



NUI Galway  
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# Membrane Mechanics

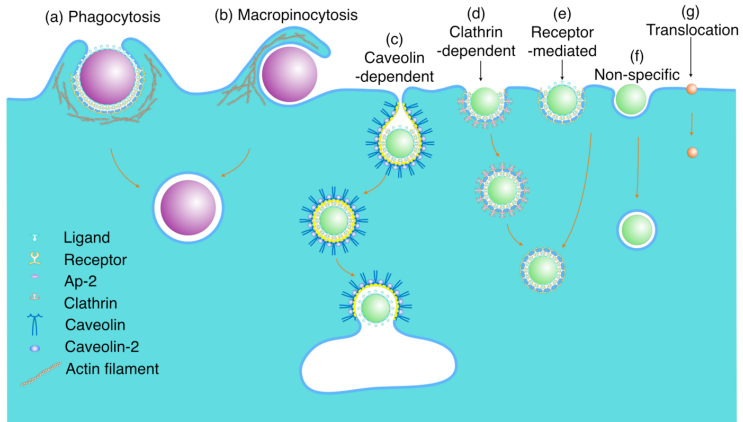
Modelling  
Research  
Group



**Paul Greaney**

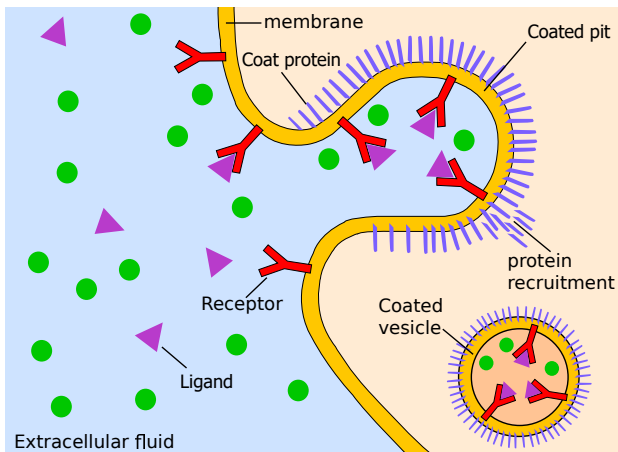
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# Endocytosis



Zhang et al., *Physical Principles of Nanoparticle Cellular Endocytosis*, ACS Nano, 9, 8655.

# Receptor-mediated Endocytosis



- Ligands on NP surface bind to receptors on cell membrane
- Signalling from receptors leads to protein recruitment and pit formation
- Pinches off to form vesicle

# Membrane Modelling

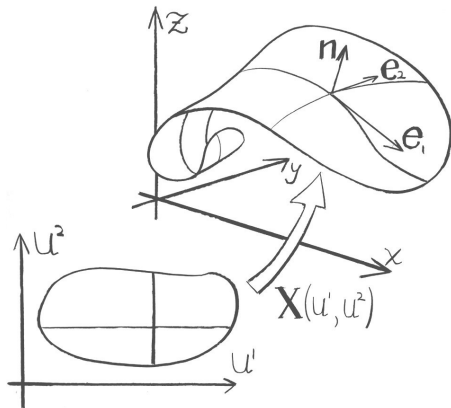
- Separation of lengthscales: lateral dimensions greatly exceed thickness.
- Parameterisation of surface: 2D coordinate system  $\{u^1, u^2\}$  with map

$$\mathbf{r} = \mathbf{X}(u^1, u^2) = \begin{pmatrix} X(u^1, u^2) \\ Y(u^1, u^2) \\ Z(u^1, u^2) \end{pmatrix}$$

- Tangent vectors

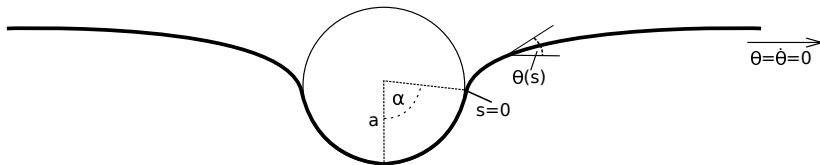
$$\mathbf{e}_a = \frac{\partial \mathbf{X}}{\partial u^a} = \partial_a \mathbf{X}, a \in \{1, 2\}$$

span local tangent plane to surface



# A Minimal Model

Consider an infinite rod, bending rigidity  $\kappa$ , in contact with a disc of radius  $a$ , contact energy  $w$  per unit length.



Require membrane to be flat far away from disc: BCs are

$$\lim_{s \rightarrow \infty} \theta(s) = \lim_{s \rightarrow \infty} \dot{\theta}(s) = 0. \quad (1)$$

Amount of stretching in bound part of membrane: (length of portion of rod in flat configuration) - (length in the wrapped configuration) =  $2\alpha a - 2a \sin(\alpha)$ . This gives the contact energy

$$E_{contact} = 2\alpha a \left( \frac{\kappa}{2a^2} - w \right) + 2a\sigma(\alpha - \sin(\alpha)).$$

# A Minimal Model

Amount of stretching in free part of the membrane is difference between length of curved piece & flat piece,  $ds - dx$ , so contribution of stretching to energy of free membrane is

$$\int_{s=0}^{s=\infty} \sigma(ds - dx) = \int_0^{\infty} \sigma \left( 1 - \frac{dx}{ds} \right) ds = \int_0^{\infty} \sigma(1 - \cos(\theta)) ds,$$

and combining this with usual expression for bending energy gives energy of free portion

$$E_{free} = 2 \int_{s=0}^{s=\infty} \left[ \sigma(1 - \cos(\theta)) + \frac{1}{2} \kappa \left( \frac{d\theta}{ds} \right)^2 \right] ds. \quad (2)$$

Thus the total energy is

$$\begin{aligned} E_{total} &= 2\alpha a \left( \frac{\kappa}{2a^2} - w \right) + \\ &\quad 2a\sigma(\alpha - \sin(\alpha)) + 2 \int_{s=0}^{s=\infty} \left[ \sigma(1 - \cos(\theta)) + \frac{1}{2}\kappa \left( \frac{d\theta}{ds} \right)^2 \right] ds \\ &= \int_{s=0}^{s=\infty} (\kappa\dot{\theta}^2 + 2\sigma(1 - \cos(\theta)) + C\dot{\theta}) ds, \end{aligned}$$

for constant  $C$ .

# A Minimal Model

Define the Lagrangian

$$L(\theta, \dot{\theta}) = \kappa \dot{\theta}^2 + 2\sigma(1 - \cos(\theta)) + C\dot{\theta},$$

from which we obtain the Euler-Lagrange equation

$$\ddot{\theta} - \frac{\sigma}{\kappa} \sin(\theta) = 0. \quad (3)$$

Solving this subject to the boundary conditions gives

$$\int \frac{d\theta}{\sqrt{1 - \cos(\theta)}} = \sqrt{\frac{2\sigma}{\kappa}} s + E, \quad (4)$$

where  $E$  is an arbitrary constant.



# A Minimal Model

Integrating and imposing  $\theta(s = 0) = \alpha$  gives

$$\theta(s) = 2 \cos^{-1}(\tanh(\tanh^{-1}(\cos(\alpha/2)) - \sqrt{\sigma/\kappa s})),$$

and the profile of the free part of the membrane can now be calculated using

$$(x(s), y(s)) = \left( a \sin(\alpha) + \int_0^s \cos(\theta(s)) ds, -a \cos(\alpha) + \int_0^s \sin(\theta(s)) ds \right).$$

where we have specified the coordinates of the first point of contact for a given degree of wrapping  $\alpha$  by

$$(x(0), y(0)) = (a \sin(\alpha), -a \cos(\alpha)).$$

# A Minimal Model

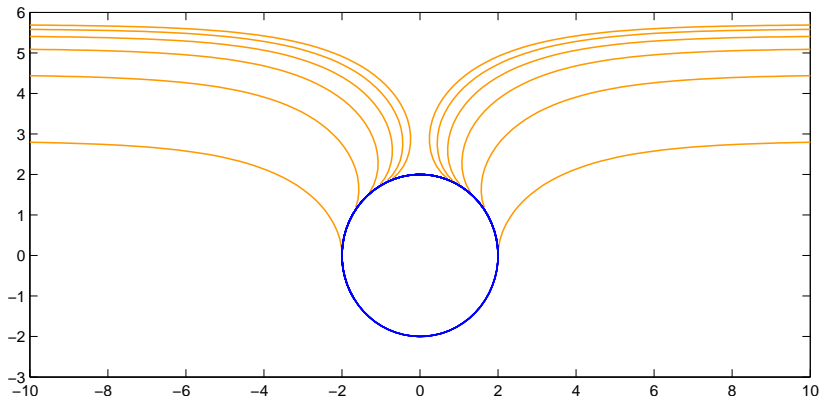


Figure: Membrane profiles for various values of wrapping angle  $\alpha$



Zhang et al.

Physical Principles of Nanoparticle Cellular Endocytosis.  
*ACS Nano*, **9**, 8655.



Markus Deserno.

Fluid lipid membranes: From differential geometry to  
curvature stresses.  
*Chemistry and Physics of Lipids*, **185** , 11–45.