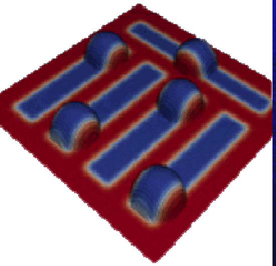
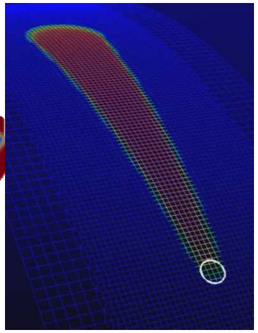
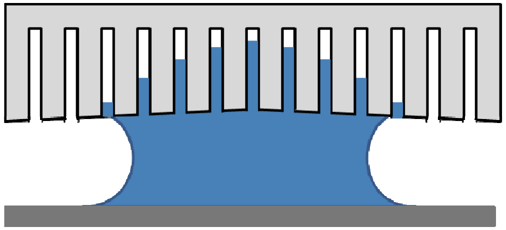
SAND2012-7471C







Reduced-order modeling techniques for understanding printing and coating processes

Scott A. Roberts, P. Randall Schunk
Sandia National Laboratories, Albuquerque, NM

Kristianto Tjiptowidjojo
University of New Mexico, Albuquerque, NM

16th International Coating Science and Technology Symposium, Atlanta, GA

September 11, 2012

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

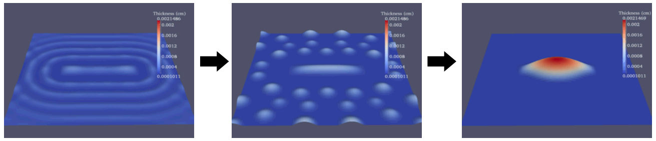
NNSA National Nuclear Security Administration

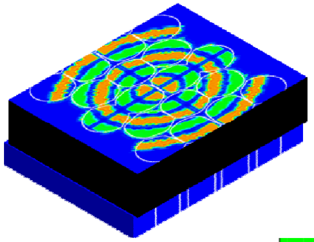
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Unclassified Unlimited Release: SAND2012-XXXX

Motivation is coating and manufacturing application driven

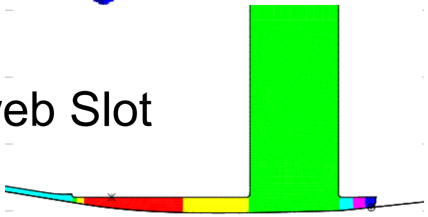
- Top-down nano-manufacturing: fluid distribution, printing, mold filling in large-aspect ratio regions

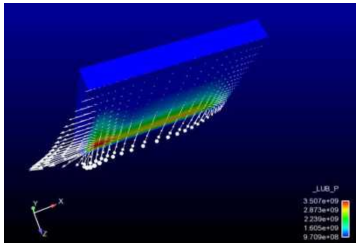




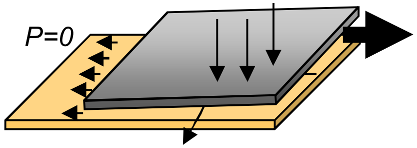
- Thin-liquid film coating: film flow, metering flows, thin metering structures

Tensioned web Slot

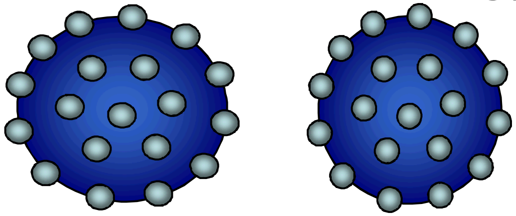


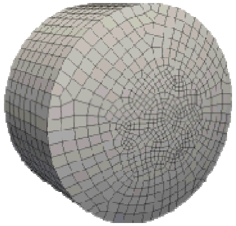


- Sliding Contacts: Lubricated bearings, electrical brush



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





- Miscellaneous: surface microprobes (Moore et al., “Comment on Hydrophilicity and the Viscosity of Interfacial Water”, Langmuir 27 (2011) 3211-3212).

What are reduced-order models?

- Begin with general 3-D governing equation (e.g. mass conservation)

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0$$

- Integrate through one dimension under a set of assumptions

$$\int_0^h \frac{\partial v_x}{\partial x} dz + \int_0^h \frac{\partial v_y}{\partial y} dz + v_z|_0^h = 0$$

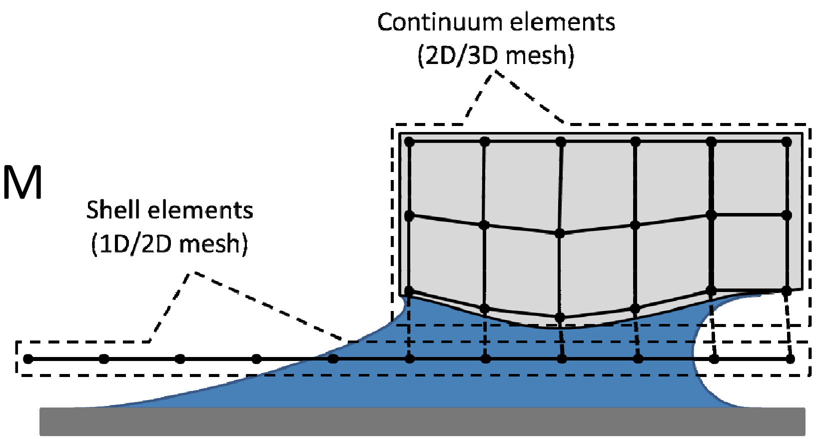
  - Reduces 3-D equation to a 2-D equation
  - Requires understanding of physics in the 3rd dimension

$$\frac{\partial \bar{v}_x}{\partial x} dz + \frac{\partial \bar{v}_y}{\partial y} dz + \bar{v}_z(h) - \bar{v}_z(0) = 0$$

$$\bar{v}_i(x, y) = \int_0^h v_i(x, y, z) dz$$

- Solve equations using shell elements with FEM

$$\boldsymbol{\nabla}_{\mathrm{II}} f = (\mathbb{I} - \boldsymbol{nn}) \cdot \boldsymbol{\nabla} f$$



Underlying assumptions of reduced-order models

- Key assumptions:
  - Material parameters (e.g. viscosity) are constant across the thickness
  - The film is thin ($\frac{\partial h}{\partial x} \ll 1$) and the flow is laminar
  - Intertial forces are negligible

- Need models for 3rd dimension:
  - Lubrication: Velocity profile is combination of Couette and Poisuelle flow, $v_x(z) = C_0 + C_1 z + C_2 z^2$
  - Porous flow: Flow in the z dimension is understood by a bundle of capillary tubes, $v_z = \frac{p_{gas} - p_{cap} - p_{lub}}{S\,h}$
  - Models need to be specifically adapted for each application

Reduced-order models

- Confined lubrication hydrodynamics
  - Roberts, Noble, Benner, & Schunk. Comp. Fluids, doi: 10.1016/j.compfluid.2012.08.009

$$\nabla_{\mathrm{II}} \cdot \left(\frac{h^3}{12\mu} \nabla_{\mathrm{II}} p + \frac{h}{2} \left(v_x(h) + v_x(0) \right) \right) = \frac{\partial h}{\partial t}$$

- Thin-film hydrodynamics
  - Tjiptowidjojo & Schunk, *in preparation*

$$\frac{\partial h}{\partial t} - \nabla_{\mathrm{II}} \cdot \left(\frac{h^3}{3\mu} \nabla_{\mathrm{II}} p - h v_x(0) \right) = 0 \qquad p + \sigma \nabla_{\mathrm{II}}^2 h = 0$$

- Porous flow through thin media
  - Roberts & Schunk, *in preparation*

$$-h\phi \frac{\partial S}{\partial t} = -\frac{h}{\mu} \nabla_{\mathrm{II}} \cdot \mathbb{K}_{II} \cdot \nabla_{\mathrm{II}} p + \frac{1}{\mu} \mathbb{K}_n \nabla_n p \Big|_{z=0}$$

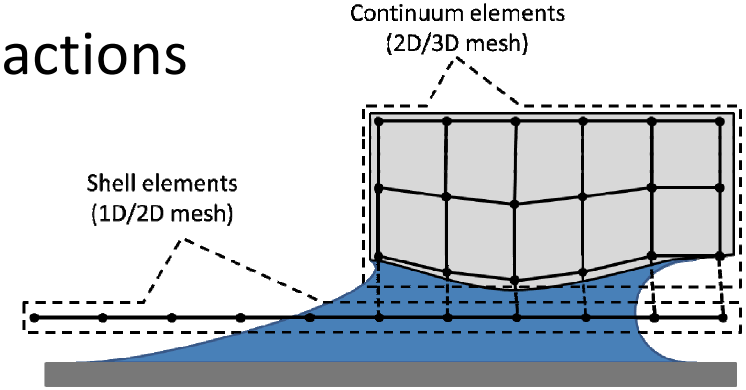
- Energy transport through thin media

$$h\rho C_p \left(\frac{\partial T}{\partial t} + \boldsymbol{v}_{II} \cdot \nabla_{\mathrm{II}} T \right) - hK \nabla_{\mathrm{II}} \cdot \nabla_{\mathrm{II}} T + Q = 0$$

Coupling to reduced-order models

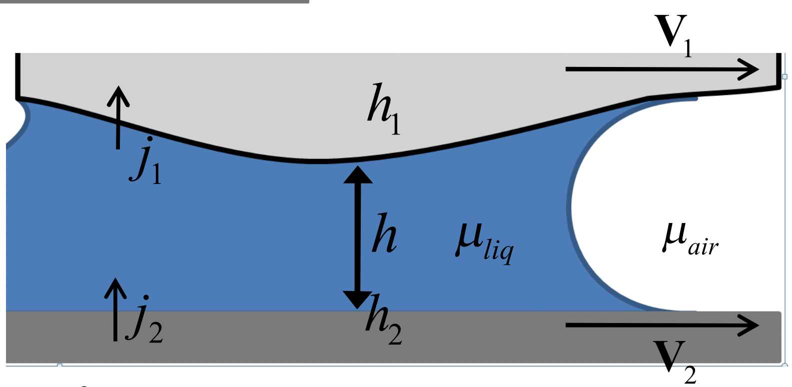
- Fluid-structural interactions

$$h = h_0 + \boldsymbol{n} \cdot \boldsymbol{d}$$

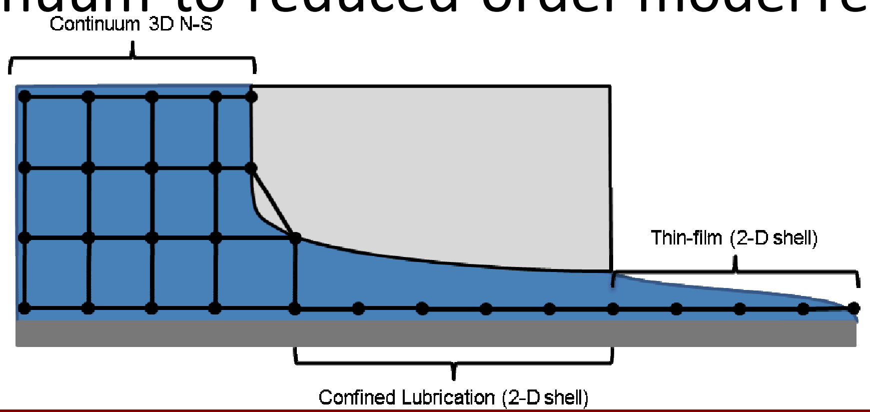


- Multiphase interfaces

$$\frac{\partial f}{\partial t} = \boldsymbol{v} \cdot \left| \boldsymbol{\nabla}_{\mathrm{II}} f \right|$$



- Continuum-to-reduced-order model regions



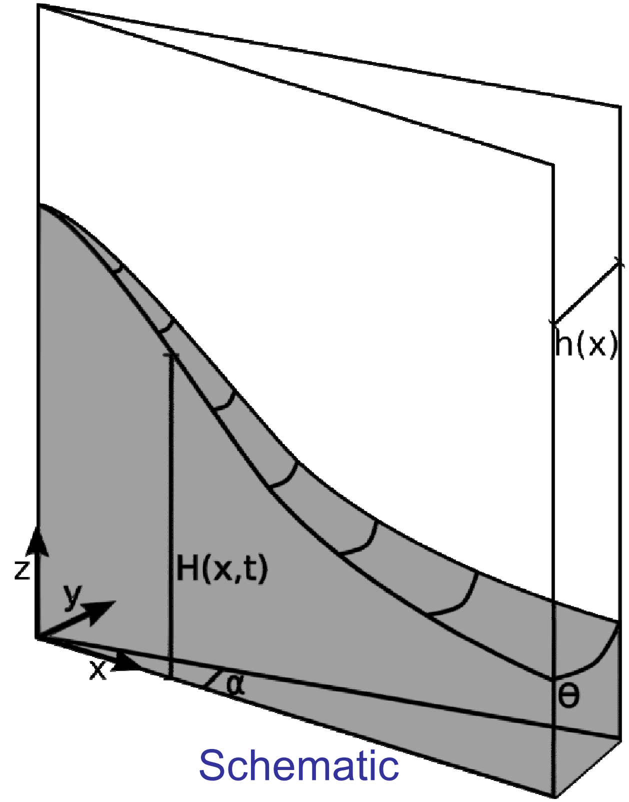
$$q_{\mathrm{continuum}} = q_{\mathrm{lubrication}}$$

Specific applications of reduced-order models

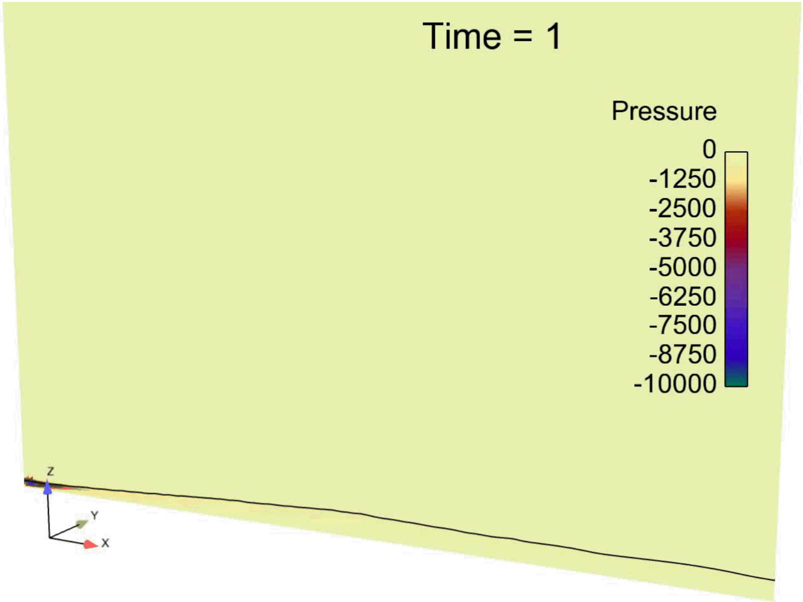
- Capillary rise of liquids
- Deformable bearings / coating processes
- Thin-film flow over patterned substrates
- Nano-imprint lithography
- Wicking porous materials
- Others …

Capillary rise of liquids

- Classic problem of capillary rise of liquids between two plates at a small angle (Taylor (1712))
- Small gap would make continuum simulations extremely difficult, due to small elements required.
- Lubrication theory allows a 2-D shell mesh and more expedient calculations
- Short-time dynamics and long-time near-steady-state profiles captured



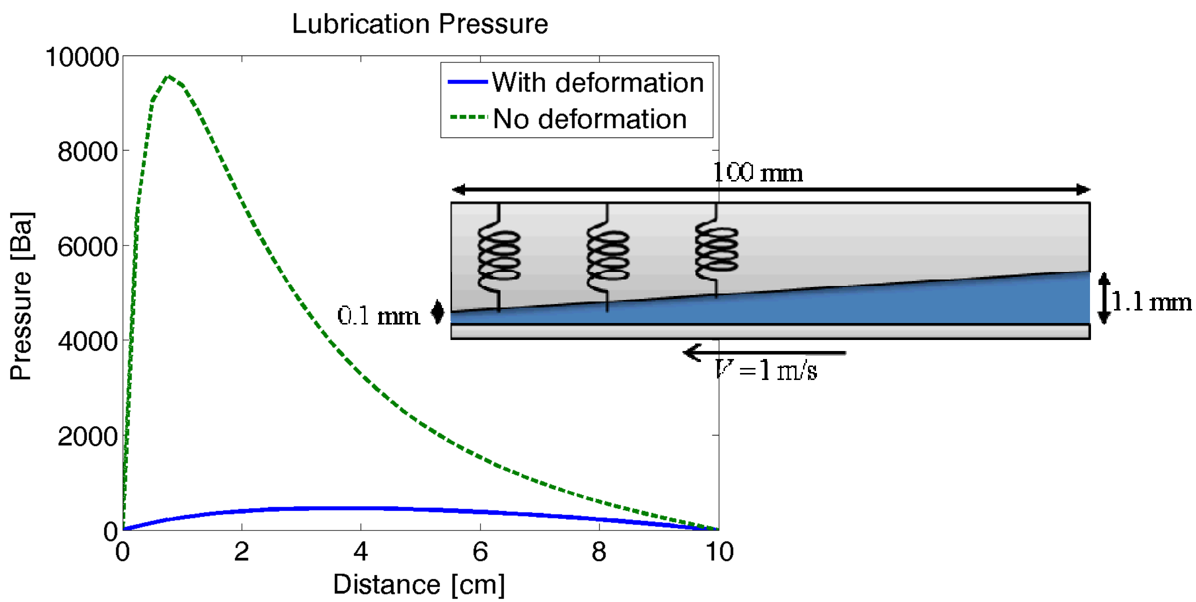
Schematic

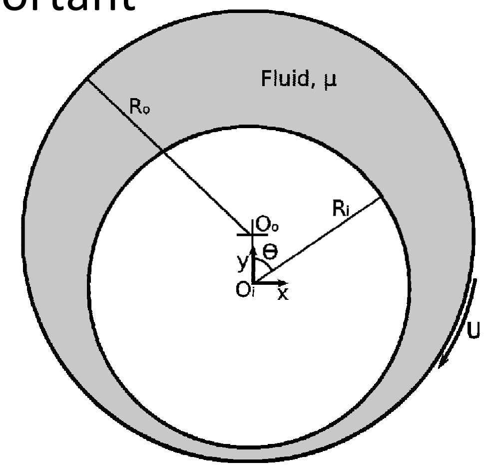


Movie of liquid rise dynamics

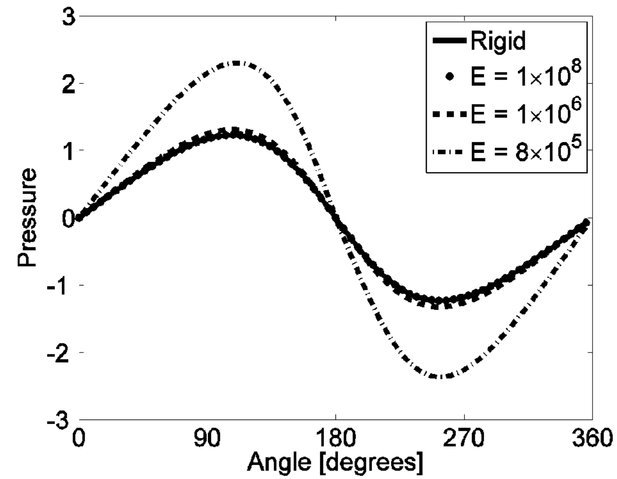
Deformable bearings / coating processes

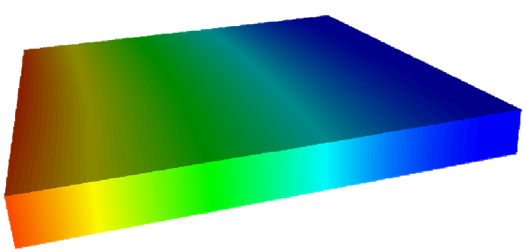
- Prototypical coating process: slot coating on tensioned web
- At high speeds and small gaps, mechanical deformation important
- Lubrication model coupled with solid mechanics (FSI)
- Deformation can reduce/shift pressure distribution





Deformable journal bearing

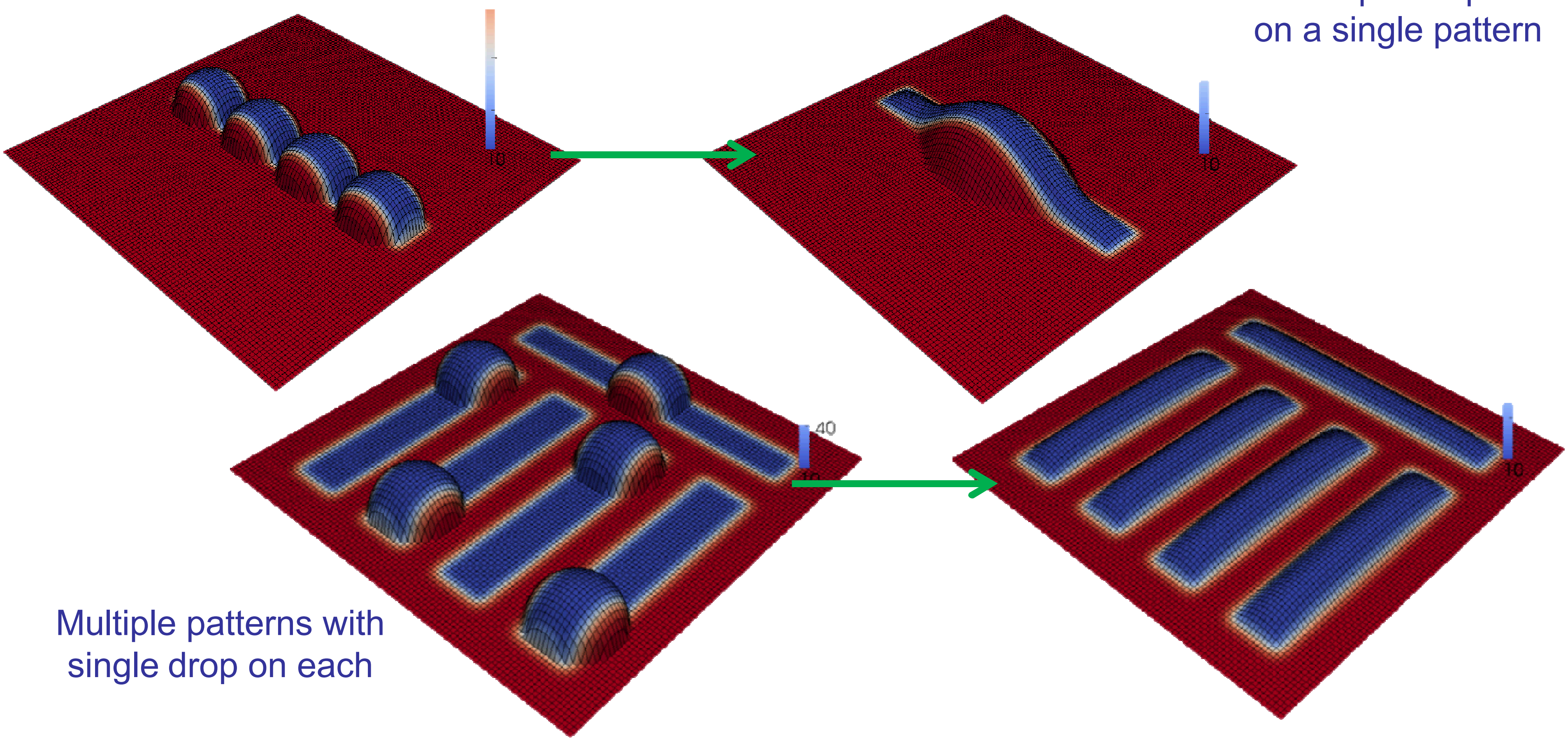




Deformable slider bearing

Thin-film flow over patterned substrates

- Substrate chemically patterned with areas of varying wettability
- Patterns are not meshed in, but an external field variable
- Drop size and pattern aspect ratio affect final liquid distribution
- Precursor film vs. contact line

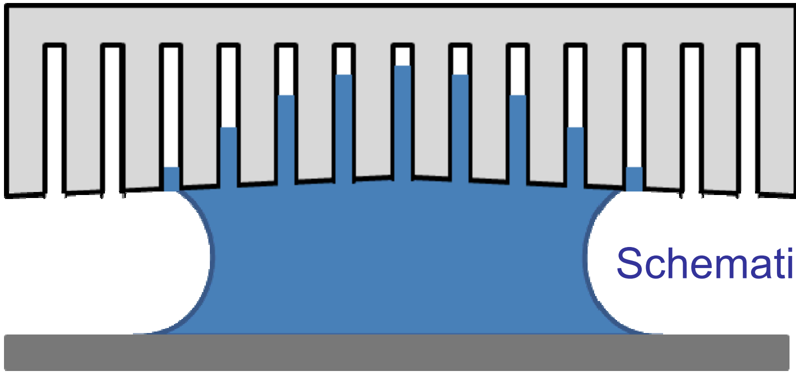


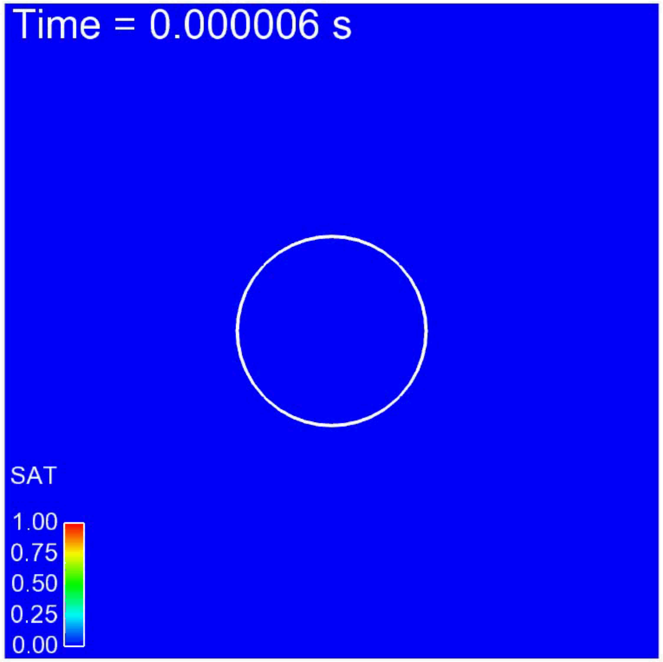
Multiple drops on a single pattern

Multiple patterns with single drop on each

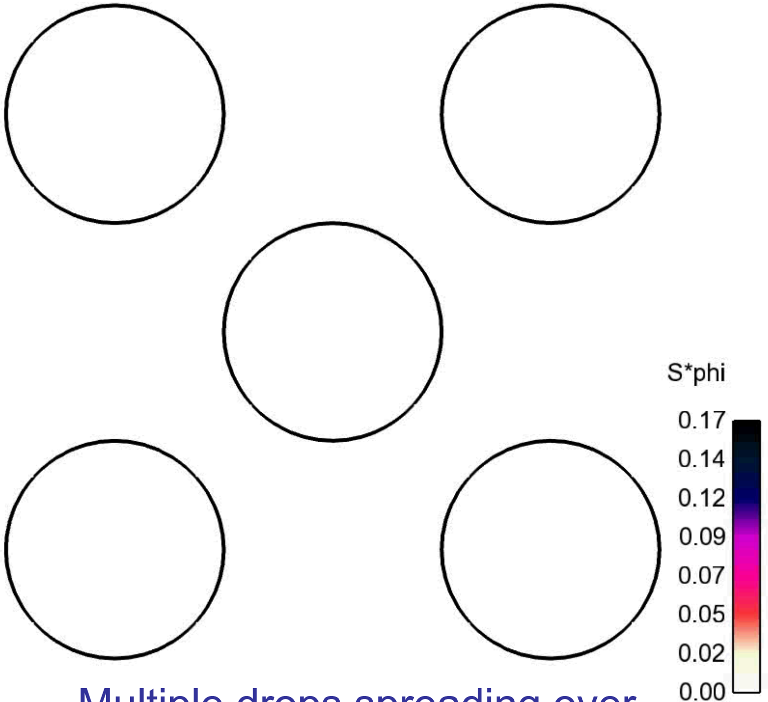
Nano-imprint lithography

- Structured, patterned, porous mask squeezed into an array of liquid drops.
- Involves lubrication and porous reduced-order models.
- Patterns in pore size and density gives different filling behaviors.





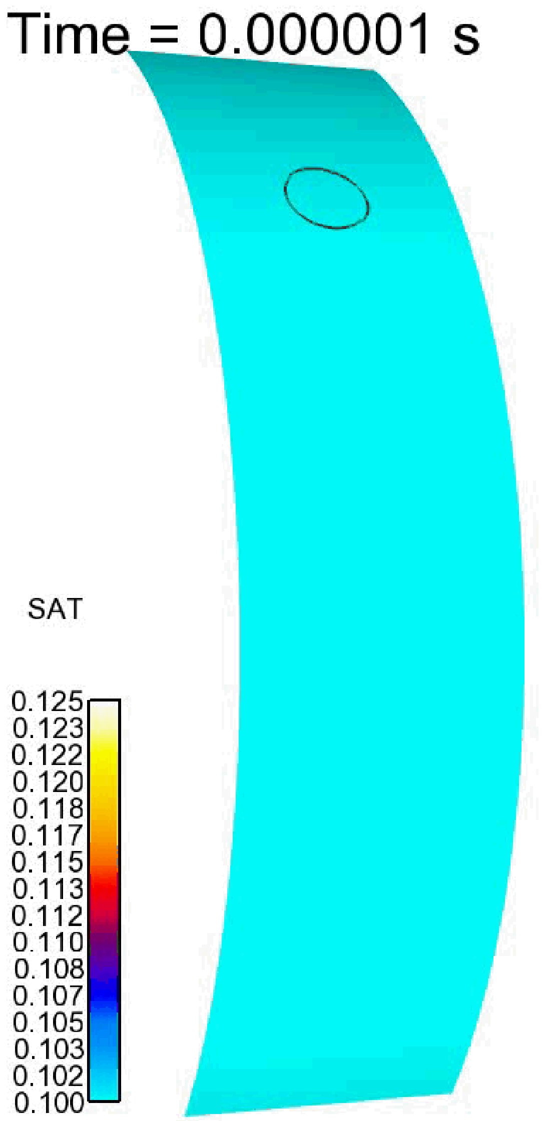
Simple spreading of a single drop



Multiple drops spreading over patterned template

Wicking porous materials

- Schematic: Drop rolling down a curved, porous substrate
- Competing effects:
  - Rolling motion under gravity
  - Liquid absorbing into porous medium
- Porous structure continues to redistribute liquid, even after drop disappears



Reduced-order models: What works, what doesn't

Advantages / Pros

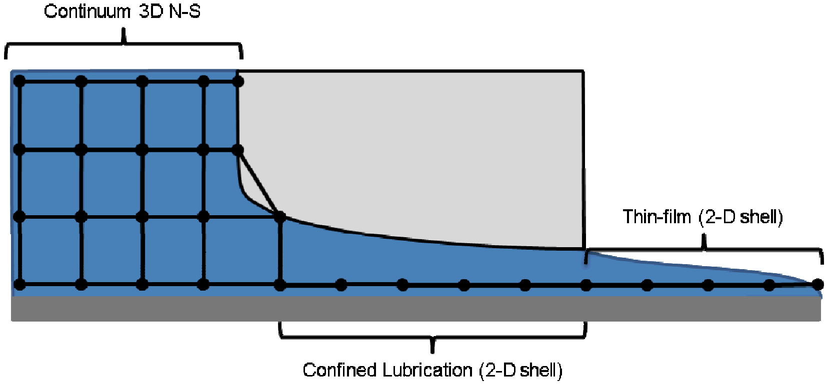
- Enables solving complex problems rendered impossible in 3D due to:
  - Small / poorly formed elements
  - Too many 3D elements
- Computationally expedient:
  - 2D shell meshes
  - Better scaling than 3D - iterative
- Simplified physics for certain problems
- Can capture complex shapes through fields rather than complex meshes

Disadvantages / Cons

- Equations / models complex to derive and code
- Models are specific to problem
  - Code changes required to change many problem parameters
  - Multiple code options / logic
- Extremely nonlinear / stiff
  - Requires more nonlinear iterations
- Shell elements not widely / completely supported in many codes

Future directions in reduced-order modeling

- Coupling confined lubrication flow to free-film flow
  - Example: Slot coating



- 3D fluid to lubrication/film coupling
- Multilayer coatings / processes
  - Multiple equations on a single shell element can represent multilayers
  - Can create custom models to handle interactions between multiple sets of reduced-order physics (lubrication, porous flow)
- Continued focus on image-to-mesh: Representing complex shapes through variations in a single field variable (height, porosity, etc.)

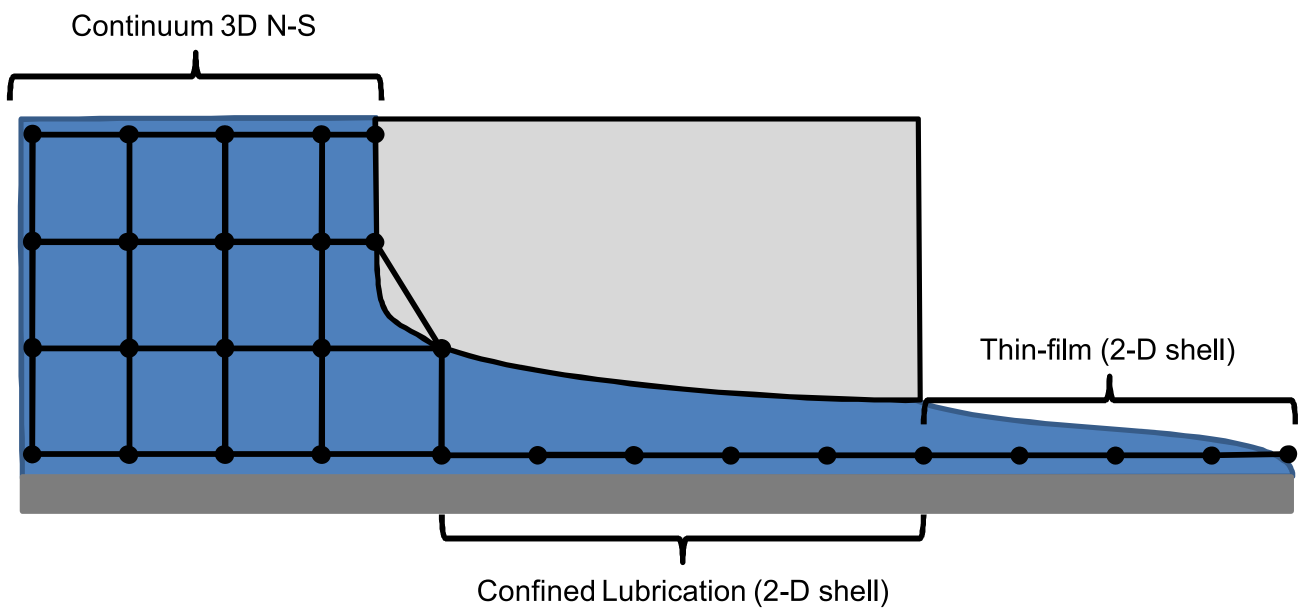
Close-up

- Final thoughts: Reduced-order models in the FEM can be enabling for problems involving fluid-flow in thin geometries. However, nonlinearities and equation complexities makes implementation non-trivial.

- Acknowledgements:

  - Sandia's Laboratory Directed Research and Development (LDRD) Program
  - D. R. Noble, E. M. Benner, Sandia National Labs
  - S. V. Sreenivasan, R. T. Bonnecaze, University of Texas at Austin
  - Molecular Imprints, Inc.

- Questions?


Continuum 3D N-S
Thin-film (2-D shell)
Confined Lubrication (2-D shell)