SAND2019-3480PE

THE UNIVERSITY of NEW MEXICO

Overview of Schunk* Research Group Activities

Department of Chemical and Biological Engineering

University of New Mexico

March 2019

Research Assistant Professor: Kristianto Tjiptowidjojo
Graduate Students: Andrew Cochrane (Ph.D), Robert Malahkov (Ph.D)
Staff: Weston Ortiz
Postdocs: hiring one or two more in the next several weeks.
Collaborators (faculty): Steve Brueck (CHTM), Roger Bonnecaze, Sang Han (UNM)
Collaborators (industry/national laboratories): NREL, ORNL, LBNL, SLAC, 3M, P&G, Corning, Avery Dennison, Ballard Inc.

*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525

Schunk Research Group Sponsors

Two Areas of Active Research – Nanomanufacturing and Complex Fluids

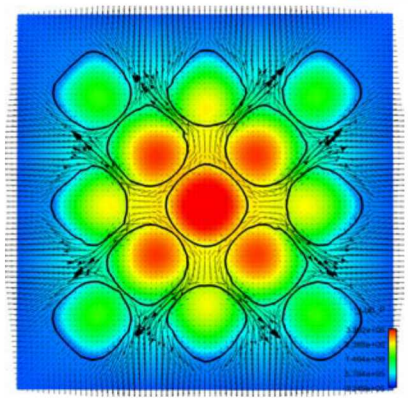
- NSF – NASCENT ERC (NASCENT-erc.org) ($130K/year)
  - NASCENT = Nanomanufacturing Systems for mobile Computing and Energy Technologies
- NSF – SNM project (thin-absorber PV) – Sang Han (PI) - $50K/year
- UNM – Matching funds for NSF ERC ($30K/year)
- Procter and Gamble (Unrestricted grants $40K and in the past $50K))
- 3M Corporation (Unrestricted grant $50K)
- Gillette (Unrestricted grant $50K)
- Sandia National Laboratories (Project funds - $200K+ consistently since 2014)

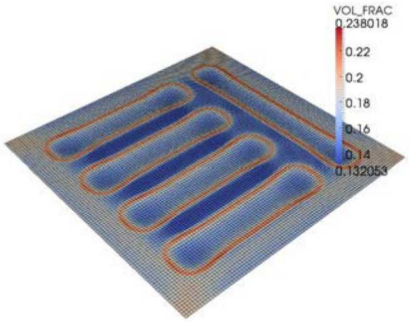
Schunk Research Group Competencies and Strengths

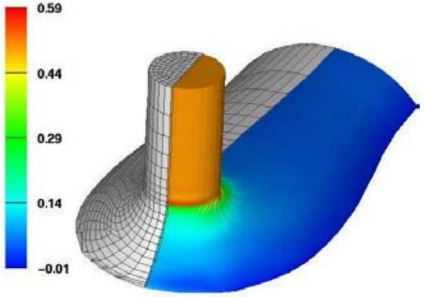
- Modeling and simulation: from code development to application.
  - Algorithm development (Finite element technology in continuum mechanics)
  - Algorithm development (Discrete element modeling technology – colloids)
  - High-performance computing (MPI-based parallel processing)
  - Matrix solver technology, preconditioner development
  - Thin-shell mechanics
- Multiphase flow (poro-elastic media, particulate flows)
- Chemically reacting systems (electrochemistry for battery performance modeling)
- Viscoelastic flow (Constitutive equation development, solver development)
- Free and moving boundary problems
- Fluid-structure interactions
- Heterogeneous materials (predictive properties)
- Manufacturing (printing thin-film coating, casting, welding/soldering/brazing,wet etching/microelectronics processing …)

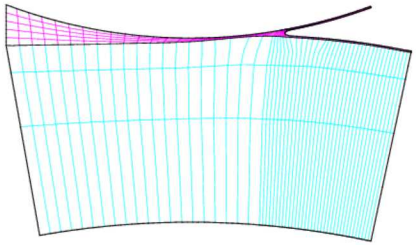
Research Group Capability: Goma 6.0

2014 R&D 100 Award Winner









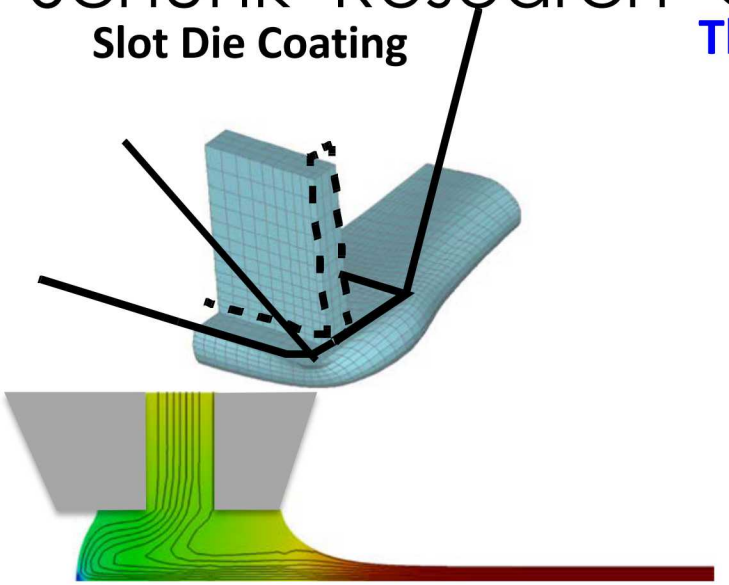
- Multiphysics ***finite element*** code, suitable for both ***research*** and ***production***
- Fully-coupled ***free*** and moving ***boundary*** parameterization – ALE, Level Set, etc.
- Modular code; ***easy to add equations*** – currently has 170+ differential equations
- ***Open source***! Available at **http://goma.github.io**
- ***Goma 6.0. training*** is available on regular basis

Goma has been used successfully in coating manufacturing for 2 decades!

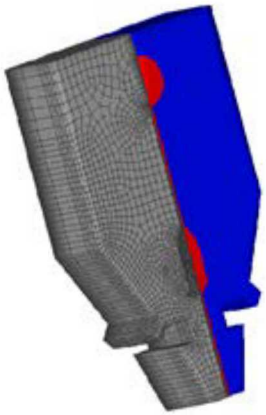
…Also a competency in LAMMPS for colloidal rheology and self/directed assembly

Schunk Research Group Modeling Capabilities

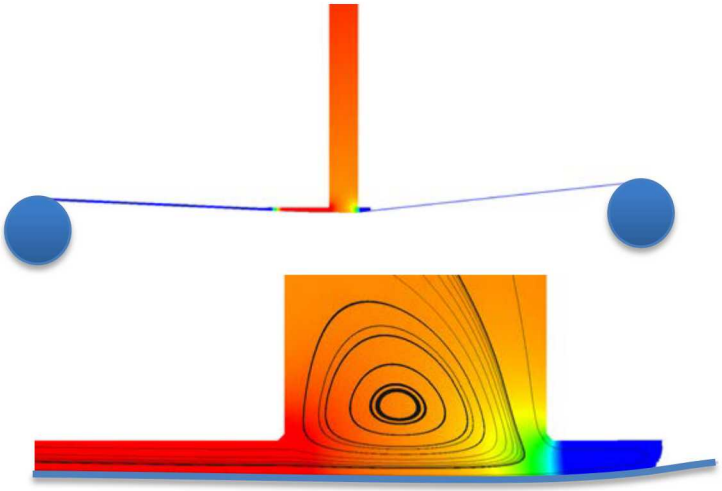
Slot Die Coating



Thin-Film Coating



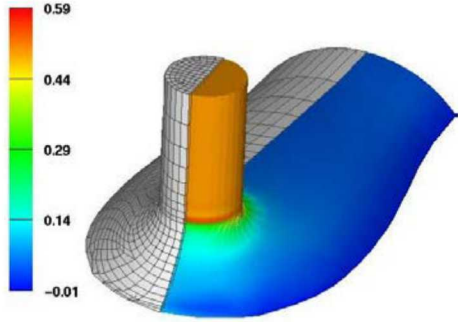
Tensioned Web over Slot Die Coating



Free Surface Tracking/Capturing

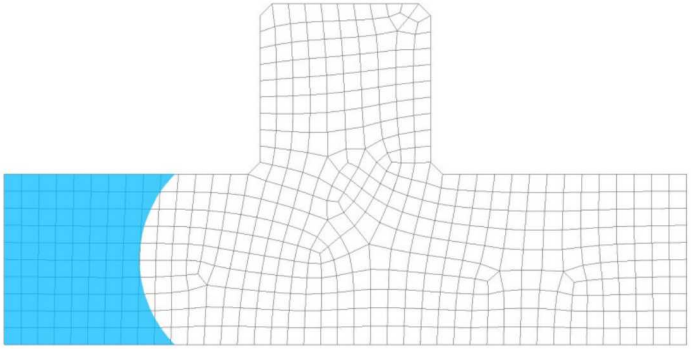
Arbitrary Lagrangian Eulerian (ALE)

Deform mesh to track free surface



Eulerian

Fixed mesh, use level set to capture free surface

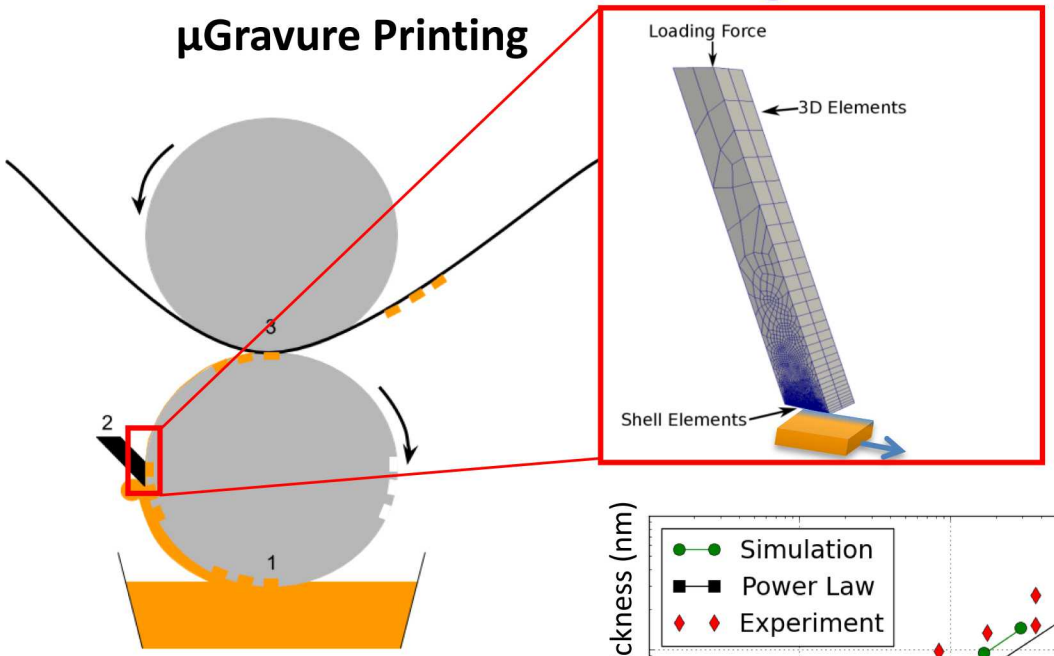


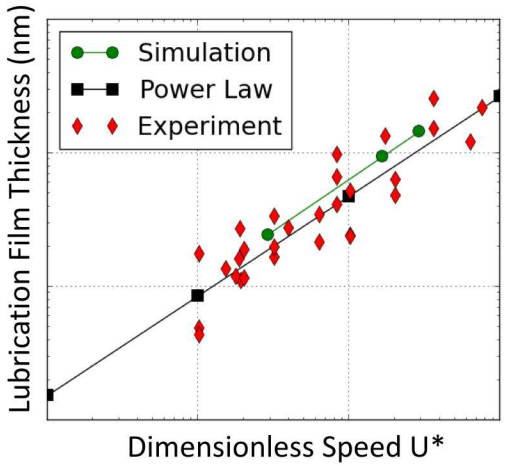
- ***Full 3-D simulation of continuous liquid film coating with finite element method***
- ***Capable of handling free surfaces two ways: ALE and level set method***

Schunk Research Group Modeling Capabilities

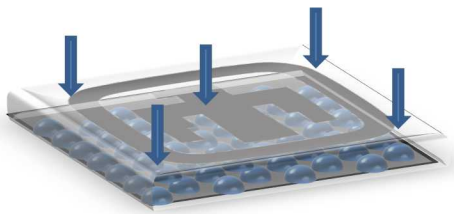
Printing and Nanopatterning

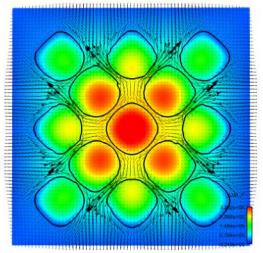
µGravure Printing

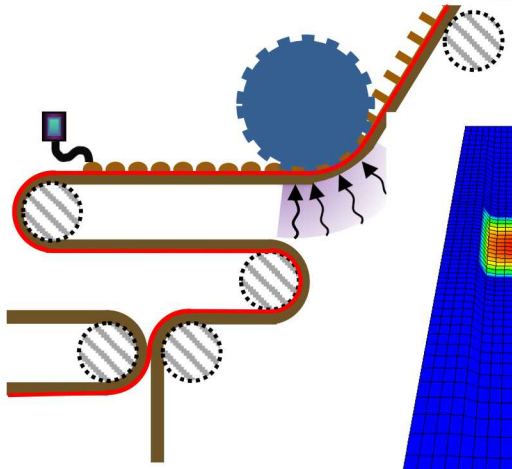




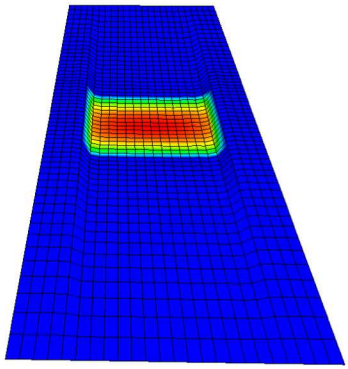
Nanoimprint Lithography







Merging drops



Substrate deflection

- ***Prediction of residual film thickness is validated with experiments***
- ***Capable of modeling fluid structural interaction (FSI) of nanopatterning process at manufacturing scale***

NASCENT Overview

THE UNIVERSITY OF TEXAS AT AUSTIN

THE UNIVERSITY of NEW MEXICO

Berkeley UNIVERSITY OF CALIFORNIA

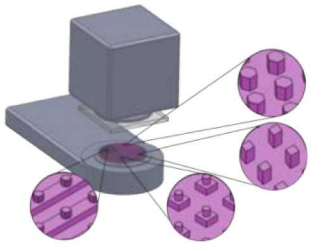
- **University research center** funded in September 2012, 10 years of expected funding from the National Science Foundation (NSF).
- NASCENT has an annual budget of >$4 million, and a **team of more than 75** graduate students, post-doctoral researchers, and faculty members.
- NASCENT Mission: To create **high throughput**, reliable and versatile **nanomanufacturing systems** and processes that will revolutionize future generations of mobile computing and energy devices.
- We are a **Nanomanufaturing R&D Center**

Courtesy of Larry Dunn Ph.D.

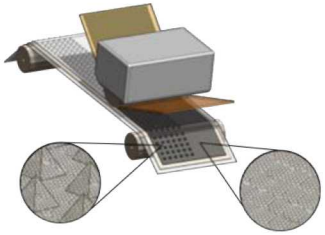
For more information, see Larry Dunn Ph.D. at the NASCENT booth

NASCENT Enabling Technologies

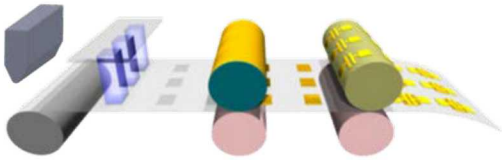
- 2D/3D Nanosculpting
  - Wafer Scale and R2R Substrates



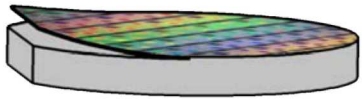
- Roll-to-roll (R2R) graphene transfer



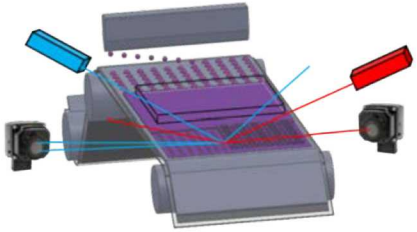
- R2R Printable Nanomaterials



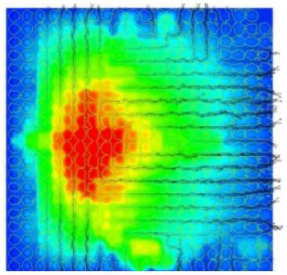
- Exfoliated crystalline materials



- In-line nanometrology



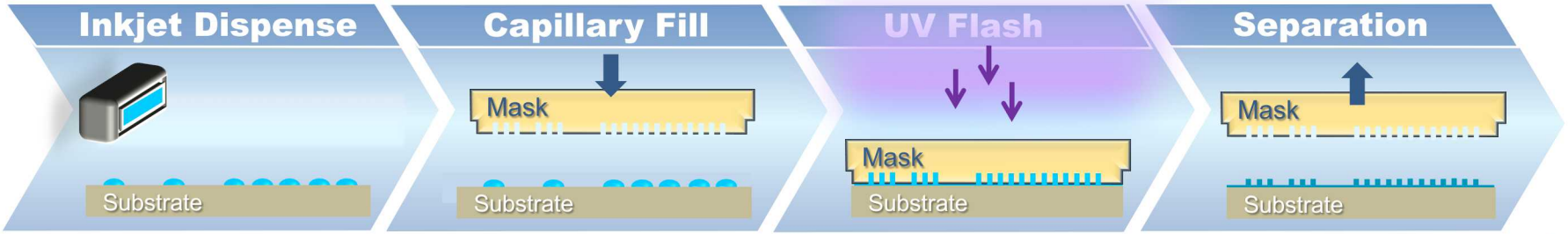
- Scale-Up and Reduced Order Model Simulators



Courtesy of Larry Dunn Ph.D.

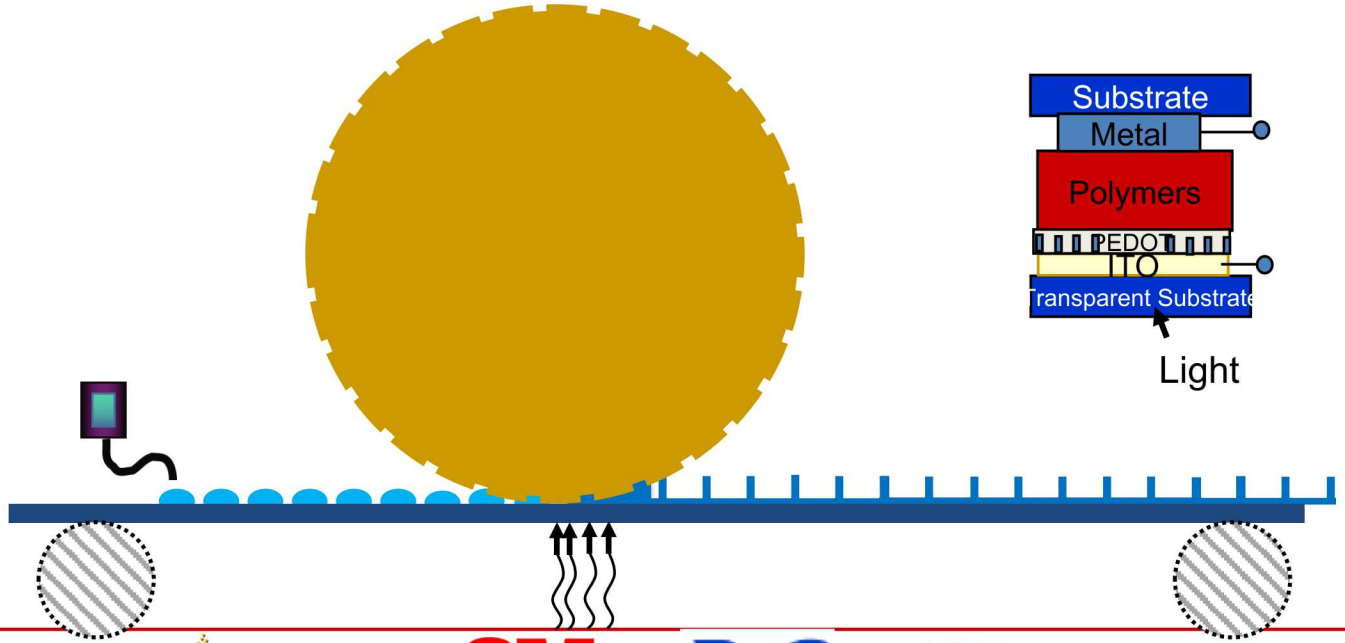
Nanosculpting: Nanoimprint Lithography

Jet Flash Imprint Lithography™ (J-FIL™)



Courtesy of MolecularImprints

Roll-to-Roll Nanoimprint Lithography (R2R_NIL)



High density storage

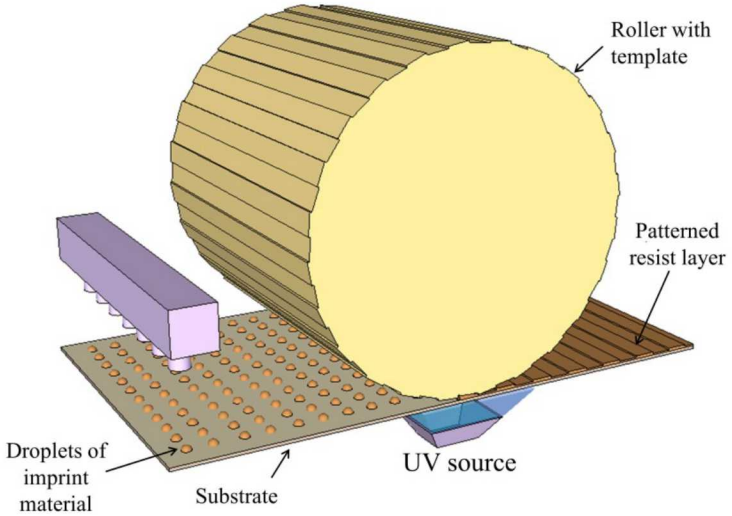
Courtesy of Akhilesh Jain

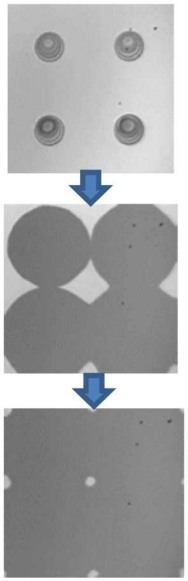
Nanoimprint Lithography

Project Goal

Optimize Rate & Yield

- Minimize Gas Trapping
- Obtain Uniform Residual Layer





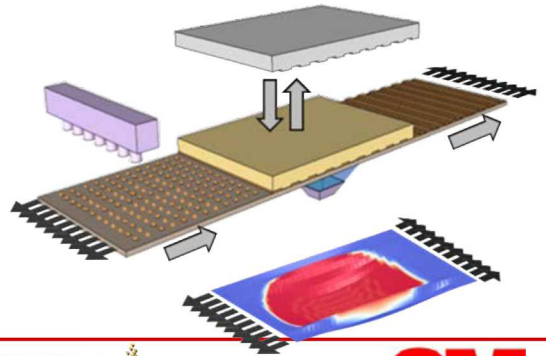
Approach

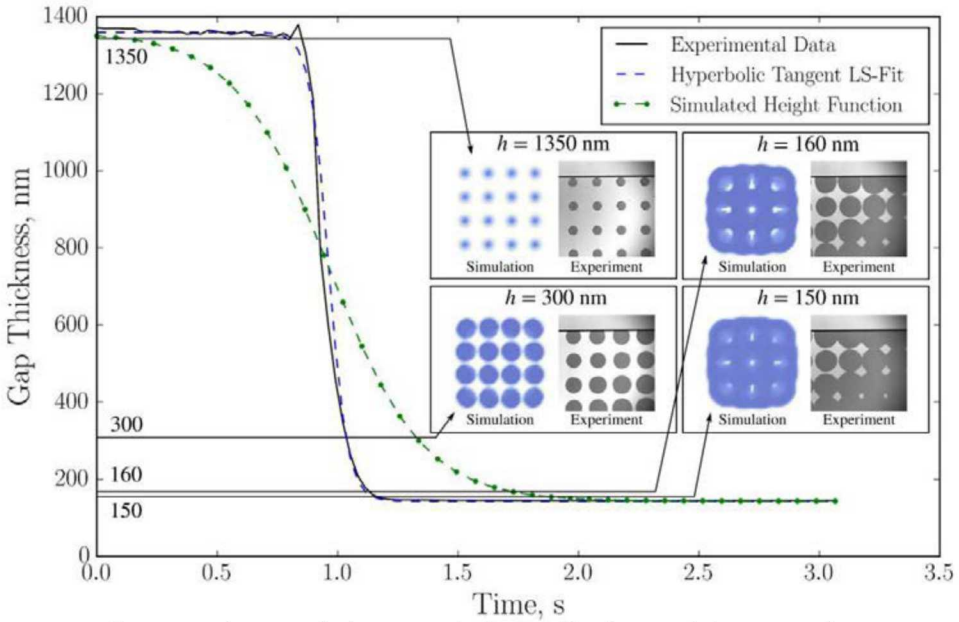
Develop a Multiphase Flow Model

- Not tracking liquid-gas interfaces
- Incorporate gas compression and dissolution

Updates

- Completed multiphase flow model
- Incorporating structure mechanics of substrates and or templates





Comparison of the model prediction with experiment

Preliminary work on coupling multiphase flow model with membrane mechanics

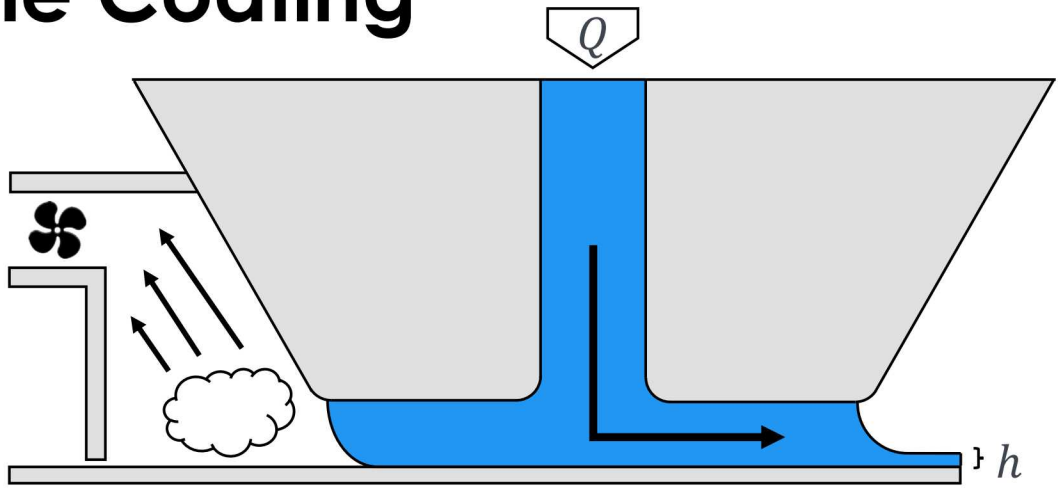
Cochrane et al. *Int. J. Multiph. Flow*, doi:10.1016/j.ijmultiphaseflow.2018.03.014

Slot-Die Coating

Project Goal

Use slot die for nanomanufacturing

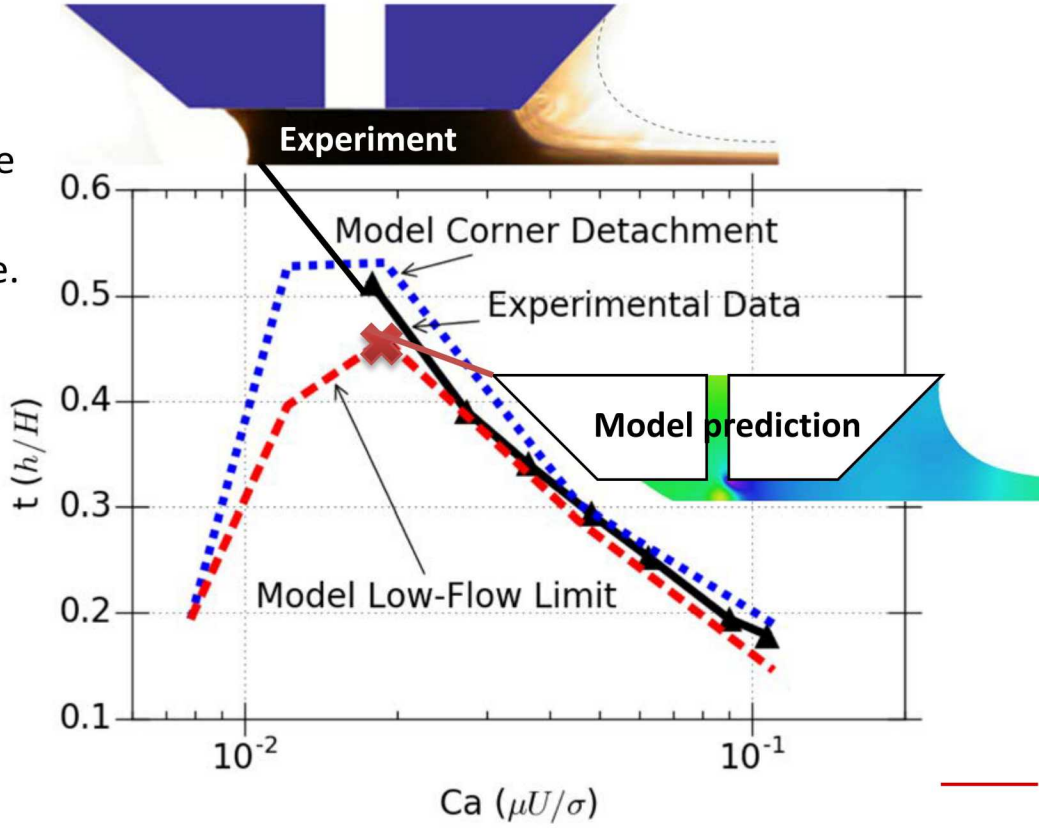
- Scale-up: Ultrathin coatings (<1µm wet thickness)
- Small-lot patch coatings



Approach

Develop slot coating flow model

- Steady 2-D Navier-Stokes with Arbitrary Lagrangian Eulerian (ALE) method to track free surface
- Predict minimum film thickness achievable, i.e. low flow limit



Updates

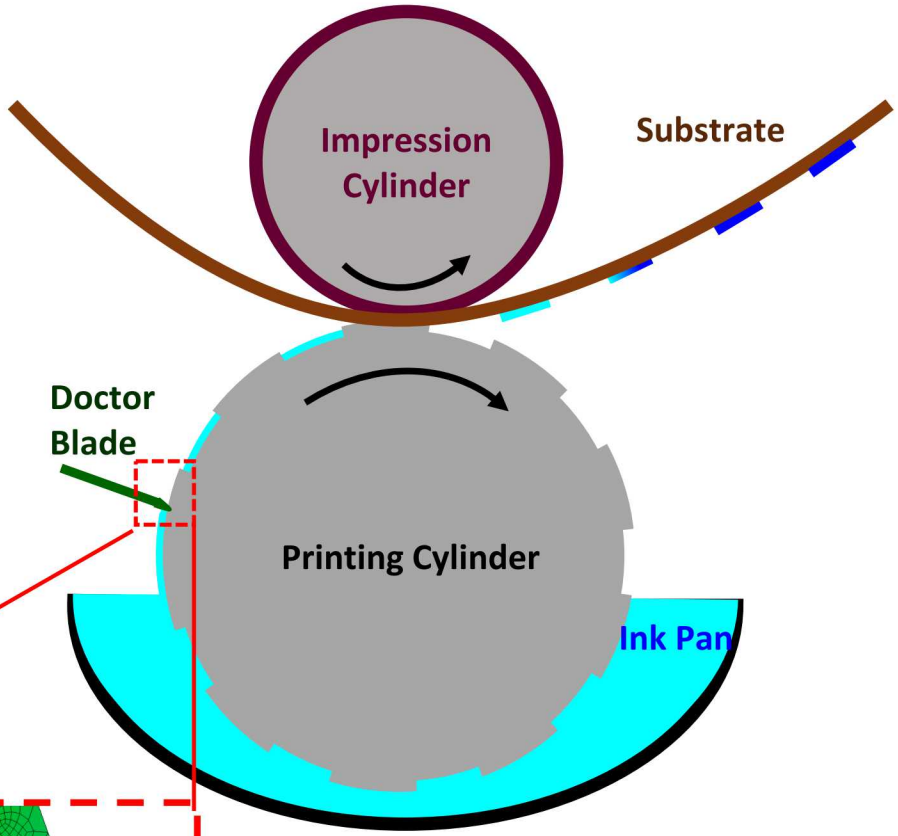
- Validated the model
- Uncovered mechanisms of low-flow limit

Gravure Printing

Project Goal

Deposit functional 0D and 1D nanomaterials

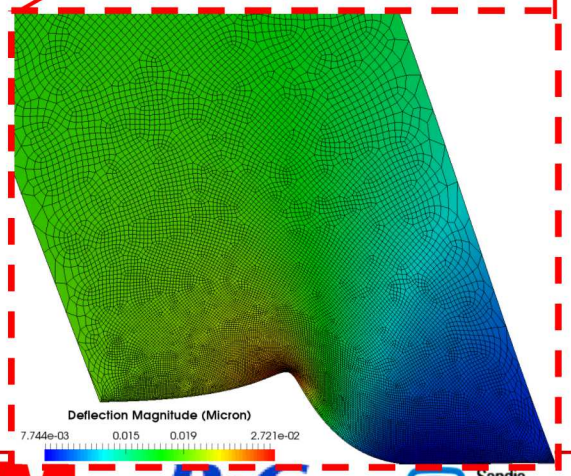
- Use gravure printer – high speed, R2R method
- Push printing resolution <1 µm



Approach

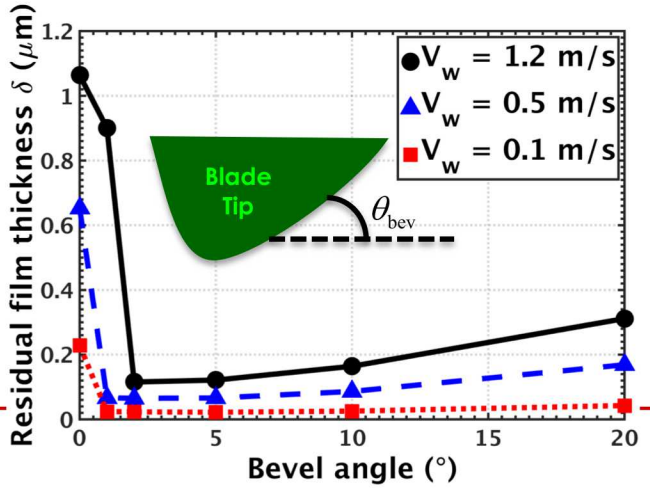
Develop gravure printer model – doctoring step

- Coupling between 3-D elasticity equation and 2-D lubrication flow
- Predict residual film thickness



Updates

- Validated the model
- Optimized blade shapes

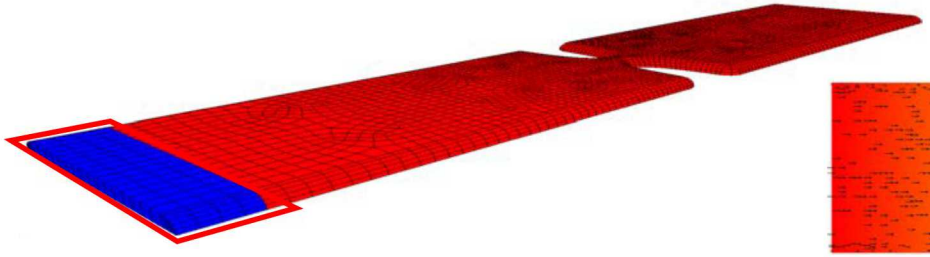


Tjiptowidjojo et al. *J. Coat.Technol. Res.*, doi:10.1007/s11998-017-0029-0

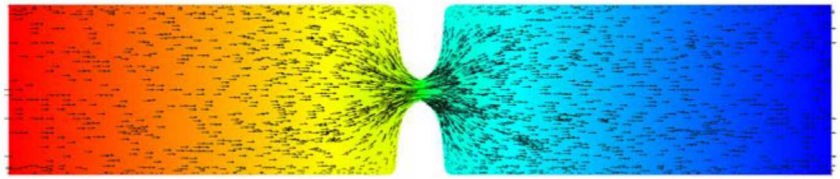
UNM NASCENT 3M P&G Sandia National Laboratories

Research in Computational Viscoelasticity

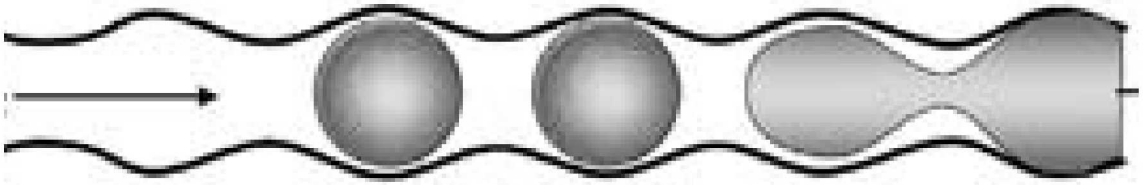
Complex Fluids (e.g. yield-stress fluids and worm-like micelle solutions) -- Sponsors P&G/Gillette

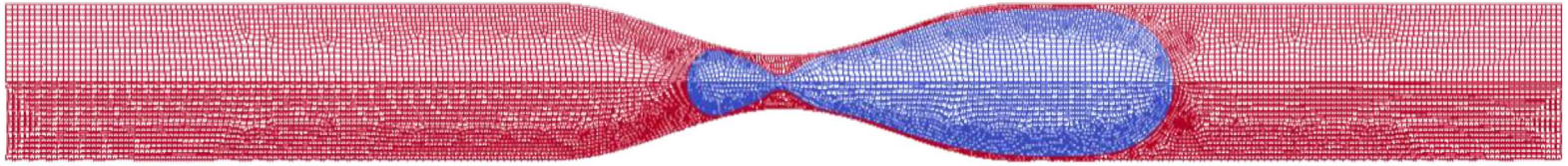


MEMS Rheometer



Viscoelastic flow application in enhanced oil recovery (assisting Prof. Matt Balhoff, Department of Petroleum Engineering, UT Austin)





Sponsor P&G, Gillette, SNL. Collaborator: UT Austin

UNM NASCENT 3M P&G Sandia National Laboratories

Roll-to-Roll Advanced Materials Manufacturing Lab Collaboration

Collaboration Lead: Claus Daniel (ORNL)
Email: danielc@ornl.gov; Phone: 865-946-1544
Argonne National Laboratory Lead: Gregory Krumdick
Lawrence Berkeley National Laboratory Lead: Vince Battaglia
National Renewable Energy Laboratory Lead: Michael Ulsh
Sandia National Laboratory: Randy Schunk
Oak Ridge National Laboratory Lead: David Wood

Presenters: Claus Daniel and Scott Mauger
2019 Hydrogen and Fuel Cells Program
Annual Merit Review
May 1, 2019

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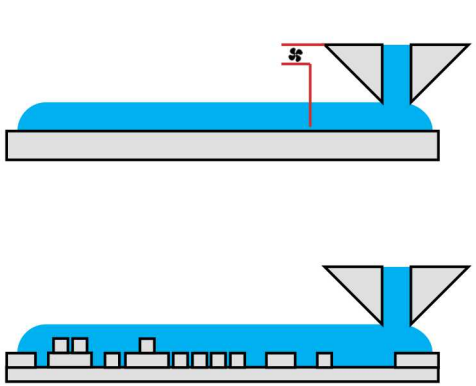

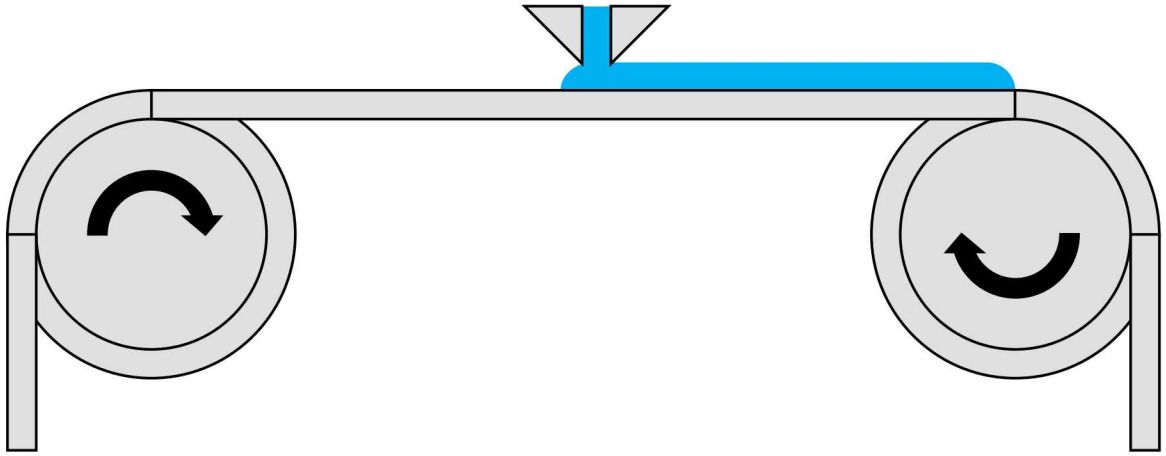

Slot Die Coating Model

Robert Malakhov[†], Kristianto Tjiptowidjojo[‡], P. Randall Schunk[‡§]

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1 University of New Mexico Albuquerque, NM 87131

[‡]Department of Chemical and Biological Engineering
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Albuquerque, NM 87185[1]

Overview

Timeline and Budget

- Project Start Date: 10/01/2016
- Project End Date: 9/30/2018
- FY18 AMO Funding: $4M
- FY18 FCTO: $0 of FCTO
- FY19 planned: $150K of FCTO for new CRADA with Proton On-Site
- $850K of FCTO contribution in negotiation

Technology Barrier

- Develop roll to roll manufacturing techniques to reduce the cost of automotive fuel cell stacks at high volume (500,000 units/year) from the 2008 value of $38/kW to $20/kW by 2025.
- Lack of high-volume MEA processes

- Project partners:
  - ORNL, NREL, ANL, LBNL, SNL
  - Proton On-Site
  - Eastman Business Park

Summary

Relevance:

- R2R is the only manufacturing process platform that will meet cost and volume targets for PEM MEAs
- Cost reduction need: 60 cents/mile in 2013 to 13 cents/mile in 2025

Approach:

- Leverage unique capabilities, facilities, expertise across the four labs
- Focus on MEA structure of industrial interest (GDEs)
- Achieve reduction in process steps and energy consumption

Collaborations:

- ORNL, ANL, LBNL, NREL, Eastman Business Park, industry

Accomplishments:

- Determined function of ionomer overlayer in spray-coated GDEs
- Characterized influence of MPL roughness on GDE performance and properties
- Developed materials and process for single-process R2R GDEs with performance better than spray-coated CCMs or GDEs – **ACHIEVED PROJECT GOAL**

Multilayer Slot/Slide Coating Process Models

Achievement

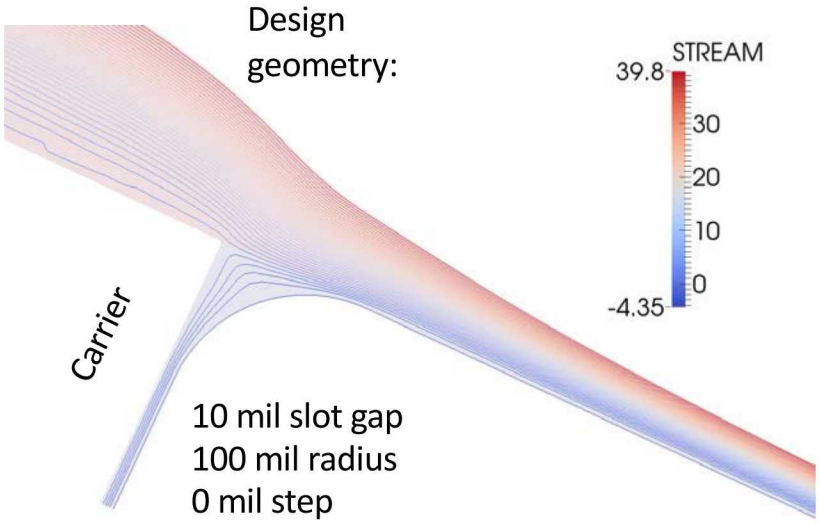
Completed workflows and demonstrated multilayer slot and slide coating process models using Goma 6.0.

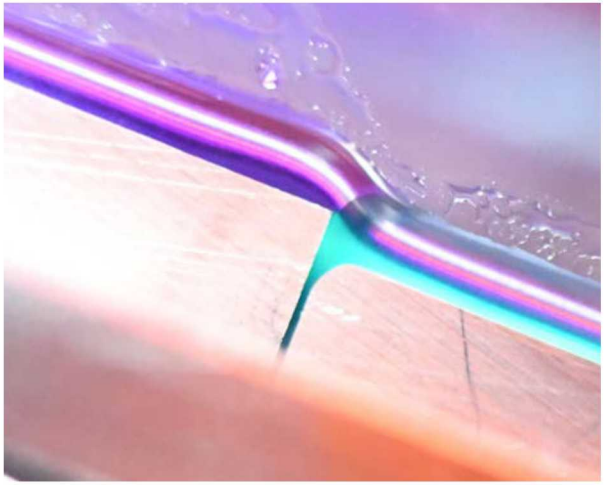
Significance and impact

-Process models of pre-metered coating flow deposition capillary hydrodynamics have proven track record of accelerated process development

-Models of consortium's slot- and slide-deposition systems with accommodation for 3+ simultaneous miscible layers has no precedence (multiple layers of varying rheology)

-Modeling and simulation of the coating process, once validated, will enable process operating windows with key parameters (layer flow rates, webspeed, slide/slot configuration etc.





Details and next steps

- Complete demonstration of 2-layer slot die coating deposition
- Complete demonstration of 1-3 layer slide-die coating deposition
- Document workflows for wider usage
- Document validation against coating trials conducted at ORNL and NREL

U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy

Future Outlook/Plans

- **NASCENT ERC in critical 7th year of 10.**
- **Growing interest from thin-film coating and consumer products industries in a research group focused on development and application of high-end simulation tools (*SNL collaborations are essential here* and part of the attraction)**
- **Grow a modeling and simulation *community of practice* at the AML and joint with several departments (at all scales, from sub-molecular to continuum to system)**
- **New partners in UMN (Derby group), EERE AMO computational mechanics**

National Laboratory Professor position mutually beneficial to UNM and Sandia: Allows for career development of key staff, widens conduit of technology exchange between two neighboring research institutions, promotes collaborations on large grants and proposals.