

**Thesis proposal 2026**

*« Investigation of the magnetic properties of interacting nanoparticles : development of a new modeling approach by Monte Carlo simulations and application to cobalt and iron oxide nanoparticles »*

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**Abstract**

This project focuses on developing a new approach to modeling, using Monte Carlo simulations, the magnetic properties (magnetization, susceptibility, heat capacity ...) of ferromagnetic (FM) nanoparticle (NP) assemblies. FM NP assemblies have applications, particularly in the fields of magnetic resonance imaging, magnetic hyperthermia, and ultra-high-density magnetic recording. This topic is therefore of interest, both in terms of fundamental research and its applications. A FM NP consists of tens of thousands of magnetic atoms (for example, cobalt). The magnetization of a NP depends on its intrinsic properties, which include its surface anisotropy, size, and shape. An assembly of NPs is a collection of NPs placed regularly or randomly within a certain volume. In an assembly of NPs, the magnetizations of the individual NPs interact with each other through dipole-dipole interactions (DDI). The magnetization of the assembly (equal to the sum of the magnetizations of the NPs) therefore depends on the intrinsic properties of each NP and the DDI. Modeling assemblies of NPs must therefore take account of the intrinsic properties and the DDI, which would require considering on the order of 100 million interacting atoms. This would lead to prohibitively long computation times given the capabilities of current supercomputers. Therefore, we propose a new modeling approach that takes account of intrinsic properties and DDI while maintaining

acceptable computation times. The aim of this modeling is to better understand the competition between the effects of intrinsic properties of NP and DDI on the magnetization of different types of NP assemblies. Our results will be compared with experimental results to optimize and control the magnetic properties of the assemblies for various applications.

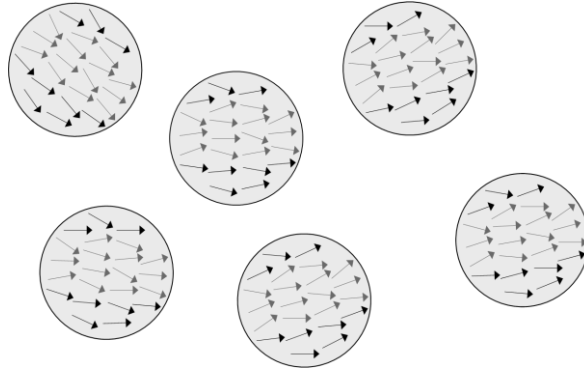


Figure : NP assembly each containing at least  $10^3$  atoms. Each arrow represents an atomic magnetic moment which interacts with all the others.

### **Goal of the thesis**

The goals of this thesis are :

- to develop a Monte Carlo simulation code based on a new modeling approach at the atomic scale capable to take into account intrinsic properties (size, shape and surface anisotropy) of each NP and long range DDI between NP regardless of their intensity ;
- to test and valid the approach ;
- to optimize the code ;
- to model the magnetic properties of realistic assemblies of cobalt and iron oxide NP and to compare with experimental results for the purpose of applications.

Keywords : nanoparticles, ferromagnetic, magnetization, Monte Carlo simulation, surface anisotropy, dipolar interactions.

Skills required : the candidate should have good skills in magnetism in solids and should be attracted to numerical simulations and programming.

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