PRISMS-PF Application Formulation
fickianDiffusion

In this example application, we implement a Fick's Law for a single component. Two time-dependent Gaussian source terms add concentration over the course of the simulation.

1 Kinetics

The Parabolic PDE for diffusion is given by:

$$\frac{\partial c}{\partial t} = -\boldsymbol{\nabla} \cdot (-D\ \boldsymbol{\nabla} c) + f \tag{1}$$

where D is the diffusion constant and f is a source term. In this example, f is given by a pair of Gaussian expressions:

$$\begin{aligned} f = A_1 \exp\left(-\left(\frac{t-t_1}{\tau_1}\right)^2\right) \exp\left(-\left(\frac{x-x_1}{L_1}\right)^2 - \left(\frac{y-y_1}{L_1}\right)^2\right) \\ + A_2 \exp\left(-\left(\frac{t-t_2}{\tau_2}\right)^2\right) \exp\left(-\left(\frac{x-x_2}{L_2}\right)^2 - \left(\frac{y-y_2}{L_2}\right)^2\right) \end{aligned} \tag{2}$$

where A_1, $_2$, t_1, t_2, τ_1, τ_2, x_1, x_2, y_1, y_2, L_1, and L_2 are constants.

2 Time discretization

Considering forward Euler explicit time stepping, we have the time discretized kinetics equation:

$$c^{n+1} = c^n + (\Delta t D)\ \Delta c^n + \Delta t f^n \tag{3}$$

3 Weak formulation

In the weak formulation, considering an arbitrary variation w, the above equation can be expressed as a residual equation:

$$\int_\Omega w c^{n+1}\ dV = \int_\Omega w c^n + w(\Delta t D)\Delta c^n + w \Delta t f^n\ dV \tag{4}$$

$$= \int_\Omega w(c^n + \Delta t f^n) - \boldsymbol{\nabla} w \cdot (\Delta t D) \boldsymbol{\nabla} c^n\ dV + \int_{\partial\Omega} w(\Delta t D) \boldsymbol{\nabla} c^n \cdot n\ dS \tag{5}$$

$$= \int_\Omega w(c^n + \Delta t f^n) - \boldsymbol{\nabla} w \cdot (\Delta t D) \boldsymbol{\nabla} c^n\ dV + \int_{\partial\Omega} w(\Delta t D) j^n\ dS \tag{6}$$

$$= \int_\Omega w(\underbrace{c^n + \Delta t f^n}_{r_c}) + \boldsymbol{\nabla} w \cdot \underbrace{(-\Delta t D) \boldsymbol{\nabla} c^n}_{r_{cx}}\ dV \quad \text{[assuming flux } j = 0\text{]} \tag{7}$$

The above values of r_c and r_{cx} are used to define the residuals in the following parameters file: *applications/fickianFlux/parameters.h*