Discretization for Radial Concentrations

- Let $\bigoplus$ denote the concatenation function.
- Let $\mathbf{rmesh} = \bigoplus_{r=r_0=50\mu m}^{r_{\max}=1000\mu m} r \equiv \bigoplus_{i=0}^{N-1} r_i$ denote the 1D array of radial distances from the aggregate. Note that rmesh is an array of length N.
- Let $c(r,t)$ denote the cAMP concentration at radial distance r at time t in nM.
- Let $pde(r,t)$ denote the PDE concentration at radial distance r at time t in nM.
- Let $F_0(t) \in [0, 200]$ nM/s be the rate of change in cAMP concentration at the aggregate at time t.
- Let $dt = 0.005s$ be the size of one time step and $dr = 1\mu m$ be the spatial resolution of $\mathbf{rmesh}$.

Then, we may compute $c(r, t + dt) = c(r, t) + dt \cdot \frac{dc}{dt}\Big|_t$, where $\frac{dc}{dt}\Big|_t$ is returned by the function `time_step`.

`time_step` is effectively defined from the following steps:

step 1: compute the face terms

- $\mathbf{dface}(t) = 0 \oplus \left(\bigoplus_{i=0}^{N-2} c(r_{i+1}, t) - c(r_i, t) \right) \oplus 0$. Note **dface** has length N+1
- $\mathbf{cp}(t) = c(r_0, t) \oplus \left(\bigoplus_{i=0}^{N-1} c(r_i, t) \right) \oplus c(r_{\max}, t)$. Note **cp** has length N+2
- $\mathbf{face}(t) = \frac{1}{2} \bigoplus_{i=0}^{N} \mathrm{cp}(r_{i+1}, t) + \mathrm{cp}(r_i, t)$. Note face has length N+1

Let $\mathrm{cp}(r_i, t)$, $\mathrm{face}(r_i, t)$, and $\mathrm{dface}(r_i, t)$ denote the i^{th} entry of $\mathbf{cp}(t)$, $\mathbf{face}(t)$, and $\mathbf{dface}(t)$, respectively.

step 2: compute the transient terms

- $\mathbf{term1}(t) = \frac{D}{dr} \bigoplus_{i=0}^{N-1} \frac{1}{r_i} \left(\mathrm{face}(r_{i+1}, t) - \mathrm{face}(r_i, t) \right)$
- $\mathbf{term2}(t) = \frac{D}{dr^2} \bigoplus_{i=0}^{N-1} \mathrm{dface}(r_{i+1}, t) - \mathrm{dface}(r_i, t)$
- $\mathbf{termDEG}(t) = -k_{PDE} \bigoplus_{i=0}^{N-1} c(r_i, t) pde(r_i, t)$
- $\mathbf{termBC}(t) = F_0 \oplus \bigoplus_{i=1}^{N-1} 0$

step 3: add the transient terms Then,

$$\frac{dc}{dt}\Big|_t = \mathbf{term1}(t) + \mathbf{term2}(t) + \mathbf{termDEG}(t) + \mathbf{termBC}(t)$$

Is the vector of rates of change of cAMP concentration at time t.

In [1]:
```
import numpy as np
```
executed in 2ms, finished 12:37:02 2020-07-14

In [2]:
```
def time_step(c, pde, rmesh, D, kPDE, dr, fluxLeft, fluxRight=0):
    '''returns d[cAMP]/dt = the rate of change of the cAMP field c
    rmesh is the 1D radial mesh,
    c = 1D array of cAMP concentrations
    pde = 1D array of PDE concentrations
    D = diffusion coefficient of cAMP
    kPDE = decay constant of cAMP due to PDE
    dr = spatial resolution, for example 1 (microns)
    fluxLeft is the rate cAMP is being added at the "left" boundary, closest t
    fluxRight is he rate cAMP is being added at the "right" boundary, furthest
    explicitely using only current state.'''
    #step one: compute the face terms
```

```
    dface = np.hstack([ 0. , np.diff(c) , 0. ])
    cp    = np.hstack([c[0], c, c[-1]])
    face  = cp[1:]*0.5 + cp[:-1]*0.5

    #step two: compute transient terms
    term1 = D*np.diff(face)/rmesh/dr
    term2 = D*np.diff(dface)/dr**2
    termDEG = -1*kPDE*c*pde
    #calculate boundary term
    termBC = np.hstack([ fluxLeft , 0*c[1:-1] , fluxRight ])

    #step three: add transient terms
    dcdt  = term1 + term2 + termBC + termDEG
    return dcdt
```

executed in 5ms, finished 12:37:02 2020-07-14