# Convergence to equilibrium for discrete gradient-like flows and An accurate method for the motion of suspended particles in a Stokes fluid

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# Convergence to equilibrium for discrete gradient-like flows and An accurate method for the motion of suspended particles in a viscous fluid

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# Abstract

The thesis has two independent parts.
The first part concerns the convergence toward equilibrium of discrete gradient flows or, with more generality, of some discretizations of autonomous systems which admit a Lyapunov function. The study is performed assuming sufficient conditions for the solutions of the continuous problem to converge toward a stationary state as time goes to infinity. It is shown that under mild hypotheses, the discrete system has the same property. This leads to new results on the large time asymptotic behavior of some known non-linear schemes.
The second part concerns the numerical simulation of the motion of particles suspended in a viscous fluid. It is shown that the most widely used methods for computing the hydrodynamic interactions between particles lose their accuracy in the presence of large non-hydrodynamic forces and when at least two particles are close from each other. This case arises in the context of medical engineering for the design of nano-robots that can swim. This loss of accuracy is due to the singular character of the Stokes flow in areas of almost contact. A new method is introduced here. Numerical experiments are realized to illustrate its better accuracy.

# Résumé

La thèse comporte deux parties.
La première traite de la convergence vers l'équilibre de flots de gradients discrets ou plus généralement de discrétisations d'un système autonome admettant une fonction de Lyapunov. En se plaçant dans une cadre pour lequel les solutions du problème continu converge vers un état stationnaire en temps grand, il est démontré sous des hypothèses générale que le système discret a la même propriété. Ce résultat conduit à des conclusions nouvelles sur le comportement en temps grand de schémas numériques anciens.
La seconde partie concerne la simulation numérique de particules en suspension dans un fluide visqueux. Il est montré que les méthodes utilisées actuellement pour simuler l'interaction hydrodynamique entre particules perdent de leur précision quand de grandes forces non-hydrodynamiques sont en jeu et que au moins deux particules sont proches l'une de l'autre. Ce cas survient, dans le contexte de l'ingénierie biomédicale, lors de la conception de nano-robots capables de nager. Cette perte de précision est due au caractère singulier de l'écoulement de Stokes dans les zones de presque contact. Une nouvelle méthode est introduite ici. Des expérimentations numériques sont effectuées pour mettre en évidence sa grande précision.

# Contents

Chapter 1

# General introduction

## 1.1 Introduction en Français

Ce manuscrit de thèse comporte deux parties indépendantes.

### 1.1.1 Objet de la première partie

Nous traiterons tout d'abord de flots de gradient discrets et plus généralement de systèmes d'EDO autonomes qui admettent une fonction de Lyapunov stricte. Nous nous intéressons au comportement en temps long de solutions discrètes de certains schémas associés à de tels systèmes. Nous nous plaçons dans des conditions où le problème continue admet une solution globale $u(t)$ qui admet une limite $\varphi$ quand le temps $t$ tend vers l'infini. Nous montrerons que pour certains schémas la solution discrète admet elle aussi une limite $\varphi^{\Delta t}$ et que dans le cas où $\varphi$ est un point de minimum local de la fonction de Lyapunov, $\varphi^{\Delta t}$ converge vers $\varphi$ quand le pas de temps $\Delta t$ converge vers 0.

#### Plan de la première partie

Le travail présenté est constitué d'une introduction et de la reproduction d'un article [19] publié conjointement avec Benoît Merlet.

### 1.1.2 Objet de la seconde partie

La seconde partie traite de l'approximation numérique des intéractions hydrostatiques entre particules en suspension dans un fluide visqueux. La motivation de ce travail vient d'une part de l'étude de suspensions denses et d'autre part de la nécessité de produire des simulations numériques précises de micro ou nano-nageurs artificiels. Dans le cas de ces derniers, comme dans le cas de nano-nageurs vivants (spermatozoïdes, bactéries ou algues mon-cellulaires) l'énergie mobilisable pour la nage est relativement grande, ce qui permet à deux parties du nageur qui sont à une distance très faible l'une de l'autre d'avoir des vitesses relatives sensiblement différentes bien que les forces hydrostatiques s'y opposent. Ces situations où deux objets à une distance $d$ faible l'un de l'autre ont des vitesses différentes créent des densités de force hydrostatique d'une part élevées et d'autre part singulières au sens où elles sont localisées dans une région de diamètre de l'ordre de $\sqrt{d}$. Le caractère localisé de ces densités de force fait qu'elles sont mal approchées par les méthodes basées sur une décomposition spectrale. C'est le cas en particulier de la dynamique Stokesienne qui est la méthode la plus utilisée pour la simulation du mouvement de particules en suspension

dans un fluide visqueux.
Nous proposons une nouvelle méthode, plus coûteuse, mais qui permet une approximation précise. Nous comparons les performances de cette méthode avec la Dynamique Stokesienne.

**Plan de la seconde partie**

Dans la Chapitre 3, nous présentons tous d'abord le système de Stokes ainsi que les espaces fonctionnels et les résultats théoriques standards (caractère bien posé des équations, régularité des solutions). Nous nous plaçons ensuite dans le cas de $N$ particules sphériques plongées dans un fluide visqueux avec des conditions de non-glissement sur le bord des particules. Nous présentons la méthode d'approximation spectrale dans ce cadre, en particulier la décomposition des vitesses et densités de force dans une base d'Harmoniques Sphériques Vectorielles (Chapitre 4). Nous expliquons ensuite à partir d'une étude numérique pourquoi cette décompositon spectrale n'est pas efficace dans le cas où deux particules proches ont des vitesses sensiblement différentes (Section 5.2). La méthode de la Dynamique Stokesienne qui palie en partie à cette faiblesse est présentée dans la Section 5.3. Nous montrons aussi les limites de cette méthodes dans le cas où une troisième particule se situe dans le voisinage d'une paire de particules proches. Nous présentons notre méthode et sa discrétisation dans les Sections 6.1 et 6.2. Les résultats numériques sont exposés dans la Section 6.3. Enfin, dans une dernière section nous discutons les choix de paramètres de discrétisation.

## 1.2 Introduction in English

This manuscript is made of two independent parts which have their own introductions.

We first study discrete gradient flows and more generally discrete schemes associated to quasi-gradient flows, that is autonomous systems of ODEs which admit a strict Lyapunov function. Under some general hypotheses, the continuous problem admits a global solution $u(t)$ which converges toward some limit $\varphi$ as the time $t$ goes to infinity. We show that under some mild hypotheses, the discrete solution associated to some standard schemes also admit a limit $\varphi^{\Delta t}$. We also prove that if moreover $\varphi$ is a local minimizer of the Lyapunov function then $\varphi^{\Delta t}$ converges to $\varphi$ as the time step $\Delta t$ goes to 0.

The second part concerns the numerical simulation of the hydrodynamic interactions between small particles in a viscous fluid. It is motivated by the study of dense suspension of particles and also by the study of the motion of living microorganisms (sperm cells, bacteria, unicellular algae) or of artificial micro or nanorobots. In these cases the energy which is available for the motion is (relatively) large and the swimmers may move close parts of their bodies with different velocities even if the hydrodynamic forces strongly oppose such movement. Such situations where two objects at a small distance $d$ from one another have different velocities create hydrostatic force densities which on the one hand have large magnitudes in a small region with a diameter of the order of $\sqrt{d}$. Due to their localized nature, these force densities are poorly approximated by methods based on a spectral decomposition (or multipole expansion). This is the case of the Stokesian Dynamics which is a widely used method to simulate the motion of particles suspended in a viscous fluid.

We propose a new method, which is more expensive, but allows accurate approximations. We compare the performance of this method with the Stokesian Dynamics.

# Part I

# Convergence to equilibrium for discrete gradient-like flows

## 1.3 Introduction to the paper [19]

In this part, we consider autonomous systems of ODE such as

$$\dot{u} \;=\; G(u), \qquad t \geq 0, \tag{1.3.1}$$

with $u(t) \in \mathbf{R}^d$ and $G \;:\; U \subset \mathbf{R}^d \to \mathbf{R}^d$.
We assume that the system admits a strict Lyapunov function $F$, that is

$$\frac{d}{dt}\left[F(u)\right](t) \;\leq\; 0 \quad \text{for every solution and every } t \geq 0,$$

and moreover,

$$\frac{d}{dt}\left[F(u)\right](t_0) \;=\; 0 \quad \Longrightarrow \quad u(t) \;=\; u(t_0) \text{ for } t \geq t_0.$$

More precisely, we study some discretizations of the system (1.3.1) and study the asymptotic behavior as $t_n \to \infty$ of the discrete solutions.

The most simple situation is the case of a gradient flow

$$G \;=\; -\nabla F.$$

In this case, if $F$ is of class $C^1$ and bounded from below, we have

$$F(u(t)) \quad \overset{t\uparrow\infty}{\longrightarrow} \quad F_\infty \in \mathbf{R}.$$

Moreover, the $\omega$-limit set

$$\omega[u] \;:=\; \Big\{ v \in \mathbf{R}^d \;:\; \exists\, (t_n) \uparrow \infty \text{ such that } u(t_n) \to v \Big\}$$

is a connected subset of the critical points of $F$.

We restrict our study to situations for which $F$ satisfies a Łojasiewicz inequality at some point $\varphi \in \omega[u]$, that is: there exists $\nu \in [0, 1/2)$, $\gamma > 0$ and $\sigma > 0$ such that

$$|v - \varphi| < \sigma \qquad \Longrightarrow \qquad |F(v) - F(\varphi)|^{1-\nu} \;\leq\; \gamma |\nabla F(v)|. \tag{1.3.2}$$

This inequality implies that $u$ has a limit at infinity:

$$u(t) \quad \overset{t\uparrow\infty}{\longrightarrow} \quad \varphi, \tag{1.3.3}$$

and we even have the stronger result

$$\int_{\mathbf{R}_+} |\dot{u}| \;<\; \infty.$$

The importance of the Łojasiewicz inequality (1.3.2) comes from a famous result by Łojasiewicz [17] which states that if $F : U \subset \mathbf{R}^d \to \mathbf{R}$ is (real) analytic then such inequality holds in the neighborhood of any point $\varphi \in U$. (This is non-trivial only when $\varphi$ is a critical point of $F$).

The convergence (1.3.3) is not true in general. As a counterexample, let us build a function $F : \mathbf{R}^2 \to \mathbf{R}$ as follows. Given a curve $\Gamma$ parameterized by $\gamma : \mathbf{R}_+ \to \mathbf{R}^2$,

$$\gamma(s) \;=\; \left(1 + \frac{1}{1+s}\right)(\cos s, \sin s)\,.$$

We define the tangent vector on this curve as $\tau(t) = \dot\gamma/|\dot\gamma|$ and the normal unit vector as $n(t) = (-\tau_2, \tau_1)$. Let us fix $\eta > 0$ small enough such that the mapping at 0, the mapping

$$\Phi \;:\; (t,s) \in \mathbf{R}_+ \times (-1,1) \quad\longmapsto\quad \gamma(t) + \frac{\eta}{1+t^2} n(t)$$

is one to one. We then set

$$F(x,y) \;=\; \begin{cases} g(t)\psi(s) & \text{if } (x,y) = \Phi(t,s) \text{ for some } (t,s) \in \mathbf{R}_+ \times (-1,1), \\ \\ 0 & \text{if } (x,y) \notin \Phi(\mathbf{R}_+ \times (-1,1)). \end{cases}$$

where $g \in C^\infty([0,+\infty],[0,1],[0,1])$ is supported in $[1/2,+\infty)$ and $g(t) = e^{1-t}$ for $t \geq 1$, and $\psi \in C_c^\infty(-1,1)$ admits a local minima at $s = 0$, with $\psi(0) = 1$ and $\psi'(0) = \psi''(0) = 0$.

We easily check that $F \in C_c^\infty(\mathbf{R}^2)$ and that the curve $\{\gamma(s) : s \geq 1\}$ is the trajectory of a solution $u$ of the gradient flow $\dot u = -\nabla F(u)$, in particular $\omega[u] \;=\; S^1$, see Figure 1.1.

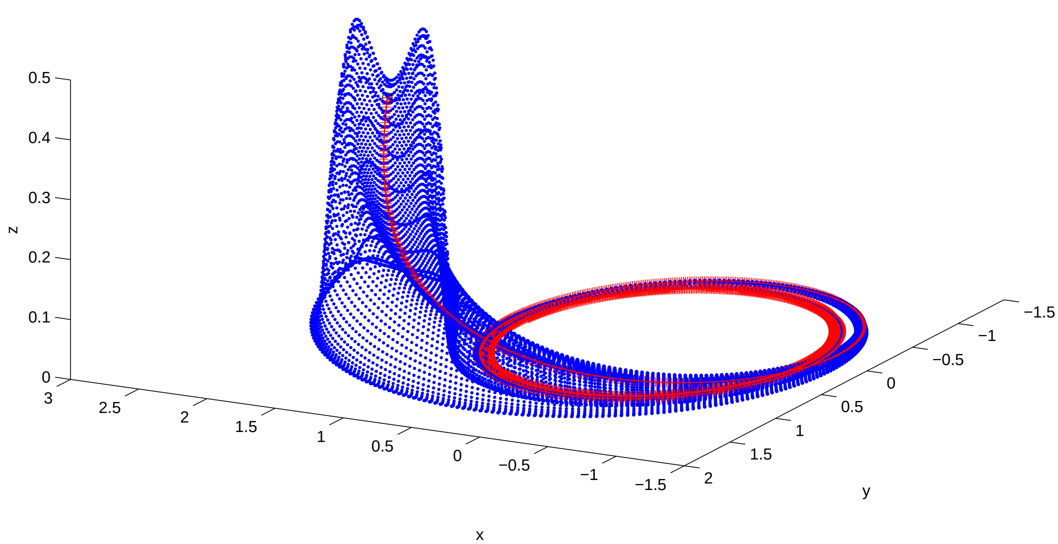


Figure 1.1: Counterexample. Graph of an energy function $F$ with a trajectory satisfying $\omega[u] = S^1$ (in red).

When (1.3.1) is not a gradient flow, we still have the following result.

**Proposition 1.3.1.** *Assume that there exists $\alpha > 0$ such that*

$$(-\nabla F, G) \;\geq\; \alpha \|\nabla F\| \, \|G\| \qquad \text{in } U, \tag{1.3.4}$$

*and that $u : \mathbf{R}_+ \to U$ solves (1.3.1). If there exists $\varphi \in \omega[u]$ such that $F$ satisfies a Łojasiewicz inequality in the neighborhood of $\varphi$, then $u(t) \to \varphi$ as $t \uparrow \infty$.*

The condition (1.3.4) is called the angle condition.

### The discrete case

In the paper reproduced after this introduction, we consider the issue whether a solution of a numerical scheme approximating (1.3.1) also satisfies these convergence properties. The practical interest of this work is to establish under mild hypotheses that if $\varphi = \lim_\infty u(t)$ is a local minimizer of $F$ and if $(u_n^{\Delta t})$ is a numerical approximation of $u(t)$ obtained by a standard numerical scheme with time step $\Delta t > 0$, then for $\Delta t$ small enough $(u_n)$ converges and

$$\lim_{\Delta t \downarrow 0} \left[ \lim_{n \uparrow \infty} u_n^{\Delta t} \right] \;=\; \varphi.$$

When $\varphi$ is not an *isolated* local minimizer of $F$, the conclusion is not trivial and may be wrong for some numerical schemes. Even for a converging and energy decreasing numerical scheme, the numerical solution could slip towards another local minimizer $\varphi^{\Delta t}$ on the same energy level $F(\varphi^{\Delta t}) = F(\varphi)$ and with $\varphi^{\Delta t} \not\to \varphi$ as $\Delta t \downarrow 0$.

In a preceding work [18], Merlet and Pierre have established that if $(u_n) \subset \mathbf{R}^d$ solves

$$u_{n+1} \in \; \text{Argmin} \left\{ F(v) + \frac{|v - u_n|^2}{2\Delta t} \;:\; v \in \mathbf{R}^d \right\}, \qquad \text{for } n \geq 0,$$

(that is $(u_n)$ solves the Euler scheme with time step $\Delta t > 0$ associated to the gradient flow $\dot{u} = -\nabla F(u)$) and if $F \in C^1(\mathbf{R}^d)$ satisfies a Łojasiewicz inequality in the neighborhood of some point $\varphi$, with

$$\varphi \;\in\; \omega[(u_n)] \;=\; \bigcap_{p \geq 0} \overline{\{u_k : p \geq k\}},$$

then $u_n \to \varphi$.
These authors also establish similar results for the $\theta$-scheme for $1/2 \leq \theta \leq 1$.

Here we continue this analysis in the case of an autonomous system which admits a strict Lyapunov function $F$. We obtain positive results assuming $(a)$ that $F$ satisfies the Łojasiewicz inequality, $(b)$ that $F$ satisfies a one-sided Lipschitz condition (i.e. $u \mapsto F(u) + \lambda |u|^2$ is convex for $\lambda$ large enough) and $(c)$ that (1.3.4) is strengthen to an angle and comparability condition: there exists $\alpha > 0$ such that

$$(-\nabla F, G) \;\geq\; \frac{\alpha}{2} \left( \|\nabla F\|^2 + \|G\|^2 \right) \qquad \text{in } \mathbf{R}^d.$$

Assuming moreover that $G$ is Lipschitz continuous, we also obtain positive results for the $\theta$-scheme.
In all these cases, we provide explicit convergence rates which are similar to the continuous case.

We also consider the case of an autonomous system on an embedded manifold $\mathcal{M} \subset \mathbf{R}^d$, i.e. we consider autonomous systems such that the condition $u(0) \in \mathcal{M}$ imply $u(t) \in \mathcal{M}$ for $t \geq 0$. In general using a standard numerical scheme, the numerical solution does not satisfy $u_n \in \mathcal{M}$ for $n \geq 1$. For this reason, we consider a family of projected $\theta$-schemes defined as $u_0 \in \mathcal{M}$ and for $n \geq 0$,

$$\begin{cases} \dfrac{v_{n+1} - u_n}{\Delta t} - \theta G(v_{n+1}) - (1-\theta)G(u_n) \ = \ 0, \\ \\ u_{n+1} \ := \ \Pi_{\mathcal{M}} v_{n+1}, \end{cases}$$

where $\Pi_{\mathcal{M}}$ denotes the orthogonal projection on the manifold $\mathcal{M}$.

We establish convergence to equilibrium results for such schemes. As an illustration, we show that they apply to some space-time discretizations of the harmonic map flow and of the Landau-Lifshitz equations of micromagnetism. For these flows, the numerical solutions are subjected to the constraint

$$u_n \in (S^2)^N,$$

where $N$ is the number of degrees of freedom associated to the space discretization.

## 1.4 Convergence to equilibrium for discretizations of gradient-like flows on Riemannian manifolds

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# Convergence to equilibrium for discretizations of gradient-like flows on Riemannian manifolds

Benoît Merlet Thanh Nhan Nguyen

## Abstract

In this paper, we consider discretizations of systems of differential equations on manifolds that admit a strict Lyapunov function. We study the long time behavior of the discrete solutions. In the continuous case, if a solution admits an accumulation point for which a Łojasiewicz inequality holds then its trajectory converges. Here we continue the work started in [18] by showing that discrete solutions have the same behavior under mild hypotheses. In particular, we consider the $\theta$-scheme for systems with solutions in $\mathbf{R}^d$ and a projected $\theta$-scheme for systems defined on an embedded manifold. As illustrations, we show that our results apply to existing algorithms: 1) Alouges' algorithm for computing minimizing discrete harmonic maps with values in the sphere; 2) a discretization of the Landau-Lifshitz equations of micromagnetism.

### 1.4.1 Introduction

In this paper, we consider time discretizations of the non-linear differential system,

$$\dot{u} \; = \; G(u), \qquad t \geq 0, \; u(t) \in M, \tag{1.4.1}$$

where $M \subset \mathbf{R}^d$ is a $C^2$-embedded manifold without boundary and $G$ is a continuous tangent vector field on $M$. More precisely, we are interested in the long-time behavior and stability properties of the global solutions of (1.4.1). If the continuous system (1.4.1) admits a strict Lyapunov function $F \in C^1(M, \mathbf{R})$ and if the set of accumulation points

$$\omega(u) \; := \; \{\varphi \in M : \exists (t_n) \uparrow \infty \text{ such that } u(t_n) \to \varphi\}$$

is non-empty, then $t \mapsto F(u(t))$ in a non-increasing function converging to $F(\varphi)$ where $\varphi \in \omega(u)$.

Under additional assumptions, namely if $F$ satisfies a Łojasiewicz inequality in a neighborhood of $\varphi$ and if $G(u)$ and $-\nabla F(u)$ satisfy an angle condition, then one can prove that $u(t)$ does indeed converge to $\varphi$ (see the papers by Lageman [16], by Chill *et al.* [10] and the more recent paper by Bárta *et al.* [7]). Under an additional comparability condition between $\|G(u)\|$ and $\|\nabla F(u)\|$, we even have convergence rates depending on the Łojasiewicz exponent.

Notice that if $\varphi$ is an isolated local minimizer of $F$, then the above convergence property is almost obvious and the Łojasiewicz inequality is not required. On the other hand these results are not trivial (and wrong in general) when a connected component of the critical set of $F$ does not reduce to a single point. A typical example is given by the function $F : \mathbf{R}^2 \mapsto \mathbf{R}$, $x \mapsto (\|x\|^2 - 1)^2$ for which the set of minimizers is $S^1$.

If we are concerned with numerical simulations, it is of interest to know whether the above asymptotic properties also hold for numerical solutions. Consider, for some time-step $\Delta t > 0$, a sequence $(u_n) \subset M$ such that $u_n$ approximates the exact solution $u$ at time $t_n = n\Delta t$. Such a sequence could be built by means of any standard or reasonable numerical scheme. Mimicking the continuous case, our first goal is to establish the following property:

**Result 1.** If $\varphi$ is an accumulation point of the sequence $(u_n)$, then $u_n \to \varphi$.

When $\varphi$ is a local minimizer of $F$, we expect a more precise stability result:

**Result 2.** Let $\varphi^* \in M$ be a local minimizer of $F$. For every $\eta > 0$ there exists $0 < \varepsilon < \eta$ such that

$$\|u_N - \varphi^*\| < \varepsilon \quad \Longrightarrow \quad \|u_n - \varphi^*\| < \eta, \ \forall n \geq N.$$

Moreover, in this case, the sequence $(u_n)$ converges to some $\varphi \in M$.

It turns out that this last property leads to a uniform convergence result. Indeed, assume that the exact solution $u$ converges to a local minimizer $\varphi^*$ of $F$, then for $T$ large enough, we have

$$\|u(t) - \varphi^*\| \ < \varepsilon/2, \qquad \forall t \geq T.$$

If the scheme is uniformly convergent on finite intervals (a reasonable query) then for $\Delta t > 0$ small enough, we have,

$$\|u_n - u(t_n)\| \ < \ \varepsilon/2, \text{ for } 0 \leq t_n \leq T + 1.$$

In particular, $\|u_N - \varphi^*\| < \varepsilon$ where $T \leq N\Delta t < T + 1$. Applying Result 2, we conclude that for $\Delta t > 0$ small enough, we have

$$\|u_n - u(t_n)\| \ \leq \ \eta, \qquad \forall n \geq N.$$

We then infer,

$$\limsup_{\Delta t \downarrow 0} \sup_{n \geq 0} \|u_n - u(t_n)\| \ = \ 0.$$

As a consequence, denoting $\varphi(\Delta t) := \lim_{n\to\infty} u_n$, we also have $\varphi(\Delta t) \to \varphi^*$ as $\Delta t \to 0$. Thus, the numerical scheme provides a method to approximate the limit $\varphi^*$. This property motivates our interest for Result 2.

Once the convergence of the sequence is known, we will try to precise the convergence rate and establish:

**Result 3.** Let $\varphi$ be the limit of Result 1. We have the estimate $\|u_n - \varphi\| \leq \kappa f(t_n)$.

The function $t \mapsto f(t)$ should decrease to 0 as $t$ goes to $+\infty$. Typically $f$ is an exponential or a rational function (see (1.4.12) below).

As in the continuous case, the background assumptions on (1.4.1) to obtain Results of type 1, 2 and 3 are a Łojasiewicz inequality, the angle condition and (for the convergence rates) the comparability condition that we will describe in the next section. For the scheme, on top of usual consistency property, the basic additional required assumption is that $F$ should be a strict Lyapunov function for the scheme with an estimate of the form

$$F(u_{n+1}) + \mu \frac{\|u_{n+1} - u_n\|^2}{\Delta t} \ \leq \ F(u_n), \tag{1.4.2}$$

for some $\mu > 0$. In the case of a gradient flow $G = -\nabla F$, and if $\nabla F$ satisfies a one-sided Lipschitz condition, this stability property is naturally satisfied by the backward Euler scheme and, under a regularity assumption on $G$, by the $\theta$-scheme for $0 \leq \theta < 1$. In this paper, we focus on these schemes and we assume that $\nabla F$ satisfies a one sided Lipschitz condition.

In a previous paper, Merlet and Pierre [18] (see also [8, Theorem 24]) have studied the long time behavior of some time-discretizations of the gradient system,

$$\dot{u} \ = \ -\nabla F(u), \qquad t \geq 0, u \in \mathbf{R}^d. \tag{1.4.3}$$

Their results have been generalized to some second order perturbations in [13]. A closely related question concerns the convergence of the proximal algorithm associated to the minimization of $F$ in finite or infinite dimension (see [1, 6, 8] and references therein). As in the present work, the key assumption for convergence results in these papers is the Łojasiewicz inequality. Here we extend the results of [18] on gradient flows in $\mathbf{R}^d$ by considering gradient-like systems on a manifold: we establish Results of type 1, 2 and 3 for the $\theta$-schemes associated to such systems.

The sequel is organized as follows. In the next section, we set the notation and the main hypotheses. We also prove the convergence result in the continuous case. Elements of this proof are used in Section 1.4.5.

Our results concerning the $\theta$-scheme and the projected $\theta$-scheme will be obtained as a consequence of general abstract results of type 1, 2 and 3 that we first establish in Section 1.4.3. We will highlight there the essential hypotheses required for these convergence to equilibrium results. We believe that this general setting enables to quickly check whether convergence to equilibrium properties in the continuous case transpose to the solutions of a numerical scheme in specific situations.

In Section 1.4.4.1, we apply the abstract situation to the $\theta$-schemes associated to (1.4.1) in the case $M = \mathbf{R}^d$.

In Section 1.4.4.2, we consider the case of an embedded manifold by paying attention to the constraint $u(t) \in M$. Of course, under usual hypotheses ensuring the unique solvability of (1.4.1) for $u(0) \in M$ (e.g. assuming that $G$ is locally Lipschitz), the trajectory of the solution will remain on $M$. This is no longer true for general time discretizations. For this reason, we introduce and study a linearized $\theta$-scheme supplemented by a projection step that enforces the constraint $u_n \in M$.

We consider the backward Euler scheme in the case $M = \mathbf{R}^d$ in a separate part (Section 1.4.5). The fact that each step of this scheme can be rewritten as a minimization problem (even in the case of the gradient-like system (1.4.1)) allows us to weaken the regularity hypotheses on $G$.

Eventually, we apply our methods to some concrete problems. First, we consider in Section 1.4.6 a scheme by Alouges [3] designed for the approximation of minimizing harmonic maps with values in the sphere $S^{l-1}$. We establish that the sequence built by the algorithm does converge to a discrete harmonic map. The original result was convergence up to extraction. Then, in Section 1.4.7, we apply our results concerning the projected $\theta$-scheme to a discretization of the Landau-Lifshitz equations of micromagnetism (again proposed by Alouges [4]). These examples illustrate our general results for in both cases the trajectories lie on a non-flat manifold ($(S^{l-1})^N$). Moreover, in the last example, the underlying continuous system is not a gradient flow but merely a system on the form (1.4.1) admiting a strict Lyapunov function.

### 1.4.2 The continuous case

From now on, $M$ is a $C^2$-Riemannian manifold without boundary. Without loss of generality, we assume that $M$ is embedded in $\mathbf{R}^d$ and that the inner product on every tangent space $T_uM$ is the restriction of the euclidian inner product on $\mathbf{R}^d$.

We consider a tangent vector field $G \in C(M, TM)$ and a function $F \in C^1(M, \mathbf{R})$. We assume that $-\nabla F$ and $G$ satisfy the *angle condition* defined below.

**Definition 1.4.1.** We say that $G$ and $\nabla F$ satisfy the *angle condition* if there exists a real number $\alpha > 0$ such that

$$\langle G(u), -\nabla F(u)\rangle \;\geq\; \alpha \|G(u)\| \|\nabla F(u)\|, \qquad \forall u \in M. \tag{1.4.4}$$

**Remark 1.4.1.** *In this definition and below, when we consider a differentiable function $F : M \to \mathbf{R}$, we write $\nabla_M F$ or simply $\nabla F$ to denote the gradient of $F$ with respect to the tangent space of $M$. In particular, $\nabla F(u) \in T_uM$. If the function $F$ is also defined on a neighborhood $\Omega$ of $M$ in $\mathbf{R}^d$, the notation $\nabla F$ is ambiguous. In this case $\nabla F(u)$ denotes the gradient of $F$ in $\mathbf{R}^d$, that is $\nabla F(u) = (\partial_{x_1} F(u), \cdots, \partial_{x_d} F(u))$ and $\nabla_M F(u) = \Pi_{T_uM} \nabla F(u)$ where $\Pi_{T_uM}$ denotes the orthogonal projection on the tangent space $T_uM \subset \mathbf{R}^d$.*

We assume moreover that $F$ is a strict Lyapunov function for (1.4.1):

**Definition 1.4.2.** We say that $F$ is a Lyapunov function for (1.4.1) if for every $u \in M$, we have $\langle G(u), -\nabla F(u)\rangle \geq 0$. If moreover, $\nabla F(u) = 0$ implies $G(u) = 0$ then we say that $F$ is a *strict* Lyapunov function.

As we already noticed, the key tool of the convergence results presented here is a Łojasiewicz inequality.

**Definition 1.4.3.** Let $\varphi \in M$.

1) We say that the function $F$ satisfies a Łojasiewicz inequality at $\varphi$ if there exists $\beta, \sigma > 0$ and $\nu \in (0, 1/2]$ such that,

$$|F(u) - F(\varphi)|^{1-\nu} \;\leq\; \beta \|\nabla F(u)\|, \qquad \forall u \in B(\varphi, \sigma) \cap M. \tag{1.4.5}$$

The coefficient $\nu$ is called a Łojasiewicz exponent.

2) The function $F$ satisfies a Kurdyka-Łojasiewicz inequality at $\varphi$ if there exists $\sigma > 0$ and a non-decreasing function $\Theta \in C(\mathbf{R}_+, \mathbf{R}_+)$ such that

$$\Theta(0) = 0, \qquad \Theta > 0 \text{ on } (0, +\infty), \qquad 1/\Theta \in L^1_{loc}(\mathbf{R}_+) \tag{1.4.6}$$

and,

$$\Theta\left(|F(u) - F(\varphi)|\right) \ \leq \ \|\nabla F(u)\|, \qquad \forall u \in B(\varphi, \sigma) \cap M. \tag{1.4.7}$$

Notice that the first definition is a particular case of the second one with $\Theta(f) = (1/\beta) f^{1-\nu}$. The interest of the first definition relies on the following fundamental result:

**Theorem 1** (Łojasiewicz [17], see also [15])**.** *If $F : \Omega \subset \mathbf{R}^d \to \mathbf{R}$ is real analytic in some neighborhood of a point $\varphi$, then $F$ satisfies the Łojasiewicz inequality at $\varphi$.*

**Remark 1.4.2.** *The Łojasiewicz inequality only provides information at critical points of $F$. Indeed, if $\varphi$ is not a critical point of $F$, then by continuity of $\nabla F$, the Łojasiewicz inequality is satisfied in some neighborhood of $\varphi$.*

It is well known that the Kurdyka-Łojasiewicz inequality implies the convergence of the bounded trajectories of the gradient flow (1.4.3) as $t$ goes to infinity. Here we state the convergence result in the more general case of a gradient-like system:

**Theorem 2.** *Assume that $F$ is a strict Lyapunov function for* (1.4.1) *and that $G, \nabla F$ satisfy the angle condition* (1.4.4)*. Let $u$ be a global solution of* (1.4.1) *and assume that there exists $\varphi \in \omega(u)$ such that $F$ satisfies the Kurdyka-Łojasiewicz inequality* (1.4.7) *at $\varphi$. Then $u(t) \to \varphi$ as $t \to +\infty$.*

**Remark 1.4.3.** *In many applications, the Kurdyka-Łojasiewicz hypothesis holds at every point. Moreover, for finite dimensional systems the fact that $\omega(u)$ is not empty is often the consequence of a coercivity condition on $F$,*

$$F(u) \longrightarrow +\infty, \qquad \textit{as } \|u\| \to \infty. \tag{1.4.8}$$

**Proof.** The proof stated here follows [10]. First we write

$$\frac{d}{dt}\left[F(u(t))\right] \ \overset{(1.4.1)}{=} \ \langle G(u(t)), \nabla F(u(t))\rangle \ \overset{(1.4.4)}{\leq} \ -\alpha \|G(u(t))\| \|\nabla F(u(t))\| \ \leq \ 0,$$

and the function $F(u)$ is non-increasing. By continuity of $F$ and since $\varphi \in \omega(u)$, $F(u(t))$ converges to $F(\varphi)$ as $t$ goes to $+\infty$. Changing $F$ by an additive constant if necessary, we may assume $F(\varphi) = 0$, so that $F(u(t)) \geq 0$ for every $t \geq 0$.

If $F(u(t_0)) = 0$ for some $t_0 \geq 0$ then $F(u(t)) = 0$ for every $t \geq t_0$ and therefore, (since $F$ is a strict Lyapunov function), $u$ is constant for $t \geq t_0$. In this case, there remains nothing to prove.

Hence we may assume $F(u(t)) > 0$ for every $t \geq 0$. Since $F$ satisfies a Kurdyka-Łojasiewicz inequality at $\varphi$, there exist $\sigma > 0$ and a function $\Theta \in C(\mathbf{R}_+, \mathbf{R}_+)$ satisfying (1.4.6) and (1.4.7). Let us define

$$\Phi(f) \ = \ \int_0^f \frac{1}{\Theta(s)} ds, \qquad f \geq 0. \tag{1.4.9}$$

Let us take $\varepsilon \in (0, \sigma)$. There exists $t_0$ large enough such that

$$\|u(t_0) - \varphi\| + \alpha^{-1}\Phi(F(u(t_0))) \;<\; \varepsilon.$$

Let us set $t_1 := \inf\{\mathrm{t} \geq \mathrm{t}_0 : \|\mathrm{u}(\mathrm{t}) - \varphi\| \geq \varepsilon\}$. By continuity of $u$ we have $t_1 > t_0$. Then for every $t \in [t_1, t_0)$, using the angle condition (1.4.4) and the Kurdyka-Łojasiewicz inequality, we have

$$-\frac{d}{dt}\Phi(F(u(t))) \;=\; \frac{\langle G(u), -\nabla F(u)\rangle}{\Theta(F(u(t)))} \;\geq\; \alpha\|G(u(t))\| \;=\; \alpha\|u'(t)\|. \tag{1.4.10}$$

Integrating on $[t_0, t)$ for any $t \in [t_0, t_1)$, we get

$$\begin{aligned}\|u(t) - \varphi\| \leq \;& \|u(t) - u(t_0)\| + \|u(t_0) - \varphi\| \leq \int_{t_0}^{t_1} \|u'(s)\|ds + \|u(t_0) - \varphi\| \\ \leq \;& \alpha^{-1}\Phi(F(u(t))) + \|u(t_0) - \varphi\| < \varepsilon.\end{aligned}$$

This inequality implies $t_1 = +\infty$. Eventually, the estimate (1.4.10) yields $\dot{u} \in L^1(\mathbf{R}_+)$ and we conclude that $u(t)$ converges to $\varphi$ as $t$ goes to infinity. □

In the case of a gradient flow and if the Łojasiewicz inequality is satisfied, we have an explicit convergence rate that depends on the Łojasiewicz exponent. In order to extend this result to gradient-like systems, the angle condition is not sufficient:

**Definition 1.4.4.** We say that $G$ and $\nabla F$ satisfy the angle and comparability condition if there exists a real number $\gamma > 0$ such that

$$\langle G(u), -\nabla F(u)\rangle \;\geq\; \frac{\gamma}{2}\left(\|G(u)\|^2 + \|\nabla F(u)\|^2\right), \qquad \forall u \in M. \tag{1.4.11}$$

**Remark 1.4.4.** *Notice that this condition implies the angle condition* (1.4.4)*. In fact* (1.4.11) *is equivalent to the fact that there exists* $\alpha > 0$ *such that for every* $u \in M$*,*

$$\langle G(u), -\nabla F(u)\rangle \geq \alpha\|G(u)\|\|\nabla F(u)\|$$

*and*

$$\alpha^{-1}\|G(u)\| \geq \|\nabla F(u)\| \geq \alpha\|G(u)\|.$$

**Theorem 3.** *Under the hypotheses of Theorem 2, assume moreover that* $\nabla F$ *and* $G$ *satisfy the angle and comparability condition* (1.4.11) *and that* $F$ *satisfies a Łojasiewicz inequality with exponent* $0 < \nu \leq 1/2$*, then there exist* $c, \mu > 0$ *such that,*

$$\|u(t) - \varphi\| \;\leq\; \begin{cases} c\,e^{-\mu t} & \text{if } \;\nu = 1/2, \\ c\,t^{-\nu/(1-2\nu)} & \text{if } \;0 < \nu < 1/2, \end{cases} \qquad \forall\, t \geq 0. \tag{1.4.12}$$

**Proof.** By Theorem 2, we know that $u(t)$ converges to $\varphi$ as $t$ goes to infinty. As in the preceding proof, we may assume $F(\varphi) = 0$ and $F(u(t)) > 0$ for every $t \geq 0$. Let $\Phi$ be defined by (1.4.9) with $\Theta(f) := (1/\beta)f^{1-\nu}$ and let us set $H(t) = \Phi(F(u(t)))$. In this case, we have the explicit formula $\Phi(f) = (\beta/\nu)f^\nu$. Next let $t_1 \geq 0$ such that $\|u(t) - \varphi\| \leq \sigma$ for every $t \geq t_1$. By (1.4.10), for every $t \geq t_1$, we have

$$\|u(t) - \varphi\| \;\leq\; \int_t^{+\infty} \|u'(s)\|\, ds \;\leq\; \int_t^{+\infty} \gamma^{-1} H'(s) ds \;=\; \gamma^{-1} H(t). \tag{1.4.13}$$

Using the angle and comparability condition (1.4.11) and the Łojasiewicz inequality (1.4.5), we compute

$$-H'(t) = \beta\,[F(u(t))]^{\nu-1}\left(-\frac{d}{dt}\,[F(u(t))]\right) \overset{(1.4.11)}{\geq} \beta\,[F(u(t))]^{\nu-1}\,\frac{\gamma}{2}\,\|\nabla F(u(t))\|^2$$
$$\overset{(1.4.5)}{\geq} \frac{\gamma\beta}{2}\,[F(u(t))]^{\nu-1}\,\frac{1}{\beta^2}\,[F(u(t))]^{2-2\nu} = \frac{\gamma}{2\beta}\,[F(u(t))]^{1-\nu} = \lambda\,[H(t)]^{\frac{1-\nu}{\nu}}.$$

where $\lambda = C(\gamma, \beta, \nu) > 0$. Summing up, we have

$$H'(t) + \lambda\,[H(t)]^{\frac{1-\nu}{\nu}} \;\leq\; 0, \qquad \forall t \geq t_1.$$

In the case $\nu = 1/2$, we get $H'(t) + \lambda H(t) \leq 0$. Writing $H(t) = e^{-\lambda t} g(t)$ we conclude that $g$ is non-increasing, so $H(t) \leq c\, e^{-\lambda t}$ for every $t \geq t_1$.
In the case $0 < \nu < 1/2$, we set $K(t) := [H(t)]^{-(1-2\nu)/\nu}$. This function satisfies $K'(t) \geq \lambda\nu/(1-2\nu)$, which implies $K(t) \geq at$ for some $a > 0$ and for $t$ large enough. Hence $H(t) \leq (at)^{-\nu/(1-2\nu)} = ct^{-\nu/(1-2\nu)}$.
Combining this estimate with (1.4.13) completes the proof. □

In the sequel, we use some tools related to Riemannian metrics on $\mathbf{R}^d$ that we introduce here.

**Definition 1.4.5.** Let $g$ be a Riemannian metric on $\mathbf{R}^d$. We recall that the gradient $\nabla_g F(u)$ of $F$ with respect to the metric $g$ at a point $u$ is defined by

$$\langle \nabla F(u), X \rangle \;=\; \langle \nabla_g F(u), X \rangle_g\,, \qquad \forall X \in \mathbf{R}^d$$

We write $\langle .,. \rangle_g$ (to be precise, we should write $\langle .,. \rangle_{g(u)}$) for the inner product on the tangent space at the point $u$. We also write $\|.\|_g$ for the induced norm.

In [7], Bárta *et al.* establish the remarkable result that when (1.4.1) admits a strict Lyapunov function then, up to a change of metric, (1.4.1) is a gradient system. The following theorem is a direct corollary of Theorem 1 and Theorem 2 in [7].

**Theorem 4.** *Assume that $F$ is a strict Lyapunov function. Then there exists a Riemannian metric $g$ on $\tilde{M} := \{u \in \mathbf{R}^d : G(u) \neq 0\}$ such that $G = -\nabla_g F$.*
*Moreover, if $\nabla F$ and $G$ satisfy the angle and comparability condition (1.4.11) then $g$ is equivalent to the Euclidean metric. Namely, there exist $c_1, c_2 > 0$ such that*

$$c_1\|X\| \leq \|X\|_{g(u)} \leq c_2\|X\|, \qquad \forall X \in \mathbf{R}^d, \forall u \in \tilde{M}. \tag{1.4.14}$$

For some numerical schemes, we are able to obtain Results 1 and 2 under the following additional assumption:

**Definition 1.4.6.** We say that $\nabla F$ satisfies the one-sided Lipschitz condition if there exists $c \geq 0$ such that:

$$\langle \nabla F(u) - \nabla F(v), u - v \rangle \ \geq \ -c\|u - v\|^2, \qquad \forall u, v \in M. \tag{1.4.15}$$

Let us define the set of accumulation points of the sequence $(u_n) \subset M$:

$$\omega((u_n)) := \left\{ \varphi \in M : \text{ there exists a subsequence } (u_{n_k}) \text{ s.t. } u_{n_k} \xrightarrow[k\to\infty]{} \varphi \right\}.$$

To end this section, we recall the main hypotheses introduced above:

- $\omega(u_n)$ is not empty. (H0)

(In applications, this hypothesis is mainly a consequence of (1.4.2) and (1.4.8).)

- The Kurdyka-Łojasiewicz inequality holds at some $\varphi \in \omega(u_n)$. (H1)
- $\nabla F$ and $G$ satisfy the angle and comparability condition (1.4.11). (H2)
- $\nabla F$ satisfies the one-sided Lipschitz condition (1.4.15). (H3)

For convergence rate results, (H1) is replaced by

- The Łojasiewicz inequality holds at some $\varphi \in \omega(u_n)$. (H1')

Other assumptions on the regularity of $G$ and $F$ will be made in the statement of the results.

### 1.4.3 Abstract convergence results

In this section we prove Results of type 1, 2 and 3 for abstract sequences $(u_n) \subset M$ satisfying the two additional conditions introduced below. In the case $M = \mathbf{R}^d$, Results of type 1 and 2 are known (see Absil *et al.* [1]). The proofs are identical in the case of an embedded manifold but we provide them for completeness and because we use them in the proof of Result 3.

Let us introduce our first condition:

$$\exists C \geq 0, \forall n \geq 0, \quad F(u_n) - F(u_{n+1}) \ \geq \ C\|\nabla_M F(u_n)\|\|u_n - u_{n+1}\|. \tag{H4}$$

We need moreover a discrete version of the strict Lyapunov hypothesis:

$$\forall n \geq 0, \quad F(u_{n+1}) = F(u_n) \quad \Longrightarrow \quad u_{n+1} = u_n. \tag{H5}$$

We first state a Result of type 1.

**Theorem 5** ([1] Theorem 3.2)**.** *Let $(u_n) \subset M$. Assume that hypotheses $(H0)$, $(H1)$, $(H4)$ and $(H5)$ hold. Then the sequence $(u_n)$ converges to $\varphi$ as $n$ goes to infinity.*

**Proof.** By (H4) the sequence $(F(u_n))$ is non-increasing, so by continuity of $F$ and hypothesis $(H0)$, we know that $F(u_n)$ converges to $F(\varphi)$ which can be assumed to be 0. By (H5), we may assume that $F(u_n)$ is decreasing, since in the other case, the sequence is constant and thus converge to $\varphi$. Since $F$ satisfies the Kurdyka-Łojasiewicz inequality at $\varphi$, there exist $\sigma > 0$ and a non-decreasing function $\Theta$ satisfying (1.4.6) and (1.4.7). Let $\Phi$ be the function defined by (1.4.9). We have for $n \geq 0$,

$$\Phi(F(u_n)) - \Phi(F(u_{n+1})) \ = \ \int_{F(u_{n+1})}^{F(u_n)} \frac{ds}{\Theta(s)} \ \geq \ \frac{1}{\Theta(F(u_n))}\left(F(u_n) - F(u_{n+1})\right).$$

Using (H4), we obtain

$$\Phi(F(u_n)) - \Phi(F(u_{n+1})) \ \geq \ C\frac{\|\nabla_M F(u_n)\|}{\Theta(F(u_n))}\|u_{n+1} - u_n\|. \tag{1.4.16}$$

By $(H0)$ and the convergence of $(F(u_n))$ to 0, there exists $\bar{n}$ such that

$$\|u_{\bar{n}} - \varphi\| + \frac{1}{C}\Phi(F(u_{\bar{n}})) \ < \ \sigma.$$

Let us define

$$N \ := \ \sup\left\{n \geq \bar{n} : \|u_k - \varphi\| < \sigma, \quad \forall \bar{n} \leq k \leq n\right\},$$

and assume by contradiction that $N$ is finite. For every $\bar{n} \leq n \leq N$, we have $\|u_n - \varphi\| < \sigma$, so we can apply (1.4.7) with $u = u_n$ and deduce from (1.4.16)

$$\|u_{n+1} - u_n\| \ \leq \ (1/C)\left\{\Phi(F(u_n)) - \Phi(F(u_{n+1}))\right\}, \qquad \forall \bar{n} \leq n < N+1. \tag{1.4.17}$$

Summing these inequalities, we get

$$\sum_{n=\bar{n}}^{N} \|u_{n+1} - u_n\| \ \leq \ \frac{1}{C}\Phi(F(u_{\bar{n}})). \tag{1.4.18}$$

In particular,

$$\|u_{N+1} - \varphi\| \ \leq \ \frac{1}{C}\Phi(F(u_{\bar{n}})) + \|u_{\bar{n}} - \varphi\| \ < \ \sigma,$$

which contradicts the definition of $N$. So $N = +\infty$, and the convergence of the sequence follows from (1.4.18). □

We now establish a result of type 2.

**Theorem 6** ([1] Proposition 3.3)**.** *Let $\varphi$ be a local minimizer of $F$ such that $F$ satisfies a Kurdyka-Łojasiewicz inequality in a neighborhood of $\varphi$. Consider a sequence $(u_n) \subset M$ and assume that* (H4) *holds. Then, for every $\eta > 0$ there exists $\varepsilon \in (0, \eta)$ only depending on $F$, $\eta$ and the constant $C$ in* (H4) *such that*

$$\|u_{\bar{n}} - \varphi\| < \varepsilon \quad \Longrightarrow \quad \|u_n - \varphi\| < \eta, \ \forall n \geq \bar{n}.$$

*Moreover, in this case, the sequence $(u_n)$ converges.*

**Proof.** We assume without loss of generality that $F(\varphi)=0$. Since $\varphi$ is a local minimizer of $F$, there exists $\rho>0$ such that

$$\forall u \in \mathbf{R}^d, \quad \|u-\varphi\|<\rho \;\Rightarrow\; F(u)\geq 0. \tag{1.4.19}$$

Moreover, since $F$ satisfies the Kurdyka-Łojasiewicz inequality at $\varphi$, there exist $\sigma>0$ and a function $\Theta$ satisfying (1.4.6) and (1.4.7).

Let $\eta>0$ and let us set

$$\bar\eta \;:=\; \min(\rho,\sigma,\eta),$$

We fix $\varepsilon\in(0,\eta)$ such that for every $u\in M$

$$\|u-\varphi\|<\varepsilon \quad\Longrightarrow\quad \|u-\varphi\|+(1/C)\Phi(F(u))<\bar\eta.$$

Then we consider a sequence $(u_n)$ satisfying (H4) and we assume that there exists $\bar n\geq 0$ such that $\|u_{\bar n}-\varphi\|<\varepsilon$. Then, as in the proof of the previous result, we define

$$N \;:=\; \sup\left\{n\geq \bar n : \|u_k-\varphi\|<\bar\eta, \quad \forall \bar n\leq k\leq n\right\},$$

and assume by contradiction that $N$ is finite. As in the proof of the preceding result, we establish and sum the Kurdyka-Łojasiewicz inequalities (1.4.17) for $\bar n\leq n\leq N$ to get:

$$\sum_{n=\bar n}^{N}\|u_{n+1}-u_n\| \;\leq\; \frac{1}{C}\left\{\Phi(F(u_{\bar n}))-\Phi(F(u_N))\right\}.$$

By definition of $N$ and (1.4.19), we have $F(u_N)\geq 0$ so that $\Phi(F(u_N))\geq 0$ and (1.4.18) holds. We deduce

$$\|u_{N+1}-\varphi\| \;\leq\; \frac{1}{C}\Phi(F(u_{\bar n}))+\|u_{\bar n}-\varphi\| \;<\; \bar\eta,$$

which contradicts the definition of $N$. The convergence of $(u_n)$ then follows from (1.4.18). $\square$

**Remark 1.4.5.** *The result does not hold if we only assume that $\varphi$ is a critical point of $F$. In this case even if $u_{\bar n}$ is very close to $\varphi$, the sequence may escape the neighborhood of $\varphi$ by taking values $F(u_n)<F(\varphi)$. In this case the proof is no more valid. Indeed, we still have the key estimate*

$$\sum_{n=\bar n}^{N}\|u_{n+1}-u_n\| \;\leq\; c\{\Phi\left(F(u_{\bar n})\right)-\Phi(F(u_N))\},$$

*but we can not bound the right hand side by $c\Phi(F(u_{\bar n}))$.*

In order to prove a convergence rate result of type 3, we need to supplement (H4) with the following hypothesis: there exists $C_2>0$ such that for every $n\geq 0$,

$$\|u_{n+1}-u_n\| \;\geq\; C_2\|\nabla F(u_n)\|. \tag{H6}$$

In the case of numerical discretizations of the gradient flow (1.4.3) (or more generally of a gradient-like system (1.4.1)), the quantity $\|u_{n+1}-u_n\|$ behaves like $\Delta t\,\|\nabla F(u_n)\|$, where $\Delta t$ is the time step. For these applications, the constant $C_2$ in the above hypothesis should scale as $\Delta t$: we expect $C_2=C_2'\Delta t$. In this context, the factors $C_2 n$ in the convergence rates (1.4.20) below, have the form $C_2' t_n$. So, these rates are uniform with respect to the time step $\Delta t$. In fact we recover the convergence rates of the continuous case (with possibly different prefactors).

**Theorem 7.** *Let $(u_n) \subset M$. Assume that hypotheses $(H0)$, $(H1')$ and $(H5)$ hold and that there exist $C, C_2 > 0$ such that* (H4) *and* (H6) *hold for $n \geq 0$. Then there exists $\bar{n} \geq 0$ such that for all $n \geq \bar{n}$*

$$\|u_n - \varphi\| \;\leq\; \begin{cases} \lambda_1 e^{-\lambda_2 C_2 n} & \textit{if} \;\; \nu = 1/2, \\ \lambda_2 \left(C_2 n\right)^{-\nu/(1-2\nu)} & \textit{if} \;\; 0 < \nu < 1/2. \end{cases} \tag{1.4.20}$$

*where $\nu$ is the Łojasiewicz exponent of $F$ at point $\varphi$ and $\lambda_1, \lambda_2$ are positive constants depending on $C, \beta$ and $\nu$.*

**Proof.** First let us recall some facts from the proof of Theorem 5. We know that $(u_n)$ converges to $\varphi$ and that the sequence $(F(u_n))$ is non-increasing and converges to $F(\varphi)$ that we assume again to be zero. Let $\tilde{n} \geq 0$ such that $\|u_n - \varphi\| < \sigma$ for $n \geq \tilde{n}$, we can apply (1.4.18) with $\bar{n} = n$ and $N = +\infty$ for every $n \geq \tilde{n}$. Here, the function $\Phi$ defined by (1.4.9) has the explicit form $\Phi(f) = (\beta/\nu) f^{\nu}$ and estimate (1.4.18) yields

$$\|u_n - \varphi\| \;\leq\; \frac{\beta}{C\nu}[F(u_n)]^{\nu}, \qquad \forall n \geq \bar{n}. \tag{1.4.21}$$

Next, let us define the function $K : (0, +\infty) \to (0, +\infty)$ by

$$K(x) \;=\; \begin{cases} -\ln x & \text{if} \;\; \nu = 1/2 \\ \dfrac{1}{(1-2\nu)x^{1-2\nu}} & \text{if} \;\; 0 < \nu < 1/2 \end{cases}$$

The sequence $(K(F(u_n)))$ is non-decreasing and tends to infinity. Using (H4) and (H6), we have

$$\begin{aligned} K(F(u_{n+1})) - K(F(u_n)) \;&=\; \int_{F(u_{n+1})}^{F(u_n)} \frac{dx}{x^{2-2\nu}} \;\geq\; \frac{F(u_n) - F(u_{n+1})}{[2F(u_{n+1})]^{2-2\nu}} \\ &\overset{(H4)(H6)}{\geq} \; CC_2 \|\nabla F(u_n)\|^2 / \left[F(u_{n+1})\right]^{2-2\nu}. \end{aligned}$$

Applying (1.4.7) in the right hand side of the last inequality, we get

$$K(F(u_{n+1})) - K(F(u_n)) \;\geq\; CC_2/\beta^2, \qquad \forall n \geq \bar{n}.$$

Summing from $\bar{n}$ to $n-1$, we get that there exists $c_1 \in \mathbf{R}$ such that

$$K(F(u_n)) \;\geq\; (CC_2/\beta^2)n + c_1, \qquad \forall n \geq \bar{n}. \tag{1.4.22}$$

Now let us consider the case $\nu = 1/2$, we have $K(F(u_n)) = -\ln(F(u_n))$, so we get

$$F(u_n) \;\leq \lambda e^{-(CC_2/\beta^2)n}, \qquad \forall n \geq \bar{n},$$

with $\lambda = e^{-c_1}$. Recalling (1.4.21), the Theorem is proved in this case.

Eventually, if $0 < \nu < 1/2$, (1.4.22) reads

$$F(u_n) \;\leq\; \left[\frac{1-2\nu}{(CC_2/\beta^2)n + c_1}\right]^{1/(1-2\nu)}, \qquad \forall n \geq \bar{n}.$$

Again, (1.4.21) completes the proof. □

### 1.4.4 The $\theta$-scheme and a projected $\theta$-scheme

In this section, we show that the convergence results of Section 1.4.3 apply to some numerical schemes associated to system (1.4.1) under the set of hypotheses $(H0)$, $(H1)$, $(H2)$, $(H3)$ ($(H0)$, $(H1')$, $(H2)$, $(H3)$ for the convergence rate). We also need some regularity assumptions on $G$ and $F$.

#### 1.4.4.1 The $\theta$-scheme in $\mathbf{R}^d$

We first consider the $\theta$-scheme in the case $M = \mathbf{R}^d$. Recall that for a fixed $\theta \in [0,1]$, the $\theta$-scheme associated to equation (1.4.1) reads:

$$\frac{u_{n+1} - u_n}{\Delta t} \;=\; \theta G(u_{n+1}) + (1-\theta)G(u_n). \tag{1.4.23}$$

**Lemma 1.4.7.** Let $\theta \in [0,1]$ and let $(u_n)$ be a sequence that complies to the $\theta$-scheme (1.4.23). Assume that $G$ is Lipschitz continuous and that hypotheses (H2) and (H3) hold. Then there exist $\mu_1, \mu_2, \Delta t' > 0$ such that for $\Delta t \in (0, \Delta t')$,

$$F(u_{n+1}) + \mu_1 \frac{\|u_{n+1} - u_n\|^2}{\Delta t} \;\leq\; F(u_n), \qquad \forall n \geq 0, \tag{1.4.24}$$

and

$$\frac{\|u_{n+1} - u_n\|}{\Delta t} \;\geq\; \mu_2 \|\nabla F(u_n)\|, \qquad \forall n \geq 0. \tag{1.4.25}$$

**Proof.** First we establish (1.4.25). We rewrite the $\theta$-scheme in the form

$$\frac{u_{n+1} - u_n}{\Delta t} \;=\; G(u_n) + \theta \left[ G(u_{n+1}) - G(u_n) \right].$$

Denoting $K \geq 0$ the Lipschitz constant of $G$ on $\mathbf{R}^d$ and using the comparability condition (1.4.11), we deduce

$$(1 + K\Delta t) \frac{\|u_{n+1} - u_n\|}{\Delta t} \;\geq\; \|G(u_n)\| \;\overset{(1.4.11)}{\geq}\; \frac{\gamma}{2} \|\nabla F(u_n)\|.$$

So (1.4.25) holds with $\mu_2 = \gamma/4$ as soon as $\Delta t \in (0, 1/K)$.

Next we prove (1.4.24). By assumption $(H2)$ we can apply Theorem 4 and there exists a metric $g$ on $\tilde{M} := \mathbf{R}^d \setminus \{v : G(v) = 0\}$ satisfying (1.4.14) and such that

$$\langle -\nabla F(u), w \rangle = \langle G(u), w \rangle_{g(u)}, \qquad \forall u \in \tilde{M}, w \in \mathbf{R}^d. \tag{1.4.26}$$

Let us set $\delta_n := u_n - u_{n+1}$ and write the Taylor expansion,

$$\begin{aligned} F(u_n) &= F(u_{n+1}) + \left\langle \int_0^1 \nabla F(u_{n+1} + t\delta_n)\, dt, \delta_n \right\rangle \\ &= F(u_{n+1}) + \langle \nabla F(u_{n+1}), \delta_n \rangle + \left\langle \int_0^1 \nabla F(u_{n+1} + t\delta_n) - \nabla F(u_{n+1}), \delta_n \right\rangle dt. \end{aligned}$$

Applying assumption (H3) with $u = u_{n+1} + t\delta_n$ and $v = u_{n+1}$, we get

$$F(u_n) - F(u_{n+1}) - \langle \nabla F(u_{n+1}), \delta_n \rangle \geq -c \int_0^1 t \|\delta_n\|^2 \, dt,$$

that is,

$$F(u_{n+1}) - F(u_n) \ \leq \ \langle \nabla F(u_{n+1}), u_{n+1} - u_n \rangle + (c/2)\|u_{n+1} - u_n\|^2.$$

If $u_{n+1} \in \tilde{M}$, then we may apply (1.4.26) with $u = u_{n+1}$ and get

$$F(u_{n+1}) - F(u_n) \ \leq \ \langle G(u_{n+1}), u_n - u_{n+1} \rangle_{g(u_{n+1})} + (c/2)\|u_{n+1} - u_n\|^2. \tag{1.4.27}$$

If $u_{n+1} \notin \tilde{M}$, then by the comparability condition we have $G(u_{n+1}) = \nabla F(u_{n+1}) = 0$ and this estimate still holds if we set $\langle \cdot, \cdot \rangle_{g(u_{n+1})}$ to be the usual scalar product. Adding the term

$$0 \ = \ \left\langle \frac{u_{n+1} - u_n}{\Delta t} - \theta G(u_{n+1}) - (1-\theta) G(u_n) \, , \, u_n - u_{n+1} \right\rangle_{g(u_{n+1})}$$

to the right hand side of (1.4.27), we get

$$\begin{aligned} F(u_{n+1}) - F(u_n) \ \leq \ & -(1/\Delta t)\|u_{n+1} - u_n\|^2_{g(u_{n+1})} \ + \ (c/2)\|u_{n+1} - u_n\|^2 \\ & + \ (1-\theta) \langle G(u_{n+1}) - G(u_n), u_n - u_{n+1} \rangle_{g(u_{n+1})} . \end{aligned}$$

Combining this estimate with (1.4.14), we obtain

$$F(u_{n+1}) - F(u_n) \ \leq \ -\mu_{\Delta t} \frac{\|u_{n+1} - u_n\|^2}{\Delta t},$$

with $\mu_{\Delta t} := c_1^2 - \Delta t(c/2 + (1-\theta) K c_2^2)$ where $K$ is the Lipschitz constant of $G$. The parameter $\mu_{\Delta t}$ being larger than the positive constant $\mu_1 := c_1^2/2$ for $\Delta t$ small enough (1.4.24) is proved. ☐

**Corollary 1.4.1.** Let $\theta \in [0,1]$ and let $(u_n)$ be the sequence defined by the $\theta$-scheme (1.4.23). Assume hypotheses $(H2)$, $(H3)$ hold, that $G$ is Lipschitz and that $\Delta t \in (0, \Delta t')$. Then:

- If $(H0)$, $(H1)$ hold, the sequence $(u_n)$ converges to $\varphi$.
- If $F$ satisfies a Kurdyka-Łojasiewicz inequality in the neighborhood of some local minimizer $\varphi$ then for every $\eta > 0$ there exists $\varepsilon \in (0, \eta)$ such that

$$\|u_{\bar{n}} - \varphi\| < \varepsilon \quad \Longrightarrow \quad \|u_n - \varphi\| < \eta, \ \forall n \geq \bar{n}.$$

- If $(H0)$, $(H1')$ hold, the sequence $(u_n)$ converges to $\varphi$ with convergence rates given by (1.4.20) with $C_2 = \mu_1 \mu_2^2 \Delta t$.

**Proof.** From (1.4.24) and (1.4.25) of Lemma 1.4.7, we easily obtain (H4), (H5) and (H6) with $C = \mu_1 \mu_2$ and $C_2 = \mu_1 \mu_2^2 \Delta t$. The result is then a consequence of Theorems 5, 6 and 7. ☐

#### 1.4.4.2 A projected $\theta$-scheme

We now consider an embedded $C^2-$manifold $M \subset \mathbf{R}^d$ without boundary and with a uniformly bounded curvature. We present a simple scheme for the approximation of (1.4.1). This scheme has two steps. The first step requires a family of mappings $\{G_u : u + T_uM \to T_uM\}_{u\in M}$. The mapping $G_u$ should approximate $G$ around $u$. Natural choices are

$$G_u(u+v) \;:=\; G(u) \qquad \text{or} \qquad G_u(u+v) \;:=\; G(u) + \langle \nabla G(u), v\rangle \quad \forall v \in T_uM.$$

Starting from $u_n \in M$, the first step of the scheme is just the computation of an approximation $v_n$ of $\dot{u}$ thanks to the classical $\theta$-scheme applied to the system $\dot{u} = G_{u_n}(u)$. We obtain an intermediate iterate $\tilde{u}_{n+1} := u_n + \Delta t\, v_n$ which does not belong to $M$ in general. The second step consists in projecting $\tilde{u}_{n+1}$ on the manifold $M$. Here, to fix the ideas, we only consider the orthogonal projection

$$\Pi_M(u) \;\in\; \operatorname{argmin}\{\|v-u\|^2 : v \in M\}.$$

Other choices are admissible as soon as (1.4.33) holds. If $M$ is the boundary of a convex set $S$, then $\tilde{u}_{n+1} \in u_n + T_{u_n}M$ belongs to $\mathbf{R}^d \setminus S$, so $\Pi_M(\tilde{u}_{n+1}) = \Pi_{\bar{S}}(\tilde{u}_{n+1})$ and the orthogonal projection is uniquely defined. This is not true for general $M$. Anyway, here $M$ is of class $C^2$ and we assume that the projection is uniquely defined as soon as $d(\tilde{u}_{n+1}, M) < \delta$ for some $\delta > 0$.

More precisely, the projected $\theta$-scheme described above is defined as follows. Let us choose a fixed parameter $\theta \in [0,1]$ and let $u_0 \in M$. Then for $n = 0, 1, 2, \ldots$

$$\left[\begin{array}{l} \textbf{step 1.} \text{ Find } v_n \in T_{u_n}M \text{ such that} \\ \qquad\qquad v_n = \theta G_{u_n}(u_n + \Delta t\, v_n) + (1-\theta) G_{u_n}(u_n). \\ \\ \textbf{step 2.} \text{ Set } u_{n+1} := \Pi_M(u_n + \Delta t\, v_n). \end{array}\right. \tag{1.4.28}$$

In this manifold context, we need to strengthen the previous regularity hypotheses. We will assume for simplicity that the family $\{G_u\}$ satisfies

$$G_u(u) \;=\; G(u) \qquad \forall u \in M. \tag{1.4.29}$$

We assume that $G$ is bounded and that $G$, $\nabla F$ and the family of mappings $\{G_u\}$ are uniformly Lipschitz continuous, *i.e.* there exist $Q, K > 0$ such that

$$\|G(u)\| \;\le\; Q, \qquad \forall u \in M, \tag{1.4.30}$$
$$\|G_u(u+v) - G_u(u+v')\| \;\le\; K\|v - v'\| \qquad \forall u \in M,\, \forall v, v' \in T_uM, \tag{1.4.31}$$
$$\|\nabla F(u) - \nabla F(u')\| \;\le\; K\|u - u'\| \qquad \forall u, u' \in M. \tag{1.4.32}$$

We also assume that the projection acts only at second order, that is there exists $\delta, R > 0$ such that

$$\|\Pi_M(u+v) - (u+v)\| \;\le\; R\|v\|^2 \qquad \forall u \in M,\, \forall v \in T_uM \text{ such that } \|v\| < \delta. \tag{1.4.33}$$

With these hypotheses, we have the analogue of Lemma 1.4.7:

**Lemma 1.4.8.** Let $\theta \in [0,1]$ and let $(u_n)$ be the sequence defined by the projected $\theta$-scheme (1.4.28). Assume that (1.4.29,1.4.30,1.4.31,1.4.32) and that (H2) hold. Then there exist $\mu_1, \mu_2, \Delta t' > 0$ such that for $\Delta t \in (0, \Delta t')$,

$$F(u_{n+1}) + \mu_1 \frac{\|u_{n+1} - u_n\|^2}{\Delta t} \;\leq\; F(u_n), \qquad \forall n \geq 0, \tag{1.4.34}$$

and

$$\frac{\|u_{n+1} - u_n\|}{\Delta t} \;\geq\; \mu_2 \|\nabla F(u_n)\|, \qquad \forall n \geq 0. \tag{1.4.35}$$

**Proof.** First we establish that the sequence $(v_n)$ is bounded. Indeed, by (1.4.29) the first step of the scheme reads,

$$v_n \;=\; G(u_n) + \theta \left[ G_{u_n}(u_n + \Delta t v_n) - G_{u_n}(u_n) \right],$$

and we deduce from (1.4.30) and (1.4.31) the estimate $(1 - K\Delta t)\|v_n\| \leq Q$. So, for $\Delta t \in (0, 1/(2K))$, we have

$$\|v_n\| \;\leq\; 2Q.$$

Next, for $\Delta t$ small enough, we have $\Delta t \|v_n\| < \delta$ and the projection step is well defined. Moreover, by (1.4.33), we have

$$v_n \;=\; \frac{u_{n+1} - u_n}{\Delta t} \;+ q_n,$$

with $\|q_n\| \leq R\Delta t \|v_n\|^2$, so there exists $\alpha \in (0,1)$ such that for $\Delta t$ small enough, we have

$$\alpha \|c\|^2 \;\leq\; \alpha \langle a, b\rangle \;\leq \alpha^{-1} \|c\|^2 \tag{1.4.36}$$

for any triplet of vectors $a, b, c$ in the set $\{v_n, (1/\Delta t)(u_{n+1} - u_n)\}$. Similarly, we deduce from the angle and comparability condition $(H2)$, that (1.4.36) holds for any choice $a, b, c$ in the set

$$\{G(u_n),\, -\nabla F(u_n),\, v_n,\, (1/\Delta t)(u_{n+1} - u_n)\}.$$

In particular, (1.4.35) holds.

Eventually, since $F$ is of class $C^{1,1}$, for $\Delta t$ small enough, we have

$$\begin{aligned} &F(u_n) - F(u_{n+1}) \\ &\qquad \geq\; \Delta t \langle -\nabla F(u_n), v_n \rangle - H(\Delta t)^2 \|v_n\|^2 \;\overset{(1.4.36)}{\geq}\; \left(\alpha - \frac{H}{\alpha}\Delta t\right) \frac{\|u_{n+1} - u_n\|^2}{\Delta t}, \end{aligned}$$

for some $H > 0$. Thus, for $\Delta t$ small enough, (1.4.34) holds with $\mu_1 = \alpha/2$. □

**Corollary 1.4.2.** Let $\theta \in [0,1]$ and let $(u_n)$ be the sequence defined by the projected $\theta$-scheme (1.4.28). Assume that (1.4.29,1.4.30,1.4.31,1.4.32) and hypothesis $(H2)$ hold and that $\Delta t \in (0, \Delta t')$. Then:

- If moreover the hypotheses $(H0)$, $(H1)$ hold, the sequence $(u_n)$ converges to $\varphi$.

- If $F$ satisfies a Kurdyka-Łojasiewicz inequality in the neighborhood of some local minimizer $\varphi$, then for every $\eta > 0$ there exists $\varepsilon \in (0, \eta)$ such that

$$\|u_{\bar{n}} - \varphi\| < \varepsilon \quad \Longrightarrow \quad \|u_n - \varphi\| < \eta, \ \forall n \geq \bar{n}.$$

- If the hypotheses $(H0)$, $(H1')$ hold, the sequence $(u_n)$ converges to $\varphi$ with convergence rates given by (1.4.20) with $C_2 = \mu_1 \mu_2^2 \Delta t$.

**Proof.** The proof is the same as the proof of Corollary 1.4.1, simply replace Lemma 1.4.7 by Lemma 1.4.8. □

### 1.4.5 The Backward Euler Scheme in $\mathbf{R}^d$

The results of the previous section are easily extended to general Runge-Kutta schemes. The counterpart of this generality is that quite strong regularity assumptions are made on $F$ , $G_u$ or $G$. Here, we show that these assumptions may be relaxed in the case of the backward Euler scheme in the case $M = \mathbf{R}^d$

We assume $M = \mathbf{R}^d$. Recall that the backward Euler scheme associated to equation (1.4.1) reads:

$$\frac{u_{n+1} - u_n}{\Delta t} \ = \ G(u_{n+1}), \qquad n \geq 0, \tag{1.4.37}$$

where $u_0 \in \mathbf{R}^d$ is the initial condition and $\Delta t > 0$ is the time step. We establish convergence Results of type 1 and 2 and a convergence rate result for these schemes under a Łojasiewicz inequality $(H1)$ (or $(H1')$), the angle and comparability condition $(H2)$, and (as unique regularity assumption) the one sided Lipschitz condition $(H3)$. These results extend Theorem 2.4 and Proposition 2.5 in [18] to gradient-like systems.

As a first step, we use Theorem 4 to show that the solution of the scheme (1.4.37) can be interpreted as a minimizer.

**Lemma 1.4.9.** Assume that $\nabla F$ and $G$ satisfy the angle and comparability condition (H2) and that $F$ satisfies the one sided Lipschitz condition (H3). There exists $\Delta t^* > 0$ such that for $\Delta t \in (0, \Delta t^*)$, if $(u_n) \subset \mathbf{R}^d$ complies with the backward Euler scheme (1.4.37), then for every $n \geq 0$, $u_{n+1}$ is the unique minimizer of the functional

$$E^n(v) \ := \ F(v) + \frac{\|v - u_n\|^2_{g(u_{n+1})}}{2\Delta t},$$

where $g$ is the Riemannian metric provided by Theorem 4.

**Remark 1.4.6.** *The above functional $E^n$ depends on the point $u_{n+1}$ through the local metric $g(u_{n+1})$ so (for a non-constant metric) the minimization problem can not be used as a definition of the scheme.*

**Proof.** Since $F$ is a strict Lyapunov function, we may apply Theorem 4. Let $g$ be the Riemannian metric on $\tilde{M} = \{u \in \mathbf{R}^d : G(u) \neq 0\}$ provided by this Theorem. For any $u \in \tilde{M}$, the map $(X,Y) \in \mathbf{R}^d \times \mathbf{R}^d \mapsto \langle X,Y\rangle_{g(u)}$ is a coercive symmetric bilinear form, so there exists a $d \times d$ symmetric positive definite matrix $A(u)$ such that

$$\langle X,Y\rangle_{g(u)} \;=\; \langle A(u)X,Y\rangle\,, \qquad \forall X,Y \in \mathbf{R}^d.$$

With this notation, the gradient of $E^n$ reads

$$\nabla E^n(v) \;=\; \nabla F(v) + (1/\Delta t)A(u_{n+1})(v-u_n).$$

Thus, for every $u,v \in \mathbf{R}^d$, $\langle \nabla E^n(u) - \nabla E^n(v), u-v\rangle$

$$\begin{aligned} &= \langle \nabla F(u) - \nabla F(v) + (1/\Delta t)A(u_{n+1})(u-v)\,,\, u-v\rangle \\ &= \langle \nabla F(u) - \nabla F(v)\,,\, u-v\rangle + (1/\Delta t)\|u-v\|^2_{g(u_{n+1})}. \end{aligned}$$

Using the one-sided Lipschitz condition (1.4.14) and (1.4.15), we get

$$\langle \nabla E^n(u) - \nabla E^n(v), u-v\rangle \;\geq\; (c_1^2 - c\Delta t)\|u-v\|^2/\Delta t.$$

So $E^n$ is strongly convex for all $\Delta t < \Delta t^* := c_1^2/c$. Hence, it admits a unique minimizer $v_{n+1}$ characterized by $\nabla E^n(v_{n+1}) = 0$, that is:

$$\begin{aligned} 0 =&\; \nabla F(v_{n+1}) + (1/\Delta t)A(u_{n+1})(v_{n+1}-u_n) \\ =&\; A(u_{n+1})\left[-G(v_{n+1}) + (1/\Delta t)(v_{n+1}-u_n)\right], \end{aligned}$$

which is equivalent to the fact that $v_{n+1}$ solves (1.4.37). Consequenlty $u_{n+1} = v_{n+1}$ is uniquely defined as the unique minimizer of $E^n$ as claimed. □

Notice that Lemma 1.4.9 implies that for $\Delta t < \Delta t^*$, if $G(u_N) = 0$ for some $N \geq 0$, then $u_n = u_N$ for every $n \geq N$. In such a case, there is nothing to prove concerning convergence. In the sequel, we assume $G(u_n) \neq 0$ (that is $u_n \in \tilde{M}$) for every $n \geq 0$.

We now state Result 1 for the backward Euler scheme.

**Theorem 8.** *Assume the set of hypotheses* $(H0)$, $(H1)$, $(H2)$, $(H3)$, *let* $\Delta t \in (0,\Delta t^*)$, *where* $\Delta t^*$ *is as in Lemma 1.4.9, and let* $(u_n)_{n\geq 0}$ *be a sequence defined by* (1.4.37), *then the sequence* $(u_n)$ *converges to* $\varphi$ *as* $n$ *goes to infinity.*

**Proof.** Assume $\Delta t < \Delta t^*$, by Lemma 1.4.9, we have $E^n(u_{n+1}) \leq E^n(u_n)$, that is

$$\frac{\|u_{n+1}-u_n\|^2_{g(u_{n+1})}}{2\Delta t} + F(u_{n+1}) \;\leq\; F(u_n) \tag{1.4.38}$$

Thus, the sequence $(F(u_n))$ is non-increasing. We assume again without loss of generality that $F(\varphi) = 0$, so $F(u_n) \downarrow 0$ as $n\ up\infty$.

Next, since $F$ satisfies the Kurdyka-Łojasiewicz inequality at $\varphi$, there exist $\sigma > 0$ and a function $\Theta$ satisfying (1.4.6) and (1.4.7). Let us fix $n \geq 0$ and consider the continuous problem

$$v(0) = u_n, \qquad \dot{v} = -\nabla F(v)$$

From the study of the continuous case, we know that if $\|u_n - \varphi\| < \varepsilon < \sigma/2$, with $\varepsilon$ small enough then $v(t)$ remains in $B(\varphi,\sigma/2)$ for any time $t > 0$. Moreover, $v(t)$ converges to

$v^* \in B(\varphi, \sigma)$ as $t$ tends to infinity. At the limit, we have $\nabla F(v^*) = 0$ and by the Kurdyka-Łojasiewicz inequality, this leads to $F(v^*) = 0$. Now, since $F(u_{n+1}) \geq 0$, there exists $T \in (0, +\infty]$ such that $F(v(T)) = F(u_{n+1})$. Then, from the optimality of $u_{n+1}$, we have $\|u_{n+1} - u_n\|_{g(u_{n+1})} \leq \|v(T) - u_n\|_{g(u_{n+1})}$. By (1.4.14), this leads to $\|u_{n+1} - u_n\| \leq c_2/c_1 \|v(T) - u_n\|$.

On the other hand, using the notation and computations of the proof of Theorem 2 (see (1.4.9), (1.4.10)), we have,

$$\begin{aligned} \Phi(F(u_n)) - \Phi(F(u_{n+1})) &= \Phi(F(v(0))) - \Phi(F(v(T))) \\ &= -\int_0^T \frac{d}{ds}\left[\Phi(F(v(s)))\right] ds \overset{(1.4.10)}{\geq} \alpha \int_0^T \|\dot{v}(s)\| ds = \alpha \|v(T) - u_n\|. \end{aligned}$$

Therefore, if $\|u_n - \varphi\| < \varepsilon < \sigma/2$, with $\varepsilon$ small enough then

$$\|u_{n+1} - u_n\| \leq c_1/(c_2\alpha)\left(\Phi(F(u_n)) - \Phi(F(u_{n+1}))\right). \tag{1.4.39}$$

Finally, using (1.4.39) and summation, we conclude as in the proof of Theorem 5 that the sequence $(u_n)$ converges to $\varphi$. □

As in Section 1.4.3, we also have a result of type 2:

**Theorem 9.** *Assume that hypotheses (H2) and (H3) hold and let $\varphi$ be a local minimizer of $F$ such that $F$ satisfies a Kurdyka-Łojasiewicz inequality in a neighborhood of $\varphi$.*

*Then, for every $\eta > 0$ there exists $\varepsilon \in (0, \eta)$ such if $\Delta t \in (0, \Delta t^*)$, where $\Delta t^*$ is as in Lemma 1.4.9, and if $(u_n)$ is a solution of the scheme (1.4.37), we have*

$$\|u_{\bar{n}} - \varphi\| < \varepsilon \quad \Longrightarrow \quad \|u_n - \varphi\| < \eta, \ \forall n \geq \bar{n}.$$

**Proof.** Theorem (9) is proved along the lines of Theorem 6. We do not repeat the arguments. □

Eventually, if the Łojasiewicz inequality holds then we can estimate the convergence rate in Theorem 8.

**Theorem 10.** *Assume that the set of hypotheses $(H0)$, $(H1')$, $(H2)$, $(H3)$ holds, let $\Delta t \in (0, \Delta t^*)$ and let $(u_n) \subset \mathbf{R}^d$ be a solution of (1.4.37). There exist $\bar{n} \geq 0$ and $\lambda_1, \lambda_2 > 0$ such that for all $n \geq \bar{n}$*

$$\|u_n - \varphi\| \leq \begin{cases} \lambda_1 e^{-\lambda_2 n \Delta t} & \text{if } \nu = 1/2 \\ \lambda_2 (n\Delta t)^{-\nu/(1-2\nu)} & \text{if } 0 < \nu < 1/2 \end{cases}$$

*where $\nu$ is the Łojasiewicz exponent of $F$ at the point $\varphi$.*

**Proof.** The proof is the same as the proof of Proposition 2.5 in [18]. □

### 1.4.6 Harmonic maps and harmonic map flow

In this section, we consider a discretization of the following problem: given $\Omega \subset \mathbf{R}^d$ a bounded domain with a Lipschitz boundary and given $g \in H^{1/2}(\partial\Omega, S^{l-1})$, find a critical point of the Dirichlet energy

$$\mathcal{D}(u) \;:=\; \frac{1}{2}\int_\Omega |\nabla u|^2,$$

under the constraint

$$u \in H^1_g(\Omega, S^{l-1}) \;:=\; \left\{ v \in H^1(\Omega, \mathbf{R}^l) : v = g \text{ on } \partial\Omega,\ |v(x)| = 1 \text{ a.e. in } \Omega \right\}.$$

**Remark 1.4.7.** *For $d = 3$ and $l = 2$, the energy $\mathcal{D}$ appears as a simplified model for the Oseen-Franck energy of nematic liquid crystals. In this context the mapping $u : \Omega \to S^2$ represents the orientation of the molecules.*

It is well known that such maps exist (for example, we may solve the minimization problem by considering a minimizing sequence and using the relative weak compactness of bounded subsets of $H^1_g$). Such maps are called harmonic maps with values in $S^{l-1}$. They are characterized by the following condition: $u \in H^1_g(\Omega, S^{l-1})$ satisfies the non- linear system:

$$-\Delta u \;=\; |\nabla u|^2 u \text{ in } \mathcal{D}'(\Omega). \tag{1.4.40}$$

During the preceding decades, many authors have considered existence and regularity problems related to these harmonic maps (see e.g. [9, 11, 14, 20] and a rather complete overview in [12]).

F. Alouges proposed in [2, 3] an efficient algorithm for finding numerical approximations of minimizing harmonic maps. In the continuous case, the algorithm reads as follows: Given an initial guess $u_0 \in H^1_g(\Omega, S^{l-1})$, compute for $n = 0, 1, \cdots$

$$\left[\begin{array}{l} \textbf{step 1.} \text{ Find } v_n \text{ minimizing } v \mapsto \mathcal{D}(u_n + v) \text{ in } K_{u_n} \text{ with} \\[1em] \qquad K_u \;:=\; \left\{ v \in H^1_0(\Omega, \mathbf{R}^l),\ u(x)\cdot v(x) = 0 \text{ for a.e. } x \in \Omega \right\}. \\[1em] \textbf{step 2.} \text{ Set } u_{n+1}(x) := \dfrac{u_n(x) + v_n(x)}{\|u_n(x) + v_n(x)\|} \quad \forall x \in \Omega. \end{array}\right. \tag{1.4.41}$$

By construction, we have $\mathcal{D}(u_n + v_n) \le \mathcal{D}(u_n)$ so the energy decreases during the first step. Notice that for every $x \in \Omega$, $\|u_n(x) + v_n(x)\|^2 = 1 + \|v_n(x)\|^2 \ge 1$, so, the second step is the projection of $u_n(x)+v_n(x)$ on the closed unit ball of $\mathbf{R}^l$. This ball being convex, this projection is a contraction and we have $\mathcal{D}(u_{n+1}) \le \mathcal{D}(u_n + v_n)$. Consequently $\mathcal{D}(u_{n+1}) \le \mathcal{D}(u_n)$ and the algorithm is energy decreasing. It is also established in [3] that, up to extraction, the sequence $(u_n)$ weakly converges to a harmonic map in $H^1(\Omega)$.

Let us now discretize in space. As in [3], we choose a finite difference approximation. Let us fix $h > 0$ and a finite subset $\Omega^h$ of $h\mathbf{Z}^d$ which stands as the discrete domain. The corresponding discrete energy is

$$\mathcal{D}^h(u^h) \;:=\; \frac{h^d}{4} \sum_{x,y\in\Omega^h,\, \|x-y\|=h} \frac{\|u^h(x) - u^h(y)\|^2}{h^2},$$

defined for any mapping $u^h \in H^h := (\mathbf{R}^d)^{\Omega^h}$. The discrete boundary is supposed to be a non-empty subset $\Gamma^h$ of $\Omega^h$ such that every point $x \in \Omega^h$ is connected to $\Gamma^h$ by a finite path in $\Omega^h$, i.e.

$$\text{there exist } x = x_0^h, x_1^h, \cdots, x_p^h \in \Omega^h \text{ with } \|x_i^h - x_{i-1}^h\| = h \text{ and } x_p^h \in \Gamma^h. \qquad (1.4.42)$$

The discrete boundary condition is a given function $g^h : \Gamma^h \to S^{l-1}$.

Our discrete problem is then: find minimizers or critical points of $\mathcal{D}^h$ in the manifold

$$M_{g^h}^h \ := \ \left\{ u^h \in H^h : u^h(x) = g^h(x), \forall x \in \Gamma^h\,;\ \|u^h(x)\| = 1,\, \forall x \in \Omega^h \right\}.$$

Let us characterized these critical points. For this, we compute the differential of $\mathcal{D}^h$ at some point $u^h : \Omega^h \to \mathbf{R}^l$. Let $u^h, v^h : \Omega^h \to \mathbf{R}^l$, we have $\mathcal{D}^h(u^h + v^h) =$

$$\mathcal{D}^h(u^h) + h^d \sum_{x\in\Omega^h} \left\langle \frac{1}{h^2} \sum_{x,y\in\Omega^h, \|x-y\|=h} \left(u^h(x) - u^h(y)\right),\, v^h(x) \right\rangle + \mathcal{D}^h(v^h),$$

so if we introduce the scalar product

$$\left\langle v^h,\, w^h \right\rangle_{H^h} \ := \ h^d \sum_{x\in\Omega^h} \left\langle v^h(x)\,,\, w^h(x) \right\rangle, \qquad v^h, w^h : \Omega^h \to \mathbf{R}^l,$$

we have by definition,

$$\left[\nabla_{H^h} \mathcal{D}^h(u^h)\right](x) \ = \ \frac{1}{h^2} \sum_{y\in\Omega^h,\, \|x-y\|=h} \left(u^h(x) - u^h(y)\right) \qquad \forall x \in \Omega^h. \qquad (1.4.43)$$

Let us consider a point $u^h \in M_{g^h}^h$. The tangent space $T_{u^h} M_{g^h}^h$ at this point is

$$K_{u^h}^h \ := \ \{v^h \in H_0^h : v^h(x) \cdot u^h(x) = 0,\, \forall x \in \Omega^h \setminus \Gamma^h\},$$

where we have set

$$H_0^h \ := \ \left\{ v^h \in H^h : v^h(x) = 0,\, \forall x \in \Gamma^h \right\}.$$

Taking into account the constraint $u^h(x) \in S^{l-1}$ for every $x \in \Omega^h$, we see that $u^h \in M_{g^h}^h$ is a critical point of $\mathcal{D}^h$ in $M_{g^h}^h$ if and only if there exists $\lambda^h : \Omega^h \setminus \Gamma^h \to \mathbf{R}$ such that

$$\left[\nabla_{H^h} \mathcal{D}^h(u^h)\right](x) + \lambda^h(x) u^h(x) \ = \ 0, \qquad \forall x \in \Omega^h \setminus \Gamma^h. \qquad (1.4.44)$$

**Definition 1.4.10.** If $u^h \in M_{g^h}^h$ satisfies (1.4.44), we say that it is a discrete harmonic map.

The scalar product $\langle\,,\,\rangle_{H^h}$ is consistent with the $L^2$-scalar product in the space $L^2(\Omega, \mathbf{R}^l)$. Another interesting bilinear form on $H^h$, associated to the energy, is

$$\left\langle v^h\,,\, w^h \right\rangle_{\mathcal{D}^h} := \ \frac{h^d}{2} \sum_{x,y\in\Omega^h,\, \|x-y\|=h} \left\langle \frac{v^h(x) - v^h(y)}{h},\, \frac{w^h(x) - w^h(y)}{h} \right\rangle.$$

With this definition, we have $\|u^h\|^2_{\mathcal{D}^h} = 2\mathcal{D}^h(u^h)$ for any $u^h \in H^h$. Under the connectivity assumption (1.4.42), this bilinear form defines a scalar product on the subspace $H^h_0$. Eventually, notice that a discrete integration by parts yields

$$\left\langle \nabla_{H^h}\mathcal{D}^h(v^h)\,,\, w^h \right\rangle_{H^h} \;=\; \left\langle v^h\,,\, w^h \right\rangle_{\mathcal{D}^h}, \qquad \forall v^h, w^h \in H^h_0. \tag{1.4.45}$$

The discretized version of (1.4.41) reads: Given an ininitial guess $u^h_0 \in M^h_{g^h}$, compute for $n = 0, 1, \cdots$

$$\left[\begin{array}{l} \textbf{step 1.}\ \text{Find } v^h_n \text{ minimizing } v^h \mapsto \mathcal{D}^h(u^h_n + v^h_n) \text{ in } K^h_{u^h_n}. \\ \\ \textbf{step 2.}\ \text{Set } u^h_{n+1}(x) := \dfrac{u^h_n(x) + v^h_n(x)}{\|u^h_n(x) + v^h_n(x)\|} \quad \forall x \in \Omega^h. \end{array}\right. \tag{1.4.46}$$

Let us state some relevant properties of this algorithm.

**Theorem 11** ([2, 3]).
*1) The algorithm (1.4.46) is well defined. We have for $n \geq 0$,*

$$0 \;\leq\; \mathcal{D}^h(u^h_{n+1}) \;\leq\; \mathcal{D}^h(u^h_n + v^h_n) \;\leq\; \mathcal{D}(u^h_n), \qquad \forall n \geq 0. \tag{1.4.47}$$

*In particular the sequence $(\mathcal{D}^h(u^h_n))$ is non-increasing and convergent.*

*Moreover, if equality occurs in one of the above inequalities, then $v^h_p = 0$ for every $p \geq 0$ and $u_n$ is a discrete harmonic map. Conversely, if $(u^h_n)$ is a discrete harmonic map, then $v^h_n = 0$ and the sequence $(u^h_n)$ is stationary.*

*2) There exists $\lambda^h_n : \Omega^h \setminus \Gamma^h \to \mathbf{R}$, such that the increment $v^h_n$ satisfies the Euler-Lagrange equation,*

$$\left[\nabla\mathcal{D}^h(u^h_n + v^h_n)\right](x) \;=\; \lambda^h_n(x)u^h_n(x), \qquad \forall x \in \Omega^h \setminus \Gamma^h. \tag{1.4.48}$$

*In particular, we have*

$$\mathcal{D}^h(v^h_n) \;=\; \mathcal{D}^h(u^h_n) - \mathcal{D}^h(u^h_n + v^h_n), \tag{1.4.49}$$

*so that*

$$\sum_{n\geq 0} \mathcal{D}^h(v^h_n) \;\leq\; \mathcal{D}^h(u^h_0) - \lim_{n\to\infty} \mathcal{D}^h(u^h_n) \;\leq\; \mathcal{D}^h(u^h_0), \tag{1.4.50}$$

*and consequently $v^h_n \to 0$ as $n$ goes to infinity.*

*3) Up to extraction, the sequence $(u^h_n)$ converges to a discrete harmonic map.*

**Proof.** The proof of all these results can be found in [3]. However, for completeness, we establish (1.4.47,1.4.48,1.4.49,1.4.50), that turn out to be useful to our purpose.

The second inequality of (1.4.47) is obvious by definition of $v^h_n$. Now, notice, that if $u^h_n(x) \in S^{l-1}$ and $v^h_n(x) \cdot u^h_n(x) = 0$, then $\|u^h_n(x) + v^h_n(x)\|^2 = 1 + \|v^h_n(x)\|^2 \geq 1$. So, the second step of the algorithm is the projection of $u^h_n(x) + v^h_n(x)$ on the closed unit ball of $\mathbf{R}^d$. By convexity of this ball, this projection is a contraction for the Euclidian distance in $\mathbf{R}^d$, so for every $x, y \in \Omega^h$, we have

$$\|u_{n+1}(x) - u_{n+1}(y)\| \;\leq\; \|(u_n + v_n)(x) - (u_n + v_n)(y)\|,$$

and the first inequality of (1.4.47) follows from the very definition of the energy $\mathcal{D}^h$.

Next, for every $n \geq 0$, $v_n^h$ minimizes the quadratic functional $v^h \mapsto \mathcal{D}^h(u_n^h + v^h)$ in the space $K^h_{u_n^h}$, so it satisfies the Euler equation (1.4.48) for some $\lambda_n^h : \Omega^h \setminus \Gamma^h \to \mathbf{R}$. We easily compute

$$\mathcal{D}(u_n^h) - \mathcal{D}(u_n^h + v_n^h) \;=\; -\left\langle \nabla \mathcal{D}^h(u_n^h + v_n^h)\,,\, v_n^h \right\rangle_{H^h} + \mathcal{D}^h(v_n^h) \;\overset{(1.4.48)}{=}\; \mathcal{D}^h(v_n^h).$$

Summing on $n = 0, \cdots$, and using (1.4.47), we obtain (1.4.50). The convergence of $(v_n^h)$ to 0 then follows from the fact that $\sqrt{\mathcal{D}}$ is a norm on $M_0^h$ (recall that $\Gamma^h$ satisfies (1.4.42)). □

We can now use the result of Section 1.4.3 to improve the convergence result Theorem 11 3/ by showing that the whole sequence converges.

**Theorem 12.** *The sequence $(u_n^h)$ built by the algorithm (1.4.46) converges to some discrete harmonic map $\varphi^h$. Moreover there exists $\nu \in (0, 1/2]$ and constants $\lambda_1, \lambda_2 > 0$, such that for every $n \geq 1$,*

$$\|u_n - \varphi\|_{H^h} \;\leq\; \begin{cases} \lambda_1 e^{-\lambda_2 n} & \text{if } \; \nu = 1/2, \\ \lambda_1 n^{-\nu/(1-2\nu)} & \text{if } \; 0 < \nu < 1/2. \end{cases}$$

**Proof.** We want to apply Theorems 5 and 7 to the sequence $(u_n) := (u_n^h)$, the manifold $M := M^h_{g^h} \subset H^h$ and the function $F := \mathcal{D}^h_{|M}$. First, recall that we use the scalar product $\langle \cdot, \cdot \rangle_{H^h}$ in the Euclidian space $H^h$. Since the manifold $M$ is analytic and $F$ is a polynomial function, we deduce (using analytical local charts of $M$) from Theorem 1 that $F$ satisfies the Łojasiewicz inequality in the neighborhood of any point of $M$. The sequence $(u_n^h)$ is bounded in the Euclidian space $H^h$ so it admits an accumulation point $\varphi^h \in M$. In order to conclude, we only have to check that (H4) and (H6) hold.

By (1.4.47) and (1.4.48), we have

$$F(u_n^h) - F(u_{n+1}^h) \;\geq\; (1/2)\|v_n^h\|^2_{\mathcal{D}^h}. \tag{1.4.51}$$

Next, using the linearity of $\nabla F$, we compute for every $w_n^h \in K^h_{u_n^h}$,

$$\left\langle \nabla F(u_n^h)\,,\, w_n^h \right\rangle_{H^h} \;=\; \left\langle \nabla_{H^h} \mathcal{D}^h(u_n^h + v_n^h)\,,\, w_n^h \right\rangle_{H^h} - \left\langle \nabla_{H^h} \mathcal{D}^h(v_n^h)\,,\, w_n^h \right\rangle_{H^h}.$$

The first term vanishes by (1.4.48) and using (1.4.45), we get

$$\left\langle \nabla F(u_n^h)\,,\, w_n^h \right\rangle_{H^h} \;=\; \left\langle v_n^h\,,\, w_n^h \right\rangle_{\mathcal{D}^h}.$$

In particular, choosing $w_n^h = \nabla F(u_n^h)$ and using the equivalence of the norms in finite dimension, there exists $\alpha > 0$ such that

$$\|\nabla F(u_n^h)\|_{\mathcal{D}^h} \;\leq\; \alpha\; \|v_n^h\|_{\mathcal{D}^h},$$

So (1.4.51) implies

$$F(u_n^h) - F(u_{n+1}^h) \;\geq\; \frac{1}{2\alpha}\|\nabla F(u_n^h)\|_{\mathcal{D}^h}\|v_n^h\|_{\mathcal{D}^h}. \tag{1.4.52}$$

Eventually, we know from (1.4.50) that $v_n^h$ tends to 0. Since

$$u_{n+1}^h(x) \;=\; u_n^h(x) + v_n^h(x) + O(\|v_n^h(x)\|^2),$$

we have for $n$ large enough

$$2\|v_n\|_{H^h} \;\geq\; \|u_{n+1} - u_n\|_{H^h}.$$

The conditions (H4) and (H6) then follow from (1.4.52), (1.4.51) and the equivalence of the norms. □

**Remark 1.4.8.** *The preceding method also applies to the discretization of the harmonic map-flow for functions $u \in L^2((0,+\infty), M_g)$ :*

$$\partial_t u - \Delta u - \|\nabla u\|^2 u \;=\; 0 \quad t \geq 0, \qquad u(0,t) = u_0 \in H^1(\Omega, S^{l-1}).$$

*The corresponding algorithm reads: Given an initial data $u_0^h \in M_{g^h}^h$ and a time step $\Delta t$, compute for $n = 0, 1, \cdots$*

$$\left[\begin{array}{l} \textbf{step 1. } \textit{Find } v_n^h \textit{ minimizing } v^h \mapsto \dfrac{\Delta t}{2}\|v_n^h\|_{H^h}^2 + \mathcal{D}^h(u_n^h + \Delta t v_n^h) \textit{ in } K_{u_n^h}^h. \\ \\ \textbf{step 2. } \textit{Set } u_{n+1}^h(x) := \dfrac{u_n^h(x) + \Delta t v_n^h(x)}{\|u_n^h(x) + \Delta t v_n^h(x)\|} \quad \forall x \in \Omega^h. \end{array}\right. \tag{1.4.53}$$

**Remark 1.4.9.** *We do not know wether Theorem 12 still holds in the continuous case. In fact, in order to reproduce the proof above in the continuous case, we should establish the following Łojasiewicz inequality*

$$|\mathcal{D}(u) - \mathcal{D}(\varphi)|^{1-\nu} \;\leq\; \beta\|\Delta u + \|\nabla u\|^2 u\|_{L^2(\Omega)},$$

*in the $H^1$-neighborhood of any harmonic map $\varphi$. This is an open issue.*

### 1.4.7 Application to the Landau-Lifshitz equations

In this section, we show that our results concerning the abstract projected $\theta$-scheme of Section 1.4.4 apply to some discretization of the Landau-Lifshitz equations. These equations describe the evolution of the magnetization $m : \Omega \times (0, +\infty) \to S^2$ inside a ferromagnetic body occupying an open region $\Omega \subset \mathbf{R}^3$. This system of equations reads

$$\alpha\partial_t m - m \times \partial_t m = (1 + \alpha^2)(\Delta m - |\nabla m|^2 m), \;\; \text{in } \Omega, \tag{1.4.54}$$

where $\alpha > 0$ is a damping parameter and $'\times'$ denotes the three dimensional cross product. It is supplemented with initial and boundary conditions

$$\left\{\begin{array}{l} \dfrac{\partial m}{\partial n} = 0 \qquad \text{on } \partial\Omega \\ m(x,0) = m_0(x) \in S^2. \end{array}\right.$$

Notice that, at least formally, this evolution system preserves the constraint $|m(x,t)| = 1, \forall x \in \Omega$.

We will consider a discretization of the following variational formulation of (1.4.54),

$$\alpha \int_\Omega \partial_t m \cdot \psi - \int_\Omega m \times \partial_t m \cdot \psi = -(1 + \alpha^2) \int_\Omega \nabla m \cdot \nabla \psi, \tag{1.4.55}$$

for every $\psi \in H^1(\Omega, \mathbf{R}^3)$ which furthermore satisfies $\psi(x).m(x) = 0$ a.e. in $\Omega$. It is known that for every initial data $m_0 \in H^1(\Omega, S^2)$, this variational formulation admits a solution for all time (see [5]).

Before coming to discretization, let us show that, formally, the Dirichlet energy $\mathcal{D}(m) = (1/2)\int_\Omega |\nabla m|^2$ is a Lyapunov function for (1.4.55). Indeed, considering a smooth solution $m(x,t)$, we compute,

$$\frac{d}{dt}\mathcal{D}(m(\cdot,t)) \;=\; \int_\Omega \nabla m \cdot \nabla \partial_t m(x,t)\, dx.$$

Since, for every $x \in \Omega$, $t \mapsto \|m(x,t)\|^2$ is constant, we have $\partial_t m(x,t) \cdot m(x,t) = 0$. So, we can choose $\psi = \partial_t m(\cdot,t)$ in (1.4.55) and deduce,

$$\frac{d}{dt}\mathcal{D}(m(\cdot,t)) \;=\; -\frac{\alpha}{1+\alpha^2}\int_\Omega \|\partial_t m\|^2(x,t)\, dx \;\leq\; 0,$$

as claimed.

#### 1.4.7.1 Space discretization

We discretize the problem in space using P1-Finite Elements. Let us introduce some notation. Let $(\tau_h)_h$ be a regular family of conformal triangulations of the domain $\Omega$ parameterized by the space step $h$. Let $(x_i^h)_i$ be the vertices of $\tau_h$ and $(\phi_i^h)_{1\leq i\leq N_{(h)}}$ the set of associated basis functions of the so-called $P^1(\tau_h)$ discretization. That is to say the functions $(\phi_i^h)_i$ are globally continuous and linear on each triangle (or tetrahedron in 3D) and satisfy $\phi_i^h(x_j^h) = \delta_{ij}$. We define

$$V^h := \left\{ m = \sum_{i=1}^{N_h} m_i \phi_i^h : \forall i, m_i \in \mathbf{R}^3 \right\}, \quad M^h := \left\{ m \in V^h : \forall i, m_i \in S^2 \right\}.$$

Notice that $M^h$ is a manifold isomorphic to $(S^2)^{N_h}$. For any $m = \sum_{i=1}^{N} m_i \phi_i^h \in M^h$, we introduce the tangent space

$$T_{m^h} M^h = \left\{ v = \sum_{i=1}^{N} v_i^h \phi_i^h : \forall i, m_i^h \cdot v_i^h = 0 \right\}.$$

The space discretization of the variational formulation (1.4.55) reads,

$$\left\{ \begin{array}{l} m^h(0) = m_0^h \in M^h, \quad \text{and} \quad \forall \psi^h \in T_{m^h(t)} M^h, \forall t > 0, \\ \alpha \displaystyle\int_\Omega \partial_t m^h.\psi^h - \sum_{i=1}^{N^h} (m_i^n \times \partial_t m_i^h) \cdot \psi_i^h \int_\Omega \phi_i^h = -(1+\alpha^2) \int_\Omega \nabla m^h.\nabla \psi^h. \end{array} \right. \tag{1.4.56}$$

**Remark 1.4.10.** *We have replaced the term $\int_\Omega (m^n \times p^n) \cdot \psi^h$ in the original scheme of [4] by*

$$\sum_{i=1}^{N^h} (m_i^n \times p_i^n) \cdot \psi_i^h \int_\Omega \phi_i^h.$$

*This modification is equivalent to using the quadrature formula:*

$$\int_\Omega f\,dx \;\simeq\; \sum_{i=1}^{N_h} f(x_i^h)\int_\Omega \phi_i^h,$$

*for the computation of this integral. The convergence to equilibrium results below are still true with an exact quadrature formula, but the proof is slightly more complicated, see Remark 1.4.11.*

We now interpret this variational formulation as a gradient-like differential system of the form (1.4.1). For this we introduce the Lyapunov functional $F : M^h \subset H^1(\Omega,\mathbf{R}^3) \to \mathbf{R}$ defined by

$$F(m^h) = \frac{1}{2}\int_\Omega |\nabla m^h|^2.$$

As usual, the gradient of this functional is $q^h = \nabla F(m^h) = A^h m^h$, where $A^h$ is the rigidity matrix associated to the $\mathrm{P}^1$-FE discretization:

$$\left\langle q^h,\psi^h\right\rangle_{L^2} \;=\; \int_\Omega \nabla m^h\cdot\nabla\psi^h \;=\; \sum_{i,j} m_i^h\psi_j^h\int \nabla\phi_i^h\cdot\nabla\phi_j^h \;=:\; \left\langle A^h m^h,\psi^h\right\rangle_{L^2}. \quad (1.4.57)$$

We also introduce the section $G:\ M^h \to TM^h$ defined by $G(m^h) := p^h$ where $p^h \in T_{m^h}M^h$ solves: $\forall \psi^h \in T_{m^h}M^h$,

$$\alpha\int_\Omega p^h\cdot\psi^h - \sum_{i=1}^{N^h}(m_i^h\times p_i^h)\cdot\psi_i^h\int_\Omega\phi_i^h = -(1+\alpha^2)\int_\Omega \nabla m^h\cdot\nabla\psi^h. \quad (1.4.58)$$

The function $G$ is well defined. Indeed, it is sufficient to check that the bilinear form $b_{m^h}$ defined on $T_{m^h}M^h\times T_{m^h}M^h$ by

$$b_{m^h}(p^h,\psi^h) = \alpha\int_\Omega p^h\cdot\psi^h - \sum_{i=1}^{N^h}(m_i^h\times p_i^h)\cdot\psi_i^h\int_\Omega\phi_i^h \quad (1.4.59)$$

has a positive symmetric part. Using $p_i^h\times p_i^h = 0$, we see that $b_{m^h}(p^h,p^h) = \alpha\|p^h\|^2_{L^2(\Omega)^2}$ and $b_{m^h}$ is coercive on $T_{m^h}M^h\times T_{m^h}M^h$. So, by definition, $m^h\in C^1(\mathbf{R}_+,M^h)$ solves the variational formulation (1.4.56) if and only if

$$\frac{d}{dt}m^h \;=\; G(m^h) \quad \forall t>0, \qquad m^h(0) \;=\; m_0^h.$$

We now check that the hypotheses of Theorem 3 hold.

**Lemma 1.4.11.** The functions $G$ and $\nabla F$ defined above satisfy the angle and comparability condition (1.4.11). Moreover, the Lyapunov function $F$ satisfies a Łojasiewicz inequality (1.4.5) in the neighborhood of any point $m^h$ of the manifold $M = M^h$.

**Proof.** For the first point, let us fix $m^h \in M^h$ and write $p^h = G(m^h)$ and $q^h = \nabla F(m^h)$. Choosing $\psi^h = q^h$ in (1.4.58) and using (1.4.57), we obtain

$$\alpha \left\langle p^h \,,\, q^h \right\rangle_{L^2} \;=\; -\sum_{i=1}^{N^h} (m_i^h \times p_i^h) \cdot q_i^h \int_\Omega \phi_i^h \;-(1+\alpha^2)\|q^h\|^2_{L^2}.$$

Then the Cauchy-Schwarz inequality, the identities $\|m_i^h\| = 1$ and the equivalence of norms in finite dimension yield

$$\|q^h\|_{L^2} \;\leq\; C\|p^h\|_{L^2}.$$

On the other hand, choosing $\psi^h = p^h$ in (1.4.58), we get

$$\alpha\|p^h\|^2_{L^2} \;=\; -(1+\alpha^2)\int_\Omega \nabla m^h \cdot \nabla p^h \;=\; -(1+\alpha^2)\left\langle q^h \,,\, p^h \right\rangle_{L^2}.$$

So, we have

$$\left\langle -q^h \,,\, p^h \right\rangle_{L^2} \;\geq\; \frac{\gamma}{2}\left(\|p^h\|^2_{L^2} + \|q^h\|^2_{L^2}\right),$$

with $\gamma = \alpha/(C(1+\alpha^2))$: i.e. the pair $(-\nabla F, G)$ satisfies the tangential angle condition and comparability condition (1.4.11).

For the second point, $F(m^h)$ is a polynomial function of $(m_i^h)_{1\leq i\leq N_h} \in (S^2)^{N_h}$, hence it is analytic. The manifold $M^h = (S^2)^{N_h}$ being analytic, we can use an analytic chart $\varphi$ (for example a product of stereographic projections) defined in a neighborhood of $m^h$. We apply Theorem 1 to the analytic function $F \circ \varphi^{-1}$ and deduce that it satisfies a Łojasiewicz inequality in the neighborhood of $\varphi(m^h)$. □

We deduce from the lemma:

**Corollary 1.4.3.** Assume $m^h(t)$ is a solution of (1.4.56). Since $M = M^h$ is compact $\omega(m^h)$ is not empty. Consequently there exists $\varphi \in M^h$ such that $u = m^h$ satisfies all the conclusions of Theorems 2, 3.

#### 1.4.7.2 Time-space discretization of the Landau-Lifshitz equations

We now consider the $\theta$-scheme proposed by F.Alouges in [4]:

$$\left\{\begin{array}{l} m^0 \in M^h \\ \text{For } n = 0,1,\ldots \\ \left[\begin{array}{l} \text{Find } p^n \in T_{m^n}M^h \text{ such that } \forall \psi^h \in T_{m^h}M^h, \\ \alpha \displaystyle\int_\Omega p^n \cdot \psi^h - \sum_{i=1}^{N^h} (m_i^n \times p_i^n)\cdot \psi_i^h \int_\Omega \phi_i^h \\ \qquad = -(1+\alpha^2)\displaystyle\int_\Omega \nabla(m^n + \theta\Delta t\, p^n)\cdot\nabla\psi^h. \\ \text{Set } m^{n+1} \;:=\; \displaystyle\sum_{i=1}^{N_h} \frac{m_i^n + \Delta t\, p_i^n}{|m_i^n + \Delta t\, p_i^n|}\phi_i^h, \quad \text{and iterate.} \end{array}\right. \end{array}\right. \tag{1.4.60}$$

Let us rewrite this scheme as a projected $\theta$-scheme of the form (1.4.28). For this we introduce the family of mappings $\{G_{m^h} : m^h + T_{m^h} \to T_{m^h}M^h\}$ defined by $G_{m^h}(u^h) = p^h$ where $p^h \in T_{m^h}M^h$ solves the variational formulation $\forall \psi^h \in T_{m^h}M^h$,

$$\alpha \int_\Omega p^h \cdot \psi^h - \sum_{i=1}^{N^h} (u_i^h \times p_i^h) \cdot \psi_i^h \int_\Omega \phi_i^h = -(1+\alpha^2) \int_\Omega \nabla u^h \cdot \nabla \psi^h.$$

Notice that $G_{m^h}$ only depends on $m^h$ through the space of test functions $T_{m^h}M^h$. As above, we see that $p^h$ is well defined and uniquely defined by this variational formulation through the coercivity of the bilinear form $b_{m^h}$ (see (1.4.59)).

**Lemma 1.4.12.** Let $m^n$, $p^n$ be defined in the scheme (1.4.60). Then,

$$p^n \;=\; \theta G_{m^n}(m^n + \Delta t p^n) + (1-\theta) G_{m^n}(m^n). \tag{1.4.61}$$

**Proof.** Let us set $q^h = G_{m^n}(m^n + \Delta t p^n)$, $r^h = G_{m^n}(m^n)$. By definition of $G_{m^n}$ and linearity, we see that the function $p^h = \theta q^h + (1-\theta) r^h$ satisfies

$$\begin{aligned} \alpha \int_\Omega p^h \cdot \psi^h - \sum_{i=1}^{N^h} (m_i^h \times p_i^h) \cdot \psi_i^h \int_\Omega \phi_i^h - \theta \Delta t \sum_{i=1}^{N^h} (p_i^n \times r_i^h) \cdot \psi_i^h \int_\Omega \phi_i^h \\ = -(1+\alpha^2) \int_\Omega \nabla (m^h + \theta \Delta t\, p^n) \cdot \nabla \psi^h, \qquad \forall \psi^h \in T_{m^h}M^h. \end{aligned}$$

We see that in the third term of the left hand side, the triple product $(p_i^n \times r_i^h) \cdot \psi_i^h$ vanishes. Indeed, the three vectors $p_i^n, r_i^h, \psi_i^h$ belong to the two dimensional tangent space $\{v_i^h \in \mathbf{R}^3 : v_i^h \cdot m_i^h = 0\}$. So, it turns out that $p^h$ and $p^n$ solve the same (well-posed) variational formulation. We conclude that $p^h = p^n$ as claimed. □

**Remark 1.4.11.** *If we had used the original variational formulation, with obvious changes in the definition of $G_{m^h}$, then the term $\theta \Delta t \int_\Omega (p^n \times r^h) \cdot \psi^h$ would not vanish in general and the identity (1.4.61) would be wrong. In this case, we can not link the scheme of [4] to our projected $\theta$-scheme. However, this term is of small magnitude and using the present ideas, it is not difficult to establish that Theorems 5, 6 and 7 apply to this scheme and conclude to the convergence to equilibrium of the sequence $(m^n)$.*

*This difficulty does not appear if we consider a Finite Difference discretization as in Section 1.4.6.*

**Lemma 1.4.13.** The functions $F$, $G$ and $\{G_{m^h}\}$ satisfy hypotheses (1.4.29,1.4.30,1.4.31, 1.4.32). Moreover, the projection $\Pi_{M^h}(z^h) := \sum_{i=1}^{N_h} \frac{z_i^h}{|z_i^h|} \phi_i^h$, satisfies (1.4.33).

**Proof.** First, the identity (1.4.29) is obvious. Next, for $m^h \in M^h$ and $p^h = G(m^h)$, using $\psi^h = p^h$ in (1.4.58), we obtain

$$\alpha \|p^h\|_{L^2}^2 \;\le\; (1+\alpha^2) \|\nabla m^h\|_{L^2} \, \|\nabla p^h\|_{L^2},$$

and we conclude from the equivalence of the norms in finite dimensional spaces, that $G$ is bounded on the compact manifold $M^h$ (that is (1.4.29) holds). The Lipschitz estimate (1.4.31) is also a consequence of this fact and of the uniform coercivity of the bilinear forms $b_{m^h}$. The Lipschitz estimate (1.4.32) on $\nabla F$ is also obvious since $F$ is smooth on the compact manifold $M^h$.

Eventually, we easily see that (1.4.33) holds. Indeed, if $v^h \in T_{m^h} M^h$, then $|m_i^h + v_i^h|^2 = |m_i^h|^2 + |v_i^h|^2 \geq 1$, so $\Pi_{M^h}(m^h + v^h)$ is just the $L^2$- projection of $(m_i^h + v_i^h)$ on the product of balls $(\overline{B}(0,1))^{N_h} \subset (\mathbf{R}^3)^{N^h}$. □

The previous Lemmas 1.4.12 and 1.4.13 show that the sequence $(u_n = m^n)$ satisfies all the hypotheses for Corollary 1.4.2. Hence, we have:

**Corollary 1.4.4.** There exists $\Delta t' > 0$ such that if $\Delta t \in (0, \Delta t')$ and $(m^n) \subset M^h$ is a sequence that complies to the scheme (1.4.60), then there exists $\varphi \in M^h$ such that $(m^n)$ converges to $\varphi$. Moreover, there exist $C_3 > 0$ and $\nu \in (0, 1/2]$ depending on $\varphi$ such that the convergence rate given by (1.4.20) holds with $C_2 = C_3 \Delta t$.

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# Part II

# An accurate method for the motion of suspended particles in a Stokes fluid

Chapter 2

# Introduction - Motivation

According to the fundamental relation of dynamics, the motion of a solid particle is given by

$$m\frac{d^2}{dt^2}v \;=\; F, \qquad I\frac{d}{dt}\omega \;=\; \mathcal{T},$$

where $m$ is the mass of the particle, $I$ is its matrix of inertia, $v$ is the velocity of the center of mass of the particle and $\omega$ is its angular velocity. The sources of the changes of the motion are total force $F$ and total torque $\mathcal{T}$ exerted on the solid.

When we study the motion of very small (say nano-scaled) objects in suspension in a viscous fluid, it is usual to neglect the inertia effects which are small compared to the hydrodynamic forces. The fundamental relation of dynamics then reads

$$F \;=\; 0, \qquad \mathcal{T} \;=\; 0.$$

The forces exerted on the solid decompose in the hydrodynamic forces which are surface forces exerted by the fluid and other forces, such as gravity (and buoyancy) forces, electrostatic forces, magnetic forces, . . . We write

$$F \;=\; F_{hydro} + F_{oth} \;=\; 0, \qquad \mathcal{T} \;=\; \mathcal{T}_{hydro} + \mathcal{T}_{oth} \;=\; 0.$$

The hydrodynamic components depend on the position $p$ and orientation $\Omega$ of the solid but also of its instantaneous velocity and angular velocity of the solid. So these equations amounts to solve the system

$$F_{hydro}(v,\omega\,;\,p,\Omega) \;=\; -F_{oth}(p,\Omega), \qquad \mathcal{T}_{hydro}(v,\omega\,;\,p,\Omega) \;=\; -\mathcal{T}_{oth}(p,\Omega).$$

Solving this $6 \times 6$ system, this allows us to determine $v$ and $\omega$ in the case of a single solid. If we consider $N$ suspended objects occupying the domains $B_i$, $i = 1, \cdots, N$, the different solids interacts through the fluid and we have to solve a $6N \times 6N$ system:

$$\left\{\begin{array}{lcl} F_{hydro}(v_1,\cdots,v_N,\omega_1,\cdots,\omega_N\,;\,p_1,\cdots,p_N,\Omega_1,\cdots,\Omega_N) &=& -F_{oth}(p_i,\Omega_i), \\ \mathcal{T}_{hydro}(v_1,\cdots,v_N,\omega_1,\cdots,\omega_N\,;\,p_1,\cdots,p_N,\Omega_1,\cdots,\Omega_N) &=& -\mathcal{T}_{oth}(p_i,\Omega_i). \end{array}\right. \tag{2.0.1}$$

The next task is to determine the coefficients of such systems, that is compute the hydrodynamic forces and torques given the positions and the velocities of the solids. Since we consider small scales and small velocities, we assume that the fluid solves the Stokes equations in the fluid domain $\Omega$,

$$\begin{cases} -\Delta\mathbf{u} + \nabla p \;=\; 0 \quad \text{in } \Omega, \\ \nabla\cdot\mathbf{u} \;=\; 0 \quad \text{in } \Omega. \end{cases}$$

where $\mathbf{u}$ and $p$ are the velocity and pressure in $\Omega$. For simplicity we assume that the fluid fills the whole space: $\Omega = \mathbf{R}^3 \setminus S$ with $S = \cup_{i=1}^N B_i$. The conditions at infinity are $\mathbf{u}(\mathbf{r})$, $p(\mathbf{r}) \to 0$ as $r \uparrow \infty$ and we consider no-slip boundary conditions on the surface of the solid:

$$\mathbf{u}(\mathbf{r}) \;=\; \mathbf{v}_i + \omega_i \times (\mathbf{r} - \mathbf{r}_i), \qquad \text{for } \mathbf{r} \in \partial B_i,\ i = 1, \cdots, N.$$

where $\mathbf{r}_i$ is an arbitrary point, $\mathbf{v}_i$ is the velocity of the frame attached to $B_i$ at point $\mathbf{r}_i$ and $\omega_i$ is the angular velocity of this frame. Denoting by $\mathbf{n}_i$ the exterior unit normal to $\Omega$ on $\partial B_i$, the surface density of hydrodynamic forces is then given (up to a multiplicative coefficient characterizing the viscosity of the fluid) by

$$\mathbf{f}(\mathbf{r}) \;=\; p\mathbf{n}_i - (\nabla \mathbf{u} + \nabla \mathbf{u}^T)\mathbf{n}_i, \qquad \text{for } \mathbf{r} \in \partial B_i,\ i = 1, \cdots, N,$$

and the total hydrodynamic force and torques exerted on $B_i$ are:

$$\begin{aligned} F_{hydro}(v_1, \cdots, v_N, \omega_1, \cdots, \omega_N\, ;\, p_1, \cdots, p_N, \Omega_1, \cdots, \Omega_N) &= \int_{\partial B_i} \mathbf{f}, \\ \mathcal{T}_{hydro}(v_1, \cdots, v_N, \omega_1, \cdots, \omega_N\, ;\, p_1, \cdots, p_N, \Omega_1, \cdots, \Omega_N) &= \int_{\partial B_i} (\mathbf{r} - \mathbf{r}_i) \times \mathbf{f}. \end{aligned}$$

From the linearity of the Stokes equations and of the force density with respect to $(\mathbf{u}, p)$, we obtain a $6N \times 6N$ friction matrix $\mathcal{F} = \mathcal{F}(p_1, \cdots, p_N, \Omega_1, \cdots, \Omega_N)$ which relates the hydrodynamic interactions to the velocities and angular velocities of the particles:

$$(F_{hydro}, \mathcal{T}_{hydro}) \;=\; \mathcal{F}(\mathbf{v}, \omega).$$

We see that (2.0.1) is a linear system. In the physical community which study the interactions of a large number of suspended (spherical) particles, the favorite numerical method for computing $\mathcal{F}$ is the so called Stokesian Dynamics introduced by Brady and Bossis in 1988 [5, 6]. This method is based on the expansion of the force density and of the velocity on $\partial S^2$ in vectorial spherical harmonics (also called moments or multipoles in the physical literature). In practice, the series of vectorial spherical harmonics are truncated at rank $L$ to obtain an approximate friction matrix $\mathcal{F}^L$. The Stokesian Dynamics method only involves six (F-T method) or eleven (F-T-S method) harmonics. Later, arbitrary values of the truncation order $L$ has been proposed in the so called multipole methods [15, 7].

One of the main challenges in the simulation of large numbers of particles in Stokes flow is the treatment of close particles with different velocities. If we consider two isolated balls separated by a small gap $d$ which are moving toward one another, the main part of the hydrodynamic forces is localized in a region of radius $O(\sqrt{d})$. For such localized densities, a large truncation number is required in order to capture the relevant phenomenon: we need $L \gg \sqrt{1/d}$, which lead to consider $N_{\text{dof}} \gg 1/d$ degrees of freedom. To avoid using large truncation orders, the idea of Brady and Bossis [6] is to correct the friction matrix by using exact values of the hydrodynamic interactions between each pair of close balls.

$$\mathcal{F}_{SD}^L \;=\; \mathcal{F}^L + \mathcal{F}_{\text{pairs}} - \mathcal{F}_{\text{pairs}}^L$$

The matrix $\mathcal{F}_{\text{pairs}}$ is the sum of the interactions between $(B_i, B_j)$ where $(B_i, B_j)$ ranges over the set of pairs of close balls (defined by the condition $d(B_i, B_j) < d_{\text{close}}$). The last term $-\mathcal{F}^L_{\text{pairs}}$ is the substraction of the poor rank $L$ approximations of these interactions which were already present in $\mathcal{F}^L$.

With the above correction, the Stokesian Dynamics and multipole methods are very efficient and accurate in many cases of interest. However, we notice that the corrections only concern pairs of close particles: a third particle in the neighborhood of two close balls is not affected by the corrections of the hydrodynamic interactions between the two first particle and we may think that it should be affected. It turns out that the friction matrices should be affected with coefficients of the order of

$$c = O(1).$$

We see that there are different situations depending on the order of the magnitude of the non-hydrodynamical forces. Let us say that the entries of the right hand side of the linear system (2.0.1) are of order of $O(K)$. When we consider two close particles $B_1$, $B_2$ with $d(B_1, B_2) = d$ then it is known that the hydrodynamic forces associated to the motion of these particles toward one another with velocity $v$ are of the order of

$$F_{hydro} \ = \ O(v/d).$$

In view of (2.0.1), this leads to

$$v \ = \ O(dK).$$

Let us assume that the truncating order $L$ is small ($L \ll \sqrt{1/d}$) so that the approximate friction matrix $\mathcal{F}^L$ is oblivious of the fine hydrodynamic phenomenons with space scale $\sqrt{d}$ between the balls $B_1$, $B_2$. In this case the error induced by this lack of accuracy on a third ball $B_3$ close to $B_1 \cup B_2$ is of the order of

$$err \ = \ O(cv) \ = \ O(cdK) \ = \ O(dK).$$

Hence, if the external forces are not too large, so that we can assume $dK \ll 1$, the Stokesian dynamic method is relevant and provides accurate results. This situation occurs for instance when we consider the sedimentation of small particles in water (or larger particles in a more viscous fluid). On the other hand, this method may be not adapted when large non-hydrodynamical forces are considered. Such (relatively) large forces occur when we consider nano-scale swimmers, such as sperm cells, swimming bacteria or unicellular algae. This is also true for artificial nanoscale swimmers designed to deliver medication from nanosized medical devices (see e.g. [9] as an example of the biomedical engineering activity in this area). In these cases, there is a need for a new numerical method which is accurate even in the presence of large forces. The object of the present work is to present a first attempt in this direction in the context of $N$ identical spherical shaped particles. In fact, this work is motivated by the numerical simulation of theoretical artificial swimmers made of a finite number of balls introduced and studied in [4, 3].

The new method that we present is designed for obtaining accurate results even in the presence of large non-hydrodynamical forces. Roughly speaking it is based on a decomposition of the velocities and angular velocities between a singular part which is responsible of the small scale interactions and a regular part which ideally creates smooth force densities. The main difference with the Stokesian Dynamics is that this new method takes into account the influence of the singular force densities between two closed particles on the neighboring particles. For this reason, it allows us to obtain a degree of accuracy not possible with previous methods. For this reason also, the computational cost is larger.

This work is a joint work with Aline Lefebvre-Lepot and Benoît Merlet.

In the sequel, we first recall well known facts about the Stokes equations (Chapter 3). Then we present the spectral approximation of the hydrodynamic interactions using Vectorial Spherical Harmonics in Chapter 4. We propose numerical evidences of the difficulties and singularities arising in the case of close particles (Chapter 5, Section 5.1). This motivates a description, via asymptotic analysis of the interactions of two isolated close particles in Section 5.2. The Stokesian dynamics is presented in Section 5.3 together with its drawbacks as discussed above. Eventually, in the last Chapter, we describe successively our new method and its discretization in Sections 6.1 and 6.2. The numerical results are presented in Section 6.3. In Section 6.4, we discuss the choice of the discretization parameters.

Chapter 3

# The Stokes problem in an exterior domain

**Contents**



In this section, we present the Stokes equations posed either a bounded subset of $\mathbf{R}^3$ or in the complement of compact subset of $\mathbf{R}^3$. We recall the basic well posedness and regularity results in these situations. Our reference for this part is mainly the book of Galdi [12].

## 3.1 Origin of the equations

We consider a viscous, incompressible and Newtonian fluid moving in a domain $\Omega$ of $\mathbf{R}^3$. The motion of the fluid is given by the momentum equation,

$$\rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) \ = \ \mu \Delta \mathbf{u} - \nabla \pi + \mathbf{F} \qquad \text{in } \Omega \times (0,T), \tag{3.1.1}$$

and the continuity equation for an incompressible fluid,

$$\nabla \cdot \mathbf{u} \ = \ 0 \qquad \text{in } \Omega \times (0,T), \tag{3.1.2}$$

Here $\rho > 0$ denotes the density of the fluid, $\mu > 0$ is the viscosity constant and $\mathbf{F} = \mathbf{F}(t,x) \in \mathbf{R}^3$ is a given density of non-hydrodynamic forces exerted on the fluid.
The unknowns of the problem are the velocity field $\mathbf{u}(t,x) \in \mathbf{R}^3$ and the pressure field $\pi(t,x) \in \mathbf{R}$.
The pressure field represents a Lagrangian multiplier associated to the constraint (3.1.2).

The system (3.1.1), (3.1.2) is the so called Navier-Stokes system. In this form, it is indefinite and must be complemented with an initial condition $\mathbf{u}(0,x) = \mathbf{u}_0(x)$ and boundary conditions.

Let us introduce a typical length $L$ and a typical velocity $V$ of the flow. Performing the change of variables, $x = L\tilde{x}$, $t = L/V\tilde{t}$, $\mathbf{u} = V\tilde{\mathbf{u}}$ we obtain the non-dimensional form of the equations,

$$\partial_{\tilde{t}}\tilde{\mathbf{u}} + \tilde{\mathbf{u}} \cdot \tilde{\nabla}\tilde{\mathbf{u}} \ = \ \frac{1}{Re}\tilde{\Delta}\tilde{\mathbf{u}} - \tilde{\nabla}\tilde{p} + \tilde{\mathbf{F}}, \tag{3.1.3}$$

where $\tilde{p} = \pi/\rho V^2$, $\tilde{\mathbf{F}} = \mathbf{F}L/\rho V^2$ and the Reynolds number is

$$Re \ = \ \rho LV/\mu.$$

We are interested in the limit of small Reynolds numbers $Re \downarrow 0$ where we can neglect the inertia effects. This limit may describe the motion of a fluid around small suspended particles or even the motion of bacteria and other micro-organisms. The limit system is given by

$$\begin{aligned} -\Delta\mathbf{u} + \nabla p \ &= \ \mathbf{F} \qquad \text{in } \Omega \times (0,T), \\ \nabla \cdot \mathbf{u} \ &= \ 0 \qquad \text{in } \Omega \times (0,T). \end{aligned}$$

We see that the time derivative has disappeared in these equations of motion. The fields $(\mathbf{u},p)(t)$ only depend on the force density and boundary conditions at time $t$. In particular, we do not need any initial condition and we can fix the time $t$ in the study.

The unkowns $\mathbf{u} = \mathbf{u}(x)$, $p = p(x)$ now solve the Stokes equations,

$$-\Delta\mathbf{u} + \nabla p \ = \ \mathbf{F} \qquad \text{in } \Omega, \tag{3.1.4}$$

$$\nabla \cdot \mathbf{u} \ = \ 0 \qquad \text{in } \Omega, \tag{3.1.5}$$

supplemented by boundary conditions and, if necessary, by conditions at infinity.

The set $\Omega$ will be an open and connected subset of $\mathbf{R}^3$ (a domain). We consider two cases: either $\Omega$ is a smooth bounded domain, either $\Omega$ is the complement in $\mathbf{R}^3$ of a smooth compact set $K$. That is $K = \Omega^c \subset B(0,R)$ for some large radius $R > 0$. In this latter case, we assume that the fluid is at rest at infinity,

$$\mathbf{u}(x) \ \to \ 0, \quad p(x) \ \to \ 0 \quad \text{as } |x| \to \infty. \tag{3.1.6}$$

On $\partial\Omega$, the velocity of the fluid is prescribed,

$$\mathbf{u} \ = \ \mathbf{g} \qquad \text{on } \partial\Omega, \tag{3.1.7}$$

where $\mathbf{g} : \partial\Omega \to \mathbf{R}^3$ is given. The boundary data $\mathbf{g}$ accounts for the displacement and shape variations of the particles occupying $K$.

Of particular interest are the forces exerted by the fluid on the particles. Denoting by $\mathbf{n}$ the exterior normal on $\partial\Omega$, the density of the forces exerted by the fluid on $\partial\Omega$ is given by

$$\mathbf{f} = \sigma \cdot \mathbf{n} \qquad \text{on } \partial\Omega,$$

where $\sigma$ is the stress tensor. Since we consider a Newtonian fluid, this stress tensor is related to the velocity and pressure fields by

$$\sigma \ := \ \nabla\mathbf{u} + \nabla\mathbf{u}^T - pId,$$

where $Id$ denotes the $3 \times 3$ identity matrix. Hence, the force density on the surface of the body $K$ is given by

$$\mathbf{f} \ = \ (\nabla\mathbf{u} + \nabla\mathbf{u}^T - pId) \cdot \mathbf{n} \ = \ \mathbf{n} \cdot \nabla\mathbf{u} + \nabla\mathbf{u} \cdot \mathbf{n} - p\mathbf{n}. \tag{3.1.8}$$

**Remark 3.1.1.** *Let us notice here that, since* $\mathbf{u}$ *is assumed to be divergence free, the momentum equation* (3.1.4) *rewrites as*

$$\nabla \cdot \sigma \ = \ \nabla \cdot (\nabla\mathbf{u} + \nabla\mathbf{u}^T - pId) \ = \ 0 \qquad \textit{in } \Omega.$$

## 3.2 Function spaces

The Sobolev spaces which are relevant for the Stokes problem described above have two particular features. First, when the domain is an exterior domain (i.e. $\mathbf{R}^3 \setminus \Omega$ is compact) we have to pay attention to the behavior at infinity of the functions. Second, the velocity fields are solenoidal vector fields: $\nabla \cdot \mathbf{u} \equiv 0$.

### 3.2.1 Spaces associated to a bounded domain.

Since we consider linear problems, we only introduce $L^2$-based Sobolev spaces. Let $\Omega \subset \mathbf{R}^3$ be a smooth bounded domain (in particular, $\Omega$ is connected). We define

$$\mathcal{D}^{1,2}(\Omega) \ := \ \left\{ \mathbf{v} \in W^{1,2}(\Omega, \mathbf{R}^3) \ : \ \nabla \cdot \mathbf{v} \equiv 0 \text{ in } \Omega \right\}.$$

Let us discuss the boundary condition

$$\mathbf{u} \ = \ \mathbf{g} \qquad \text{on } \partial\Omega. \tag{3.2.1}$$

Since $\Omega$ is a bounded and connected domain, the divergence free condition implies

$$0 \ = \ \int_\Omega \nabla \cdot \mathbf{u} \ = \ \int_{\partial\Omega} \mathbf{g} \cdot \mathbf{n} \ =: \ \Phi.$$

In this case, the condition of vanishing total flux $\Phi \equiv 0$ is a necessary condition for the existence of a solution of the Stokes problem in $\Omega$ with boundary condition (3.2.1). In fact, if $\mathbf{g}$ is smooth enough, it is also a sufficient condition.

Let us introduce the fractional Sobolev space:

$$W^{1/2,2}(\partial\Omega, \mathbf{R}^3) \;:=\; \left\{\mathbf{g} \in L^2(\partial\Omega) \;:\; \mathbf{g} \text{ is the trace on } \partial\Omega \text{ of some } \mathbf{v} \in W^{1,2}(\Omega \cap B(0,R), \mathbf{R}^3)\right\},$$

endowed with the inner product

$$(\mathbf{g}, \mathbf{h})_{W^{1/2,2}} \;:= (\mathbf{g}, \mathbf{h})_{L^2} + \int_{\partial\Omega\times\partial\Omega} \frac{(\mathbf{g}(x) - \mathbf{g}(y)) \cdot (\mathbf{h}(x) - \mathbf{h}(y))}{|x-y|^3}\, d\sigma(x)\, d\sigma(y),$$

$W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ is a Hilbert space.
Under the condition $\Phi \equiv 0$, we can find a lifting of $\mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ in $\mathcal{D}^{1,2}(\Omega)$.

**Proposition 3.2.1.** *Let $\Omega \subset \mathbf{R}^3$ be a smooth bounded domain (we can in fact only assume that $\Omega$ has Lipschitz regularity). For any $\mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ such that $\Phi(\mathbf{g}) = 0$, there exists $\mathbf{u} \in \mathcal{D}^{1,2}(\Omega)$ such that (3.2.1) holds. Moreover, there exists a constant $C = C(\Omega)$ such that*

$$\|\mathbf{u}\|_{W^{1,2}} \;\leq\; C\|\mathbf{g}\|_{W^{1/2,2}}.$$

The pressure field associated to the Stokes problem in a bounded domain is not unique. If the pair $(\mathbf{u}, p)$ solves the Stokes equation then $(\mathbf{u}, p + c)$ is also a solution for any constant $c \in \mathbf{R}$. To fix this constant, we will impose $\int_\Omega p = 0$. For this, we introduce the space

$$L^2_0(\Omega) \;=\; \left\{q \in L^2(\Omega) : \quad \int_\Omega q = 0\right\}.$$

### 3.2.2 Pressure fields. Homogeneous Sobolev spaces in an exterior domain

Let us now consider that $\Omega$ is a smooth exterior domain of $\mathbf{R}^3$. In particular, $\Omega$ is connected and there exists $R > 0$ such that $\Omega^c \subset B(0, R)$. We set

$$D^{1,2} \;=\; D^{1,2}(\Omega) \;:=\; \left\{q \in L^2_{loc}(\Omega) \;:\; \nabla q \in L^2(\Omega)\right\}.$$

The functions of $D^{1,2}$ admit a limit at infinity. More precisely, for every $q \in D^{1,2}$, there exists a real number $q_0$ such that for every $r > R$,

$$\int_{S^2} |q(r\sigma) - q_0|^2)\, d\sigma \;\leq\; \frac{1}{r}\int_{|x|>r} |\nabla q|^2 \;\to\; 0 \quad \text{as } r \uparrow \infty. \tag{3.2.2}$$

We consider the subspace $\hat{D}^{1,2}$ of $D^{1,2}$ formed by functions $q \in D^{1,2}$ such that $q_0 = 0$. The space $\hat{D}^{1,2}(\Omega)$ equipped with the inner product $(q, q')_{D^{1,2}} \;:=\; \int_\Omega \nabla q \cdot \nabla q'$ is a Hilbert space.

By definition, the elements of $\hat{D}^{1,2}$ satisfy (3.2.2) with $q_0 = 0$. We also have, for every $q \in \hat{D}^{1,2}$,

$$\frac{q}{|x|} \in L^2\left(\mathbf{R}^3 \setminus \overline{B(0,R)}\right) \quad \text{with} \quad \int_{\mathbf{R}^3\setminus B(0,R)} \left(\frac{q}{|x|}\right)^2 \leq 4\int_{\mathbf{R}^3\setminus B(0,R)} |\nabla q|^2 . \qquad (3.2.3)$$

Moreover, by Gagliardo-Nirenberg estimate, for every $q \in \hat{D}^{1,2}$,

$$q \in L^6(\Omega) \quad \text{with} \quad \|q\|_{L^6} \leq C(\Omega)\|q\|_{D^{1,2}} . \qquad (3.2.4)$$

Notice that the space $\hat{D}^{1,2}$ is strictly larger that $W^{1,2}(\Omega)$. For example, if $\Omega = \mathbf{R}^3 \setminus \overline{B(0,1)}$, then $x \mapsto |x|^{-\alpha} \in \hat{D}^{1,2}(\Omega) \setminus L^2(\Omega)$ for every $\alpha > 1/2$. The conditions (3.2.3) or (3.2.4) characterize $\hat{D}^{1,2}(\Omega)$:

$$\begin{aligned} \hat{D}^{1,2}(\Omega) &= \left\{q \in L^1_{loc}(\Omega),\ \nabla q \in L^2(\Omega),\ q/\sqrt{1+|x|^2} \in L^2(\Omega)\right\} \\ &= \left\{q \in L^1_{loc}(\Omega),\ \nabla q \in L^2(\Omega),\ q \in L^6(\Omega)\right\} . \end{aligned}$$

### 3.2.3 Homogeneous Sobolev spaces of velocity fields in exterior domains

We now consider solenoidal vector fields $\mathbf{v} : \Omega \to \mathbf{R}^3$. The velocity fields solving the above Stokes equations will lie in the following space:

$$\mathcal{D}^{1,2}(\Omega) := \left\{\mathbf{v} \in \hat{D}^{1,2}(\Omega)^3 \ : \ \nabla \cdot \mathbf{v} \equiv 0 \text{ in } \Omega\right\} .$$

Let us introduce the inner product

$$(\mathbf{v}, \mathbf{w})_{\mathcal{D}^{1,2}} := \int_\Omega \nabla \mathbf{v} : \nabla \mathbf{w} .$$

The space $(\mathcal{D}^{1,2}(\Omega), (\cdot,\cdot)_{\mathcal{D}^{1,2}})$ is a Hilbert space.
As in the scalar case, we have the following equivalent definitions,

$$\begin{aligned} \mathcal{D}^{1,2}(\Omega) &= \left\{\mathbf{v} \in L^1_{loc}(\Omega, \mathbf{R}^3) \ : \ \nabla \cdot \mathbf{v} \equiv 0,\ \nabla \mathbf{v} \in L^2(\Omega),\ \mathbf{v}/\sqrt{1+|x|^2} \in L^2(\Omega)\right\} \\ &= \left\{\mathbf{v} \in L^1_{loc}(\Omega, \mathbf{R}^3) \ : \ \nabla \cdot \mathbf{v} \equiv 0,\ \nabla \mathbf{v} \in L^2(\Omega),\ \mathbf{v} \in L^6(\Omega)\right\} . \end{aligned}$$

For further use we also introduce the space $\mathcal{D}^{1,2}_0(\Omega)$ defined as the closure of compactly supported smooth vector fields in $\mathcal{D}^{1,2}(\Omega)$.

Let us now consider the boundary condition (3.2.1). In the case of an exterior domain the total flux $\int_{\partial\Omega} \mathbf{g} \cdot \mathbf{n} = \Phi$ may be arbitrary. For instance, if $\Omega$ is the complement of the closed unit ball, the velocity field defined, in spherical coordinates, by

$$\mathbf{v}(\mathbf{r}) := r^{-2}\mathbf{e}_r ,$$

solves the Stokes equations (3.1.4)(3.1.5)(3.2.1) with $p \equiv 0$, $\mathbf{F} \equiv 0$ and boundary condition $\mathbf{g} = \mathbf{e}_r$. Moreover, we have $\mathbf{v}(\mathbf{r}) \to 0$ as $\mathbf{r} \to 0$ and

$$\mathbf{v} \in \mathcal{D}^{1,2}(\Omega).$$

We easily see that the total flux on the boundary of $\Omega$ does not vanish. We have $\Phi = -4\pi$ (and by conservation of the flux, for every $r > 1$, $\int_{\partial B(0,r)} \mathbf{v} \cdot \mathbf{e}_r = 4\pi$).

Let us return to the case of a general smooth exterior domain $\Omega$. The more general boundary conditions that we will consider are given by the traces of the element of $\mathcal{D}^{1,2}(\Omega)$.

$$\left\{\mathbf{g} \in L^2(\partial\Omega) \ : \ \mathbf{g} \text{ is the trace on } \partial\Omega \text{ of some } \mathbf{v} \in \mathcal{D}^{1,2}(\Omega)\right\}$$

The linear constraint $\nabla \cdot \mathbf{v} \equiv 0$ does not play any role here. We have:

**Proposition 3.2.2.** *Let $\Omega \subset \mathbf{R}^3$ be a smooth exterior domain (we can in fact only assume that $\Omega$ has Lipschitz regularity). For any $\mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ there exists $\mathbf{u} \in \mathcal{D}^{1,2}(\Omega)$ such that (3.2.1) holds. Moreover, there exists a constant $C = C(\Omega)$ such that*

$$\|\mathbf{u}\|_{\mathcal{D}^{1,2}} \ \leq \ C\|\mathbf{g}\|_{W^{1/2,2}}.$$

*Proof.* To establish this proposition, we first invoke the fact that there exists $\mathbf{u}_1 \in W^{1,2}(\Omega)$ compactly supported in $B(0,R) \cap \overline{\Omega}$ such that $\mathbf{u}_1 = \mathbf{g}$ on $\partial\Omega$ and

$$\|\mathbf{u}_1\|_{W^{1,2}} \ \leq \ C'(\Omega)\|\mathbf{g}\|_{W^{1/2,2}}.$$

By Theorem III.3.4 in [12], there exists $\mathbf{w} \in \mathcal{D}_0^{1,2}(\Omega)$ satisfying $\nabla \cdot \mathbf{w} = -\nabla \cdot \mathbf{u}_1$ in $\Omega$ with the estimate

$$\|\mathbf{w}\|_{\mathcal{D}^{1,2}} \ \leq \ C''(\Omega)\|\nabla \cdot \mathbf{u}_1\|_{L^2}.$$

The vector field $\mathbf{u} = \mathbf{u}_1 + \mathbf{w}$ then satisfies the requirements of the proposition with $C = C' + C''$. □

## 3.3 Well-posedness and regularity results

We consider the Stokes problem (3.1.4)(3.1.5) in a smooth domain $\Omega \subset \mathbf{R}^3$ with compact boundary $\partial\Omega$, i.e. $\Omega$ is either a bounded domain or an exterior domain. In the last case, we impose the condition at infinity (3.1.6). In both cases, we consider the boundary condition (3.1.7). We assume that $\mathbf{g} \in W^{1/2,2}(\Omega, \mathbf{R}^3)$ with $\Phi = 0$ if $\Omega$ is bounded and that $\mathbf{F} \in \mathcal{D}^{-1,2}(\Omega, \mathbf{R}^3) := \left[\mathcal{D}^{1,2}(\Omega, \mathbf{R}^3)\right]'$. We look for a solution of the variational formulation:

$$\text{Find} \ \ \mathbf{v} \in \left\{\mathbf{w} \in \mathcal{D}^{1,2}(\Omega) \ : \ \mathbf{w} = \mathbf{g} \text{ on } \partial\Omega\right\} \tag{3.3.1}$$

such that

$$\int_\Omega \nabla\mathbf{v} : \nabla\mathbf{w} - \int_\Omega \mathbf{F} \cdot \mathbf{w} \ = \ 0 \qquad \forall\, \mathbf{w} \in \mathcal{D}_0^{1,2}(\Omega). \tag{3.3.2}$$

or equivalently, using the divergence free condition,

$$\frac{1}{2}\int_\Omega (\nabla\mathbf{v} + \nabla\mathbf{v})^T : (\nabla\mathbf{w} + \nabla\mathbf{w}^T) - \int_\Omega \mathbf{F} \cdot \mathbf{w} \ = \ 0 \qquad \forall\, \mathbf{w} \in \mathcal{D}_0^{1,2}(\Omega).$$

Using the lifting $\mathbf{u}$ of $\mathbf{g}$ provided by Proposition 3.2.1 or by Proposition 3.2.2, the existence of a unique solution $\mathbf{v}$ of the variational formulation follows from the Lax-Milgram Theorem.

The existence of a pressure field then follows from an instance of De Rham Theorem. The pressure field is unique up to a constant. In order to fix this constant, we impose

$$p \in \begin{cases} L^2(\Omega), & \text{when } \Omega \text{ is an exterior domain,} \\ L^2_0(\Omega) := \left\{ q \in L^2(\Omega) \ : \ \int_\Omega q = 0 \right\}, & \text{when } \Omega \text{ is a bounded domain.} \end{cases}$$

**Theorem 13.** *Given $\Omega$, $\mathbf{F}$ and $\mathbf{g}$ as above, there exists a unique solution to the variational formulation (3.3.1)(3.3.2). Moreover there exists a unique pressure $p$ in the space $L^2(\Omega)$ (or $L^2_0(\Omega)$ if $\Omega$ is bounded) such that the momentum equation (3.1.4) holds in the sense of distributions in $\Omega$. Eventually, there exists $C = C(\Omega)$ such that*

$$\|\mathbf{v}\|_{\mathcal{D}^{1,2}} + \|p\|_{L^2} \ \leq \ C \left( \|\mathbf{g}\|_{W^{1/2,2}} + \|\mathbf{F}\|_{\mathcal{D}^{-1,2}} \right).$$

### 3.3.1 The fundamental solution and the Stokes equations in $\mathbf{R}^3$

In the case $\Omega = \mathbf{R}^3$, we have an explicit formula for the solution $\mathbf{v} \in \mathcal{D}^{1,2}(\mathbf{R}^3)$ of the variational formulation and the associated pressure field:

$$\mathbf{v}(\mathbf{r}) \ = \ \int_{\mathbf{R}^3} G(\mathbf{r} - \mathbf{r}')\mathbf{F}(r')\, d\mathbf{r}', \qquad p(\mathbf{r}) \ = \ \int_{\mathbf{R}^3} \Pi(\mathbf{r} - \mathbf{r}') \cdot \mathbf{F}(\mathbf{r}')\, d\mathbf{r}', \tag{3.3.3}$$

where

$$G(\mathbf{r}) \ := \ \frac{1}{8\pi r} \left( Id + \mathbf{e}_r \otimes \mathbf{e}_r \right)$$

is the fundamental solution of the Stokes problem, and

$$\Pi(\mathbf{r}) \ := \ \frac{1}{4\pi r^2} \mathbf{e}_r.$$

From these formulas, we deduce as in the case of the Laplace equation, the following regularity result:

**Theorem 14.** *Let $\mathbf{F} \in W^{m,2}(\mathbf{R}^3)$, then the associated solution of the Stokes problem given by (3.3.3) satisfy $\mathbf{v} \in W^{m+2,2}_{loc}(\mathbf{R}^3)$, $p \in W^{m+1,2}_{loc}(\mathbf{R}^3)$. Moreover, for $0 \leq l \leq m$, $D^{l+1}\mathbf{v} \in \mathcal{D}^{1,2}(\mathbf{R}^3)$, $D^l p \in \hat{D}^{1,2}(\mathbf{R}^3)$, with the estimates*

$$\|D^{l+2}\mathbf{v}\|_{L^2} + \|D^{l+1}p\|_{L^2} \ \leq \ C\|D^l\mathbf{F}\|_{L^2}.$$

### 3.3.2 Local regularity

Using truncation arguments, and Theorem 14, we can derive interior estimates for solutions of the Stokes problem in $\Omega \subset \mathbf{R}^3$. For regularity results up to the boundary, we can rely on the Nirenberg translation method (see Temam [18]) or apply the general regularity theory for elliptic problems of Agmon, Douglis and Nirenberg [1, 2]. In [12], the boundary regularity is obtained by first studying the Stokes problem in $\mathbf{R}^2 \times \mathbf{R}_+$.

**Theorem 15** (Sobolev regularity). *If $\Omega$ is of class $C^{m+2}$, if $\mathbf{F} \in W^{m,2}_{loc}(\overline{\Omega})$, $\mathbf{g} \in W^{m+3/2,2}_{loc}(\Omega)$ and $(\mathbf{v}, p)$ is a weak solution of the Stokes equations (3.1.4),(3.1.5) and (3.2.1) in $\Omega$, then $\mathbf{v} \in W^{m+2,2}_{loc}(\overline{\Omega})$ and $p \in W^{m+1,2}_{loc}(\Omega)$. Moreover, for $r' > r > 0$ there exists $C = C(r, r', \Omega)$ such that, noting $\Omega_s = \Omega \cap B(0, s)$, we have*

$$\begin{aligned}&\|D^{m+2}\mathbf{v}\|_{L^2(\Omega_r)} + \|D^{m+1}p\|_{L^2(\Omega_r)}\\ &\quad\le\; C\left(\|D^m\mathbf{F}\|_{L^2(\Omega_{r'})} + \|D^{m+1}\mathbf{g}\|_{W^{1,2}(\partial\Omega\cap B(0,r'))} + \|D^{m+1}\mathbf{v}\|_{L^2(\Omega_{r'})} + \|D^m p\|_{L^2(\Omega_{r'})}\right).\end{aligned}$$

In particular, if $\mathbf{F} \in C^\infty_c(\overline{\Omega})$ and $\mathbf{g} \in C^\infty(\partial\Omega)$, the variational solution $(\mathbf{v}, p)$ of the Stokes equations is smooth in $\overline{\Omega}$.

### 3.3.3 Asymptotics as $|x| \to \infty$

In the sequel, we are mainly interested by the case of an exterior domain with $\mathbf{F} \equiv 0$ or $\mathbf{F}$ compactly supported. In this case the behavior at infinity of $\mathbf{v}$ and $p$ follows the behavior of the fundamental solution of the Stokes problem in $\mathbf{R}^3$ and global regularity results follow from local regularity and the following decay estimates.

**Theorem 16.** *Let $\Omega \subset \mathbf{R}^3$ be a smooth exterior domain, let $\mathbf{g} \in W^{1/2,m}(\partial\Omega)$ and $\mathbf{F} \in D^{-1,2}(\Omega)$ be compactly supported in $\overline{\Omega}$. Let $(\mathbf{v}, p) \in \mathcal{D}^{1,2}(\Omega) \times L^2(\Omega)$ be the variational solution of (3.1.4),(3.1.5),(3.2.1), then*

$$\mathbf{v}(x) \;=\; G(x)\mathbf{F}_0 + \mathbf{v}_1(x), \qquad p(x) \;=\; \Pi(x)\mathbf{F}_0 + p_1(x),$$

*with*

$$\mathbf{F}_0 = \int_\Omega \mathbf{F} - \int_{\partial\Omega} (\nabla\mathbf{v} + \nabla\mathbf{v}^T - pId)\cdot\mathbf{n} \;\in \mathbf{R}^3.$$

*and for every $\alpha \in \mathbf{N}^3$,*

$$|D^\alpha \mathbf{v}_1(x)| \;\le\; C_\alpha |x|^{-(2+|\alpha|)}, \qquad |D^\alpha p_1(x)| \;\le\; C'_\alpha |x|^{-(3+|\alpha|)}.$$

## 3.4 Dirichlet-to-Neumann and Neumann-to-Dirichlet operators

Let us consider a variational solution $(\mathbf{u}, p)$ of the homogeneous Stokes equations in a smooth domain $\Omega$ with non-homogeneous boundary condition $\mathbf{u} = \mathbf{g}$ on $\partial\Omega$. If $(\mathbf{u}, p)$ is sufficiently smooth, the surface density of forces applied by the boundary of $\Omega$ on the fluid is defined as

$$\mathbf{f} \;=\; (\nabla\mathbf{u} + \nabla\mathbf{u}^T - pId)\cdot\mathbf{n}. \tag{3.4.1}$$

The purpose of this section is to extend this definition to the case of general variational solutions and to describe some properties of the Dirichlet to Neumann operators $\mathbf{g} \mapsto \mathbf{f}$. In the next two parts, we consider successively the case of a bounded domain and the case of an exterior domain. In the third part, we consider the case of the whole space $\mathbf{R}^3$ with exterior forces applied on a closed surface of $\Gamma \subset \mathbf{R}^3$.

### 3.4.1 The Dirichlet to Neumann operator in a bounded domain

Let $\Omega \subset \mathbf{R}^3$ be a smooth and bounded domain (recall that $\Omega$ is connected) and let $\mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ such that $\displaystyle\int_{\partial\Omega} \mathbf{g} \cdot \mathbf{n} \;=\; 0$. Let $(\mathbf{u}, p)$ be the associated solution of the homogeneous Stokes problem provided by Theorem 13. If $(\mathbf{u}, p)$ are sufficiently smooth, say $(\mathbf{u}, p) \in W^{2,2}(\Omega, \mathbf{R}^3) \times W^{1,2}(\Omega)$, the traces of $\nabla\mathbf{u}$ and $p$ on $\partial\Omega$ are well defined and we can use formula (3.4.1) to define the density of surface forces.
In order to extend the notion of surface force density to weaker solutions, we proceed by duality. Let us introduce $\mathbf{h} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ and let us choose an arbitrary lifting $\varphi \in W^{1,2}(\Omega, \mathbf{R}^3)$ of $\mathbf{h}$ subjected to the constraint that $\nabla \cdot \varphi$ is constant in $\Omega$. Such lifting does exist. Indeed, let $\Phi := \int_{\partial\Omega} \mathbf{h} \cdot \mathbf{n}$ and let us set $\mathbf{h}_0(x) := \mathbf{h}(x) - (\Phi/3|\Omega|)x$. We have

$$\int_{\partial\Omega} \mathbf{h}_0 \cdot \mathbf{n} \;=\; \Phi\left(1 - \frac{1}{3|\Omega|}\int_{\partial\Omega} x \cdot \mathbf{n}\right) \;=\; \Phi\left(1 - \frac{1}{3|\Omega|}\int_{\Omega} \nabla \cdot x\right) \;=\; 0.$$

Hence, by Proposition 3.2.1, there exists $\varphi_0 \in \mathcal{D}^{1,2}(\Omega)$ such that $\varphi_0 = \mathbf{h}_0$ on $\partial\Omega$. We conclude by setting $\varphi(x) = \varphi_0(x) + (\Phi/3|\Omega|)x$. We have $\varphi = \mathbf{h}$ on $\partial\Omega$ and $\nabla \cdot \varphi = \Phi/|\Omega|$ is constant in $\Omega$. Notice also that with this construction, we have

$$\|\nabla\varphi\|_{L^2(\Omega)} \;\leq\; C(\Omega)\|\mathbf{h}\|_{W^{1/2,2}}.$$

Let us now return to the definition of the force density. Taking the dot product of $\mathbf{f}$ with $\mathbf{h}$ and integrating on $\partial\Omega$ we set

$$a_{int}(\mathbf{g}, \mathbf{h}) \;:=\; \int_{\partial\Omega} \mathbf{f} \cdot \mathbf{h}.$$

Integrating by parts, we compute

$$a_{int}(\mathbf{g}, \mathbf{h}) \;=\; \int_{\partial\Omega} (\nabla\mathbf{u} + \nabla\mathbf{u}^T - pId) : (\mathbf{n} \otimes \mathbf{h}) \;=\; \int_{\Omega} \nabla \cdot \left[(\nabla\mathbf{u} + \nabla\mathbf{u}^T - pId)\varphi\right].$$

Expending this expression, and using the fact that $\mathbf{u}$ solves the Stokes equations, we obtain,

$$a_{int}(\mathbf{g}, \mathbf{h}) \;=\; \int_{\Omega} \left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right) : \nabla\varphi - \left(\int_{\Omega} p\right) \nabla \cdot \varphi.$$

Since $\int_\Omega p = 0$, the last term vanishes. Symmetrizing the expression, we end with

$$a_{int}(\mathbf{g}, \mathbf{h}) \;=\; \frac{1}{2}\int_{\Omega} \left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right) : \left(\nabla\varphi + \nabla\varphi^T\right). \tag{3.4.2}$$

Consequently,

$$a_{int}(\mathbf{g}, \mathbf{h}) \;\leq\; 2\|\nabla\mathbf{u}\|_{L^2(\Omega)}\|\nabla\varphi\|_{L^2(\Omega)} \;\leq\; C(\Omega)\|\mathbf{g}\|_{W^{1/2,2}(\partial\Omega)}\|\mathbf{h}\|_{W^{1/2,2}(\partial\Omega)}.$$

Hence $a_{int}$ extends as a continuous bilinear form on

$$\left\{\mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3) \;:\; \int_{\Omega} \mathbf{g} \cdot \mathbf{n} = 0\right\} \times W^{1/2,2}(\partial\Omega, \mathbf{R}^3).$$

From the definition $a_{int}(\mathbf{g}, \mathbf{h}) = \int_{\partial\Omega} \mathbf{f} \cdot \mathbf{h}$, we deduce the following result.

**Proposition 3.4.1.** *Let $\Omega \subset \mathbf{R}^3$ be a smooth and bounded domain. There exists a linear and continuous mapping,*

$$\mathcal{DN}_{int} \ : \ \left\{ \mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3) \ : \ \int_\Omega \mathbf{g}\cdot\mathbf{n} = 0 \right\} \ \longrightarrow \ W^{-1/2,2}(\partial\Omega, \mathbf{R}^3), \qquad \mathbf{g} \ \longmapsto \ \mathbf{f}.$$

*which extends the classical definition of surface force density. Namely, if* $\mathbf{g}$ *is smooth and if* $\mathbf{f}$ *is defined by* (3.4.1)*, we have*

$$\langle \mathcal{DN}_{int}\,\mathbf{g}\,;\,\mathbf{h}\rangle_{W^{-1/2,2},W^{1/2,2}} = \int_{\partial\Omega} \mathbf{f}\cdot\mathbf{h} \qquad \textit{for every } \mathbf{h} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3).$$

The mapping $\mathcal{DN}_{int}$ is not one to one. Indeed, from the identity

$$\left\langle \mathcal{DN}_{int}\,\mathbf{g}\,;\,\mathbf{v}_{|\partial\Omega}\right\rangle_{W^{-1/2,2},W^{1/2,2}} \ = \ \int_\Omega (\nabla\mathbf{u} + \nabla\mathbf{u}^T)\cdot\nabla\mathbf{v}, \qquad \text{for every } \mathbf{v} \in \mathcal{D}^{1,2}(\Omega),$$

we see that $\mathcal{DN}_{int}\,\mathbf{g} = 0$ if and only if $\nabla\mathbf{u} + \nabla\mathbf{u}^T$ vanishes on $\Omega$, that is, by Korn inequality, if and only if $\mathbf{u}$ is the velocity field of a rigid motion. We conclude that

$$\ker(\mathcal{DN}_{int}) \ = \ \left\{ \mathbf{g} : \partial\Omega \to \mathbf{R}^3 \ : \mathbf{g}(x) \ = \ \mathbf{e} + \omega\times x \text{ for some } \mathbf{e}, \omega \in \mathbf{R}^3 \right\}.$$

Let us now compute the range of $\mathcal{DN}_{int}$. First, we notice that for every

$$\mathbf{g} \in \left\{ \mathbf{h} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3) \ : \ \int_\Omega \mathbf{h}\cdot\mathbf{n} = 0 \right\},$$

we have

$$\left\langle \mathcal{DN}_{int}\,\mathbf{g}\,;\,\mathbf{v}_{|\partial\Omega}\right\rangle_{W^{-1/2,2},W^{1/2,2}} = 0,$$

for every velocity field $\mathbf{v}$ corresponding to the combination of a rigid displacement and an expansion $\mathbf{v}(x) = \lambda x + \mathbf{e} + \omega\times x$. Indeed, we have in this case $\nabla\mathbf{v} + \nabla\mathbf{v}^T = 2\lambda Id$ and we deduce from the above computation,

$$\left\langle \mathcal{DN}_{int}\,\mathbf{g}\,;\,v_{|\partial\Omega}\right\rangle_{W^{-1/2,2},W^{1/2,2}} \ = \ \frac{1}{2}\int_\Omega (\nabla\mathbf{u} + \nabla\mathbf{u}^T)\cdot(\nabla\mathbf{v} + \nabla\mathbf{v}^T) \ = \ \lambda\int_\Omega \nabla\cdot\mathbf{u} \ = \ 0.$$

Consequently,

$$\text{Range}\,(\mathcal{DN}_{int}) \ \subset \ \mathcal{R} \ := \ \Big\{ \mathbf{f} \in W^{-1/2,2}(\partial\Omega, \mathbf{R}^3) \ : \ \langle \mathbf{f}\,;\,\mathbf{v}\rangle_{W^{-1/2,2},W^{1/2,2}} = 0$$
$$\text{for test functions of the form: } \ \mathbf{v}(x) = x, \ \mathbf{v}(x) = \mathbf{e} \in \mathbf{R}^3 \text{ and } \mathbf{v}(x) = \omega\times x, \ \omega \in \mathbf{R}^3 \Big\}.$$

Conversely, let $\mathbf{f} \in \mathcal{R}$ and let us consider the homogeneous Stokes equations with non-homogeneous "Neumann" boundary conditions:

$$\left\{ \begin{array}{rcll} -\Delta\mathbf{u} + \nabla p & = & 0 & \text{in } \Omega, \\ \nabla\cdot\mathbf{u} & = & 0 & \text{in } \Omega, \\ (\nabla\mathbf{u} + \nabla\mathbf{u}^T - p\,Id)\cdot\mathbf{n} & = & \mathbf{f} & \text{on } \partial\Omega. \end{array} \right. \tag{3.4.3}$$

The solution of this problem, if it exists, is not unique. Indeed, we can add to the velocity any velocity field corresponding to a rigid displacement. To enforce uniqueness of the velocity, we impose the conditions,

$$\int_\Omega \mathbf{u}(x) \;=\; \int_\Omega x \times \mathbf{u}(x) \;=\; 0. \tag{3.4.4}$$

From (3.4.2), we see that a natural variational formulation for this problem is : find $\mathbf{u} \in \mathcal{D}^{1,2}(\Omega)$ satisfying (3.4.4) such that

$$\frac{1}{2}\int_\Omega (\nabla\mathbf{u} + \nabla\mathbf{u}^T) : (\nabla\mathbf{v} + \nabla\mathbf{v}^T) \;=\; \big\langle \mathbf{f}\,;\,\mathbf{v}_{|\partial\Omega}\big\rangle_{W^{-1/2,2},W^{1/2,2}} \qquad \forall\,\mathbf{v} \in \mathcal{D}^{1,2}(\Omega). \tag{3.4.5}$$

Thanks to the Korn inequality, this variational formulation admits a unique solution $\mathbf{u}$ in

$$\mathcal{E} \;:=\; \left\{ \mathbf{v} \in \mathcal{D}^{1,2}(\Omega) : \int_\Omega \mathbf{v}(x) \;=\; \int_\Omega x \times \mathbf{v}(x) \;=\; 0 \right\}.$$

The identity (3.4.5) holds for every $\mathbf{v} \in \mathcal{E}$ and since $\mathbf{u} \in \mathcal{E}$ and $\mathbf{f} \in \mathcal{R}$, this identity also holds for every $\mathbf{v} \in \mathcal{D}^{1,2}(\Omega)$. In particular,

$$\int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v} \;=\; 0 \quad \text{ for every } \mathbf{v} \in \mathcal{D}^{1,2}(\Omega) \cap C_c^\infty(\Omega).$$

By de Rham's Theorem, there exists a unique pressure $p \in L^2_0(\Omega)$ such that

$$-\Delta\mathbf{u} + \nabla p \;=\; 0 \quad \text{in the sense of distributions in } \Omega.$$

This solution defines the Neumann to Dirichlet operator

$$\mathcal{ND}_{int}\mathbf{f} \;:=\; \mathbf{u}_{|\partial\Omega} \in W^{1/2,2}(\Omega, \mathbf{R}^3).$$

By construction, we see that the composition $\mathcal{DN}_{int} \circ \mathcal{ND}_{int}$ is the identity operator on $\mathcal{R}$. We have established:

**Proposition 3.4.2.** *The operator $\mathcal{DN}_{int}$ defines a continuous isomorphism from*

$$\mathcal{S} \;=\; \left\{ \mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3) : \int_{\partial\Omega} \mathbf{g}\cdot\mathbf{n} = 0,\; \int_{\partial\Omega} \mathbf{g} \;=\; \int_{\partial\Omega} x \times \mathbf{g} = 0 \right\}$$

*onto $\mathcal{R} \subset W^{-1/2,2}(\partial\Omega, \mathbf{R}^3)$.*

### 3.4.2 The Dirichlet to Neumann operator in an exterior domain

We consider the corresponding operators in the case of an exterior domain $\Omega \subset \mathbf{R}^3$. Let $\mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ and let $(\mathbf{u}, p) \in \mathcal{D}^{1,2}(\Omega) \times L^2(\Omega)$ be the variational solution of the Stokes problem. For every $\mathbf{h} \in W^{1/2,2}(\Omega, \mathbf{R}^3)$, there exists a lifting $\varphi$ of $\mathbf{h}$ in $\mathcal{D}^{1.2}(\Omega)$ (see Proposition 3.2.2). The bilinear form

$$a_{ext}(\mathbf{g}, \mathbf{h}) \;=\; \int_\Omega (\nabla\mathbf{u} + \nabla\mathbf{u}^T) : \nabla\varphi$$

is well defined. Indeed, for every $\mathbf{v} \in \mathcal{D}_0^{1,2}(\Omega)$, we have $\int_\Omega (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : \nabla \mathbf{v} = 0$, so the above quantity does not depend on the particular lifting $\varphi$. We have

$$a_{ext}(\mathbf{g}, \mathbf{h}) \;\leq\; 2\|\nabla \mathbf{u}\|_{L^2} \|\nabla \varphi\|_{L^2} \;\leq\; C\|\mathbf{g}\|_{W^{1/2,2}} \|\mathbf{h}\|_{W^{1/2,2}}.$$

Hence there exists a continuous linear operator $\mathcal{DN}_{ext} \,:\, W^{1/2,2}(\partial\Omega, \mathbf{R}^3) \to W^{-1/2,2}(\partial\Omega, \mathbf{R}^3)$ such that

$$\langle \mathcal{DN}_{ext}\, \mathbf{g}\, ;\, \mathbf{h} \rangle_{W^{-1/2,2}, W^{1/2,2}} \;=\; a_{ext}(\mathbf{g}, \mathbf{h}) \qquad \forall\, \mathbf{g}, \mathbf{h} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3).$$

When $\mathbf{g} \in W^{3/2,2}(\partial\Omega, \mathbf{R}^3)$, $D^2\mathbf{u}$ and $\nabla p$ belong to $L^2(\Omega)$ and the surface force density

$$\mathbf{f} \;=\; (\nabla \mathbf{u} + \nabla \mathbf{u}^T - p\, Id) \cdot \mathbf{n} \tag{3.4.6}$$

is well defined on $\partial\Omega$, with $\mathbf{f} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$. In this case, we have, as in the case of a bounded domain,

$$\int_{\partial\Omega} \mathbf{f} \cdot \mathbf{h} \;=\; \int_\Omega (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : \nabla \varphi \;-\; \int_\Omega p \nabla \cdot \varphi.$$

Since $\varphi \in \mathcal{D}^{1,2}(\Omega, \mathbf{R}^3)$, the last term vanishes and we see that

$$\int_{\partial\Omega} \mathbf{f} \cdot \mathbf{h} \;=\; \langle \mathcal{DN}_{ext}\, \mathbf{g}\, ;\, \mathbf{h} \rangle_{W^{-1/2,2}, W^{1/2,2}}\, .$$

We have established:

**Proposition 3.4.3.** *For any smooth exterior domain $\Omega \subset \mathbf{R}^3$, there exists a continuous Dirichlet to Neumann operator $\mathcal{DN}_{ext} \,:\, \mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3) \to \mathbf{f} \in W^{-1/2,2}(\partial\Omega, \mathbf{R}^3)$ which extends the definition of surface force density* (3.4.6)*.*

For every $\mathbf{g} \in W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$, we have

$$\langle \mathcal{DN}_{ext} \mathbf{g}\, ;\, \mathbf{g} \rangle_{W^{-1/2,2}, W^{1/2,2}} \;=\; \frac{1}{2} \int_\Omega |\nabla \mathbf{u} + \nabla \mathbf{u}^T|^2.$$

By Korn's inequality, the right hand side is bounded from below by $(1/C(\Omega))\|\nabla \mathbf{u}\|_{L^2}^2$. Hence,

$$\langle \mathcal{DN}_{ext} \mathbf{g}\, ;\, \mathbf{g} \rangle_{W^{-1/2,2}, W^{1/2,2}} \;\geq\; (1/C(\Omega))\|\mathbf{g}\|_{W^{1/2,2}}^2.$$

We deduce from the Lax Milgram Theorem that the operator $\mathcal{DN}_{ext}$ is one to one and onto.

**Proposition 3.4.4.** *For any smooth exterior domain $\Omega \subset \mathbf{R}^3$, the Dirichlet to Neumann operator $\mathcal{DN}_{ext}$ is a linear continuous isomorphism from $W^{1/2,2}(\partial\Omega, \mathbf{R}^3)$ onto $W^{-1/2,2}(\partial\Omega, \mathbf{R}^3)$ and we denote by $\mathcal{ND}_{ext}$ its inverse.*

It is easy to check that the inverse operator satisfies $\mathcal{ND}_{ext}\mathbf{f} = \mathbf{u}_{|\partial\Omega}$ where $\mathbf{u} \in \mathcal{D}^{1,2}(\Omega)$ is the unique solution of the variational formulation

$$\int_\Omega (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : \nabla \mathbf{v} \;-\, \big\langle \mathbf{f}\, ;\, \mathbf{v}_{|\partial\Omega} \big\rangle_{W^{-1/2,2}, W^{1/2,2}} \;=\; 0 \qquad \forall\, \mathbf{v} \in \mathcal{D}^{1,2}(\Omega).$$

### 3.4.3 Jump of forces through an interface. A new Neumann to Dirichlet operator

Let us now consider an open set $\Omega \subset \mathbf{R}^3$ which is the union of a finite number of smooth bounded domains $\Omega_1, \cdots, \Omega_N$. We assume moreover that the closures $\overline{\Omega}_i$ are pairwise disjoint. We note $\Gamma_i$ the boundary of $\Omega_i$ and $\Gamma = \partial\Omega = \cup_i \Gamma_i$. We denote by $\mathbf{n} : \Gamma \to S^2$ the unit exterior normal to $\Omega$ and $\mathbf{n}_i$ its restriction on $\Gamma_i$. We consider Dirichlet boundary data in the space,

$$H \;=\; \left\{ \mathbf{g} \in W^{1/2,2}(\Gamma, \mathbf{R}^3) \;:\; \text{such that } \mathbf{g}_i = \mathbf{g}_{|\Gamma_i} \text{ satisfies } \int_{\Gamma_i} \mathbf{g}_i \cdot \mathbf{n}_i \;= 0 \text{ for } i = 1, \cdots, N \right\}.$$

Eventually, we define $\Omega_0$ as the exterior domain,

$$\Omega_0 \;:=\; \mathbf{R}^3 \setminus \overline{\Omega}.$$

Let $\mathbf{g} \in H$, for $i = 0, \cdots, N$, we denote by $\mathbf{u}_i \in \mathcal{D}^{1,2}(\Omega_i)$ the unique solution of the variational problem: $\mathbf{u}_i = \mathbf{g}_i$ on $\Gamma_i$ if $i \geq 1$ or $\mathbf{u} = \mathbf{g}$ on $\Gamma$ if $i = 0$ and

$$\int_{\Omega_i} (\nabla \mathbf{u}_i + \nabla \mathbf{u}_i^T) : \nabla \mathbf{v} \;=\; 0 \qquad \forall\, \mathbf{v} \in \mathcal{D}_0^{1,2}(\Omega_i).$$

We denote by $p_0 \in L^2(\Omega_0)$ and $p_i \in L_0^2(\Omega_i)$, $i = 1, \cdots, N$ the corresponding pressure fields. We define the following operator as

$$[\mathcal{DN}_\Gamma\, \mathbf{g}]_{|\Gamma_i} \;:=\; \mathcal{DN}_{int}\, \mathbf{g}_i + [\mathcal{DN}_{ext}\, \mathbf{g}]_{|\Gamma_i}, \qquad \text{for } i = 1, \cdots, N.$$

This defines a continuous linear operator from $H$ in $W^{-1/2,2}(\Gamma, \mathbf{R}^3)$.

Alternatively, we can define this operator without explicit reference to the operators $\mathcal{DN}_{int}$ and $\mathcal{DN}_{ext}$. For every $\mathbf{g} \in H$, we can define $\mathbf{u} \in \mathcal{D}^{1,2}(\mathbf{R}^3)$ as the the unique solution of the variational problem $\mathbf{u} = \mathbf{g}$ on $\Gamma$ and

$$\int_{\Omega} \nabla \mathbf{u} : \nabla \mathbf{v} \;=\; 0 \qquad \text{for every } \mathbf{v} \in \mathcal{D}^{1,2}(\mathbf{R}^3) \text{ such that } \mathbf{v}_{|\Gamma} \equiv 0.$$

Obvioulsy, we have $\mathbf{u}_{|\Omega_i} = \mathbf{u}_i$ for $i = 0, \cdots, N$. Then, for $\mathbf{h} \in H$, we choose a lifting $\varphi$ of $\mathbf{h}$ in $\mathcal{D}^{1,2}(\mathbf{R}^3)$ and we set:

$$a_\Gamma(\mathbf{g}, \mathbf{h}) \;:=\; \int_{\mathbf{R}^3} \nabla \mathbf{u} : \nabla \varphi.$$

The bilinear form $a_\Gamma$ is continuous on $H \times H$ and since we can choose $\varphi$ as the variational solution of the Stokes equations in $\mathbf{R}^3 \setminus \Gamma$ with boundary condition $\varphi = \mathbf{h}$ on $\Gamma$, we see that $a_\Gamma$ is symmetric and nonnegative. Let us consider an element $L \in H'$ and let us extend it on $W^{1/2,2}(\Gamma, \mathbf{R}^3)$ by setting

$$L\left(\mathbf{h} + \sum_{i=1}^{N} c_i \mathbf{1}_{|\Gamma_i} \mathbf{n}_i\right) \;=\; L(\mathbf{h}) \qquad \text{for every } \mathbf{h} \in H,\, c_1, \cdots, c_N \in \mathbf{R}.$$

There exists a unique $\mathbf{f} \in W^{-1/2,2}(\Gamma, \mathbf{R}^3)$ such that

$$L(\mathbf{h}) \;=\; \langle \mathbf{f}\,;\mathbf{h} \rangle_{W^{-1/2,2}, W1/2,2} \qquad \text{for every } \mathbf{h} \in W^{1/2,2}(\Gamma, \mathbf{R}^3).$$

Choosing $\mathbf{h} = \mathbf{1}_{|\Gamma_i}\mathbf{n}_i$, we see that $\langle \mathbf{f}\,;\mathbf{n}_i\rangle_{W^{-1/2,2},W1/2,2} = 0$ for $i = 1,\cdots,N$ and it turns out that we can make the identification

$$H' \;=\; \Big\{\mathbf{f} \in W^{-1/2,2}(\Gamma,\mathbf{R}^3)\;:\;\langle \mathbf{f}\,;\mathbf{n}\rangle_{W^{-1/2,2},W1/2,2} \;=\; 0\Big\}.$$

Applying this to the linear form $L(\mathbf{h}) = a_\Gamma(\mathbf{g},\mathbf{h})$, there exists a unique $\mathbf{f} \in H'$ such that

$$\langle \mathbf{f}\,;\mathbf{h}\rangle_{W^{-1/2,2},W1/2,2} \;=\; a_\Gamma(\mathbf{g},\mathbf{h}) \qquad \text{for every } \mathbf{h} \in W^{1/2,2}(\Gamma,\mathbf{R}^3).$$

We set

$$\mathcal{DN}_\Gamma\,\mathbf{g} \;:=\; \mathbf{f}. \tag{3.4.7}$$

Eventually, for every $\mathbf{g}$ in $H$, we have with obvious notation,

$$a_\Gamma(\mathbf{g},\mathbf{g}) \;=\; \langle \mathcal{DN}_\Gamma\,\mathbf{g}\,;\mathbf{g}\rangle_{W^{-1/2,2},W1/2,2} \;=\; \int_{\mathbf{R}^3} |\nabla \mathbf{u}|^2.$$

We see that $a_\Gamma$ is coercive on $H$. Hence, the linear operator $\mathcal{DN}_\Gamma : H \to H'$ is a continuous linear isomorphism.

**Proposition 3.4.5.** *Let $\Omega = \cup_{i=1}^N \Omega_i$ be a finite union of smooth open subsets of $\mathbf{R}^3$ such that the $\overline{\Omega}_i$ are pairwise disjoint. Let $\Gamma = \partial\Omega$. The operator $\mathcal{DN}_\Gamma$ defined by (3.4.7) is a continuous linear isomorphism from*

$$H \;=\; \left\{\mathbf{g} \in W^{1/2,2}(\Gamma,\mathbf{R}^3)\;:\;\int_{\partial\Omega_i} \mathbf{g}\cdot\mathbf{n}_i \;=\; 0,\ \textit{for every } i = 1,\cdots,N\right\}$$

*onto $H'$ where we identify $H'$ with the closure of $H$ in $W^{-1/2,2}(\Gamma,\mathbf{R}^3)$.*

Now, let us consider the inverse problem. Let $\mathbf{f} \in H'$, and let us consider the solution $\mathbf{u} \in \mathcal{D}^{1,2}(\mathbf{R}^3)$ of the variational problem

$$\int_{\mathbf{R}^3} \nabla\mathbf{u} : \nabla\mathbf{v} \;=\; \big\langle \mathbf{f}\,;\mathbf{v}_{|\Gamma}\big\rangle_{W^{-1/2,2},W^{1/2,2}} \qquad \forall\,\mathbf{v} \in \mathcal{D}^{1,2}(\mathbf{R}^3).$$

Notice that the linear form $\mathbf{v} \in \mathcal{D}^{1,2}(\mathbf{R}^3) \mapsto \big\langle \mathbf{f}\,;\mathbf{v}_{|\Gamma}\big\rangle_{W^{-1/2,2},W^{1/2,2}}$ is continuous. Hence, the existence of a unique solution to the variational formulation relies on Theorem 13. We also know that this solution is obtained by convolution with the fundamental solution of the Stokes equations in $\mathbf{R}^3$:

$$\mathbf{u}(x) \;=\; \langle \mathbf{f}\,;G(\cdot - x)\rangle_{W^{-1/2,2}(\Gamma),W^{1/2,2}(\Gamma)}\,, \qquad \text{for } x \in \mathbf{R}^3.$$

Identifying $\mathbf{f}$ with the distribution $\varphi \in C_c^\infty(\mathbf{R}^3,\mathbf{R}^3) \mapsto \big\langle \mathbf{f}\,;\varphi_{|\Gamma}\big\rangle_{W^{-1/2,2}(\Gamma),W^{1/2,2}(\Gamma)}$, this formula rewrites as

$$\mathbf{u} \;=\; G\star\mathbf{f},$$

where we recall the definition of the Stokeslet,

$$G(\mathbf{r}) \;=\; \frac{1}{8\pi r}\left(Id + \mathbf{e}_r\otimes\mathbf{e}_r\right).$$

Now we define

$$\mathcal{ND}_\Gamma \, \mathbf{f} \ := \ [G \star \mathbf{f}]_{|\Gamma} \, .$$

This operator maps $H'$ in $H$ and we easily see that $\mathcal{ND}_\Gamma \circ \mathcal{DN}_\Gamma = Id_H$. We see that $\mathbf{u}$ solves the variational formulation $\mathbf{u} = \mathcal{ND}_\Gamma \, \mathbf{f}$ on $\Gamma$ and

$$\int_{\mathbf{R}^3} \nabla \mathbf{u} : \nabla \mathbf{v} \ = \ 0 \qquad \text{for every } \mathbf{v} \in \mathcal{D}^{1,2}(\mathbf{R}^3) \text{ such that } \mathbf{v}_{|\Gamma} \equiv 0.$$

By definition, we have $\mathcal{DN}_\Gamma[\mathcal{ND}_\Gamma \, \mathbf{f}] = \mathbf{f}$. Hence $\mathcal{ND}_\Gamma$ is the inverse of $\mathcal{DN}_\Gamma$.

**Proposition 3.4.6.** *Let $\Omega = \cup_{i=1}^N \Omega_i$ be a finite union of smooth open subsets of $\mathbf{R}^3$ such that the $\overline{\Omega}_i$ are pairwise disjoint. Let $\Gamma = \partial\Omega$. The "Neumann to Dirichlet" operator defined as*

$$\mathcal{ND}_\Gamma \, \mathbf{f} \ = \ [G \star \mathbf{f}]_{|\Gamma} \qquad \textit{for every } \mathbf{f} \in H'$$

*is the inverse of the "Dirichlet to Neumann" operator $\mathcal{DN}_\Gamma$.*

Chapter 4

# Spectral discretization of the hydrodynamic interactions

Contents



## 4.1 The hydrodynamic interactions

### 4.1.1 Setting of the problem

We consider $N$ non intersecting particles immersed in a viscous fluid. For simplicity, the particles are identical balls $B_1$, $B_2$,...,$B_N$ with radius 1 and centers $\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_N \in \mathbf{R}^3$, respectively. We assume that the closed balls $B_i$ do not intersect and that the fluid fills the rest of the space. The fluid occupies the domain

$$\Omega := \mathbf{R}^3 \backslash \left( \bigcup_{i=1}^{N} B_i \right).$$

We assume moreover that the fluid inertia effects are negligible compared to the viscosity (i.e. the Reynolds number is very small $\mathrm{Re} \ll 1$) so that the velocity $\mathbf{u}$ and the pressure $p$ solve the stationary Stokes equations in the fluid domain,

$$\left\{ \begin{array}{ll} \nabla \cdot \sigma = 0 & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega, \end{array} \right. \tag{4.1.1}$$

where $\sigma = \nabla \mathbf{u} + \nabla \mathbf{u}^T - p\mathrm{Id}$ is the stress tensor in the fluid and Id is the identity matrix.

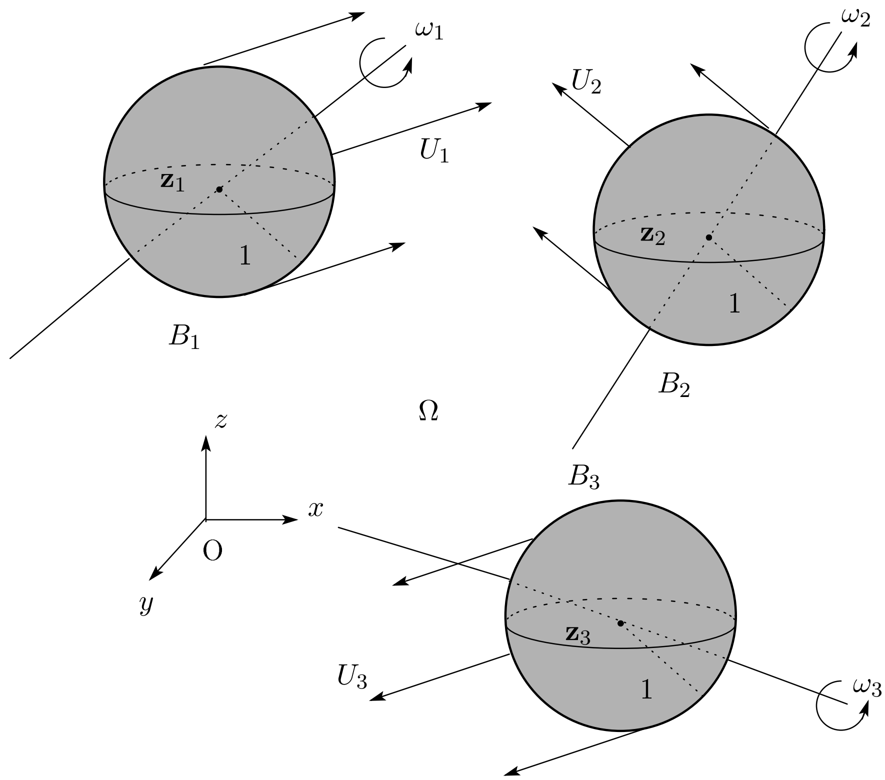


Figure 4.1: Example with three particles.

On the surfaces of the particles, we consider a no-slip condition,

$$\mathbf{u} \;=\; \mathbf{u}_i \quad \text{on } \partial B_i, \quad i = 1, 2, ..., N.$$

where the velocity $\mathbf{u}_i$ corresponds to a rigid displacement. It is characterized by the velocity $\mathbf{U}_i$ at the center $\mathbf{z}_i$ of the ball $B_i$ and by the angular velocity $\omega_i$ ($\mathbf{U}_i, \omega_i \in \mathbf{R}^3$),

$$\mathbf{u}_i(\mathbf{r}) \;:=\; \mathbf{U}_i + \omega_i \times (\mathbf{r} - \mathbf{z}_i), \quad \text{for } \mathbf{r} \in \mathbf{R}^3, \quad i = 1, 2, ..., N. \tag{4.1.2}$$

We are interested in solutions $\mathbf{u}$ which decay at infinity, i.e., which fulfills

$$\mathbf{u}(\mathbf{r}) \to 0, \quad \text{as } |\mathbf{r}| \to \infty.$$

As recalled in the preceding section, the existence and uniqueness of a solution to (4.1.1) is classical in the Hilbert space

$$\mathcal{D}^{1,2}(\Omega) \;:=\; \left\{ \mathbf{u} \in \mathcal{D}'(\Omega, \mathbf{R}^3) : \; \nabla \mathbf{u} \in L^2(\Omega), \frac{\mathbf{u}}{\sqrt{1 + r^2}} \in L^2(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega \right\},$$

endowed with the scalar product

$$(\mathbf{u}, \mathbf{v})_{\mathcal{D}} \;:=\; \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v}.$$

The surface density of force exerted on the fluid at some point $\mathbf{r}$ of the surface $\partial B_i$ is given by

$$\mathbf{f}_i(\mathbf{r}) \;=\; \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - p\mathrm{Id}\right).\mathbf{n}_i, \tag{4.1.3}$$

where $\mathbf{n}_i$ denotes the exterior normal on the surface of the i-est particle $B_i$.

The total force and total torque exerted by the particle $B_i$ on the fluid are given by the following formulas,

$$\mathbf{F}_i \;=\; \int_{\partial B_i} \mathbf{f}_i(\mathbf{r}) dS(\mathbf{r}),$$

$$\mathcal{T}_i \;=\; \int_{\partial B_i} (\mathbf{r} - \mathbf{z}_i) \times \mathbf{f}_i(\mathbf{r}) dS(\mathbf{r}).$$

The main goal of our work is to propose a numerical method for computing accurate approximations of the friction operator,

$$\mathcal{F} :\; (\mathbf{R}^3)^{2N} \longrightarrow (\mathbf{R}^3)^{2N}, \quad (\mathbf{U}_i, \omega_i)_{1\le i\le N} \longmapsto (\mathbf{F}_i, \mathcal{T}_i)_{1\le i\le N},$$

which describes the hydrodynamic interactions between the particles.

### 4.1.2 The boundary integral method

Let us first make a crucial remark: any velocity field associated to a rigid displacement $\mathbf{w}(\mathbf{r}) = \mathbf{U} + \omega \times \mathbf{r}$ solves the Stokes equations with a constant pressure field $p = p_\infty \in \mathbf{R}$. Indeed, direct computations show that $\nabla \cdot \mathbf{w}(\mathbf{r}) = 0$ and that the stress tensor $\sigma$ reduces to the uniform tensor $-p_\infty \mathrm{Id}$. Hence, it is reasonable to extend the velocity and pressure fields inside the particles by setting,

$$\mathbf{u}(\mathbf{r}) \;:=\; \mathbf{u}_i(\mathbf{r}) \;\text{ and }\; p(\mathbf{r}) \;:=\; p_i = \frac{1}{4\pi}\int_{\partial B_i} p(\mathbf{r}')dS(\mathbf{r}'), \quad \text{for } \mathbf{r} \in B_i,\; i = 1, 2, ..., N.$$

The extended fields solve

$$\nabla \cdot \sigma \;=\; 0 \quad \text{in } \mathbf{R}^3 \setminus \cup \partial B_i, \qquad \nabla \cdot \mathbf{u} \;=\; 0 \quad \text{in } \mathbf{R}^3, \tag{4.1.4}$$

with the jump condition,

$$[\sigma] \cdot \mathbf{n}_i \;=\; \tilde{\mathbf{f}}_i \quad \text{on } \partial B_i, \quad i = 1, 2, ..., N, \tag{4.1.5}$$

where $\tilde{\mathbf{f}}_i$ is a surface density of forces on $\partial B_i$. These force densities do not identify with the surface density $\mathbf{f}_i$ introduced in (4.1.3). In fact, we have for $\mathbf{r}$ on the surface of $\partial B_i$,

$$\tilde{\mathbf{f}}_i(\mathbf{r}) \;=\; [\sigma(\mathbf{r};\Omega) - \sigma(\mathbf{r}; B_i)] \cdot \mathbf{n}_i(\mathbf{r}) \;=\; \mathbf{f}_i - \sigma(\mathbf{r}; B_i) \cdot \mathbf{n}_i(\mathbf{r}),$$

with $\sigma(\mathbf{r}; B_i) = \nabla \mathbf{u}_i + \nabla \mathbf{u}_i^T - p_i \mathrm{Id}$. However, since this stress tensor corresponds to a rigid motion, it does not contribute to the total force and torque exerted by the surface of $B_i$, that is

$$\int_{\partial B_i} \sigma(\mathbf{r}; B_i) \cdot \mathbf{n}_i(\mathbf{r}) dS(\mathbf{r}) \;=\; \int_{\partial B_i} \mathbf{n}_i(\mathbf{r}) \times [\sigma(\mathbf{r}; B_i) \cdot \mathbf{n}_i(\mathbf{r})] dS(\mathbf{r}) \;=\; 0.$$

Hence, the total forces and torques can be rewritten as follows

$$\mathbf{F}_i \;=\; \int_{\partial B_i} \tilde{\mathbf{f}}_i(\mathbf{r})dS(\mathbf{r}), \qquad \mathcal{T}_i \;=\; \int_{\partial B_i} \mathbf{n}_i \times \tilde{\mathbf{f}}_i(\mathbf{r})dS(\mathbf{r}). \tag{4.1.6}$$

The unique solution $\mathbf{u} \in \mathcal{D}^{1,2}(\mathbf{R}^3)$ of (4.1.4), (4.1.5) is given by convolution of the surface density forces $\tilde{\mathbf{f}}_i$ with the Green tensor associated to the Stokes equations in $\mathbf{R}^3$,

$$\mathbf{u}(\mathbf{r}) \;=\; \sum_{i=1}^{N} \int_{\partial B_i} G(\mathbf{r}-\mathbf{r}') \cdot \tilde{\mathbf{f}}_i(\mathbf{r}')dS(\mathbf{r}'), \qquad \mathbf{r} \in \mathbf{R}^3, \tag{4.1.7}$$

where the tensor $G$ is the Stokeslet

$$G(\mathbf{r}) \;:=\; \frac{1}{8\pi}\left(\frac{\mathrm{Id}}{r} + \frac{\mathbf{r}\otimes\mathbf{r}}{r^3}\right).$$

The explicit formula (4.1.7) gives the velocity field everywhere as soon as the force densities $\tilde{\mathbf{f}}_i$ are known. However, the data of the problem are the velocity fields $\mathbf{u}_i$, not these force densities. We are then led to consider the following “Neumann to Dirichlet” operator introduced in Section 3.4:

$$\begin{aligned}\mathcal{ND} \;:\; \quad H_0^{-1/2}(\partial B_1)\times ...\times H_0^{-1/2}(\partial B_N) \;&\longrightarrow\; H_0^{1/2}(\partial B_1)\times ...\times H_0^{1/2}(\partial B_N)\\ (\tilde{\mathbf{f}}_1, ..., \tilde{\mathbf{f}}_N) \;&\longmapsto\; (\mathbf{u}_{|\partial B_1}, ..., \mathbf{u}_{|\partial B_N}),\end{aligned}$$

where for every $i = 1, .., N$, the spaces $H_0^{1/2}(\partial B_i)$ and $H_0^{-1/2}(\partial B_i)$ are defined by

$$\begin{aligned}H_0^{1/2}(\partial B_i) \;&=\; \left\{\mathbf{g} \in H^{1/2}(\partial B_i) : \quad \int_{\partial B_i} \mathbf{g}\cdot\mathbf{n}_i = 0\right\},\\ H_0^{-1/2}(\partial B_i) \;&=\; \left\{\mathbf{f} \in H^{-1/2}(\partial B_i) : \quad \langle \mathbf{f}, \mathbb{1}_{\partial B_i}\mathbf{n}_i\rangle = 0\right\}.\end{aligned}$$

This operator is positive and symmetric, its inverse is the corresponding “Dirichlet to Neumann” operator,

$$\begin{aligned}\mathcal{DN} := \mathcal{ND}^{-1} \;:\; \quad H_0^{1/2}(\partial B_1)\times ...\times H_0^{1/2}(\partial B_N) \;&\longrightarrow H_0^{-1/2}(\partial B_1)\times ...\times H_0^{-1/2}(\partial B_N)\\ (\mathbf{u}_{|\partial B_1}, ..., \mathbf{u}_{|\partial B_N}) \;&\longmapsto\; (\tilde{\mathbf{f}}_1, ..., \tilde{\mathbf{f}}_N).\end{aligned}$$

In the initial problem, we only need to compute approximations of this operator when $(\mathbf{u}_{i|\partial B_i})_{1\le i\le N}$ is a finite sequence of rigid motions. Moreover we do not need a complete description of $(\tilde{\mathbf{f}}_i)_{1\le i\le N}$ but only the projections of these force densities given by (4.1.6). In short, we only need a projection of the operator $\mathcal{DN}$ on a finite dimensional space of dimensions $6N$, that is a $6N \times 6N$ matrix. This operator,

$$\mathcal{F} \;:\; \mathbf{R}^{6N} \longrightarrow \mathbf{R}^{6N}, \quad (\mathbf{U}_i, \omega_i)_{1\le i\le N} \longmapsto (\mathbf{F}_i, \mathcal{T}_i)_{1\le i\le N}$$

is called the friction operator and its representation in a basis of translations and rotations of individual particles is called the friction or resistance matrix. The inverse of this matrix is called the mobility matrix

$$\mathcal{M} \;:\; \mathbf{R}^{6N} \longrightarrow \mathbf{R}^{6N}, \quad (\mathbf{F}_i, \mathcal{T}_i)_{1\le i\le N} \longmapsto (\mathbf{U}_i, \omega_i)_{1\le i\le N}.$$

Unfortunately, we do not have a nice explicit expression for $\mathcal{DN}$ such as (4.1.7). To compute accurate approximations of $\mathcal{F}$ starting from (4.1.7), the naive method consists in 1/ approximating $\mathcal{ND}$ by a finite dimensional discrete operator, 2/ inverse this approximate operator, 3/ project this inverse on the space of rigid motions. In the next section we describe this idea in the case of a spectral discretization.

### 4.1.3 Spectral approximation

To approximate the operator $\mathcal{ND}$, we use a Galerkin method. For this, let us rewrite this operator in variational form. For simplicity, let us define

$$\begin{aligned} H_0^{1/2}(\partial\Omega) &:= H_0^{1/2}\left(\partial B_1, \mathbf{R}^3\right) \times ... \times H_0^{1/2}\left(\partial B_N, \mathbf{R}^3\right), \\ H_0^{-1/2}(\partial\Omega) &:= H_0^{-1/2}\left(\partial B_1, \mathbf{R}^3\right) \times ... \times H_0^{-1/2}\left(\partial B_N, \mathbf{R}^3\right). \end{aligned}$$

Given $\mathbf{u}_i := \mathbf{u}_{|\partial B_i} \in H_0^{1/2}\left(\partial B_i, \mathbf{R}^3\right)$, for $i = 1, 2, ..., N$, we define for $\mathbf{f}, \mathbf{g} \in H_0^{-1/2}(\partial\Omega)$ the bilinear form

$$a(f,g) = \sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\partial B_i}\int_{\partial B_j} g_i^T(\mathbf{r}) \cdot G(\mathbf{r}-\mathbf{r}') \cdot f_j(\mathbf{r}')dS(\mathbf{r}')dS(\mathbf{r}),$$

and the linear form,

$$L(g) = \sum_{i=1}^{N}\int_{\partial B_i} g_i^T(\mathbf{r}) \cdot \mathbf{u}(\mathbf{r})dS(\mathbf{r}).$$

In particular, $a(\cdot,\cdot)$ is a bounded and coercive bilinear form (see Section 3.4) and $L$ is a bounded linear functional on $H_0^{-1/2}(\partial\Omega)$.

The surface density forces $\tilde{\mathbf{f}} = \left(\tilde{\mathbf{f}}_1, ..., \tilde{\mathbf{f}}_N\right)$ in $H_0^{-1/2}(\partial\Omega)$ solves the problem:

$$\text{Find } f \in H_0^{-1/2}(\partial\Omega) \text{ such that: } \quad a(f,g) = L(g),\ \forall g \in H_0^{-1/2}(\partial\Omega). \tag{4.1.8}$$

Therefore we can approximate the solution of equation (4.1.8) by a Galerkin method. For $i = 1, ..., N$, choose subspaces $V_i^K \subset H_0^{1/2}\left(\partial B_i, \mathbf{R}^3\right)$ of dimension $K$ and then solve the projected problem on $V_i^K$:

$$\text{Find } f^K \in V_1^K \times ... \times V_N^K \text{ such that: } \quad a\left(f^K, g^K\right) = L\left(g^K\right), \quad \forall g^K \in V_1^K \times ... \times V_N^K. \tag{4.1.9}$$

Let $\{\phi_{i,\alpha}\}_{\alpha=1,...,K}$ be a basis of $V_i^K$, for $i = 1, ..., N$. The unknown $f^K = (f_1^K, ..., f_N^K)$ can be decomposed as $f_i^K = \sum_{\alpha=1}^K F_{i,\alpha}^K \phi_{i,\alpha}$. The discrete problem (4.1.9) can be rewritten in the matrix form

$$A^K F^K = L^K,$$

where

$$A_{i,\alpha,j,\beta}^K = \int_{\partial B_i}\int_{\partial B_j} \phi_{j,\beta}^T(\mathbf{r}) \cdot G(\mathbf{r}-\mathbf{r}') \cdot \phi_{i,\alpha}(\mathbf{r}')dS(\mathbf{r}')dS(\mathbf{r}), \tag{4.1.10}$$

$$L_{i,\alpha}^K = u_{i,\alpha}, \qquad \text{with } i,j \in \{1,...,N\}, \text{ and } \alpha,\beta \in \{1,...,K\}. \tag{4.1.11}$$

The first difficulty is that the integral in (4.1.10) is singular if $i = j$. In order to overcome this problem, it is convenient to use a spectral decomposition method. More precisely, for every $i = 1, ..., N$, we choose the finite dimensional subspace $V_i^h$ to be the space generated by the first eigenvectors of the following operator,

$$\begin{aligned} \mathcal{G}_i \ : \quad H^{-1/2}(\partial B_i, \mathbf{R}^3) &\longrightarrow H^{1/2}(\partial B_i, \mathbf{R}^3) \\ \phi &\longmapsto \int_{\partial B_i} G(. - \mathbf{r}') \cdot \phi(\mathbf{r}') dS(\mathbf{r}'). \end{aligned}$$

In other words, for $i = 1, ..., N$ and $\alpha = 1, ..., K$, $\phi_{i,\alpha}$ satisfies

$$\int_{\partial B_i} G(\mathbf{r} - \mathbf{r}') \cdot \phi_{i,\alpha}(\mathbf{r}') dS(\mathbf{r}') = \frac{1}{\lambda_\alpha} \phi_{i,\alpha}(\mathbf{r}), \qquad \text{for all } \mathbf{r} \in \partial B_i. \tag{4.1.12}$$

Using this spectral decomposition, self interactions are diagonal and the other terms do not include singular integrals. Indeed, by (4.1.12), when $i = j$ the formula (4.1.10) becomes

$$A^h_{i,\alpha,i,\beta} = \frac{\delta_{\alpha\beta}}{\lambda_\alpha}.$$

Moreover, when $i \neq j$ the integrals in (4.1.10) do not include singular integrals, since

$$|\mathbf{r} - \mathbf{r}'| \geq d(B_i, B_j) > 0, \quad \forall \mathbf{r} \in \partial B_i, \ \forall \mathbf{r}' \in \partial B_j.$$

It turns out that the basis $\{\phi_{i,\alpha}\}_{\alpha=1,...,K}$ is a basis of vectorial spherical harmonics associated to the sphere. We describe this basis and the decomposition of the Dirichlet to Neumann operator $\mathcal{DN}$ in the next section.

## 4.2 Decomposition in vectorial spherical harmonics

In this section we describe the basis of vectorial spherical harmonics. We follow the notation of Nédélec in [17] where these objects are introduced in the context of electromagnetism. Then we present the decomposition of the solution of the Stokes problem and of the corresponding Dirichlet to Neumann operator $\mathcal{DN}$ in vectorial spherical harmonics.

### 4.2.1 The basis of vectorial spherical harmonics

#### 4.2.1.1 Spherical harmonics

Let us recall the definition and some properties of vectorial spherical harmonics. We consider the unit sphere $S^2$ in $\mathbf{R}^3$. The case of a sphere of arbitrary radius follows by a change of scale. In this geometry, it is natural to define a point of $\mathbf{R}^3$ by its spherical coordinates $(r, \theta, \varphi)$, where $r$ is the radius and $\theta, \varphi$ the two Euler angles. These coordinates are related to the euclidean coordinates $(x_1, x_2, x_3)$ by

$$\left\{ \begin{aligned} x_1 &= r \sin\theta \cos\varphi, \\ x_2 &= r \sin\theta \sin\varphi, \\ x_3 &= r \cos\theta. \end{aligned} \right. \tag{4.2.1}$$

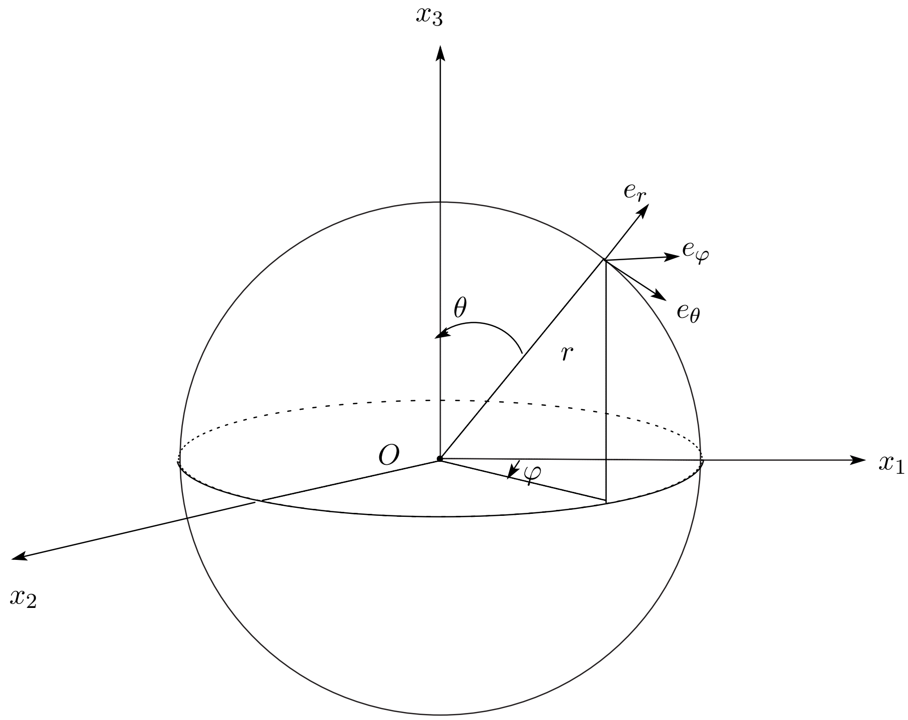


Figure 4.2: Coordinate systems.

The corresponding moving frame is $\{\vec{e}_r, \vec{e}_\theta, \vec{e}_\varphi\}$, where the unitary vectors $\vec{e}_r$, $\vec{e}_\theta$ and $\vec{e}_\varphi$ can be determined as

$$\begin{aligned}\vec{e}_r &= (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)\,,\\ \vec{e}_\theta &= (\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta)\,,\\ \vec{e}_\varphi &= (-\sin\varphi, \cos\varphi, 0)\,.\end{aligned}$$

In these coordinates, the surface gradient of the function $\mathbf{u}$, denoted $\nabla_{S^2}\mathbf{u}$, is defined as

$$\nabla_{S^2}\mathbf{u} \;=\; \frac{1}{\sin\theta}\frac{\partial\mathbf{u}}{\partial\varphi}\vec{e}_\varphi + \frac{\partial\mathbf{u}}{\partial\theta}\vec{e}_\theta. \tag{4.2.2}$$

Let $H^1(S^2)$ denotes the Hilbert space

$$H^1(S^2) \;=\; \Big\{\mathbf{u}\in L^2(S^2,\mathbb{C}):\ \nabla_{S^2}\mathbf{u}\in\big(L^2(S^2)\big)^3\Big\},$$

with its hermitian product

$$(\mathbf{u},\mathbf{v})_{H^1(S^2)} \;=\; \frac{1}{4}\int_{S^2}\mathbf{u}\bar{\mathbf{v}}d\sigma + \int_{S^2}\nabla_{S^2}\mathbf{u}\cdot\nabla_{S^2}\bar{\mathbf{v}}d\sigma.$$

More generally, for $n\geq 0$, we denote by

$$H^n(S^2) \;=\; \Big\{\mathbf{u}\in L^2(S^2,\mathbb{C}):\ \nabla^k_{S^2}\mathbf{u}\in L^2(S^2)\text{ for }0\leq k\leq n\Big\}.$$

The Laplace operator has the expression

$$\Delta\mathbf{u} \;=\; \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\mathbf{u}}{\partial r}\right)+\frac{1}{r^2}\left(\frac{1}{\sin^2\theta}\frac{\partial^2\mathbf{u}}{\partial\varphi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\mathbf{u}}{\partial\theta})\right).$$

We will denote by $\Delta_{S^2}$ the Laplace-Beltrami operator on the unit sphere $S^2$, defined as

$$\Delta_{S^2}\mathbf{u} \;=\; \frac{1}{\sin^2\theta}\frac{\partial^2\mathbf{u}}{\partial\varphi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\mathbf{u}}{\partial\theta}\right).$$

The area element on the sphere is: $d\sigma = \sin\theta d\theta d\varphi$. The operator $\Delta_{S^2}$ is self-adjoint for the hermitian product in $L^2(S^2)$ given by

$$\int_{S^2}\mathbf{u}\bar{\mathbf{v}}d\sigma \;=\; \int_0^{2\pi}\int_0^{\pi}\mathbf{u}(\theta,\varphi)\bar{\mathbf{v}}(\theta,\varphi)\sin\theta d\theta d\varphi.$$

This can be seen using an integration by parts

$$\begin{aligned}\int_{S^2}\Delta_{S^2}\mathbf{u}\bar{\mathbf{v}}d\sigma &= -\int_0^{2\pi}\int_0^{\pi}\left(\frac{1}{\sin\theta}\frac{\partial\mathbf{u}}{\partial\varphi}\frac{\partial\bar{\mathbf{v}}}{\partial\varphi}+\sin\theta\frac{\partial\mathbf{u}}{\partial\theta}\frac{\partial\bar{\mathbf{v}}}{\partial\theta}\right)d\theta d\varphi\\ &= -\int_0^{2\pi}\int_0^{\pi}\left(\frac{1}{\sin\theta}\frac{\partial\mathbf{u}}{\partial\varphi}\frac{1}{\sin\theta}\frac{\partial\bar{\mathbf{v}}}{\partial\varphi}+\frac{\partial\mathbf{u}}{\partial\theta}\frac{\partial\bar{\mathbf{v}}}{\partial\theta}\right)\sin\theta d\theta d\varphi\\ &= \int_{S^2}\mathbf{u}\Delta_{S^2}\bar{\mathbf{v}}d\sigma.\end{aligned}$$

The following Green's formula holds

$$\int_{S^2}\nabla_{S^2}\mathbf{u}.\nabla_{S^2}\bar{\mathbf{v}}d\sigma \;=\; -\int_{S^2}\Delta_{S^2}\mathbf{u}\bar{\mathbf{v}}d\sigma \quad \text{for } \mathbf{u}\in C^2(S^2),\ \mathbf{v}\in C^1(S^2).$$

By density this formula also holds for $\mathbf{u}\in H^2(S^2)$ and $\mathbf{v}\in H^1(S^2)$.

The Laplace-Betrami operator is self-adjoint in the space $L^2(S^2)$ and it is coercive on the space $H^1(S^2)\cap L_0^2(S^2)$. It admits a family of eigenfunctions which constitutes an orthogonal Hilbert basis of the space $L^2(S^2)$. This basis is also orthogonal for the scalar product in $H^1(S^2)$. These eigenfunctions are called spherical harmonics. They are described in Theorem 4.2.1.

Let $\mathcal{H}_l$ be the space of homogeneous polynomials of degree $l$ in three variables that are moreover harmonic in $\mathbf{R}^3$, i.e., that satisfy

$$\Delta P \;=\; 0.$$

Let $\mathcal{Y}_l$ be the space of the restrictions to the unit sphere $S^2$ of polynomials in $\mathcal{H}_l$.

**Theorem 4.2.1** ([17]). *Let $Y_l^m$, $-l\le m\le l$, denote an orthonormal basis of $\mathcal{Y}_l$ for the hermitian product of $L^2(S^2)$. The functions $Y_l^m$, for $l\ge 0$ and $-l\le m\le l$, form an orthogonal basis in $L^2(S^2)$, which is also orthogonal in $H^1(S^2)$. Moreover, $\mathcal{Y}_l$ coincides with the subspace spanned by the eigenfunctions of the Laplace-Beltrami operator associated with the eigenvalue $-l(l+1)$, i.e.,*

$$\Delta_{S^2}Y_l^m + l(l+1)Y_l^m \;=\; 0.$$

*The eigenvalue $-l(l+1)$ has multiplicity $2l+1$.*

For $s \geq 0$, we have

$$H^s(S^2) = \left\{ Y = \sum_{l,m} c_{l,m} Y_l^m : \ |Y|^2_{H^s(S^2)} = \sum_{l,m} \{l(l+1)\}^s |c_{l,m}|^2 < \infty \right\}.$$

By Theorem 4.2.1 and the above Green's formula, we have

$$\|\nabla_{S^2} Y_l^m\|^2_{L^2} = l(l+1).$$

#### 4.2.1.2 Legendre polynomials

We consider the segment $[-1,1]$ and the space $L^2([-1,1])$. The Legendre polynomials $\mathbb{P}_l$ are the orthogonal polynomials defined on this segment for the usual scalar product in $L^2([-1,1])$ and constructed with the Gram-Schmidt orthonormalization process, when starting form the usual basis $1, x, x^2, \ldots$. The usual normalization consists in fixing $\mathbb{P}_l(1) = 1$. The Rodrigues formula then gives the expression of the Legendre polynomial $\mathbb{P}_l$:

$$\mathbb{P}_l(x) = \frac{(-1)^l}{2^l l!} \frac{d^l}{dx^l}(1-x^2)^l.$$

The associated Legendre functions $\mathbb{P}_l^m$, for $0 \leq m \leq l$, are given by

$$\mathbb{P}_l^m = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} \mathbb{P}_l(x).$$

The spherical harmonics of order $l$ are the $2l+1$ functions which are given by: for $l \geq 0, -l \leq m \leq l$

$$\begin{aligned} Y_l^m(\theta,\varphi) &= \sqrt{2} C_l^m P_l^m(\cos\theta)\cos(m\varphi), \text{ if } m > 0, \\ Y_l^m(\theta,\varphi) &= \sqrt{2} C_l^m P_l^{|m|}(\cos\theta)\sin(|m|\varphi), \text{ if } m < 0, \\ Y_l^m(\theta,\varphi) &= C_l^m P_l^0(\cos\theta), \text{ if } m = 0, \end{aligned}$$

where

$$C_l^m = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}}.$$

#### 4.2.1.3 Vectorial spherical harmonics

To describe the spaces $L^2(S^2, \mathbf{R}^3)$ or $H^1(S^2, \mathbf{R}^3)$ we could simply use the basis given by

$$Y_{l_1}^{m_1} e_1 + Y_{l_2}^{m_2} e_2 + Y_{l_3}^{m_3} e_3, \quad l_1, l_2, l_3 \geq 0, |m_i| \leq l_i.$$

However in the context of the Maxwell equations and of the Stokes equation (see [13]), it is more convenient to use different combinations of the scalar spherical harmonics called vectorial spherical harmonics.

Let $l \geq 0$ and $H \in \mathcal{H}_l$, we define

$$\begin{aligned} H_A(x) &:= \nabla H(x) \wedge x, \\ H_B(x) &:= \nabla H(x), \\ H_C(x) &:= -|x|^2 \nabla H(x) + (2l+1) H(x) x. \end{aligned}$$

We show that $H_A \in \mathcal{H}_l(\mathbf{R}^3, \mathbf{R}^3)$ for $l \geq 0$, $H_B \in \mathcal{H}_{l-1}(\mathbf{R}^3, \mathbf{R}^3)$ for $l \geq 1$ and $H_C \in \mathcal{H}_{l+1}(\mathbf{R}^3, \mathbf{R}^3)$ for $l \geq 0$. First, we check immediately that $H_A$ is a homogeneous polynomial of degree $l$ and we compute

$$\Delta H_A(x) = \nabla \Delta H(x) \wedge x + 2 \sum_{n=1}^{3} \nabla \partial_{x_n} H(x) \wedge \partial_{x_n} x + \nabla H(x) \wedge \Delta x = 2 \sum_{n=1}^{3} \nabla \partial_{x_n} H(x) \wedge \partial_{x_n} x$$

Then, for $1 \leq k \leq 3$ and using the three-dimensional antisymmetric Levi-Civita symbol $\varepsilon_{ijk}$ to express the cross product, we compute

$$\begin{aligned} [\Delta H_A]_k(x) &= 2 \left( \sum_{1 \leq i,j,n \leq 3} \varepsilon_{ijk} \partial_{x_i} \partial_{x_n} H(x) \partial_{x_n} x_j \right)_k \\ &= 2 \left( \sum_{1 \leq i,j,n \leq 3} \varepsilon_{ijk} \partial_{x_i} \partial_{x_j} H(x) \right)_k \overset{\varepsilon_{ijk} = -\varepsilon_{jik}}{=} 0. \end{aligned}$$

Clearly, $H_B$ is a homogeneous polynomial of degree $l-1$ and $\Delta H_B = 0$. Finally, $H_C$ is a homogeneous polynomial of degree $l+1$ and we have

$$\Delta H_C(x) = -6 \nabla H(x) - 4(x \cdot \nabla) \nabla H + 2(2l+1) \nabla H.$$

But since $\nabla H$ is a homogeneous polynomial of degree $l-1$, we have $(x \cdot \nabla) \nabla H = (l-1) \nabla H$ and we obtain $\Delta H_C = 0$.

For $x \in S^2$, we respectively define $T_{l,m}, I_{l,m}, N_{l,m}$ as the traces on $S^2$ of the harmonic polynomials $\{H_{l,m}\}_A$, $\{H_{l+1,m}\}_B$ and $\{H_{l-1,m}\}_C$:

$$\begin{aligned} T_{l,m}(x) &:= \{H_{l,m}\}_A(x), && -l \leq m \leq l,\ l \geq 1, \\ I_{l,m}(x) &:= \{H_{l+1,m}\}_B(x), && -l-1 \leq m \leq l+1,\ l \geq 0, \\ N_{l,m}(x) &:= \{H_{l-1,m}\}_C(x), && -l+1 \leq m \leq l-1,\ l \geq 1. \end{aligned}$$

Notice that by construction the components of $T_{l,m}, I_{l,m}, N_{l,m}$ belong to $\mathcal{Y}_l$, that is

$$\Delta_{S^2} Y + l(l+1) Y = 0, \quad \text{for } Y = T_{l,m}, I_{l,m}, N_{l,m}.$$

Using the tangential gradient defined by (4.2.2) and the Euler relation for the normal derivatives, we obtain

$$T_{l,m}(x) = \nabla_{S^2} Y_{l,m}(x) \wedge x =: \nabla_{S^2}^{\perp} Y_{l,m}(x) \in TS^2, \tag{4.2.3}$$

$$I_{l,m}(x) = \nabla_{S^2} Y_{l+1,m}(x) + (l+1) Y_{l+1,m}(x) x, \tag{4.2.4}$$

$$N_{l,m}(x) = -\nabla_{S^2} Y_{l-1,m}(x) + l Y_{l-1,m}(x) x. \tag{4.2.5}$$

**Theorem 4.2.2** ([17]). *For each $l \geq 0$, the family $\{(T_{l,m})_{|m|\leq l}; (I_{l,m})_{|m|\leq l+1}; (N_{l,m})_{|m|\leq l-1}\}$ forms an orthogonal basis of $\left(H^1(S^2)\right)^3$ and of $(L^2(S^2))^3$. Further, they satisfy*

$$\begin{aligned}\int_{S^2} |T_{l,m}(x)|^2 d\sigma &= l(l+1),\\ \int_{S^2} |I_{l,m}(x)|^2 d\sigma &= (l+1)(2l+3),\\ \int_{S^2} |N_{l,m}(x)|^2 d\sigma &= l(2l-1).\end{aligned}$$

In summary, let $\mathbf{u} \in L^2(S^2, \mathbf{R}^3)$, then $\mathbf{u}$ decomposes as

$$\mathbf{u}(x) = \sum_{l\geq 1}\sum_{m=-l}^{l} i_{l,m}T_{l,m}(x) + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} j_{l,m}I_{l,m}(x) + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} k_{l,m}N_{l,m}(x),$$

and for $s \geq 0$ we have

$$\begin{aligned}\|\mathbf{u}\|_s^2 := &\sum_{l\geq 1}\sum_{m=-l}^{l} [l(l+1)]^s l(l+1)|i_{l,m}|^2 + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} [l(l+1)]^s (2l+3)(l+1)|j_{l,m}|^2\\ &+ \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} [l(l+1)]^s l(2l-1)|k_{l,m}|^2.\end{aligned}$$

### 4.2.2 The Stokes problem in a ball or in the complement of a ball

We now show that the vectorial spherical harmonic basis diagonalizes the operator $\mathcal{ND}$ defined on a single particle. For this, we consider the Stokes problem in the domain $\Omega_0 \cup B(0,1)$ where $\Omega_0 := \mathbf{R}^3 \setminus \overline{B(0,1)}$. Given a velocity field $\mathbf{g}$ defined on $S^2 := \partial B(0,1)$, we seek the velocity and pressure fields $(\mathbf{u}, p)$ satisfying

$$\begin{cases} -\Delta \mathbf{u} + \nabla p = 0 & \text{in } \Omega_0 \cup B(0,1),\\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega_0 \cup B(0,1),\\ \mathbf{u} = \mathbf{g} & \text{on } S^2. \end{cases} \tag{4.2.6}$$

#### 4.2.2.1 Decomposition of velocity and pressure field

**Proposition 4.2.1.** *Let $\mathbf{g} \in H_0^{1/2}(S^2, \mathbf{R}^3)$ and let $(\mathbf{u}, p)$ be the variational solution of (4.2.6) ($\mathbf{u} \in \mathcal{D}(\Omega_0 \cup B(0,1))$, $p \in L^2(\Omega_0 \cup B(0,1))$ and $\int_{B(0,1)} p = 0$). If the decomposition of $\mathbf{g}$ in the basis of vectorial spherical harmonics reads*

$$\mathbf{g}(x) = \sum_{l\geq 1}\sum_{m=-l}^{l} g_{l,m}^T T_{l,m}(x) + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} g_{l,m}^I I_{l,m}(x) + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} g_{l,m}^N N_{l,m}(x), \tag{4.2.7}$$

*then we obtain the decompositions of the velocity field* $\mathbf{u}$ *and of the pressure field* $p$ *in vectorial spherical harmonics for* $r > 1$*, as follows,*

$$\begin{aligned}\mathbf{u}(x) &= \sum_{l\geq 1}\sum_{m=-l}^{l} g^T_{l,m} r^{-(l+1)} T_{l,m} + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} g^I_{l,m} r^{-(l+1)} I_{l,m} \\ &\quad + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1}\left[\frac{(2l-3)(l-1)}{2l} g^I_{l-2,m}(r^2-1) + g^N_{l,m}\right] r^{-(l+1)} N_{l,m},\end{aligned} \quad (4.2.8)$$

$$p(x) = \sum_{l\geq 1}\sum_{m=-l}^{l} \frac{(2l-1)l}{l+1} g^I_{l-1,m} r^{-(l+1)} \left[I_{l_1,m}(x/r) + N_{l+1,m}(x/r)\right]\cdot e_r. \quad (4.2.9)$$

*Proof.* Since $\Delta p = 0$, we put

$$p(x) = \sum_{l\geq 0}\sum_{m=-l}^{l} \alpha_{l,m} r^{-(l+1)} Y_{l,m}(x/r).$$

We decompose $\mathbf{u}$ in the form

$$\begin{aligned}\mathbf{u}(x) &= \sum_{l\geq 1}\sum_{m=-l}^{l} i_{l,m}\left(r^{-(l+1)}T_{l,m}(x)\right) + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} j_{l,m}\left(r^{-(l+1)}I_{l,m}(x)\right) \\ &\quad + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} k_{l,m}\left(r^{-(l+1)}N_{l,m}(x)\right).\end{aligned}$$

This form is chosen because $r^{-(l+1)}T_{l,m}(x)$, $r^{-(l+1)}I_{l,m}(x)$ and $r^{-(l+1)}N_{l,m}(x)$ are harmonics. Using (4.2.3), (4.2.4), (4.2.5) and the formula

$$\operatorname{div}(ae_r) = \partial_r a + (2/r)a,$$

we obtain

$$\begin{aligned}\operatorname{div}\mathbf{u}(x) &= \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} (l+1) r^{-(l+2)}\left(r j'_{l,m} - (2l+1) j_{l,m}\right) Y_{l+1,m} \\ &\quad + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} l r^{-(l+1)} k'_{l,m} Y_{l-1,m}.\end{aligned}$$

Since $\operatorname{div}\mathbf{u} = 0$, we deduce

$$k'_{1,0} = 0, \quad (4.2.10)$$

$$(l+1)\left(r^2 j'_{l,m} - r(2l+1) j_{l,m}\right) + (l+2) k'_{l+2,m} = 0, \quad l \geq |m| \geq 0. \quad (4.2.11)$$

We now decompose the first relation of equations (4.2.6). We have by (4.2.5),

$$\begin{aligned}\nabla p(x) &= \sum_{l\geq 0}\sum_{m=-l}^{l} \alpha_{l,m} r^{-(l+2)} \left(\nabla_{S^2} Y_{l,m}(x/r) - (l+1)Y_{l,m}(x/r)e_r\right)\\ &= \sum_{l\geq 1}\sum_{m=-l+1}^{l} (-\alpha_{l-1,m}) r^{-(l+1)} N_{l,m}(x/r),\end{aligned}$$

and

$$\begin{aligned}\Delta \mathbf{u}(x) &= \sum_{l\geq 1}\sum_{m=-l}^{l} r^{-(l+2)} \left(r i''_{l,m} - 2l i'_{l,m}\right) T_{l,m}\\ &\quad + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} r^{-(l+2)} \left(r j''_{l,m} - 2l j'_{l,m}\right) I_{l,m}\\ &\quad + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} r^{-(l+2)} \left(r k''_{l,m} - 2l k'_{l,m}\right) N_{l,m}.\end{aligned}$$

Identifying these expansions in vectorial spherical harmonics, we obtain

$$r i''_{l,m} - 2l i'_{l,m} = 0, \qquad l \geq 1,\ |m| \leq l, \tag{4.2.12}$$

$$r j''_{l,m} - 2l j'_{l,m} = 0, \qquad l \geq 0,\ |m| \leq l+1, \tag{4.2.13}$$

$$r k''_{l,m} - 2l k'_{l,m} = -\alpha_{l-1,m} r, \qquad l \geq 1,\ |m| \leq l-1. \tag{4.2.14}$$

We deduce from (4.2.12), (4.2.13), the boundary condition $\mathbf{u} = \mathbf{g}$ on $\partial\Omega_0$ and the condition of decay at infinity that

$$\begin{aligned} i_{l,m}(r) &= g^T_{l,m}, \qquad l \geq 1,\ |m| \leq l,\\ j_{l,m}(r) &= g^I_{l,m}, \qquad l \geq 0,\ |m| \leq l+1.\end{aligned}$$

The relations (4.2.10), (4.2.11) lead to

$$\begin{aligned} k_{1,0} &= g^N_{1,0}, \quad \alpha_{0,0} = 0,\\ k_{l,m} &= \frac{(2l-3)(l-1)}{2l} g^I_{l-2,m}(r^2-1) + g^N_{l,m}, \quad l \geq 2,\ 0 \leq |m| \leq l-1.\end{aligned}$$

From (4.2.14) we get

$$\alpha_{l,m} = \frac{(2l+1)(2l-1)l}{l+1} g^I_{l-1,m}, \qquad l \geq 1,\ 0 \leq |m| \leq l.$$

Eventually, with the convention $g^I_{-1,0} = 0$ and all of the above equalities, we obtain the decompositions of $p$ and $\mathbf{u}$ in vectorial spherical harmonics as in (4.2.9) and (4.2.8).

□

#### 4.2.2.2 Decomposition of Neumann to Dirichlet operator

**Proposition 4.2.2.** *Let* $\mathbf{g} \in H^{1/2}(S^2, \mathbf{R}^3)$ *and let* $(\mathbf{u}, p)$ *be a solution of* (4.2.6)*. Then the vectorial spherical harmonic basis diagonalizes the Neumann to Dirichlet operator* $\mathcal{ND}$ *defined on* $\partial B(0,1)$*.*

*In particular, if the decomposition of* $\mathbf{g}$ *in the basis of vectorial spherical harmonics is given by* (4.2.7)*, then we have*

$$\mathcal{ND}\mathbf{g} \;=\; \sum_{l\geq 1}\sum_{m=-l}^{l} \frac{1}{2l+1} g^T_{l,m} T_{l,m} + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} \frac{l+2}{4l^2+8l+3} g^I_{l,m} I_{l,m} + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} \frac{l-1}{4l^2-1} g^N_{l,m} N_{l,m}. \quad (4.2.15)$$

*Proof.* Let us first decompose the following operator

$$\mathcal{DN}_{jump}\mathbf{g} \;:=\; \left[-e_r \cdot \left(\nabla \mathbf{u} + \nabla \mathbf{u}^t\right) + p e_r\right]_{|S^2}.$$

We have

$$\mathcal{DN}_{jump}\mathbf{g} \;=\; \mathcal{DN}_{ext}\mathbf{g} + \mathcal{DN}_{int}\mathbf{g}, \quad (4.2.16)$$

where $\mathcal{DN}_{ext}$ and $\mathcal{DN}_{int}$ correspond to the exterior and interior solutions.

Let us first decompose $\mathcal{DN}_{ext}$. We have

$$\mathcal{DN}_{ext} \;=\; \left[-e_r \cdot \left(\nabla \mathbf{u} + \nabla \mathbf{u}^t\right) + p e_r\right]_{|S^2_{ext}}.$$

For $x \in S^2$, we compute

$$\begin{aligned} -(\nabla \mathbf{u} \cdot e_r)(x) \;=\;& \sum_{l\geq 1}\sum_{m=-l}^{l} (l+1) g^T_{l,m} (T_{l,m}\cdot e_r) e_r + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} (l+1) g^I_{l,m} (I_{l,m}\cdot e_r) e_r \quad (4.2.17)\\ &+ \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} \left[-\frac{(2l-3)(l-1)}{l} g^I_{l-2,m} + (l+1) g^N_{l,m}\right] (N_{l,m}\cdot e_r) e_r \\ &- \sum_{l\geq 1}\sum_{m=-l}^{l} g^T_{l,m} \{\nabla_{S^2} T_{l,m}\}\cdot e_r - \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} g^I_{l,m} \{\nabla_{S^2} I_{l,m}\}\cdot e_r \\ &- \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} g^N_{l,m} \{\nabla_{S^2} N_{l,m}\}\cdot e_r \end{aligned}$$

To reduce the three first terms, we use (4.2.3), (4.2.4) and (4.2.5) and obtain

$$T_{l,m}\cdot e_r = 0, \qquad I_{l,m}\cdot e_r = (l+1) Y_{l+1,m}, \qquad N_{l,m}\cdot e_r = l Y_{l-1,m}.$$

For the three remaining terms, we remark that for a regular vector field $V$ of $TS^2$ and a spherical harmonic $Y$ of $S^2$ in $\mathbf{R}^3$, we have

$$\{\nabla_{S^2} V\}\cdot e_r \;=\; -V, \qquad \{\nabla_{S^2}(Y e_r)\}\cdot e_r \;=\; \nabla_{S^2} Y.$$

Combining to (4.2.3), (4.2.4) and (4.2.5), it leads

$$\begin{aligned}\{\nabla_{S^2} T_{l,m}\}\cdot e_r &= -T_{l,m},\\ \{\nabla_{S^2} I_{l,m}\}\cdot e_r &= l\nabla_{S^2} Y_{l+1,m},\\ \{\nabla_{S^2} N_{l,m}\}\cdot e_r &= (l+1)\nabla_{S^2} Y_{l-1,m}.\end{aligned}$$

The equality (4.2.17) then becomes

$$\begin{aligned}-(\nabla \mathbf{u}\cdot e_r)(x) &= \sum_{l\geq 0}\sum_{m=-l-1}^{l+1}(l+1)^2 g^I_{l,m} Y_{l+1,m} e_r - \sum_{l\geq 2}\sum_{m=-l+1}^{l-1}(2l-3)(l-1) g^I_{l-2,m} Y_{l-1,m} e_r\\ &+ \sum_{l\geq 1}\sum_{m=-l+1}^{l-1}(l+1) l g^N_{l,m} Y_{l-1,m} e_r + \sum_{l\geq 1}\sum_{m=-l}^{l} g^T_{l,m} T_{l,m}\\ &+ \sum_{l\geq 0}\sum_{m=-l-1}^{l+1}(-l) g^I_{l,m}\nabla_{S^2} Y_{l+1,m} + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1}(-l-1) g^N_{l,m}\nabla_{S^2} Y_{l-1,m}.\end{aligned}$$

After simlifying and using again (4.2.3), (4.2.4) and (4.2.5), we obtain,

$$-(\nabla \mathbf{u}\cdot e_r)(x) = \sum_{l\geq 1}\sum_{m=-l}^{l} g^T_{l,m} T_{l,m} - \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} l g^I_{l,m} I_{l,m} + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1}(l+1) g^N_{l,m} N_{l,m}.$$

With the same kind of computation, we obtain (see L. Halpern in [13])

$$\Lambda \mathbf{g}(x) = \sum_{l\geq 1}\sum_{m=-l}^{l}(l+1) g^T_{l,m} T_{l,m} + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1}\frac{3(l+1)^2}{l+2} g^I_{l,m} I_{l,m} + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1}(l+1) g^N_{l,m} N_{l,m},$$

where $\Lambda \mathbf{g}(x) := \left(-e_r\cdot\nabla \mathbf{u}^t + p e_r\right)_{|S^2_{ext}}$. Eventually, we get

$$\begin{aligned}\mathcal{DN}_{ext}\mathbf{g}(x) &= \sum_{l\geq 1}\sum_{m=-l}^{l}(l+2) g^T_{l,m} T_{l,m} + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1}\frac{2l^2+4l+3}{l+2} g^I_{l,m} I_{l,m}\\ &\qquad + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} 2(l+1) g^N_{l,m} N_{l,m}, \quad (4.2.18)\end{aligned}$$

To decompose $\mathcal{DN}_{int}$, we solve the interior problem (4.2.6) in the unit ball $B(0,1)$ with $\mathbf{g} = T_{l,m}$, $\mathbf{g} = I_{l,m}$ and then $\mathbf{g} = N_{l,m}$.

For $\mathbf{g} = T_{l,m}$, since $x \mapsto r^l T_{l,m}(x/r)$ is harmonic and divergence free, we have a solution of the form $\mathbf{u} = r^l T_{l,m}(x/r)$ and $p = 0$. Using the above formulas, it is easy to check that

$$p e_r - (\nabla \mathbf{u} + \nabla \mathbf{u}^T)\cdot e_r = (l-1) T_{l,m}.$$

For $\mathbf{g} = I_{l,m}$, we still have a solution of the form $\mathbf{u} = r^l I_{l,m}(x/r)$ and $p = 0$. Similarly, we calculate

$$p e_r - (\nabla \mathbf{u} + \nabla \mathbf{u}^T)\cdot e_r = 2l I_{l,m}.$$

For $\mathbf{g} = N_{l,m}$, the mapping $x \mapsto r^l N_{l,m}(x/r)$ is not divergence free. Proceeding as in the case of the exterior domain, we look for a solution of the form,

$$\mathbf{u} \;=\; r^l N_{l,m} + \alpha r^{l-2}(1-r^2) I_{l-2,m}, \qquad p \;=\; \beta r^{l-1} Y_{l-1,m}.$$

The condition $\nabla \cdot \mathbf{u} = 0$ yields

$$\alpha \;=\; \frac{l(2l+1)}{2(l-1)}.$$

Using the first equation of (4.2.6), we get

$$\beta \;=\; -2(2l-1)\alpha \;=\; -\frac{l(4l^2-1)}{l-1}.$$

Then we compute

$$pe_r - (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot e_r \;=\; \frac{2l^2+1}{l-1} N_{l,m}.$$

We remark that the coefficient of $N_{1,0}$ is zero.

Eventually, $\mathcal{DN}_{int}$ writes as:

$$\mathcal{DN}_{int}\mathbf{g}(x) \;=\; \sum_{l\geq 1}\sum_{m=-l}^{l} (l-1) g^T_{l,m} T_{l,m} + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} 2l g^I_{l,m} I_{l,m} + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} \frac{2l^2+1}{l-1} g^N_{l,m} N_{l,m}. \tag{4.2.19}$$

Finally, the decomposition of the Dirichlet to Neumann operator is obtained by (4.2.16), (4.2.18) and (4.2.19),

$$\begin{aligned}\mathcal{DN}_{jump}\mathbf{g}(x) \;=\; & \sum_{l\geq 1}\sum_{m=-l}^{l} (2l+1) g^T_{l,m} T_{l,m} + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} \frac{4l^2+8l+3}{l+2} g^I_{l,m} I_{l,m} \\ & + \sum_{l\geq 1}\sum_{m=-l+1}^{l-1} \frac{4l^2-1}{l-1} g^N_{l,m} N_{l,m}.\end{aligned} \tag{4.2.20}$$

This is de desired decomposition. □

### 4.2.3 Practical implementation of the boundary integral method in the basis of vectorial spherical harmonnics

#### 4.2.3.1 Truncation order $L_{max}$

Firstly, we rewrite the problems (4.1.1) as the boundary integral problems (4.1.4), (4.1.5), whose unknowns are the surface force densities $\tilde{\mathbf{f}}_i$ on the boundary of the particles. Let us define the basis of vectorial spherical harmonics $VSH_i$ associated to the sphere $\partial B_i$ as follows:

$$VSH_i = \left\{ (T^i_{l,m})_{|m|\leq l};\; (I^i_{l,m})_{|m|\leq l+1};\; (N^i_{l,m})_{|m|\leq l-1} \right\}_{l\geq 0,\; i=1,2,\ldots,N}.$$

Noting that by Theorem 4.2.2 the solution satisfy $(\tilde{\mathbf{f}}_i, T^i_{0,0}) = 0$, so we ignore the $T^i_{0,0}$ from the basis. Then, the six first terms of this basis are

$$I^i_{0,-1}(\mathbf{z}_i + x) \;=\; \frac{1}{\sqrt{4\pi}} e_y, \quad I^i_{0,0}(\mathbf{z}_i + x) \;=\; \frac{1}{\sqrt{4\pi}} e_z, \quad I^i_{0,1}(\mathbf{z}_i + x) \;=\; -\frac{1}{\sqrt{4\pi}} e_x, \tag{4.2.21}$$

$$T^i_{1,-1}(\mathbf{z}_i + x) \;=\; \sqrt{\frac{3}{8\pi}} e_y \times x, \quad T^i_{1,0}(\mathbf{z}_i + x) \;=\; \sqrt{\frac{3}{8\pi}} e_z \times x, \quad T^i_{1,1}(\mathbf{z}_i + x) \;=\; -\sqrt{\frac{3}{8\pi}} e_x \times x, \tag{4.2.22}$$

where $e_x, e_y, e_z$ denote three unit normal vectors of coordinates system.

We decompose the unknown $\tilde{\mathbf{f}}_i$ in $VSH_i$ as,

$$\tilde{\mathbf{f}}_i \;=\; \sum_{l\geq 1} \sum_{m=-l}^{l} f^{T,i}_{l,m} T^i_{l,m} + \sum_{l\geq 0} \sum_{m=-l-1}^{l+1} f^{I,i}_{l,m} I^i_{l,m} + \sum_{l\geq 1} \sum_{m=-l+1}^{l-1} f^{N,i}_{l,m} N^i_{l,m}. \tag{4.2.23}$$

The discretization step consists in truncating the series (4.2.23) up to order $l = L_{max}$ which we call the truncation order in this thesis. The elements $I^i_{0,m}$, for $m = -1, 0, 1$, in (4.2.21) correspond to the components of the total forces and $T^i_{1,m}$, for $m = -1, 0, 1$, in (4.2.22) correspond to the components of the total torques. Hence the total force and torque exerted by the particle $B_i$ on the fluid are obtained by projection of the force density $\tilde{\mathbf{f}}_i$ on the space generated by $\left\{ I^i_{0,m}, T^i_{1,m} : \; |m| \leq 1 \right\}$. The discretization proposed by Durlofsky and Brady [10, 11] was a truncation of the series (4.2.23) up to order $l = 1$, including 11 terms: total forces, torques and the stresslets $I^i_{1,m}$, $|m| \leq 2$. To improve the accuracy of the method, other authors [15], [7] have considered truncations up to arbitrary order.

#### 4.2.3.2 Computation of discrete Neumann to Diriclet matrix $\mathcal{ND}^{L_{max}}$

It is convenient to rewrite the basis $VSH_i$ with the notation $VSH_i = (\phi_{i,\alpha})_{\alpha\geq 0, i=1,\ldots,N}$. The components of the operator $\mathcal{ND}$ in the Hilbert basis $VSH_i$ are given by

$$\mathcal{ND}_{i,\alpha;j,\beta} \;=\; \int_{\partial B_j} \int_{\partial B_i} \phi^T_{i,\alpha}(x) \cdot G(x - y) \cdot \phi_{j,\beta}(y) dS(y) dS(x).$$

In fact, the velocity field $\mathbf{u}_{j,\beta}(x) = \int_{\partial B_j} G(x - y) \cdot \phi_{j,\beta}(y)$ generated by a force distribution $\phi_{i,\beta}$ is explicitly known so the above formula simplifies to

$$\mathcal{ND}_{i,\alpha;j,\beta} \;=\; \int_{\partial B_i} \phi^T_{i,\alpha}(x) \cdot \mathbf{u}_{j,\beta}(x) dS(x). \tag{4.2.24}$$

The nice feature of the vectorial spherical harmonics basis is that it diagonalizes self interactions: we have, for $i = 1, 2, \ldots, N$,

$$\mathcal{ND}_{i,\alpha;i,\beta} \;=\; \delta_{\alpha,\beta} \lambda_\alpha. \tag{4.2.25}$$

The sequence of positive real numbers $(\lambda_\alpha)_{\alpha\geq 0}$ is the list of the eigenvalues of the Neumann to Dirichlet operator corresponding to an isolated spherical particle in $\mathbf{R}^3$.

Recall that the discretization consists in truncating the series up to some truncation order $l = L_{max}$. Correspondingly, we denote by $M_{max}$ the number of vectorial spherical harmonics in the discrete basis. In fact, up to the truncation order $L_{max}$, the number of vectorial spherical harmonics are determined exactly,

$$M_{max} \; = \; 3\,(L_{max}+1)^2 - 1.$$

The discrete matrix of the Neumann to Dirichlet operator $\mathcal{ND}_{dis.}$ computed in the basis $(\phi_{i,\alpha})_{1\le\alpha\le M_{max},1\le i\le N}$ can be written as $N \times N$ blocks as follows,

$$\mathcal{ND}^{L_{max}}_{dis.} \; = \; \begin{pmatrix} \mathcal{ND}^{L_{max}}_{1,1} & \mathcal{ND}^{L_{max}}_{1,2} & \cdots & \mathcal{ND}^{L_{max}}_{1,N} \\ \mathcal{ND}^{L_{max}}_{2,1} & \mathcal{ND}^{L_{max}}_{2,2} & \cdots & \mathcal{ND}^{L_{max}}_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{ND}^{L_{max}}_{N,1} & \mathcal{ND}^{L_{max}}_{N,2} & \cdots & \mathcal{ND}^{L_{max}}_{N,N} \end{pmatrix}.$$

The $N$ diagonal blocks $\mathcal{ND}^{L_{max}}_{i,i}$, for $i = 1, 2, ..., N$, are explicitly known diagonal matrices given by (4.2.25),

$$\mathcal{ND}^{L_{max}}_{i,i} \; = \; \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_{L_{max}} \end{pmatrix}.$$

For the extra-diagonal blocks $\mathcal{ND}^{L_{max}}_{i,j}$ $(i \neq j)$, we use formula (4.2.24). We have tested two methods to approximate the integrals on the spheres in the right hand side of (4.2.24): first is using the quadrature formula of Hannay and Nye in [14], second is using the quadrature formula of Lebedev in [16].

#### 4.2.3.3 The discrete friction and mobility matrices

The $6N \times 6N$ discretized friction matrix $\mathcal{F}_{dis.}$ is obtained by inversing the matrix $\mathcal{ND}^{L_{max}}_{dis.}$ and then extracting the entries with indices $(i, \alpha; j, \beta)$ for $1 \le \alpha, \beta \le 6$, $1 \le i, j \le N$:

$$(\mathcal{F}_{dis.})_{i,\alpha;j,\beta} \; := \; \left( \left[ \mathcal{ND}^{L_{max}}_{dis.} \right]^{-1} \right)_{i,\alpha;j,\beta}.$$

As the definition of the mobility matrix in Section 4.1.2, the discrete mobility matrix $\mathcal{M}_{dis.}$ is defined as the inverse of the discrete friction matrix $\mathcal{F}_{dis.}$,

$$\mathcal{M}_{dis.} \; := \; \mathcal{F}^{-1}_{dis.}.$$

Throughout this thesis, the method for approximating the total forces and torques using this discrete approximation of the mobility matrix is called the direct method. In the next section, we perform some numerical tests to illustrate the performance of this method.

Chapter 5

# The Stokesian dynamic method for close particles

## Contents



## 5.1 First numerical tests. Difficulties for close particles

For a fixed position of the particles, the spectral decomposition method has a very good behavior as we send the truncating order to infinity. Indeed, the force distribution $\tilde{\mathbf{f}}_i$ are smooth and the spectral expansion has an exponential rate of convergence.

On the contrary, if we consider a sequence of configurations with at least two particles $B_i, B_j$ getting closer and closer ($d_{(i,j)} \to 0$) and with different prescribed velocities $\mathbf{u}_i \neq \mathbf{u}_j$, the distributions of forces $\tilde{\mathbf{f}}_i, \tilde{\mathbf{f}}_j$ concentrate near the contact points. In this case the convergence of the spectral expansion degenerates. The goal of this section is to illustrate this phenomenon.

Let us consider a simple case with two identical spheres $\partial B_1, \partial B_2$ of unit radius. We denote by $d$ the distance between these particles. We assume that the two centers lie on the vertical axis with coordinates $\mathbf{z}_1 = (0, 0, -1 - d/2)$ and $\mathbf{z}_2 = (0, 0, 1 + d/2)$. The velocity and pressure $\mathbf{u}, p$ in the surrounding fluid solve the Stokes equations

$$\begin{cases} -\Delta \mathbf{u} + \nabla p \ = \ 0 & \text{in } \Omega := \mathbf{R}^3 \setminus (B_1 \cup B_2), \\ \nabla \cdot \mathbf{u} \ = \ 0 & \text{in } \mathbf{R}^3 \setminus (B_1 \cup B_2), \\ \mathbf{u} \ = \ \mathbf{u}_i & \text{on } \partial B_i, \ i = 1, 2, \\ \mathbf{u}, p \ \to \ 0 & \text{at } \infty. \end{cases} \tag{5.1.1}$$

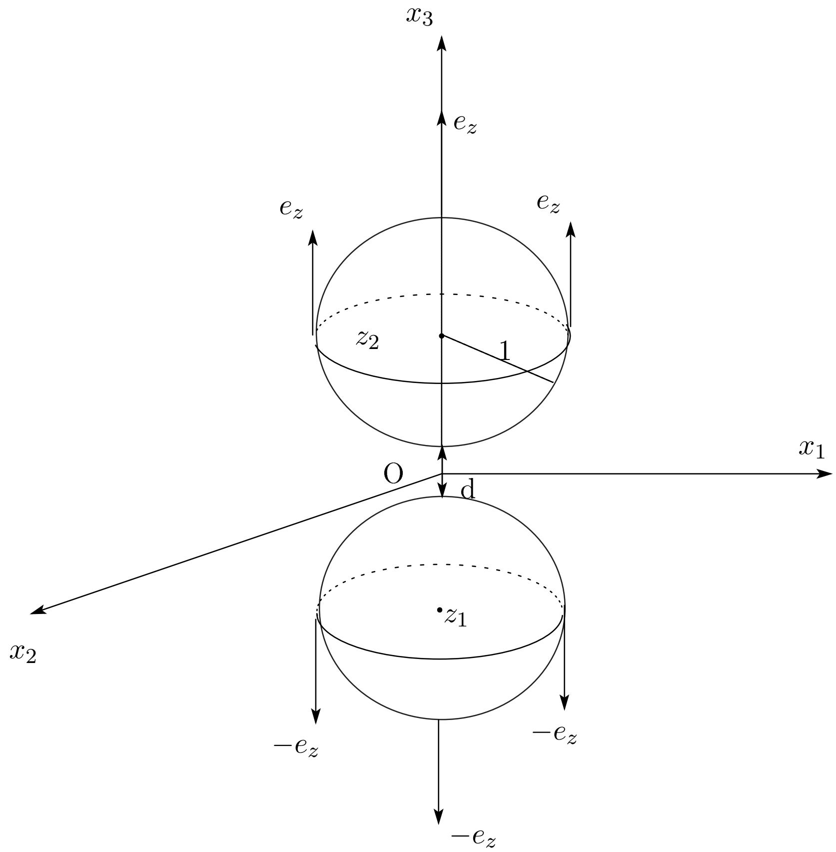


Figure 5.1: The prescribed velocities of two close particles.

We consider the case of opposite translational motions along the vertical axis, i.e, the prescribed velocities of the two balls are respectively $\mathbf{u}_1 = -e_z, \mathbf{u}_2 = e_z$ (see Figure 5.1). In cylindrical coordinates $(r, \theta, z)$, the velocity has the form

$$\mathbf{u} \;=\; u_r e_r + u_\theta e_\theta + u_z e_z.$$

For $\rho > 0$ small, we consider the domain (see Figure 5.2)

$$\Omega_\rho \;:=\; \{(r, \theta, z): \; |z| < 1 + d/2, \; r < \rho\} \cap \Omega.$$

The boundary of this domain can be decomposed in three parts as follows

$$\partial\Omega_\rho \;=\; \Gamma \cup C_1 \cup C_2, \tag{5.1.2}$$

where

$$\begin{aligned} \Gamma \;&=\; \{(r, \theta, z): \; |z| < 1 + d/2, \; r = \rho\}, \\ C_1 \;&=\; \left\{(r, \theta, z): \; z = -d/2 - 1 + \sqrt{1 - r^2}, \; r < \rho\right\}, \\ C_2 \;&=\; \left\{(r, \theta, z): \; z = d/2 + 1 - \sqrt{1 - r^2}, \; r < \rho\right\} \end{aligned}$$

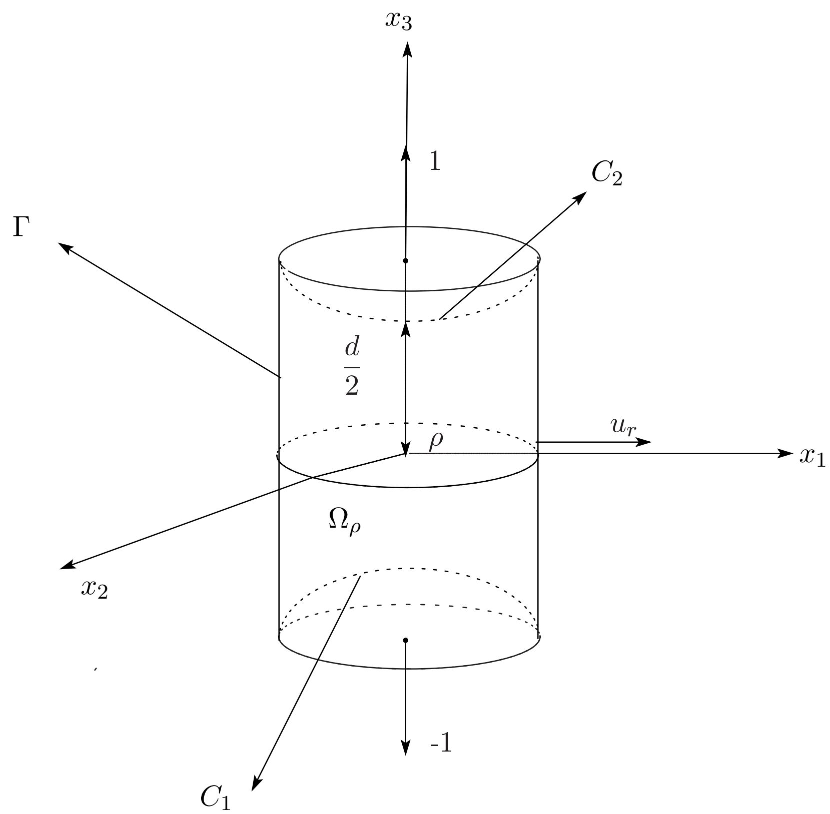


Figure 5.2: The domain $\Omega_\rho$.

Let us define the mean value of $u_r$ on $\Gamma$ by $\bar{u}_r(\rho)$,

$$\bar{u}_r(\rho) \ := \ \frac{1}{|\Gamma|}\int_\Gamma u_r,$$

where $|\Gamma|$ denotes the area of the surface $\Gamma$. We want to show that

$$\bar{u}_r(\rho) \ \simeq \ \frac{\rho}{d+\rho^2}, \qquad \text{for } \rho \lesssim \sqrt{d} \ll 1. \tag{5.1.3}$$

First, the area $|\Gamma|$ can be estimated as

$$|\Gamma| \ = \ 2\pi\rho.2\left(\frac{d}{2}+1-\sqrt{1-\rho^2}\right) \ \simeq 2\pi\rho(d+\rho^2).$$

Next, from the conservation of matter, we have

$$\int_{\partial\Omega_\rho} \mathbf{u}\cdot\mathbf{n} \ = \ \int_{\Omega_\rho} \nabla\cdot\mathbf{u} \ = \ 0. \tag{5.1.4}$$

We thus have

$$\int_\Gamma \mathbf{u}\cdot\mathbf{n} + \int_{C_1} \mathbf{u}\cdot\mathbf{n} + \int_{C_2} \mathbf{u}\cdot\mathbf{n} \ = \ 0. \tag{5.1.5}$$

Since the velocities on $C_2$ and $C_1$ are respectively $\pm e_z$, by symmetry we obtain that

$$\int_{C_2} \mathbf{u}\cdot\mathbf{n} \;=\; \int_{C_1} \mathbf{u}\cdot\mathbf{n} \;=\; -|C_1| \;=\; -\pi\rho^2.$$

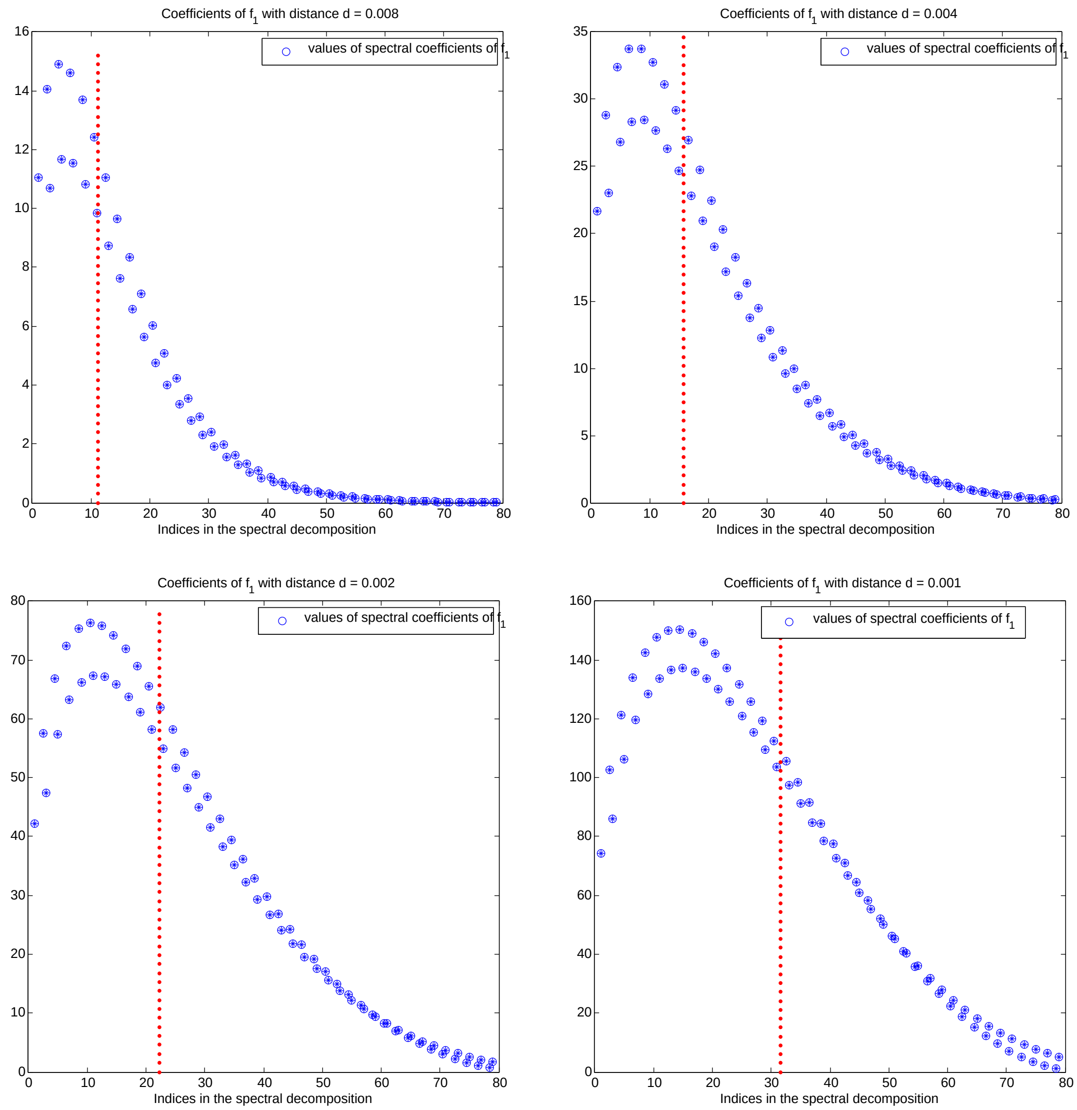


Figure 5.3: Behavior of spectral expansion of force density: the blue line presents the spectral coefficients of $\mathbf{f}_1$, the red line presents $1/\sqrt{d}$.

Therefore, the mean value $\bar{u}_r$ satisfies

$$\bar{u}_r(\rho) \;\simeq\; \frac{2\pi\rho^2.1}{2\pi\rho\,(d+\rho^2)}.$$

Hence, $\bar{u}_r \;\simeq\; \dfrac{\rho}{d+\rho^2}$, as claimed. This formula implies that if $\rho \propto \sqrt{d}$ then $\bar{u}_r \propto \dfrac{1}{\sqrt{d}}$. In view of this asymptotic behavior and taking into account the boundary condition $\mathbf{u} = 0$ on

$C_1$ and $C_2$, we expect

$$\frac{\partial}{\partial z}u_r \propto \frac{1}{d^{3/2}} \quad \text{and} \quad \frac{\partial^2}{\partial^2 z}u_r \propto \frac{1}{d^2}.$$

Using the Stokes momentum equations, we deduce

$$\frac{\partial}{\partial r}p \propto \frac{1}{d^2}.$$

Hence, a natural ansatz is to assume that the leading part of the flow in the region $r \lesssim \sqrt{d}$, $|z| \lesssim d$ is given by:

$$u_r = \frac{1}{\sqrt{d}}U_r\left(\frac{r}{\sqrt{d}}, \frac{z}{d}\right); \quad u_z = U_z\left(\frac{r}{\sqrt{d}}, \frac{z}{d}\right); \quad p = \frac{1}{d^2}P\left(\frac{r}{\sqrt{d}}, \frac{z}{d}\right).$$

Under this ansatz, the surface density of force scales as

$$\mathbf{f} \propto d^{-2}\phi\left(\frac{r}{\sqrt{d}}\right). \tag{5.1.6}$$

According to this formula, when we consider a finite element approximation $\mathbf{f}^h$ of $\mathbf{f}$, this approximation could be accurate only if the step size of the mesh is substantially smaller than $\sqrt{d}$. This leads to expensive computations in the case of a small gap $d$.

In order to check the validity of the formula (5.1.6), we have performed numerical simulations and compute accurate spectral expansions of $\mathbf{f}$ for various gaps $d$. The results given in Figure 5.3 and Figure 5.4 confirm that the force density concentrates on a region of radius of order $\sqrt{d}$ near the contact points. Since the density $\mathbf{f}$ is defined on a surface, this means that for an approximation based on the finite element or a spectral decomposition, at least $O(1/d) = O\left(\frac{1}{\sqrt{d}} \times \frac{1}{\sqrt{d}}\right)$ degrees of freedom are required.

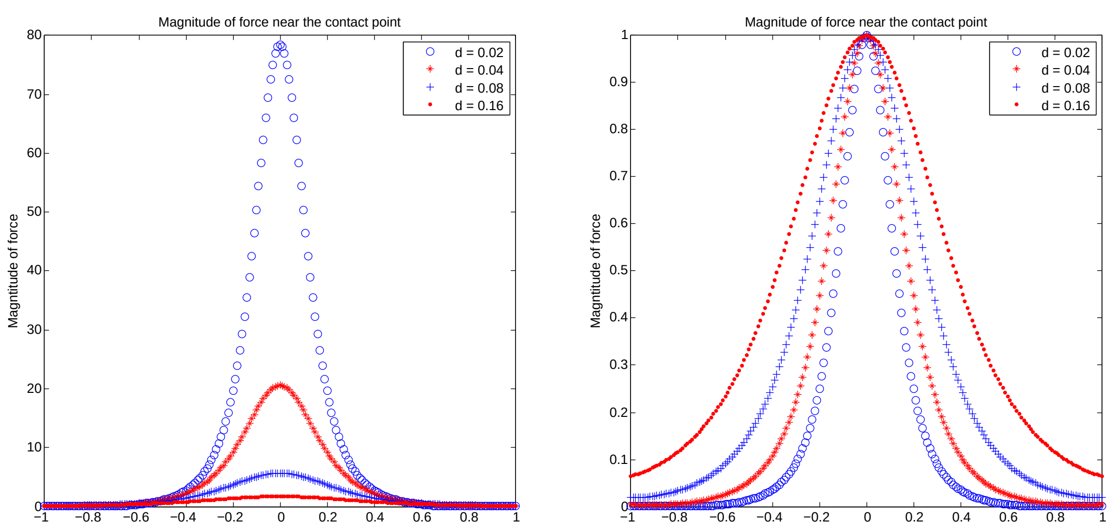


Figure 5.4: Magnitude of force near the contact point on $\partial B_1$ in natural units (left) and in rescaled units (right).

The singular behavior of the force density can not be neglected. Indeed, the leading part of the total hydrodynamic forces comes from the small region $r \lesssim \sqrt{d}$ and the resulting total force is large:

$$\int_{\partial B_1} \mathbf{f} \cdot e_z \ \propto \ \frac{A}{d}.$$

This singular behavior only depends on the relative positions and relative motions. It causes slow convergence of the multipole approximation of the matrix $\mathcal{F}$. Of course, this problem persists for $N$-particles. The singular behavior of the lubrication forces and torques in the limit of small gaps between particles causes a slow convergence of the spectral decomposition. We establish asymptotic formulas for the total forces and torques for close particles in the next section.

## 5.2 Asymptotics for two close particles

In this section, we give asymptotic formulas for the forces and torques of two close particles as the gap $d$ tends to 0. These results are taken from [8].

Let us consider the problem (5.1.1), with prescribed velocities corresponding to rigid displacements:

$$\mathbf{u}_i(x) \ = \ \mathbf{U}_i + \omega_i \times (x - \mathbf{z}_i), \qquad \text{for } i = 1, 2, \tag{5.2.1}$$

where $\mathbf{U}_i, \omega_i$ are respectively the velocities and angular velocities of $B_i$.

### 5.2.1 Decomposition of the motion

We decompose these displacements as follows:

$$\begin{aligned}
\mathbf{u}_1(x) \ &= \ \frac{\mathbf{U}_1 + \mathbf{U}_2}{2} + \frac{\mathbf{U}_1 - \mathbf{U}_2}{2} + \frac{\omega_1 + \omega_2}{2} \times (x - \mathbf{z}_1) + \frac{\omega_1 - \omega_2}{2} \times (x - \mathbf{z}_1),\\
\mathbf{u}_2(x) \ &= \ \frac{\mathbf{U}_1 + \mathbf{U}_2}{2} + \frac{\mathbf{U}_2 - \mathbf{U}_1}{2} + \frac{\omega_1 + \omega_2}{2} \times (x - \mathbf{z}_2) + \frac{\omega_2 - \omega_1}{2} \times (x - \mathbf{z}_2),
\end{aligned}$$

To lighten motion, let us introduce the mean values:

$$\bar{\mathbf{U}} \ := \ \frac{\mathbf{U}_1 + \mathbf{U}_2}{2}, \quad \bar{\omega} \ := \ \frac{\omega_1 + \omega_2}{2}, \quad \bar{\mathbf{z}} \ := \ \frac{\mathbf{z}_1 + \mathbf{z}_2}{2}.$$

The two rigid velocities $\mathbf{u}_1$ and $\mathbf{u}_2$ can be decomposed as sums of singular and regular part as follows

$$\mathbf{u}_i(x) \ = \ \mathbf{u}^{rigid}(x) + \mathbf{u}_i^{singular}(x), \qquad \text{for } i = 1, 2, \tag{5.2.2}$$

where

$$\begin{aligned}
\mathbf{u}^{rigid}(x) \ &= \ \bar{\mathbf{U}} + \bar{\omega} \times (x - \bar{\mathbf{z}}),\\
\mathbf{u}_1^{singular}(x) \ &= \ \frac{\mathbf{U}_1 - \mathbf{U}_2}{2} + \bar{\omega} \times \frac{\mathbf{z}_2 - \mathbf{z}_1}{2} + \frac{\omega_1 - \omega_2}{2} \times (x - \mathbf{z}_1),\\
\mathbf{u}_2^{singular}(x) \ &= \ \frac{\mathbf{U}_2 - \mathbf{U}_1}{2} - \bar{\omega} \times \frac{\mathbf{z}_2 - \mathbf{z}_1}{2} + \frac{\omega_2 - \omega_1}{2} \times (x - \mathbf{z}_2).
\end{aligned}$$

It is convenient to set $\mathbf{V} = \dfrac{\mathbf{U}_1 - \mathbf{U}_2}{2} + \bar{\omega} \times \dfrac{\mathbf{z}_2 - \mathbf{z}_1}{2}$ and $\omega = \dfrac{\omega_1 - \omega_2}{2}$, then the singular parts of the velocities rewrite as

$$\begin{aligned} \mathbf{u}_1^{singular}(x) &= \mathbf{V} + \omega \times (x - \mathbf{z}_1), \\ \mathbf{u}_2^{singular}(x) &= -\mathbf{V} - \omega \times (x - \mathbf{z}_2). \end{aligned}$$

By linearity, the corresponding force densities are given by

$$\mathbf{f}_i = \mathbf{f}^{rigid} + \mathbf{f}_i^{singular}.$$

We note that in the decomposition (5.2.2), since the first term $\mathbf{u}^{rigid}$ corresponds to a rigid displacement of the object formed by the two balls, we do not expect it to lead to a singular force density. We have $\mathbf{f}^{rigid} = O(1)$. For simplicity, we assume $\mathbf{u}^{rigid} = 0$, that is:

$$\mathbf{u}_i(x) = \pm \mathbf{V} \pm \omega \times (x - \mathbf{z}_i). \tag{5.2.3}$$

Let us consider the total force $\mathbf{F}$ and torque $\mathcal{T}$ exerted by the fluid on the first particle. The total force and torque on the other particle are obtained by symmetry. Recall that $F$ and $\mathcal{T}$ are given by

$$\mathbf{F} = \int_{\partial B_1} \mathbf{f}_1 dS, \qquad \mathcal{T} = \int_{\partial B_1} \mathbf{n} \times \mathbf{f}_1 dS. \tag{5.2.4}$$

where $\mathbf{n}$ is the unit normal to the surface and $dS$ is the element of area of the surface.

The main goal of this section is to establish the following asymptotic formulas for the total force and torque given by (5.2.4),

$$\begin{aligned} F_1^{asympt} &= 2\pi V_1 \ln d + O(d^0), \\ F_2^{asympt} &= 2\pi V_2 \ln d + O(d^0), \\ F_3^{asympt} &= -3\pi V_3 d^{-1} + O(\ln d), \\ \mathcal{T}_1^{asympt} &= \left(-2\pi V_2 + \frac{6\pi}{5}\omega_1\right) \ln d + O(d^0), \\ \mathcal{T}_2^{asympt} &= \left(2\pi V_1 + \frac{6\pi}{5}\omega_2\right) \ln d + O(d^0), \\ \mathcal{T}_3^{asympt} &= O(d^0). \end{aligned}$$

To do this, we first expand the velocity $\mathbf{u}$ and pressure $p$ in the power series of the distance $d$. Next, we form the equations of the leading terms based on a decomposition into inner and outer region of expansion. By linearity of the equations, we decompose the total force (torque) as a sum of several forces (torques) which correspond to simple motions. The detailed process is described in the two next sections.

### 5.2.2 Inner and outer region of expansion

It is known that the expansions of velocity $\mathbf{u}$ and pressure $p$ are singular in terms of the distance $d$. So we consider two regions of expansion. An outer region of expansion is defined using the outer variables $(x_1, x_2, x_3)$ in euclidean coordinates. In these coordinate systems, the velocity $\mathbf{u}$ and the pressure $p$ have the forms

$$\mathbf{u} = (u_1(x), u_2(x), u_3(x)) \quad \text{and } p = p(x),$$

with $x = (x_1, x_2, x_3)$. The system of equations (4.1.1) is valid in this region. For some very small distances $d \downarrow 0$, the particles are almost in contact and the point of contact will be a singular point for the flow. So it is necessary to build a new coordinates system for inner region of expansion.

As the discussion in Section 5.1, the variations in the inner region of expansion are described using the inner variables $(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)$:

$$\tilde{x}' = d^{-1/2}x', \qquad \tilde{x}_3 = d^{-1}x_3,$$

where $x' = (x_1, x_2)$, $\tilde{x}' = (\tilde{x}_1, \tilde{x}_2)$. In this coordinate system, the velocity and pressure fields are given by

$$\begin{aligned} \tilde{u}_1(\tilde{x}) &= d^{1/2-k}u_1(x), \qquad & \tilde{u}_2(\tilde{x}) &= d^{1/2-k}u_2(x), \\ \tilde{u}_3(\tilde{x}) &= d^{-k}u_3(x), \qquad & \tilde{p}(\tilde{x}) &= d^{2-k}p(x), \end{aligned}$$

where $x = (x_1, x_2, x_3)$, $\tilde{x} = (\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)$ and $k$ is a real constant which is defined later. We have

$$\nabla_x \mathbf{u} = \begin{pmatrix} d^{k-3/2}\nabla_{\tilde{x}}\tilde{u}_1 \\ d^{k-3/2}\nabla_{\tilde{x}}\tilde{u}_2 \\ d^{k-1}\nabla_{\tilde{x}}\tilde{u}_3 \end{pmatrix} \cdot \begin{pmatrix} d^{1/2} & 0 & 0 \\ 0 & d^{1/2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

From the scaling relations between inner and outer variables we have:

$$\begin{aligned} \nabla_x p &= \left(d^{k-5/2}\partial_{\tilde{x}_1}\tilde{p},\ d^{k-5/2}\partial_{\tilde{x}_2}\tilde{p},\ d^{k-3}\partial_{\tilde{x}_3}\tilde{p}\right)^T, \\ \Delta_x u_1 &= d^{k-3/2}\nabla^2_{\tilde{x}'}\tilde{u}_1 + d^{k-5/2}\frac{\partial^2 \tilde{u}_1}{\partial \tilde{x}_3^2}, \\ \Delta_x u_2 &= d^{k-3/2}\nabla^2_{\tilde{x}'}\tilde{u}_2 + d^{k-5/2}\frac{\partial^2 \tilde{u}_2}{\partial \tilde{x}_3^2}, \\ \Delta_x u_3 &= d^{k-1}\nabla^2_{\tilde{x}'}\tilde{u}_3 + d^{k-2}\frac{\partial^2 \tilde{u}_3}{\partial \tilde{x}_3^2}. \end{aligned}$$

We then expand formally $\tilde{\mathbf{u}}$ and $\tilde{p}$ on the forms

$$\begin{aligned} \tilde{\mathbf{u}} &= \tilde{\mathbf{u}}^0 + d\tilde{\mathbf{u}}^1 + d^2\tilde{\mathbf{u}}^2 + ... \\ \tilde{p} &= \tilde{p}^0 + d\tilde{p}^1 + d^2\tilde{p}^2 + ... \end{aligned}$$

Plugging these expansions in (4.1.1) and identifying the terms of the power series in $d^i$, $i = k - 5/2, k - 2, k - 3/2, ...$, we obtain that the flow field $(\tilde{\mathbf{u}}^0, \tilde{p}^0)$ satisfies

$$\frac{\partial^2 \tilde{u}_1^0}{\partial \tilde{x}_3^2} - \frac{\partial \tilde{p}^0}{\partial \tilde{x}_1} = 0, \quad \frac{\partial^2 \tilde{u}_2^0}{\partial \tilde{x}_3^2} - \frac{\partial \tilde{p}^0}{\partial \tilde{x}_2} = 0, \quad \frac{\partial \tilde{p}^0}{\partial \tilde{x}_3} = 0, \quad \frac{\partial \tilde{u}_1^0}{\partial \tilde{x}_1} + \frac{\partial \tilde{u}_2^0}{\partial \tilde{x}_2} + \frac{\partial \tilde{u}_3^0}{\partial \tilde{x}_3} = 0. \qquad (5.2.5)$$

The flow field $(\tilde{\mathbf{u}}^1, \tilde{p}^1)$ satisfies

$$\frac{\partial^2 \tilde{u}_1^1}{\partial \tilde{x}_3^2} - \frac{\partial \tilde{p}^1}{\partial \tilde{x}_1} = -\nabla^2_{\tilde{x}'} \tilde{u}_1^0, \quad \frac{\partial^2 \tilde{u}_2^1}{\partial \tilde{x}_3^2} - \frac{\partial \tilde{p}^1}{\partial \tilde{x}_2} = -\nabla^2_{\tilde{x}'} \tilde{u}_2^0, \quad \frac{\partial \tilde{p}^1}{\partial \tilde{x}_3} = \frac{\partial^2 \tilde{u}_3^0}{\partial \tilde{x}_3^2}, \quad \frac{\partial \tilde{u}_1^1}{\partial \tilde{x}_1} + \frac{\partial \tilde{u}_2^1}{\partial \tilde{x}_2} + \frac{\partial \tilde{u}_3^1}{\partial \tilde{x}_3} = 0. \tag{5.2.6}$$

There is no difficulty in principle which prevents us from now proceeding to calculate further terms in the expansion, but for the purpose of the analysis, we only need to consider the leading order given by (5.2.5).

Now, it is convenient to change variables

$$y_1 \;=\; \tilde{x}_1, \quad y_2 \;=\; \tilde{x}_2, \quad y_3 \;=\; \tilde{x}_3 + \frac{1}{2} + \frac{1}{2}\left(\tilde{x}_1^2 + \tilde{x}_2^2\right).$$

The surfaces of the particles near the contact point respectively satisfy

$$\partial B_1^{inner}: \quad y_3 \;=\; O(d), \tag{5.2.7}$$

$$\partial B_2^{inner}: \quad y_3 \;=\; 1 + y_1^2 + y_2^2 + O(d) =: h(y_1, y_2) + O(d). \tag{5.2.8}$$

For $\tilde{x} = (\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)$ and $y = (y_1, y_2, y_3)$, let us set

$$\mathbf{v}(y) \;:=\; \tilde{u}_0(\tilde{x}), \quad q(y) \;:=\; \tilde{p}_0(\tilde{x}).$$

With these new variables and $\mathbf{v}(y) = (v_1(y), v_2(y), v_3(y))$, the equation (5.2.5) reads as follows

$$\frac{\partial^2 v_1}{\partial y_3^2} - \frac{\partial q}{\partial y_1} = 0, \quad \frac{\partial^2 v_2}{\partial y_3^2} - \frac{\partial q}{\partial y_2} = 0, \quad \frac{\partial q}{\partial y_3} = 0, \tag{5.2.9}$$

$$\frac{\partial v_1}{\partial y_1} + \frac{\partial v_2}{\partial y_2} + \frac{\partial v_3}{\partial y_3} + y_1 \frac{\partial v_1}{\partial y_3} + y_2 \frac{\partial v_2}{\partial y_3} = 0. \tag{5.2.10}$$

Let us consider the force $F$ and torque $\mathcal{T}$ exerted by the fluid on the first particle. The force and torque on the other particle can be obtained by symmetry. In inner variables, the unit normal $\mathbf{n}$ to the surface and the element of area of the surface $dS$ are given by

$$\mathbf{n} \;=\; \left(d^{1/2} y_1 + O(d), d^{1/2} y_2 + O(d), 1 + O(d)\right),$$

$$dS \;=\; d.dy_1 dy_2 (1 + O(d)).$$

We note that the singular terms of force and torque are contained in the leading term of the inner expansion. Moreover the asymptotic formulas of force $\mathbf{F}^{asympt}$ and torque $\mathcal{T}^{asympt}$ at small gaps are only generated on the area of surface around the contact points. Hence we may compute $\mathbf{F}^{asympt}$ and $\mathcal{T}^{asympt}$ on the small surface $\left\{x \in \partial B_1 :\ x_1^2 + x_2^2 \le \varepsilon^2\right\}$, where $\varepsilon$ is a small real number. In inner variables, this surface becomes

$$S_\varepsilon \;=\; \left\{y \in \partial B_1^{inner} :\ y_1^2 + y_2^2 \le d^{-1}\varepsilon^2\right\}.$$

Then we obtain

$$F_1^{asympt} \;=\; d^{k-1/2} \int_{S_\varepsilon} \left(-y_1 q + \frac{\partial v_1}{\partial y_3}\right) dy_1 dy_2 + O(d^k),$$

$$F_2^{asympt} \;=\; d^{k-1/2} \int_{S_\varepsilon} \left(-y_2 q + \frac{\partial v_2}{\partial y_3}\right) dy_1 dy_2 + O(d^k),$$

$$F_3^{asympt} \;=\; d^{k-1} \int_{S_\varepsilon} (-q)\, dy_1 dy_2 + O(d^k), \tag{5.2.11}$$

$$\begin{aligned}
\mathcal{T}_1^{asympt} &= d^{k-1/2}\int_{S_\varepsilon}\left(-\frac{\partial v_2}{\partial y_3}\right)dy_1dy_2 + O(d^k),\\
\mathcal{T}_2^{asympt} &= d^{k-1/2}\int_{S_\varepsilon}\left(\frac{\partial v_1}{\partial y_3}\right)dy_1dy_2 + O(d^k),\\
\mathcal{T}_3^{asympt} &= d^{k}\int_{S_\varepsilon}\left(y_1\frac{\partial v_2}{\partial y_3} - y_2\frac{\partial v_1}{\partial y_3}\right)dy_1dy_2 + O(d^{k+1/2}).
\end{aligned} \tag{5.2.12}$$

The boundary conditions for $\mathbf{v}$ in inner variables read

$$\begin{aligned}
v_1 &= V_1 d^{1/2-k} - \omega_3 y_2 d^{1-k} + O(d^{3/2-k}),\\
v_2 &= V_2 d^{1/2-k} + \omega_3 y_1 d^{1-k} + O(d^{3/2-k}),\\
v_3 &= V_3 d^{-k} + (\omega_1 y_2 - \omega_2 y_1)\, d^{1/2-k}, \quad \text{on } \partial B_1^{inner},
\end{aligned} \tag{5.2.13}$$

and

$$\begin{aligned}
v_1 &= -V_1 d^{1/2-k} + \omega_3 y_2 d^{1-k} + O(d^{3/2-k}),\\
v_2 &= -V_2 d^{1/2-k} - \omega_3 y_1 d^{1-k} + O(d^{3/2-k}),\\
v_3 &= -V_3 d^{-k} - (\omega_1 y_2 - \omega_2 y_1)\, d^{1/2-k}, \quad \text{on } \partial B_2^{inner},
\end{aligned} \tag{5.2.14}$$

where $\mathbf{V}$ and $\omega$ in (5.2.3) have components $\mathbf{V} = (V_1, V_2, V_3)$ and $\omega = (\omega_1, \omega_2, \omega_3)$.

### 5.2.3 Asymptotic formulas of the total force and torque

Since $(\mathbf{v}, q)$ linearly depends on $\mathbf{V}$ and $\omega$, we may decompose the velocity field $(\mathbf{v}, q)$ in three parts

$$\mathbf{v} = \mathbf{v}_A + \mathbf{v}_B + \mathbf{v}_C, \qquad q = q_A + q_B + q_C,$$

where the first part $(\mathbf{v}_A, q_A)$ is the flow resulting from the translational motion of surfaces along the vertical axis, the second part $(\mathbf{v}_B, q_B)$ is the flow resulting from the tangential and rolling motion of surfaces and the last part $(\mathbf{v}_C, q_C)$ is the flow resulting from the rotational motion of surfaces about normal. More precisely, three flow fields $(\mathbf{v}_A, q_A)$, $(\mathbf{v}_B, q_B)$ and $(\mathbf{v}_C, q_C)$ satisfy (5.2.9), (5.2.10) with the following boundary conditions

$$(v_A)_1 = (v_A)_2 = 0, \quad (v_A)_3 = \pm V_3 d^{-k} \quad \text{on } \partial B_i^{inner}, \tag{5.2.15}$$

$$\begin{aligned}
&(v_B)_1 = \pm V_1 d^{1/2-k} + O(d^{3/2-k}), \quad (v_B)_2 = \pm V_2 d^{1/2-k} + O(d^{3/2-k}),\\
&\qquad (v_B)_3 = \pm(\omega_1 y_2 - \omega_2 y_1)\, d^{1/2-k} \quad \text{on } \partial B_i^{inner},
\end{aligned} \tag{5.2.16}$$

$$(v_C)_1 = \mp\omega_3 y_2 d^{1-k}, (v_C)_2 = \pm\omega_3 y_1, \quad (v_C)_3 = 0 \quad \text{on } \partial B_i^{inner}, \tag{5.2.17}$$

From the boundary condition (5.2.15), (5.2.16) and (5.2.17) we deduce that in order to calculate $(\mathbf{v}_A, q_A)$ one must take $k = 0$, $k = 1/2$ for $(\mathbf{v}_B, q_B)$ and $k = 1$ for $(\mathbf{v}_C, q_C)$. Next we build the asymptotic formulas of force and torque which are correspondingly decomposed as

$$\mathbf{F}^{asympt} = \mathbf{F}_A + \mathbf{F}_B + \mathbf{F}_C, \quad \mathcal{T}^{asympt} = \mathcal{T}_A + \mathcal{T}_B + \mathcal{T}_C.$$

#### 5.2.3.1 Translation motion of spheres

Since $(\mathbf{v}_A, q_A)$ satisfies (5.2.9), (5.2.10), we obtain

$$q_A = q_A(y_1, y_2), \quad (v_A)_1 = \frac{1}{2}\frac{\partial q_A}{\partial y_1} + Ay_3 + C, \quad (v_A)_2 = \frac{1}{2}\frac{\partial q_A}{\partial y_2} + By_3 + D,$$

where $A, B, C$ and $D$ are arbitrary functions of $y_1$ and $y_2$. These terms may be determined from the above boundary conditions of $\mathbf{v}_A$ as

$$A = -\frac{1}{2}\frac{\partial q_A}{\partial y_1}h(y_1, y_2), \quad B = -\frac{1}{2}\frac{\partial q_A}{\partial y_2}h(y_1, y_2), \quad C = D = 0. \tag{5.2.18}$$

Hence, $(v_A)_1$ and $(v_A)_2$ become

$$(v_A)_1 = \frac{1}{2}\left(y_3^2 - y_3 h\right)\frac{\partial q_A}{\partial y_1}, \qquad (v_A)_2 = \frac{1}{2}\left(y_3^2 - y_3 h\right)\frac{\partial q_A}{\partial y_2}. \tag{5.2.19}$$

Substituting the expressions of $(v_A)_1$, $(v_A)_2$ given by (5.2.19) into (5.2.10) and then integrating with respect to $y_3$ we get

$$(v_A)_3 = -\frac{1}{6}\left(\frac{\partial^2 q_A}{\partial y_1^2} + \frac{\partial^2 q_A}{\partial y_2^2}\right)y_3^3 - \frac{1}{2}\left(\frac{\partial A}{\partial y_1} + \frac{\partial B}{\partial y_2} + y_1\frac{\partial q_A}{\partial y_1} + y_2\frac{\partial q_A}{\partial y_y}\right)y_3^2 - (Ay_1 + By_2)y_3 + E, \tag{5.2.20}$$

where $E$ is an function of $y_1$ and $y_2$. Since $(v_A)_3 = -V_3$ on the surface $y_3 = 0$ in the limit of $d \downarrow 0$, it follows that $E = -V_3$. Similarly, since $(v_A)_3 = 1$ on the surface $y_3 = h$, we get

$$-2V_3 = -\frac{1}{6}\left(\frac{\partial^2 q_A}{\partial y_1^2} + \frac{\partial^2 q_A}{\partial y_2^2}\right)h^3 - \frac{1}{2}\left(\frac{\partial A}{\partial y_1} + \frac{\partial B}{\partial y_2} + y_1\frac{\partial q_A}{\partial y_1} + y_2\frac{\partial q_A}{\partial y_2}\right)h^2 - (Ay_1 + By_2)h,$$

After substituting the values of $A$ and $B$ from (5.2.18) into the above equality and then simplifying we obtain

$$\nabla.\left(h^3 \nabla q_A\right) = -24V_3. \tag{5.2.21}$$

In order to solve this equation, we use the polar coordinates

$$y_1 = \hat{r}\cos\theta, \qquad y_2 = \hat{r}\sin\theta,$$

so that the equation (5.2.21) takes the form

$$\hat{r}^2\frac{\partial^2 q_A}{\partial \hat{r}^2} + \frac{\partial^2 q_A}{\partial \theta^2} + \left(\hat{r} + \frac{6\hat{r}^3}{1+\hat{r}^2}\right)\frac{\partial q_A}{\partial \hat{r}} = \frac{-24V_3\hat{r}^2}{(1+\hat{r}^2)^3}. \tag{5.2.22}$$

If we assume that $q_A$ is of order $\hat{r}^n$ as $\hat{r} \to \infty$, then $(v_A)_1, (v_A)_2$ are $O(\hat{r}^{n-1})$ and $(v_A)_3$ is of the form $-1 + O(\hat{r}^n)$ as $\hat{r} \to \infty$. By expressing these qualities in outer variables and noting that the pressure and velocity in the outer region of expansion can not contain any terms which tend to infinity as $d$ tends to 0, this shows that $n \leq -4$. Hence

$$q_A = O(\hat{r}^{-4}) \quad \text{as } \hat{r} \to \infty.$$

The solution of (5.2.22) which satisfies the above condition could be

$$q_A = \frac{3}{(1+\hat{r}^2)^2} + O(d). \tag{5.2.23}$$

The error term of order $d$ in the expression of $q_A$ arises from the fact that the expressions given in the boundary conditions have an error of order $d$.

From (5.2.11) and (5.2.12), the asymptotic formulas $\mathbf{F}_A$ and $\mathcal{T}_A$ generated from the flow field $(\mathbf{v}_A, q_A)$ are given by

$$\begin{aligned}
(F_A)_1 &= d^{-1/2}\int_{S_\varepsilon}\left(-y_1 q_A + \frac{\partial (v_A)_1}{\partial y_3}\right) dy_1 dy_2 + O(d^0),\\
(F_A)_2 &= d^{-1/2}\int_{S_\varepsilon}\left(-y_2 q_A + \frac{\partial (v_A)_2}{\partial y_3}\right) dy_1 dy_2 + O(d^0),\\
(F_A)_3 &= d^{-1}\int_{S_\varepsilon}(-q_A)\, dy_1 dy_2 + O(d^0),
\end{aligned}$$

and

$$\begin{aligned}
(\mathcal{T}_A)_1 &= d^{-1/2}\int_{S_\varepsilon}\left(-\frac{\partial (v_A)_2}{\partial y_3}\right) dy_1 dy_2 + O(d^0),\\
(\mathcal{T}_A)_2 &= d^{-1/2}\int_{S_\varepsilon}\left(\frac{\partial (v_A)_1}{\partial y_3}\right) dy_1 dy_2 + O(d^0),\\
(\mathcal{T}_A)_3 &= \int_{S_\varepsilon}\left(y_1\frac{\partial (v_A)_2}{\partial y_3} - y_2\frac{\partial (v_A)_1}{\partial y_3}\right) dy_1 dy_2 + O(d^{1/2}).
\end{aligned}$$

We can see that if $y_1, y_2$ are replaced by $-y_1, -y_2$ respectively, the value of $q_A$ given by (5.2.23) is unchanged whereas $(v_A)_1, (v_A)_2$ given by (5.2.19) become $-(v_A)_1, -(v_A)_2$ respectively. Hence the force $\mathbf{F}_A$ and $\mathcal{T}_A$ can be estimated by

$$(F_A)_1 = O(d^0), \quad (F_A)_2 = O(d^0), \quad (F_A)_3 = d^{-1}\int_{S_\varepsilon}(-q_A)\, dy_1 dy_2 + O(\ln d), \tag{5.2.24}$$

and

$$(\mathcal{T}_A)_1 = O(d^0), \quad (\mathcal{T}_A)_2 = O(d^0), \quad (\mathcal{T}_A)_3 = \int_{S_\varepsilon}\left(y_1\frac{\partial (v_A)_2}{\partial y_3} - y_2\frac{\partial (v_A)_1}{\partial y_3}\right) dy_1 dy_2 + O(d^{1/2}). \tag{5.2.25}$$

Substituting the formula of $q_A$ given by (5.2.22), we have

$$\begin{aligned}
(F_A)_3 &= -d^{-1}\int_{\hat{r}=0}^{d^{-1/2}\varepsilon}\int_{\theta=0}^{2\pi}\hat{r} q_A d\hat{r} d\theta + O(\ln d)\\
&= 6\pi d^{-1}\int_{\hat{r}=0}^{d^{-1/2}\varepsilon}\hat{r}(1+\hat{r}^2)^{-2} d\hat{r} + O(\ln d).
\end{aligned}$$

Moreover, we have

$$\int_{\hat{r}=0}^{d^{-1/2}\varepsilon}\hat{r}(1+\hat{r}^2)^{-2} d\hat{r} = \frac{1}{2}\left(1 - \frac{1}{1+d^{-1}\varepsilon}\right) \to \frac{1}{2}, \qquad \text{as } d \text{ tends to } 0.$$

It implies

$$(F_A)_3 = 3\pi d^{-1} + O(\ln d).$$

Substituting $(v_A)_1$ and $(v_A)_2$ given by (5.2.19) into the expression of $\mathcal{T}_A$ in (5.2.25), we get

$$(\mathcal{T}_A)_3 \;=\; \int_{S_\varepsilon} h\left(y_2\frac{\partial q_A}{\partial y_1} - y_1\frac{\partial q_A}{\partial y_2}\right) dy_1 dy_2 + O(d^0).$$

Using polar coordinates $y_1 = \hat{r}\cos\theta$, $y_2 = \hat{r}\sin\theta$, we obtain

$$(\mathcal{T}_A)_3 \;=\; \frac{1}{2}\int_{\hat{r}=0}^{d^{-1/2\varepsilon}} \int_{\theta=0}^{2\pi} \hat{r}(1+\hat{r}^2)O(d)d\hat{r}d\theta + O(d^0) = f(\varepsilon) + O(d^0),$$

where $f(\varepsilon)$ tends to 0 as $\varepsilon$ tends to 0. Therefore we get $(\mathcal{T}_A)_3 = O(d^0)$.

### 5.2.3.2 Tangential and rolling motion of spheres

Since $(\mathbf{v}_B, q_B)$ satisfies (5.2.9) and (5.2.10), we can do similar to the previous section, the value of the flow field $(\mathbf{v}_B, q_B)$ is given by

$$q_B \;=\; q_B(y_1,y_2), \quad (v_B)_1 \;=\; \frac{1}{2}\frac{\partial q_B}{\partial y_1}y_3^2 + Ay_3 + V_1, \quad (v_B)_2 \;=\; \frac{1}{2}\frac{\partial q_B}{\partial y_2}y_3^2 + By_3 + V_2, \tag{5.2.26}$$

$$(v_B)_3 \;=\; -\frac{1}{6}\left(\frac{\partial^2 q_B}{\partial y_1^2} + \frac{\partial^2 q_B}{\partial y_2^2}\right)y_3^3 - \frac{1}{2}\left(\frac{\partial A}{\partial y_1} + \frac{\partial B}{\partial y_2} + y_1\frac{\partial q_B}{\partial y_1} + y_2\frac{\partial q_B}{\partial y_2}\right)y_3^2 - (Ay_1 + By_2)y_3 + \omega_1 y_2 - \omega_2 y_1, \tag{5.2.27}$$

where $A, B$ are the functions of $y_1, y_2$ and are given by

$$A \;=\; \frac{-2V_1}{h} - \frac{1}{2}\frac{\partial q_B}{\partial y_1}h, \qquad B \;=\; \frac{-2V_2}{h} - \frac{1}{2}\frac{\partial q_B}{\partial y_2}h.$$

Substituting the value of $(v_B)_3$ into the last boundary condition we obtain

$$\nabla\cdot(h^3\nabla q_B) \;=\; 24(\omega_2 y_1 - \omega_1 y_2), \tag{5.2.28}$$

We use the polar coordinates again, the above equation has the form

$$\hat{r}^2\frac{\partial^2 q_B}{\partial \hat{r}^2} + \frac{\partial^2 q_B}{\partial \theta^2} + \left(\hat{r} + \frac{6\hat{r}^3}{1+\hat{r}^2}\right)\frac{\partial q_B}{\partial \hat{r}} \;=\; 24\left(\omega_2 cos\theta - \omega_1 sin\theta\right)\frac{\hat{r}^3}{(1+\hat{r}^2)^3}. \tag{5.2.29}$$

Here we just need the asymptotic expansion of $q_B$ for large $\hat{r}$, so we only requires the form of $q_B$ by using the limiting form of (5.2.29), we have

$$\hat{r}^2\frac{\partial^2 q_B}{\partial \hat{r}^2} + \frac{\partial^2 q_B}{\partial \theta^2} + 7\hat{r}\frac{\partial q_B}{\partial \hat{r}} \;=\; 24\left(\omega_2 cos\theta - \omega_1 sin\theta\right)\hat{r}^{-3}. \tag{5.2.30}$$

Similar to the case of $q_A$, we requires $q_B$ to satisfy

$$q_B \;=\; O(\hat{r}^{-3}) \quad \text{as } \hat{r}\to\infty. \tag{5.2.31}$$

The solution of (5.2.30) satisfying (5.2.31) is

$$q_B \;=\; -\frac{12}{5}\hat{r}^{-3}\left(\omega_2 cos\theta - \omega_1 sin\theta\right). \tag{5.2.32}$$

Due to the approximation in (5.2.30) that $\hat{r}$ was very large, (5.2.32) for $q_B$ gives really the first term in the asymptotic expansion of $q_B$ for large $\hat{r}$. Also since the expressions in the boundary condition have an error of order $d$, so $q_B$ is given by

$$q_B \;=\; -\frac{12}{5}\hat{r}^{-3}\left(\omega_2 cos\theta - \omega_1 sin\theta\right) + O(\hat{r}^{-2}) + O(d). \tag{5.2.33}$$

If we replace $y_1, y_2$ by $-y_1, -y_2$ respectively or equivalently $\theta$ by $\pi+\theta$, the value $q_B$ becomes $-q_B$, whilst $(v_B)_1$ and $(v_B)_2$ are unchanged. Using these symmetric properties of the flow, the force $\mathbf{F}_B$ and torque $G_B$ on $\partial B_1$ generated by the flow $(\mathbf{v}_B, q_B)$ are calculated from (5.2.11) and (5.2.12) as

$$\begin{aligned}
(F_B)_1 &= \int_{S_\varepsilon}\left(-y_1 q_B + \frac{\partial(v_B)_1}{\partial y_3}\right) dy_1 dy_2 + O(d^{1/2}),\\
(F_B)_2 &= \int_{S_\varepsilon}\left(-y_2 q_B + \frac{\partial(v_B)_2}{\partial y_3}\right) dy_1 dy_2 + O(d^{1/2}),\\
(F_B)_3 &= O(d^0),
\end{aligned}$$

and

$$\begin{aligned}
(\mathcal{T}_B)_1 &= \int_{S_\varepsilon}\left(-\frac{\partial(v_B)_2}{\partial y_3}\right) dy_1 dy_2 + O(d^{1/2}),\\
(\mathcal{T}_B)_2 &= \int_{S_\varepsilon}\left(\frac{\partial(v_B)_1}{\partial y_3}\right) dy_1 dy_2 + O(d^{1/2}),\\
(\mathcal{T}_B)_3 &= O(d^0).
\end{aligned} \tag{5.2.34}$$

Substituting the values of $(v_B)_1$ and $(v_B)_2$ from (5.2.26) into these expressions, we obtain

$$\begin{aligned}
(F_B)_1 &= \int_{S_\varepsilon}\left(-y_1 q_B + \frac{-2V_1}{h} - \frac{1}{2}h\frac{\partial q_B}{\partial y_1}\right) dy_1 dy_2 + O(d^{1/2}),\\
(F_B)_2 &= \int_{S_\varepsilon}\left(-y_2 q_B + \frac{-2V_2}{h} - \frac{1}{2}h\frac{\partial q_B}{\partial y_2}\right) dy_1 dy_2 + O(d^{1/2}).
\end{aligned} \tag{5.2.35}$$

These integrals can be evaluated by changing from $(y_1, y_2)$ to polar coordinates $(\hat{r}, \theta)$ and by substituting the value of $q_B$ from (5.2.33), the above expression for $(F_B)_1$ becomes

$$(F_B)_1 \;=\; \frac{\pi}{2}\int_0^{d^{-1/2}\varepsilon}\left(\frac{24\omega_2}{5}\hat{r}^{-1} - 8V_1\frac{\hat{r}}{1+\hat{r}^2} - \frac{24\omega_2}{5}\frac{1+\hat{r}^2}{\hat{r}^3}\right) d\hat{r} + O(d^0). \tag{5.2.36}$$

So we get the asymptotic form of $(F_B)_1$ as

$$(F_B)_1 \;=\; 2\pi V_1 \ln d + O(d^0).$$

By performing the similar computations for $(F_B)_2, (\mathcal{T}_B)_1$, and $(\mathcal{T}_B)_2$, we also obtain

$$(F_B)_2 \;=\; 2\pi V_2 \ln d + O(d^0),$$

and

$$(\mathcal{T}_B)_1 \;=\; \left(-2\pi V_2 + \frac{6\pi}{5}\omega_1\right)\ln d + O(d^0),$$

$$(\mathcal{T}_B)_2 \;=\; \left(2\pi V_1 + \frac{6\pi}{5}\omega_2\right)\ln d + O(d^0).$$

#### 5.2.3.3 Rotational motion of spheres

As in two previous sections, since $(\mathbf{v}_C, q_C)$ satisfies (5.2.9), and (5.2.10) we obtain

$$q_C \;=\; q_C(y_1, y_2), \quad (v_C)_1 \;=\; \frac{1}{2}\frac{\partial q_C}{\partial y_1}y_3^2 + Ay_3 - \omega_3 y_2, \quad (v_C)_2 \;=\; \frac{1}{2}\frac{\partial q_C}{\partial y_2}y_3^2 + By_3 - \omega_3 y_1, \tag{5.2.37}$$

$$(v_C)_3 \;=\; -\frac{1}{6}\left(\frac{\partial^2 q_C}{\partial y_1^2} + \frac{\partial^2 q_C}{\partial y_2^2}\right)y_3^3 - \frac{1}{2}\left(\frac{\partial A}{\partial y_1} + \frac{\partial B}{\partial y_2} + y_1\frac{\partial q_C}{\partial y_1} + y_2\frac{\partial q_C}{\partial y_2}\right)y_3^2 - (Ay_1 + By_2)y_3, \tag{5.2.38}$$

where $A$ and $B$ are functions of $y_1, y_2$ and are given by

$$A \;=\; \frac{2\omega_3}{h}y_2 - \frac{1}{2}\frac{\partial q_C}{\partial y_1}h, \qquad B = -\frac{2\omega_3}{h}y_1 - \frac{1}{2}\frac{\partial q_C}{\partial y_2}h.$$

Using the last boundary condition on $(v_C)_3$ we obtain an equation for $q_C$ as follows

$$\nabla \cdot (h^3 \nabla q_C) \;=\; 0. \tag{5.2.39}$$

This implies that $q_C = O(d)$. Hence, we can see that the force $\mathbf{F}_C$ and torque $\mathcal{T}_C$ are no longer singular being of order $d^0$, it means

$$\mathbf{F}_C = O(d^0), \qquad \mathcal{T}_C = O(d^0).$$

Combining with the results in Section 5.2.3.1 and Section 5.2.3.2, we obtain the asymptotic formulas of the force $\mathbf{F}$ and torque $\mathcal{T}$ on $\partial B_1$ as claimed.

## 5.3 Stokesian Dynamic method

In this section, we first summarize the Stokesian dynamic method which is developed by Durlofsky and Brady in [10, 11]. This is a general method to calculate the friction matrix for the lubrication effects. Then we perform some numerical tests to illustrate the efficiency and to show a limitations of this method.

### 5.3.1 Main idea

The method assumes that, in the case of two spherical particles the friction matrix is known exactly. This is not true, we do not have any explicit analytic formula for the friction matrix. In practice, we can compute accurate approximations of the friction matrix for two balls at different values of the distance $d \in \{d_0, \lambda d_0, \lambda^2 d_0, ...\}$ for some small $d_0$ and some $\lambda > 1$. For this we use a number of vectorial spherical harmonics in order to reach a given accuracy. We also know the asymptotic bebavior of the friction matrix as $d \downarrow 0$. Tabulating these data and using an interpolation method, we can indeed assume that the friction matrix for two particles is known within a given accuracy.

For a larger number $N$ of particles, we need to make some approximations. Starting from the fundametal solution of the Stokes equations, the friction matrix $\mathcal{F}_{L_{max}}$ is built by expanding the force density on the surface of each particle in a series of vectorial spherical harmonics truncated at level $L_{max}$. The Stokesian dynamics consists in modifying the friction matrix by adding the “exact” lubrication forces $\tilde{\mathcal{F}}_p$ between each pair of close particles. The friction matrix already contained a poor approximation of these short range interactions. In order to avoid counting these interactions twice, we substract a poor approximation $\mathcal{F}_{p,L_{max}}$,

$$\mathcal{F}^{St.Dyn.} = \mathcal{F}_{L_{max}} + \sum_p \left(\tilde{\mathcal{F}}_p - \mathcal{F}_{p,L_{max}}\right).$$

This two-sphere friction matrix $\mathcal{F}_{p,L_{max}}$ is computed with the truncation order $L_{max}$ as $\mathcal{F}_{L_{max}}$.

In Stokesian dynamics, the short range interactions are exact for two spheres. However, by construction, the correction $\tilde{\mathcal{F}}_p - \mathcal{F}_{p,L_{max}}$ only modifies the interaction between the balls of the pair $p = (B_1, B_2)$. If the third ball $B_3$ is close to one of the balls $B_1, B_2$ then the fact that $B_1$ and $B_2$ are close also affects the hydrodynamic interactions $B_1 \longleftrightarrow B_3$ and $B_2 \longleftrightarrow B_3$. The Stokesian dynamic corrections are oblivious of these secondary lubrication effect. In the next section, we expose numerical evidences of this fact.

### 5.3.2 Limitation of the Stokesian Dynamics

Let us consider three particles $B_1, B_2$ and $B_3$. We assume that their centers lie on the vertical axis with the coordinates $\mathbf{z}_1 = (0, 0, 0)$, $\mathbf{z}_2 = (0, 0, 2+d)$ and $\mathbf{z}_3 = (0, 0, 4+2d)$, where $d$ is the distance between two consecutive particles. We assume moreover that these particles translate along the vertical axis with velocities $\mathbf{u}_1 = -e_z$, $\mathbf{u}_2 = \mathbf{u}_3 = e_z$ (see Figure 5.5).

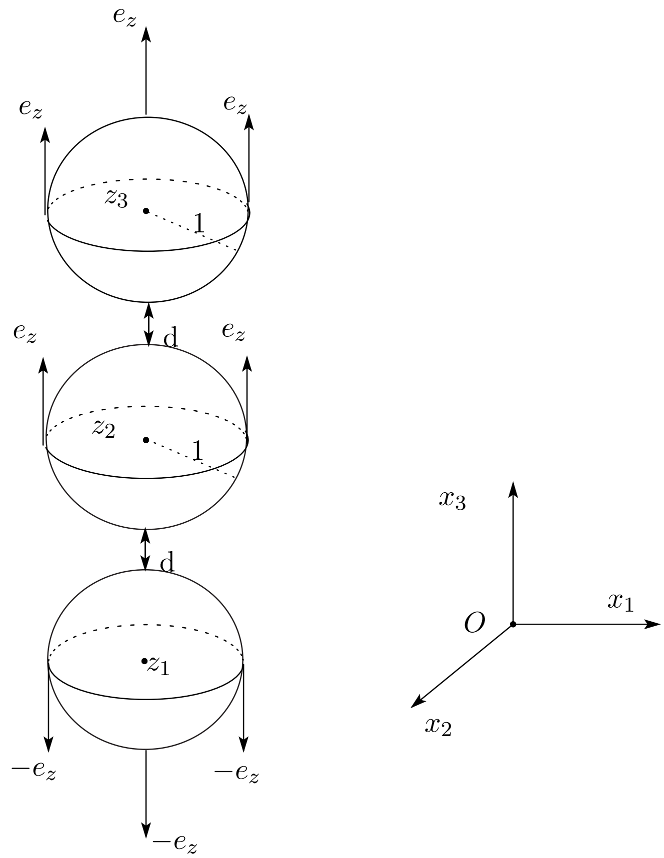


Figure 5.5: Example with three particles.

We compute approximations of the total forces exerted by the surface of the particles on the fluid. We use and compare two methods: the direct method (spectral discretization of the Neumann to Dirichlet operator) and the Stokesian dynamic method as described above.

As expected (see Figure 5.6) the Stokesian dynamic method provide a good approximation of the force exerted by $B_1$: the main part of this force coming from the singular part due to the difference between the velocities $\mathbf{u}_1$ and $\mathbf{u}_2$.

On the other hand, $B_2$ and $B_3$ have the same velocity and the force densities in area between $B_2$ and $B_3$ are smooth. In this case we see that the Stokesian dynamic correction does not lead to any improvement (see Figure 5.7). In fact, the behavior of the approximated force using both methods is exactly the same. Here the Stokesian Dynamics only modifies the interactions between $B_1$ and $B_2$.

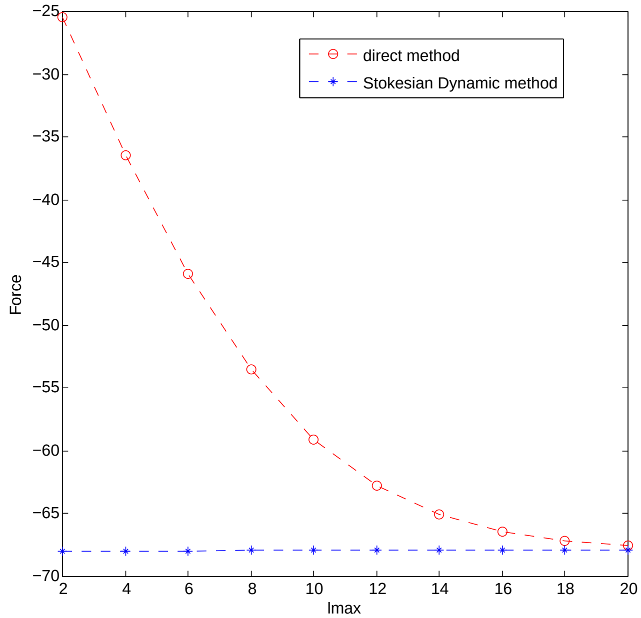


Figure 5.6: The total forces on $B_1$ computed by the Stokesian Dynamics (blue line) and direct method (red line) with $d = 0.05$.

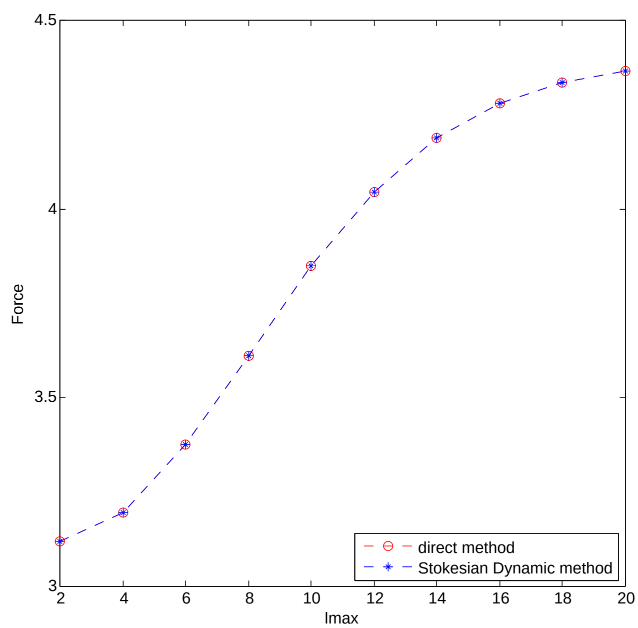


Figure 5.7: The total forces on $B_3$ computed by the Stokesian Dynamics (blue line) and direct method (red line) with $d = 0.05$.

Eventually, the force exerted by the ball $B_2$ combine the situations of the ball $B_1$ and $B_3$. The leading part of this force is due to the lubrication forces between $B_1$ and $B_2$ (different velocities). This leading part is well approximated by the Stokesian dynamic method. On the other hand, the method is oblivious to the influence of the closeness of $B_3$. We observe the same order of magnitude for the error on the force exerted by $B_2$ as for the force exerted by $B_3$ (see Figure 5.8).

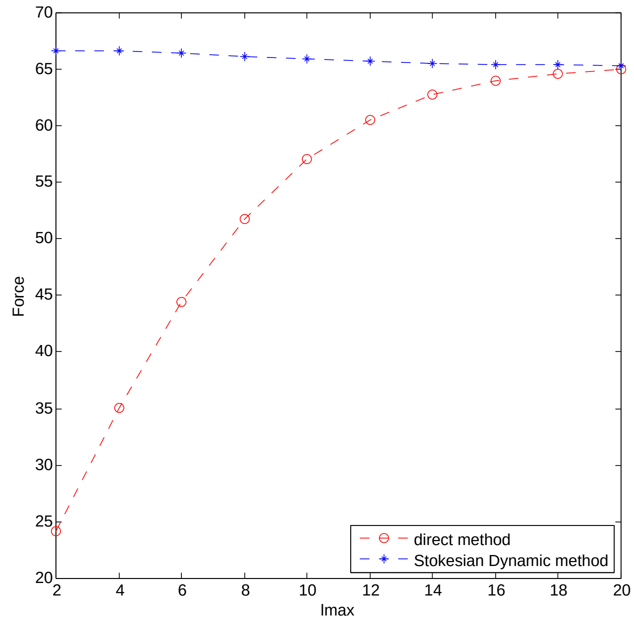


Figure 5.8: The total forces on $B_2$ computed by the Stokesian Dynamics (blue line) and direct method (red line) with $d = 0.05$.

In order to overcome this problem, we propose a new method which we call the correction method. This new method is based on the singular-regular splitting of the hydrodynamic interactions of particles. We present this method in the next chapter.

Chapter 6

# The correction method

### Contents



## 6.1 Singular-regular splitting of the hydrodynamic interactions

We consider $N$ particles as described in Section 4.1.1. Let us start with some notation. Firstly, let us introduce a cut-off distance $\delta > 0$. Denoting by $d_{(i,j)}$ the distance between two particles $B_i$ and $B_j$, $d_{(i,j)} = |\mathbf{z}_i - \mathbf{z}_j| - 2$, the set of pairs of close particles is defined as

$$\mathcal{P} \;=\; \left\{(i,j) \in \{1,...,N\}^2, i \neq j : \quad d_{(i,j)} < \delta\right\}.$$

Our method consists in taking advantage of the linearity of the Stokes equations for rewriting the fields $(\mathbf{u}, p)$ as a superposition

$$\mathbf{u} \;=\; \mathbf{u}^0 + \sum_{c\in\mathcal{P}} \mathbf{u}^c, \qquad p \;=\; p^0 + \sum_{c\in\mathcal{P}} p^c,$$

where each couple $(\mathbf{u}^0, p^0)$ solves the Stokes equations in $\Omega$ and $(\mathbf{u}^c, p^c)$ solves the Stokes equations in the fictitious fluid domain:

$$\Omega^c \;=\; \mathbf{R}^3 \setminus \{B_i \cup B_j\}, \qquad \text{for } c = (i,j) \in \mathcal{P}.$$

The couple $(\mathbf{u}^c, p^c)$ handle the large variations of $(\mathbf{u}, p)$ localized in the small gap between $B_i$ and $B_j$ which are due to the difference between the prescribed velocities on $\partial B_i$ and $\partial B_j$. Precisely, for $c = (i,j) \in \mathcal{P}$, we introduce the velocity field

$$\mathbf{w}^c(x) \;:=\; \frac{1}{2}[\mathbf{u}_j(x) - \mathbf{u}_i(x)],$$

which vanishes if and only if the solid $B_i \cup B_j$ follows a rigid motion. The "singular" field $(\mathbf{u}^c, p^c)$ are defined as the unique solution of the problem

$$\begin{cases} -\Delta \mathbf{u}^c + \nabla p^c \;=\; 0 \quad \text{in } \Omega^c, \\ \nabla \cdot \mathbf{u}^c \;=\; 0 \quad \text{in } \Omega^c, \\ \mathbf{u}^c \;= -\mathbf{w}^c \quad \text{on } \partial B_i, \\ \mathbf{u}^c \;= \mathbf{w}^c \quad \text{on } \partial B_j, \\ \mathbf{u}^c(x) \to 0,\; p^c(x) \to 0 \quad \text{as } |x| \to +\infty. \end{cases} \tag{6.1.1}$$

By linearity, the remaining part $(\mathbf{u}^0, p^0)$ solves the Stokes problem in $\Omega$. The boundary conditions $\mathbf{u}^0$ for this problem are set so that the total velocity field satisfies the boundary conditions $\mathbf{u}_i$ specified in the original problem

$$\begin{cases} -\Delta \mathbf{u}^0 + \nabla p^0 \;=\; 0 \quad \text{in } \Omega, \\ \nabla \cdot \mathbf{u}^0 \;=\; 0 \quad \text{in } \Omega, \\ \mathbf{u}^0 \;=\; \mathbf{w}^0 \quad \text{on } \partial B_i,\; i = 1, 2, ..., N, \\ \mathbf{u}^0(x) \to 0,\; p^0(x) \to 0 \quad \text{as } |x| \to +\infty, \end{cases} \tag{6.1.2}$$

with,

$$\mathbf{w}^0(x) \;:=\; \mathbf{u}_i(x) - \sum_{c \in \mathcal{P}} \mathbf{u}^c(x) \quad \text{for } x \in \partial B_i,\; i = 1, 2, ..., N. \tag{6.1.3}$$

At the end we aggregate the different contributions. With obvious notation,

$$F_k = F_k^0 + \sum_{c \in \mathcal{P}} F_k^c, \qquad \mathcal{T}_k = \mathcal{T}_k^0 + \sum_{c \in \mathcal{P}} \mathcal{T}_k^c, \qquad k = 1, 2, ..., N.$$

Notice that the singular solution $(\mathbf{u}^c, p^c)$ associated to a pair of close particles $c = (i, j) \in \mathcal{P}$ do not contribute to the forces and torques exerted by the surface of a third particle $B_k$, $k \notin \{i, j\}$ : we have $F_k^c = \mathcal{T}_k^c = 0$. Indeed, in this case, $B_k \subset \Omega^c$, so that by the Stokes formula,

$$F_k^c \;=\; \int_{\partial B_k} \sigma^c(x) \cdot \mathbf{n}_k(x) dS \;=\; \int_{B_k} \nabla \cdot \sigma^c(x) dx = 0.$$

Similarly, using the Levi-Civita antisymmetric symbol $\varepsilon_{\alpha\beta\gamma}$ and Einstein summation convention on greek indices, we compute,

$$\begin{aligned} \mathcal{T}_k^c \;&=\; \int_{\partial B_k} \mathbf{n}_k(x) \times (\sigma^c \cdot \mathbf{n}_k(x)] dS \\ &=\; \varepsilon_{\alpha\beta\gamma} \int_{\partial B_k} \mathbf{n}_\beta \sigma^c_{\gamma\zeta} \mathbf{n}_\zeta dS \;=\; \varepsilon_{\alpha\beta\gamma} \int_{B_k} \frac{\partial}{\partial x_\zeta} \left[ (x - \mathbf{z}_i)_\beta \sigma^c_{\gamma\zeta} \right] dx \\ &=\; \varepsilon_{\alpha\beta\gamma} \int_{B_k} (x - \mathbf{z}_i)_\beta \underbrace{(\nabla \cdot \sigma^c)_\gamma}_{=0} dx + \int_{B_k} \underbrace{\varepsilon_{\alpha\beta\gamma} \sigma^c_{\gamma\beta}}_{=0} dx \;=\; 0. \end{aligned}$$

As a consequence, the total force and torque exerted by the particle $B_k$ on the fluid are given by

$$F_k \;=\; F_k^0 + \sum_{\substack{c=(i,j)\in\mathcal{P}, \\ k \in \{i,j\}}} F_k^c, \qquad \mathcal{T}_k \;=\; \mathcal{T}_k^0 + \sum_{\substack{c=(i,j)\in\mathcal{P}, \\ k \in \{i,j\}}} \mathcal{T}_k^c. \tag{6.1.4}$$

The advantage of decomposing the solution resides in the possibility of using different methods for solving problems (6.1.1) and (6.1.2). The singular parts are solution of the Stokes equations (6.1.1) around only two solid particles. We will approximate these singular parts by interpolating in pre-computed tables. The remaining parts solves the Stokes equations (6.1.2) in the original domain but with modified boundary conditions which do not necessarily correspond to rigid motions of the particles. The remaining regular part may be approximated by using any standard numerical method.

Let us first consider problem (6.1.1). For $c = (i, j) \in \mathcal{P}$, by changing coordinates, we may assume that $\mathbf{z}_i = -(1 + d_c/2)e_z$ and $\mathbf{z}_j = (1 + d_c/2)e_z$. In the new coordinates, the velocity $\mathbf{w}^c$ uniquely decomposes as

$$\mathbf{w}^c(x) \;=\; U_z^c e_z + U_{xy}^c e_1 + \omega_z^c e_z \times x + \omega_{xy}^c e_2 \times x,$$

where $e_1$ and $e_2$ are two unit vectors orthogonal to $e_z$. Hence, the solution of (6.1.1) can be decomposed as

$$(\mathbf{u}^c, p^c) \;=\; U_z^c(\mathbf{u}_A, p_A) + U_{xy}^c(\mathbf{u}_B, p_B) + \omega_{xy}^c(\mathbf{u}_{B'}, p_{B'}) + \omega_z^c(\mathbf{u}_C, p_C), \tag{6.1.5}$$

where, for $Z = A, B, B'$, or $C$, the couple $(\mathbf{u}_Z, p_Z)$ solves the Stokes equations in the domain

$$\Omega^{d_c} \;:=\; \mathbf{R}^3 \setminus \left[B_+^{d_c} \cup B_-^{d_c}\right], \tag{6.1.6}$$

where $B_\pm^{d_c}$ denotes the solid sphere with unit radius and center $\pm(1 + d_c/2)e_z$. The difference between these problems comes from the specific boundary conditions,

$$\mathbf{u}_Z \;=\; \mathbf{w}_Z \qquad \text{on } \partial B_+^{d_c} \cup \partial B_-^{d_c},$$

where $\mathbf{w}_Z$ are defined as follows, for $x \in \partial B_\pm^{d_c}$,

$$\mathbf{w}_A(x) \;:=\; \pm e_z, \quad \mathbf{w}_B(x) \;:=\; \pm e_1, \quad \mathbf{w}_{B'}(x) \;:=\; \pm e_2 \times x, \quad \mathbf{w}_C(x) \;:=\; \pm e_z \times x. \tag{6.1.7}$$

When solving independently the second or the third problem, we may rotate the frame so that $e_1$ or $e_2$ coincide with $e_x$. We end with four family of problems only depending on the distance $d_c$. More precisely, in view of (6.1.4), we need approximations of

$$F_Z(d_c) \;:=\; \int_{\partial B_+^{d_c}} \sigma_Z(x) \cdot \mathbf{n}(x) dS(x), \tag{6.1.8}$$

$$\mathcal{T}_Z(d_c) \;:=\; \int_{\partial B_+^{d_c}} \mathbf{n}(x) \times [\sigma_Z(x) \cdot \mathbf{n}(x)] dS(x). \tag{6.1.9}$$

Using the symmetries of the problems, the corresponding total forces and torques on $\partial B_-^{d_c}$ are deduced from the former. For the computation of the boundary conditions (6.1.3) satisfied by the remaining "regular part" $(\mathbf{u}^0, p^0)$, we also need approximations of

$$\mathbf{v}_Z(x, d_c) \;:=\; \mathbf{u}_Z(x), \qquad \text{for } x \in \Omega^{d_c} \text{ and } Z = A, B, B', C.$$

In the next section, we describe a procedure for computing these quantities. The method is based on known asymptotic as $d_c \to 0$, direct computations and interpolation in the parameter $d_c$.

Let us now consider problem (6.1.2). It is of the same nature as the original problem: solve the Stokes equations in the fluid domain surrounding the particles. The new problem looks even more complex since we have substituted the function $\mathbf{w}^0$ for the simple rigid motions $\mathbf{u}_i$ that can be described with $6N$ parameters. However, by construction, $(\mathbf{u}^0, p^0)$ is a very regular vector field, even in the limit of touching particles. As a consequence, applying standard numerical methods to problem (6.1.2), we can compute approximations of $(\mathbf{u}^0, p^0)$ with an accuracy that does not depend on the distance $d_c$ between close particles.

## 6.2 Discretization

As in the previous section, we split the solution into a regular and a singular field. In this section, we describe a procedure for computing the approximations of the singular part and the boundary condition for the regular part. The main idea is to interpolate the needed quantities into a grid of known values which has been computed once for all during a preprocessing step.

### 6.2.1 The interpolation method for computing the singular fields

As explained in the discussions at the end of Section 6.1, for each $c = (i, j) \in \mathcal{P}$, the singular part $(\mathbf{u}^c, p^c)$ can be decomposed as a combination of four parts $(\mathbf{u}_Z, p_Z)$ which are solutions of four family of problems only depending on the distance $d_c$,

$$\begin{cases} -\Delta \mathbf{u}_Z + \nabla p_Z \ = \ 0, \quad \nabla \cdot \mathbf{u}_Z \ = \ 0 \qquad \text{in } \Omega^{d_c}, \\ \mathbf{u}_Z \ = \ \mathbf{w}_Z \qquad \text{on } \partial\Omega^{d_c}, \end{cases} \tag{6.2.1}$$

where $\Omega^{d_c}$ and $\mathbf{w}_Z$ are given by (6.1.6) and (6.1.7) respectively. Recall that the fluid domain $\Omega^{d_c}$ only depends on the distance $d_c$. We need to compute approximations of $\mathbf{F}_Z$ and $\mathcal{T}_Z$ given by (6.1.8), (6.1.9). Our method is based on asymptotic formulas for the total force and torque at small distance, direct computations and interpolation in the parameter $d_c$.

In a preprocessing step, we decompose $(\tilde{\mathbf{f}}_Z)_k$ and $(\mathbf{w}_Z)_k$, for $k = B_-^{d_c}, B_+^{d_c}$, in the basis of vectorial spherical harmonics as follows,

$$\begin{aligned} (\tilde{\mathbf{f}}_Z)_k \ &= \ \sum_{\alpha \geq 0} f_{k,\alpha}^Z \phi_{k,\alpha}, \\ (\mathbf{w}_Z)_k \ &= \ \sum_{\alpha \geq 0} w_{k,\alpha}^Z \phi_{k,\alpha}. \end{aligned}$$

By truncating the above series up to order $M_{max}$, with $M_{max}$ large, the discrete Neumann to Dirichlet matrix $\mathcal{ND}_{Z,dis.}$ is computed as described in Section 4.2.3.2. Then we compute accurate approximations of the surface force density $\mathbf{f}_Z^{dis.}$ by solving the linear problem,

$$ND_{Z,dis.}.\mathbf{f}_Z^{dis.} \ = \ W_Z,$$

where $W_Z = \left(w_{i,\alpha}^Z\right)_{k=i,j,\alpha=1,\ldots,M_{max}}$. By this direct method, we may compute $\mathbf{f}_Z^{dis.}$ as a function of $d_c$ for a finite number of distances, say $d_c \in \mathcal{D}^{dis} := \{d_0, \lambda d_0, \lambda^2 d_0, \ldots\}$ for some small $d_0$ and some $\lambda > 1$. Combining the explicit asymptotic formula of the force density with this discrete set of accurately computed values, we obtain approximations of $\mathbf{f}_Z^{dis.}(d_c)$ by interpolation for every $0 < d_c < \delta$.

For instance, let us consider the first problem $Z = A$. We are interested in the total force and torque exerted by the first particles $B_-^{d_c}$. In this case, from the symmetries and the asymptotic formulas given in Section 5.2, we have,

$$\mathbf{F}^A(d_c) \;=\; \left(\frac{3\pi}{d_c} + O(\ln d_c)\right) e_z, \qquad \text{and} \;\; \mathcal{T}_A(d_c) \;=\; 0,$$

We guess that $\mathbf{F}^A(d_c)$ expands as

$$\mathbf{F}^A(d_c) \;=\; \left[\frac{3\pi}{d_c} + C_1 \ln d_c + C_2 + C_3(d_c \ln d_c) + C_4 d_c + \mathcal{R}_A(d_c)\right] e_z.$$

The constants $C_1, C_2, C_3$ and $C_4$ are then determined by using a least square approximation based on highly accurate numerical simulations performed for a small number of small values of $d_c$. The Figure 6.1 shows the behavior of the rest term $\mathcal{R}_A(d_c)$.

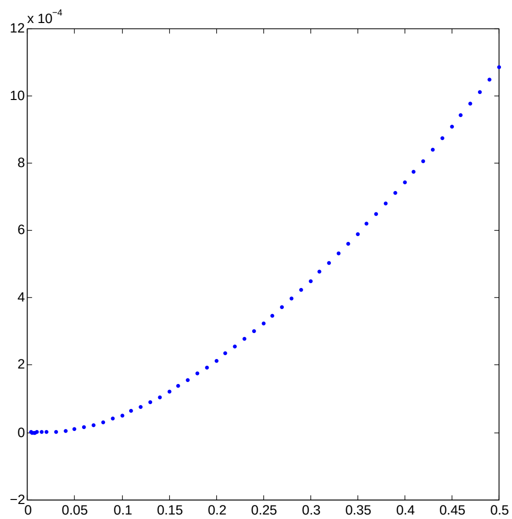


Figure 6.1: The term $\mathcal{R}_A(d_c)$ in a function of $d_c$.

Table 6.1: The absolute errors of interpolation.

| $d_c$ | 0.475 | 0.355 | 0.275 | 0.135 | 0.0135 |
|---|---|---|---|---|---|
| $L_{max}$ | 50 | 50 | 50 | 70 | 150 |
| absolute error (total force) | 4.4e-13 | 2.2e-12 | 3.5e-12 | 7.4e-12 | 3.1e-10 |

In a second step we build a table of values of $\mathcal{R}_A(d_c)$ for $d_c$ ranging in a finite subset of $(0, \delta)$. These values are obtained by the direct method with a very large $L_{max}$.

In practice, we have preformed accurate simulations with the following distances:

$$d_c = 0.001,\ 0.002,\ ...,\ 0.009,\ 0.01,\ 0.02,\ ...,\ 0.5.$$

This ends the preprocessing step.
Eventually, when needed, we use the cubic spline interpolation method to estimate $\mathcal{R}_A(d_c)$ for any non-tabulated distance $d_c \in (0, \delta)$ from the tabulated values. In Table 6.1, we show the result of some numerical tests realized in order to estimate the error due to the interpolation method.

### 6.2.2 Computation of correction velocities

In this section, we present the interpolation method to compute the coefficients of the correction velocities.

We consider again the problem (6.2.1). Let $B_R$ be the ball of radius $R = 3$ centered at the origin of the coordinate system. This ball contains the two balls $B_-^{d_c}$ and $B_+^{d_c}$. We want to determine the velocity $\mathbf{U}_Z(\mathbf{r}, d_c)$ for $\mathbf{r} \in \mathbf{R}^3 \setminus B_R$.

We first compute the force densities on the boundary of $B_+^{d_c}$ and $B_-^{d_c}$ using the direct method with a large truncating order. Then, we can deduce the velocity field $\mathbf{U}_Z$ everywhere using the explicit formula (4.1.7). On the other hand, we know that the velocity field in $\mathbf{R}^3 \setminus B_R$ reads

$$\begin{aligned}\mathbf{U}_Z(\mathbf{r}, d_c) \;=\; &\sum_{l\geq 1}\sum_{m=-l}^{l} g^T_{Z,l,m}(d_c) r^{-(l+1)} T_{l,m} + \sum_{l\geq 0}\sum_{m=-l-1}^{l+1} g^I_{Z,l,m}(d_c) r^{-(l+1)} I_{l,m} \\ &+ \sum_{l\geq 1}\sum_{m=-l+1}^{l-1}\left[\frac{(2l-3)(l-1)}{2l} g^I_{Z,l-2,m}(d_c)(r^2-1) + g^N_{Z,l,m}(d_c)\right] r^{-(l+1)} N_{l,m}, \quad (6.2.2)\end{aligned}$$

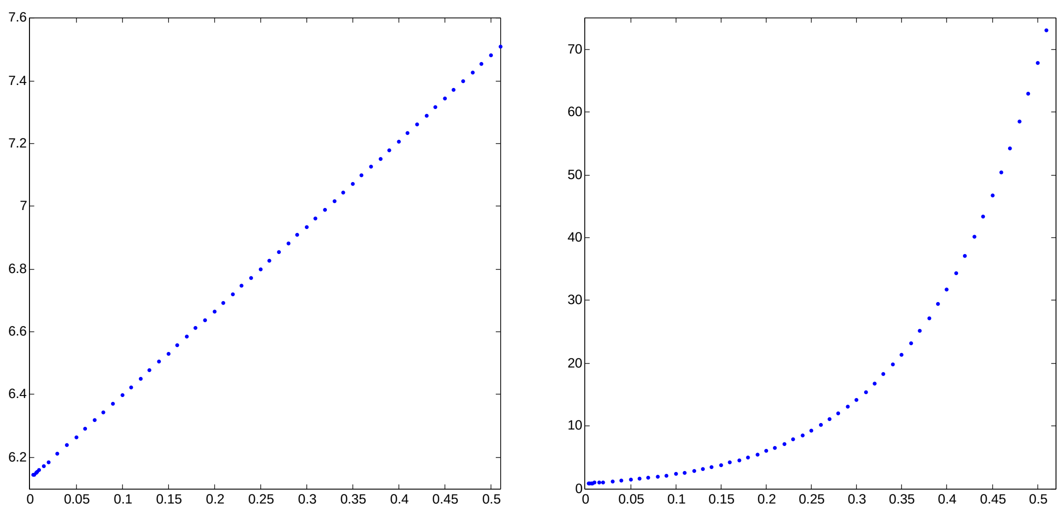


Figure 6.2: The coefficients $g^I_{Z,0,0}(d_c)$ (left) and $g^N_{Z,5,0}(d_c)$ (right) in functions of $d_c$ in the case $Z = A$.

We then only have to tabulate the coefficients $g^T_{Z,l,m}, g^I_{Z,l,m}, g^N_{Z,l,m}$. These coefficients are obtained by projecting $\mathbf{U}_Z(\cdot, d_c)$ on the basis of rescaled vectorial spherical harmonics on

$\partial B_R$. In a last step, we use (6.2.2) to obtain the corresponding coefficients in the vectorial spherical harmonic basis on $\partial B(0,1)$.

In practice, the series (6.2.2) is truncated at some order $\tilde{L}_{max}$. We call $\tilde{L}_{max}$ the correction truncation order. Notice that this truncation order may be different than $L_{max}$ defined in Section 4.2.3.1. The choice of $\tilde{L}_{max}$ will be discussed in Section 6.4.

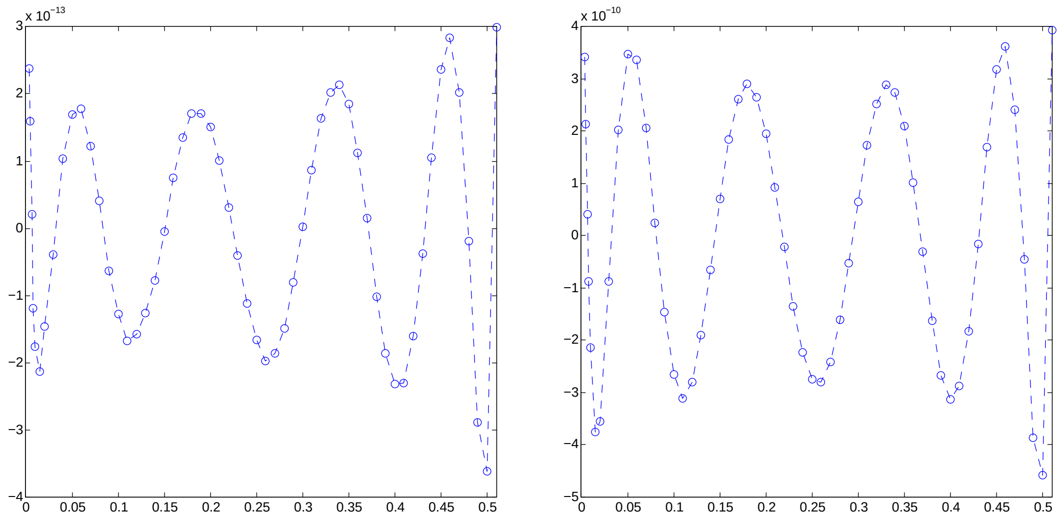


Figure 6.3: The absolute errors of interpolation correspond to the coefficients $g^I_{Z,0,0}(d_c)$ (left) and $g^N_{Z,5,0}(d_c)$ (right) in function of $d_c$ in the case $Z = A$.

Finally, using a polynomial interpolation of these computed coefficients, we can estimate the coefficients of the correction velocities on the unit sphere for any $d_c \in \mathcal{D}^{dis}$.

These coefficients are computed as functions of the distance $d_c$ in the four cases corresponding to $Z = A, B, B', C$. As an example, we show the behavior of $g^I_{Z,0,0}(d_c)$ and $g^N_{Z,5,0}(d_c)$ in the case $Z = A$ in Figure 6.2. The absolute errors of the polynomial interpolation corresponding to these coefficients are also shown (Figure 6.3).

## 6.3 Numerical results

In this section, we perform some numerical tests to compare the three methods: the direct method, the Stokesian Dynamics and the correction method. Recall that in the case of two particles, the correction method and the Stokesian Dynamics are exactly the same. Hence we just consider the cases with more than two particles.

### 6.3.1 Three particles

Let us again consider three spheres with different velocities as decribed in Section 5.3. The Stokesian Dynamics and the correction method are really better than the direct method as shown by the representation of the approximation of the forces $\mathbf{F}_1, \mathbf{F}_2, \mathbf{F}_3$ applied by the balls $B_1, B_2, B_3$ on the fluid using the three different methods (see Figure 6.4).

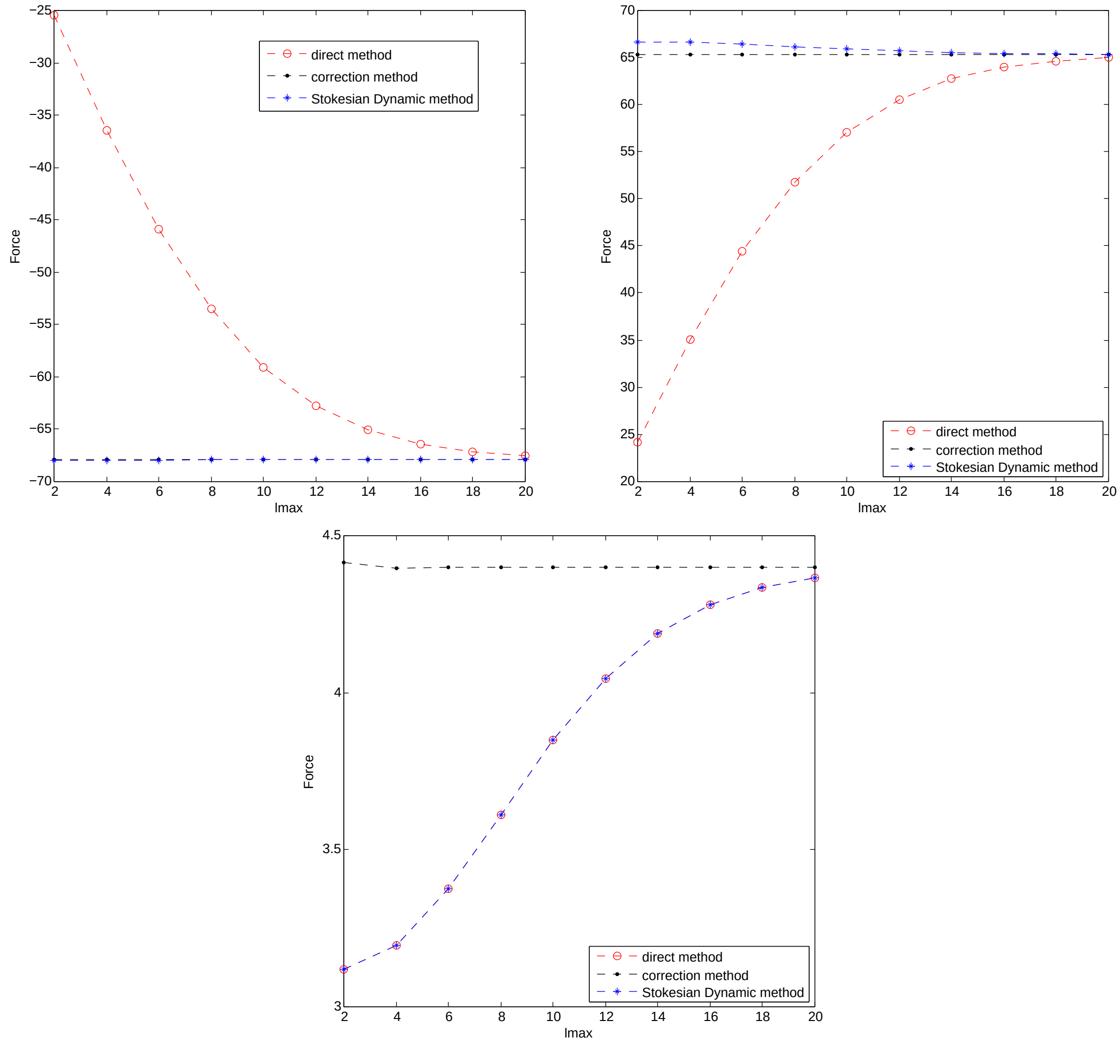


Figure 6.4: Comparison of the three methods with 3 particles: $B_1$ (first), $B_2$ (second) and $B_3$ (third) with $d = 0.05$.

Zooming on the results of the Stokesian Dynamics and the correction method (see Figure 6.5), we see that the latter has a better behavior. With $L_{max} = 8$, the relative error for the correction is $6.10^{-6}$. So we conclude that even in the presence of several particles the correction method also improves the approximation of the interactions with neighboring particles.

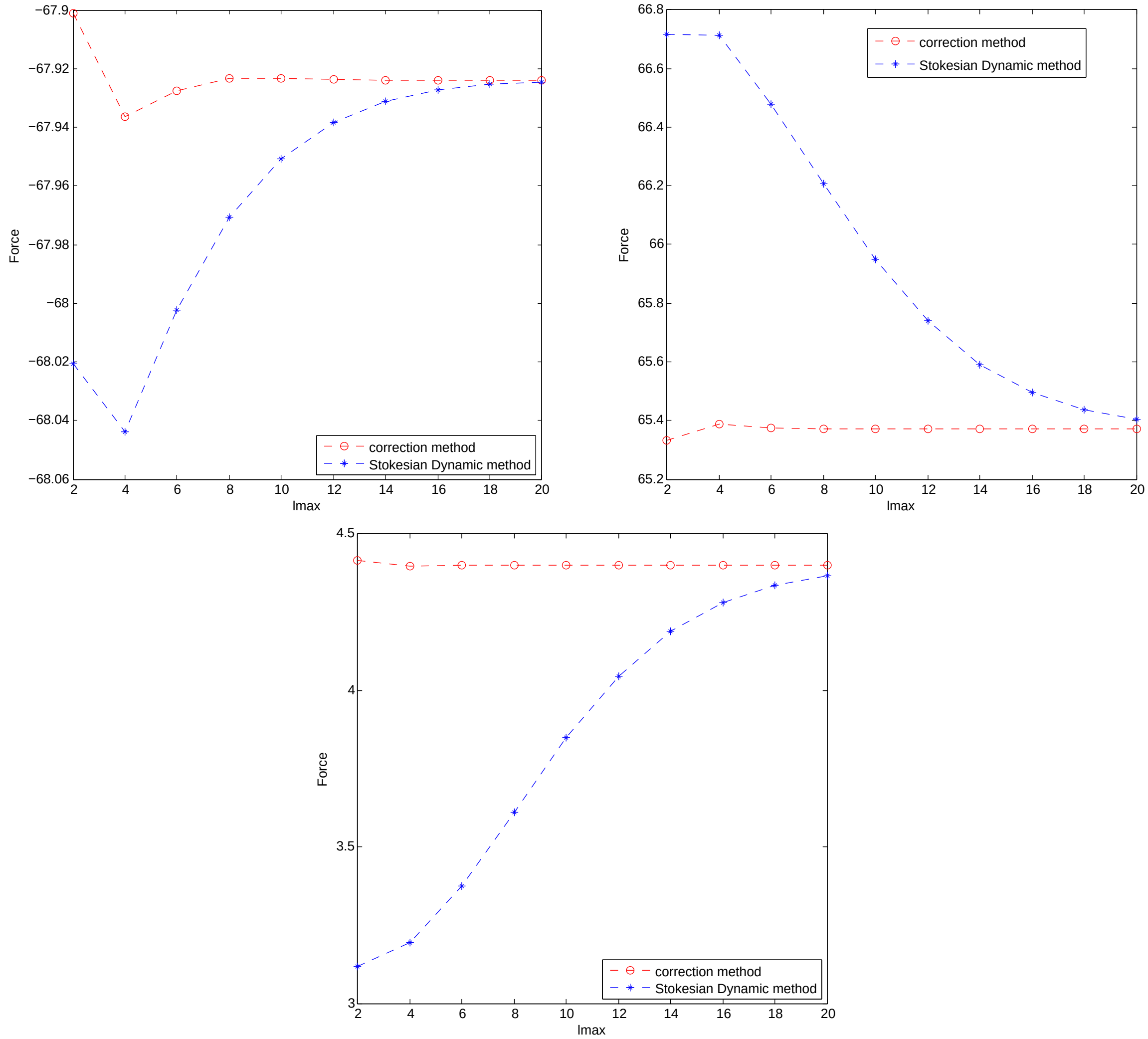


Figure 6.5: Comparison of the Stokesian Dynamics and of the correction method with 3 particles: $B_1$ (first), $B_2$ (second) and $B_3$ (third) with $d = 0.05$.

Let us state again the main difference between these methods. The Stokesian Dynamics modifies the interaction of each pair of close particles independently. The correction method also modifies the interactions with neighboring particles. Hence at the same level of truncation order, the computational time of the correction method is larger. But the correction method converges very fast and requires a small level of truncation order to get an accurate result.

### 6.3.2 Four particles

We perform some numerical test in a more complicated configuration. We consider four particles such that their centers are not on a straight line. These centers are respectively

$$\mathbf{z}_1 = 0, \quad \mathbf{z}_2 = (2+d)e_a, \quad \mathbf{z}_3 = \mathbf{z}_2 + (2+d)e_b, \quad \mathbf{z}_4 = \mathbf{z}_3 + (2+d)e_c,$$

where $d = 0.05$ is the distance of particles and $e_a, e_b, e_c$ are unit vectors as follows

$$e_a = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right), \quad e_b = \left(\frac{1}{\sqrt{4}}, \frac{1}{\sqrt{5}}, \sqrt{\frac{11}{20}}\right), \quad e_c = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{3}}\right).$$

The rigid displacements $\mathbf{u}_i$ are given by (4.1.2), where the corresponding velocities $\mathbf{U}_i$ and angular velocities $\omega_i$ are given by

$$\mathbf{U}_1 = (1,-2,3), \quad \mathbf{U}_2 = (-2,3,0), \quad \mathbf{U}_3 = (3,0,-1), \quad \mathbf{U}_4 = (-1,-1,1),$$

$$\omega_1 = (2,0,-3), \quad \omega_2 = (-1,-2,0), \quad \omega_3 = (2,1,-2), \quad \omega_4 = (-1,-1,1).$$

As in the previous section, we show the numerical results in two steps: first we compare the three methods in Figure 6.6 and then we compare the two best methods in Figure 6.7.

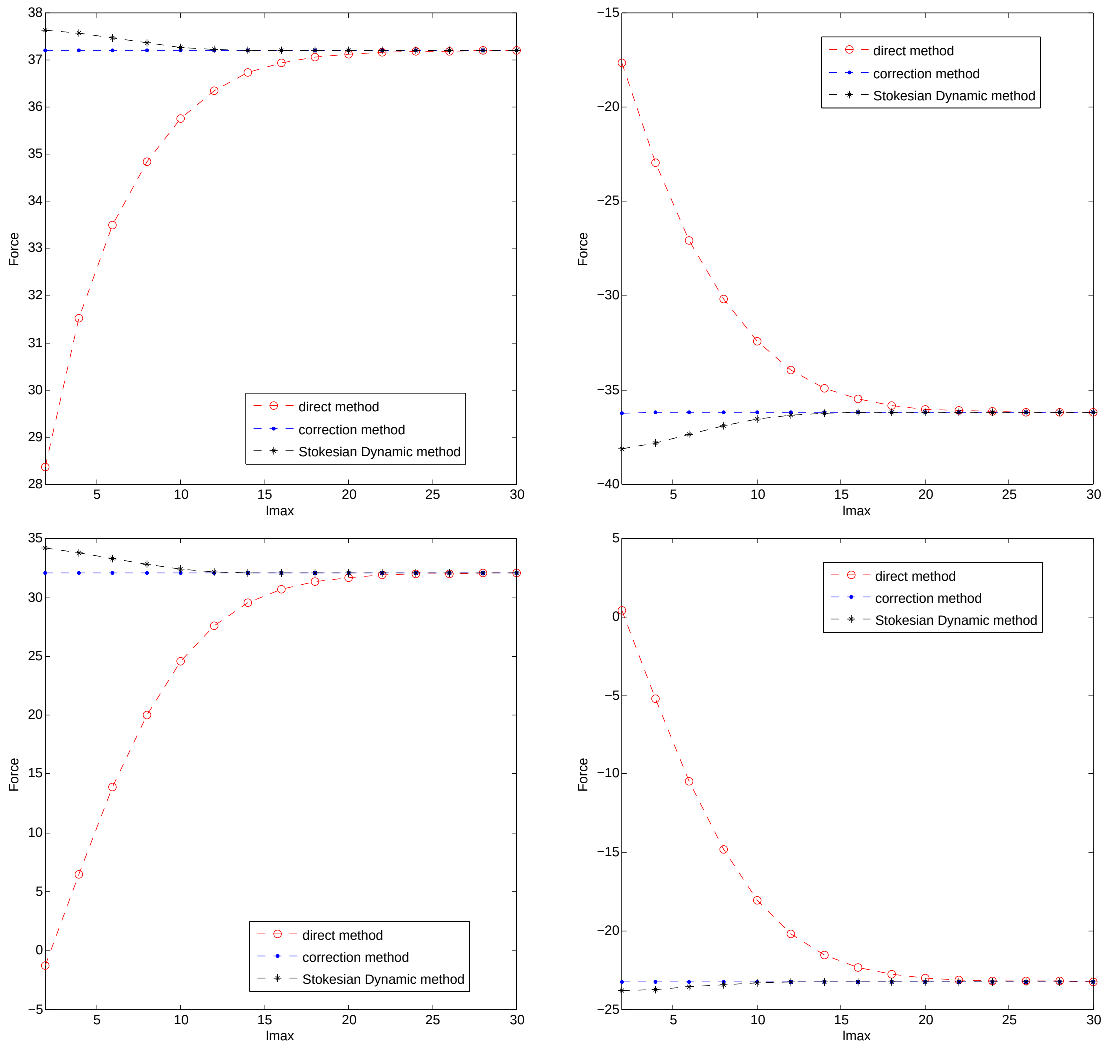


Figure 6.6: Forces on the four particles in $z$ direction computed with the three methods: $B_1$ (first), $B_2$ (second), $B_3$ (third) and $B_4$ (fourth). $d = 0.05$.

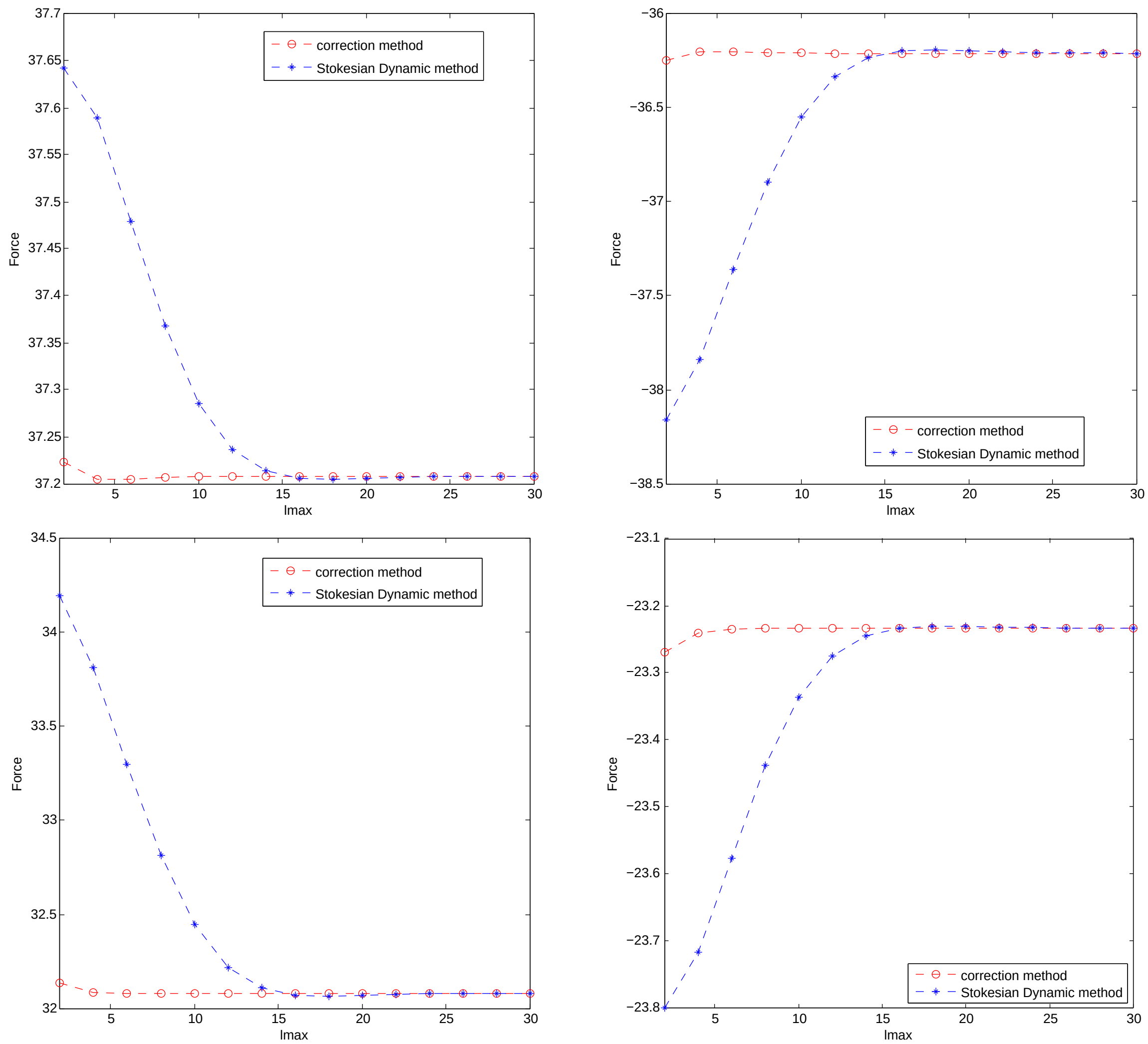


Figure 6.7: Forces on the four particles in $z$ direction computed with the Stokesian Dynamics and the correction method: $B_1$ (first), $B_2$ (second), $B_3$ (third) and $B_4$ (fourth). $d = 0.05$.

The results are similar to the three sphere case. The correction method provides an accurate result for $L_{max} = 8$.

## 6.4 Numerical determination of the truncation orders

In the correction method, when we approximate the correction $\mathbf{w}^0$ determined by (6.1.3) and the Neumann to Dirichlet matrix $\mathcal{DN}$, we have to choose two truncating parameters: $L_{max}$ for approximating the Neumann to Dirichlet matrix and $\tilde{L}_{max}$ for approximating the velocity corrections. These quantities prescribe the number of vectorial spherical harmonics used for the discretization. The natural question is how can we choose these parameters such that the solution has a given accuracy? How do they depend on the distances between the particles? In this section, we present a numerical estimation of these parameters.

### 6.4.1 Correction truncation order

Let us consider the problem (4.1.1) with three unit balls. We assume that their centers lie on the vertical axis with corresponding coordinates $\mathbf{z}_1 = (0,0,0)$, $\mathbf{z}_2 = (0,0,2+d)$, and $\mathbf{z}_3 = (0,0,4+d+D)$. We assume moreover that the two first balls translate along the vertical axis with opposite velocities and that the third particle moves with the same velocity of the second one, i.e., the given velocities of three balls are respectively $\mathbf{u}_1 = -e_z$ and $\mathbf{u}_2 = \mathbf{u}_3 = e_z$.

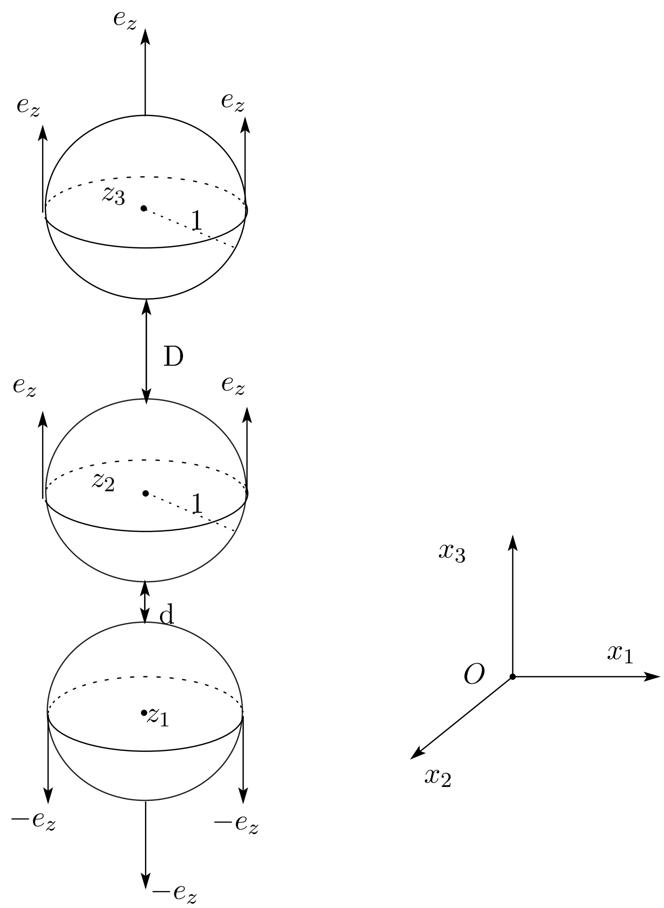


Figure 6.8: Example with three particles.

Firstly, we write the surface densities as functions of the distances between the particles and of the truncating parameters

$$\mathbf{f}^{dis.} = \mathbf{f}^{dis.}\left(d, D, L, \tilde{L}\right),$$

where $L$ and $\tilde{L}$ are respectively the truncation orders used for approximating the Neumann to Dirichlet matrix and for the velocity corrections.

Since the correction method converges very fast, we may fix a large enough value of the truncation order $L = L_0$ for estimating $\tilde{L}_{max}$. In numerical tests we choose $L_0 = 20$. Then for every $\tilde{L} \in \left[1, \tilde{L}_\infty\right)$, we define the error for the surface density as follows

$$Err\left(d, D, \tilde{L}\right) \ := \ \left|\mathbf{f}^{dis.}\left(d, D, L_0, \tilde{L}\right) - \mathbf{f}^{dis.}\left(d, D, L_0, \tilde{L}_\infty\right)\right|,$$

where $\tilde{L}_\infty$ is very large.

Given a real small number $\varepsilon > 0$, the truncation order $\tilde{L}_{max}$ is chosen as follows

$$\tilde{L}_{max}(d, D) \ := \ \min\left\{\tilde{L} \in \left[1, \tilde{L}_\infty\right) : \quad Err\left(d, D, \tilde{L}\right) < \varepsilon\right\}.$$

In our numerical experiments, we set $\varepsilon = 10^{-6}$. Moreover, we only consider $d < \delta$, where $\delta = 2$ is the cut-off distance defined in Section 6.1. Then we numerically calculate $\tilde{L}_{max}(d, D)$ as a function of $d$ and $D$ (see Figure 6.9).

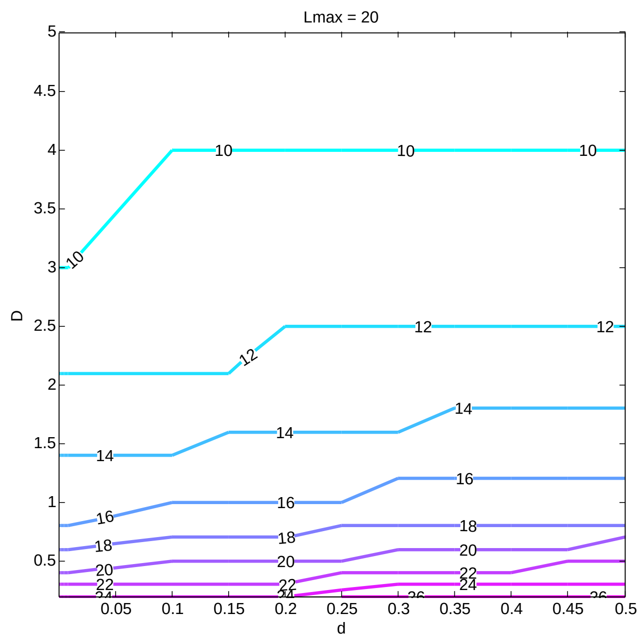


Figure 6.9: $\tilde{L}_{max}(d, D)$.

Figure 6.9 shows that the truncation order $\tilde{L}_{max}$ for computing the velocity correction mainly depends on $D$. This truncation order can be used to estimate the other truncation order $L_{max}$ in the next section.

Here we perform the tests with $D$ varify from 0.1 to 5. We can choose

$$\tilde{L}_{max}(D) = \begin{cases} 10 & \text{for } D \geq 3, \\ 12 & \text{for } 2 \leq D < 3, \\ 14 & \text{for } 1.5 \leq D < 2, \\ 16 & \text{for } 0.7 \leq D < 1.5, \\ 18 & \text{for } 0.6 \leq D < 0.7, \\ 22 & \text{for } 0.3 \leq D < 0.6, \\ 24 & \text{for } 0.1 \leq D < 0.3. \end{cases}$$

### 6.4.2 Truncation order for solving the problem

We now consider the same three-sphere configuration as in the previous section. For computational time problem, we could not calculate $\mathbf{f}^{dis.}\left(d, D, L, \tilde{L}_{max}\right)$ for very large values of $L$. The error on the surface force density is estimated by the difference between two consecutive values of $L$ with $\tilde{L}_{max}$ determined in the previous section. For every $L \geq 1$, we define

$$Err\,(d, D, L) \;:=\; \left|\mathbf{f}^{dis.}\left(d, D, L, \tilde{L}_{max}(D)\right) - \mathbf{f}^{dis.}\left(d, D, L-1, \tilde{L}_{max}(D)\right)\right|, \qquad (6.4.1)$$

The truncation order $L_{max}$ is chosen as follows, for a given small real number $\varepsilon > 0$,

$$L_{max}(d, D) \;:=\; \min\left\{L \in [1, \infty) : \quad Err\,(d, D, L) < \varepsilon\right\}.$$

In fact, the truncation order $L_{max}$ can be also estimated with another definition of the density error,

$$\widetilde{Err}\,(d, D, L) \;=\; \left|\mathbf{f}^{dis.}\left(d, D, L, \tilde{L}_{\infty}\right) - \mathbf{f}^{dis.}\left(d, D, L-1, \tilde{L}_{\infty}\right)\right|,$$

where $\tilde{L}_{\infty}$ is very large. The two errors are very close in the numerical computation. Hence, it is more convenient to use the first definition (6.4.1).

We also choose $\varepsilon = 10^{-6}$ and the cut-off distance $\delta = 2$. We consider two cases: $D > \delta$ and $D < \delta$.

- The first case: $D = D_0 > \delta$,

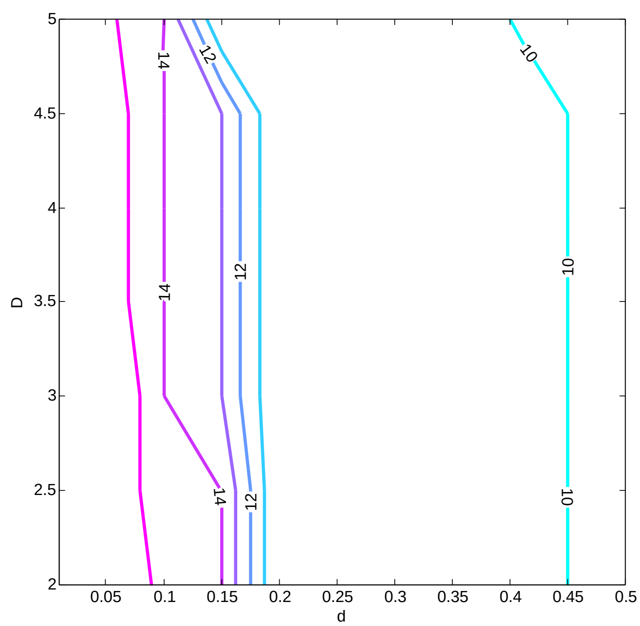


Figure 6.10: $L_{max}(d, D)$ for $D \geq \delta = 2$.

In this case, the truncation order mainly depends on the distance $d$. We conclude that for isolated pairs of particles $D \geq \delta$, we see that the critical truncation level is a monotonic increasing function of $d$.

We can choose

$$L_{max}(d) = \begin{cases} 10 & \text{for } d \geq 0.5, \\ 11 & \text{for } 0.2 \leq d < 0.5, \\ 12 & \text{for } 0.18 \leq d < 0.2, \\ 13 & \text{for } 0.15 \leq d < 0.18, \\ 14 & \text{for } 0.1 \leq d < 0.15, \\ 15 & \text{for } 0.01 \leq d < 0.1. \end{cases}$$

We made these tests with $d$ varying from 0.01 to 0.5. Even for $d = 0.01$, the truncation order $L_{max} = 15$ lead to an error smaller than $\varepsilon = 10^{-6}$ (see Figure 6.10).

- The second case: $D = D_0 < \delta$,

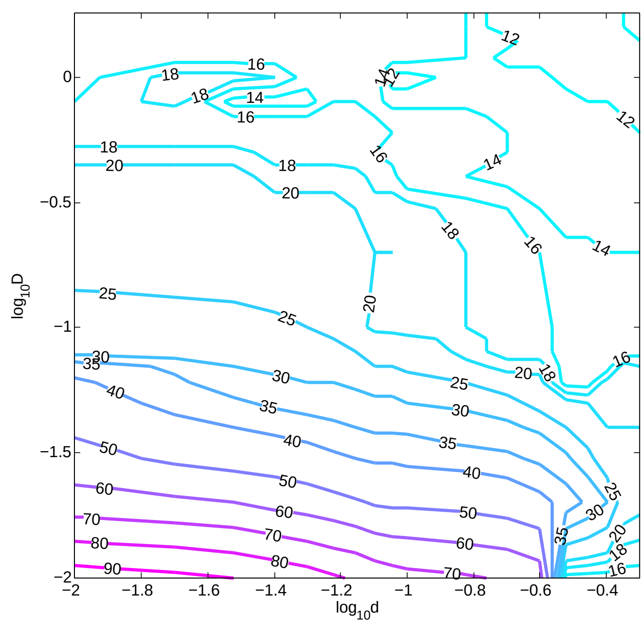


Figure 6.11: $L_{max}(d, D)$ for $D \leq \delta = 2$.

In this case, the optimal truncation order depends on both $d$ and $D$. This truncation order tends to infinity as both $d$ and $D$ go to 0.

In practice, we see on the graphic that we can choose $L_{max}$ as an affine function of $log_{10}D$ and $log_{10}d$ in the region of $[L_{max,opt} \geq 40]$ (see Figure 6.11).

## 6.5 Conclusions and perpectives

In conclusion, we have proposed an accurate method for the computations of hydrodynamic forces between spherical particles suspended in a Stokes fuild. The main improvement of this new method compared with the Stokesian Dynamics is that the influence of the singular force densities between two closed particles on the neighboring particles is also computed. For this reason, the computational cost for this method is larger. The main part of the computational time is due to the computation of the correction velocities and their projection on the vectorial spherical harmonics basis. On the other hand, these computations are independent from one sphere to another and could be easily parallelized. This should solve the main drawback of the method.

In this thesis, we only consider spherical particles. The main advantage of this shape is that the computation can be based on the vectorial spherical harmonics basis. The methods generalize to arbitrary smooth particles. In this case, we should use a boundary finite element method instead of the decomposition in vectorial spherical harmonics.

Our method is just built for some very special domains for which the minimal fictitious sphere enclosing two neighboring particles does not intersect any other particle. We have not yet a definite method for treating the general case.

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# List of Figures