

Charged tracer particle in a diffusive environment

A mock-up multiphysics model

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Ingredients:

1. Two dimensional diffusion equation for density field $\rho(\mathbf{r}, t)$ governed by PDE

$$\frac{\partial \rho}{\partial t} = D \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right). \quad (1)$$

2. Tracer particle satisfies ODE

$$m\ddot{\mathbf{R}} = \mathbf{F} - \alpha(\rho)\dot{\mathbf{R}}, \quad (2a)$$

where m is the mass, \mathbf{F} is a force acting on the particle and the friction constant α is proportional to the viscosity, and is density dependent.

- Ad hoc form for density dependent friction constant α :

$$\alpha(\rho) = \alpha_0(1 + a\rho). \quad (2b)$$

- Ad hoc form for force, like a constant electric field:

$$\mathbf{F} = qE\hat{\mathbf{x}}. \quad (2c)$$

3. And let's say we have periodic boundary conditions in all directions, i.e.,

$$\mathbf{r} \sim \mathbf{r} + L(k\hat{\mathbf{x}} + l\hat{\mathbf{y}}). \quad (3)$$

where L is the length of the side of the square periodic box, and k and l are integers. Positional coordinates can thus be restricted to lie between $-L/2$ and $L/2$.

4. Initial conditions:

$$\rho(\mathbf{r}) = \exp \left[-\frac{\|\mathbf{r}\|^2}{2\sigma_0^2} \right], \quad (4a)$$

$$\mathbf{R}(0) = \mathbf{R}_0, \quad (4b)$$

$$\dot{\mathbf{R}}(0) = \mathbf{V}_0. \quad (4c)$$

5. Values for the parameters (arbitrary) are

$$D = 1; m = 1; \alpha_0 = 1; a = 15; qE = 1; L = 10; \sigma_0 = 1; \mathbf{R}_0 = \mathbf{0}; \mathbf{V}_0 = 10\hat{\mathbf{y}} \quad (5)$$