COMSOL CONFERENCE 2020 NORTH AMERICA

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Simulating a photothermal elastic capsule as a drug delivery device

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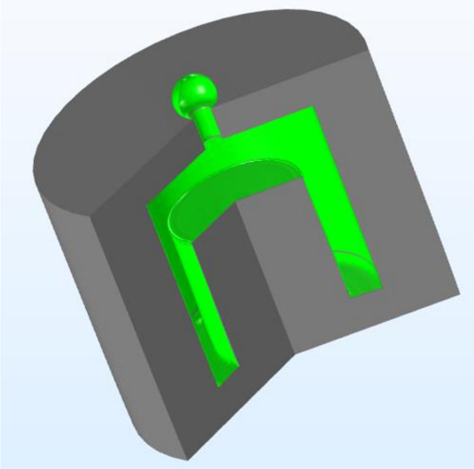
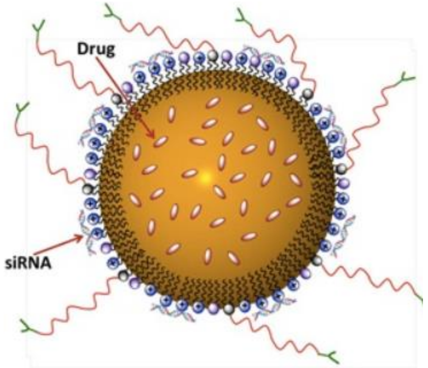


Drug delivery systems

a) Conventional delivery systems

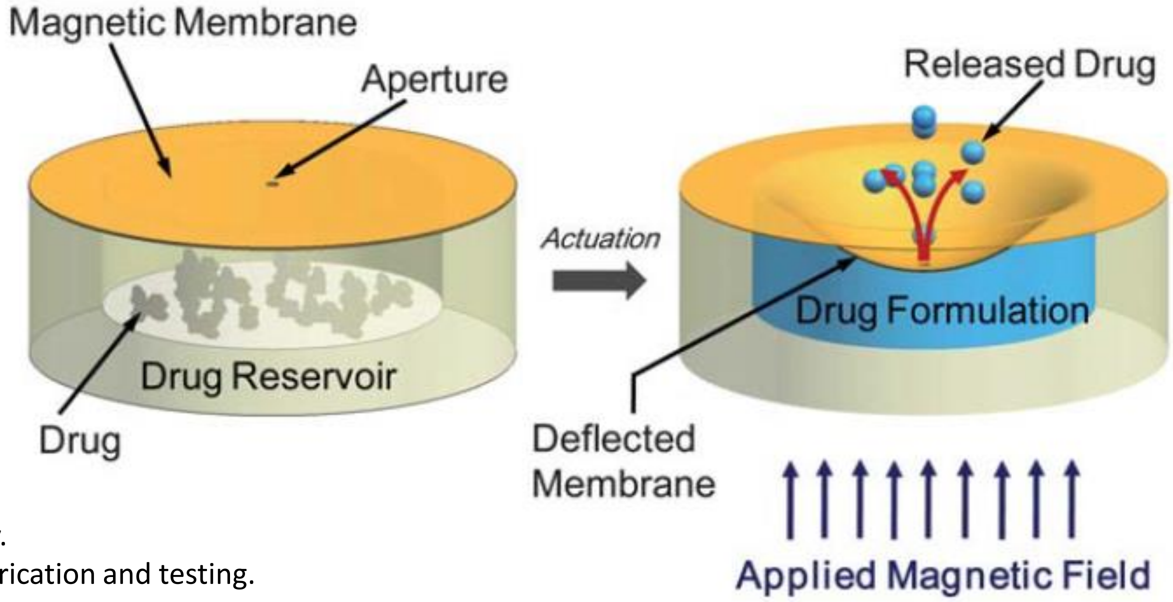
b) Advanced delivery systems: engineering of carrier agents such as nano-colloids



- ✓ improve stability, selectivity, bioavailability
- ✓ maintain or control drug concentration in plasma

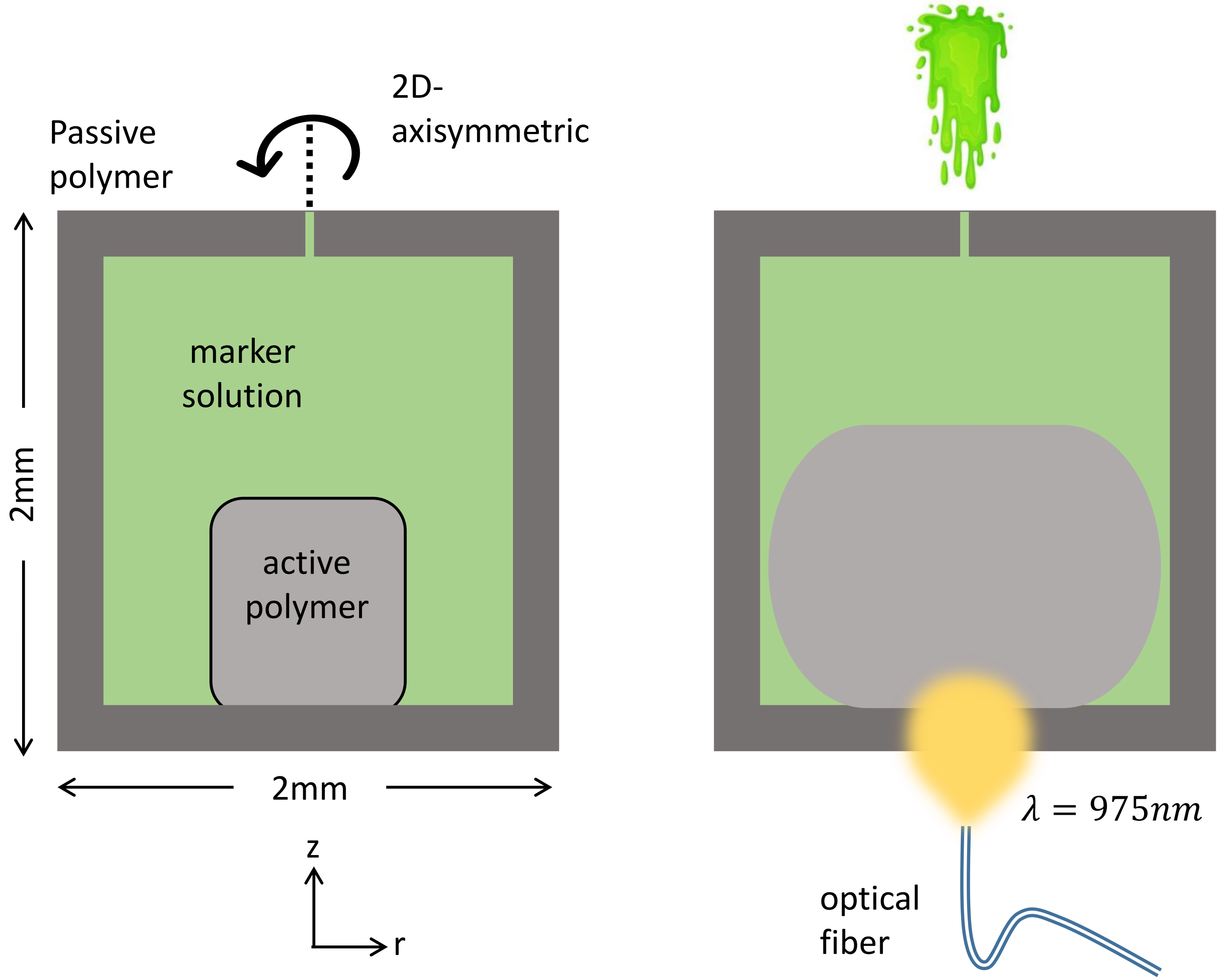
c) External devices or Bio-MEMS

- ✓ Control of plasma concentrations on-demand in chronic diseases
- ✓ External control: invasive or non invasive (magnetic or electromagnetic fields)

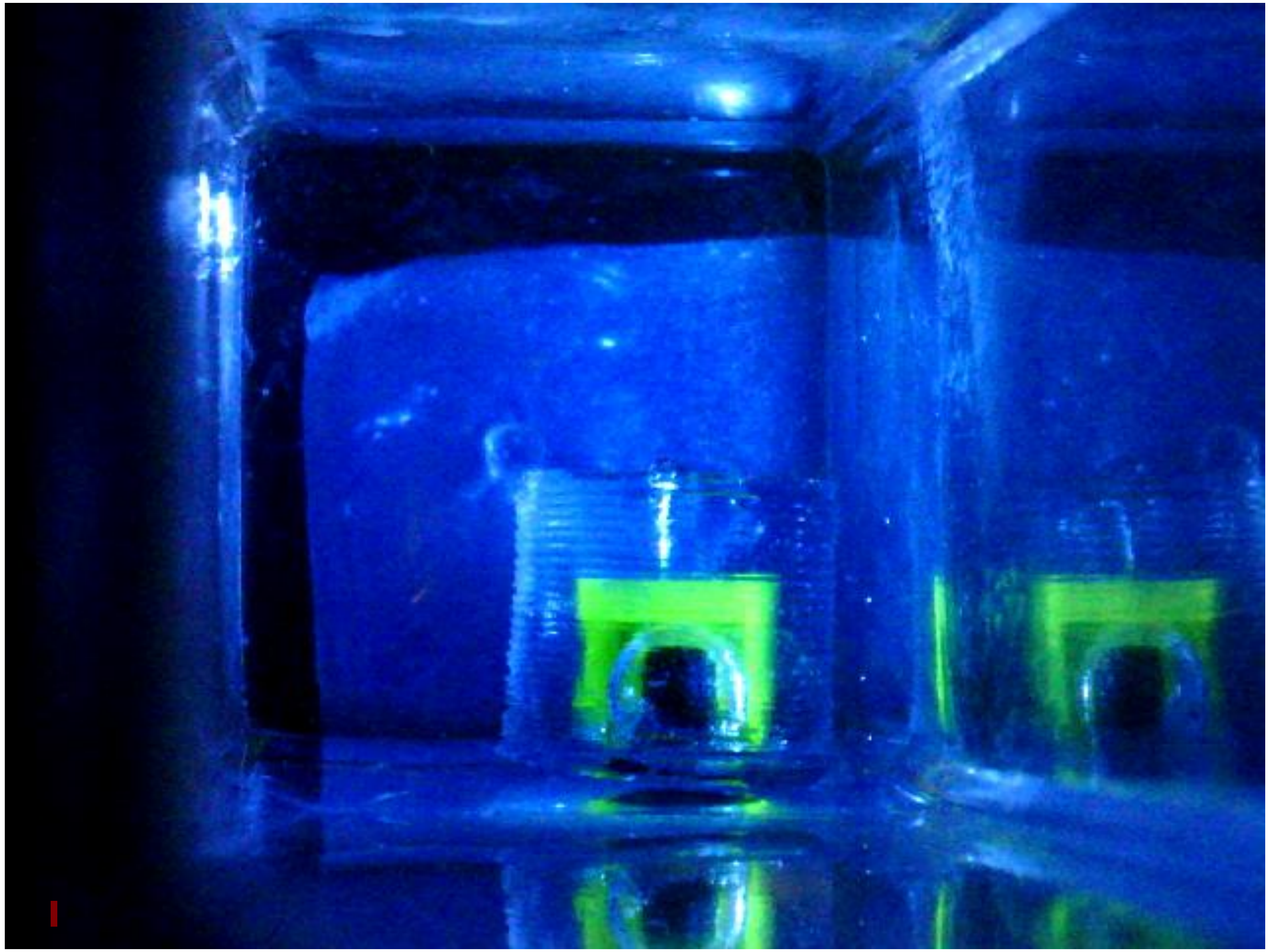


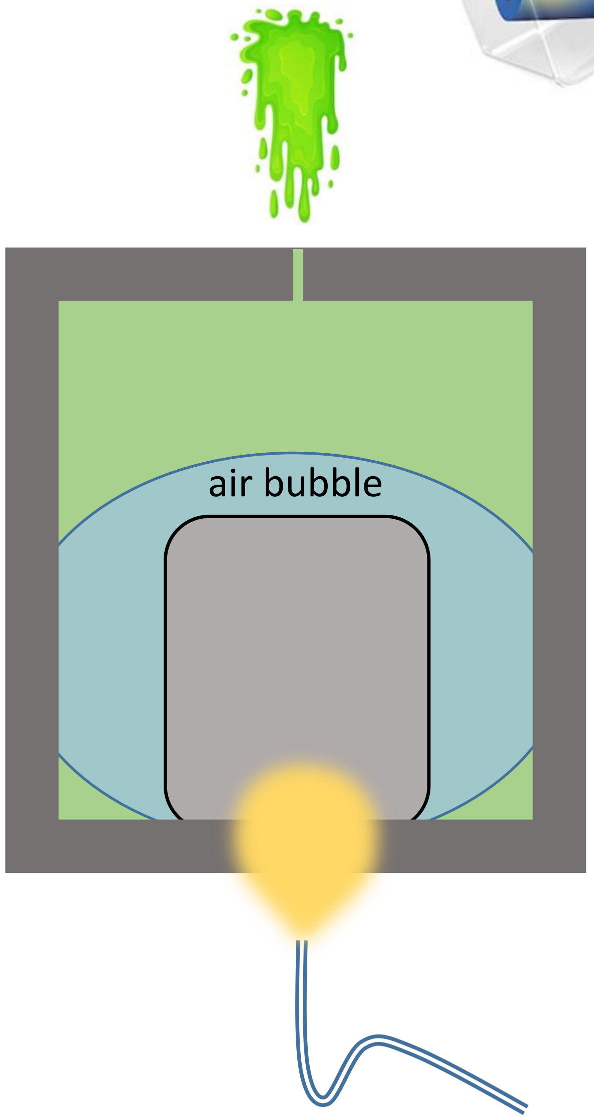
- ❑ Bandopadhyay etal. (2020) Overview of different carrier systems for advanced drug delivery.
- ❑ Pirmoradi etal. (2011) A magnetically controlled MEMS device for drug delivery: design, fabrication and testing.
- ❑ Polymer microspheres for drug delivery to the bladder.

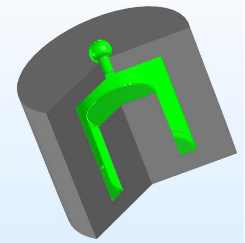
Photothermal capsule



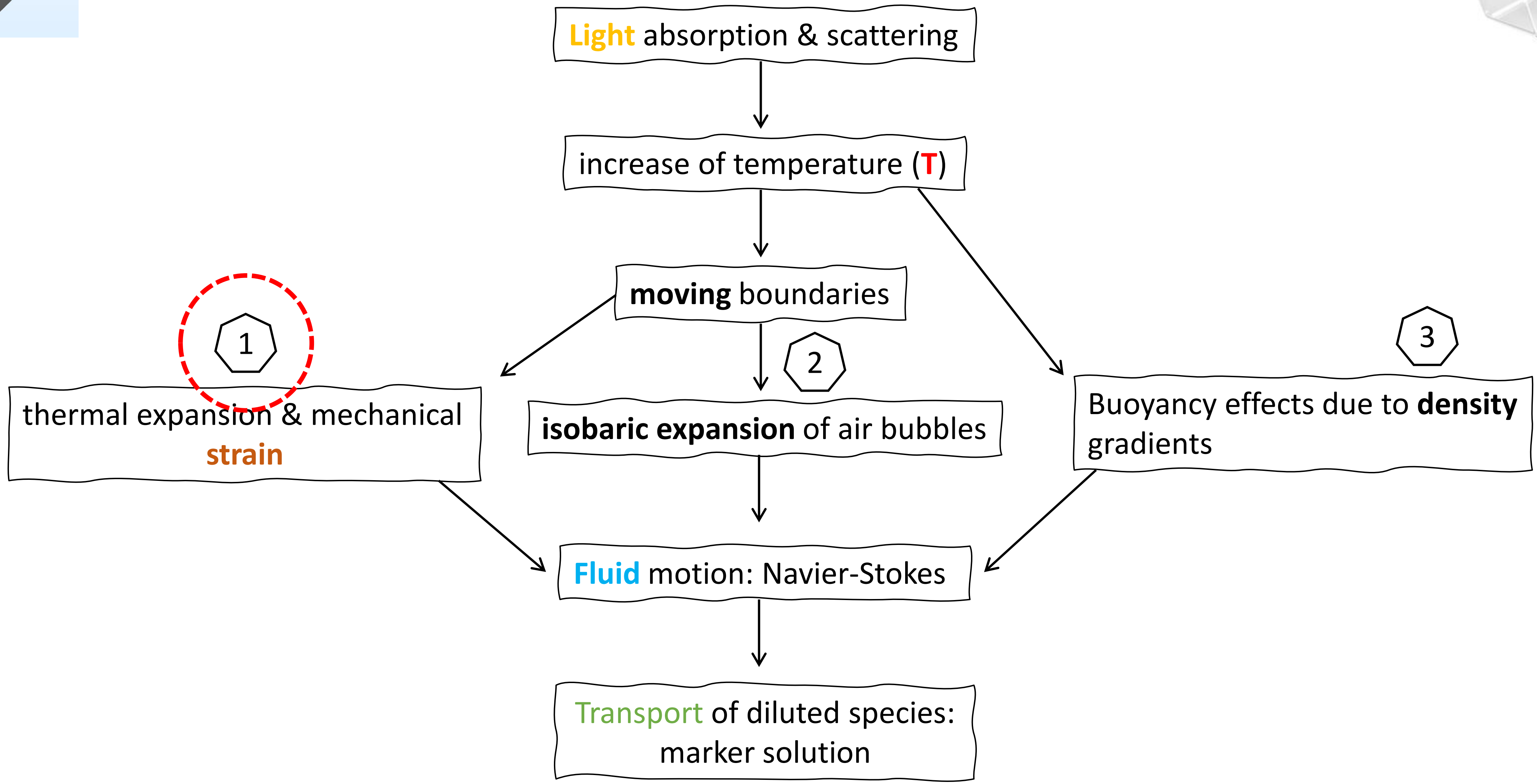
Photothermal capsule: experimental realization

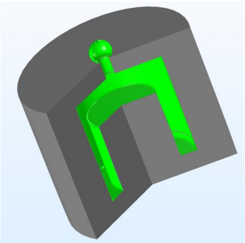






Photothermal capsule: general context





Finding the photothermal conversion efficiency η_{eff}

Conservation of energy (steady state)

$$\nabla \cdot (-\kappa \, \nabla T) = Q_{gen}$$

Light intensity profile neglecting scattering (gaussian beam)

$$Q_{gen} = \boldsymbol{\eta_{eff}} \kappa_{ext} I_0 exp[-\kappa_{ext} z - r^2/A]$$

$$I_0 = P_0/\pi A \qquad A = w^2/2$$

beam waist

$$w = w_o + z \tan(\theta)$$

Stationary mechanical stresses

$$\nabla \cdot \sigma_{ij} = 0$$

$$\nabla \cdot (F_{ij} S_{kl}) = 0$$

$$F_{ij} = \mathbb{I} + \nabla \boldsymbol{y}$$

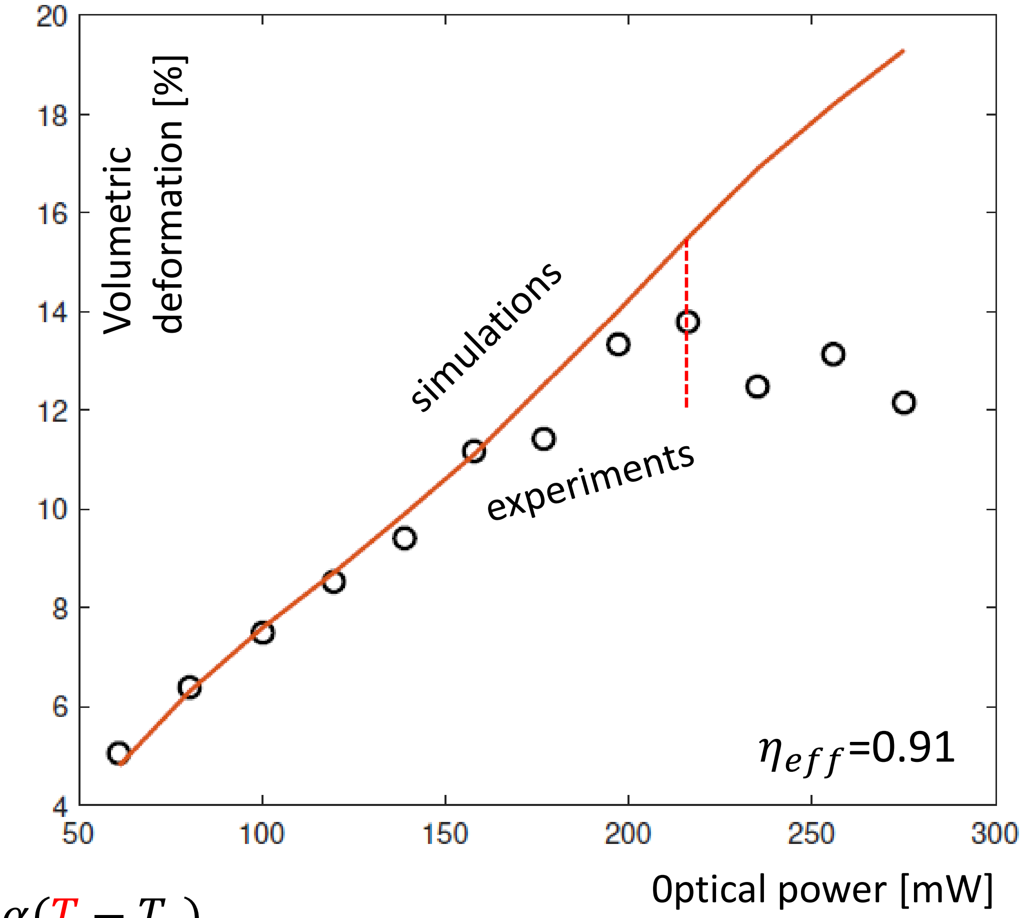
$$S_{kl} = \mathcal{C} : \boldsymbol{E}_{elast}$$

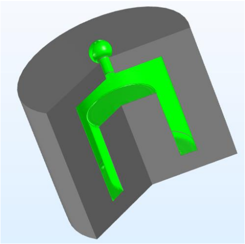
$$\mathcal{C} = \mathcal{C}(E_{Young}, \upsilon) \ldots$$

elasticity matrix

$$\boldsymbol{E}_{elast} = \boldsymbol{E} - E_{inelas} = \boldsymbol{E} - \alpha(T - T_o)$$

$$\boldsymbol{E} = \frac{1}{2}\left[(\nabla \boldsymbol{y})^T + \nabla \boldsymbol{y} + \mathcal{O}(\nabla \boldsymbol{y})^2\right]$$





Photothermal capsule: one-way fluid structure interaction

- ✓ Conservation of energy (transient) @216.mW
- ✓ Solid mechanics (transient)
- ✓ Fluid dynamics (transient)

$$\rho \frac{\partial u}{\partial t} + \rho[(u - u_{mesh}) \cdot \nabla]u = \nabla \cdot [-pI + \mu(\nabla u + (\nabla u)^T)]$$

$$\nabla \cdot u = 0$$

- ✓ Convection of diluted species

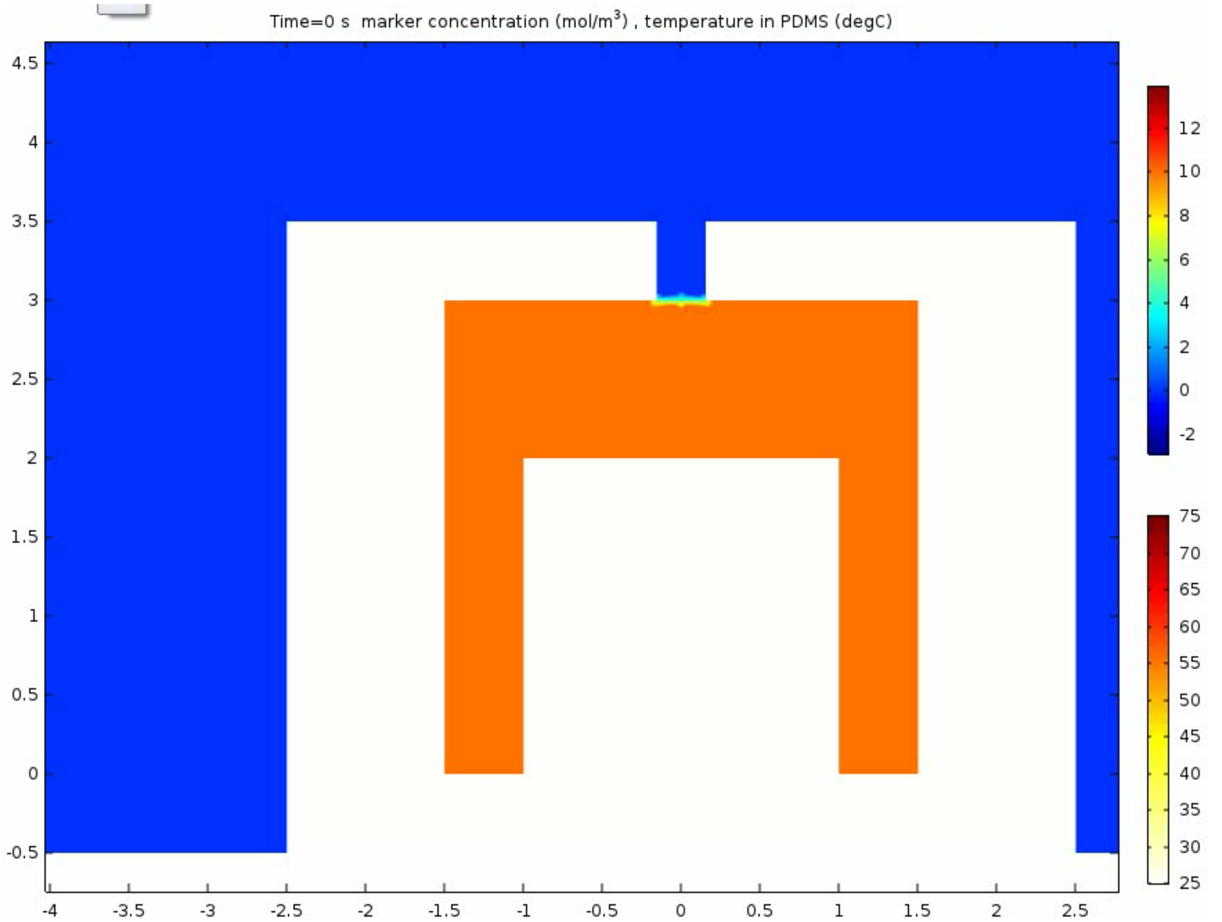
$$\frac{\partial c}{\partial t} + \nabla \cdot [(u - u_{mesh})c] = 0$$

+ Boundary and initial conditions

$$u = \frac{dy}{dt}$$

$$\sigma_{solid} \cdot n = [-pI + \mu(\nabla u + (\nabla u)^T)]$$

$$j = c(u_{mesh} \cdot n)$$



Photothermal capsule: air bubble expansion

1st study

✓ Conservation of energy (transient) @216.mW

Compute average *T(t)* in fixed bubble

$$\rho(t) = p \cdot M_w / RT(t)$$

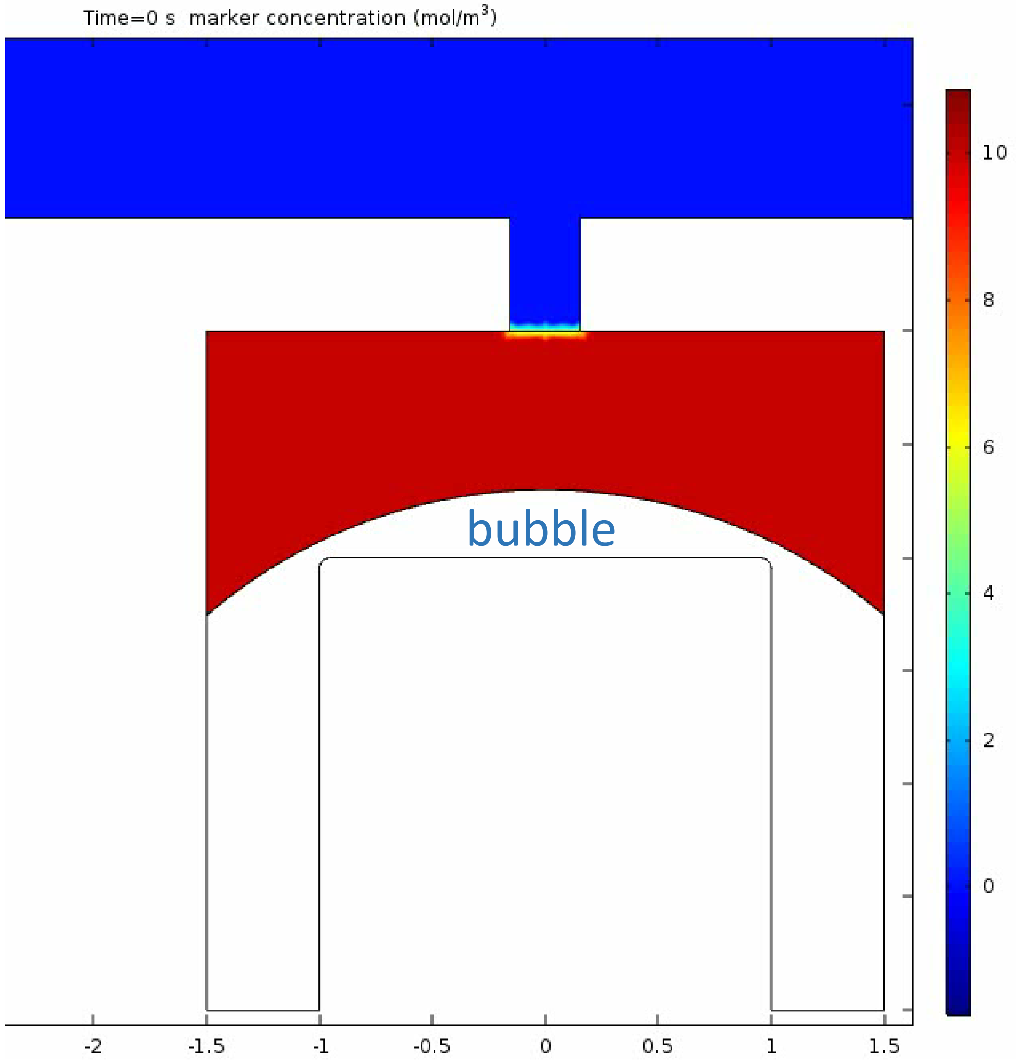
2nd study

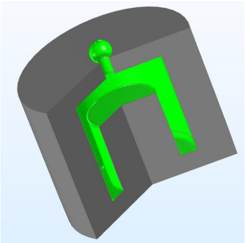
✓ Fluid dynamics (transient, moving mesh)

$$\frac{\partial \rho(t)}{\partial t} + \nabla \cdot (\rho u) = 0$$

✓ Convection of diluted species

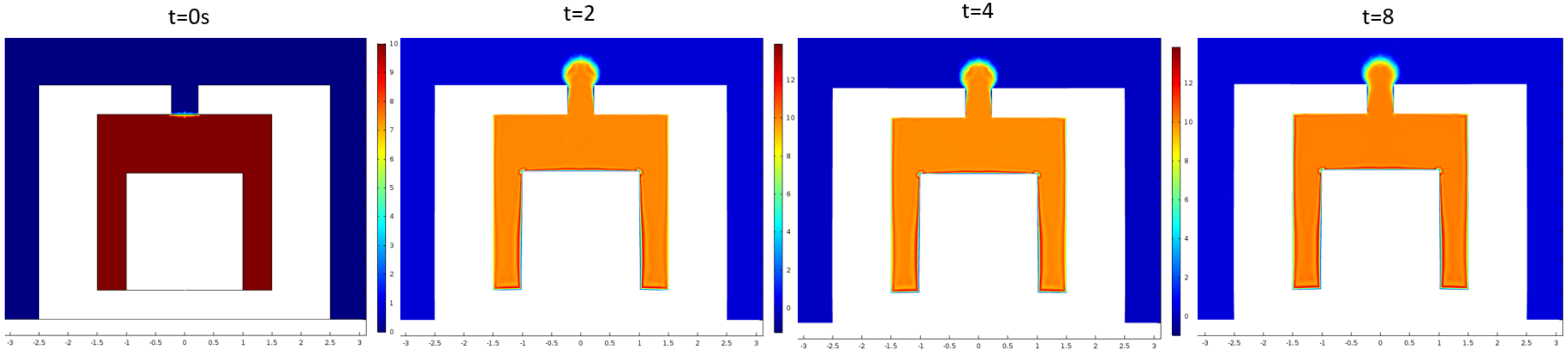
+ Boundary and initial conditions



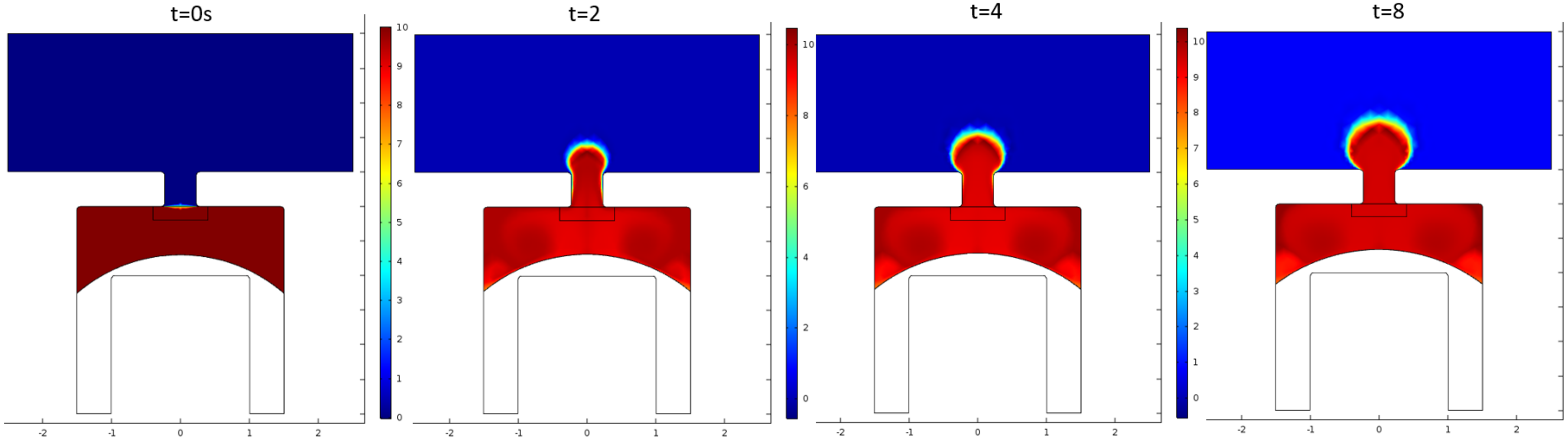


Conclusions

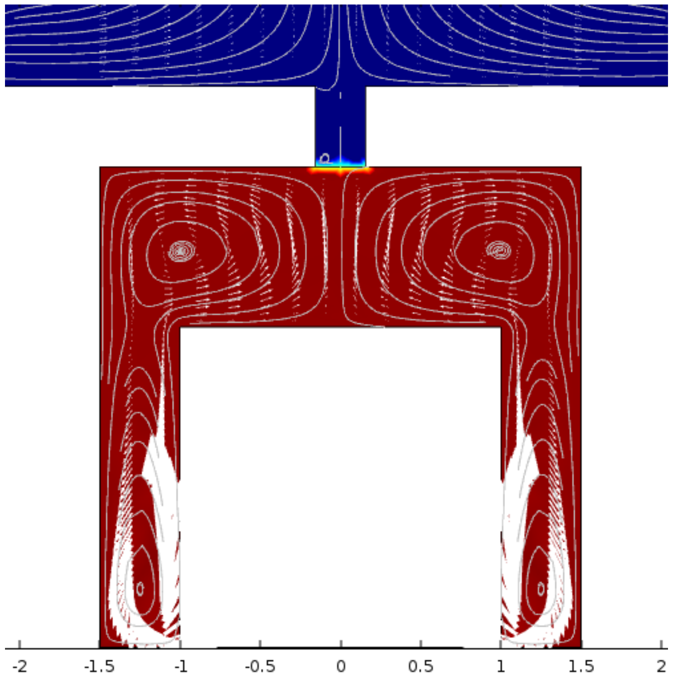
Content delivery by elastic deformation: fast release



Content delivery by bubble expansión: prolonged release



Buoyancy forces are not important



THANKS !

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