PDE units

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1 Introduction

We have fundamental units of

- time: T

- length: L

- amount: A

and we want to simulate the d-dimensional reaction diffusion equation

$$\frac{\partial u}{\partial t} = D\nabla^2 u + R(u) \tag{1}$$

where

- t is time, with units $[t] = T$

- u is (a vector of) species concentration, with units $[u] = AL^{-d}$

- D is the diffusion constant, with units $[D] = L^2 T^{-1}$

- R is the reaction term, with units $[R] = [u]T^{-1} = AL^{-d}T^{-1}$

To fully define the problem we need to specify the geometry of the compartment where u lives, and the boundary conditions on u at the boundaries of this compartment.

We choose to start with zero-flux Neumann boundary conditions at all surfaces, to which we can add flux terms $\Gamma(u)$, which specify the rate at which species *amount* crosses unit area of the surface,

- $\Gamma(u)$ is a flux term, with units $[\Gamma] = AL^{1-d}T^{-1}$

Systems with multiple compartments have a reaction diffusion equation for each compartment, which are coupled to each other via the flux terms at the surfaces where compartments meet.

2 Alternative concentration units

To allow the use of common units of concentration for the species density, we introduce an additional (derived) unit

- volume: $V = \alpha L^d$,

where α is a dimensionless scalar, along with an alternative definition for species concentration u', where

- u' is (a vector of) species concentration, with units $[u'] = AV^{-1}$

so the units of concentration are related by the constant factor α,

$$[u'] = A(\alpha L^d)^{-1} = \alpha^{-1} A L^{-d} = \alpha^{-1}[u] \tag{2}$$

and the dimensionless part of the variables are related by

$$u' = \alpha u \tag{3}$$

Inserting this into Eq.(1) gives

$$\frac{\partial u'/\alpha}{\partial t} = D\nabla^2 u'/\alpha + R(u'/\alpha) \tag{4}$$

and multiplying by α gives

$$\Rightarrow \frac{\partial u'}{\partial t} = D\nabla^2 u' + \alpha R(u'/\alpha) \tag{5}$$

Comparing this with a reaction diffusion equation for u'

$$\Rightarrow \frac{\partial u'}{\partial t} = D\nabla^2 u' + R'(u') \tag{6}$$

we find the reaction terms R and R' are related by

$$R(x) = \frac{1}{\alpha} R'(\alpha x) \tag{7}$$

3 What the user provides

In the GUI, the user provides

- u': initial species concentrations, with units $[u'] = AV^{-1}$

- $R'(u')$: reaction terms, with units $[R'] = [u']/T = AV^{-1}T^{-1}$

- $\Gamma'(u')$: membrane flux terms, with units $[\Gamma'] = AL^{1-d}T^{-1}$

(note the different units for the membrane flux terms vs the reaction terms - this is unfortunate and results in confusion for the user)

4 Dune implementation

For Dune simulations, we need to provide Eq.(1), along with the flux terms for the boundaries between compartments.

1. The user provides

   - u': species concentrations, with units $[u'] = AV^{-1}$
   - $R'(u')$: reaction terms, with units $[R'] = [u']/T = AV^{-1}T^{-1}$
   - $\Gamma'(u')$: membrane reaction terms, with units $[\Gamma'] = AL^{1-d}T^{-1}$

2. The GUI (internally) converts these to

   - $u = u'/\alpha$: species concentrations, with units $[u'] = AL^{-d}$
   - $R(u) = R'(\alpha u)/\alpha$: reaction terms, with units $[R] = [u]/T = AL^{-d}T^{-1}$
   - $\Gamma(u) = \Gamma'(\alpha u)$: membrane reaction terms, with units $[\Gamma] = AL^{1-d}T^{-1}$

3. DUNE simulates Eq.(1), i.e. the reaction-diffusion equation for u

4. The GUI converts the results back to u'

   - $u' = \alpha u$: species concentrations, with units $[u'] = AV^{-1}$

5 Pixel implementation

For Pixel simulations, we implement the membrane as a thin but finite-width d-dimensional compartment, rather than a $(d-1)$-dimensional surface. This means that for each membrane pixel, a change in amount due to a flux into/out of the pixel can then be converted into an equivalent change in concentration within the pixel. Taking advantage of this, we convert the flux terms into reaction terms for the membrane pixels, and then directly simulate Eq.(6) with zero-flux boundary conditions at all boundaries.

Assuming a pixel in the membrane has surface area S and width w,

- rate at which *amount* enters the pixel: $\Gamma'(u')S$

- $\Rightarrow \partial u/\partial t$ contribution in the pixel: $\Gamma'(u')S/(Sw) = \Gamma'(u')/w$

- $\Rightarrow \partial u'/\partial t$ contribution in the pixel: $\alpha\Gamma'(u')/w$

so we replace the membrane flux term with the following extra reaction term (for the membrane pixels in the compartment only):

$$R'(u') \mathrel{+}= \alpha\Gamma'(u')/w \tag{8}$$

6 Open questions

- are these methods correct (and equivalent)?

- can we make the units more intuitive for the user?