Supplementary: On the Accurate Large-scale Simulation of Ferrofluids

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S1 SINGLE PARTICLE MAGNETIC FIELD

In this section, we provide the detailed derivation of the magnetic field $\boldsymbol{H}$ generated by a particle with a spherically symmetric distribution W:

$$\begin{aligned} \boldsymbol{M}(\boldsymbol{r}) &= \boldsymbol{m}W(\boldsymbol{r}) = \boldsymbol{m}W(|\boldsymbol{r}|)\,, \\ \nabla\cdot\boldsymbol{H} &= -\nabla\cdot\boldsymbol{M}\,, \\ \nabla\times\boldsymbol{H} &= 0\,, \\ \boldsymbol{H}|_\infty &= 0\,. \end{aligned}$$

Since $\boldsymbol{H}$ is curl-free, it can be represented by a negative gradient of a potential field ϕ:

$$\boldsymbol{H}(\boldsymbol{r}) = -\nabla\phi(\boldsymbol{r})\,.$$

We substitute the gradient representation into the divergence equation and obtain

$$\begin{aligned} \Delta\phi &= \nabla\cdot\boldsymbol{M}\,, \qquad \text{(S1)} \\ \phi|_\infty &= 0\,. \end{aligned}$$

In order to solve this problem, we borrow ideas from electrostatics since Eq. (S1) resembles the Poisson's equation for an electric potential with dipole sources. We first need to realize that the dipole is simply a superposition of positive and negative charges. Let $\boldsymbol{m} = q\,\boldsymbol{l}$ be constant, where q is the amount of charge, and $\boldsymbol{l}$ is the separation of two charges. The larger the distance, the less charges they have. Let there be a positive charge distribution $q_1(\boldsymbol{r})$ centered at $\boldsymbol{l}$, and a negative charge distribution $q_2(\boldsymbol{r})$ centered at the origin:

$$\begin{aligned} q_+(\boldsymbol{r}) &= qW(|\boldsymbol{r}-\boldsymbol{l}|)\,, \\ q_-(\boldsymbol{r}) &= -qW(|\boldsymbol{r}|)\,. \end{aligned}$$

In electrostatics, the potential formed by a point charge distribution $p\delta(\boldsymbol{r})$ at the origin satisfies the following Poisson's equation:

$$\begin{aligned} \Delta\varphi &= -\frac{p}{\varepsilon_0}\delta(\boldsymbol{r})\,, \\ \boldsymbol{E} &= -\nabla\varphi\,, \end{aligned}$$

where ε_0 is the vacuum permittivity constant. We investigate the total potential ϕ_t formed by two opposite charges by changing the point charge distribution to our charge distribution:

$$\begin{aligned} \Delta\phi_+ &= -q_+(\boldsymbol{r}) = -qW(|\boldsymbol{r}-\boldsymbol{l}|)\,, \\ \Delta\phi_- &= -q_-(\boldsymbol{r}) = qW(|\boldsymbol{r}|)\,, \\ \phi_t &= \phi_+ + \phi_-\,, \\ \Delta\phi_t &= -q(W(|\boldsymbol{r}-\boldsymbol{l}| - W(|\boldsymbol{r}|))) \\ &= ql\frac{W(|\boldsymbol{r}|) - W(|\boldsymbol{r}-\boldsymbol{l}|)}{l}\,, \\ \phi_t &= 0 \text{ at infinity}\,. \end{aligned}$$

When the center of the positive charge shrinks to the origin, using $\boldsymbol{m} = q\boldsymbol{l}$ the total potential becomes the dipole potential:

$$\begin{aligned} \lim_{l\to 0}\Delta\phi_t &= \lim_{l\to 0} ql\frac{W(|\boldsymbol{r}|) - W(|\boldsymbol{r}-\boldsymbol{l}|)}{l} \\ &= \boldsymbol{m}\cdot\nabla W(\boldsymbol{r}) \\ &= \nabla\cdot\boldsymbol{m}W \\ &= \nabla\cdot\boldsymbol{M}(\boldsymbol{r}) \\ &= \Delta\phi\,. \end{aligned}$$

Therefore we observe that a dipole's equation and two opposite charges' equation have the same right hand side. In addition, they have the same vanishing boundary condition, so they have the same solution due to the uniqueness of solutions.

We ultimately need to find the negative gradient of the potential:

$$\begin{aligned} \boldsymbol{H}_+ &= -\nabla\phi_+\,, \\ \boldsymbol{H}_- &= -\nabla\phi_-\,. \end{aligned}$$

For an electric point charge $p\delta(\boldsymbol{r})$, the solution to the electrostatics equation is

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{\boldsymbol{r}}{4\pi\varepsilon_0|\boldsymbol{r}|^3}p\,.$$

The field generated by charges with spherically symmetric distributions has a closed-form solution. It is equivalent to the field generated by a point charge at the center of the distribution with the equivalent charge being the sum of all charges within the radius of $r = |\boldsymbol{r}|$:

$$\begin{aligned} \boldsymbol{H}_-(\boldsymbol{r}) &= \frac{-\boldsymbol{r}\,\frac{m}{l}}{4\pi|\boldsymbol{r}|^3}\int_{|\boldsymbol{r}'|<|\boldsymbol{r}|} W(|\boldsymbol{r}'|)\,\mathrm{d}\boldsymbol{r}' \\ &= \frac{-\boldsymbol{r}\,\frac{m}{l}}{4\pi|\boldsymbol{r}|^3}\int_0^{|\boldsymbol{r}|}\xi^2 W(\xi)\,\mathrm{d}\xi\int_0^{2\pi}\int_0^{\pi}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi \\ &= \frac{-\boldsymbol{r}\,\frac{m}{l}}{|\boldsymbol{r}|^3}\int_0^{|\boldsymbol{r}|}\xi^2 W(\xi)\,\mathrm{d}\xi\,, \\ \boldsymbol{H}_+(\boldsymbol{r}) &= \frac{(\boldsymbol{r}-\boldsymbol{l})\frac{m}{l}}{4\pi|\boldsymbol{r}-\boldsymbol{l}|^3}\int_{|\boldsymbol{r}'-\boldsymbol{l}|<|\boldsymbol{r}-\boldsymbol{l}|} W(|\boldsymbol{r}'-\boldsymbol{l}|)\,\mathrm{d}\boldsymbol{r}' \\ &= \frac{(\boldsymbol{r}-\boldsymbol{l})\frac{m}{l}}{|\boldsymbol{r}-\boldsymbol{l}|^3}\int_0^{|\boldsymbol{r}-\boldsymbol{l}|}\xi^2 W(\xi)\,\mathrm{d}\xi\,, \end{aligned}$$

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$$
\begin{aligned}
\boldsymbol{H}(\boldsymbol{r}) &= \lim_{l\to 0} \boldsymbol{H}_+(\boldsymbol{r}) + \boldsymbol{H}_-(\boldsymbol{r}) \\
&= \lim_{l\to 0} \frac{(\boldsymbol{r}-\boldsymbol{l})\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}-\boldsymbol{l}|^3} \int_0^{|\boldsymbol{r}-\boldsymbol{l}|} \xi^2 W(\xi)\,\mathrm{d}\xi \\
&\quad -\frac{\boldsymbol{r}\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}|^3} \int_0^{|\boldsymbol{r}|} \xi^2 W(\xi)\,\mathrm{d}\xi \\
&= \lim_{l\to 0} \frac{\boldsymbol{r}\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}-\boldsymbol{l}|^3} \int_0^{|\boldsymbol{r}-\boldsymbol{l}|} \xi^2 W(\xi)\,\mathrm{d}\xi \\
&\quad -\frac{\boldsymbol{r}\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}|^3} \int_0^{|\boldsymbol{r}|} \xi^2 W(\xi)\,\mathrm{d}\xi \\
&\quad -\frac{\boldsymbol{l}\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}-\boldsymbol{l}|^3} \int_0^{|\boldsymbol{r}-\boldsymbol{l}|} \xi^2 W(\xi)\,\mathrm{d}\xi\,. \qquad \text{(S2)}
\end{aligned}
$$

The last term has a trivial limit:

$$
\lim_{l\to 0} \frac{\boldsymbol{l}\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}-\boldsymbol{l}|^3} \int_0^{|\boldsymbol{r}-\boldsymbol{l}|} \xi^2 W(\xi)\,\mathrm{d}\xi = \frac{\boldsymbol{m}}{|\boldsymbol{r}|^3} \int_0^{|\boldsymbol{r}|} \xi^2 W(\xi)\,\mathrm{d}\xi\,.
$$

We consider the first two terms on the right-hand side of Eq. (S2):

$$
\begin{aligned}
&\lim_{l\to 0} \frac{\boldsymbol{r}\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}-\boldsymbol{l}|^3} \int_0^{|\boldsymbol{r}-\boldsymbol{l}|} \xi^2 W(\xi)\,\mathrm{d}\xi \\
&\quad -\frac{\boldsymbol{r}\frac{\boldsymbol{m}}{l}}{|\boldsymbol{r}|^3} \int_0^{|\boldsymbol{r}|} \xi^2 W(\xi)\,\mathrm{d}\xi \\
&= \boldsymbol{m}\boldsymbol{r} \lim_{l\to 0} \frac{1}{l} \left(\frac{\int_0^{|\boldsymbol{r}-\boldsymbol{l}|} \xi^2 W(\xi)\,\mathrm{d}\xi}{|\boldsymbol{r}-\boldsymbol{l}|^3} - \frac{\int_0^{|\boldsymbol{r}|} \xi^2 W(\xi)\,\mathrm{d}\xi}{|\boldsymbol{r}|^3} \right). \qquad \text{(S3)}
\end{aligned}
$$

Let us set up

$$
\begin{aligned}
f(\eta) &= \frac{\int_0^{\eta} \xi^2 W(\xi)\,\mathrm{d}\xi}{\eta^3}\,, \\
\eta &= |\boldsymbol{r}-\boldsymbol{l}|\,.
\end{aligned}
$$

The limit in Eq. (S3) is actually given by the derivative $\frac{\mathrm{d}f}{\mathrm{d}\eta}\frac{\mathrm{d}\eta}{\mathrm{d}l}$ when $l = 0$:

$$
\begin{aligned}
\frac{\mathrm{d}f}{\mathrm{d}\eta} &= -3\frac{\int_0^{\eta} \xi^2 W(\xi)\,\mathrm{d}\xi}{\eta^4} + \frac{\eta^2 W(\eta)}{\eta^3}\,, \\
\frac{\mathrm{d}\eta}{\mathrm{d}l} &= \frac{\mathrm{d}|\boldsymbol{r}-\boldsymbol{l}|}{\mathrm{d}l} \\
&= \frac{\mathrm{d}(r^2 - 2rl\cos\theta + l^2)^{1/2}}{\mathrm{d}l}\Big|_{l=0} \\
&= -r\cos(\theta)/r \\
&= -\cos\theta \\
&= -\frac{\boldsymbol{r}\cdot\boldsymbol{l}}{rl}\,,
\end{aligned}
$$

$$
\frac{\mathrm{d}f}{\mathrm{d}\eta}\frac{\mathrm{d}\eta}{\mathrm{d}l} = \left(\frac{\boldsymbol{r}}{r}\cdot\frac{\boldsymbol{l}}{l}\right)\left(3\frac{\int_0^{r} \xi^2 W(\xi)\,\mathrm{d}\xi}{r^4} - \frac{W(r)}{r}\right).
$$

Note that although l reduces to zero, its direction (which is also the dipole's direction) is kept. By combining all the results above, we obtain the total dipole field:

$$
\begin{aligned}
\boldsymbol{H}_t &= \lim_{l\to 0} \boldsymbol{H}_+(\boldsymbol{r}) + \boldsymbol{H}_-(\boldsymbol{r}) \\
&= \boldsymbol{r}m\left(\frac{\boldsymbol{r}}{r}\cdot\frac{\boldsymbol{l}}{l}\right)\left(3\frac{\int_0^{r} \xi^2 W(\xi)\,\mathrm{d}\xi}{r^4} - \frac{W(r)}{r}\right) \\
&\quad -\frac{\boldsymbol{m}}{|\boldsymbol{r}|^3} \int_0^{x} \xi^2 W(\xi)\,\mathrm{d}\xi\,.
\end{aligned}
$$

We set $\hat{\boldsymbol{r}} := \boldsymbol{r}/|\boldsymbol{r}|$. The previous equation can be further simplified:

$$
\begin{aligned}
\boldsymbol{H} &= \frac{\boldsymbol{r}}{r}m\left(\frac{\boldsymbol{r}}{r}\cdot\frac{\boldsymbol{l}}{l}\right)\left(3\frac{\int_0^{r} \xi^2 W(\xi)\,\mathrm{d}\xi}{r^3} - W(r)\right) \\
&\quad -\frac{\boldsymbol{m}}{|\boldsymbol{r}|^3} \int_0^{r} \xi^2 W(\xi)\mathrm{d}\xi \\
&= \hat{\boldsymbol{r}}(\hat{\boldsymbol{r}}\cdot\boldsymbol{m})\left(3\frac{\int_0^{r} \xi^2 W(\xi)\,\mathrm{d}\xi}{r^3} - W(r)\right) \\
&\quad -\frac{\boldsymbol{m}}{|\boldsymbol{r}|^3} \int_0^{r} \xi^2 W(\xi)\,\mathrm{d}\xi \\
&= \hat{\boldsymbol{r}}(\hat{\boldsymbol{r}}\cdot\boldsymbol{m})(W_{\mathrm{avr}}(r) - W(r)) \\
&\quad -W_{\mathrm{avr}}(r)\frac{\boldsymbol{m}}{3}\,, \qquad \text{(S4)}
\end{aligned}
$$

where we introduce an intermediate variable

$$
\begin{aligned}
W_{\mathrm{avr}}(r) &= \frac{\int_0^{2\pi}\int_0^{\pi} \sin\theta \int_0^{r} \xi^2 W(\xi)\,\mathrm{d}\xi\,\mathrm{d}\theta\,\mathrm{d}\phi}{\frac{4\pi}{3}r^3} \\
&= \frac{3\int_0^{r} \xi^2 W(\xi)\,\mathrm{d}\xi}{r^3}\,.
\end{aligned}
$$

The quantity $W_{\mathrm{avr}}(r)$ can be considered as the average of the density function $W(r)$ within the radius of r. It is well defined for $r = 0$. Therefore, $\boldsymbol{H}(\boldsymbol{r})$ has no singularity and is well defined even for $\boldsymbol{r} = \boldsymbol{0}$ unless $W(0)$ is singular. This formula is valid for all spherically symmetric density functions $W(|\boldsymbol{r}|)$.

Eq. (S4) is the field generated by a dipole particle with spherically symmetric density distribution.

S2 FAST MULTIPOLE METHOD DETAILS

The theory of the fast multipole method is well covered in academic literature [Beatson and Greengard 1997]. Hence, we focus on some modifications in this section. The source-to-multipole transfer is explained in the main article. Here, we present the cumbersome formula for the force gradient in the far-field.

The fast multipole program evaluates the potential Φ at $\boldsymbol{P}$ using

$$
\begin{aligned}
\Phi(P) &= \sum_{j=0}^{\infty}\sum_{k=-j}^{j} L_j^k \cdot Y_j^k(\theta,\phi)\cdot r^j\,, \\
Y_n^m(\theta,\phi) &= \sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\cdot P_n^{|m|}(\cos\theta)e^{im\phi}\,,
\end{aligned}
$$

where L_j^k are the local expansion coefficients, and (r,θ,ϕ) represents the spherical coordinates of $\boldsymbol{P}$ with the origin being the center of the local expansion, Y_n^m is the spheric harmonics, P_n^m is the associated Legendre polynomial.

This expression results in a scalar field in the neighborhood of the local expansion center. In order to evaluate the force, we need the negative gradient $\boldsymbol{H} = -\nabla\Phi$ and the negative Hessian $\nabla\boldsymbol{H} = -\nabla\nabla\Phi$.

Since the potential field is represented in spherical coordinates, there is additional work to do in order to convert it into its Cartesian representation:

$$\begin{aligned}
\frac{\partial}{\partial x} &= \cos\phi\sin\theta\frac{\partial}{\partial r} + \frac{\cos\phi\cos\theta}{r}\frac{\partial}{\partial\theta} \\
&\quad -\frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}, \\
\frac{\partial}{\partial y} &= \sin\phi\sin\theta\frac{\partial}{\partial r} + \frac{\sin\phi\cos\theta}{r}\frac{\partial}{\partial\theta} \\
&\quad +\frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}, \\
\frac{\partial}{\partial z} &= \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}, \\
\boldsymbol{H}(P) &= -\nabla\Phi(P), \\
-H_x(P) &= \frac{\partial\Phi(P)}{\partial x} \\
&= \cos\phi\sin\theta\frac{\partial\Phi(P)}{\partial r} + \frac{\cos\phi\cos\theta}{r}\frac{\partial\Phi(P)}{\partial\theta} \\
&\quad -\frac{\sin\phi}{r\sin\theta}\frac{\partial\Phi(P)}{\partial\phi}, \\
-H_{x,r} &= \cos\phi\sin\theta\frac{\partial^2\Phi(P)}{\partial r^2} + \frac{\cos\phi\cos\theta}{r}\frac{\partial^2\Phi(P)}{\partial r\partial\theta} \\
&\quad -\frac{\cos\phi\cos\theta}{r^2}\frac{\partial\Phi(P)}{\partial\theta} + \frac{\sin\phi}{r^2\sin\theta}\frac{\partial\Phi(P)}{\partial\phi} \\
&\quad -\frac{\sin\phi}{r\sin\theta}\frac{\partial^2\Phi(P)}{\partial r\partial\phi}, \\
-H_{x,\theta} &= \cos\phi\cos\theta\frac{\partial\Phi(P)}{\partial r} + \cos\phi\sin\theta\frac{\partial^2\Phi(P)}{\partial\theta\partial r} \\
&\quad +\frac{-\cos\phi\sin\theta}{r}\frac{\partial\Phi(P)}{\partial\theta} + \frac{\cos\phi\cos\theta}{r}\frac{\partial^2\Phi(P)}{\partial\theta^2} \\
&\quad \frac{\cos\theta\sin\phi}{r\sin^2\theta}\frac{\partial\Phi(P)}{\partial\phi} - \frac{\sin\phi}{r\sin\theta}\frac{\partial^2\Phi(P)}{\partial\theta\partial\phi}, \\
-H_{x,\phi} &= -\sin\phi\sin\theta\frac{\partial\Phi(P)}{\partial r} + \cos\phi\sin\theta\frac{\partial^2\Phi(P)}{\partial\phi\partial r} \\
&\quad +\frac{-\sin\phi\cos\theta}{r}\frac{\partial\Phi(P)}{\partial\theta} + \frac{\cos\phi\cos\theta}{r}\frac{\partial^2\Phi(P)}{\partial\phi\partial\theta} \\
&\quad -\frac{\cos\phi}{r\sin\theta}\frac{\partial\Phi(P)}{\partial\phi} - \frac{\sin\phi}{r\sin\theta}\frac{\partial^2\Phi(P)}{\partial\phi^2}, \\
-H_y(P) &= \frac{\partial\Phi(P)}{\partial y} \\
&= \sin\phi\sin\theta\frac{\partial\Phi(P)}{\partial r} + \frac{\sin\phi\cos\theta}{r}\frac{\partial\Phi(P)}{\partial\theta} \\
&\quad +\frac{\cos\phi}{r\sin\theta}\frac{\partial\Phi(P)}{\partial\phi}, \\
-H_{y,r} &= \sin\phi\sin\theta\frac{\partial^2\Phi(P)}{\partial r^2} - \frac{\sin\phi\cos\theta}{r^2}\frac{\partial\Phi(P)}{\partial\theta} \\
&\quad +\frac{\sin\phi\cos\theta}{r}\frac{\partial^2\Phi(P)}{\partial r\partial\theta} - \frac{\cos\phi}{r^2\sin\theta}\frac{\partial\Phi(P)}{\partial\phi} \\
&\quad +\frac{\cos\phi}{r\sin\theta}\frac{\partial^2\Phi(P)}{\partial r\partial\phi}, \\
-H_{y,\theta} &= \sin\phi\cos\theta\frac{\partial\Phi(P)}{\partial r} + \sin\phi\sin\theta\frac{\partial^2\Phi(P)}{\partial\theta\partial r} \\
&\quad +\frac{-\sin\phi\sin\theta}{r}\frac{\partial\Phi(P)}{\partial\theta} + \frac{\sin\phi\cos\theta}{r}\frac{\partial^2\Phi(P)}{\partial\theta^2} \\
&\quad -\frac{\cos\theta\cos\phi}{r\sin^2\theta}\frac{\partial\Phi(P)}{\partial\phi} + \frac{\cos\phi}{r\sin\theta}\frac{\partial^2\Phi(P)}{\partial\theta\partial\phi}, \\
-H_{y,\phi} &= \cos\phi\sin\theta\frac{\partial\Phi(P)}{\partial r} + \sin\phi\sin\theta\frac{\partial^2\Phi(P)}{\partial\phi\partial r} \\
&\quad +\frac{\cos\phi\cos\theta}{r}\frac{\partial\Phi(P)}{\partial\theta} + \frac{\sin\phi\cos\theta}{r}\frac{\partial^2\Phi(P)}{\partial\phi\partial\theta} \\
&\quad +\frac{-\sin\phi}{r\sin\theta}\frac{\partial\Phi(P)}{\partial\phi} + \frac{\cos\phi}{r\sin\theta}\frac{\partial^2\Phi(P)}{\partial\phi^2}, \\
-H_z(P) &= \frac{\partial\Phi(P)}{\partial z} = \cos\theta\frac{\partial\Phi(P)}{\partial r} - \frac{\sin\theta}{r}\frac{\partial\Phi(P)}{\partial\theta}, \\
-H_{z,r} &= \cos\theta\frac{\partial^2\Phi(P)}{\partial r^2} + \frac{\sin\theta}{r^2}\frac{\partial\Phi(P)}{\partial\theta} \\
&\quad -\frac{\sin\theta}{r}\frac{\partial^2\Phi(P)}{\partial r\partial\theta}, \\
-H_{z,\theta} &= -\sin\theta\frac{\partial\Phi(P)}{\partial r} + \cos\theta\frac{\partial^2\Phi(P)}{\partial\theta\partial r} \\
&\quad -\frac{\cos\theta}{r}\frac{\partial\Phi(P)}{\partial\theta} - \frac{\sin\theta}{r}\frac{\partial^2\Phi(P)}{\partial\theta^2}, \\
-H_{z,\phi} &= \cos\theta\frac{\partial^2\Phi(P)}{\partial\phi\partial r} - \frac{\sin\theta}{r}\frac{\partial^2\Phi(P)}{\partial\phi\partial\theta}.
\end{aligned}$$

When evaluating Eq. (S5), a crucial step is to evaluate the associated Legendre polynomial function value. Although the analytical formulas for every degree n and order m are known, it is more efficient to deduce the value for different degree n and order m but keep the same variables θ and ϕ using its recurrence formulas. The (first and second) derivatives of the Legendre polynomials $P_n^m(\cos(\theta))$ are also obtained using recurrence formulas. After the function values of the Legendre polynomials and their derivatives are calculated, they are multiplied with the expansion coefficients L_j^k and summed up to get the potential, the gradient (using the first order derivative), and the Hessian (using the second order derivatives).

All the derivatives in spherical coordinates need to be converted into Cartesian coordinates using the formula provided in the first set of equations. The evaluation of $\Phi_{\theta\theta}$ requires the second order derivative of the Legendre polynomial. Its recurrence formulas are

$$\begin{aligned}
\frac{d^2P_n^0}{d\theta^2} &= \frac{\mathrm{d}\mathrm{P}_n^1(x)}{d\theta}, \\
\frac{d^2P_n^m(\cos\theta)}{d\theta^2} &= \frac{-1}{2}\Bigg((n+m)(n-m+1)\frac{\mathrm{d}\mathrm{P}_n^{m-1}(x)}{d\theta} \\
&\qquad -\frac{\mathrm{d}\mathrm{P}_n^{m+1}(x)}{d\theta}\Bigg), \\
\frac{d^2P_n^n}{d\theta^2} &= -n\frac{dP_n^{n-1}}{d\theta},
\end{aligned}$$

in which $x = \cos\theta$; see Bösch [2000].

The three formulas above are direct results of

$$\sqrt{1-x^2}\,\frac{d}{dx}P_\ell^m(x) = \frac{1}{2}\left((\ell+m)(\ell-m+1)P_\ell^{m-1}(x) - P_\ell^{m+1}(x)\right) .$$

The first order derivative is obtained by

$$(x^2-1)\frac{d}{dx}P_\ell^m(x) = \ell x P_\ell^m(x) - (\ell+m)P_{\ell-1}^m(x) .$$

S3 FITTED FORCE DETAILS

In this section, we provide further details with respect to our force model described in Section 3.2 of our main article.The total force $\boldsymbol{f}_{s\to t}$ from the source (s) to the target (t) is given by

$$\boldsymbol{f}_{s\to t} = \mu_0 \boldsymbol{m}_t \cdot \int W(\boldsymbol{r}-\boldsymbol{r}_t, h)\nabla \boldsymbol{H}(\boldsymbol{r}-\boldsymbol{r}_s, \boldsymbol{m}_s)\,\mathrm{d}\boldsymbol{r} , \qquad \text{(S5)}$$

where the integration only covers regions in which $W(\boldsymbol{r}-\boldsymbol{r}_t, h) \neq 0$. The source and target center locations are given by $\boldsymbol{r}_s$ and $\boldsymbol{r}_t$, and $\boldsymbol{m}_s$ and $\boldsymbol{m}_t$ denote the total magnetic moments of the source and target particle respectively.

For $|\boldsymbol{r}_t-\boldsymbol{r}_s| > 4h$, Eq. (S5) has a closed-form solution as explained in the main article. For $|\boldsymbol{r}_t-\boldsymbol{r}_s| \leq 4h$, $\boldsymbol{H}_s$ is not always harmonic, so that we employ numerical integration. However, the numerical integration is expensive. Our motivation is to treat the integration as a black-box system, and find an economic way to parameterize this black-box system. The integral Eq. (S5) is equivalent to a black-box function $\boldsymbol{F}_0$:

$$\boldsymbol{f}_{s\to t} = \boldsymbol{F}_0(\boldsymbol{r}_t-\boldsymbol{r}_s, h, \boldsymbol{m}_t, \boldsymbol{m}_s) .$$

In the following steps, we tear down the multi-variable function $\boldsymbol{F}_0$ to a single-variable function which we can measure and fit.

In the first step, the black-box $\boldsymbol{F}_0$ depends not only on the distance between two particles, but also on the direction. We can remove the directional dependency by choosing a proper coordinate system to calculate the integral in Eq. (S5).

We set the origin at the center of the source particle. Let $\hat{\xi}, \hat{\eta}, \hat{\zeta}$ be the unit vectors of the axes and the target particle is on the ζ axis. Let $\boldsymbol{R}$ be the rotation matrix. A possible choice is given by

$$\text{if}(|\boldsymbol{r}_t-\boldsymbol{r}_s| > \varepsilon): \ \hat{\zeta} = \frac{\boldsymbol{r}_t-\boldsymbol{r}_s}{|\boldsymbol{r}_t-\boldsymbol{r}_s|}, \quad \text{else}: \ \hat{\zeta} = \hat{\boldsymbol{z}},$$

$$\text{if}(|\hat{\zeta}\times\hat{\boldsymbol{z}}| > \varepsilon): \ \hat{\eta} = \frac{\hat{\zeta}\times\hat{\boldsymbol{z}}}{|\hat{\zeta}\times\hat{\boldsymbol{z}}|}, \quad \text{else}: \ \hat{\eta} = \hat{\boldsymbol{y}},$$

$$\hat{\xi} = \hat{\eta}\times\hat{\zeta}, \quad \boldsymbol{R} = (\hat{\xi}, \hat{\eta}, \hat{\zeta}),$$

where $\hat{\boldsymbol{z}}$ and $\hat{\boldsymbol{y}}$ are the unit vectors of $\boldsymbol{z}$ and $\boldsymbol{y}$ axis respectively, and ε is a small number to ensure numerical stability. We call this the local coordinates. A vector in the world coordinate $\boldsymbol{m}$ is connected to its local coordinate counterpart $\tilde{\boldsymbol{m}}$ by $\boldsymbol{m} = \boldsymbol{R}\tilde{\boldsymbol{m}}$ and $\tilde{\boldsymbol{m}} = \boldsymbol{R}^\mathsf{T}\boldsymbol{m}$. A tilde indicates that it is the local coordinate vector. In this coordinate system, the same physical law from Eq. (S5) holds:

$$\tilde{\boldsymbol{f}}_{s\to t} = \mu_0 \tilde{\boldsymbol{m}}_t \cdot \int W(\tilde{\boldsymbol{r}} - (0,0,|\boldsymbol{r}_t-\boldsymbol{r}_s|)^\mathsf{T}, h)\nabla \boldsymbol{H}(\tilde{\boldsymbol{r}}, \tilde{\boldsymbol{m}}_s)\,\mathrm{d}\tilde{\boldsymbol{r}} . \qquad \text{(S6)}$$

The above integration can be written as

$$\tilde{\boldsymbol{f}}_{s\to t} = \boldsymbol{F}_1(|\boldsymbol{r}_t-\boldsymbol{r}_s|, h, \tilde{\boldsymbol{m}}_s, \tilde{\boldsymbol{m}}_t),$$

where the function $\boldsymbol{F}_1$ depends only on the distance.

In the second step, the dependency on $\tilde{\boldsymbol{m}}_s, \tilde{\boldsymbol{m}}_t$ from $\boldsymbol{F}_1$ is removed. $\boldsymbol{F}_1$ is a function of both source and target moments $\tilde{\boldsymbol{m}}_s, \tilde{\boldsymbol{m}}_t$. Fortunately, the force $\tilde{\boldsymbol{f}}_{s\to t}$ is linear in the target moment $\tilde{\boldsymbol{m}}_t$, meanwhile, $\tilde{\boldsymbol{f}}_{s\to t}$ is linear in the gradient of magnetic field $\nabla \boldsymbol{H}(\tilde{\boldsymbol{r}}, \tilde{\boldsymbol{m}}_s)$, which is further linear in the source moment $\tilde{\boldsymbol{m}}_s$. Therefore, the force is bilinear in both moments, and Eq. (S6) states a mapping: $\mathbb{R}^3\times\mathbb{R}^3 \mapsto \mathbb{R}^3$. This relationship can be described by a third-order tensor with 27 entries. $\tilde{\Lambda}$ denotes this tensor in the local coordinate system.

$\boldsymbol{F}_1(|\boldsymbol{r}_t-\boldsymbol{r}_s|, h, \tilde{\boldsymbol{m}}_s, \tilde{\boldsymbol{m}}_t)$ is then reduced to a tensor $\tilde{\Lambda}(|\boldsymbol{r}_t-\boldsymbol{r}_s|, h)$:

$$\tilde{f}_{s\to t}^\alpha = \sum_{\beta=1}^{3}\sum_{\gamma=1}^{3}\tilde{\Lambda}^{\alpha\beta\gamma}(|\boldsymbol{r}_t-\boldsymbol{r}_s|, h)\tilde{m}_s^\beta \tilde{m}_t^\gamma , \quad \alpha\in\{1,2,3\} , \qquad \text{(S7)}$$

where α, β, γ denote vector (tensor) components in local coordinates. The equation above is a generalization of the matrix-vector multiplication:

$$y^\alpha = \sum_{\beta=1}^{3} A^{\alpha\beta}x^\beta .$$

The first dimension of $\tilde{\Lambda}^{\alpha\beta\gamma}$ outputs the force, the second dimension takes source moments, and the third dimension takes target moments.

In the third step, the integral formula Eq. (S6) is used to determine the tensor $\tilde{\Lambda}^{\alpha\beta\gamma}$ numerically. After h is fixed, the tensor $\tilde{\Lambda}^{\alpha\beta\gamma}(|\boldsymbol{r}_t-\boldsymbol{r}_s|, h)$ consists of 27 curves as functions of the particle distance $|\boldsymbol{r}_t-\boldsymbol{r}_s|$. First, the kernel size h is fixed, and the normalized distance is looped q from 0 to 4. The target particle is then placed on $(0,0,qh)^\mathsf{T}$. The source moment $\tilde{\boldsymbol{m}}_s$ loops over three directions: $(1,0,0)^\mathsf{T}$, $(0,1,0)^\mathsf{T}$, and $(0,0,1)^\mathsf{T}$. The target moment $\tilde{\boldsymbol{m}}_t$ loops over the same three directions. For each of the combination, the force $\tilde{\boldsymbol{f}}_{s\to t}$ is determined by Eq. (S6) (explained below). After 9 measurements, the tensor value $\tilde{\Lambda}^{\alpha\beta\gamma}$ for this distance qh is obtained. For example, $\tilde{\boldsymbol{m}}_s = (0,1,0)^\mathsf{T}$, $\tilde{\boldsymbol{m}}_t = (1,0,0)^\mathsf{T}$, the three tensor entries are determined by

$$\tilde{\Lambda}^{\alpha 21}(qh, h) = \tilde{f}_{s\to t}^\alpha$$

for $\alpha\in\{1,2,3\}$.

To measure the force $\tilde{\boldsymbol{f}}_{s\to t}$ given a pair of source-target moments $\tilde{\boldsymbol{m}}_s$, $\tilde{\boldsymbol{m}}_t$, and distance qh, the integration formula Eq. (S6) is used. The target particle at $\tilde{\boldsymbol{r}}_t = (0,0,qh)^\mathsf{T}$ is contained in a cube with an edge length of $4h$ because the weight function we choose has a support of diameter $4h$. The container cube is divide into $10\times10\times10$ cells. Each cell is centered at $\tilde{\boldsymbol{r}}_{\text{cell}}$ and has an edge length of $0.4h$. We calculate the magnetic force on each cell as

$$\tilde{\boldsymbol{f}}_{\text{cell}} = \mu_0(0.4h)^3\, W(\tilde{\boldsymbol{r}}_{\text{cell}} - \tilde{\boldsymbol{r}}_t, h)\tilde{\boldsymbol{m}}_t \cdot \nabla \boldsymbol{H}(\tilde{\boldsymbol{r}}_{\text{cell}}, \tilde{\boldsymbol{m}}_s) .$$

We sum over all cells for the total force $\tilde{\boldsymbol{f}}_{s\to t} = \sum_{\text{cell}} \tilde{\boldsymbol{f}}_{\text{cell}}$.

After the measurements for various q and h, we discovered that when we fix the normalized distance q, the tensor is proportional to h^{-4}. Most of the 27 entries in $\tilde{\Lambda}^{\alpha\beta\gamma}$ are zeros. Finally, the six of the seven non-zero entries share the same curve $C_1 : q \mapsto C_1(q)$, and one obtains an unique curve $C_2 : q \mapsto C_2(q)$:

$$\tilde{\Lambda}^{311}, \tilde{\Lambda}^{322}, \tilde{\Lambda}^{113}, \tilde{\Lambda}^{223}, \tilde{\Lambda}^{131}, \tilde{\Lambda}^{232} = C_1(q)h^{-4} ,$$

$$\tilde{\Lambda}^{333} = C_2(q)h^{-4} .$$

We fit the measured tensor entries using piece-wise polynomials

$$C(q) = a_4 q^4 + a_3 q^3 + a_2 q^2 + a_1 q + a_0 \ .$$

We use fourth order polynomials according to Occam's razor since we found that third order ones are not sufficient to fit very well. The polynomial coefficients are listed in Table 3 and 4 in the appendix of the main paper.

In the forth step, we change the summation variable from forces to force tensors. Given the tensor $\tilde{\Lambda}^{\alpha\beta\gamma}$, it is clear how to calculate the force $\tilde{\boldsymbol{f}}_{s\to t}$ in local coordinates using $\tilde{\boldsymbol{m}}_s, \tilde{\boldsymbol{m}}_t$, and how to transform it back. The total force on one particle $\boldsymbol{f}_t$ is given by the summation of all forces from every source particle $\boldsymbol{f}_t = \sum_s \boldsymbol{f}_{s\to t}$.

However, in the large-scale summation, we use the fast multipole method to accelerate the computations. The fast multipole method can only work with the positions of the target particles, but summing the force requires target moments. Therefore we must change the force to a quantity independent of the target magnetic moment $\boldsymbol{m}_t$.

In order to do so, the summation in Eq. (S7) is divided into two parts by introducing a 3×3 source force tensor $\tilde{\boldsymbol{T}}_s$:

$$\begin{aligned} \tilde{\boldsymbol{f}}_{s\to t} &= \tilde{\boldsymbol{T}}_s \tilde{\boldsymbol{m}}_t \ , \\ \tilde{f}^{\alpha}_{s\to t} &= \sum_{\gamma=1}^{3} \tilde{T}^{\alpha\gamma}_s \tilde{m}^{\gamma}_t \ , \\ \tilde{T}^{\alpha\gamma}_s &= \sum_{\beta=1}^{3} \tilde{\Lambda}^{\alpha\beta\gamma}(|\boldsymbol{r}_t - \boldsymbol{r}_s|, h) \tilde{m}^{\beta}_s \ . \end{aligned}$$

Since $\tilde{\Lambda}$ is sparse, we can directly write the force tensor $\tilde{\boldsymbol{T}}_s$ in local coordinates:

$$\begin{aligned} \tilde{\boldsymbol{T}}_s &= \begin{pmatrix} \tilde{\Lambda}^{131}\tilde{m}^3_s & 0 & \tilde{\Lambda}^{113}\tilde{m}^1_s \\ 0 & \tilde{\Lambda}^{232}\tilde{m}^3_s & \tilde{\Lambda}^{223}\tilde{m}^2_s \\ \tilde{\Lambda}^{311}\tilde{m}^1_s & \tilde{\Lambda}^{322}\tilde{m}^2_s & \tilde{\Lambda}^{333}\tilde{m}^3_s \end{pmatrix} \\ &= h^{-4} \begin{pmatrix} \tilde{m}^3_s C_1(q) & 0 & \tilde{m}^1_s C_1(q) \\ 0 & \tilde{m}^3_s C_1(q) & \tilde{m}^2_s C_1(q) \\ \tilde{m}^1_s C_1(q) & \tilde{m}^2_s C_1(q) & \tilde{m}^3_s C_2(q) \end{pmatrix} , \end{aligned}$$

where the superscripts denote the components.

The rotation matrix $\boldsymbol{R}$ is used to transform the force tensor $\tilde{\boldsymbol{T}}_s$ to world coordinates:

$$\begin{aligned} \boldsymbol{f}_{s\to t} &= \boldsymbol{R}\tilde{\boldsymbol{f}}_{s\to t} = \boldsymbol{R}\tilde{\boldsymbol{T}}_s \tilde{\boldsymbol{m}}_t = \boldsymbol{R}\tilde{\boldsymbol{T}}_s \boldsymbol{R}^{\mathsf{T}} \boldsymbol{m}_t = \boldsymbol{T}_s \boldsymbol{m}_t \ , \\ \boldsymbol{T}_s &= \boldsymbol{R}\tilde{\boldsymbol{T}}_s \boldsymbol{R}^{\mathsf{T}} \ , \end{aligned}$$

where $\boldsymbol{T}_s$ is the force tensor in world coordinates. $\boldsymbol{T}_s$ only depends on target position, so that it is suitable for the summation to use the fast multipole method:

$$\boldsymbol{f}_t = \left(\sum_{s=1}^{N} \boldsymbol{T}_s(\boldsymbol{r}_t) \right) \boldsymbol{m}_t \ .$$

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