Institute of High Performance Computing (IHPC)

Dr. Zishun Liu (Z.S. Liu)

April 5, 2011 XJTU

Using Polymeric Gel Theory to Explain Plant Phyllotaxis

Z.S. Liu
IHPC, Singapore
National University of Singapore

Collaborators:

W. Hong: Iowa State University
Z.G. Suo: Harvard University
S. Swaddiwudhipong: National University of Singapore

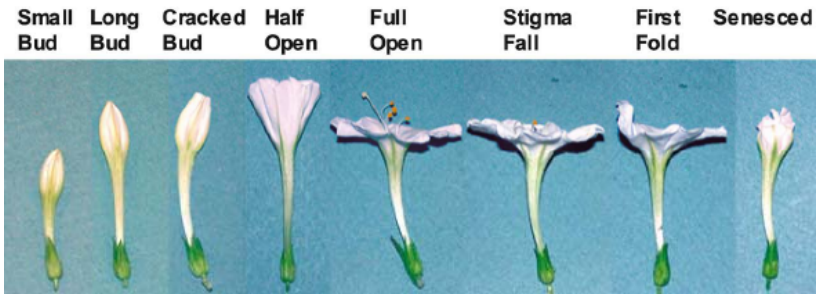
Using Polymeric Gel Theory to Explain Plant Phyllotaxis

OUTLINE

- Introduction
- Gel theories
- Modeling & Simulation of Gel Deformation
- Governing Equations of Film Gel Wrinkling
- Botanical plants modeling
- Future Study & Discussion

A*STAR IHPC

Introduction



Fascinating complex patterns and shapes & interesting undulating surface morphology

In plants, interesting undulating surface morphology is often observed across a large scale

Phyllotaxis: (namely the arrangement of phylla)
has intrigued natural scientists for over 400 years

Introduction

Question:

What are the physical mechanisms of this natural structure deformation?

How to explain the mechanism of flower opening and closure?

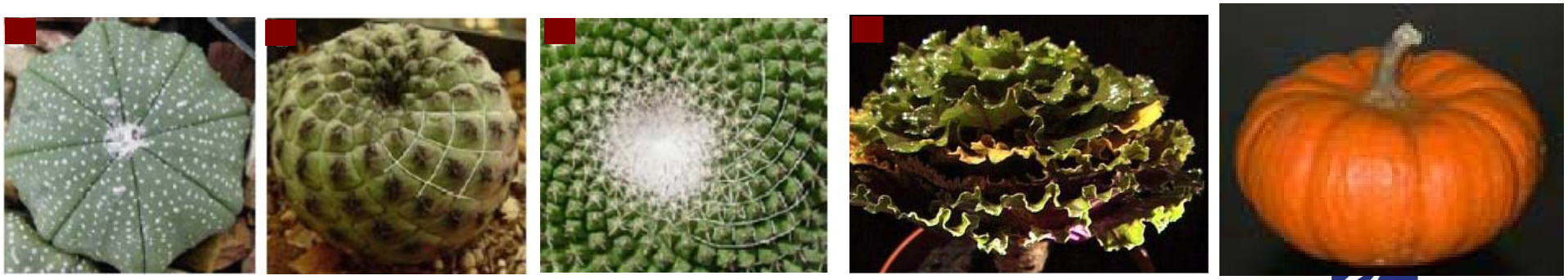
How to explain the morphogenesis of the natural growth of some leaves, flowers and vesicles?

The challenge:

How to provide a rational explanation for the formation of such patterns, a mechanism or combination of mechanisms which capture natural phenomena

Many natural tissues of plants and animals are to some extent polymeric gels.

Polymeric gel theory may be used to explain the formation of phyllotactic patterns at plant



Various phyllotactic lattice and tiling patterns

Newell et al, *J. Theoy. Boil.* 251, 2008

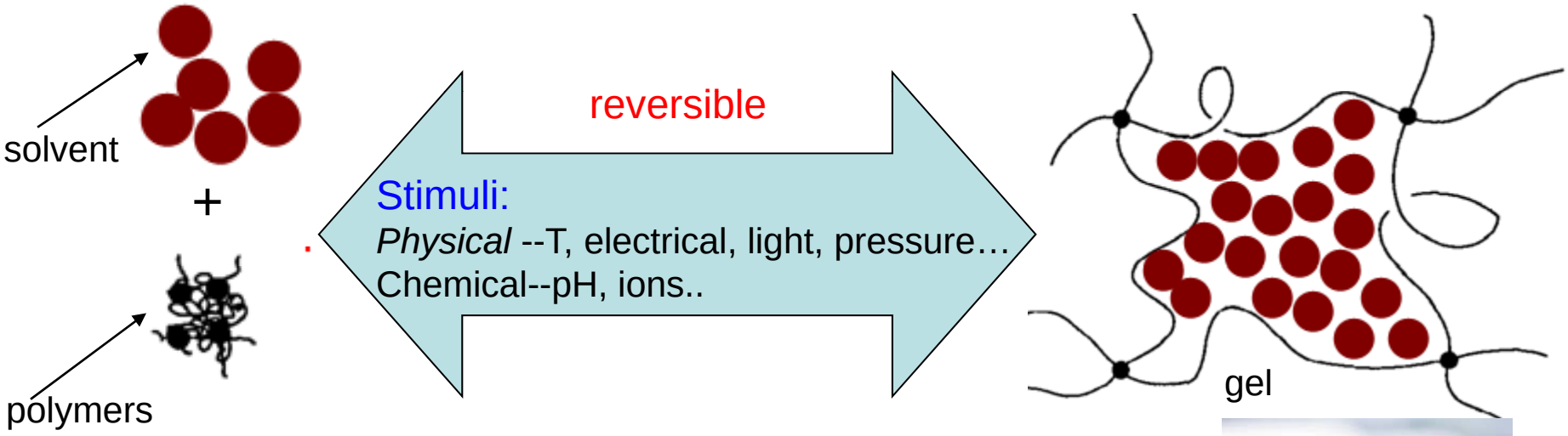
IHPC A*STAR

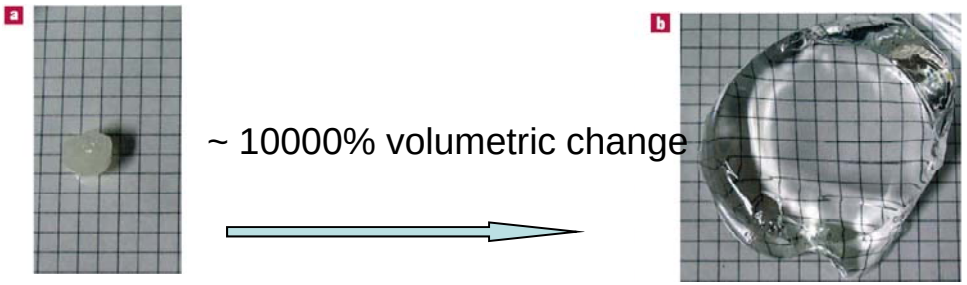
Introduction

What is Gel?

Gel= elastomer + solvent

- Elasticity: long polymers are cross-linked by strong bonds.
- Fluidity: polymers and solvent molecules aggregate by weak bonds.



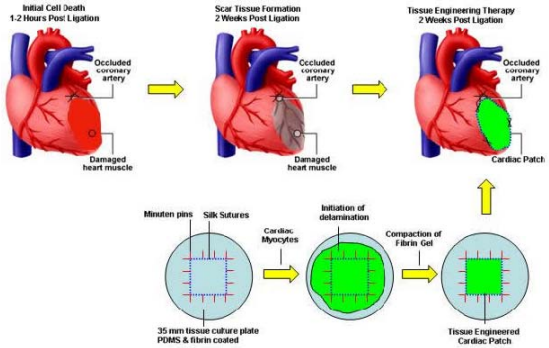


Polyelectrolyte gels

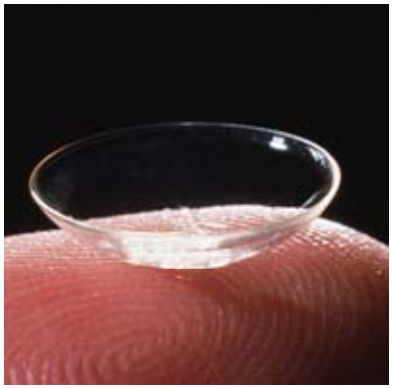
Introduction

Applications of Gels

Soft robots; Drug delivery; Tissue engineering; Water treatment; Sealing in oil wells; Sensor & actuator…

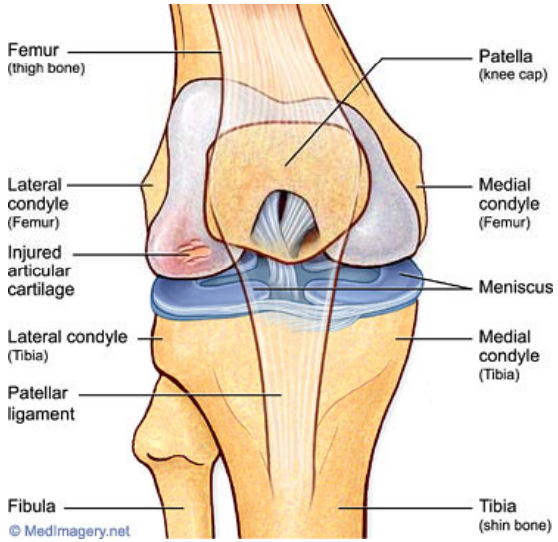


Repair damaged heart muscle

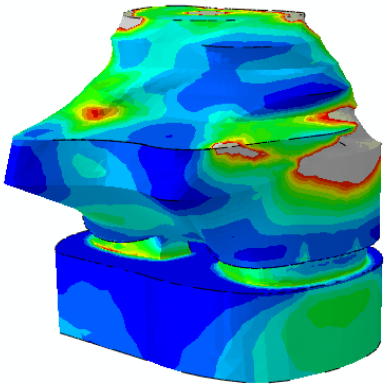


Contact lenses

Wichterie, Lim, Nature 185, 117 (1960)

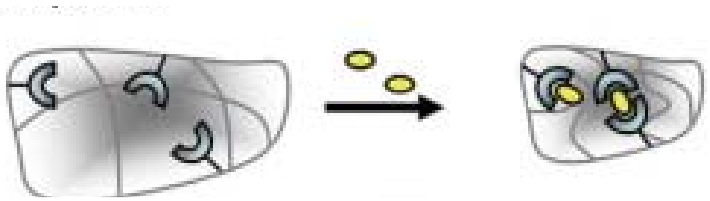


Tissues, natural or engineered



National University Hospital

Cartilage & Meniscus

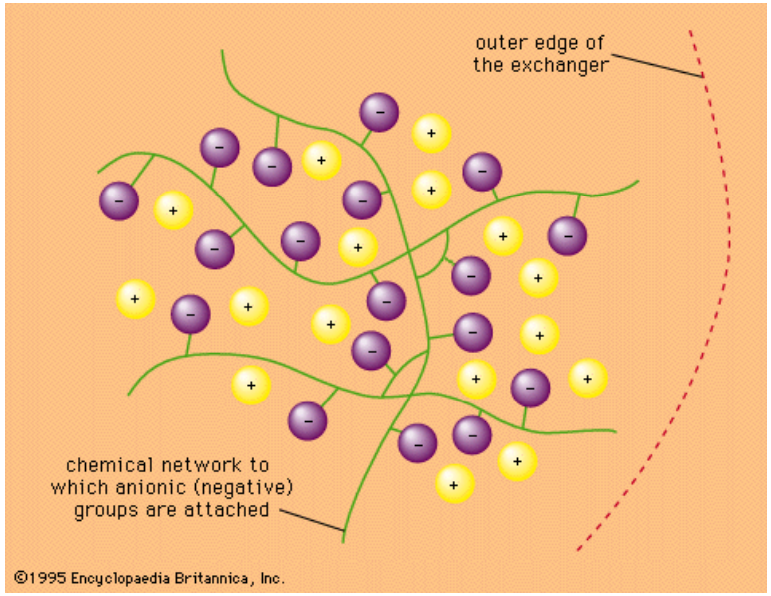


Nanogel & Drug delivery

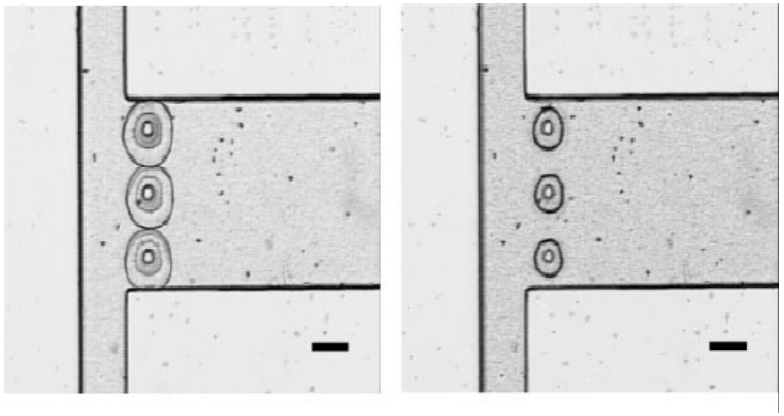
Ulijn et al. Materials Today 10, 40 (2007)

Introduction

Applications of Gels

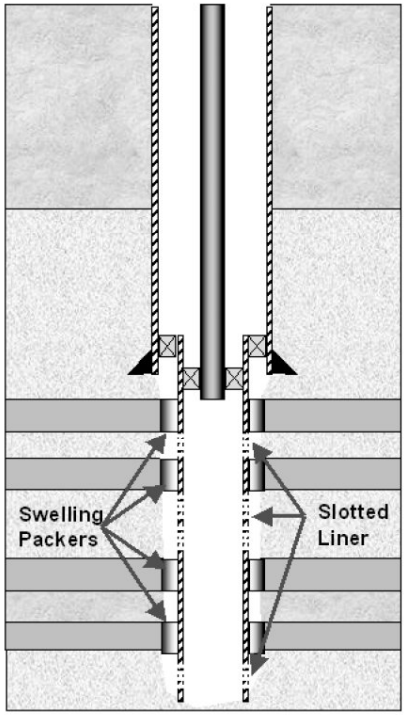


Ion exchange for water treatment



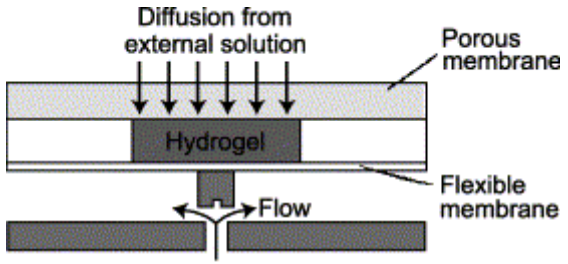
Beebe, Moore, Bauer, Yu, Liu, Devadoss, Jo, Nature 404, 588 (2000)

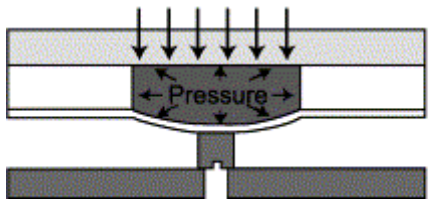
Valves in fluidics



Sealing in oil wells

Shell, 2003



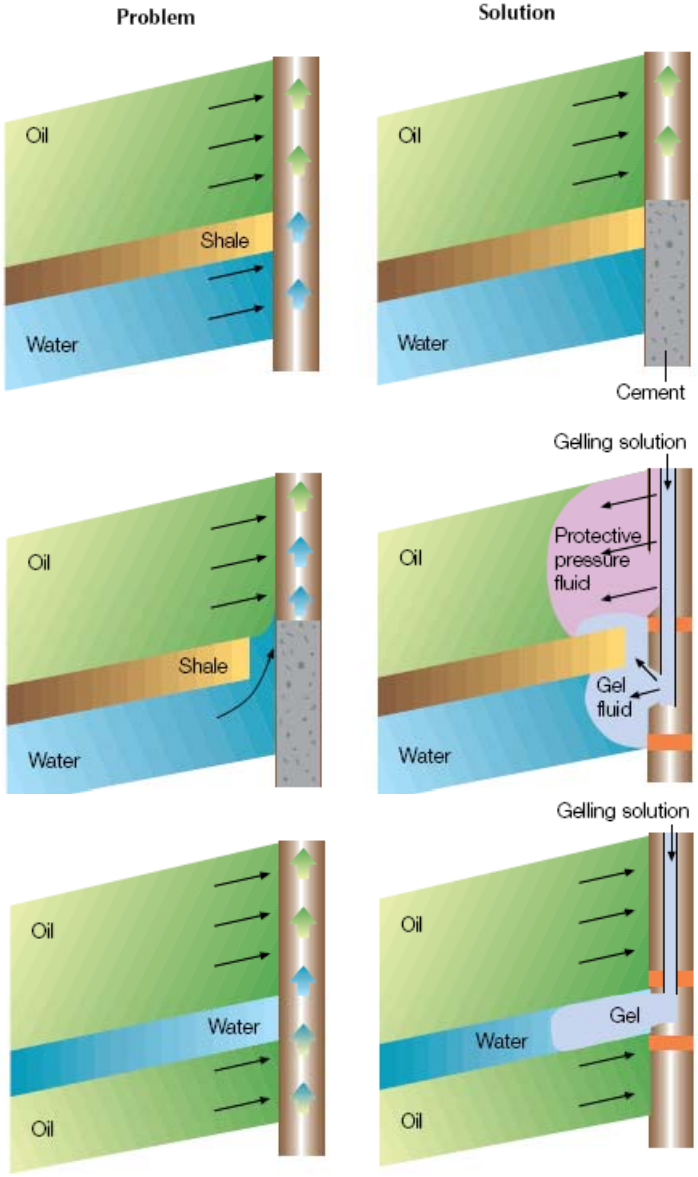


Hydrogel gate valve

IHPC

Introduction

Gelling System in Oil Well



1. Watered-out zone separated from an oil zone by an impermeable shale barrier-the solution is to cement in bottom zone.

2. Shale doesn't reach to production well. Solution is inject gel into the lower zone.

3. Watered-out high permeability zone sandwiched between two oil zones-the solution is to isolate the zone and inject gel

IHPC
A*STAR

Introduction

Challenges of Gel Applications

1. A lack of understanding of the relationship between gel composition and response kinetics

2. The majority of previous research efforts of gel are experimental-based

3. More complex shapes are required and the accurate dimensional measurements of their volume transition behaviors are not convenient in experimental analysis

4. A lack of completed analytical theory for Gel

5. The prediction of gel performance by modeling and simulation will thus be critical for understanding the characteristics of gel

A*STAR IHPC

Theories of Gel Deformation

THB Theory: Tanaka, Hocker, and Benedek, J. Chem. Phys. (1973)

Multiphasic theory

Biphasic theory: Bowen, Int. J. Eng. Sci. (1980)

Triphasic model: Lai, Hou, Mow, J. Biomech. Eng. Trans. (1991)

Mixture theory: Shi, Rajagopal, Wineman, Int. J. Eng. Sci. (1981)

Limitations

- No instant response to loads
- Linear theory, small deformation
- Basic principles are unclear, hard to extend

- View solvent and solute as two or three phases
- Unclear physical picture.
- Unmeasurable quantities.

Monophasic theory:

- Regard a gel as a single phase
- Start with thermodynamics
- Analogy to solid mechanics

Hong, Zhao, Zhou, Suo, JMPS (2007)

$$\int\left(\frac{\partial}{\partial X_K}\frac{\partial W}{\partial F_{iK}}+B_i\right)\delta x_i dV+\int\left(T_i-\frac{\partial W}{\partial F_{iK}}N_K\right)\delta x_i dA+\int\left(\mu-\frac{\partial W}{\partial C}\right)\delta C dV=0$$

Gibbs, The Scientific Papers of J. Willard Gibbs, 184, 201, 215 (1878): Derive equilibrium theory from thermodynamics.
Biot, JAP 12, 155 (1941): Use Darcy's law to model migration.
……
Hong, Zhao, Zhou, Suo, JMPS (2008)
Hong, Liu, Suo, IJSS (2009)
Liu, Hong, Suo, Somsak, Zhang, COMMAT, (2010)
Liu, Somsak, Cui, Hong, Suo, IJAM (2011)

PC

Theory of Gel Deformation

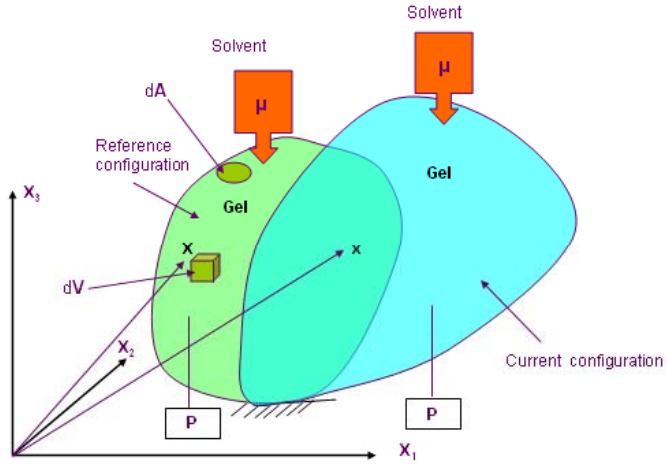
3D inhomogeneous fields:

$\mathbf{F} = \dfrac{\partial \mathbf{x}(\mathbf{X})}{\partial \mathbf{X}}$ Deformation gradient

$C(\mathbf{X}, t)$ Concentration of solvent

μ Chemical potential

$W(\mathbf{F}, C)$



A gel is in contact with a solvent of a fixed chemical potential, and subject to a mechanical load and geometric constraint

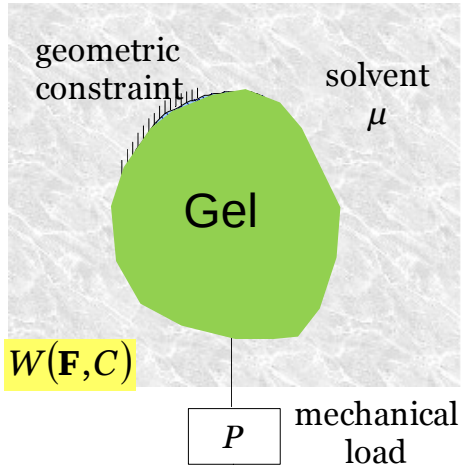
In equilibrium, the change in the free energy of the gel, associated with arbitrary change in displacement field and concentration field , equals the work done by the mechanical loads and the environment

Free-energy of system changes by

$$\delta G = \int \delta W dV - \int B_i \delta x_i dV - \int T_i \delta x_i dA - \mu \int \delta C dV$$

Free-energy density changes

$$\delta W = \frac{\partial W(\mathbf{F}, C)}{\partial F_{iK}} \delta F_{iK} + \frac{\partial W(\mathbf{F}, C)}{\partial C} \delta C$$



System = gel + load+ solvent

Hong, Zhao, Zhou, Suo, JMPS (2008)

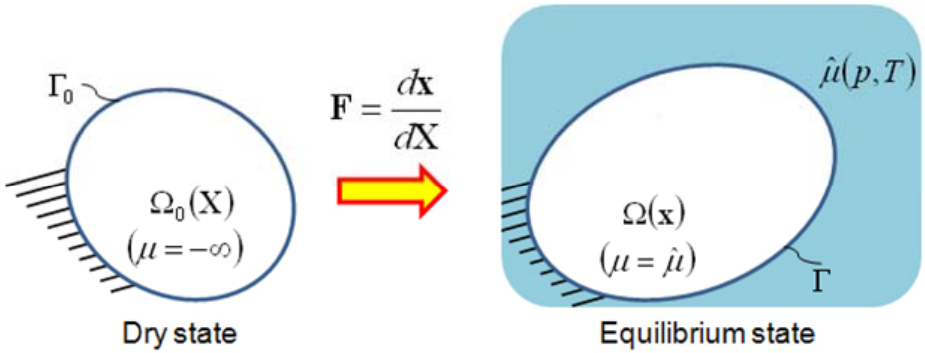
Chemical Potential

The chemical potential definition:

$$\mu = \frac{\partial U(S,V,N)}{\partial N} = \frac{\partial F(T,V,N)}{\partial N} = \frac{\partial G(T,p,N)}{\partial N}$$

Introducing the energy, entropy and volume per molecular u, s, and v

$$\mu = u - Ts + pv \qquad \delta\mu = -s\delta T + v\delta p$$



The chemical potential of the solvent (μ) in general depends on the temperature (T) and pressure (p) $\mu = \mu(T, p)$

In equilibrium: the chemical potential inside the gel be a constant and equal to the chemical potential of the external solvent $\mu = \hat{\mu}$

For constant Temperature

$\hat{\mu} = \hat{\mu}(p_0, T) + v(T)(p - p_0)$ for incompressible liquid phase

$\hat{\mu} = \hat{\mu}(p_0, T) + k_B T \log(p / p_0)$ for ideal gas

$$\hat{\mu} = \begin{cases} v(p - p_0) & if \quad p > p_0 \\ k_B T \log(p / p_0) & if \quad p < p_0 \end{cases}$$

where p_0 is the equilibrium vapor pressure and depends on the temperature,
At the equilibrium vapor pressure ($p = p_0$), the external chemical potential: $\hat{\mu} = 0$
In a vacuum (p = 0): $\hat{\mu} = -\infty$

IHPC
A*STAR

Theory of Gel Deformation

In equilibrium condition

$$\delta G = \int \delta W dV - \int B_i \delta x_i dV - \int T_i \delta x_i dA - \mu \int \delta C dV = 0$$

Free-energy density changes

$$\delta W = \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} \delta F_{iK} + \frac{\partial W(\mathbf{F},C)}{\partial C} \delta C$$

Applying the divergence theorem $\int_V \nabla \cdot \mathrm{G} dV = \int_\Gamma \mathrm{G} \cdot d\mathrm{A}$

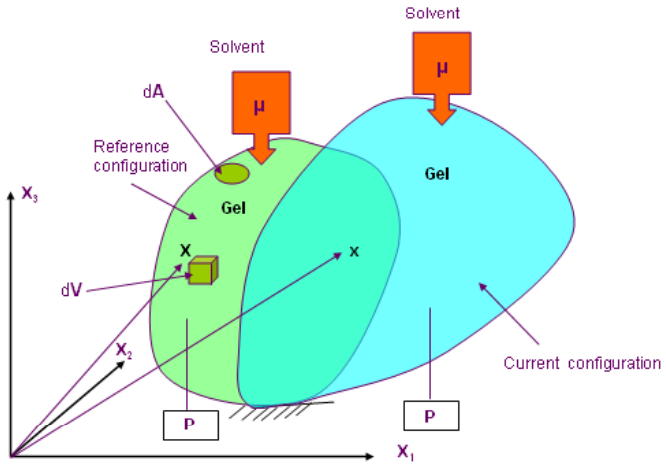
$$\int \left(\frac{\partial}{\partial X_K} \frac{\partial W}{\partial F_{iK}} + B_i \right) \delta x_i dV + \int \left(T_i - \frac{\partial W}{\partial F_{iK}} N_K \right) \delta x_i dA$$

$$+ \int \left(\mu - \frac{\partial W}{\partial C} \right) \delta C dV = 0$$

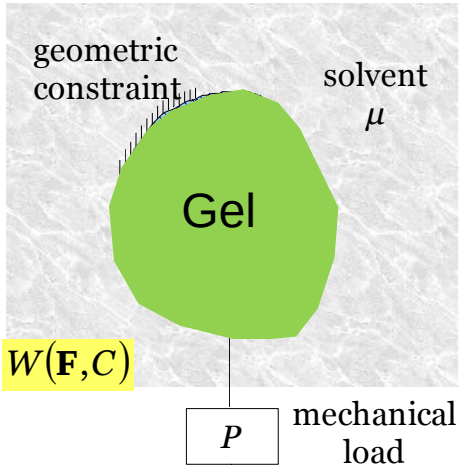
$$\frac{\partial}{\partial X_K} \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} + B_i = 0$$

$$\frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} N_K = T_i$$

$$\mu = \frac{\partial W(\mathbf{F},C)}{\partial C}$$



A gel is in contact with a solvent of a fixed chemical potential, and subject to a mechanical



System = gel + load+ solvent

Hong, Zhao, Zhou, Suo, JMPS (2008)

Theory of Gel Deformation

Introduce a new free-energy function $\hat{W}$ by a Legendre transform

$$\hat{W}(\mathbf{F},\mu) = W(\mathbf{F},C) - \mu C$$

New Equilibrium condition:

$$\int \delta \hat{W} dV = \int B_i \delta x_i dV + \int T_i \delta x_i dA$$

Define nominal stress as the work conjugate to the deformation gradient

$$s_{iK} = \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}}$$

The change in free energy

$$\delta W = \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} \delta F_{iK} + \frac{\partial W(\mathbf{F},C)}{\partial C} \delta C$$

$$\delta W = s_{iK} \delta F_{iK} + \mu \delta C$$

$$\delta \hat{W} = s_{iK} \delta F_{iK} - C \delta \mu$$

$$s_{iK} = \frac{\partial \hat{W}(\mathbf{F},\mu)}{\partial F_{iK}}$$

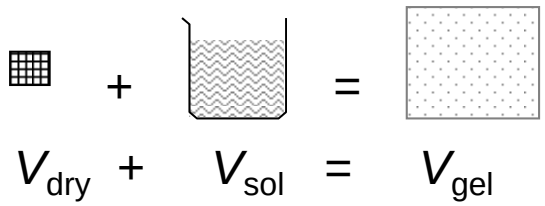
$$C = -\frac{\partial \hat{W}(\mathbf{F},\mu)}{\partial \mu}$$

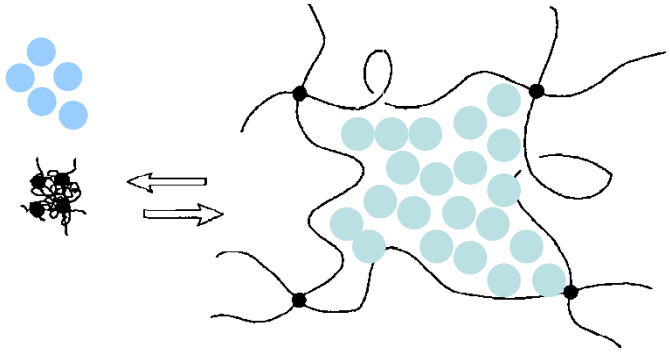
The true stress

$$\sigma_{ij} = \frac{F_{jK}}{\det \mathbf{F}} s_{iK} = \frac{F_{jK}}{\det \mathbf{F}} \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} = \frac{F_{jK}}{\det \mathbf{F}} \frac{\partial \hat{W}(\mathbf{F},\mu)}{\partial F_{iK}}$$

A*STAR IHPC

Molecular Incompressibility in Gels





$1 + vC = \det \mathbf{F}$ v – volume per solvent molecule

Assumptions:

- Individual solvent molecule and polymer are incompressible.
- Gel has no voids.

This molecular incompressibility condition can be enforced as a constraint by introducing a Lagrange multiplier Π

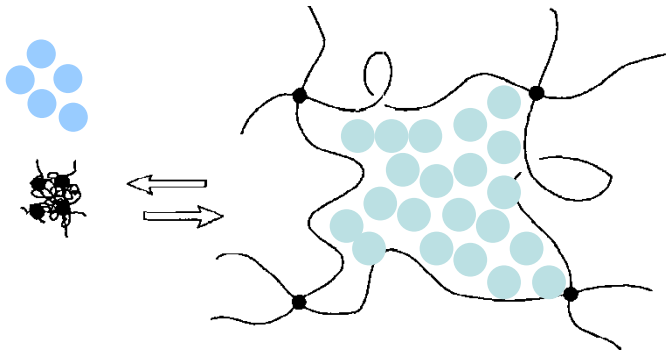
$$W(\mathbf{F}, C) = W(\mathbf{F}, C) + \Pi(1 + vC - \det \mathbf{F})$$

IHPC A*STAR

Theory of Gel Deformation

Flory-Rehner Free Energy in Gels

Swelling increases entropy by mixing solvent and polymers, but decreases entropy by straightening the polymers.



Following Flory and Rehner, the free energy density can be written as

Free-energy function $$W(\mathbf{F},C)=W_s(\mathbf{F})+W_m(C)$$

$$s_{iK}=\frac{\partial W}{\partial F_{iK}} \qquad \mu=\frac{\partial W}{\partial C}$$

Free energy of stretching $$W_s(\mathbf{F})=\frac{1}{2}NkT\left[F_{iK}F_{iK}-3-2\log(\det\mathbf{F})\right]$$

Free energy of mixing $$W_m(C)=-\frac{kT}{v}\left[vC\log\left(1+\frac{1}{vC}\right)+\frac{\chi}{1+vC}\right]$$

Flory, Rehner, J. Chem. Phys., 11, 521 (1943)

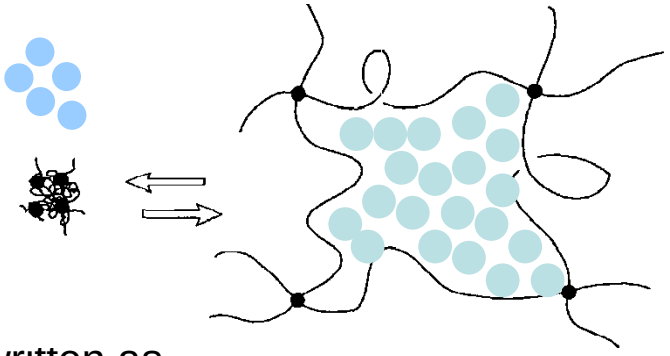
Flory-Huggins polymer theory

IHPC A*STAR

Theory of Gel Deformation

Flory-Rehner Free Energy in Gels

Consider the molecular incompressibility condition as a constraint by introducing a Lagrange multiplier Π



Following Flory and Rehner, the free energy density can be written as

Free-energy function $W(\mathbf{F},C)=W_s(\mathbf{F})+W_m(C)+\Pi(1+\upsilon C-\det\mathbf{F})$ $+\Pi_1(F,C)$

$$s_{iK}=\frac{\partial W}{\partial F_{iK}}=\frac{\partial W_s}{\partial F_{iK}}-\Pi H_{iK}\det\mathbf{F} \qquad \mu=\frac{\partial W}{\partial C}=\frac{\partial W_m}{\partial C}+\Pi\upsilon$$

Consider other energy terms

Open Space

....

$$s_{iK}=\frac{\partial W}{\partial F_{iK}}=\frac{\partial W_s}{\partial F_{iK}}-\Pi H_{iK}\det\mathbf{F}+\frac{\partial \Pi_1}{\partial F_{iK}} \qquad \mu=\frac{\partial W}{\partial C}=\frac{\partial W_m}{\partial C}+\Pi\upsilon+\frac{\partial \Pi_1}{\partial C}$$

A*STAR IHPC

Theory of Gel Deformation

Free energy $$W(\mathbf{F},C)=W_s(\mathbf{F})+W_m(C)+\Pi(1+\upsilon C-\det\mathbf{F})$$

$$W_s(\mathbf{F})=\frac{1}{2}NkT\left[F_{iK}F_{iK}-3-2\log(\det\mathbf{F})\right] \qquad W_m(C)=-\frac{kT}{\upsilon}\left[\upsilon C\log\left(1+\frac{1}{\upsilon C}\right)+\frac{\chi}{1+\upsilon C}\right]$$

$$s_{iK}=\frac{\partial W_s}{\partial F_{iK}}-\Pi H_{iK}\det\mathbf{F} \qquad \mu=\frac{\partial W_m}{\partial C}+\Pi\upsilon$$

Assume the principal nominal stresses are $s_1=s_{11}$ $s_2=s_{22}$ $s_3=s_{33}$ $\mathbf{F}=\begin{bmatrix}\lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3\end{bmatrix}$

$$s_1=NkT(\lambda_1-\lambda_1^{-1})-\Pi\lambda_2\lambda_3$$
$$s_2=NkT(\lambda_2-\lambda_2^{-1})-\Pi\lambda_1\lambda_3$$
$$s_3=NkT(\lambda_3-\lambda_3^{-1})-\Pi\lambda_1\lambda_2$$

$$\mu=kT\left[\log\left(\frac{\upsilon C}{1+\upsilon C}\right)+\frac{1}{1+\upsilon C}+\frac{\chi}{(1+\upsilon C)^2}\right]+\Pi\upsilon$$

Constitutive equations:

$$\frac{\upsilon s_1}{kT}=N\upsilon\left(\lambda_1-\frac{1}{\lambda_1}\right)+\left[\lambda_1\lambda_2\lambda_3\log\left(1-\frac{1}{\lambda_1\lambda_2\lambda_3}\right)+1+\frac{\chi}{\lambda_1\lambda_2\lambda_3}-\frac{\mu}{kT}\lambda_1\lambda_2\lambda_3\right]\frac{1}{\lambda_1}$$

$$\frac{\upsilon s_2}{kT}=N\upsilon\left(\lambda_2-\frac{1}{\lambda_2}\right)+\left[\lambda_1\lambda_2\lambda_3\log\left(1-\frac{1}{\lambda_1\lambda_2\lambda_3}\right)+1+\frac{\chi}{\lambda_1\lambda_2\lambda_3}-\frac{\mu}{kT}\lambda_1\lambda_2\lambda_3\right]\frac{1}{\lambda_2}$$

$$\frac{\upsilon s_3}{kT}=N\upsilon\left(\lambda_3-\frac{1}{\lambda_3}\right)+\left[\lambda_1\lambda_2\lambda_3\log\left(1-\frac{1}{\lambda_1\lambda_2\lambda_3}\right)+1+\frac{\chi}{\lambda_1\lambda_2\lambda_3}-\frac{\mu}{kT}\lambda_1\lambda_2\lambda_3\right]\frac{1}{\lambda_3}$$

A*STAR IHPC

Theory of Gel Deformation

General Form of Equations of State in Gels

Enforce molecular incompressibility as a constraint by introducing a Lagrange multiplier P

$$s_{iK} = \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} - \Pi H_{iK} \det(\mathbf{F}) \qquad \mu = \frac{\partial W(\mathbf{F},C)}{\partial C} + \Pi v$$

Use the Flory-Rehner free energy

$$s_{iK} = NkT(F_{iK} - H_{iK}) - \Pi H_{iK} \det \mathbf{F} \qquad \mu = kT\left[\log\frac{vC}{1+vC} + \frac{1}{1+vC} + \frac{\chi}{(1+vC)^2}\right] + \Pi v$$

Constitutive Equations

$$\frac{vs_{iK}}{kT} = Nv(F_{iK} - H_{iK}) + \left[\det(\mathbf{F})\log\left(1 - \frac{1}{\det \mathbf{F}}\right) + 1 + \frac{\chi}{\det \mathbf{F}} - \frac{\mu}{kT}\det \mathbf{F}\right] H_{iK}$$

A*STAR IHPC

FEM Implementation for Deformation in Gels

Constitutive equations (Equation of State)

$$\frac{\upsilon s_{iK}}{kT} = Nv\left(F_{iK} - H_{iK}\right) + \left[\det(\mathbf{F})\log\left(1 - \frac{1}{\det\mathbf{F}}\right) + 1 + \frac{\chi}{\det\mathbf{F}} - \frac{\mu}{kT}\det\mathbf{F}\right]H_{iK}$$

We select new reference state of the gel by free swelling $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_o$

$$\mathbf{F} = \mathbf{F}' \cdot \mathbf{F}_o \qquad \mathbf{F}_o = \begin{bmatrix} \lambda_o & & \\ & \lambda_o & \\ & & \lambda_o \end{bmatrix} \qquad I' = F'_{iK} F'_{iK} \qquad J' = \det\mathbf{F}'$$

$$\hat{W}(\mathbf{F},\mu) = \frac{1}{2}NkT\left(\lambda_o^2 I' - 3 - 2\log J' - 6\log\lambda_o\right) - \frac{kT}{\upsilon}\left[\left(\lambda_o^3 J' - 1\right)\log\frac{J'}{J' - \lambda_o^{-3}} + \frac{\chi}{\lambda_o^3 J'}\right] - \frac{\mu}{\upsilon}\left(\lambda_o^3 J' - 1\right)$$

Constitutive equations (Equation of state)

$$\frac{\upsilon s'_{iK}}{kT} = Nv\left(\lambda_o^2 F'_{iK} - H'_{iK}\right) + \lambda_o^3\left[\det(\mathbf{F}')\log\left(1 - \frac{1}{\lambda_o^3\det\mathbf{F}'}\right) + \frac{1}{\lambda_o^3} + \frac{\chi}{\lambda_o^6\det\mathbf{F}'} - \frac{\mu}{kT}\det\mathbf{F}'\right]H'_{iK}$$

ABAQUS UMAT ABAQUS UHYPE

Hong, Liu, Suo: IJSS (2009)

Liu, Hong, Suo, Somsak, Zhang, Com. Mat. Sci. (2010)

Theory of Gel

Neutral Gel Theory:

$\mathbf{F} = \dfrac{\partial \mathbf{x}(\mathbf{X})}{\partial \mathbf{X}}$ Deformation gradient

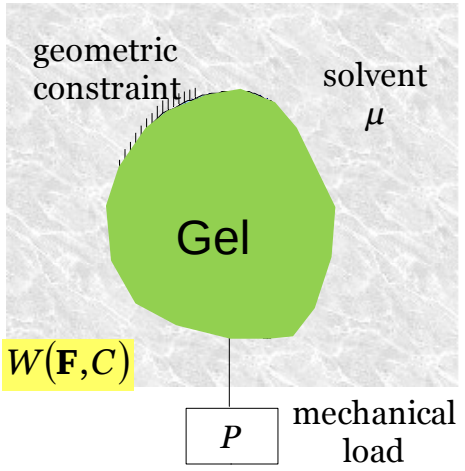
$C(\mathbf{x},t)$ Concentration of solvent

μ Chemical potential

$$1 + vC = \det \mathbf{F}$$

incompressible constraint

v – volume per solvent molecule



The change of free-energy of system

$$\delta G = \int \delta W dV - \int B_i \delta x_i dV - \int T_i \delta x_i dA - \mu \int \delta C dV$$

$$\int \left(\frac{\partial}{\partial X_K} \frac{\partial W}{\partial F_{iK}} + B_i \right) \delta x_i dV + \int \left(T_i - \frac{\partial W}{\partial F_{iK}} N_K \right) \delta x_i dA + \int \left(\mu - \frac{\partial W}{\partial C} \right) \delta C dV = 0$$

System = gel + load+ solvent

Hong, Zhao, Zhou, Suo, JMPS (2007)

$$\frac{\partial}{\partial X_K} \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} + B_i = 0$$

$$\frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} N_K = T_i$$

$$\mu = \frac{\partial W(\mathbf{F},C)}{\partial C}$$

Define nominal stress

$$s_{iK} = \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}}$$

$$\delta W = \frac{\partial W(\mathbf{F},C)}{\partial F_{iK}} \delta F_{iK} + \frac{\partial W(\mathbf{F},C)}{\partial C} \delta C$$

Flory, Rehner, J. Chem. Phys., (1943)

$$W(\mathbf{F},C) = W_{net}(\mathbf{F}) + W_{sol}(C) + \Pi(1 + vC - \det \mathbf{F})$$

$$W_{net}(\mathbf{F}) = \frac{1}{2} NkT \left[F_{iK} F_{iK} - 3 - 2 \log(\det \mathbf{F}) \right]$$

$$W_{sol}(C) = -\frac{kT}{v} \left[vC \log\left(1 + \frac{1}{vC}\right) + \frac{\chi}{1 + vC} \right]$$

$$1 + vC = \det \mathbf{F}$$

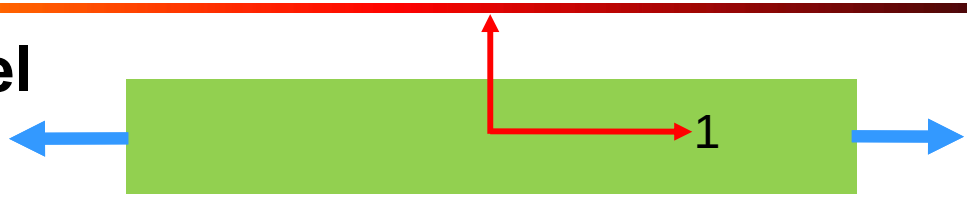
Constitutive Equations

$$\frac{v s_{iK}}{kT} = Nv(F_{iK} - H_{iK}) + \left[\det(\mathbf{F}) \log\left(1 - \frac{1}{\det \mathbf{F}}\right) + 1 + \frac{\chi}{\det \mathbf{F}} - \frac{\mu}{kT} \det \mathbf{F} \right] H_{iK}$$

Hong, Liu, Suo, IJSS, (2009)

Analytical solution of 1-D beam gel buckling

Incremental Modulus of the Gel



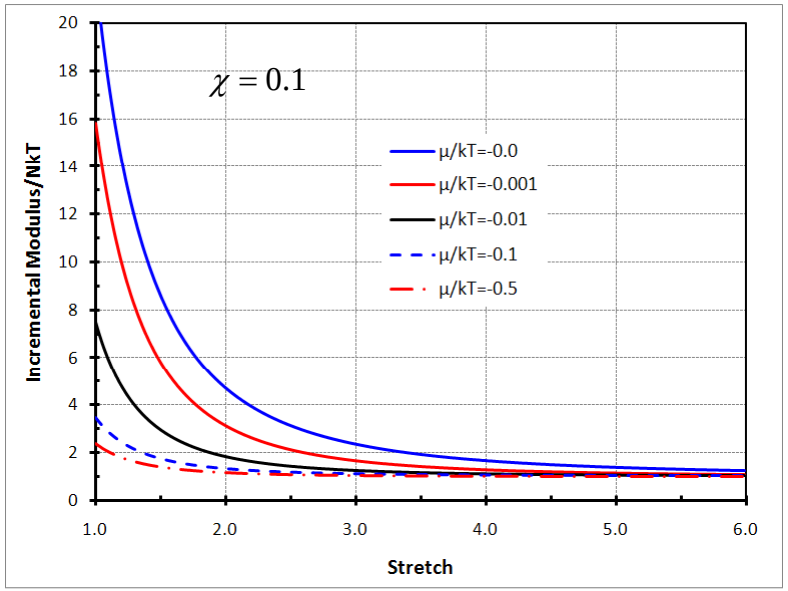
For column or bean case

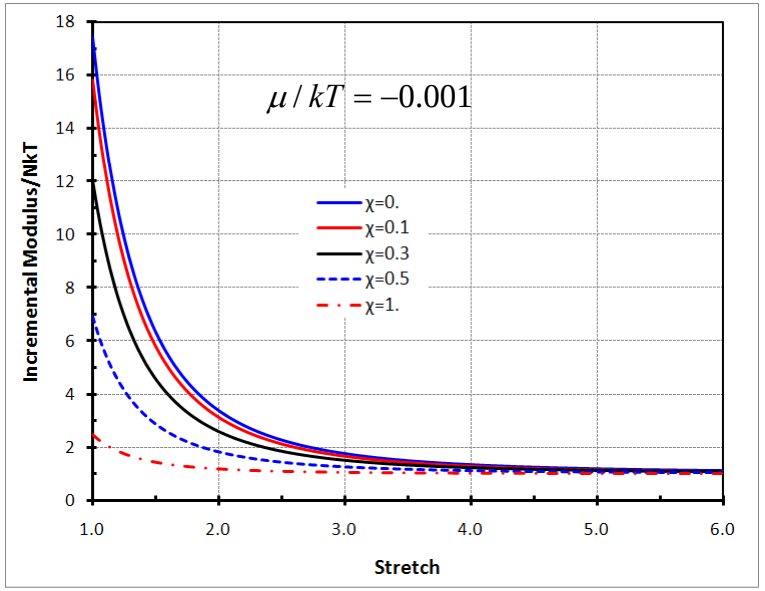
$$\frac{\upsilon s_1}{kT} = N\upsilon\left(\lambda_1 - \frac{1}{\lambda_1}\right) + \left[\lambda_1\lambda_2^2 \log\left(1 - \frac{1}{\lambda_1\lambda_2^2}\right) + 1 + \frac{\chi}{\lambda_1\lambda_2^2} - \frac{\mu}{kT}\lambda_1\lambda_2^2\right]\frac{1}{\lambda_1}$$

$$N\upsilon\left(\lambda_2 - \frac{1}{\lambda_2}\right) + \left[\lambda_1\lambda_2^2 \log\left(1 - \frac{1}{\lambda_1\lambda_2^2}\right) + 1 + \frac{\chi}{\lambda_1\lambda_2^2} - \frac{\mu}{kT}\lambda_1\lambda_2^2\right]\frac{1}{\lambda_2} = 0$$

$$\tilde{E} = \partial s_1 / \partial \varepsilon_1 = \partial s_1 / \partial \lambda_1$$

$$\frac{\upsilon}{kT}\tilde{E} = N\upsilon\left(1 + \frac{\lambda_2^2}{\lambda_1^2}\right)$$





Incremental modulus of gel varying with stretch for a) various initial chemical potentials b) various dimensionless measures of the enthalpy of mixing

Liu, Somsak, Cui, Hong, Suo, Zhang, IJAM, (2011)

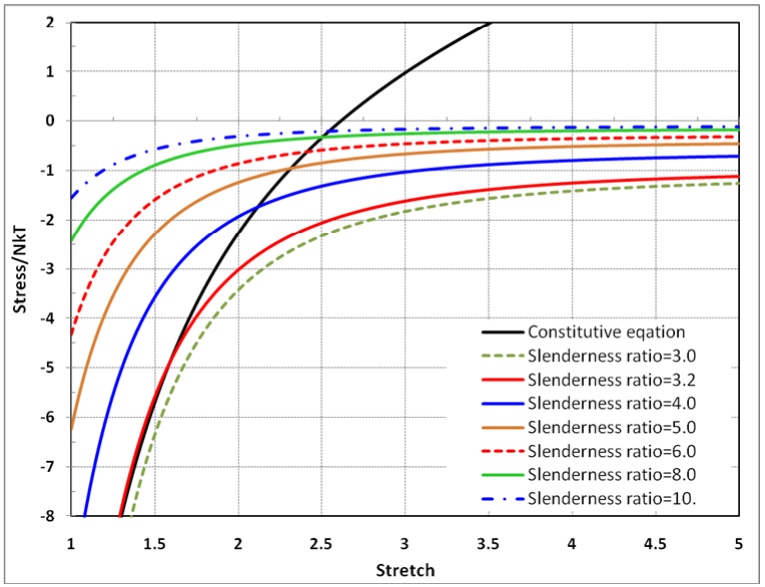
Analytical solution of 1-D beam gel buckling

Critical values of beam gel under buckling

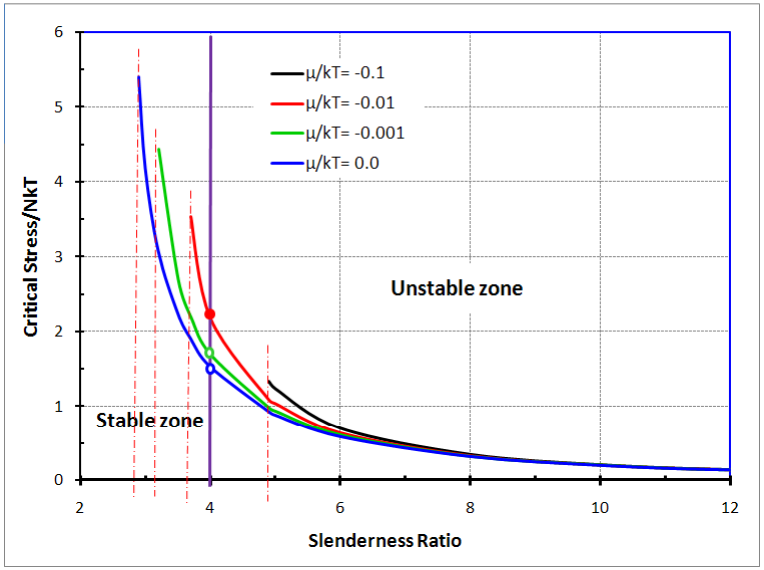
the critical stress of a column with hinged ends (Timoshenko and Gere)

$$(s)_{cr} = \frac{\pi^2 \tilde{E}}{(l/r)^2}$$

$$\frac{kT}{v}\left\{Nv\left(\lambda_1 - \frac{1}{\lambda_1}\right) + \left[\lambda_1\lambda_2^2 \log\left(1 - \frac{1}{\lambda_1\lambda_2^2}\right) + 1 + \frac{\chi}{\lambda_1\lambda_2^2} - \frac{\mu}{kT}\lambda_1\lambda_2^2\right]\frac{1}{\lambda_1}\right\} = \frac{\pi^2 NkT}{(l/r)^2}\left(1 + \frac{\lambda_2^2}{\lambda_1^2}\right)$$



Different stress curves varying with stretch



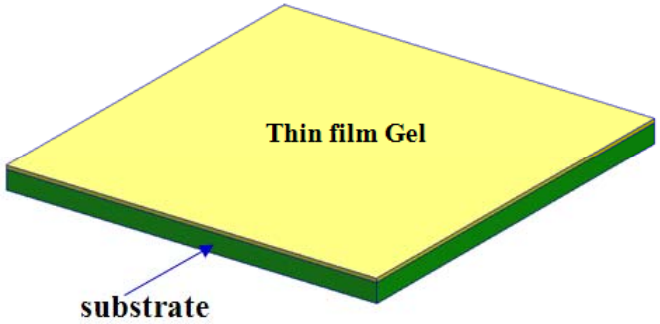
Stability diagram showing normalized critical stress of gel beam varying with its slenderness ratio of beam for different chemical potentials

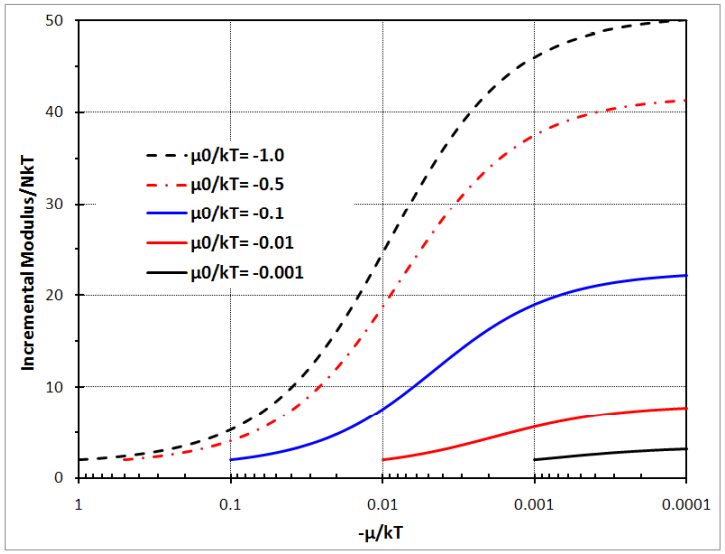
Liu, Somsak, Cui, Hong, Suo, Zhang, IJAM, (2011)

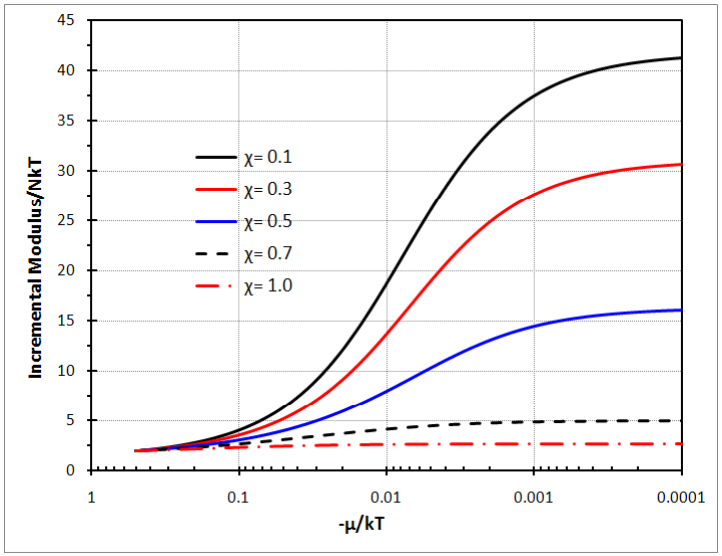
Thin Film Gel with Wrinkle Mode

In-plane Incremental Modulus of thin film gel

$$\frac{v}{kT}\tilde{E} = Nv\left(1+\frac{\lambda_3^2}{\lambda_1^2}\right) \qquad \frac{v}{kT}\tilde{E} = Nv\left(1+\lambda^2\right)$$



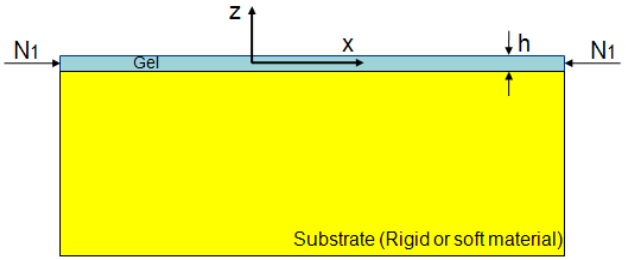


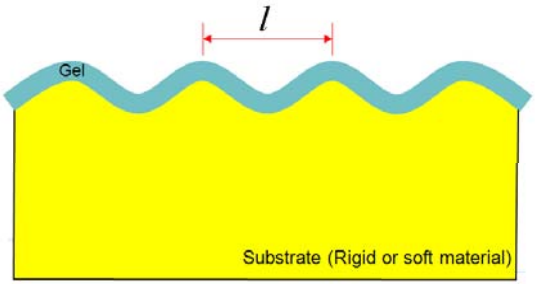


In-plane incremental modulus of thin film gel varying with chemical potential for a) different initial chemical potentials, b) different dimensionless measures of the enthalpy of mixing

Thin Film Gel with Wrinkle Mode

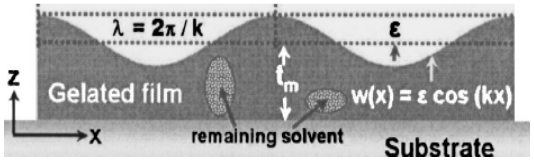
The buckling stress and wave length of thin film gel

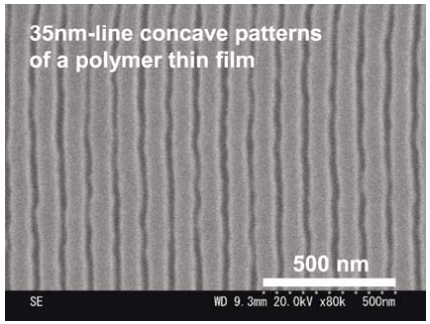




Schematics of thin gel film before and after bucking

Wrinkling of a sol-gel-derived thin film





$$D\nabla^4 w-(N_1)\nabla^2 w=-bq \qquad w=w_m\sin\frac{2\pi x}{l} \qquad q=\frac{2A}{l}w_m\sin\frac{2\pi x}{l}$$

$$\sigma_1=\frac{4\pi^2 D}{bh_0^3}\left(\frac{h_0}{l}\right)^2+\frac{A}{2\pi^2}\left(\frac{l}{h_0}\right)=\frac{4\pi^2 D}{bh_0^3}\left(\frac{1}{\phi}\right)^2+\frac{A}{2\pi^2}\phi$$

To minimize $\dfrac{\partial\sigma_1}{\partial\phi}=0$

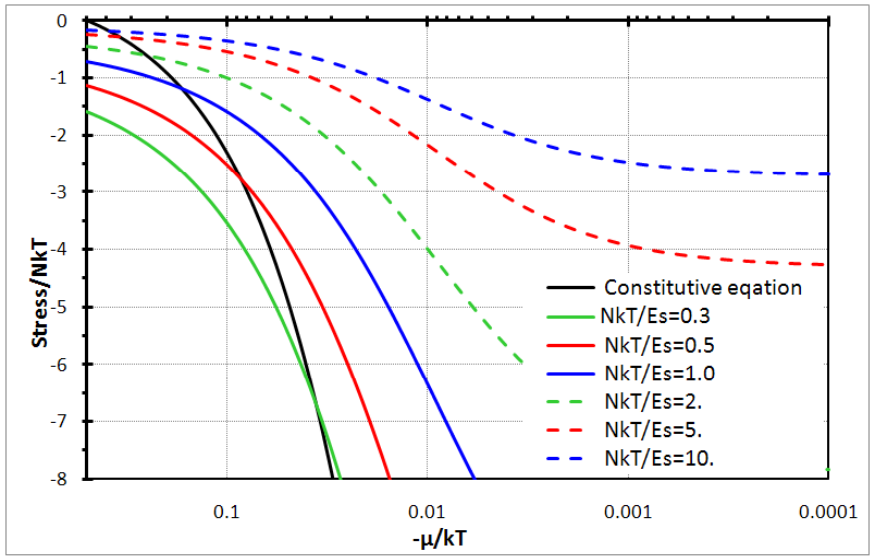
$$\phi_{cr}=\left(\frac{l}{h_0}\right)_{cr}=\left(\frac{4\pi^4 NkT(1+\lambda^2)\lambda^3}{3A}\right)^{1/3}$$

$$\sigma_{1cr}=\frac{\pi^2 NkT(1+\lambda^2)\lambda^3}{3}\left(\frac{4\pi^4 NkT(1+\lambda^2)\lambda^3}{3A}\right)^{-2/3}+\frac{A}{2\pi^2}\left(\frac{4\pi^4 NkT(1+\lambda^2)\lambda^3}{3A}\right)^{1/3}$$

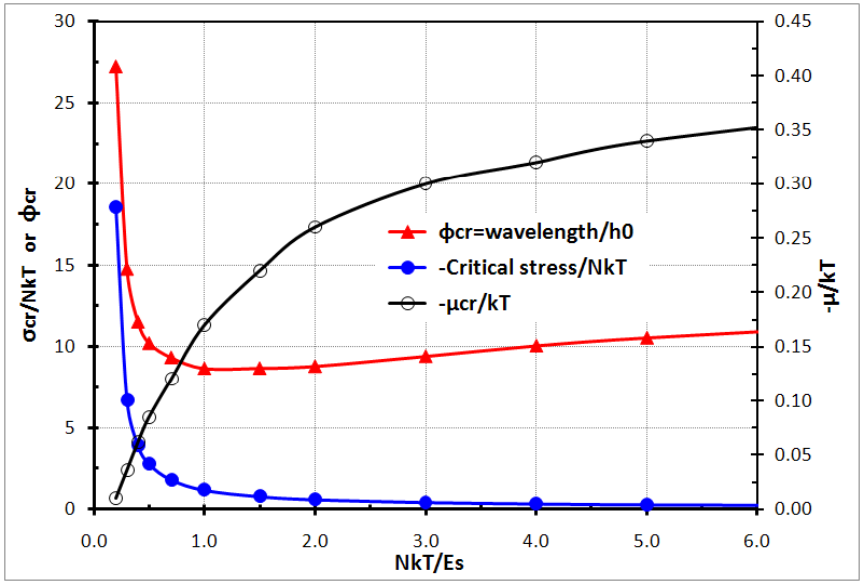
Liu, Somsak, Cui, Hong, Suo, Zhang, IJAM, (2011)

Thin Film Gel with Wrinkle Mode

The buckling stress and wave length of thin film gel



Normalized stresses varying with chemical potential for different gel film and substrate stiffness factor of NkT/Es

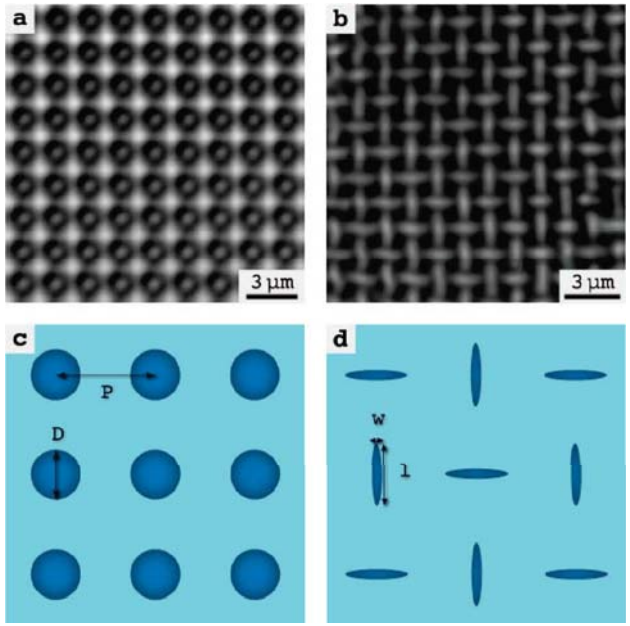


Normalized critical stress, normalized wavelength and critical chemical potential of thin film gel varying with gel film and substrate stiffness factor of NkT/Es

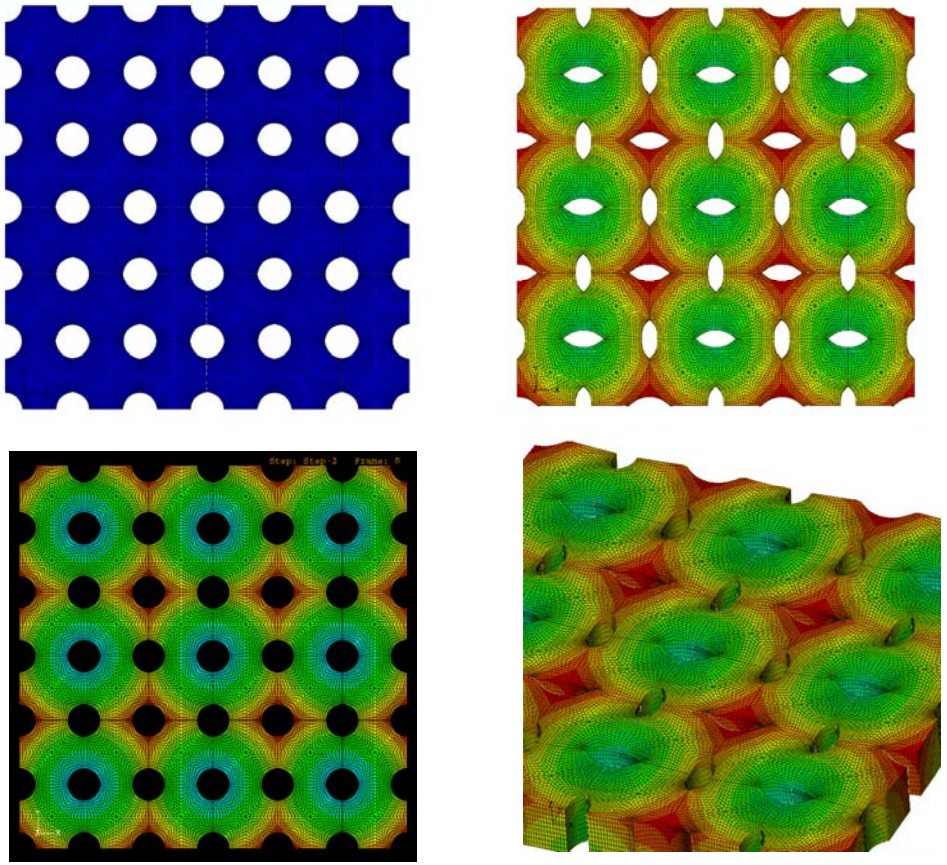
Liu, Somsak, Cui, Hong, Suo, Zhang, IJAM, (2011)

PDMS membrane gel on substrate in swelling

Swelling-induced bifurcation



Zhang Y et. al. Nano Letter 2008

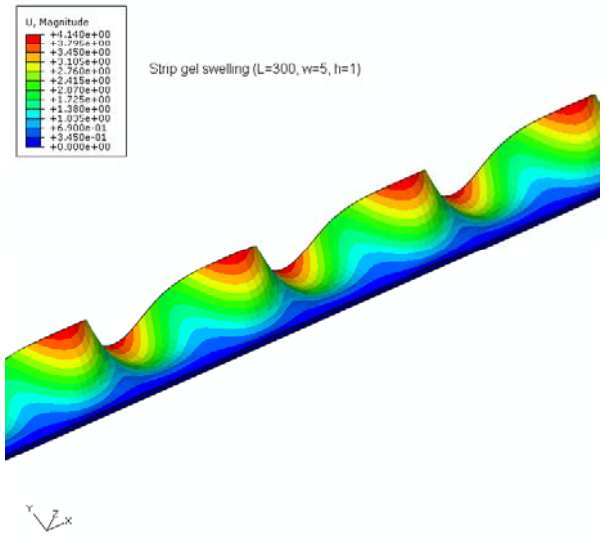


The pattern of PDMS membrane gel with a square lattice of holes before and after swelling

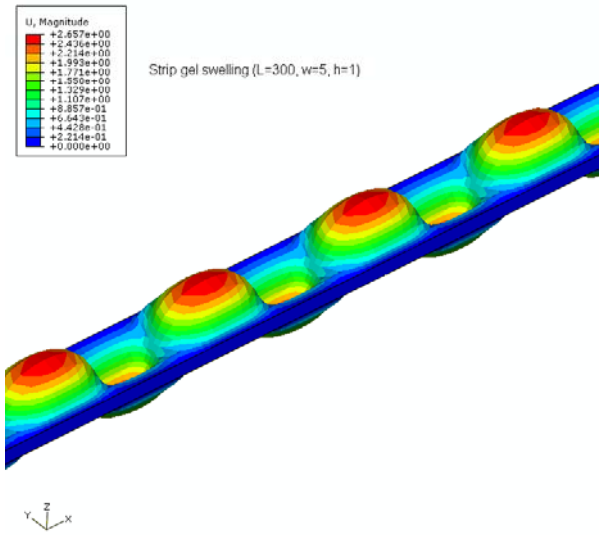
A square lattice of cylindrical holes bifurcates into a periodic structure of ellipses with alternating directions

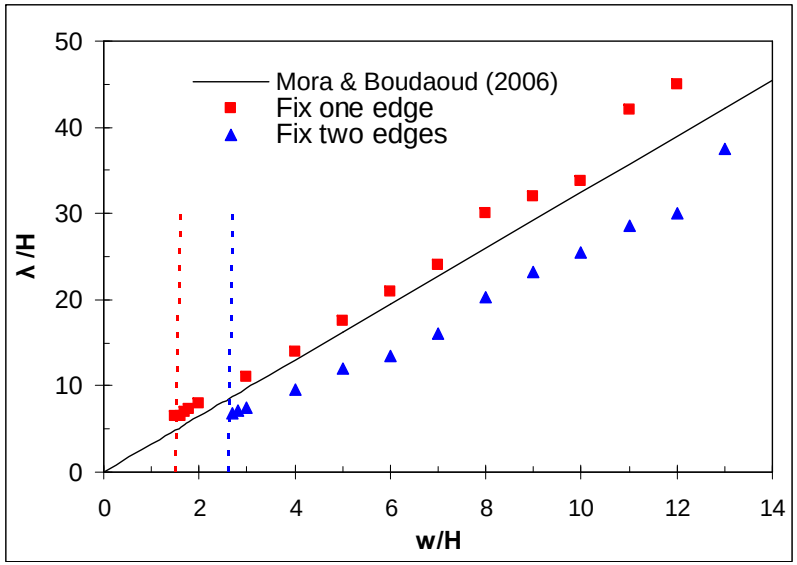
Hong, Liu, Suo, IJSS, (2009)

Rectangular Strip Membrane Gel



http://www.lmm.jussieu.fr/~audoly/research/ssw/index.htm



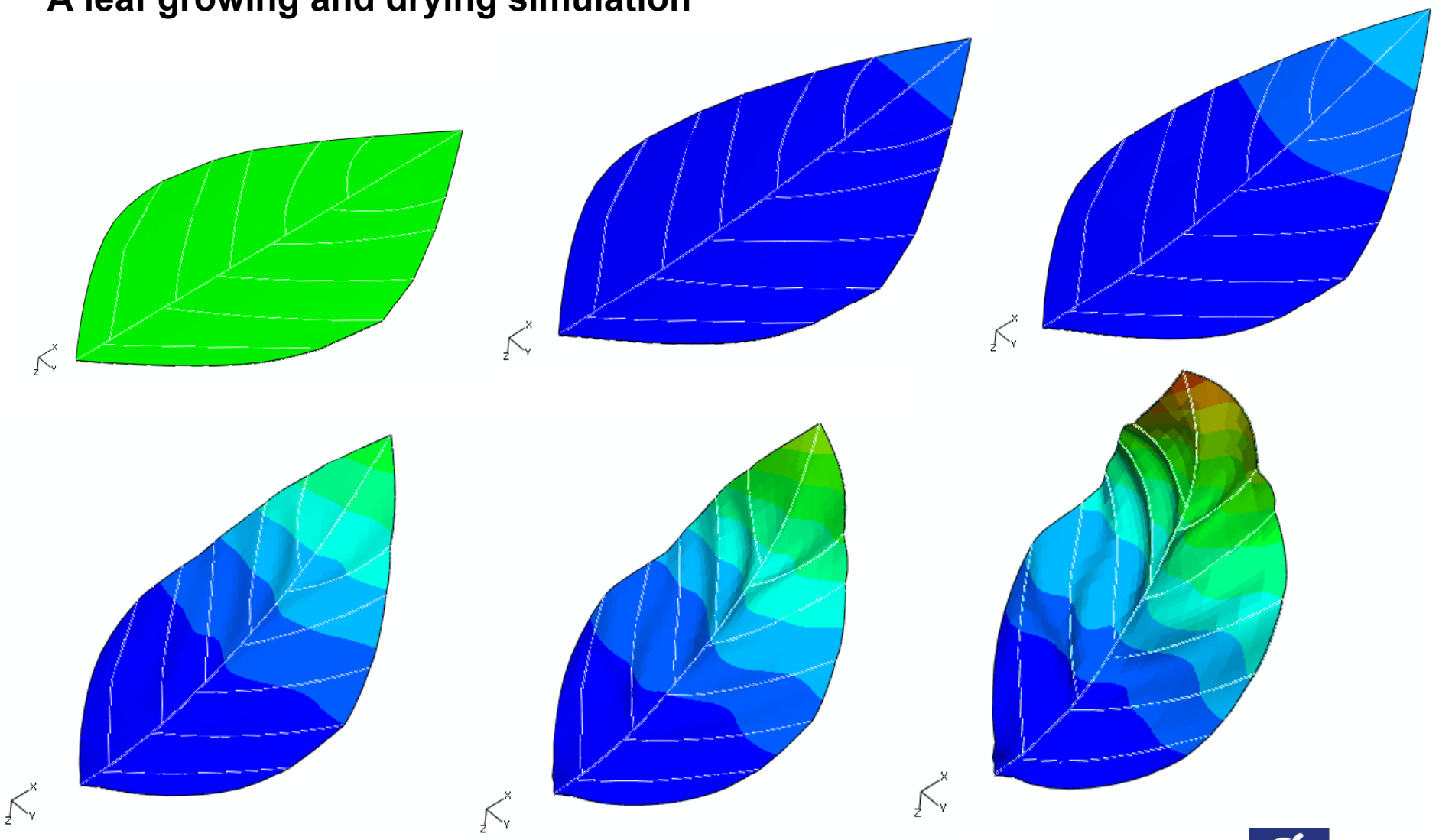


The instability wavelength λ as a function of the width w of the swollen rectangular membrane gel strip for constraining one edge and two edges

Liu, Hong, Suo, Somsak, Zhang, Com. Mat. Sci. (2010)

How To Explain Various Phyllotactic Patterns

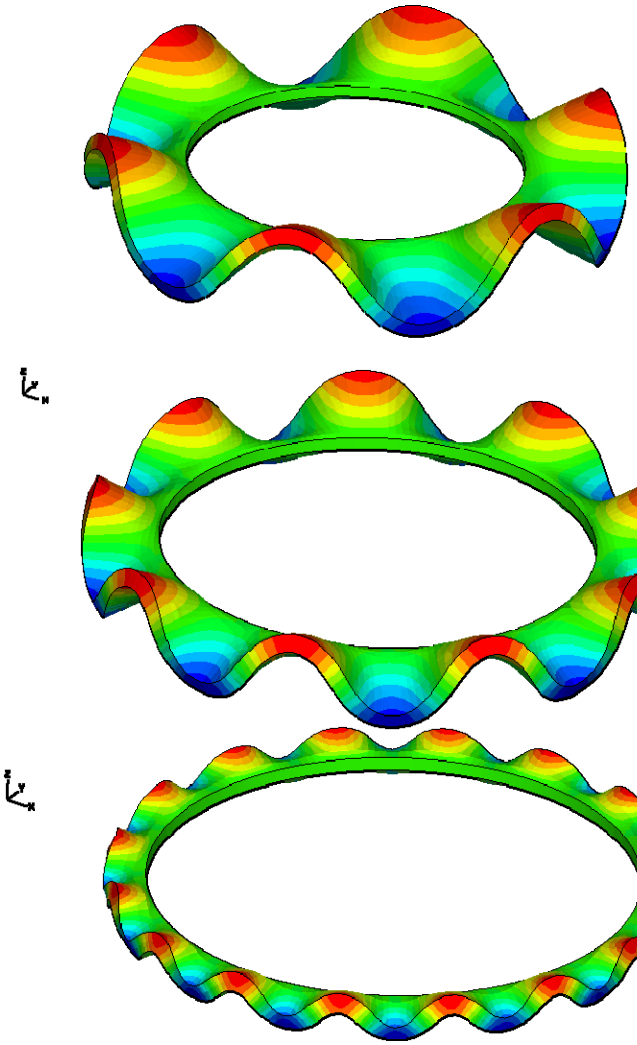
A leaf growing and drying simulation



The deformation pattern of a leaf when drying by using membrane gel

IHPC A*STAR

Swelling of Corona membrane Gel in Equilibrium



$R_i / H = 14$

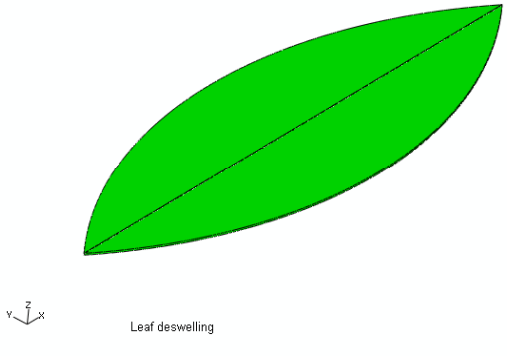
$R_i / H = 16$

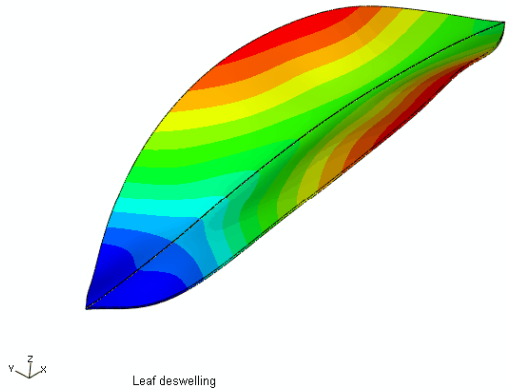
$R_i / H = 18$

The buckling shapes of corona membrane gel for different inner radius (the ratio of outer radius and thickness $R_0 / H = 20$, initial chemical potential, $\frac{\mu_0}{kT} = -0.001394203$)

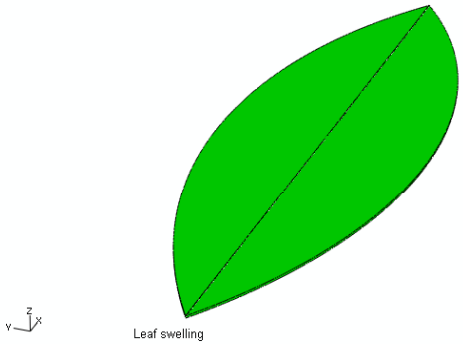
IHPC A*STAR

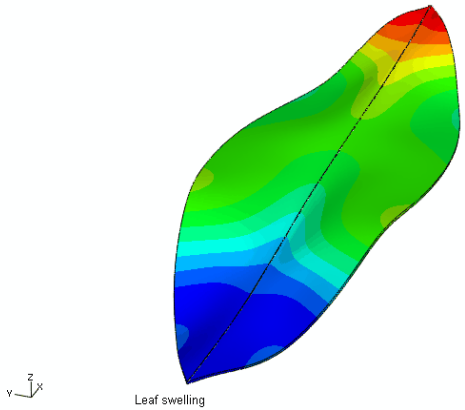
A leaf growing and drying simulation





The deformation pattern of a leaf is drying by using membrane gel deswelling



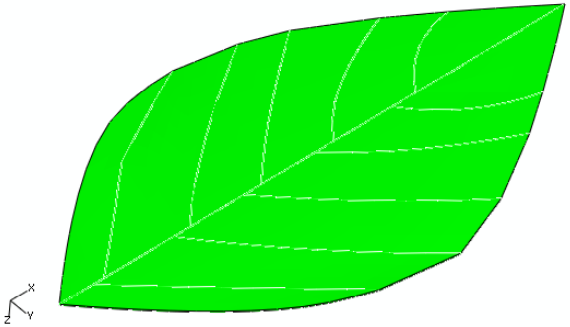


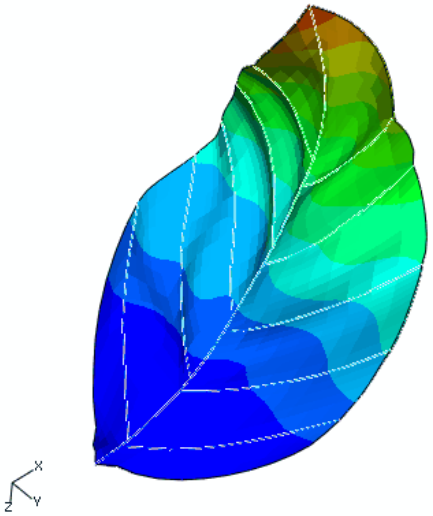
The deformation pattern of a leaf is growing by using membrane gel swelling

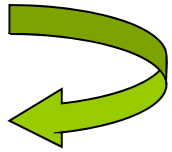
IHPC
A*STAR

How To Explain Various Phyllotactic Patterns

A leaf growing and drying simulation



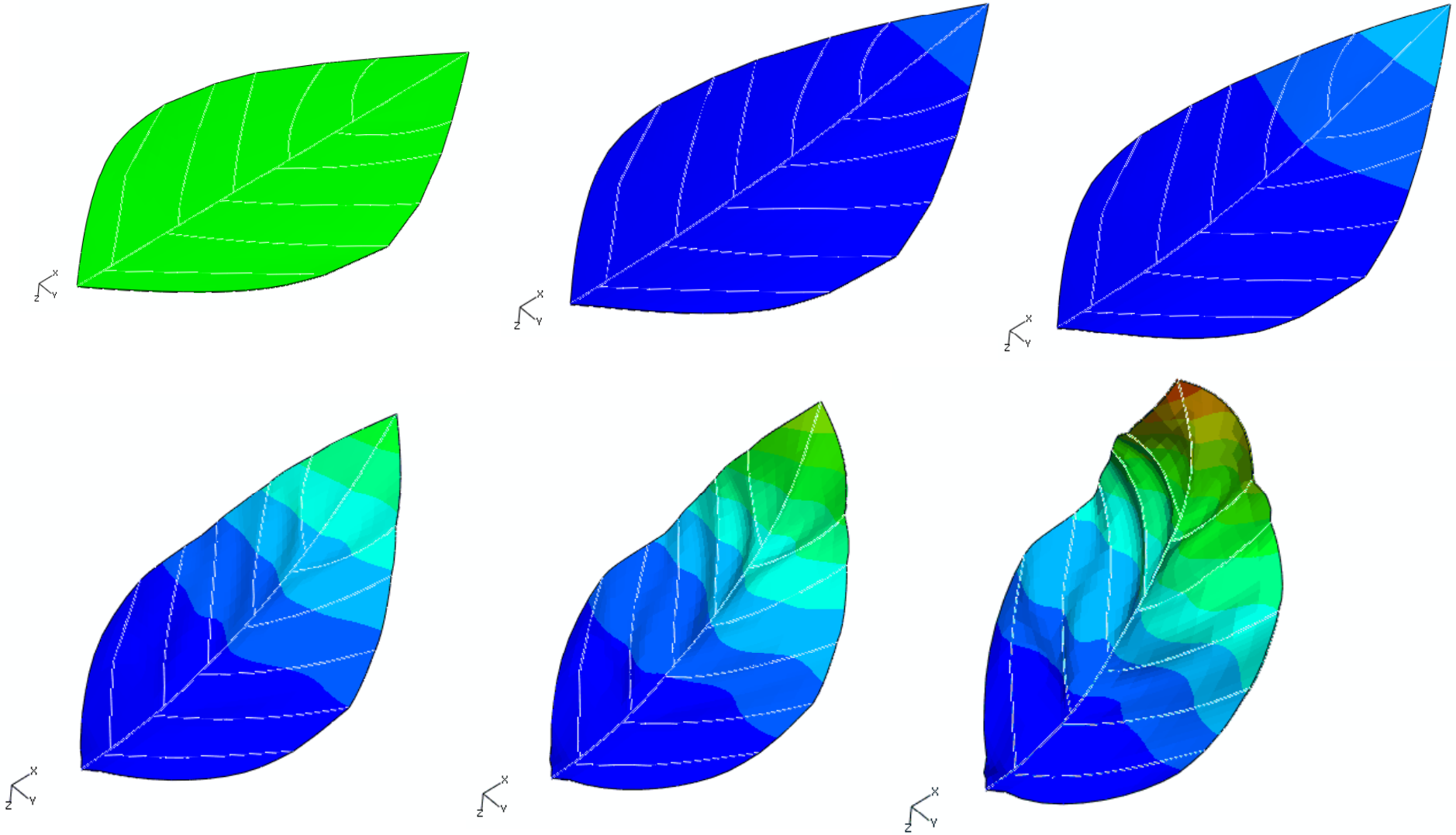




The deformation pattern of a leaf when drying by using membrane gel

IHPC
A*STAR

A leaf growing and drying simulation



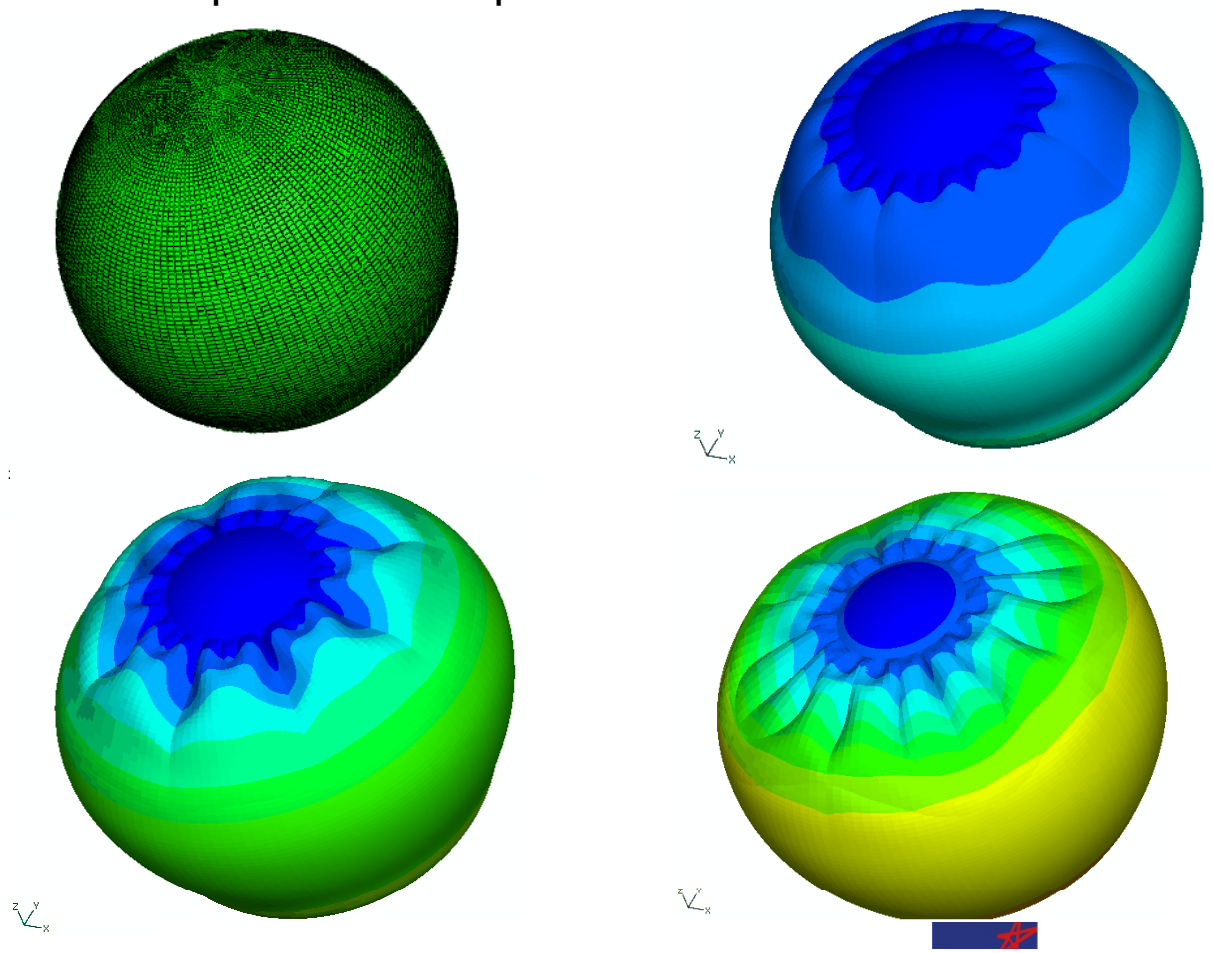
The deformation pattern of a leaf when drying by using membrane gel pH change

IHPC
A*STAR

A Swelling of Spherical Shape Shell Gel

Phyllotaxis:

How to provide a rational explanation for the formation of friut patterns, a mechanism or combination of mechanisms which capture natural phenomena?

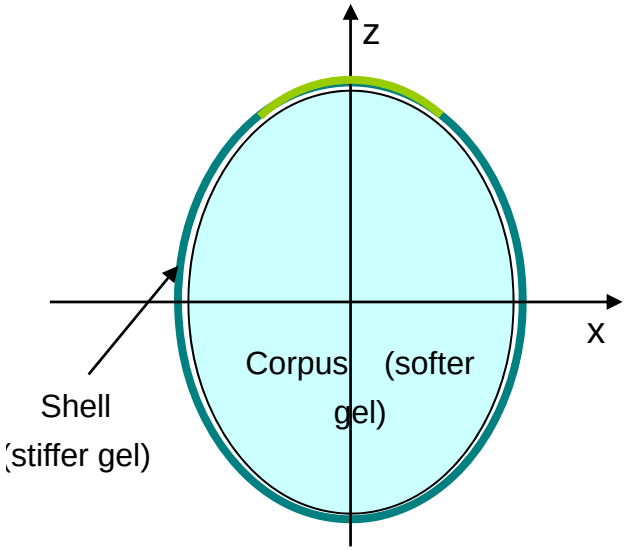


A swelling of spheroidal thin layer of gel to represent the growing process of plant (pH effect)

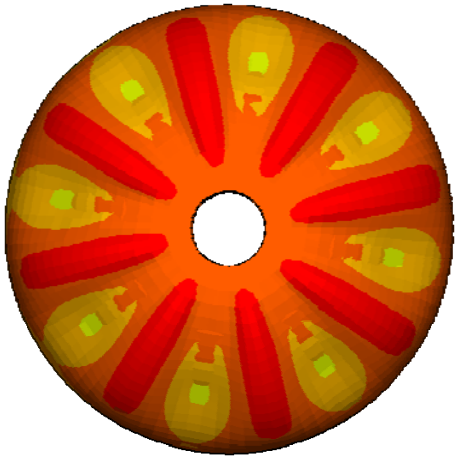
IHPC
A*STAR

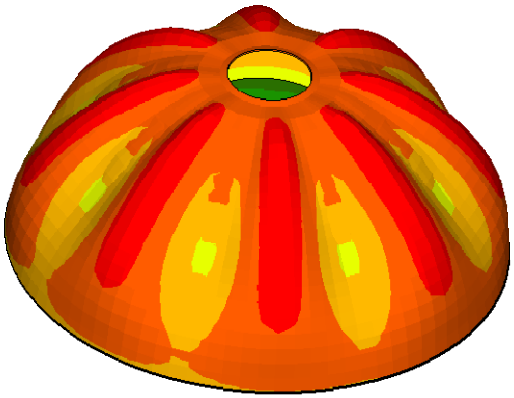
How To Explain Various Phyllotactic Patterns

A Swelling of Spherical Annulus Gel Shell



Schematic of the geometry of spheroid model



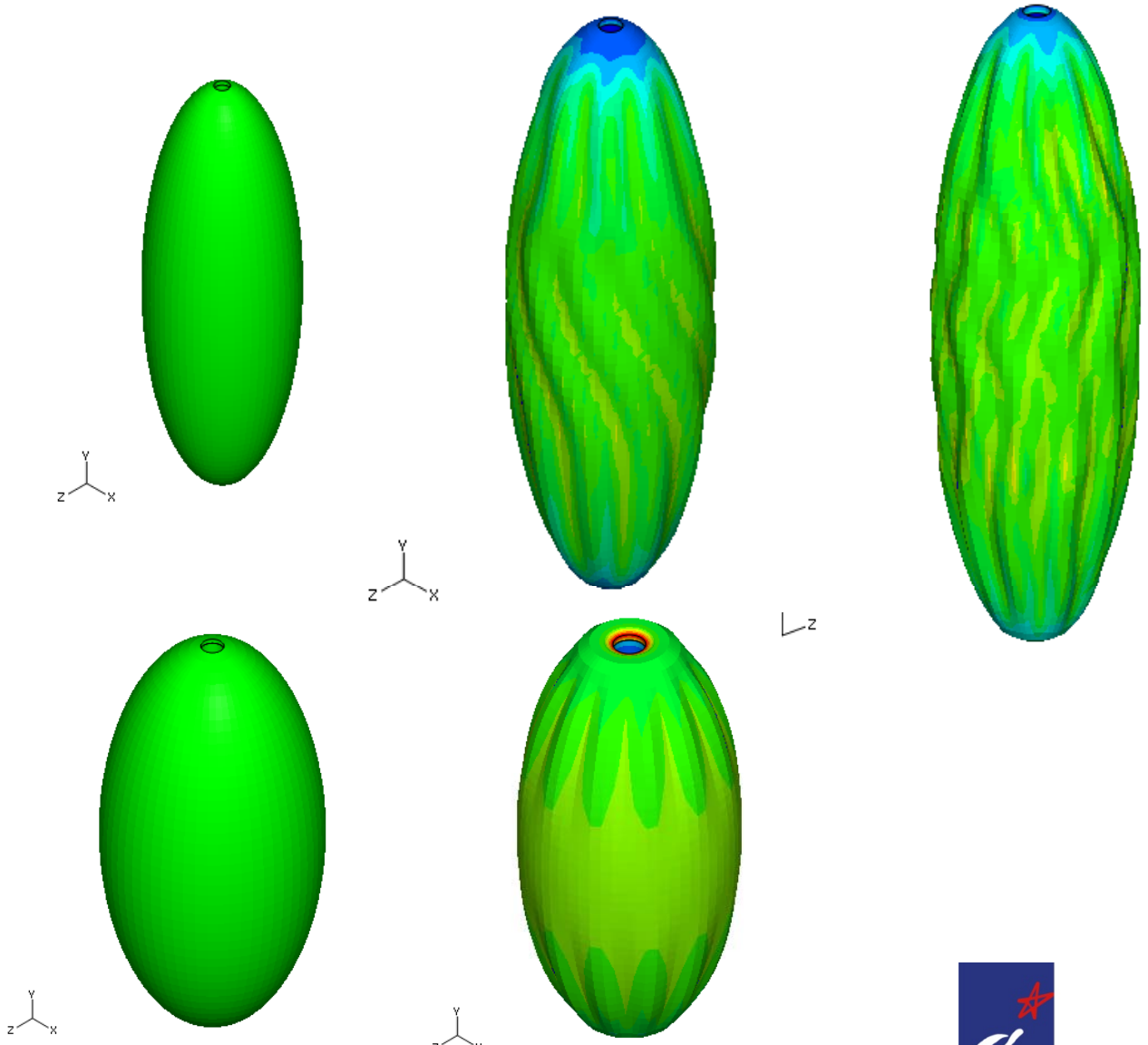


Phyllotactic pattern lattice and tiling pattern of plant

A swelling of spheroidal thin film/substrate system of gel to represent the growing process of plants

IHPC
A*STAR

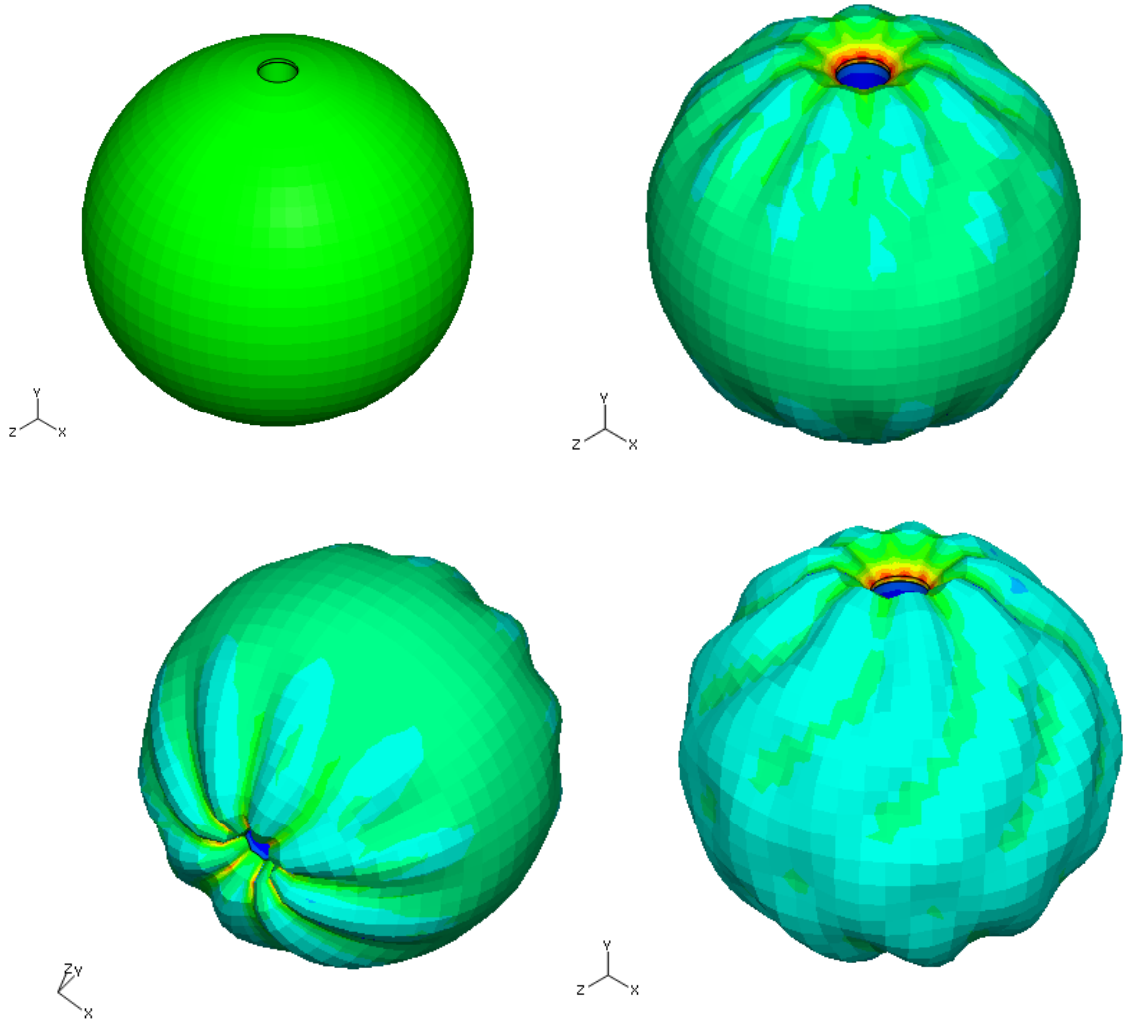
How To explain Various Phyllotactic Patterns



Cucumber growing can be simulated by gel swelling with changing the chemical potential

IHPC
A*STAR

How To explain Various Phyllotactic Patterns

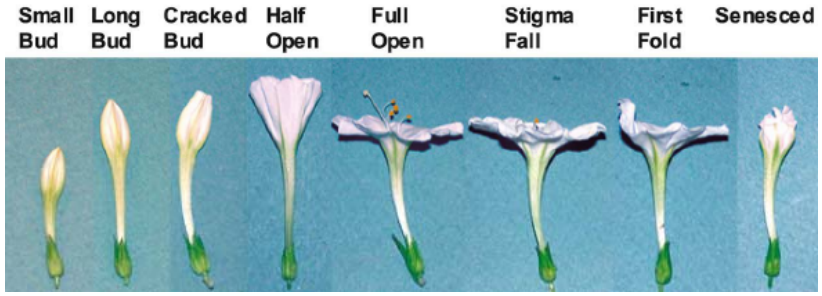


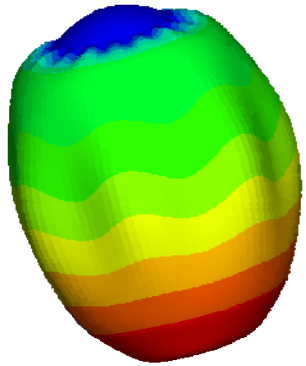
Apple growing can be simulated by gel swelling with changing the chemical potential

IHPC
A*STAR

Concluding remarks & Future Work

- Modeling and simulation results are inspiring
- Some natural phenomena can be explained by gel theory
- Acidic Leaves (actual dimension and components)
- Acidic fruits (actual dimension and components)
- Natural or engineered tissues; bio-material





Various phyllotactic lattice and tiling patterns

Newell et al, *J. Theoy. Boil.* 251, 2008

IHPC
A*STAR

Thank You