Finite difference algorithm for diffusion equations in non-uniform media with different composition ranges

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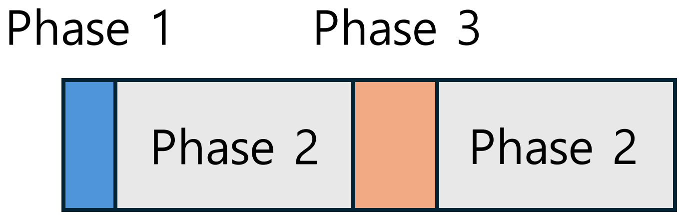
Algorithm overview



A simple diffusion equation: $\frac{\partial c}{\partial t} = -\mathrm{div}(\vec{j}) = -\mathrm{div}(-M\nabla c)$

Composition ranges: $[c_{min}^{1}, c_{max}^{1}]$, within phase 1
$[c_{min}^{2}, c_{max}^{2}]$, within phase 2
$[c_{min}^{3}, c_{max}^{3}]$, within phase 3

- Estimate $c_{i,j}^{NEW}$ by finite difference Euler method. i, j: spatial grid index along x and y axis
- Check if $c_{i,j}^{NEW}$ is in valid composition range or not.
- If $c_{i,j}^{NEW}$ exceeds the valid composition range, multiply so-called ‘flow factor’, $\alpha_{i,j}$ by $M_{i,j}$ to compute the effective mobility $M'_{i,j} = \alpha_{i,j} M_{i,j}$ so that $c_{i,j}^{NEW}$ does not exceed the valid composition range.
- Solve the diffusion equation with $M'_{i,j}$.

Discretized diffusion equation with Euler method

$$\frac{\partial c_{i,j}}{\partial t} = -\frac{(J_{x+} - J_{x-})}{\Delta x} - \frac{(J_{y+} - J_{y-})}{\Delta y}$$

$$J_{x+} = -M_{i+\frac{1}{2},j}\left(c_{i+1,j} - c_{i,j}\right)/\Delta x$$

$$J_{x-} = -M_{i-\frac{1}{2},j}\left(c_{i,j} - c_{i-1,j}\right)/\Delta x$$

$$J_{y+} = -M_{i,j+\frac{1}{2}}\left(c_{i,j+1} - c_{i,j}\right)/\Delta y$$

$$J_{y-} = -M_{i,j-\frac{1}{2}}\left(c_{i,j} - c_{i,j-1}\right)/\Delta y$$

$$c_{i,j}^{NEW} = c_{i,j} + \frac{\partial c_{i,j}}{\partial t}\Delta t = c_{i,j} + \Delta t\left[-\frac{(J_{x+} - J_{x-})}{\Delta x} - \frac{(J_{y+} - J_{y-})}{\Delta y}\right]$$

How about considering arithmetic mean?

$$M_{i+\frac{1}{2},j} = \frac{M_{i,j} + M_{i+1,j}}{2} \qquad M_{i-\frac{1}{2},j} = \frac{M_{i,j} + M_{i-1,j}}{2} \qquad M_{i,j+\frac{1}{2}} = \frac{M_{i,j} + M_{i,j+1}}{2} \qquad M_{i,j-\frac{1}{2}} = \frac{M_{i,j} + M_{i,j-1}}{2}$$

When $c_{i,j}^{NEW}$ is out of valid range, considering multiplying the flow factor $\alpha_{i,j}$ by $M_{i,j}$ and let:

$$\begin{aligned}
&\Delta c_{max} = c_{max} - c_{i,j} \\
&= \frac{\Delta t}{\Delta x}\left[\left(\frac{\alpha_{i,j}M_{i,j} + M_{i+1,j}}{2}\right)\frac{\left(c_{i+1,j} - c_{i,j}\right)}{\Delta x} - \left(\frac{\alpha_{i,j}M_{i,j} + M_{i-1,j}}{2}\right)\frac{\left(c_{i,j} - c_{i-1,j}\right)}{\Delta x}\right] \\
&+ \frac{\Delta t}{\Delta y}\left[\left(\frac{\alpha_{i,j}M_{i,j} + M_{i,j+1}}{2}\right)\frac{\left(c_{i,j+1} - c_{i,j}\right)}{\Delta y} - \left(\frac{\alpha_{i,j}M_{i,j} + M_{i,j-1}}{2}\right)\frac{\left(c_{i,j} - c_{i,j-1}\right)}{\Delta y}\right]
\end{aligned}$$

$$\begin{aligned}
&\Delta c_{max} \\
&= \Delta c - \frac{\Delta t}{\Delta x}\left[\left(\frac{(1-\alpha_{i,j})M_{i,j}}{2}\right)\frac{\left(c_{i+1,j} - c_{i,j}\right)}{\Delta x} - \left(\frac{(1-\alpha_{i,j})M_{i,j}}{2}\right)\frac{\left(c_{i,j} - c_{i-1,j}\right)}{\Delta x}\right] \\
&+ \frac{\Delta t}{\Delta y}\left[\left(\frac{(1-\alpha_{i,j})M_{i,j}}{2}\right)\frac{\left(c_{i,j+1} - c_{i,j}\right)}{\Delta y} - \left(\frac{(1-\alpha_{i,j})M_{i,j}}{2}\right)\frac{\left(c_{i,j} - c_{i,j-1}\right)}{\Delta y}\right]
\end{aligned}$$

How about considering arithmetic mean?

$$\Delta c_{max} = \Delta c - \frac{\Delta t}{\Delta x}(1-\alpha_{i,j})M_{i,j}\left[\frac{\left(c_{i+1,j}+c_{i-1,j}-2c_{i,j}\right)}{2\Delta x}\right] + \frac{\Delta t}{\Delta y}(1-\alpha_{i,j})M_{i,j}\left[\frac{\left(c_{i,j+1}+c_{i,j-1}-2c_{i,j}\right)}{2\Delta y}\right]$$

$$\Delta c_{max} = \Delta c - \left(1-\alpha_{i,j}\right)M_{i,j}\Delta t\left[\frac{1}{\Delta x}\frac{\left(c_{i+1,j}+c_{i-1,j}-2c_{i,j}\right)}{2\Delta x} + \frac{1}{\Delta y}\frac{\left(c_{i,j+1}+c_{i,j-1}-2c_{i,j}\right)}{2\Delta y}\right]$$

$$\frac{\Delta c - \Delta c_{max}}{\Delta t} = \left(1-\alpha_{i,j}\right)M_{i,j}\left[\frac{1}{\Delta x}\frac{\left(c_{i+1,j}+c_{i-1,j}-2c_{i,j}\right)}{2\Delta x} + \frac{1}{\Delta y}\frac{\left(c_{i,j+1}+c_{i,j-1}-2c_{i,j}\right)}{2\Delta y}\right]$$

$$\alpha_{i,j} = 1 - \frac{\dfrac{c_{i,j}^{NEW} - c_{max}}{\Delta t}}{\dfrac{M_{i,j}}{2}\left[\dfrac{1}{\Delta x}\dfrac{\left(c_{i+1,j}+c_{i-1,j}-2c_{i,j}\right)}{\Delta x} + \dfrac{1}{\Delta y}\dfrac{\left(c_{i,j+1}+c_{i,j-1}-2c_{i,j}\right)}{\Delta y}\right]}$$

Works very well

$$\alpha_{i,j} = 1 - \frac{\left(c_{i,j}^{NEW} - c_{max}\right)}{0.5M_{i,j}\Delta t\left[\left(c_{i+1,j}+c_{i-1,j}-2c_{i,j}\right)/\Delta x^2 + \left(c_{i,j+1}+c_{i,j-1}-2c_{i,j}\right)/\Delta y^2\right]}$$

Diffusion equation with harmonic average mobility estimation at ½ grids

$$J_{x+} = -M_{i+\frac{1}{2},j}\left(c_{i+1,j} - c_{i,j}\right)/\Delta x$$

$$J_{x-} = -M_{i-\frac{1}{2},j}\left(c_{i,j} - c_{i-1,j}\right)/\Delta x$$

$$J_{y+} = -M_{i,j+\frac{1}{2}}\left(c_{i,j+1} - c_{i,j}\right)/\Delta y$$

$$J_{y-} = -M_{i,j-\frac{1}{2}}\left(c_{i,j} - c_{i,j-1}\right)/\Delta y$$

$$M_{i+\frac{1}{2},j} = \frac{2M_{i,j}M_{i+1,j}}{M_{i,j} + M_{i+1,j}} \qquad M_{i-\frac{1}{2},j} = \frac{2M_{i,j}M_{i-1,j}}{M_{i,j} + M_{i-1,j}}$$

$$M_{i,j+\frac{1}{2}} = \frac{2M_{i,j}M_{i,j+1}}{M_{i,j} + M_{i,j+1}} \qquad M_{i,j-\frac{1}{2}} = \frac{2M_{i,j}M_{i,j-1}}{M_{i,j} + M_{i,j-1}}$$

$$\frac{\partial c_{i,j}}{\partial t} = -\frac{(J_{x+} - J_{x-})}{\Delta x} - \frac{\left(J_{y+} - J_{y-}\right)}{\Delta y} = -M_{i,j}\left[\frac{(J_{x+} - J_{x-})}{M_{i,j}\Delta x} + \frac{\left(J_{y+} - J_{y-}\right)}{M_{i,j}\Delta y}\right]$$

$$= -M_{i,j}\left[\frac{(j_{x+} - j_{x-})}{\Delta x} + \frac{\left(j_{y+} - j_{y-}\right)}{\Delta y}\right]$$

$$c_{i,j}^{NEW} = c_{i,j} + \frac{\partial c_{i,j}}{\partial t}\Delta t = c_{i,j} + \Delta t M_{i,j}\left[-\frac{(j_{x+} - j_{x-})}{\Delta x} - \frac{\left(j_{y+} - j_{y-}\right)}{\Delta y}\right]$$

Composition range: $[c_{min}, c_{max}]$

$$c_{i,j}^{NEW} = c_{i,j} + \frac{\partial c_{i,j}}{\partial t}\Delta t = c_{i,j} + \Delta t M_{i,j}\left[-\frac{(j_{x+} - j_{x-})}{\Delta x} - \frac{(j_{y+} - j_{y-})}{\Delta y}\right] = c_{i,j} + \Delta c$$

If $c_{i,j}^{NEW}$ became greater than c_{max}, we need to modify $M_{i,j}$ so that $c_{i,j}^{NEW}$ does not exceed the range.

The maximum amount of Δc allowed: $\Delta c_{max} = c_{max} - c_{i,j} > 0$.
Let, $c_{i,j}^{NEW} - c_{i,j} = \Delta c$.
To ensure not to be out of bound, $\frac{\Delta c_{max}}{\Delta c} \geq 1$. If this inequality violated, we need to adjust k, a multiplier of $M_{i,j}$.

$$\Delta c_{max} \geq \Delta c = \Delta t\left[-\frac{(J_{x+} - J_{x-})}{\Delta x} - \frac{(J_{y+} - J_{y-})}{\Delta y}\right]$$

$$\begin{aligned}
&\Delta c_{max} \\
&= -\frac{\Delta t}{\Delta x}\left[-\frac{2\alpha M_{i,j}M_{i+1,j}}{\alpha M_{i,j} + M_{i+1,j}}\frac{(c_{i+1,j} - c_{i,j})}{\Delta x} + \frac{2\alpha M_{i,j}M_{i-1,j}}{\alpha M_{i,j} + M_{i-1,j}}\frac{(c_{i,j} - c_{i-1,j})}{\Delta x}\right] \\
&- \frac{\Delta t}{\Delta y}\left[-\frac{2\alpha M_{i,j}M_{i,j+1}}{\alpha M_{i,j} + M_{i,j+1}}\frac{(c_{i,j+1} - c_{i,j})}{\Delta y} + \frac{2\alpha M_{i,j}M_{i,j-1}}{\alpha M_{i,j} + M_{i,j-1}}\frac{(c_{i,j} - c_{i,j-1})}{\Delta y}\right]
\end{aligned}$$

$$\Delta c_{max} = \\ = \frac{\Delta t}{\Delta x}\left[\frac{2\alpha M_{i,j}M_{i+1,j}}{\alpha M_{i,j}+M_{i+1,j}}\frac{(c_{i+1,j}-c_{i,j})}{\Delta x} - \frac{2\alpha M_{i,j}M_{i-1,j}}{\alpha M_{i,j}+M_{i-1,j}}\frac{(c_{i,j}-c_{i-1,j})}{\Delta x}\right] \\ + \frac{\Delta t}{\Delta y}\left[\frac{2\alpha M_{i,j}M_{i,j+1}}{\alpha M_{i,j}+M_{i,j+1}}\frac{(c_{i,j+1}-c_{i,j})}{\Delta y} - \frac{2\alpha M_{i,j}M_{i,j-1}}{\alpha M_{i,j}+M_{i,j-1}}\frac{(c_{i,j}-c_{i,j-1})}{\Delta y}\right]$$

Hmmm difficult....

Think in different way. k is not necessarily exact value to meet the equality. It should be OK with some value to satisfy the inequality.

Considering the ratio of Δc_{max} to Δc: $\frac{\Delta c_{max}}{\Delta c} = \xi$. If we find proper k to make ξ greater than 1, it should be fine.

Ratio: $$\frac{2\alpha M_{i,j}M_{i+1,j}}{\alpha M_{i,j}+M_{i+1,j}}\frac{M_{i,j}+M_{i+1,j}}{2M_{i,j}M_{i+1,j}} \\ = \frac{2\alpha M_{i,j}M_{i+1,j}}{\alpha M_{i,j}+M_{i+1,j}}$$

$$\Delta c' = \xi\Delta c \\ = \frac{\Delta t}{\Delta x}\left[\frac{2\alpha M_{i,j}M_{i+1,j}}{\alpha M_{i,j}+M_{i+1,j}}\frac{(c_{i+1,j}-c_{i,j})}{\Delta x} - \frac{2\alpha M_{i,j}M_{i-1,j}}{\alpha M_{i,j}+M_{i-1,j}}\frac{(c_{i,j}-c_{i-1,j})}{\Delta x}\right] \\ + \frac{\Delta t}{\Delta y}\left[\frac{2\alpha M_{i,j}M_{i,j+1}}{\alpha M_{i,j}+M_{i,j+1}}\frac{(c_{i,j+1}-c_{i,j})}{\Delta y} - \frac{2\alpha M_{i,j}M_{i,j-1}}{\alpha M_{i,j}+M_{i,j-1}}\frac{(c_{i,j}-c_{i,j-1})}{\Delta y}\right]$$

$$\max\left(\frac{\alpha(M_{i,j}+M_{i+1,j})}{\alpha M_{i,j}+M_{i+1,j}}, \frac{\alpha(M_{i,j}+M_{i-1,j})}{\alpha M_{i,j}+M_{i-1,j}}, \frac{\alpha(M_{i,j}+M_{i,j+1})}{\alpha M_{i,j}+M_{i,j+1}}, \frac{\alpha(M_{i,j}+M_{i,j-1})}{\alpha M_{i,j}+M_{i,j-1}}\right) \le \xi$$

$$\frac{\alpha_{x+}\left(M_{i,j} + M_{i+1,j}\right)}{\alpha_{x+}M_{i,j} + M_{i+1,j}} \leq \xi$$

$$\alpha_{x+}\left(M_{i,j} + M_{i+1,j}\right) \leq \xi\left(\alpha_{x+}M_{i,j} + M_{i+1,j}\right)$$

$$\alpha_{x+}\left(M_{i,j} + M_{i+1,j} - \xi M_{i,j}\right) \; = \xi\left(M_{i+1,j}\right)$$

$$\alpha_{x+} \leq \frac{\xi M_{i+1,j}}{(1-\xi)M_{i,j} + M_{i+1,j}}$$

$$\alpha_{x+} \leq \frac{\xi M_{i+1,j}}{(1-\xi)M_{i,j} + M_{i+1,j}} = \alpha_{x+}^{max} \qquad \alpha_{y+} \leq \frac{\xi M_{i,j+1}}{(1-\xi)M_{i,j} + M_{i,j+1}} = \alpha_{y+}^{max}$$

$$\alpha_{x-} \leq \frac{\xi M_{i-1,j}}{(1-\xi)M_{i,j} + M_{i-1,j}} = \alpha_{x-}^{max} \qquad \alpha_{y-} \leq \frac{\xi M_{i,j-1}}{(1-\xi)M_{i,j} + M_{i,j-1}} = \alpha_{y-}^{max}$$

$$\alpha = \min\left(\alpha_{x+}^{max}, \alpha_{x-}^{max}, \alpha_{y+}^{max}, \alpha_{y-}^{max}\right)$$

Composition range: $[c_{min}, c_{max}]$

$$c_{i,j}^{NEW} = c_{i,j} + \frac{\partial c_{i,j}}{\partial t}\Delta t = c_{i,j} + \Delta t M_{i,j}\left[-\frac{(j_{x+} - j_{x-})}{\Delta x} - \frac{(j_{y+} - j_{y-})}{\Delta y}\right] = c_{i,j} + \Delta c$$

If $c_{i,j}^{NEW}$ became lesser than c_{min}, we need to modify $M_{i,j}$ so that $c_{i,j}^{NEW}$ does not go below the range.

The maximum amount of Δc (< 0) allowed: $\Delta c_{min} = c_{min} - c_{i,j} < 0$

To ensure not to be out of bound, $\frac{\Delta c_{min}}{\Delta c} \geq 1$. If this inequality violated, we need to adjust k.

Considering the ratio of Δc_{max} to Δc: $\frac{\Delta c_{min}}{\Delta c} = \xi$. If we find proper k to make ξ greater than 1, it should be fine.

$$\begin{aligned}
&\Delta c' = \xi \Delta c \\
&= \frac{\Delta t}{\Delta x}\left[\frac{2\alpha M_{i,j} M_{i+1,j}}{\alpha M_{i,j} + M_{i+1,j}} \frac{(c_{i+1,j} - c_{i,j})}{\Delta x} - \frac{2\alpha M_{i,j} M_{i-1,j}}{\alpha M_{i,j} + M_{i-1,j}} \frac{(c_{i,j} - c_{i-1,j})}{\Delta x}\right] \\
&+ \frac{\Delta t}{\Delta y}\left[\frac{2\alpha M_{i,j} M_{i,j+1}}{\alpha M_{i,j} + M_{i,j+1}} \frac{(c_{i,j+1} - c_{i,j})}{\Delta y} - \frac{2\alpha M_{i,j} M_{i,j-1}}{\alpha M_{i,j} + M_{i,j-1}} \frac{(c_{i,j} - c_{i,j-1})}{\Delta y}\right]
\end{aligned}$$

Which becomes the same condition as reducing the amount of flux so that Δc do not exceed the allowed bounds.

$$\frac{\alpha_{x+}\left(M_{i,j}+M_{i+1,j}\right)}{\alpha_{x+}M_{i,j}+M_{i+1,j}} \le \xi$$

$$\alpha_{x+}\left(M_{i,j}+M_{i+1,j}\right) \le \xi\left(\alpha_{x+}M_{i,j}+M_{i+1,j}\right)$$

$$\alpha_{x+}\left(M_{i,j}+M_{i+1,j}-\xi M_{i,j}\right) \; = \xi\left(M_{i+1,j}\right)$$

$$\alpha_{x+} \le \frac{\xi M_{i+1,j}}{(1-\xi)M_{i,j}+M_{i+1,j}}$$

$$\alpha_{x+} \le \frac{\xi M_{i+1,j}}{(1-\xi)M_{i,j}+M_{i+1,j}} = \alpha_{x+}^{max} \qquad \alpha_{y+} \le \frac{\xi M_{i,j+1}}{(1-\xi)M_{i,j}+M_{i,j+1}} = \alpha_{y+}^{max}$$

$$\alpha_{x-} \le \frac{\xi M_{i-1,j}}{(1-\xi)M_{i,j}+M_{i-1,j}} = \alpha_{x-}^{max} \qquad \alpha_{y-} \le \frac{\xi M_{i,j-1}}{(1-\xi)M_{i,j}+M_{i,j-1}} = \alpha_{y-}^{max}$$

$$\alpha = \min\left(\alpha_{x+}^{max}, \alpha_{x-}^{max}, \alpha_{y+}^{max}, \alpha_{y-}^{max}\right)$$