

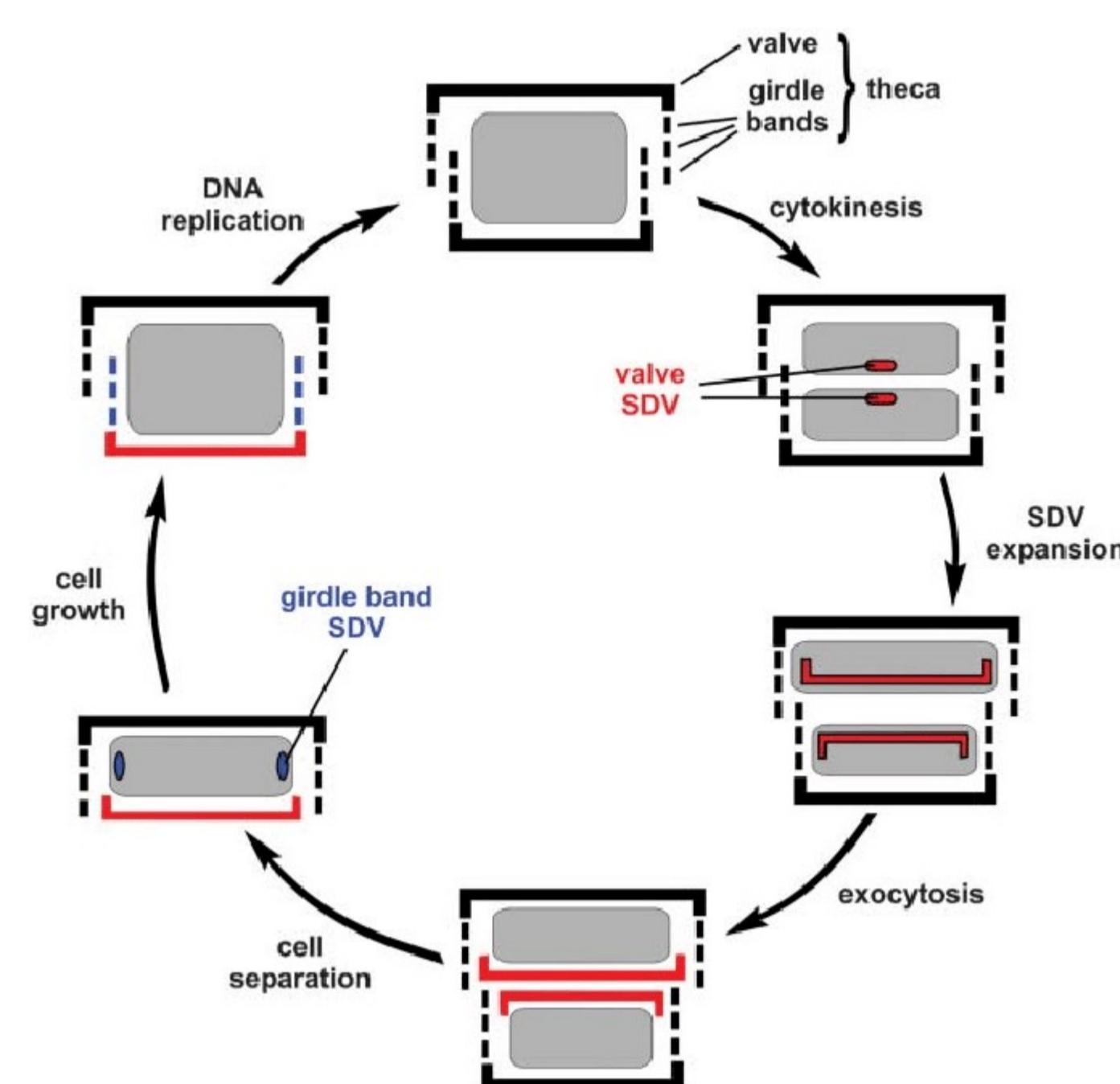
# Modelling of biosilica patterns formation in diatoms

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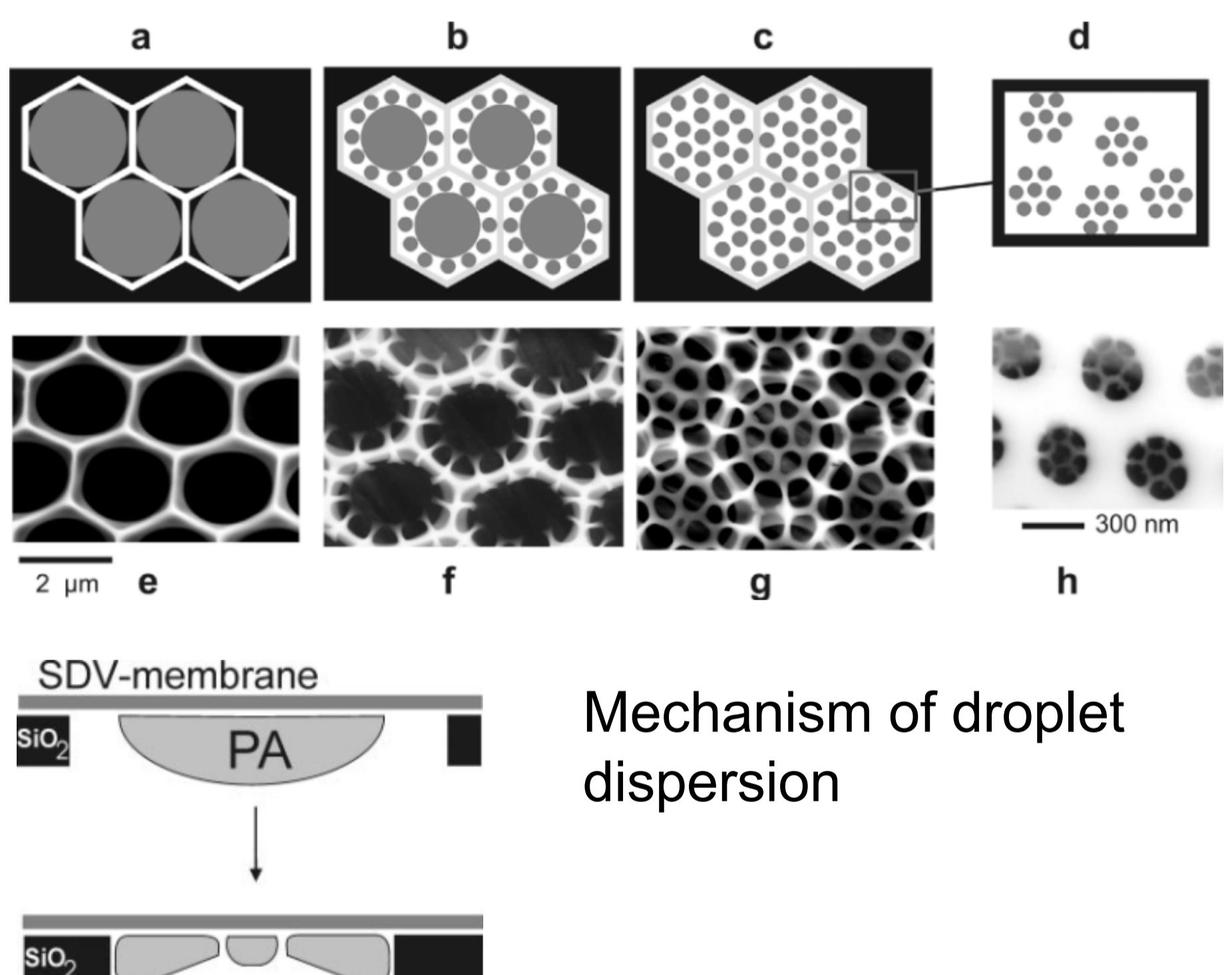
## The diatom cell cycle



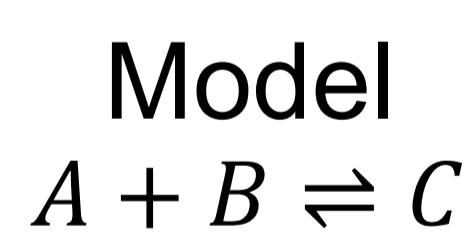
[M.Sumper and N.Kroger. Silica formation in diatoms: the function of long-chain polyamines and silaffins. 2004]

Schematic cross-sections of the diatom cell. The biosilica cell wall is depicted by black or red bars

## Templating mechanism



[M.Sumper. A Phase Separation Model for the Nanopatterning of Diatom Biosilica. 2002]



$A$  – organic molecules (unable to phase separate),  
 $B$  – phosphate ions,  $C$  – formed organic component

Phase separation process. Gibbs energy functional:

$$G(\varphi) = \int dV \left[ g(\varphi) + \frac{1}{2} \kappa (\nabla \varphi)^2 \right]$$

where  $\varphi$  – volume fraction of phase separating component,  $g(\varphi)$  - Gibbs energy of mixing,  $\kappa$  – gradient energy coefficient.

$$\begin{aligned} \frac{\partial c_A}{\partial t} &= \nabla \cdot D_A \nabla c_A - \alpha c_A c_B + \beta \varphi \\ \frac{\partial c_B}{\partial t} &= \nabla \cdot D_B \nabla c_B - \alpha c_A c_B + \beta \varphi \\ \frac{\partial \varphi}{\partial t} &= \nabla \cdot M \nabla (g'(\varphi) - \nabla^2 \varphi) + \alpha c_A c_B - \beta \varphi \end{aligned}$$

Where  $c_A, c_B$  - concentrations and  $D_A, D_B$  - diffusion coefficients of corresponding components,  $\alpha$  – reaction velocity of components  $A$  and  $B$ ,  $\beta$  – backward reaction

## Influence of free energy form, initial concentration and dissociation rate

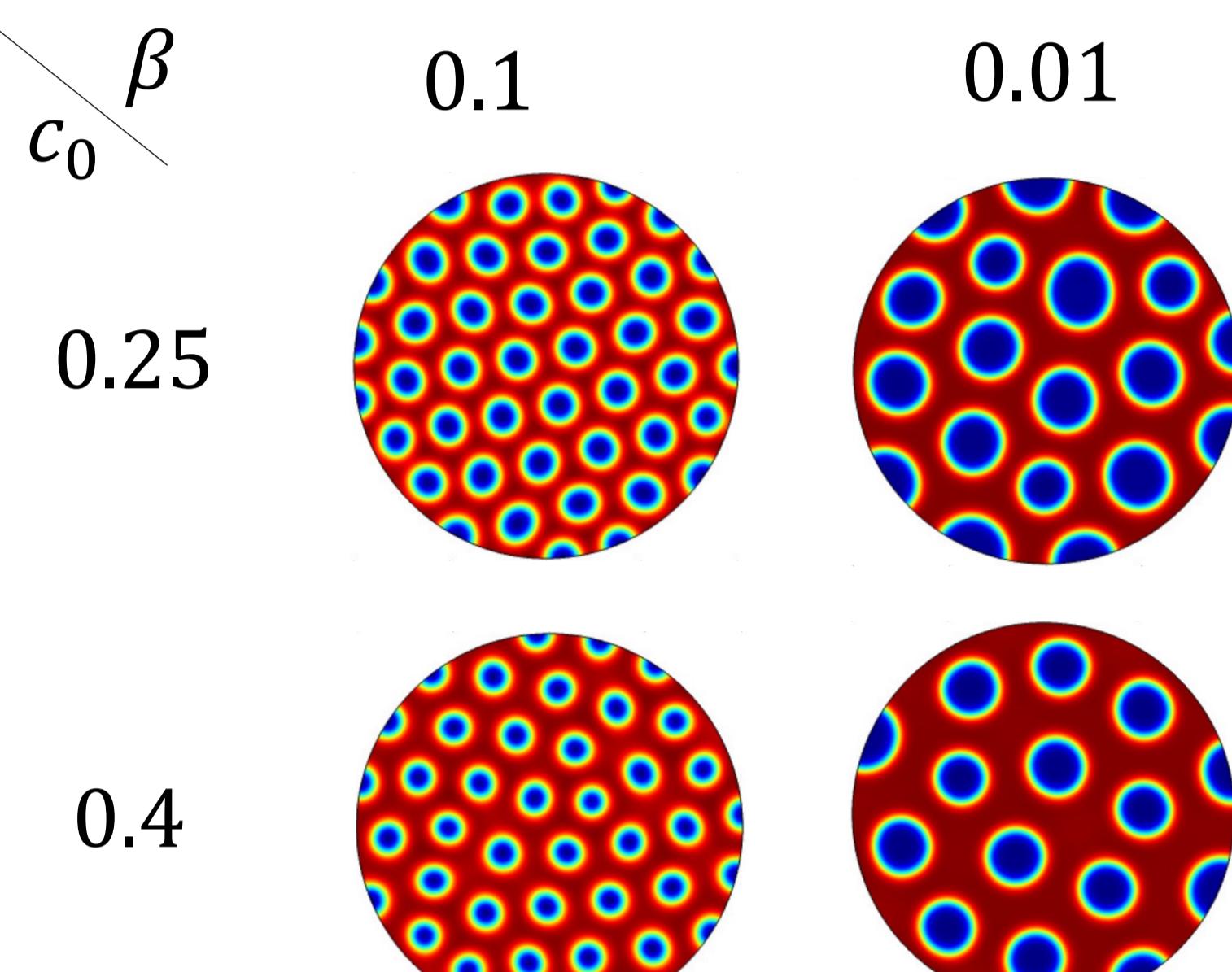
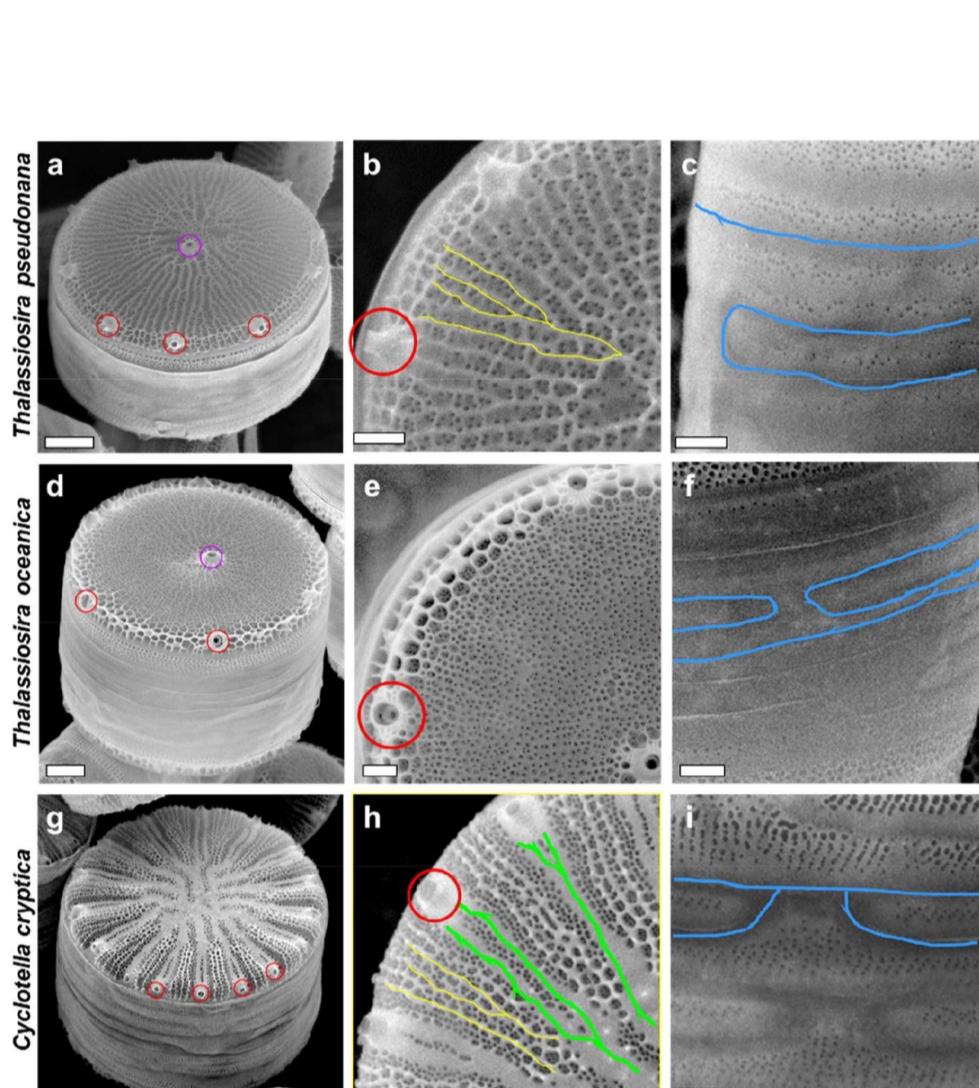
Cahn-Hilliard equation:

$$\frac{\partial \varphi}{\partial t} = \nabla \cdot \frac{M\lambda}{\varepsilon^2} \nabla (-\nabla \cdot \varepsilon^2 \nabla \varphi + (\varphi^2 - 1)\varphi)$$

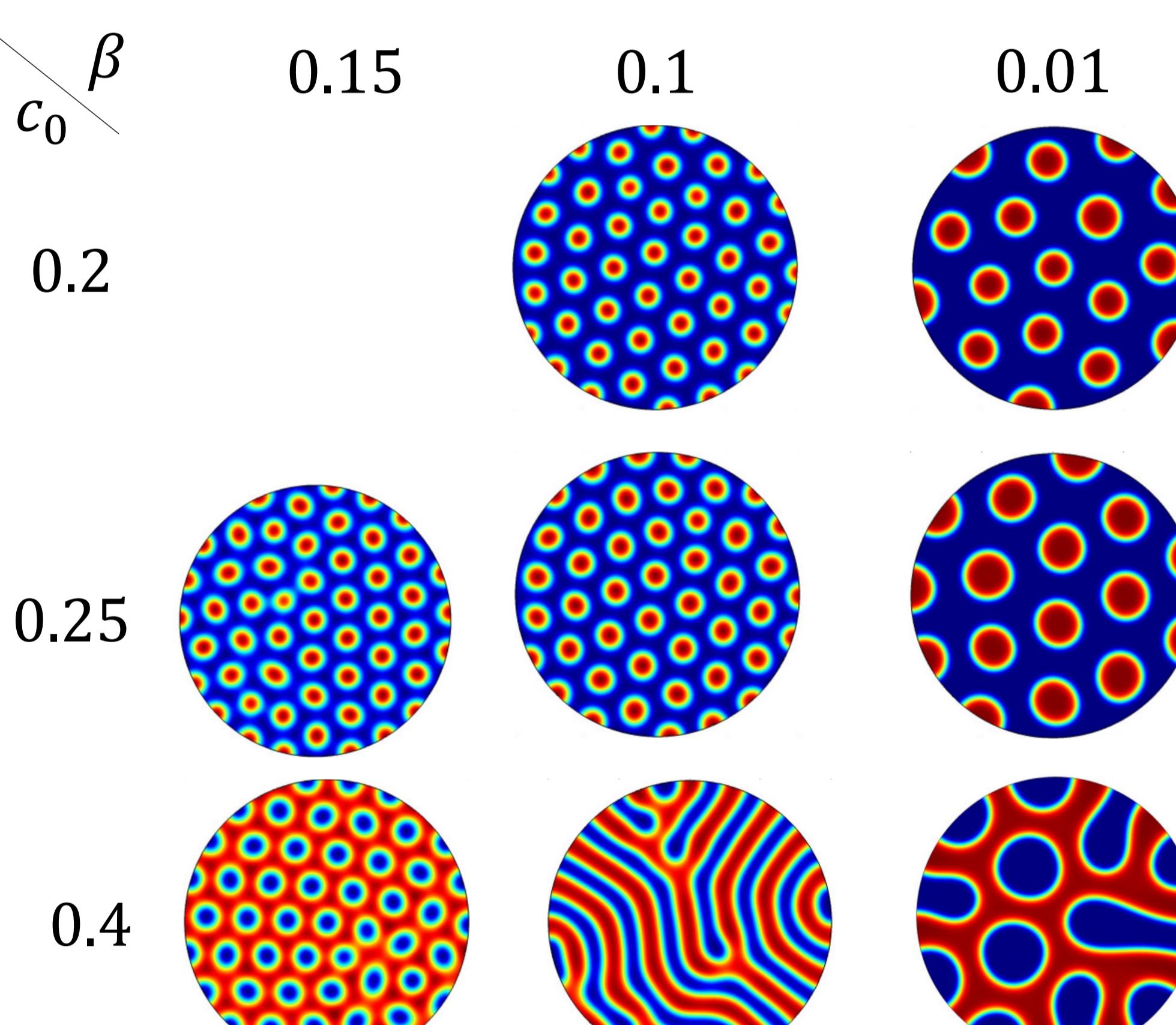
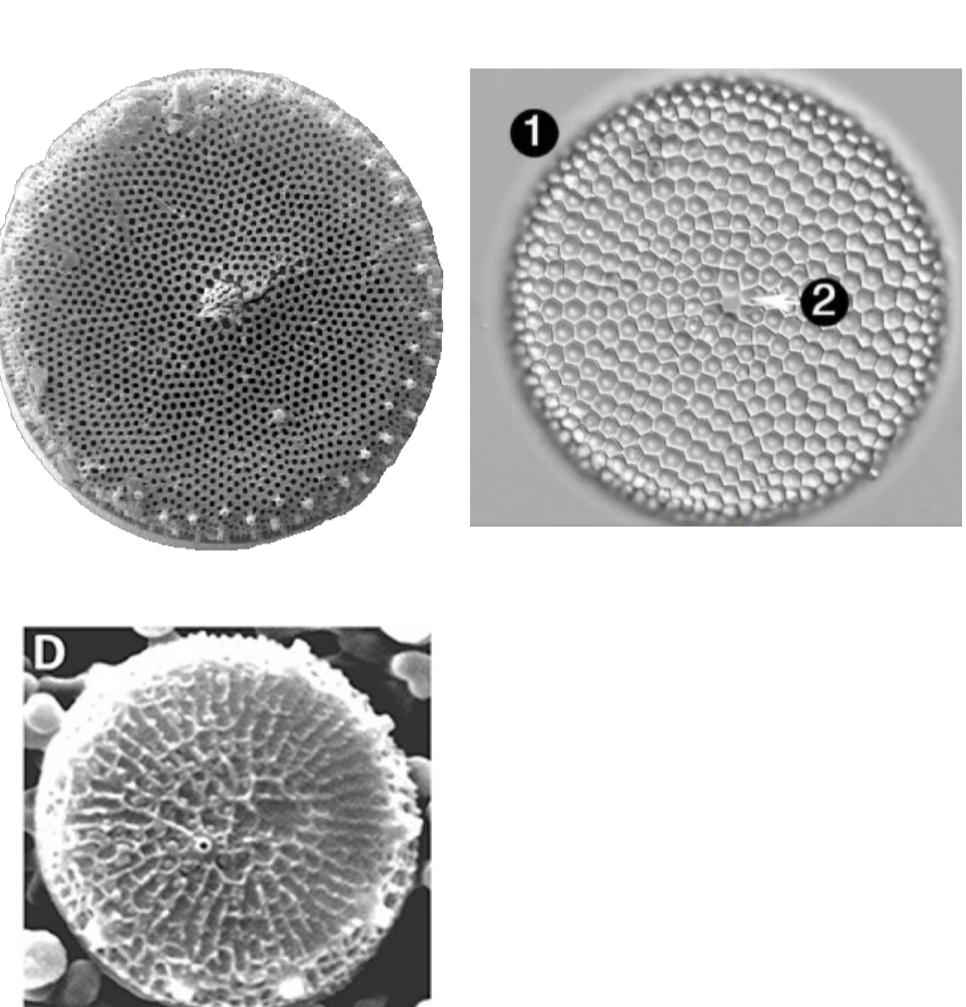
Flory-Huggins model:

$$g(\varphi) = g_0 \left( \frac{1}{N} \varphi \ln \varphi + (1 - \varphi) \ln (1 - \varphi) + \chi \varphi (1 - \varphi) \right)$$

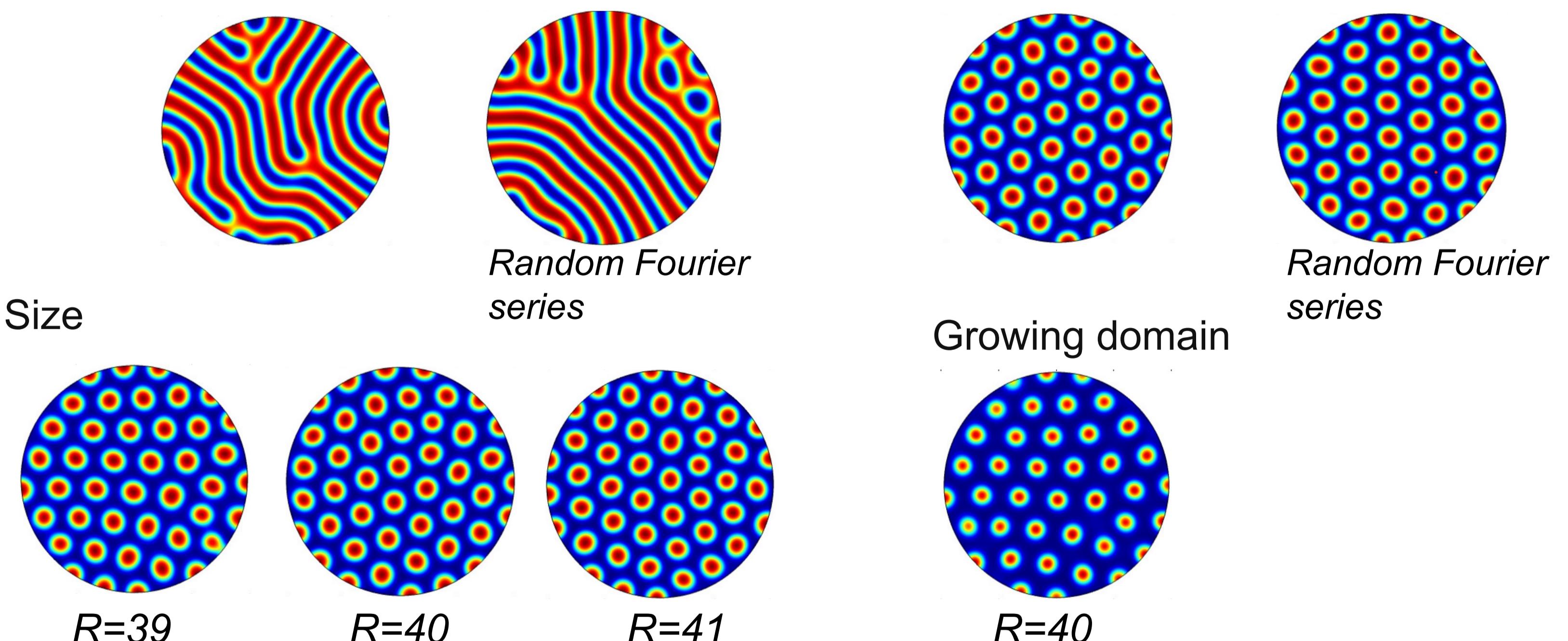
Where  $g_0$  - prefactor,  $N$  – degree of polymerization,  $\chi$  – Flory-Huggins interaction parameter



Flory-Huggins model:



## Initial Perturbations



## Future project/Interests:

- Expand such coupled problem to electro-
- Complex geometry
- Diffusion-controlled growth
- Polyamine enthalpy

