SAND2011-1530C

Multiphase hydrodynamics of free and confined thin films with fluid-structural interactions

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16th International Conference on Finite Elements in Flow Problems (FEF 11)
Minisymposium: Computational fluid mechanics for fluid surface flows
Munich, Germany

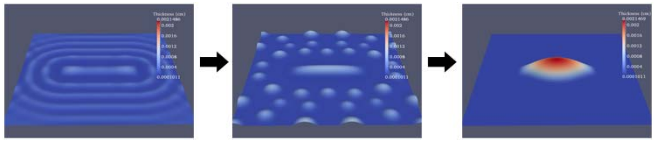
March 25, 2011

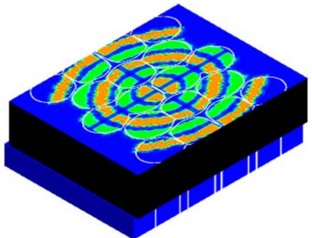
NNSA National Nuclear Security Administration

Sandia National Laboratories

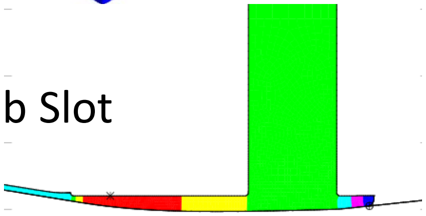
Motivation is application driven

Top-down nano-manufacturing: fluid distribution, printing, mold filling in large-aspect ratio regions



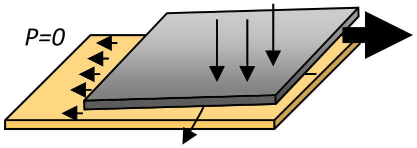


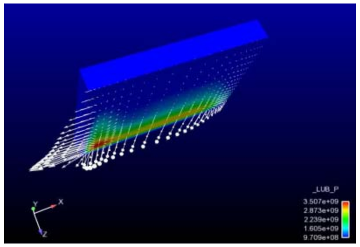
Thin-liquid film coating: film flow, metering flows, thin metering structures



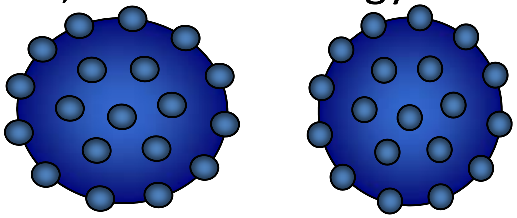
Tensioned web Slot

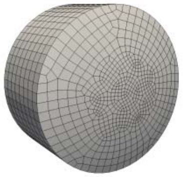
Sliding Contacts: Lubricated bearings, electrical brush





Capillary surface microstructure, surface rheology: emulsions, surface rheometry, oil recovery



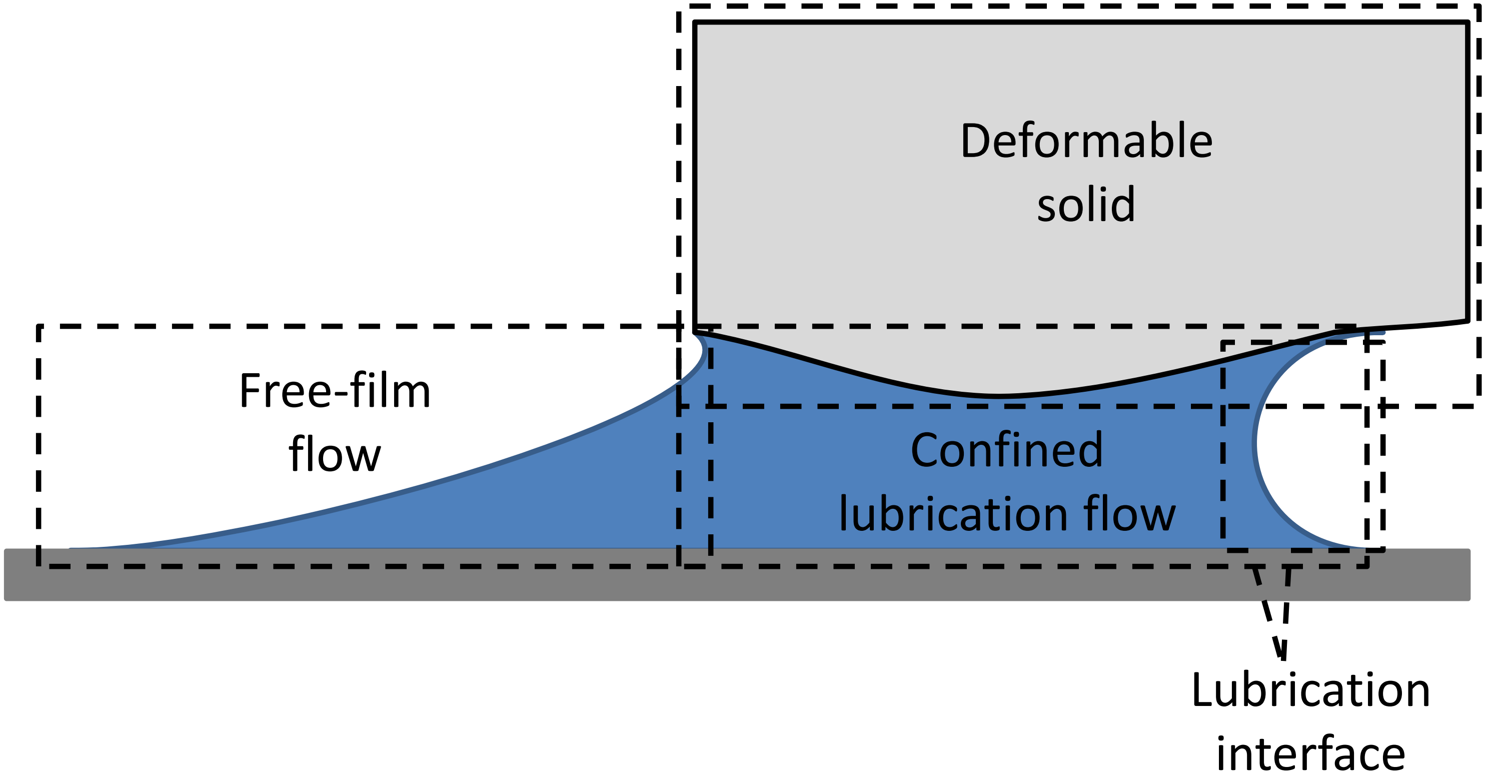


Miscellaneous: surface microprobes (Moore et al., “Hydrophilicity and the Viscosity of Interfacial Water”, Langmuir (2011) ASAP).

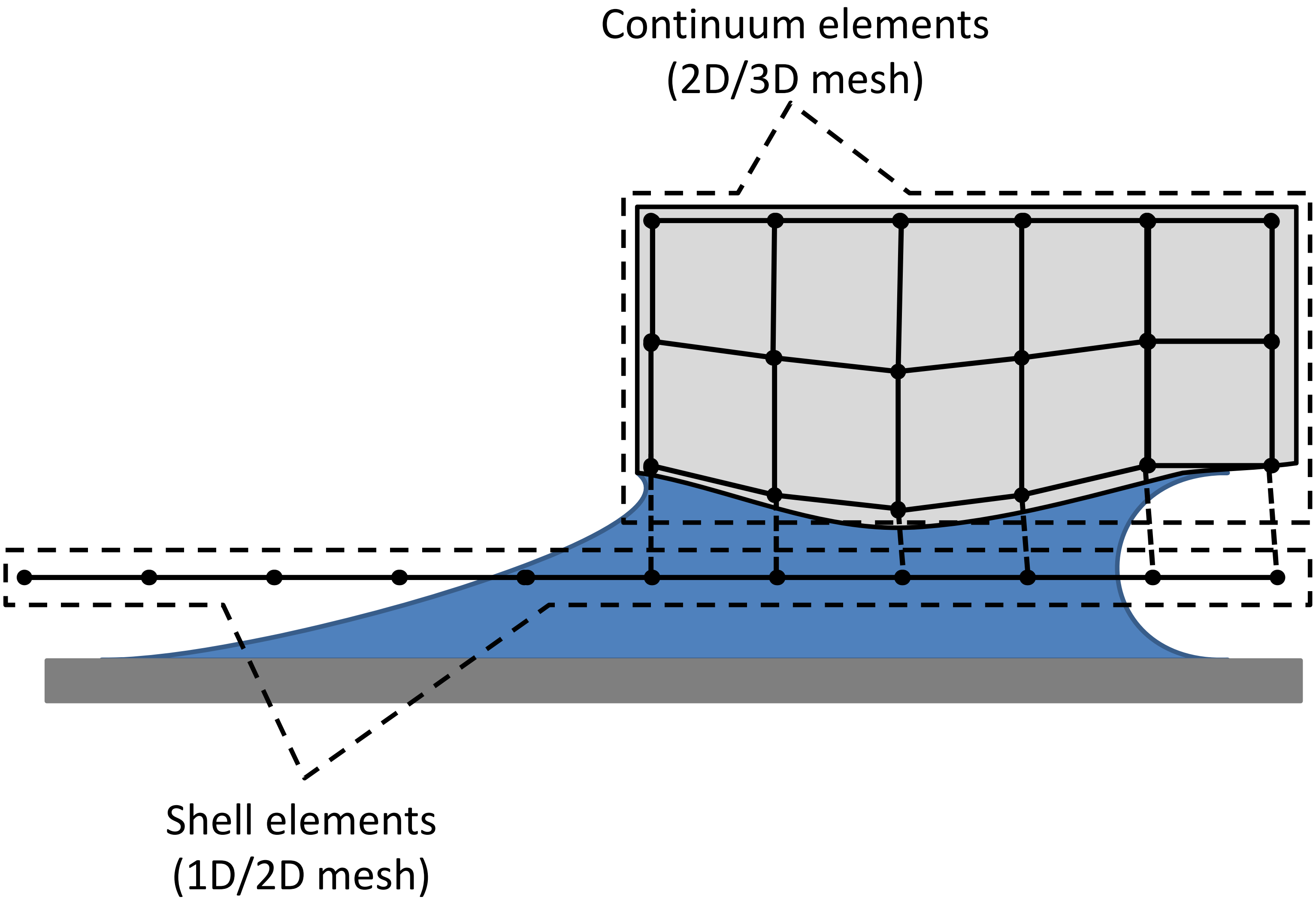
Presentation outline

- Model components
- Governing equations and implementation
  - Free film flow
  - Confined lubrication flow
  - Balanced-force multiphase lubrication
- Demonstrations
  - Film flow over patterned substrate
  - Deformable slider bearing
  - Multi-drop spreading
- Summary

Model geometry

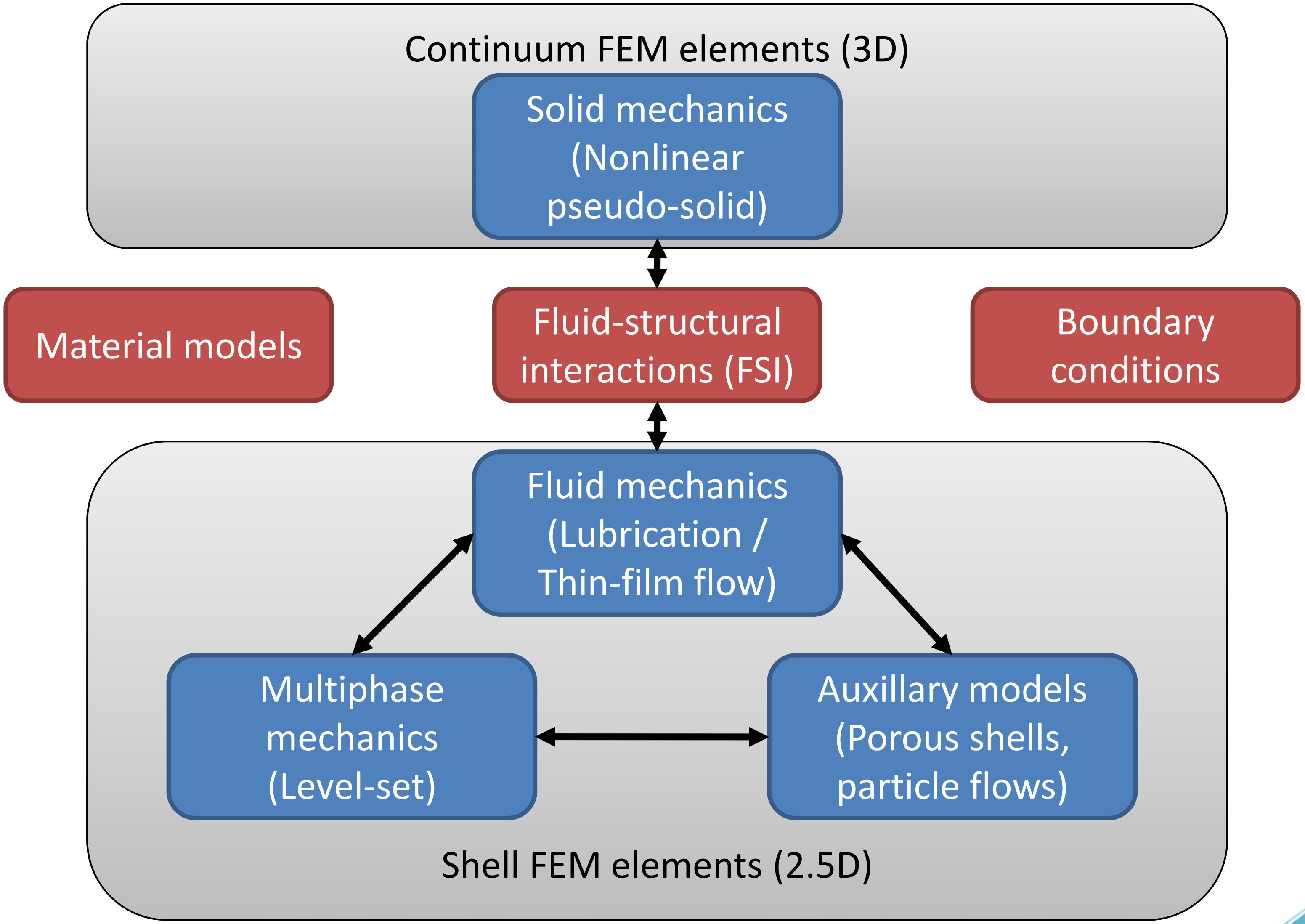


Model geometry


Continuum elements
(2D/3D mesh)

Shell elements
(1D/2D mesh)

Model components



Continuum FEM elements (3D)

Solid mechanics (Nonlinear pseudo-solid)

Material models

Fluid-structural interactions (FSI)

Boundary conditions

Fluid mechanics (Lubrication / Thin-film flow)

Multiphase mechanics (Level-set)

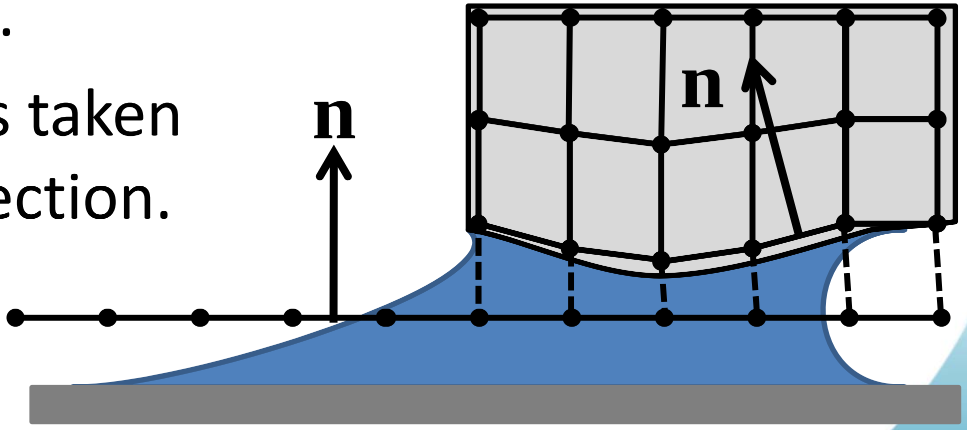
Auxillary models (Porous shells, particle flows)

Shell FEM elements (2.5D)

Model equations: Shell elements

- Traditionally rooted in solid-mechanics community:
  - Structural shells developed to provide more accurate response to thin-structure mechanics (membranes, cylindrical shells, plates, bars, etc.)
  - Shells given a finite-thickness assumed much less than the inverse radius of curvature
- The concepts however extend to fluid-thermal problems and even species transport.
- In shell elements, gradients taken only along the in-plane direction.

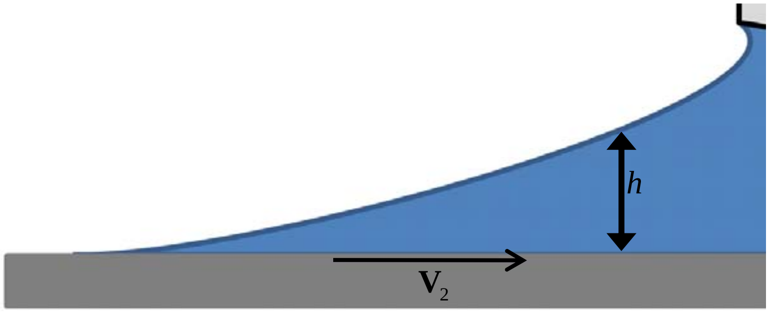
$$\nabla_{II} f = (\mathbf{I} - \mathbf{nn}) \cdot \nabla f$$



Model equations: Free film

- Film profile evolution

$$\underbrace{\frac{\partial h}{dt}}_{\text{Height change}} = \underbrace{-\nabla_{II}\cdot\left[\frac{h^3}{3\mu}\nabla_{II}P - \mathbf{V}_2 h\right]}_{\text{Convection inflow}} + \underbrace{\dot{E}}_{\text{Evaporation}}$$



- Pressure coupling definition

$$P = \underbrace{-\sigma\nabla^2_{II}h}_{\text{Capillary pressure}} + B\left[\underbrace{\left(\frac{h_*}{h}\right)^n}_{\text{Disjoining pressure}} - \underbrace{\left(\frac{h_*}{h}\right)^m}_{\text{Conjoining pressure}}\right]$$

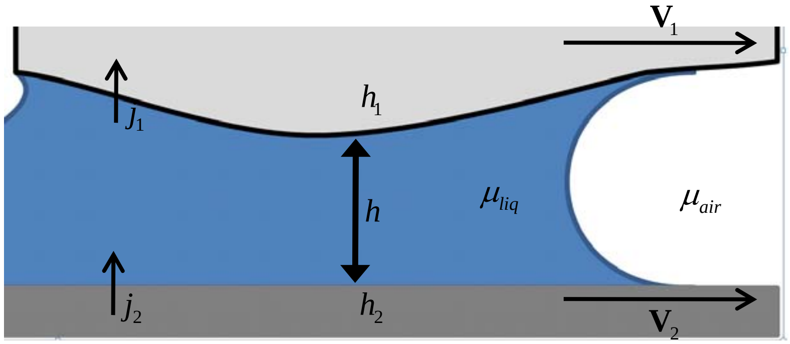
$$B = \frac{\sigma}{h_*}\frac{(n-1)(m-1)}{n-n}\left(\cos(\theta)-1\right)$$

Precursor film thickness

Contact angle

Model equations: Confined film flow

- Reynolds’ lubrication equation:



$$\overbrace{\frac{\partial h}{dt}}^{\text{Squeezing flow}} + \underbrace{j_1 - j_2}_{\text{Porous boundary flux}} = \overbrace{-\nabla_{II}\cdot\mathbf{q}}^{\text{Couette + Poiseuille flow}} + \underbrace{\mathbf{V}_1\cdot\nabla_{II}h_1 - \mathbf{V}_2\cdot\nabla_{II}h_2}_{\text{Sliding “bearing” flow}}$$

- Liquid flux:

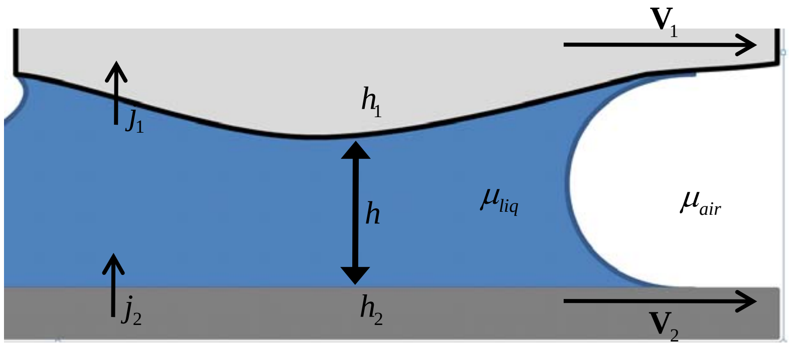
$$\mathbf{q} = \frac{h^3}{\underbrace{k_{turb}}_{\text{Turbulent mixing param.}}\mu}\left(\overbrace{\nabla_{II}P}^{\text{Pressure gradient}} - \underbrace{\rho\mathbf{g}}_{\text{Gravity/body force}} + \overbrace{F_{CSF}}^{\text{Capillary force}}\right) + \underbrace{\frac{h}{2}\left(\mathbf{V}_1 + \mathbf{V}_2\right)}_{\text{Couette flow}}$$

$$k_{turb} = \begin{cases} 12 & \text{Re} < 2000 \\ 0.3\left(2\,\text{Re}\right)^{0.75} & \text{Re} > 2000 \end{cases}$$

Model equations: Level set method

- Level-set advection equation governs location of liquid-air interface:

$$\frac{\partial f}{dt} = \mathbf{v} \cdot \left| \nabla_{II} f \right| \qquad \mathbf{v} = \frac{\mathbf{q}}{h}$$



- Balanced-force approach utilizes node-based heaviside

$$F_{CSF} = \sigma\kappa\nabla_{II} H \qquad H = \sum_i \phi_i H_i \qquad H_i = \begin{cases} 0 & f_i < -\alpha \\ \frac{1}{2}\left(1 + \frac{f_i}{\alpha} + \frac{\sin(\pi f_i / \alpha)}{\pi}\right) & -\alpha < f_i < \alpha \\ 1 & f_i > \alpha \end{cases}$$

- Curvature includes in-plane and “height” directions

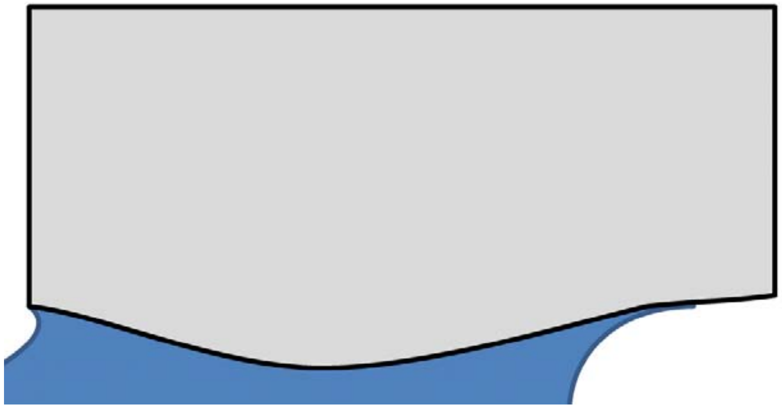
$$\kappa = \frac{1}{h}\left[\underbrace{\cos\left(\pi - \theta_1 - \arctan(\mathbf{n}_{\text{int}} \cdot \nabla_{II} h_1)\right)}_{\text{Top contact angle}} + \underbrace{\cos\left(\pi - \theta_2 - \arctan(\mathbf{n}_{\text{int}} \cdot \nabla_{II} h_2)\right)}_{\text{Bottom contact angle}}\right] + \underbrace{\nabla_{II} \cdot \mathbf{n}_{\text{int}}}_{\text{In-plane}}$$

Model equations: Fluid-structural interactions

- Compressible Hooke's Law models solid deformation

$$\nabla \cdot \boldsymbol{\sigma} = 0$$

$$\boldsymbol{\sigma} = \lambda \varepsilon \mathbf{I} + 2\mu \mathbf{E}$$



- Neo-Hookean constitutive model

$$\mathbf{E} = (\nabla \mathbf{d}) + (\nabla \mathbf{d})^T + (\nabla \mathbf{d})^T (\nabla \mathbf{d}) \qquad \varepsilon = 3\left(\det\left((\mathbf{I} - \nabla \mathbf{d})^{-1} \right)^{1/3} - 1 \right)$$

- Continuum and shell elements coupled through the lubrication pressure

$$\mathbf{n} \cdot \boldsymbol{\sigma} = \mathbf{n}P + (\mathbf{I} - \mathbf{nn}) \cdot \left(\frac{h}{12} \nabla P + \frac{\mu}{h} \mathbf{v} \right)$$

Model equations: Auxiliary capabilities

- Pattern-to-mesh tool:
  - Spatially and time-varying material parameters and external fields without meshing in separate regions
- Porous shells:
  - Liquid uptake from lubrication layer with in-plane transport
- Particle transport:
  - Convection/diffusion of particles in thin films, with evaporation
- Energy transport:
  - Shell model for convection/diffusion of heat in liquid layers
- Phase-change models:
  - Heat/friction can melt adjoining solids, transferring mass into and out of the liquid phase
- Interfacial / surface rheology:
- Many others ….

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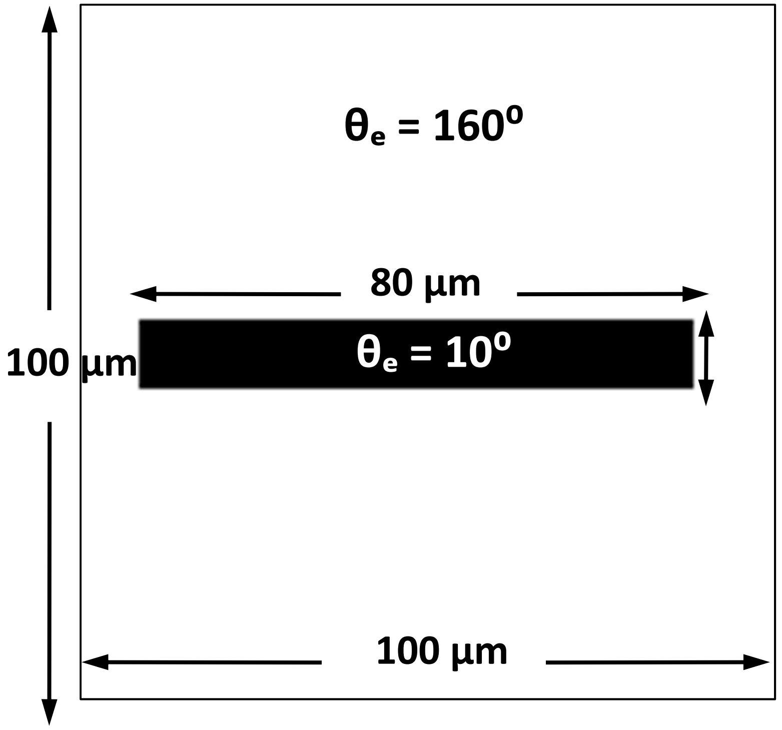
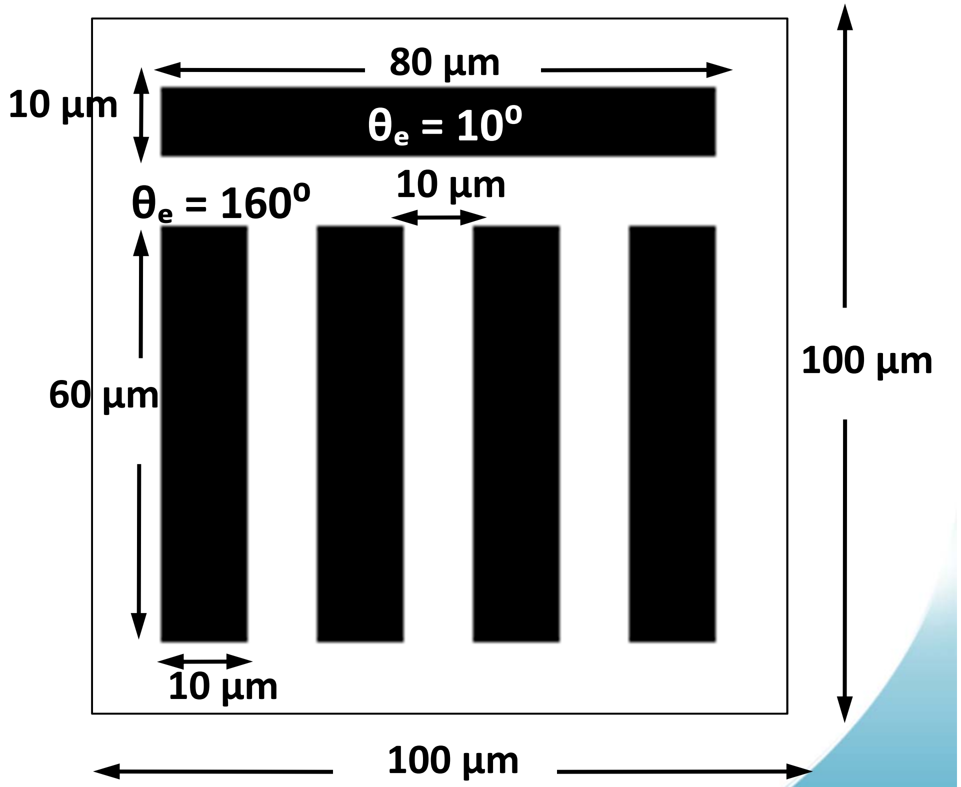
Film flow over patterned substrate

- Substrate chemically patterned with areas of varying wetability
- Patterns are not meshed in, but an external field variable

Single-feature pattern

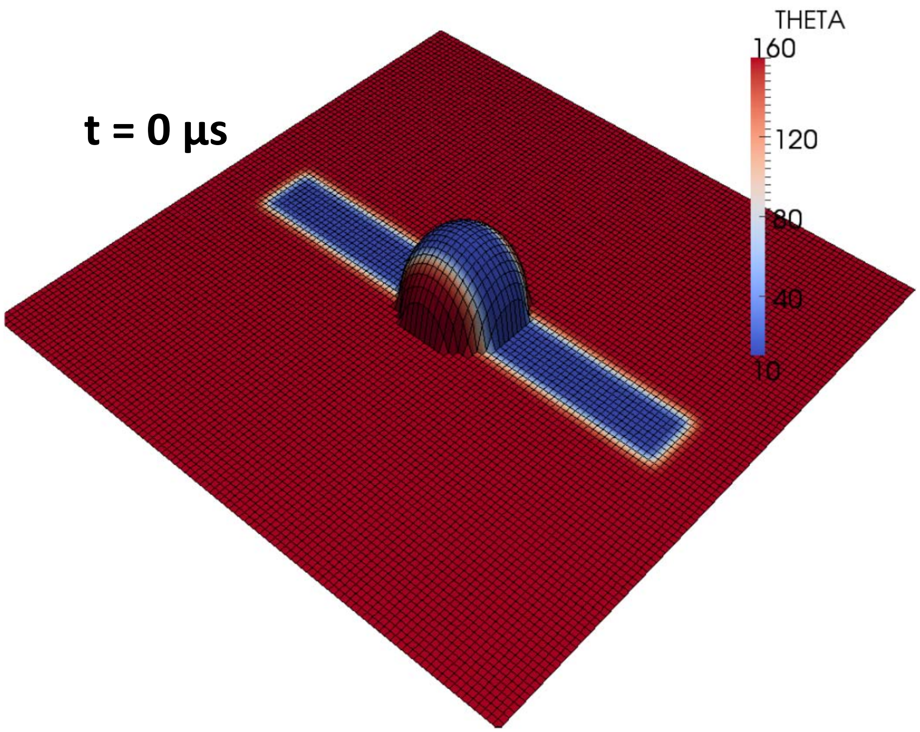


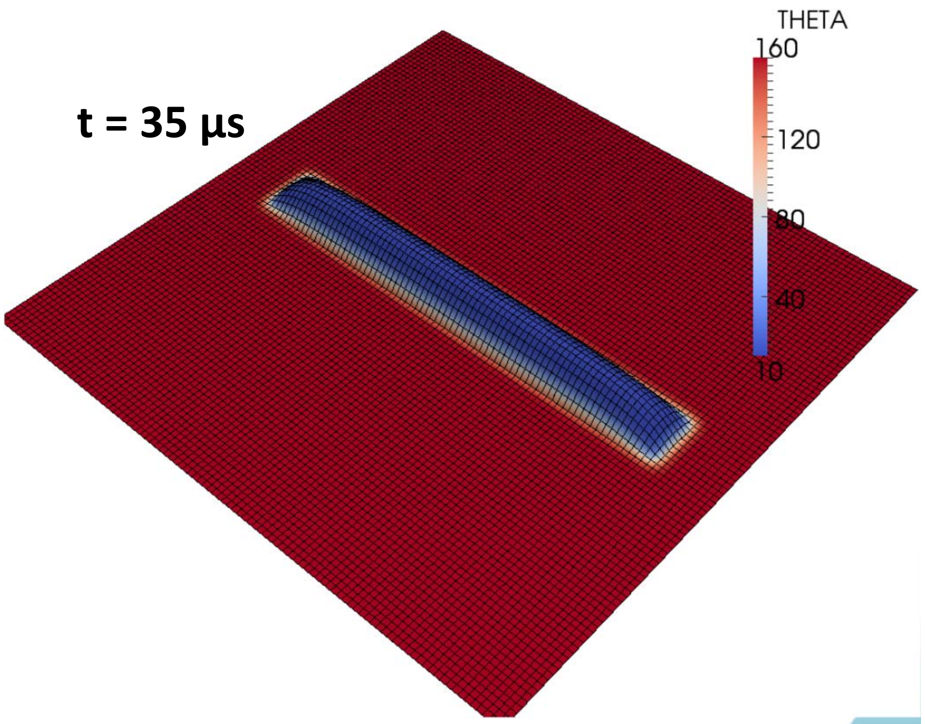
Multiple-feature pattern



Film flow over patterned substrate

Single-feature pattern initialized with a single 2 pL drop (ink-jet deposited)

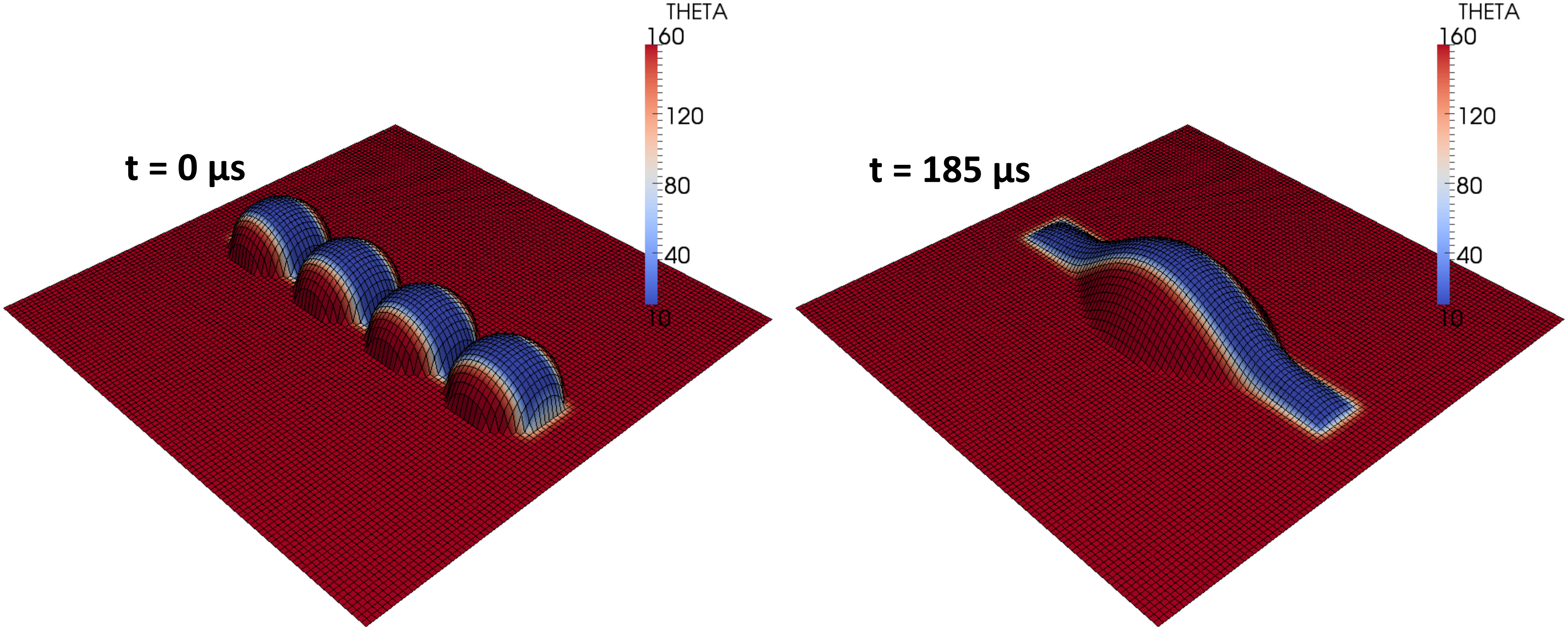




Droplet quickly spreads to cover the entire pattern

Film flow over patterned substrate

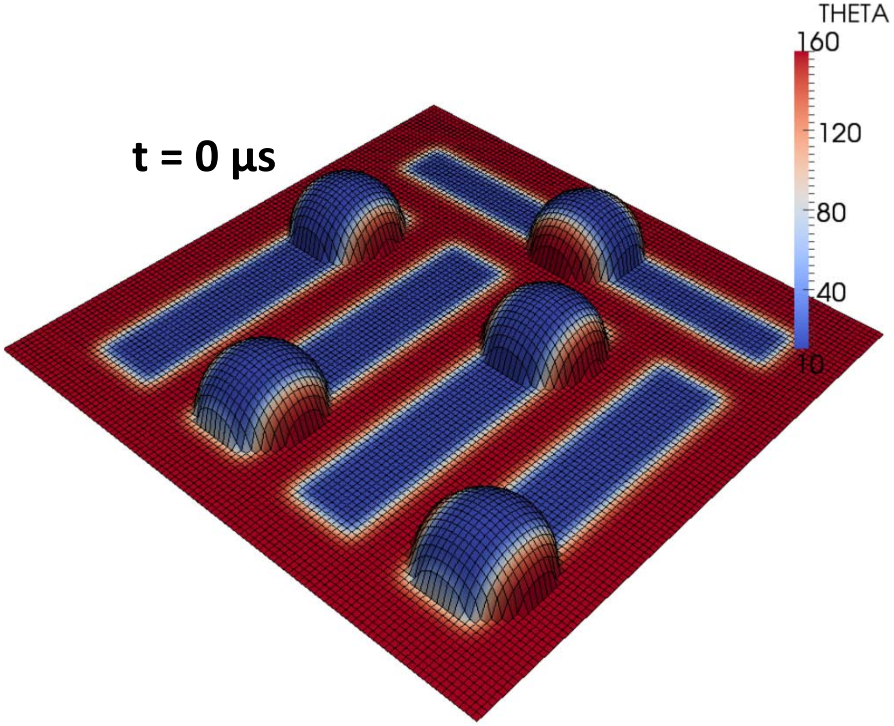
Single-feature pattern initialized with FOUR 2 pL drops



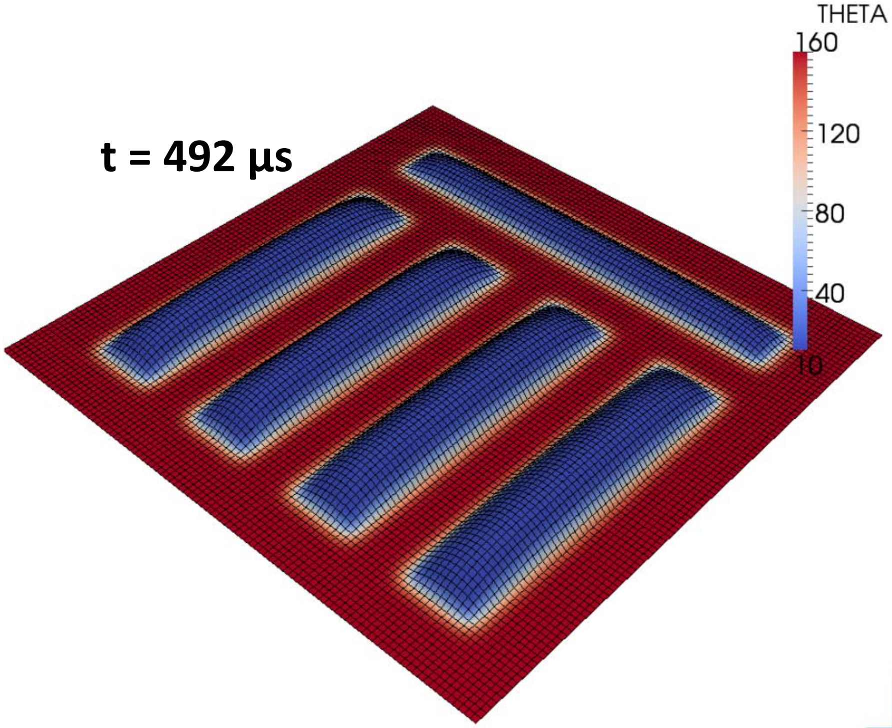
Resulting droplet does not conform to the pattern due to excess liquid deposited

Film flow over patterned substrate

Complicated multiple-feature patterns can also be studied



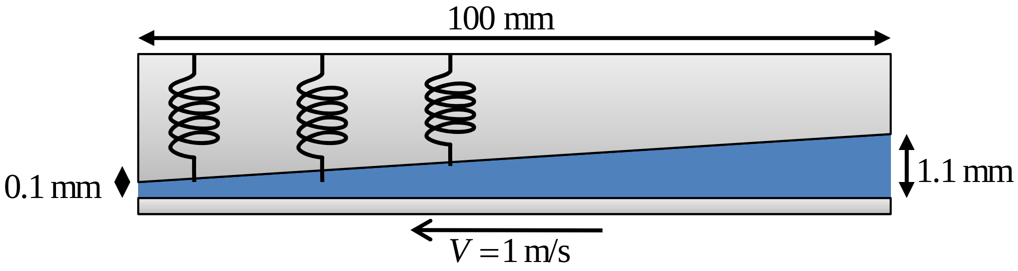
t = 0 μs

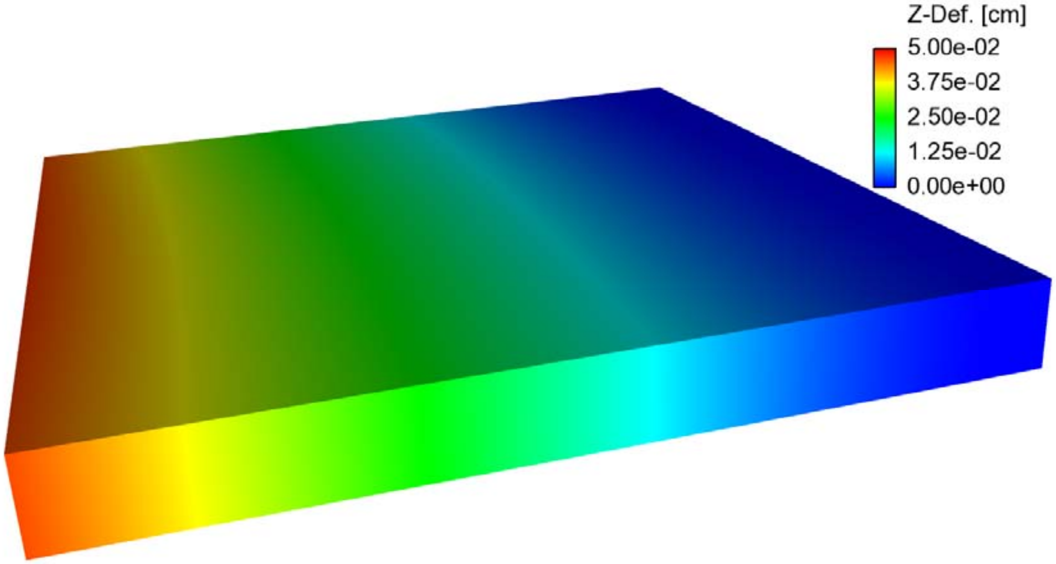


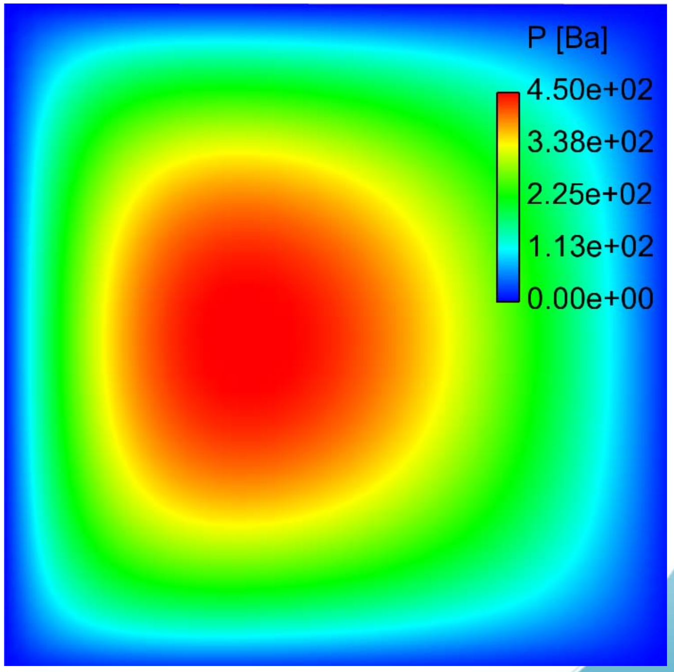
t = 492 μs

Droplets spread to cover patterned areas

Deformable slider bearing

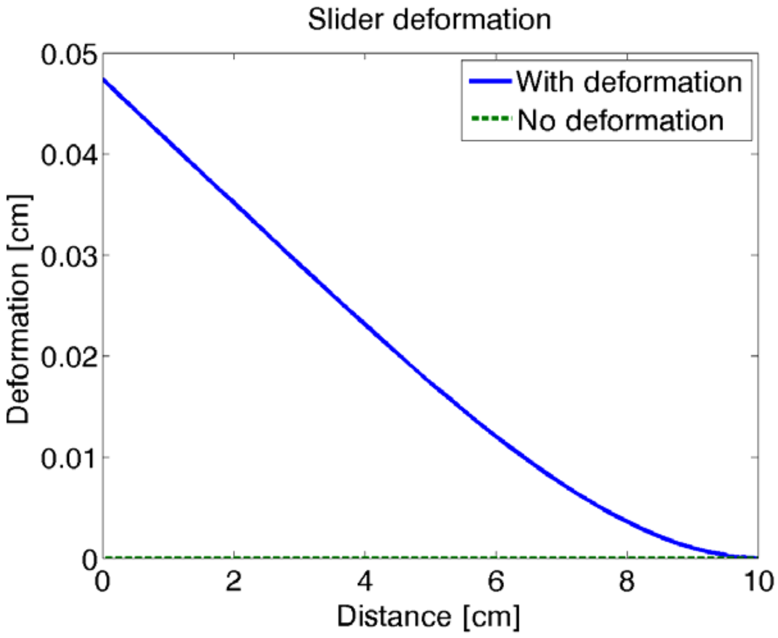


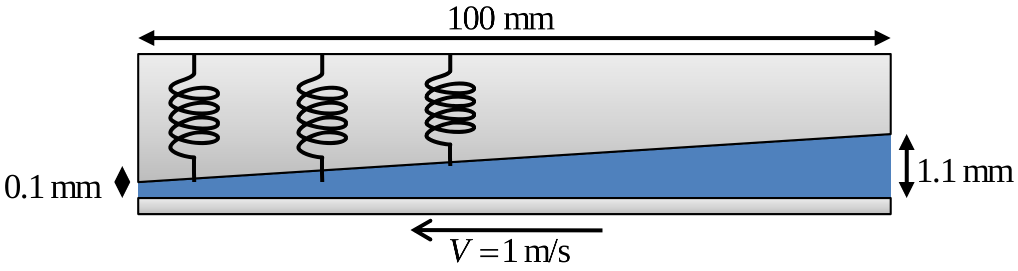


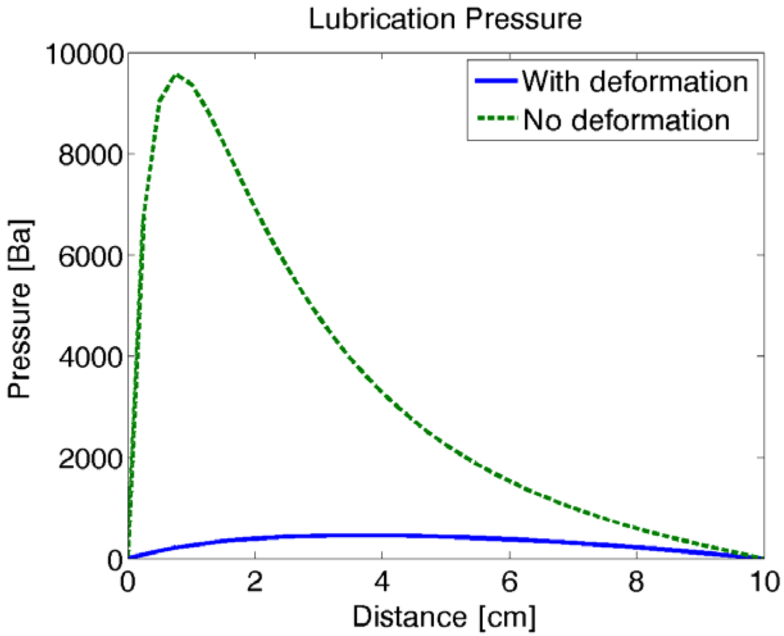


Slider deforms under the strong lubrication forces

Deformable slider bearing



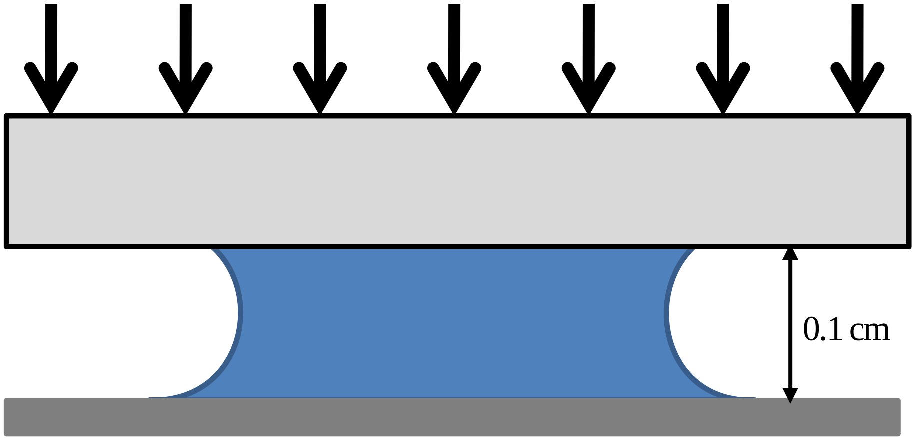




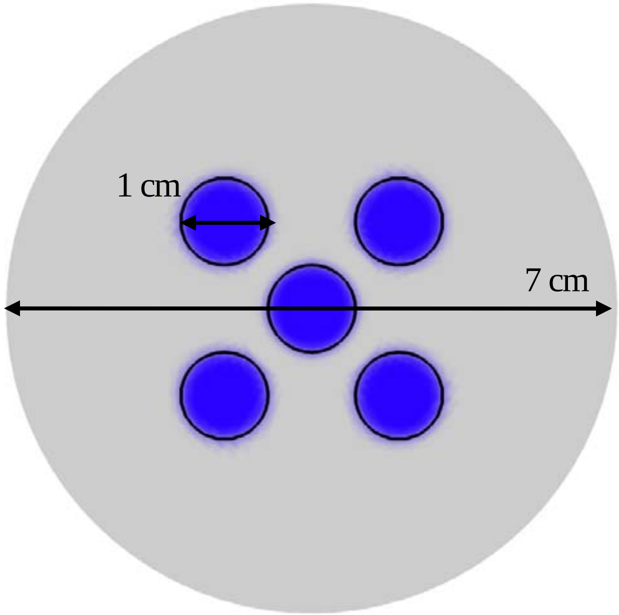
Lubrication pressure is greatly decreased when the slider is allowed to deform.

Multi-drop squeezing

- Squeezing liquid drops between two plates
  - Top plate deformable
  - Lubrication with level-set representation of liquid

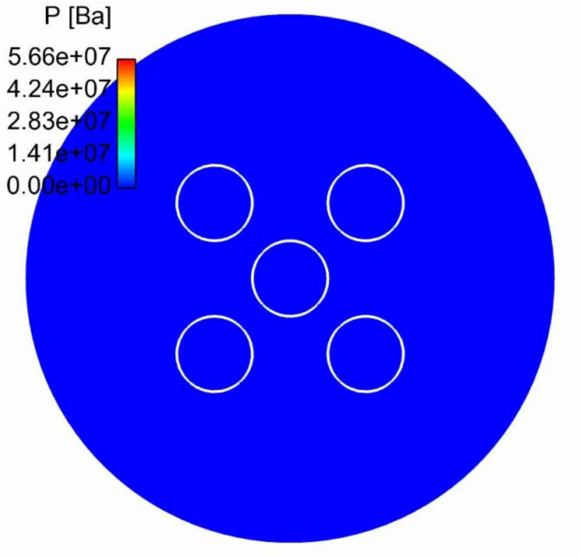


- Initial distribution:

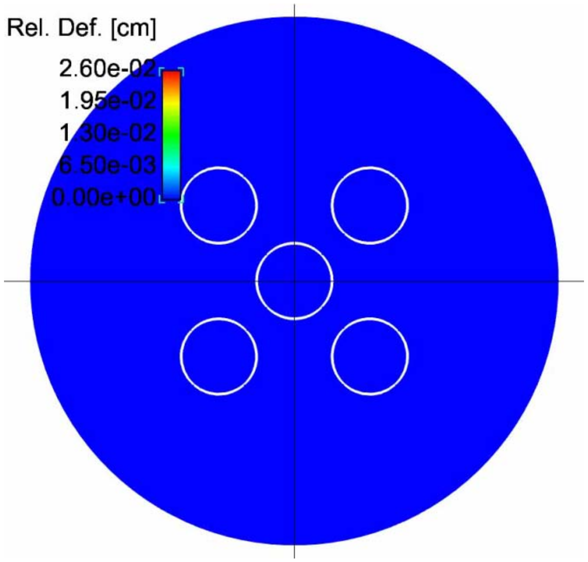


Multi-drop squeezing

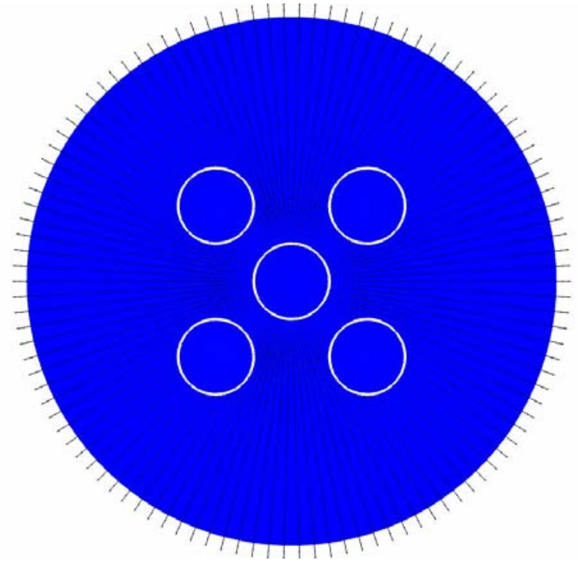
Lubrication pressure



Relative deformation



Fluid/gas velocity



- Drops spread and merge under the significant squeezing force
- Mesh deforms under the buildup of lubrication pressure
- Gas must move quickly to get out from under plates

Summary

- Many industrial applications have regions with **thin fluid flows** involving **free boundaries**.
- **Reduced-order models** / shell models can greatly simplify computational analysis of these processes.