This notebook demonstrates that filling a phase-field according to the distance function of (circle, sphere) has an error of $O(W^2)$ compared to the sharp interface volume one would expect, with W an interface width parameter. We first show this analytically for the circle, followed by numerical illustration, and then derive the relevant expression for the sphere as employed in the paper.

We assume that a shape is given as a distance field $d(r, R) = R - r$ from its center, with $d > 0$ being inside the shape and $d < 0$ being outside the shape; hence the 0.5 level set of the phase-field is located at $d = 0$. For a particular shape its size may be scaled by a scalar R, representing an appropriate linear extent. Hence we may write

$$\phi(r, R, W) = \phi_{1d}(-r + R, W) \tag{1}$$

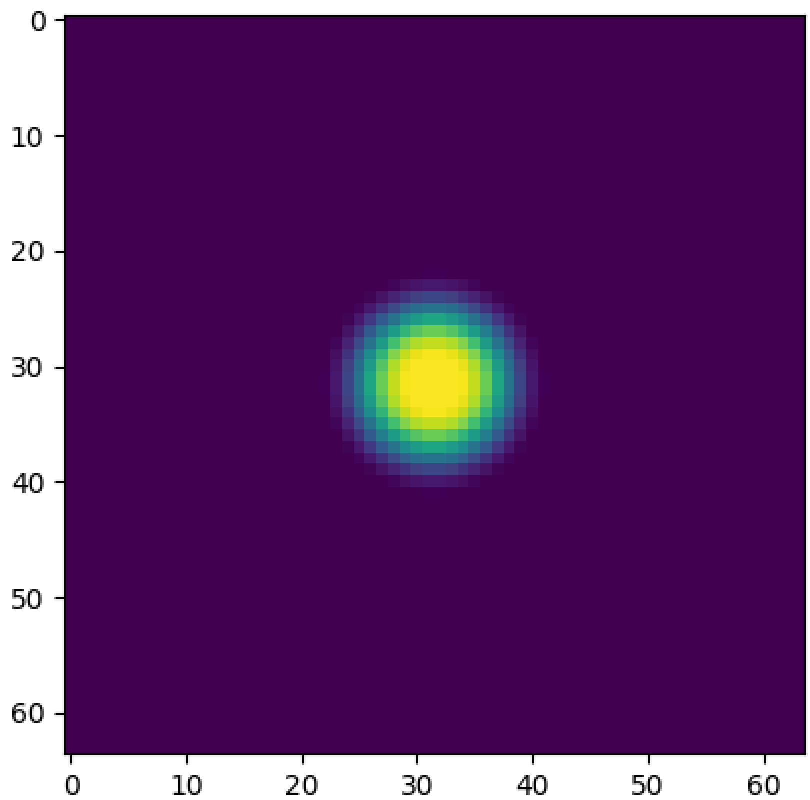
$$\phi_{1d}(d, W) = \frac{1}{2}(1 + \sin\frac{d}{W}) \tag{2}$$

with the obstacle potential's equilibrium profile $\phi_{1d}(d, W)$. Since that is valid for $d \in \{-\pi W/2, \pi W/2\}$ with constant values outside of this interval, the volume integral is split into a section of constant value 1 for $d \geq \pi W/2$ and one of variable value $-\pi W/2 \leq d < \pi W/2$, with values beyond this being trivially zero.

We note that it is likely that well-types of potentials with a hyperbolic tangent profile suffer from a similar error. Since the area integral it yields isn't easily analytically evaluated however we restrict ourselves to the obstacle potential profile.

$$\int\limits_0^{2\pi} \int\limits_0^{R} \phi(r)\, dr\, d\theta = \pi R^2 + W^2 \left(-2\pi + \frac{\pi^3}{4}\right)$$

The above shows that we have errors of $O(W^2)$ for the volume of a circle compared to the sharp interface picture. Hence if $R \gg W$, then these are negligible. We next give some numerical illustration as to the size of this effect in practice.



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<matplotlib.image.AxesImage at 0x7f81d9862390>
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Numerical value vs. predicted with O(W^2) error: -1.41893680581304e-6
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Relative error wrt. the sharp interface solution: 0.0810962286599858
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Here we have a 8.1% relative error in the area for $R/W = 2.4$ which is used for the simulations of immobile particles in the paper, with the 3D error being even larger (24%). In order to fix this we simply equate the analytical phase-field volume with an unknown radius R to the volume of the shape we desire, parametrized by its own radius r, and pick the real, positive solution, e.g. for a circle:

$$\frac{\sqrt{-\pi^2 W^2 + 8W^2 + 4r^2}}{2}$$

The 3D derivation doesn't have anything new safe for a different volume element. We obtain three solutions of which only one is real and positive.

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Relative error of the volume in 3D: 0.243438073058510
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$$\frac{-8W^2+\pi^2W^2-\left(-4r^3+\sqrt{-W^6\left(8-\pi^2\right)^3+16r^6}\right)^{\frac{2}{3}}}{2\sqrt[3]{-4r^3+\sqrt{-W^6\left(8-\pi^2\right)^3+16r^6}}}$$

The above is the function $R=f(r,W)$ s.t. $\int_V \phi(-r+f(R,W))dV$ is equal to the sharp interface volume $4/3\pi R^3$ when r is L^2 distance field from the center of a sphere.