Introduction to Virtual Cell

Yingjie Liu
Applied Mathematics and Statistics
SUNY at Stony Brook

References

University of Connecticut Health Center

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Outline of the Talk

- background
- Physical infrastructure
- Computational methods
- Summary

Background

Physical Infrastructure

State variables

- C_i: concentration of the ith molecular specie
- V: electric potential

Flux and source term

- molecular flux J_i
- electric flux density D
- current density I
- source term from reaction
- membrane transaction

Reaction-Diffusion Equations

Molecular flux

$$J_i = -D_i \nabla C_i - z_i \mu_i C_i \nabla V$$

- D_i diffusion constant
- z_i ionic valence
- $\mu_i = D_i F/(RT)$ mobility
- F Faraday's constant
- R gas constant
- T absolute temperature

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot J_i + S_i(C_1, C_2, \cdots, C_N)$$

Example:

$$A + B \qquad C$$

$$S_C = k_1[A][B] - k_{-1}[C]$$

Implicit Finite Volume Scheme

$$\frac{\partial C_i}{\partial t} \rightarrow \text{volume} \cdot (C_i - C_i^0)/\Delta t$$

$$\oint_S J_i \cdot n dS = \text{Area} \cdot$$
$$[J_x|_{x+} - J_x|_{x-} + J_y|_{y+} - J_y|_{y-} +$$
$$J_z|_{z+} - J_z|_{z-}]_i$$

Linearize the source term:

$$S_i \rightarrow S_i^C + S_i^P \cdot C_i$$

Discrete Molecular Flux

Interface between similar elements

$$J_x|_{x+} = -D_i[C_i(x+\Delta x) - C_i(x)]/\Delta x -$$
$$z_i \mu_i \cdot C_i|_{x+} \cdot [V(x+\Delta x) - V(x)]/\Delta x$$

Interface between dissimilar elements (membrane)

$$J_x|_{x+} = f(C_1, C_2, \cdots, C_N, V)$$

Simulation boundary

$$J_x|_{x+} = J_{\text{boundary}}$$

Line-by-Line Method ("ADI")

$$a_P C_P = a_E C_E + a_W C_W + a_N C_N + a_S C_S + b$$

where coefficients $a, b's$ depending on C and

$$b = S_C \Delta x \Delta y + a_P^0 C_P^0$$

$$a_P = a_E + a_W + a_N + a_S + a_P^0 - S_P \Delta x \Delta y$$

Line-by-Line Method

$$a_P^* C_P = a_E^* C_E + a_W^* C_W + a_N^* C_N^* + a_S^* C_S^* + b^*$$

$*$ means the value is taken from previous iteration

$$a_P^* C_P = a_E^* C_E^* + a_W^* C_W^* + a_N^* C_N + a_S^* C_S + b^*$$

Stability and Underrelaxation

Iteration:

$$a_P C_P = \sum a_k C_k^* + b$$

A Sufficient Stability Condition:

$$\sum |a_k| \leq |a_P|$$

and the inequality is strict for at least one equation

Relaxation:

$$C_P - C_P^* = \frac{\sum a_k C_k^* + b}{a_P} - C_P^*$$

replaced by

$$C_P - C_P^* = \theta \cdot [\frac{\sum a_k C_k^* + b}{a_P} - C_P^*]$$

Separation of Fast and Slow Reaction

$$\frac{\partial C_i}{\partial t} = D_i \Delta C_i + S_i, \quad i = 1, \cdots, n$$

$$S_i = \sum_{j=1}^{m} \alpha_{ij} \nu_j (C_i, \cdots, C_n), \quad \alpha_{ij} \text{ intergers}$$

Let $\nu_1, \cdots, \nu_k, \ k \leq m$ be the fast reactions, the remaining are slow. From time t_n to t_{n+1}

Step 1: solve for time Δt

$$\frac{\partial C_i}{\partial t} = \sum_{j=1}^{k} \alpha_{ij} \nu_j, \quad i = 1, \cdots, n$$

with initial value $C_i(x, t_n)$ to get $\tilde{C}_i(x)$

Step 2: with initial value $\tilde{C}_i(x)$, solve for time Δt

$$\frac{\partial C_i}{\partial t} = D_i \Delta C_i + \sum_{j=k+1}^{m} \alpha_{ij} \nu_j, \quad i = 1, \cdots, n$$

to get $C_i(x, t_{n+1})$