Exercise: molecular dynamics in a harmonic potential

Implement the velocity Verlet algorithm (bottom) to sample positions in the x/y-plane where we assume that the particle of mass 1 moves in the potential ϕ (given on the right).

$$\phi(x, y) = \frac{x^2 + y^2}{2}$$

To this aim, we start at a given position and momentum, and propagate these quantities using a small time steps Δt.

$$\mathbf{r} = \begin{pmatrix} x \\ y \end{pmatrix}, \quad \mathbf{p} = m \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix}$$

Before you start implementing, write some unit tests to check that, e.g., your potential and its gradient are correctly evaluated.

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \frac{\Delta t}{m}\mathbf{p}(t) - \frac{\Delta t^2}{2m}\nabla\phi(\mathbf{r}(t))$$

$$\mathbf{p}(t + \Delta t) = \mathbf{p}(t) - \frac{\Delta t}{2}\left(\nabla\phi(\mathbf{r}(t)) + \nabla\phi(\mathbf{r}(t + \Delta t))\right)$$