitious domain/one–domain approach in a moving coordinate frame,
- a splitting scheme to decouple the particle movement from the computation of the velocity field,
- the subspace projection method to account for the rigid body motion of the particles,
- a novel mesh smoothing/moving mesh method to explicitly adapt a triangulation to the particle boundary without the need for remeshing.

The advantages of the proposed method are the high approximation quality of the discrete solution obtained due to the sharp representation of the particles’ boundaries and the simple, modularized structure which allows for an easy and efficient implementation of the method in an existing moving mesh / ALE based Navier–Stokes solver.

We demonstrated the advantages of the proposed approach by giving an error bound for the discrete solution. It was proved that by representing the particles’ boundaries using linear edges of the triangulation, first order convergence can be achieved (as opposed to a $h^{1/2}$ result which holds if no mesh alignment is performed). Using isoparametric elements and a quadratic representation of the geometry was shown to result in an optimal (second order) convergence rate.

We have evaluated the error bound and its sharpness with a quasi–stationary numerical example and demonstrated the potential of the method by simulating a lid–driven cavity problem with 100 particles.

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PREPRINTS

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