Most General Forward Problem

The Forward Problem

$$\partial_t \rho = D_0 \nabla^2 \rho - c_{Flow} \nabla \cdot (\rho \mathbf{w}_{Flow}) + c_{ext} \nabla \cdot (\rho \nabla V_{ext}) + \gamma \nabla \cdot \int_\Omega \rho(r)\rho(r') \nabla V_2(|r - r'|) dr'$$
$$+ c_w w_{Force} + c_{Force} f \qquad \text{in} \quad \Omega,$$

$\rho = \rho_0 \quad \text{at} \quad t = 0.$

Possible Boundary Conditions include:

No-Flux

$$D_0 \frac{\partial \rho}{\partial n} - c_{Flow} \rho \mathbf{w}_{Flow} \cdot \mathbf{n} + c_{ext} \rho \frac{\partial V_{ext}}{\partial n} + \gamma \int_\Omega \rho(r)\rho(r') \frac{\partial V_2(|r - r'|)}{\partial n} dr' = 0 \qquad \text{on} \quad \partial\Omega,$$

Dirichlet

$$\rho = 0 \qquad \text{on} \quad \partial\Omega,$$

PDE-Constrained Optimization Problem 1: Flow Control

$$\min_{\rho, \mathbf{w}_{Flow}} \quad \frac{1}{2} \|\rho - \hat{\rho}\|^2_{L^2} + \frac{\beta}{2} \|\mathbf{w}_{Flow}\|^2_{L^2},$$

subject to the Forward Problem

Adjoint Equation

$$\begin{aligned} \partial_t p &= \rho - \hat{\rho} - c_{Flow} \nabla p \cdot \mathbf{w}_{Flow} - D_0 \nabla^2 p + c_{ext} \nabla p \cdot \nabla V_{ext} \\ &\quad + \gamma \int_\Omega (\nabla p(r) + \nabla p(r')) \rho(r') \nabla V_2(|r - r'|) dr', \qquad \text{in} \quad \Omega, \\ p(r, T) &= 0, \end{aligned}$$

Possible Boundary Conditions include:

No-Flux

$$\frac{\partial p}{\partial n} = 0, \quad \text{on} \quad \partial\Omega,$$

Dirichlet

$$p = 0, \quad \text{on} \quad \partial\Omega.$$

Gradient Equation

$$c_{Flow}\mathbf{w}_{Flow} = -\frac{1}{\beta}\rho\nabla p$$

PDE-Constrained Optimization Problem 2: Force Control

$$\min_{\rho, fw_{Force}} \quad \frac{1}{2}\|\rho - \hat{\rho}\|^2_{L^2} + \frac{\beta}{2}\|w_{Force}\|^2_{L^2},$$

subject to the Forward Problem

Adjoint Equation

$$\begin{aligned}
\partial_t p &= \rho - \hat{\rho} - c_{Flow}\nabla p \cdot \mathbf{w}_{Flow} - D_0\nabla^2 p + c_{ext}\nabla p \cdot \nabla V_{ext} \\
&\quad + \gamma \int_\Omega (\nabla p(r) + \nabla p(r'))\rho(r')\nabla V_2(|r - r'|)dr', \qquad \text{in} \quad \Omega, \\
p(r, T) &= 0,
\end{aligned}$$

Possible Boundary Conditions include:

$$\begin{aligned}
&\text{No-Flux} \\
&\qquad \frac{\partial p}{\partial n} = 0, \quad \text{on} \quad \partial\Omega, \\
&\text{Dirichlet} \\
&\qquad p = 0, \quad \text{on} \quad \partial\Omega.
\end{aligned}$$

Gradient Equation

$$c_w w_{Force} = -\frac{1}{\beta}p$$