

M | S | R | F

Sandia National Laboratories

An Overview

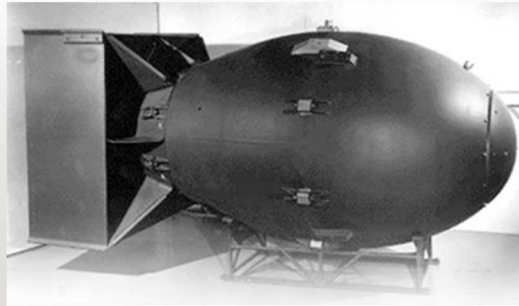


*Exceptional
service
in the
national
interest*



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. SAND NO. 2011-XXXXP

Sandia's History



THE WHITE HOUSE
WASHINGTON
May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the construction of a laboratory at Albuquerque, New Mexico.

This operation, which is a vital part of the atomic national defense, and should have the highest national direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. C. E. Duskley.

Very sincerely yours,
Harry Truman

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

exceptional service in the national interest.





Governance of Sandia Laboratories

Sandia Corporation

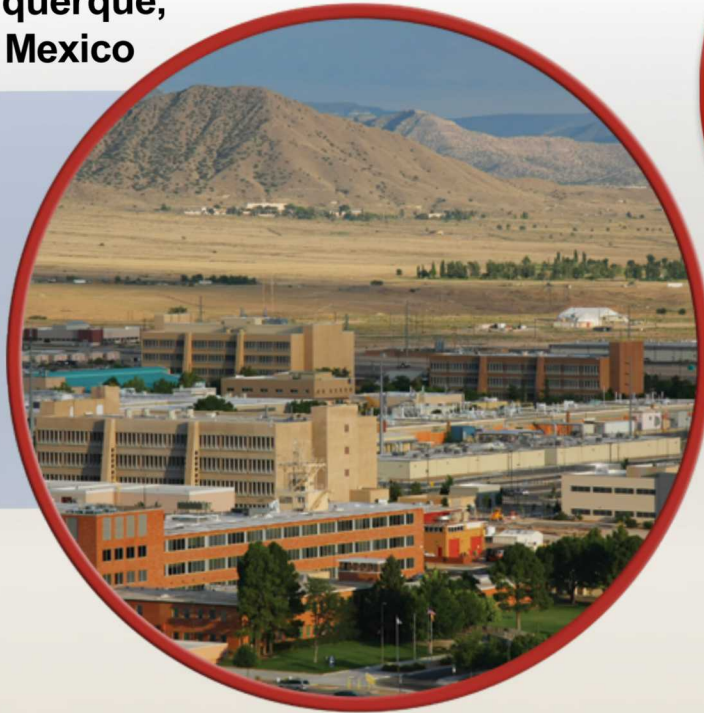
- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–2017
- National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc.: 2017-present
- Government owned, contractor operated

Federally funded
research and development center



Sandia's Sites

**Albuquerque,
New Mexico**



**Livermore,
California**



Tonopah, Nevada



**Waste Isolation Pilot Plant,
Carlsbad, New Mexico**

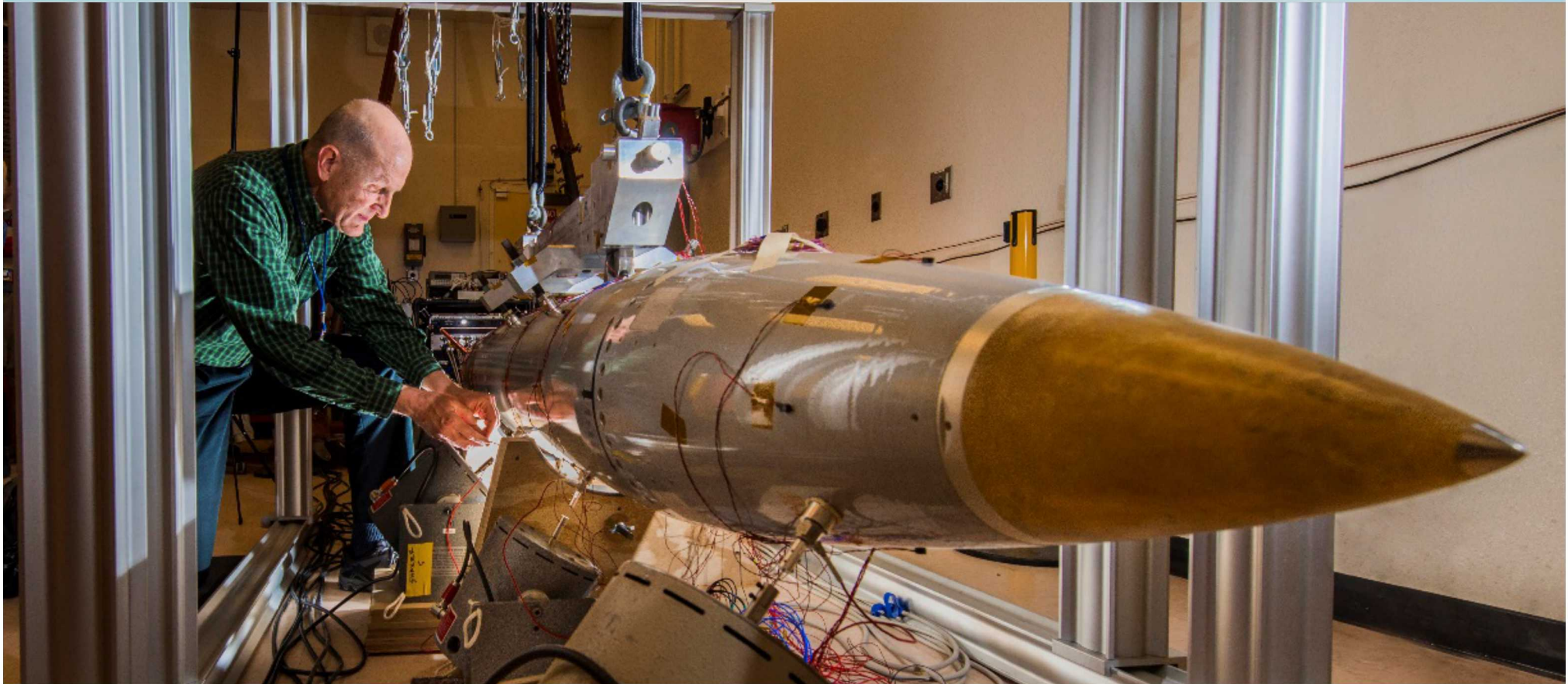


Pantex, Texas



Purpose Statement

Sandia develops advanced technologies to ensure global peace





Sandia Addresses National Security Challenges

1950s

Nuclear weapons

Production and manufacturing engineering



1960s

Development engineering

Vietnam conflict



1970s

Multiprogram laboratory

Energy crisis



1980s

Missile defense work

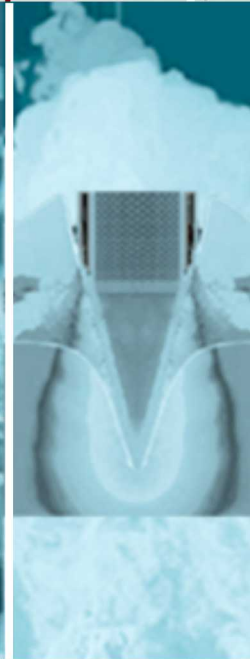
Cold War



1990s

Post-Cold War transition

Stockpile stewardship



2000s

START
Post 9/11

National security



2010s

LEPs
Cyber, biosecurity proliferation

Evolving national security challenges



Sandia's Current Nuclear Weapons Activities



Warhead Systems Engineering and Integration



Gas Transfer systems



Design Agency for Nonnuclear Components



Arming, fuzing, and firing systems

Safety systems



An extensive suite of multi-disciplinary capabilities are required for Design, Qualification, Production, Surveillance, Experimentation / Computation

Major Environmental Test Facilities and Diagnostics



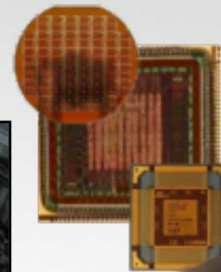
Light Initiated High Explosive



Z Machine

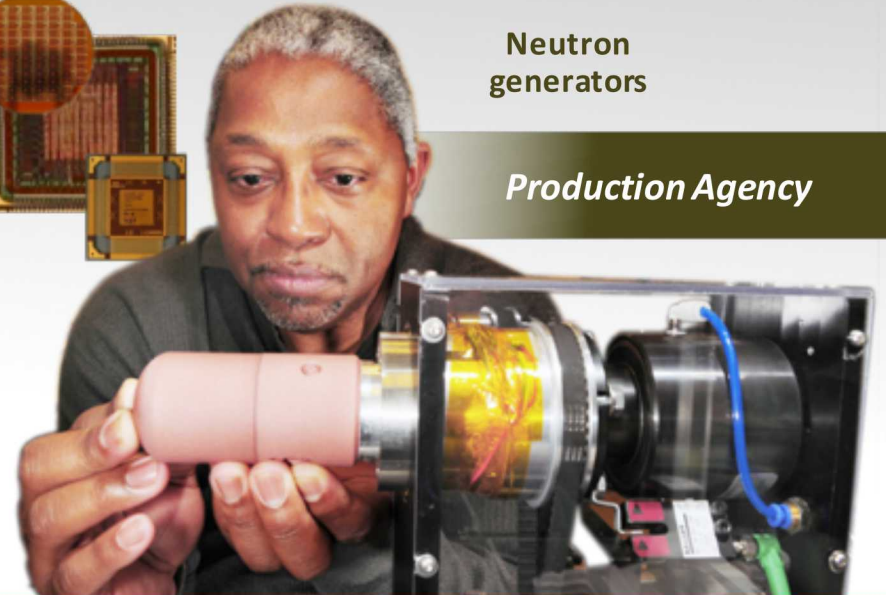
Annular core research reactor

MESA Microelectronics



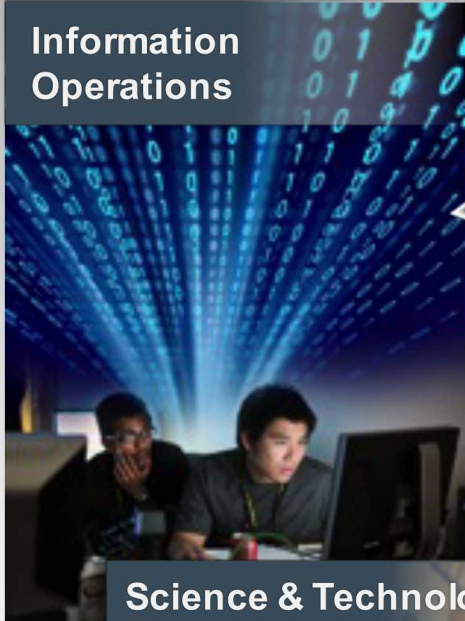
Neutron generators

Production Agency



National Security and Defense Nuclear Nonproliferation Programs

Information
Operations



Surveillance &
Reconnaissance



Remote Sensing
and Verification



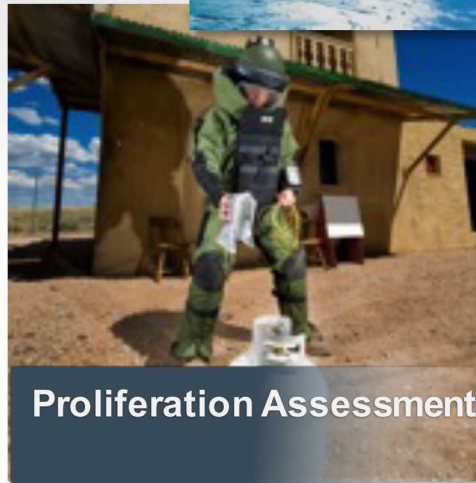
Space Mission



Science & Technology
Products



Proliferation Assessment



Integrated Military Systems



Energy

Energy Research

ARPAe, BES Chem Sciences, ASCR, CINT, Geo Bio Science, BES Material Science

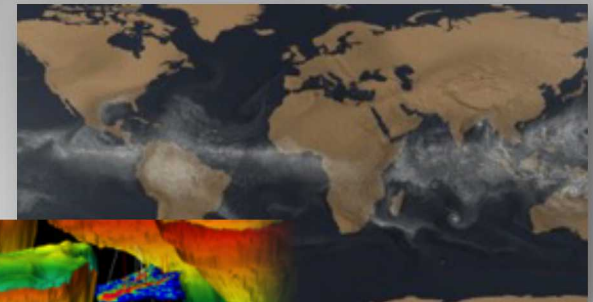
Climate & Environment

Measurement & Modeling, Carbon Management, Water & Environment, and Biofuels



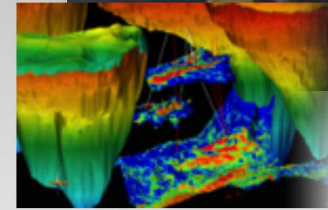
Nuclear Energy & Fuel Cycle

Commercial Nuclear Power & Fuel, Nuclear Energy Safety & Security, DOE Managed Nuclear Waste Disposal



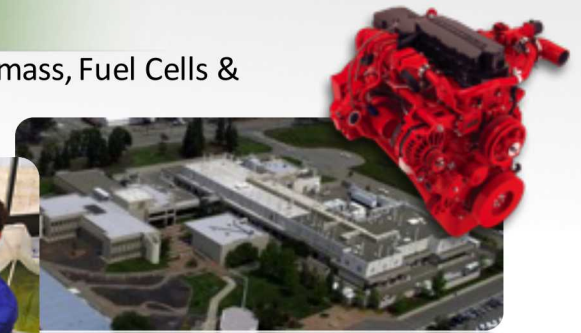
Renewable Systems & Energy Infrastructure

Renewable Energy, Energy Efficiency, Grid and Storage Systems



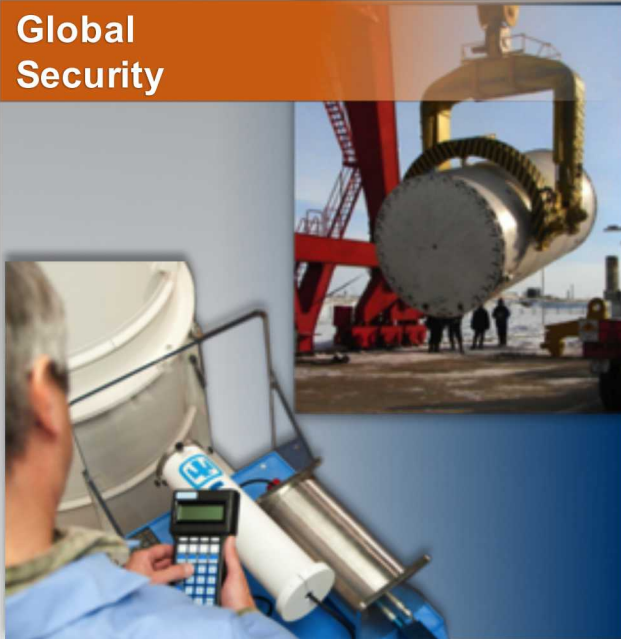
Transportation Energy & Systems

Vehicle Technologies, Biomass, Fuel Cells & Hydrogen Technology

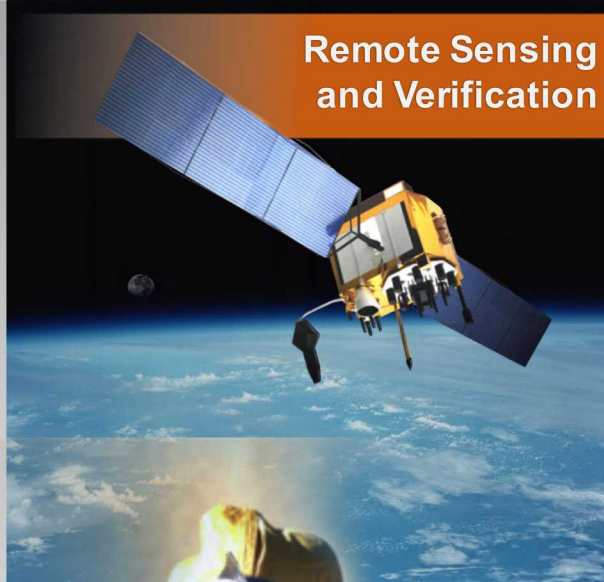


Global and Homeland Security

Global
Security



Remote Sensing
and Verification



Homeland
Security Programs



Cyber and
Infrastructure Security



WMD
Counterterrorism
and Response



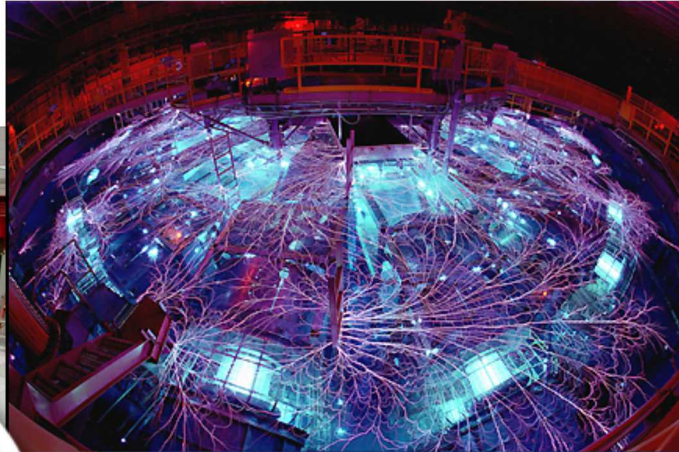
Homeland Defense
and Force Protection



Our Research Framework

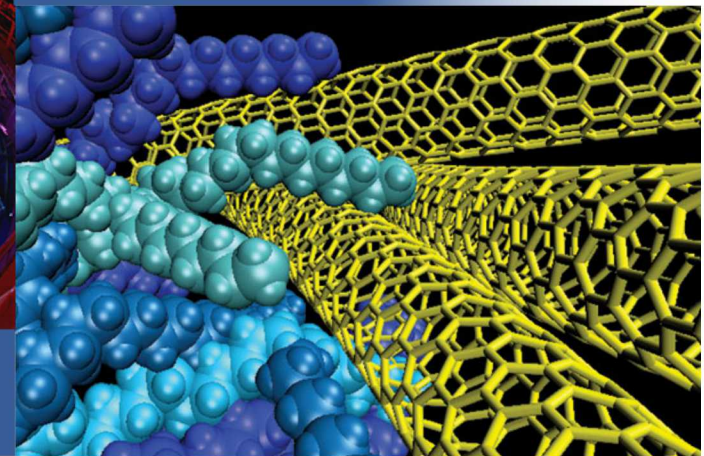
Strong research foundations play a differentiating role in our mission delivery

Computing & Information Sciences

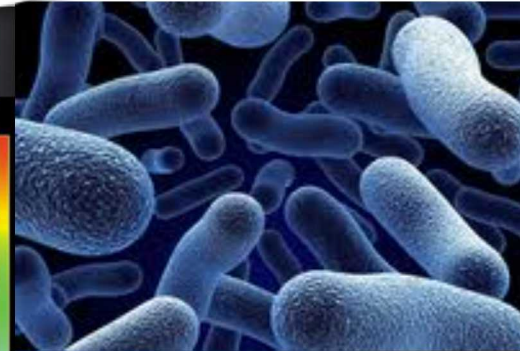
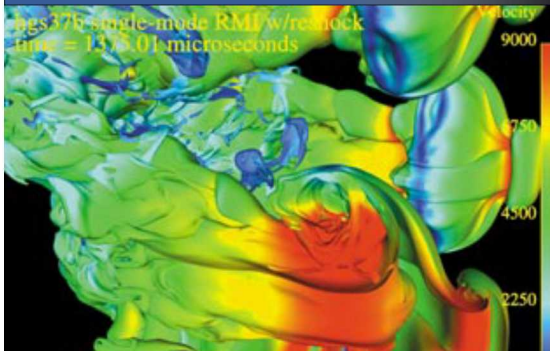


Radiation Effects & High Energy Density Science

Materials Sciences

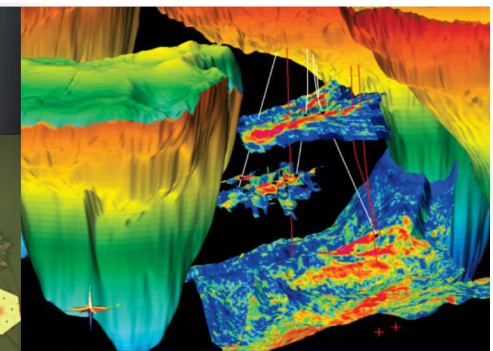


Engineering Sciences



Bioscience

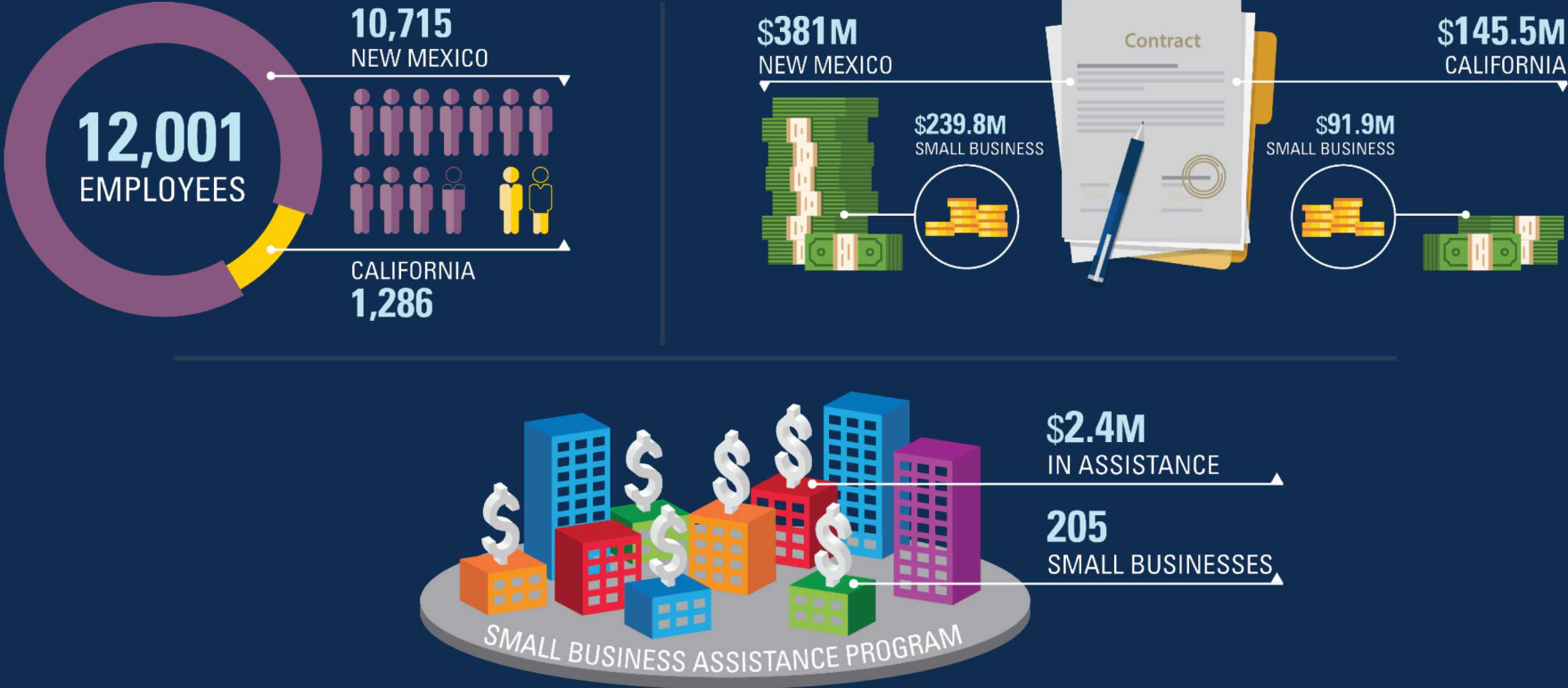
Nanodevices & Microsystems



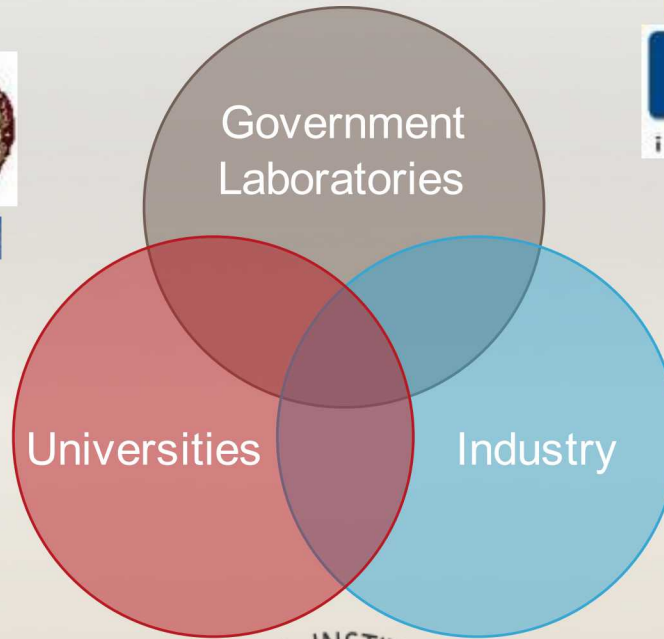
Geoscience

FY 2016: Impacting the local economy

Workforce: 12,001 employees (10,715 NM, 1,286 CA)



Partnerships and Collaboration Accelerate Innovation





Doing Business with Sandia



Sandia
National
Laboratories

*Exceptional
service
in the
national*



Partnerships Agreements Sandia National Laboratories

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under contract DE-AC04-94AL85000.

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Types of Agreements

- Other Federal Agency Agreements (OFAs)
- Cooperative Research and Development Agreements (CRADAs)
- Commercial Licenses
- Funds-in (Non Federal Entity)
- Designated Capability (DC)
- User Facility (UF)



Cooperative Research and Development Agreements (CRADAs)

- Governs collaborative R&D between SNL and industry
- Can be 100% funded by partner, must include “in-kind” contribution
- DOE approval required
- Each party can take title to its own CRADA generated IP
- Partner has option to license joint inventions



P&G/Sandia CRADAs

- Coating and Related Manufacturing Processes (multiparty consortium) 1996-2007
- Nanoparticle Flow Project (multiparty consortium) 2007-2011

Umbrella CRADA 1672

- Fluid-handling product modeling 2003
- Structural modeling (body, product, garment) 2003
- Material modeling 2003
- Micromechanical analysis of Foam Structures 2005
- Shaving cartridge models and design 2005
- Tensioned web slot coating models 2006
- Surface rheology modeling 2007
- Nanofiber production 2008
- Bottle-filling models 2009
- Porous flow in thin-sheets modeling 2010
- Battery performance modeling 2013
- Battery microstructure modeling 2013
- Thin-sheet performance models 2014-pre

Project Task Statement (Ver. 05-12-08)
PTS 1672.01.13 Version 10/20/11

Page 1

PROJECT TASK STATEMENT
No. 1672.01.13

BETWEEN
Sandia Corporation

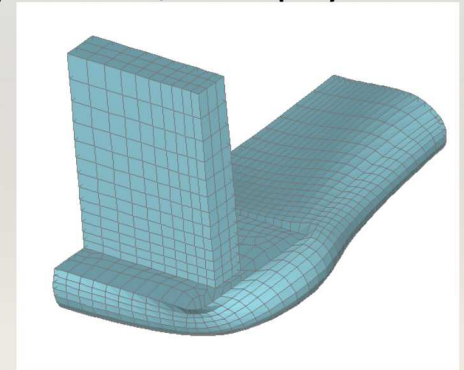
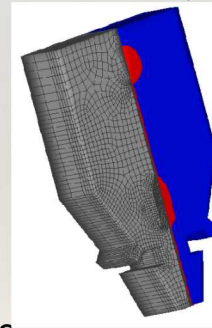
AND
Procter and Gamble Company
a corporation of the State of Ohio
having a principal office in Cincinnati, Ohio
(hereinafter "Participant")

October 20, 2011

Fluid-Structure Interaction of Deforming Porous Media

CRMPC-Coating and Related Manufacturing Processes Consortium

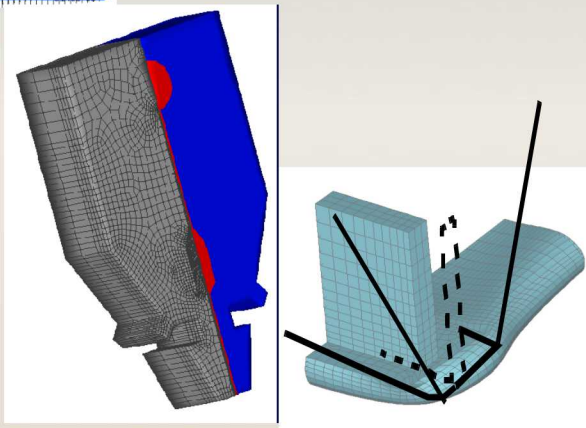
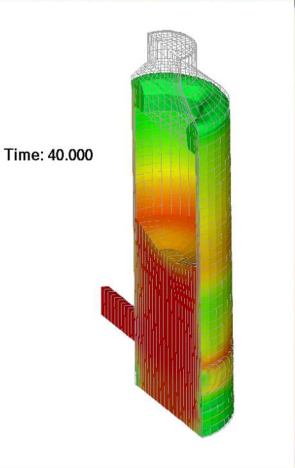
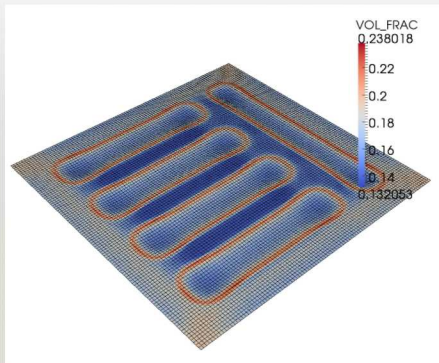
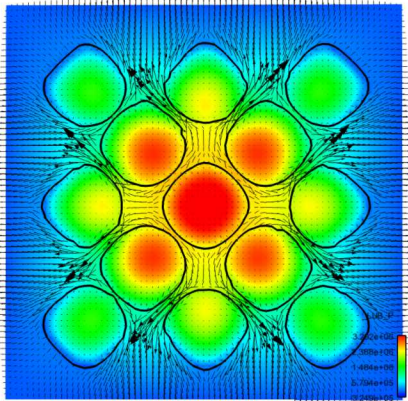
- CRMPC initiated in 1994-1996 timeframe. (3M, Xerox, P&G, Corning, Polaroid, Imation, Kodak, Avery Dennison). Industry estimated to be \$600 billion/year in value of coated products (1992). Well over \$2T/year in 2012.
- Started with seven companies, dues were \$75,000/year with matching dollars from Sandia.
- CRMPC contract funded research and development of Goma, an incompressible, multiphysics code in the following areas:
 - Research of free and boundaries algorithms
 - Wetting on Deformable Substrates
 - Algorithms for manufacturing window prediction
 - Extensive Porous Media Capability
 - Automated Geometry, 3D Meshing
 - Issue Tracking, QA Testing, Software Distribution, etc.
- Work on Goma development through the CRMPC occurred over a five year period.
- Upon completion of these core capabilities (2002) within Goma, subset of the CRMPC companies invested in a three year extension that shifted the focus to Eulerian Front Tracking Algorithms
- CRADA ended circa 2008 with new capability in level-set technology and porous absorbent media. --
- Follow-on CRADA established with 5 companies in the area of Nanoparticle composite manufacturing. The NPFC (NanoParticle Flow Consortium) still ongoing.





Goma 6.0

2014 R&D 100 Award Winner



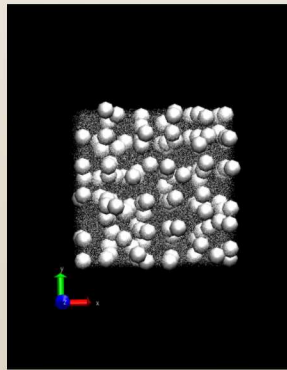
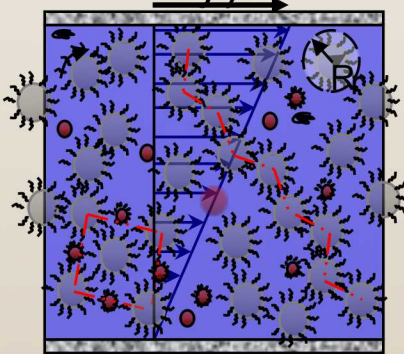
- Multiphysics *finite element* code, suitable for both *research* and *production*
- Fully-coupled *free* and moving *boundary* parameterization – ALE, Level Set, etc.
- Modular code; *easy to add equations* – currently has 170+ differential equations
- *Open source!* Available at <http://goma.github.io>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

Nanoparticle Flow Project

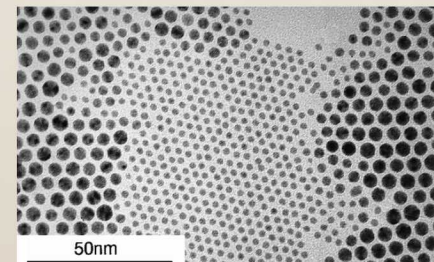
“nanoparticle” is colloidal in nature with characteristic size of 10 nm - 500 nm.

- Project Description - “CAE Tools For NanoManufacturing”
 - Disperse nanoparticles in films, fibers, monolithic bulk structures for material engineering
 - Fluidization in liquid followed by traditional processing techniques (coating, casting, spinning) allows control of nano-building blocks at the macroscale.
 - Modeling and simulation of flow of dense suspensions to build process understanding and control.
- Partners: 3M, Corning, Procter and Gamble, BASF, ICI (Materials Manufacturing Industry)
- Product: Production software framework for dispersion design (rheology, stability)



*Dispersion stability:
Melting of a bi-
disperse lattice of
nanoparticles*

E.G.: Coating into functional films



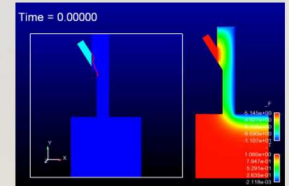
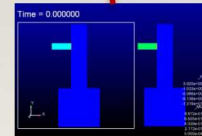
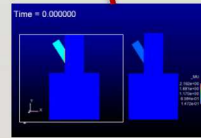
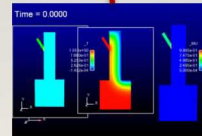
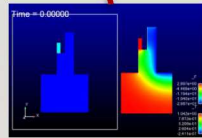
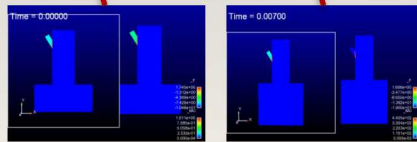
Factor Space Comparison

Non-isothermal

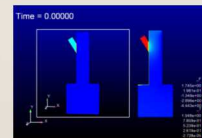
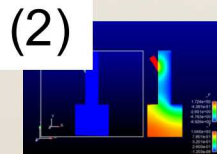
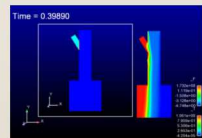
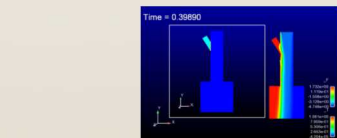
2D_Nufiber

WideAir | Standard | truparallel | thingap | shortlan | perpen | parallel | insetup | insetdown

case0 | case1

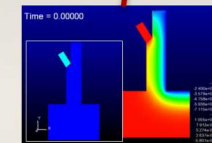


case0 | case1 | case2 | case3

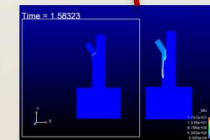


(2)

(2)



(1)

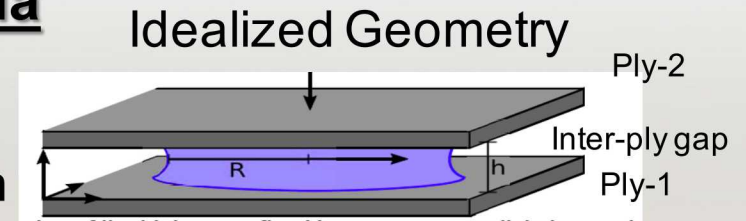


Takeaways: (1) “case-hardening” leads to Kelvin-Helmholtz like wave shape. Air grabs more liquid. (2) Thin warm layer on die (slightly less than base viscosity of isothermal case) very critical to behavior. *Die-Temperature Matters!* (3) More representative/certain temperature shifts should be measured.

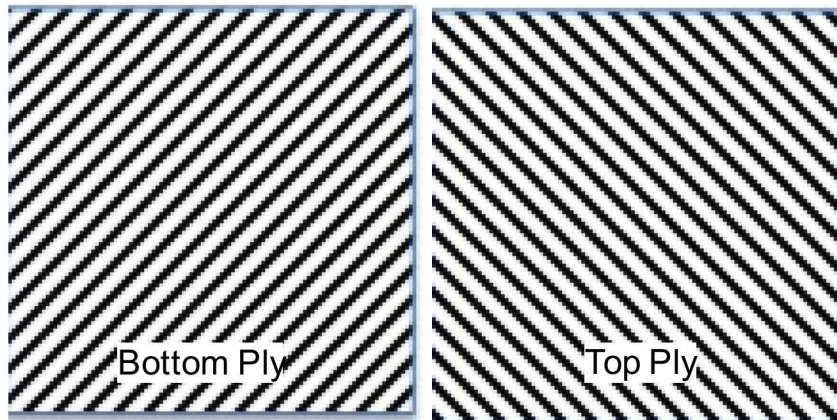
Paper Design Tool

Thin Multi-layer Free-Surface + Porous Media

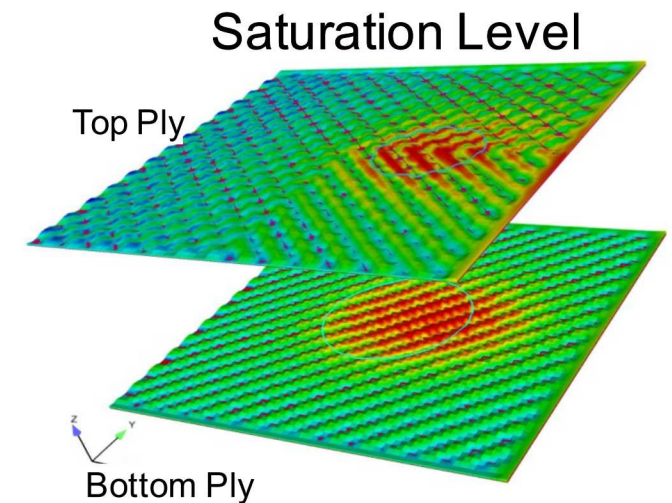
- New to the World Capability
- P&G / Sandia Proprietary Technology
- Enables High Aspect Ratio Parallel Simulation
- Direct Pattern to Mesh



Pattern to Simulation Automation



Pixel
 →
 To
 Mesh



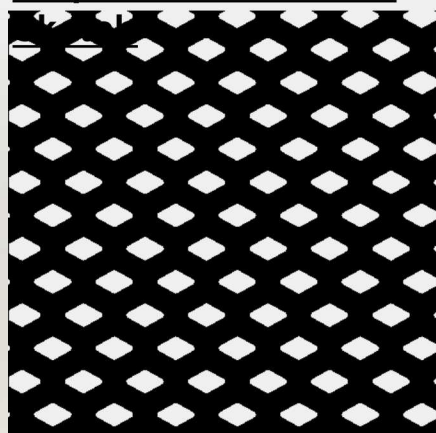
Inter-ply Free Surface Not Shown



**Jpeg, gif files

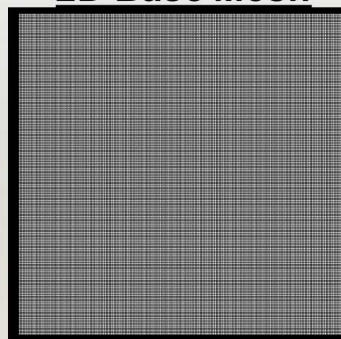
Paper Design Tool / Single Ply

Step # 1: Create a 2D

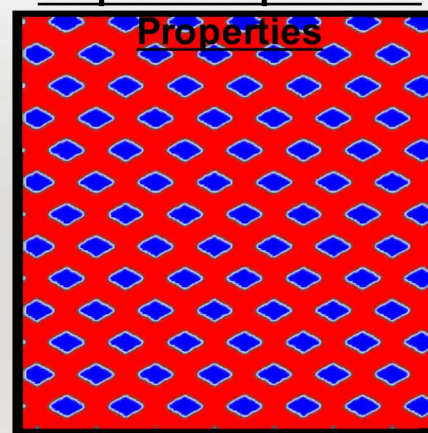


Rule: Pillows → Black

2D Base Mesh



Step # 2: Map Porous

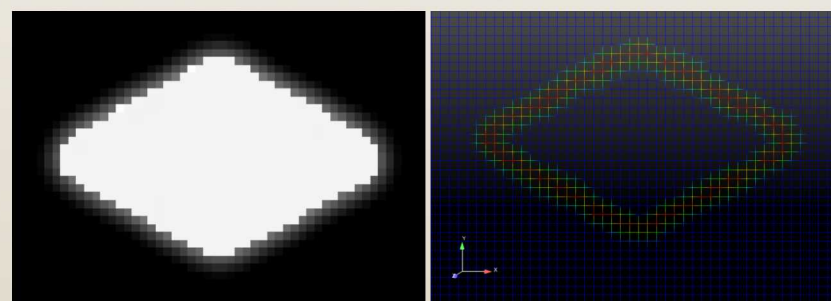


Properties

Porosity
Permeability
Rel Permeability
Thickness
Pc-S Curve Coeff
+
Cellulose Capacity

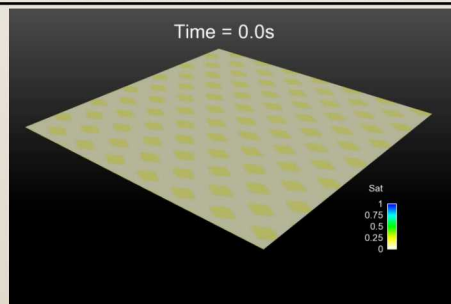
Image To Mesh

Step # 3: Volume & Drag Correction Step



**** Require 3D Volume or Surface Area ****

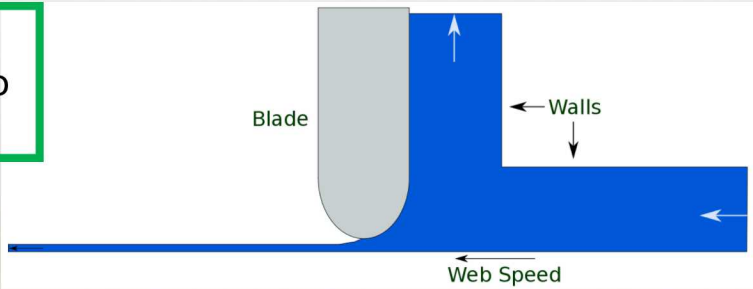
Step # 4: Simulation + Post-Processing



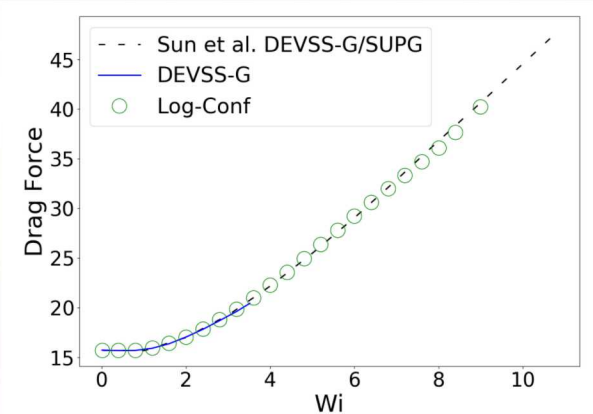
**** Mass Uptake & Wicking Distance ****

Viscoelastic Modeling of Blade Coating for Gillette

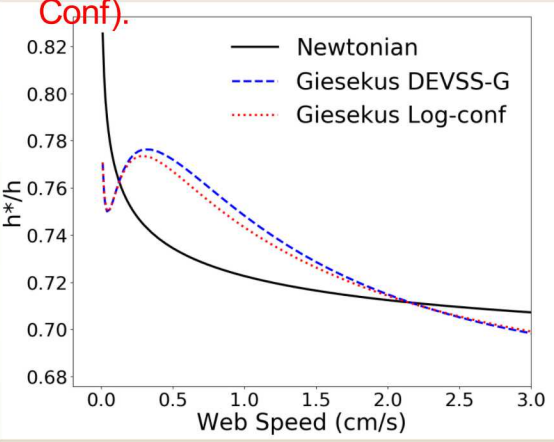
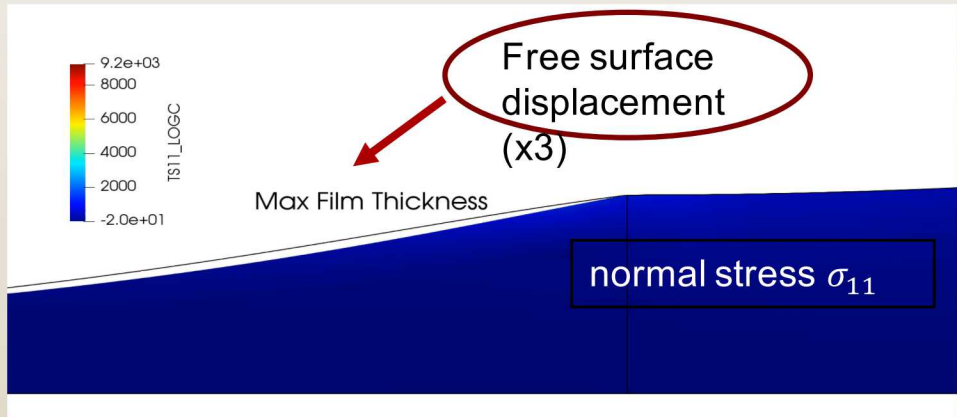
GOMA 6.0 with log-conformation formulation to improve performance



- For Newtonian fluids, the film thins as the web speed increases.
- Viscoelastic film **thickness** is **non-monotonic**, thickens and then thins

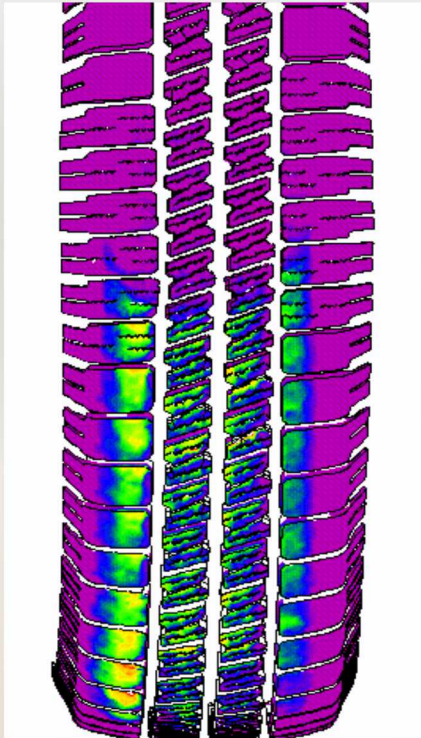


Log-conformation tensor increases maximum Wi obtained in flow over a cylinder. **3.5 (DEVSS-G), 9.0 (Log-Conf).**

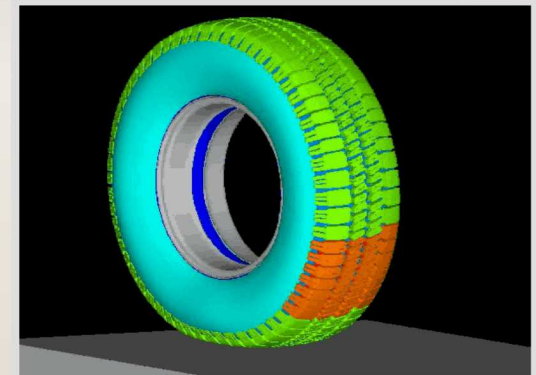
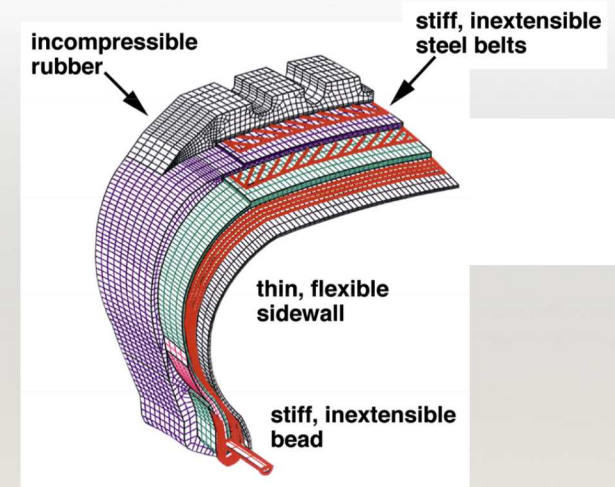


Martin et al, Viscoelastic Blade Coating, submitted C&F, 2018

Goodyear/Sandia Interaction

GOODYEAR

- Increase Model Complexity by Several Orders of Magnitude
- Decrease Computational Run Times by 2 Orders of Magnitude (day)
- Automatic Coupling between Solid Geometry, Meshing, Mechanics Codes, and Visualization of Results
- Reduce Prototype Tire Builds from 3 – 4 to 1
- **Reduced yearly R&D Costs by \$100M!**
- **M&S investment led to best sales quarter in 7 years and 3rd best in company history**



The Goodyear/Sandia interaction is mutually beneficial. Goodyear gets “rocket science” applied to tires. Sandia gets real-world development and testing of simulation technology.

M | S | R | F

Advanced Materials Laboratory

Department 1815 Overview and Outlook

P. Randall Schunk, Manager

8 November 2016



*Exceptional
service
in the
national
interest*



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AML Mission, Focus, and Vision

- The Advanced Materials Laboratory (AML) provides unique materials discovery solutions coupled with materials demonstration/deployment.
- AML's materials focus centers around synthetic chemistry routes with novel precursors and catalysts to explore new materials with solvo-thermal, solution-precipitation, and sol-gel routes.
- AML's rapidly advancing materials processing capability enables materials delivery ready for functional prototyping
Integrated materials synthesis and materials processing breadth unique to the complex



Advanced Materials Laboratory

Advanced Materials Laboratory (AML) – a Sandia-leased facility on the campus of the University of New Mexico

Original Vision: Foster substantive collaborative/partnering relationships in material science with UNM

Strategic Advantages:

- Access to students
- Greater opportunity for collaborations with UNM faculty
- Access to campus resources – equipment, library, computer resources
- Funding sources not readily available to Sandia (NSF)
- Technology transfer
- Joint purchase/maintenance of novel instrumentation



The Advanced Materials Laboratory, a part of Sandia National Labs since August, 1992
29,295 sq ft. (~14,000 sq ft lab space)

Developing materials science and engineering technology in the National Interest

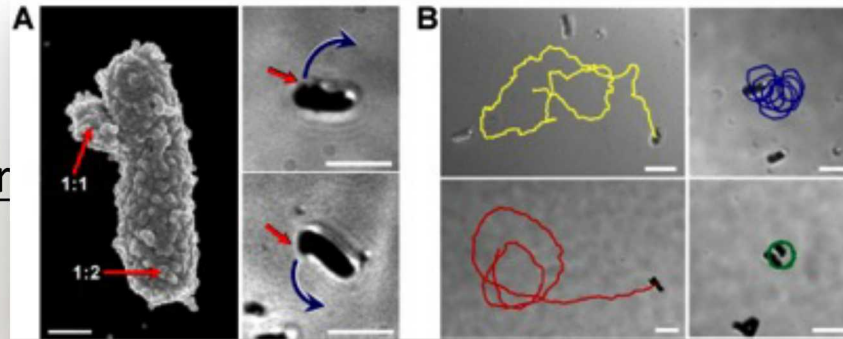
The AML has a wide range of capabilities important to Sandia's missions

Synthetic Chemistry

- Novel inorganic precursor
- Catalysts
- Sol-gel
- Solvothermal
- Solution precipitation

Ceramic/glass processing

- science of sintering
- composite materials
- unique fabrication
- novel characterization



Nano-scale materials

- Nanoparticle synthesis (0D,1D,2D)
- Surface functionalization
- characterization

Bio-, Nano-materials capability

- BSL-2 Laboratory
- Surface functionalization

Characterization

- Diffractometry: SAXS, XRD, XPS
- Thermal (TGA, DSC)
- Spectroscopy (mass, FTIR, ICP)
- Multispectral ellipsometer

Materials processing

- Self- and directed-assembly
- Films (dip, spin coat, gravure)
- Fibers (electrospinning)
- Bulk materials (sintering)
- Multiphoton lithography
- Direct/aerosol write, inkjet
- R2R printing (gravure, flexo)



AML and its diverse residents

- Advanced Materials Laboratory Department (13 staff, 4 techs, 8 postdocs, 13 intern students)
- Other Sandia residents (1816 Electronic, optical and nanomaterials 2; 1832 Coatings and AM – 3)
- UNM collaborators – ~30 year around
- Other university working visitors, PO contractors ~5
- Student programs (STAR, STEP, REU, RET, MAC, APS) - 6
- Other temporary workers from at least 5 other Sandia organizations: 1100, 1700, 1500, 6000, 8600

80 (approx 25 full time) year around workers, over 100 in summer



Bernadette Hernandez-Sanchez



Tim Boyle



Madison Casillas





From nano-materials to components at the AML

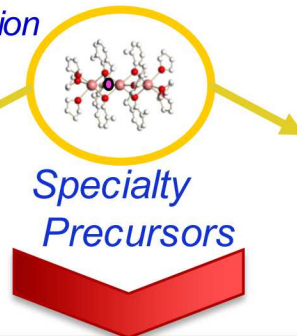
Solution Precipitation



Solvothermal



Specialty Precursors



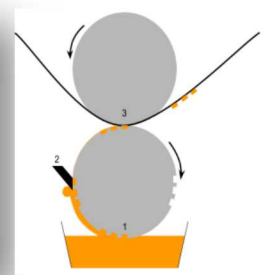
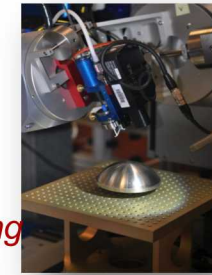
Colloidal Chemistry

Specialty Inks



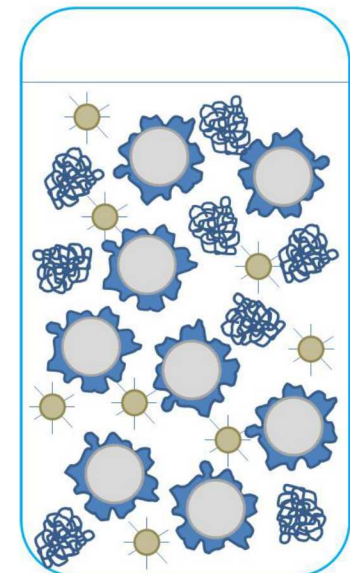
Process Engineering

Direct Write Printed Parts

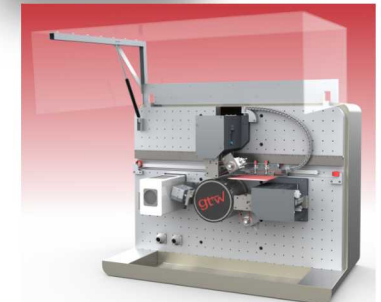


Ink Characterization

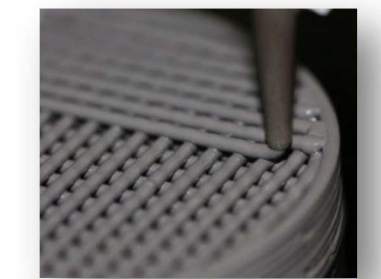
Specialized Nanomaterials



Ink Rheology Tailoring



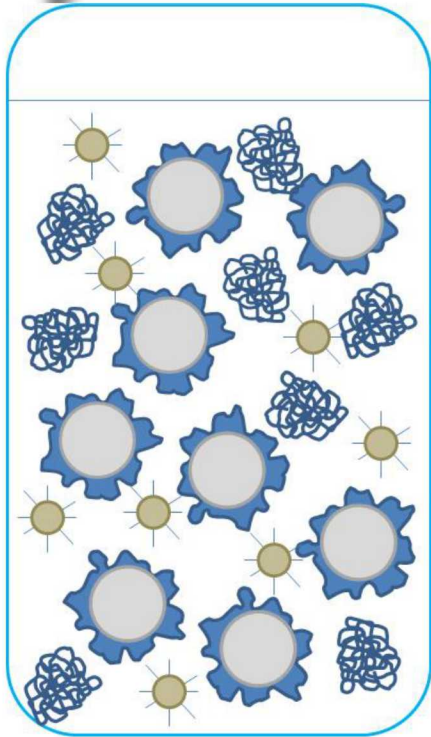
Micro-gravure printing



Aerosol, Inkjet, extrusion

From specialized, tailored nano-materials to process-able inks requires chemical synthesis, colloidal chemistry, rheology/characterization, process engineering

Development of Ink Compositions for Printing



Ink Systems are formed from multiple components:

- Solvents (s), wetting agents, soluble polymers or micelles, & nanoparticle(s)
- Control over viscosity, surface tension, drying rate, and wetting are required.

$$Ca = \mu V / \sigma$$

$$We = \rho V^2 d / \sigma$$

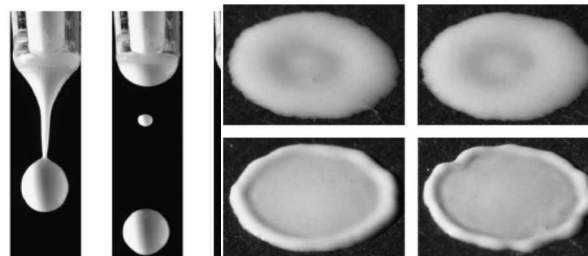
B. Effective dispersion is critical for printing using DOD or gravure/flexo printers.

- Solids loading increased by proper dispersant choice, up to ~15-20%
- Surface tensions are low : between 15 – 40 mN/m
- Viscosity vary from 1-10 mPas.
- Surfactant concentrations tailored to surface area

$$\mu_{rel} = \mu_{\text{solvent}} / \mu_{\text{ink}} = (1 - \phi / \phi_m)^{-n}$$

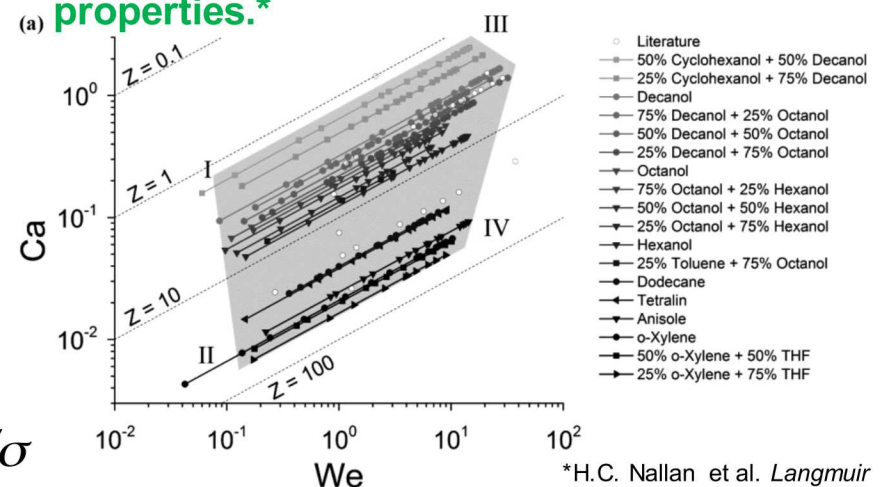
C. Adjust wetting and drying agents to minimize satellite drops and surface wetting concerns.

Dependent on surface interactions with substrate, and drying rate.



R. Guo et al. *JECerS* **23** (2003) 115-122.
 X. Zhao, et al. *Ceram.Intl.* **29** (2003) 887-892.
 N. Ramakrishnan, et al. *J. Mat. Proc. Tech.* **169** (2005) 372-381.
 P.S.R. Krishna Prasad et al. *J. Mat. Proc. Tech.* **176** (2006) 222-229.

A. Develop solvent compositions within the printing window of fluid properties.*



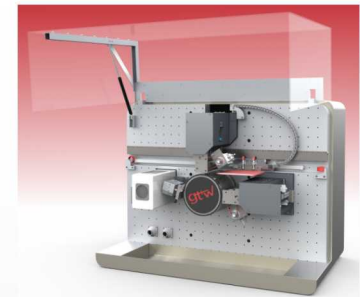
All experimental capabilities and SMEs exist at the AML!

Ink-based, Polymer Based Additive Manufacturing, and Precision coating and Printing Laboratories at the AML

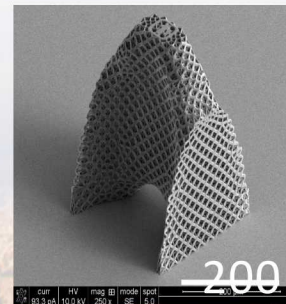
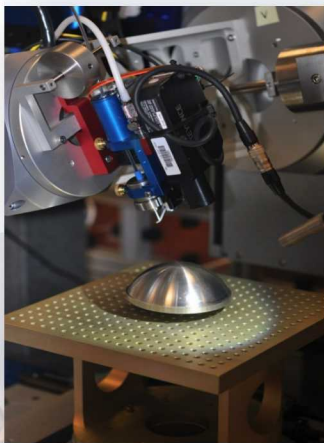
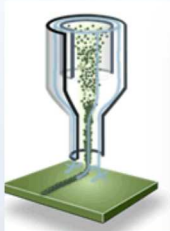
- FY16 ~\$900k investment to equip a new Precision Digital Printing & Coating AM lab at the Adv. Materials Lab (AML)
 - Feature length scales from ~ 100 nanometers to macro-scale
 - Deposit wide variety of nanoinks and solid-state materials for precision applications and with scalable throughput
 - Film thicknesses to <1 micron, and throughputs of 100 cm²/s
- Applications -- thin-film transistors, fuel-cell membranes, photonic devices, gas sensors, printed electronics, power sources, and more
- Potential customers across all Sandia missions and industry
- **Materials->Part demonstration of low-cost, printed devices**



Precision N-Tact slot-die coating tool

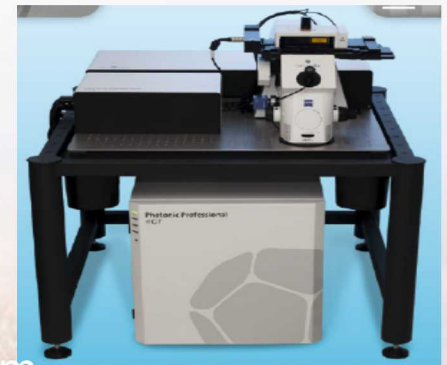


SuperProofer multilayer printing tool



200 μm

Microscale lattice structure designed w PLATO & printed w new 3D photolithography at AML



NanoScribe™ Maskless 3D Lithography Tool

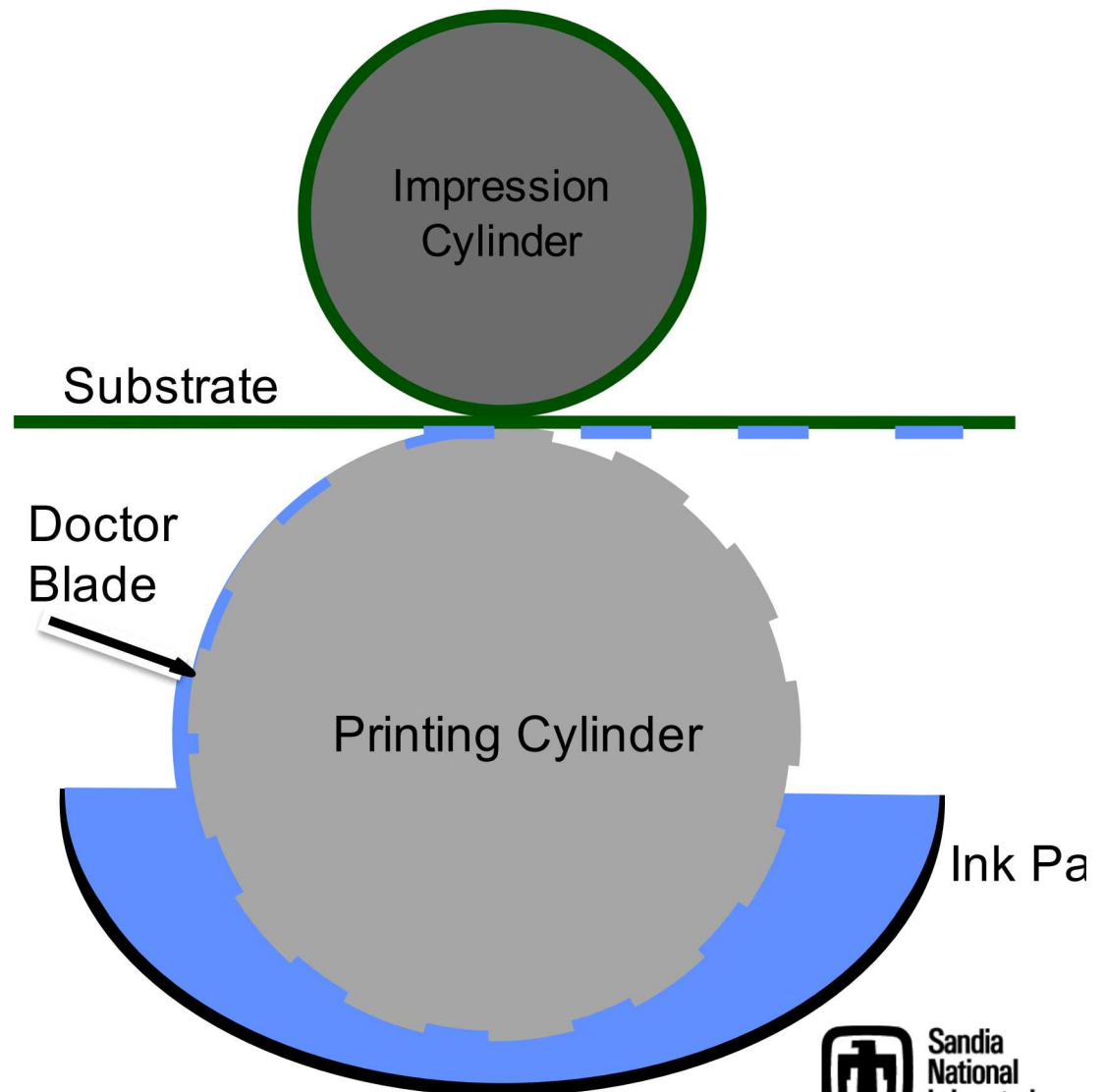
Schunk Research Group Competencies and Strengths

- 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 (wet etching, printing thin-film coating, casting, welding/soldering/brazing, ...)



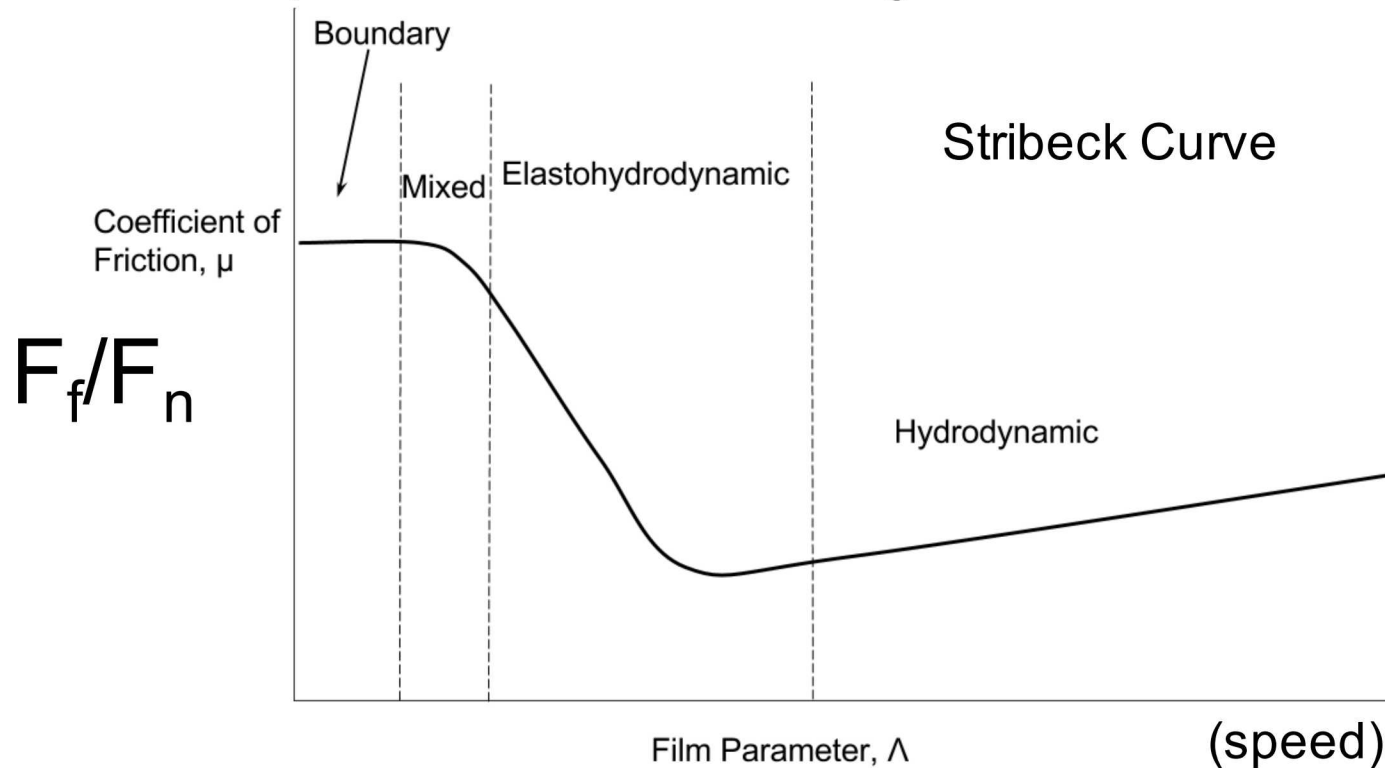
Gravure Printing Process

- Gravure printing is a high throughput (10-15 m/s), high-fidelity (10-15 μm) printing technique
- Involves three steps:
 1. Filling – Fill template with ink
 2. Doctoring – Remove excess ink
 3. Transfer – Transfer ink to substrate
- *Micro*-gravure has pushed this process to sub-5 micron features (Grau et al. 2016)
- Many challenges of *micro*-gravure, e.g., design of printing cylinder, effects of nanoinks
- One challenge is that doctoring presents a fundamental limit for feature resolution



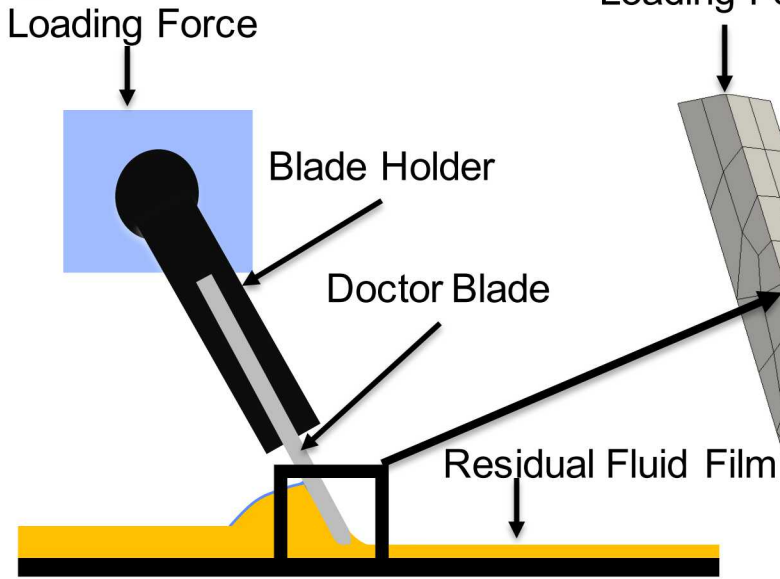
Regimes of Lubrication

- As gap is decreased, elastohydrodynamic lubrication occurs
- Standard problem in tribology, the study of friction and wear
- Typically, Hertzian contact mechanics are considered coupled to the Reynolds equation
- As the gap is further decreased, boundary lubrication occurs, which is problematic for doctoring

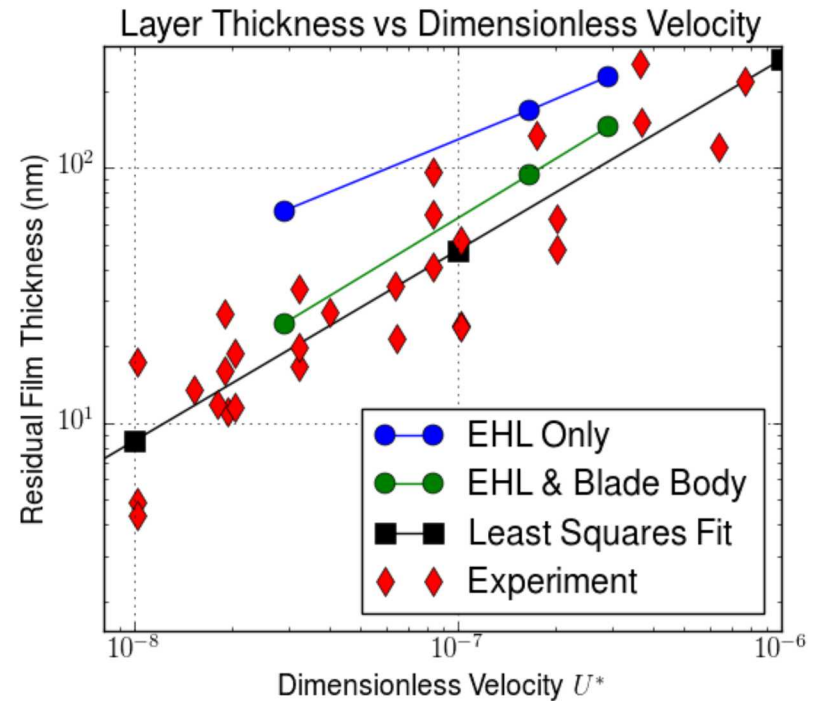
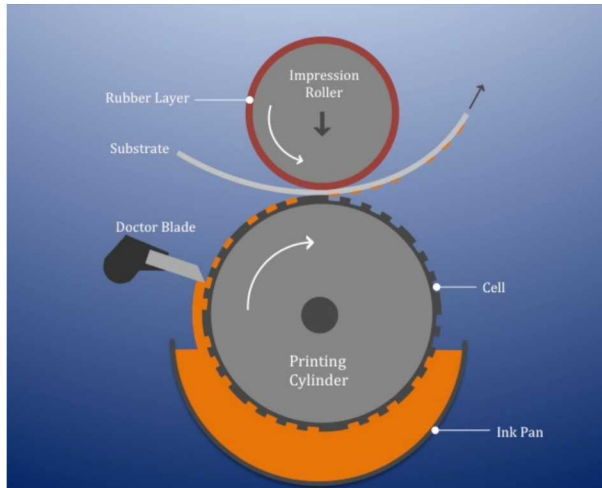
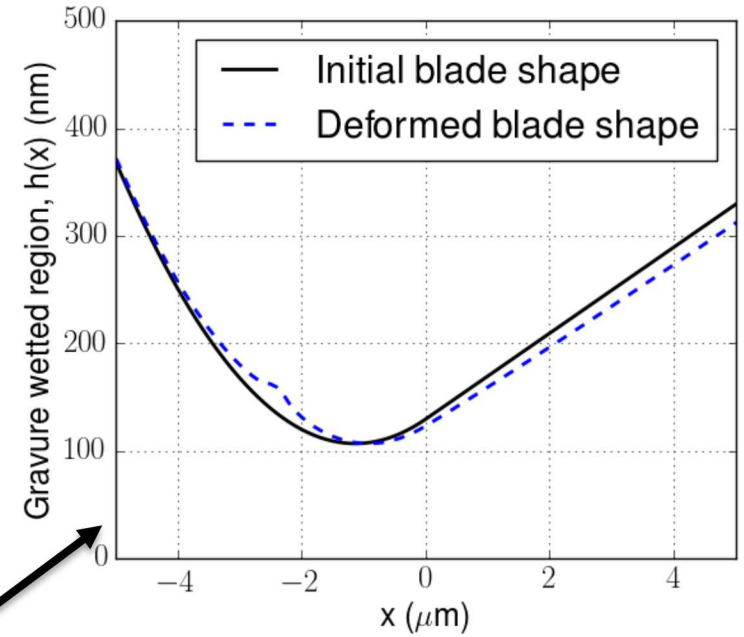
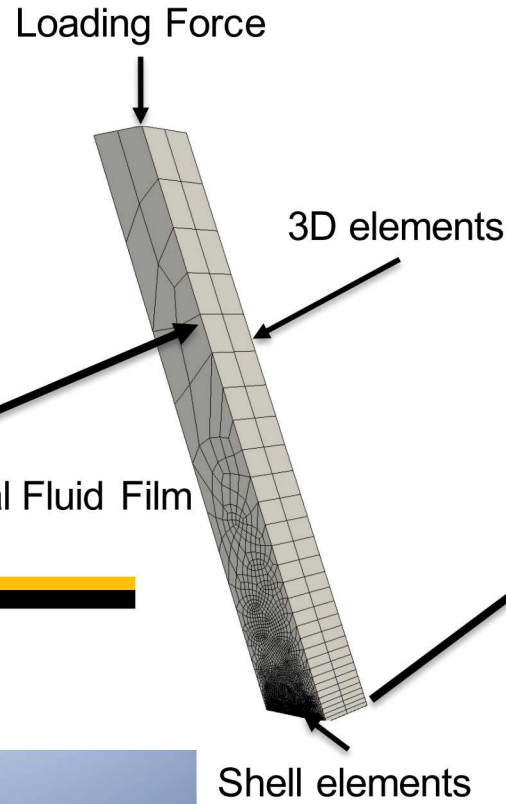


Doctoring in gravure printing

Doctoring process



Doctoring Model





BACKUPS

SLOT-COATING SIMULATOR

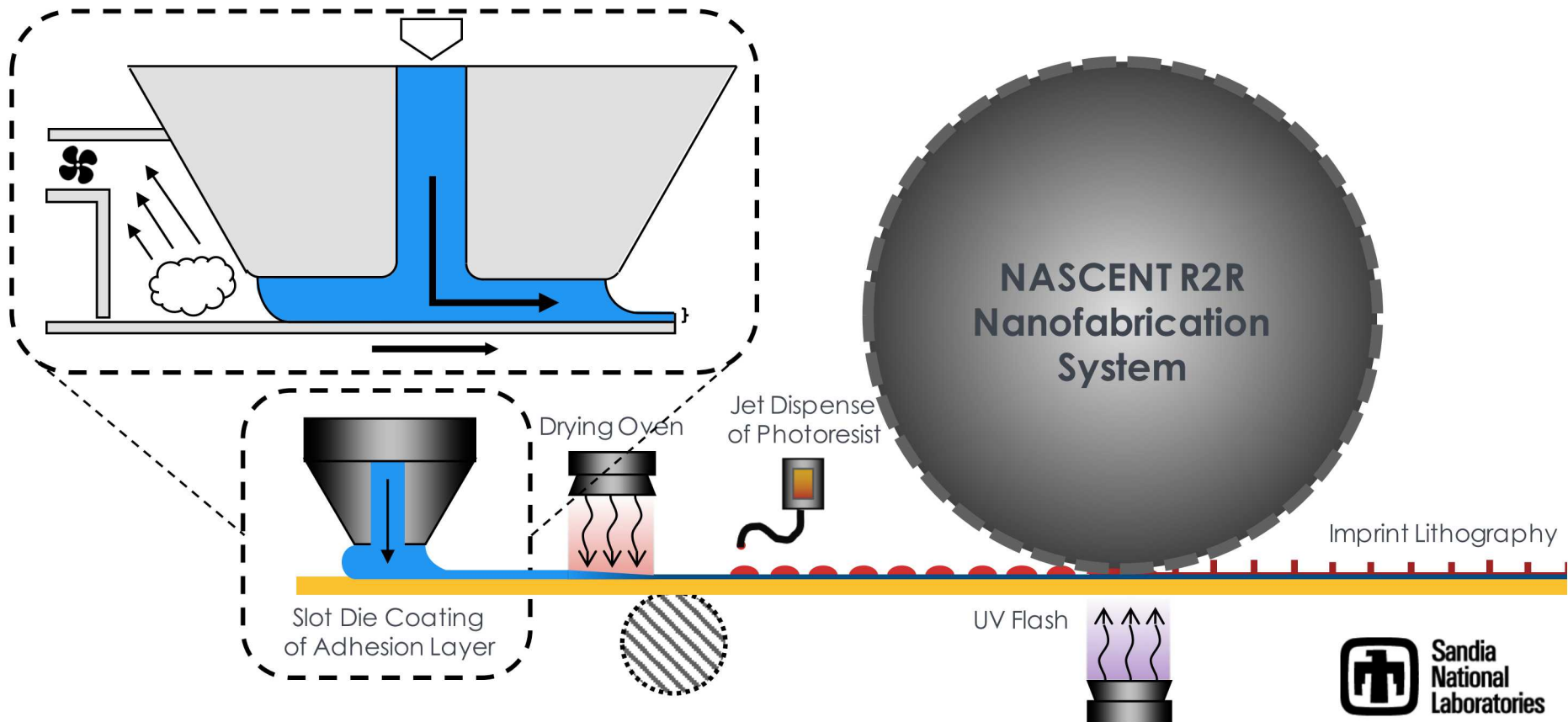
Robert Malakhov, Kris Tjiptowidjojo, Randall Schunk [UNM] (P-2E.1-K)

Goals

- Slot Die Simulator
 - Scale-up: Ultrathin coatings ($1 < \mu\text{m}$)
 - Small-lot: Continuous coatings
 - Prepare surfaces for nano-imprint lithography with films of desired thickness and uniformity

Research Methods

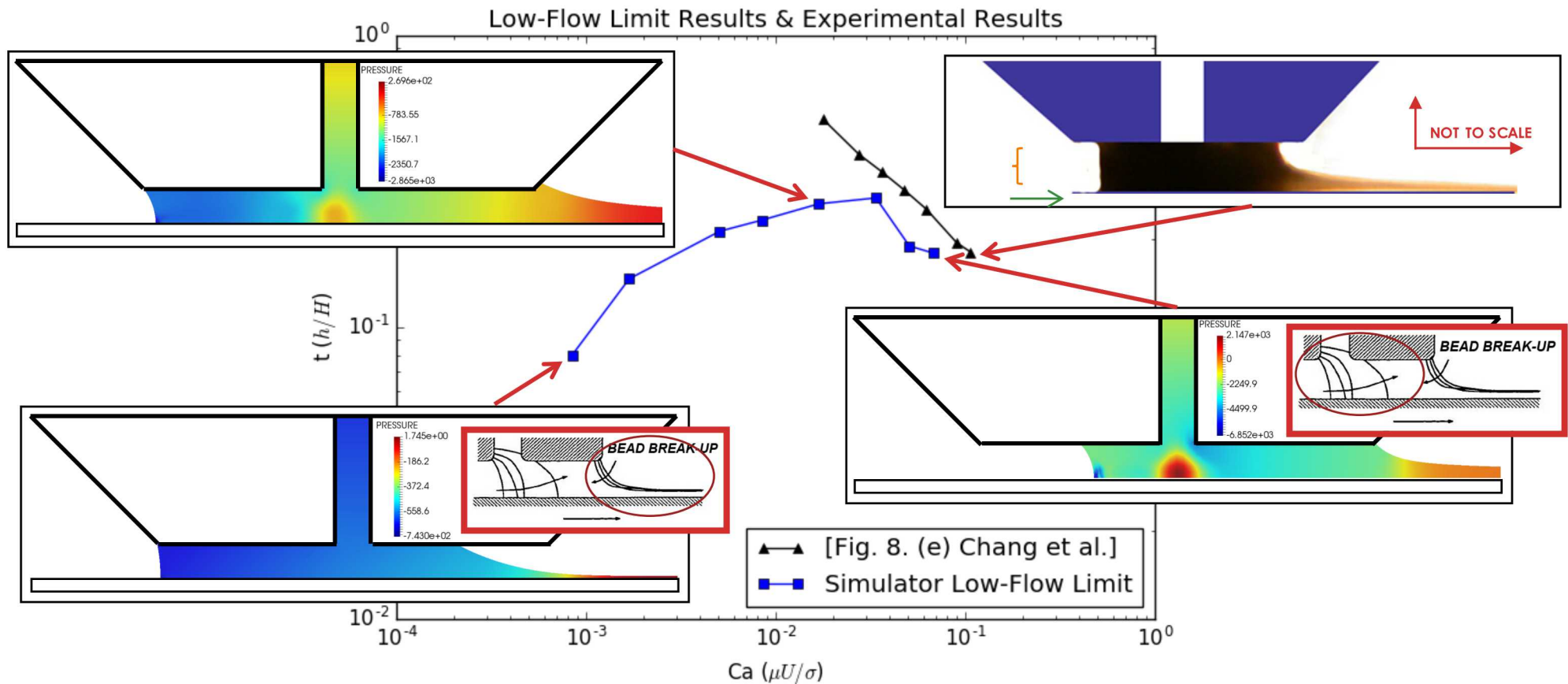
- Navier-Stokes w/BC's model
 - Solved via FEM
Goma 6.0
- Experimental Validation



PROGRESS REPORT

Low-Flow limit comparison to experimental results

- Computational results reproduce experimental film thicknesses, meniscus topologies, and failure modes



Low-Flow limit three region coexistence analysis

- Region 1 and 3 identified but region 2 not clear



Sandia and Industrial Partnership for CAE tool development to assist ink design: The NanoParticle Flow Consortium (NPFC)

Comp. Part. Mech. (2014) 1:321–356
DOI 10.1007/s40571-014-0007-6

Particle dynamics modeling methods for colloid suspensions

Dan S. Bolintineanu · Gary S. Grest ·
Jeremy B. Lechman · Flint Pierce ·
Steven J. Plimpton · P. Randall Schunk

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	Explicit Solvents		Implicit Solvents
	DPD	MPCD	SD-based (FLD, BD)
PREDICTIVE ABILITIES FOR SIMPLE SUSPENSIONS OF SPHERICAL PARTICLES			
Diffusion and viscosity	Well-established, but minor challenges remain in accuracy/boundary conditions; large polydispersity ratios can be computationally challenging		Well-established, but large polydispersity ratios still problematic
Microstructure prediction	Finite size of DPD particles problematic at high volume fractions/close particle contact.	Depletion effects introduce artificial inter-particle interactions.	Excellent agreement with experimental data for simple systems.
Direct mapping to physical properties	Often difficult, not all properties can be achieved simultaneously. Inherently problematic due to low Schmidt numbers and high fluid compressibility.		Simple solvent properties (e.g. viscosity, temperature) are directly input.
ADVANCED CAPABILITIES			
Non-spherical particles	DPD-colloid coupling relies on centrosymmetric potential; problematic for general case	Minor challenges exist with regard to boundary conditions/accuracy	Some simple shapes tractable. Near-field only applicable to spheres, spheroids, or particles composed of spheres; crude approximations possible for far-field.
Non-Newtonian solvent rheology	Modified algorithms can achieve certain solvent rheological properties; mapping to exact given rheology difficult		No attempts reported; requires significant development, e.g. coupling to mesh-based continuum solvers (FEM/FDM)
Complex flow geometries	Minor challenges with regard to boundary conditions/collision detection.		Boundary condition development required for confined and flow through systems. Not suitable for arbitrary geometries.
Solvent removal (drying) and/or curing	Solvent can be readily removed to simulate drying. Capillary forces must be added. Viscosity cannot easily be adjusted during simulation.		Only simple slow drying models possible (e.g. moving wall). Capillary forces must be added. Solvent curing can be simulated by changing viscosity.

Speed dependence in hopper coating – Weak speed dependence

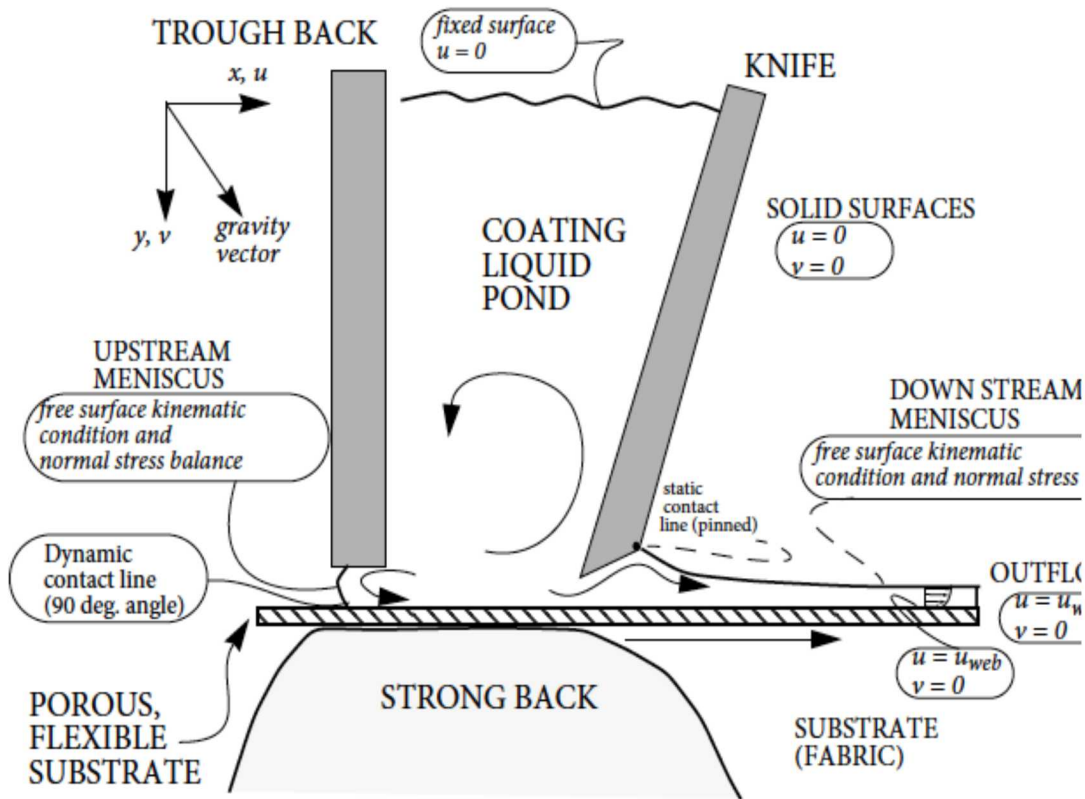


Figure 1 Generic coating head configuration.

Film Thickness vs. Web speed

Visc = 0.3 Pa-s; V-Trough

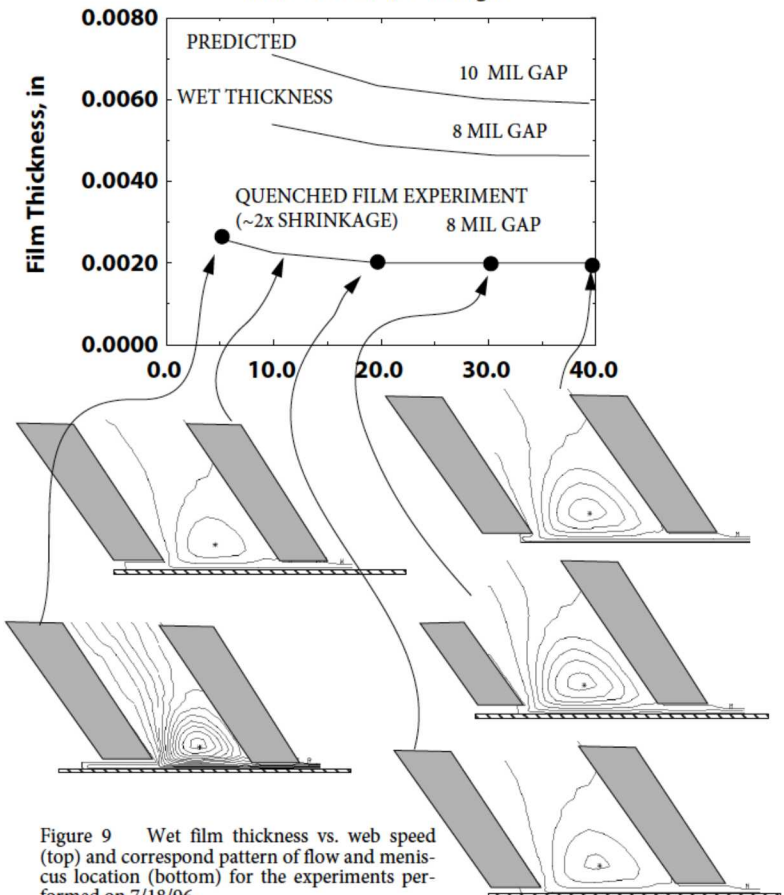
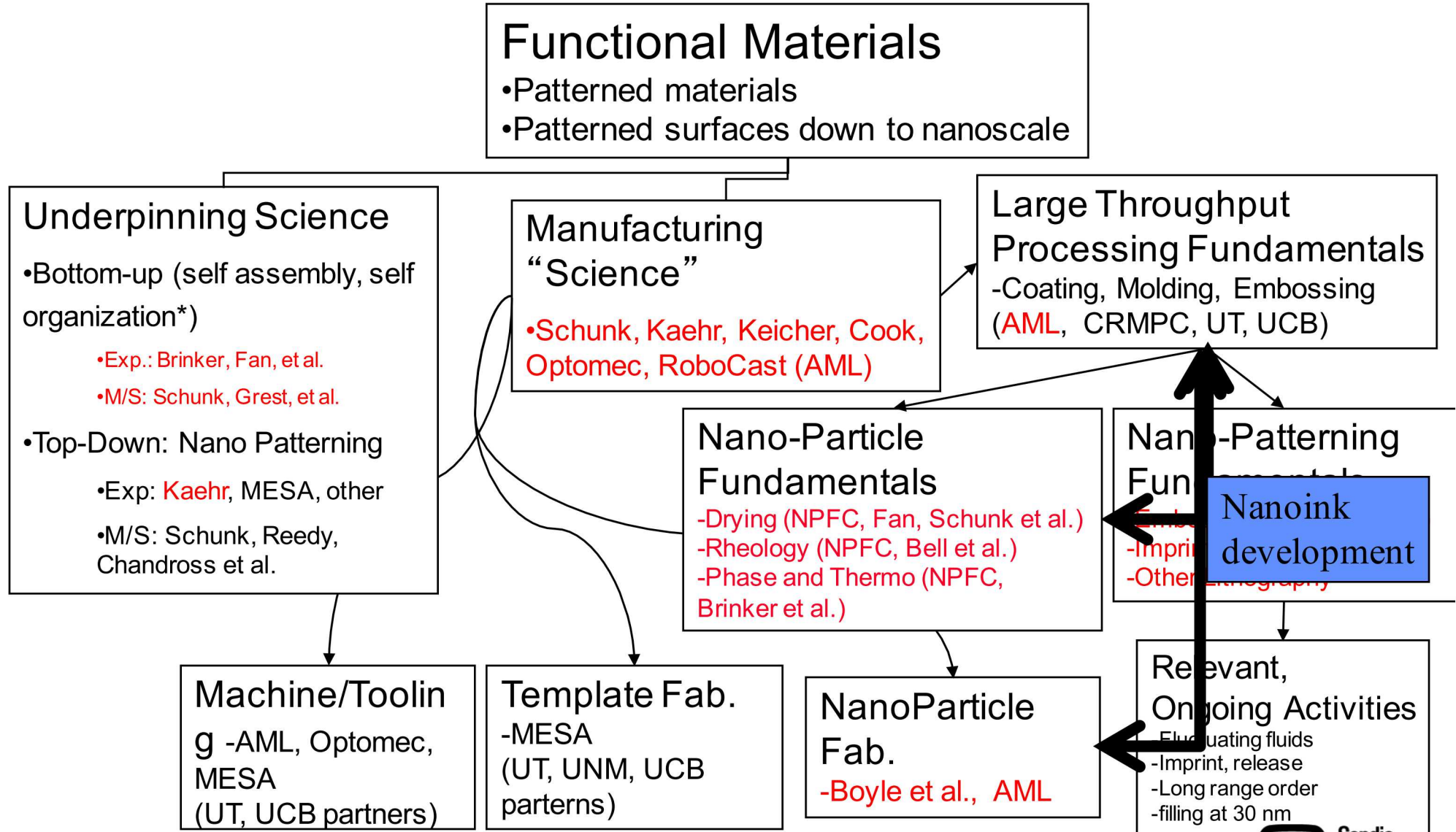


Figure 9 Wet film thickness vs. web speed (top) and correspond pattern of flow and meniscus location (bottom) for the experiments performed on 7/18/96.



Meeting these challenges at Sandia's Advanced Materials Laboratory



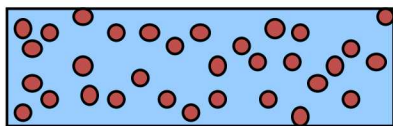
*Made practical by Pre-Processing to Concentrated form, before thermo takes over

Effective dispersion is critical for printing using DOD printers

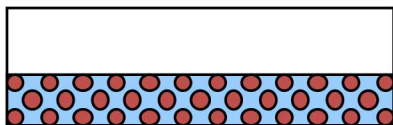
Dispersed

Discrete Particle Behavior

- Long range repulsion or screened van der Waals.
- At high ϕ , exhibit yield stress and higher viscosity



Disordered



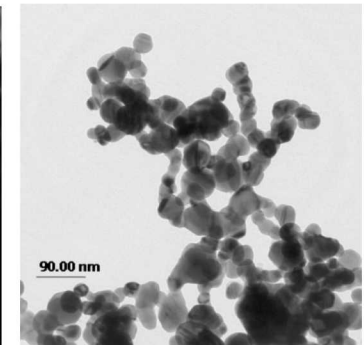
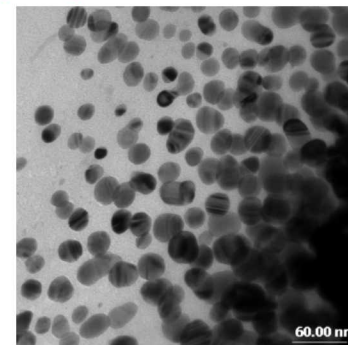
Ordered



Uniform, well packed particles

Particle dispersion affects ink stability and lifetime, packing density of the printed line, & consolidated properties.

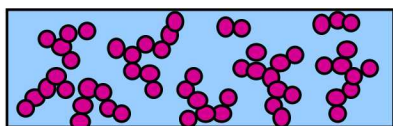
Dispersed vs. agglomerated silver nanoparticles illustrate the ability of the materials to pack due to capillary forces during drying.



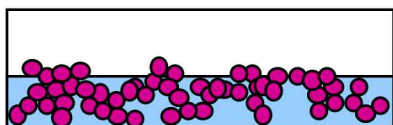
Flocculated

Elastic Network

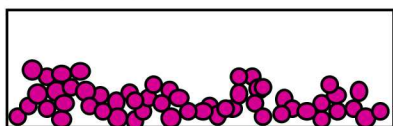
- Little or no repulsive barrier or attractive forces.
- Shear thinning, difficult to achieve high solids loading.



Fractal floc formation



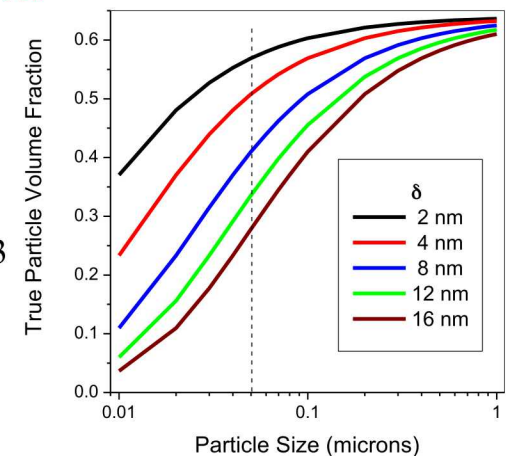
Percolating network at 16 Vol%



Porous, poorly packed particles

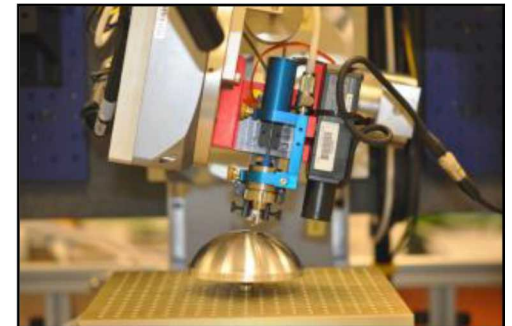
Inkjet compositions must be low viscosity at solid loadings of 10-20 %.

$$\phi_{eff} = \phi \left(1 + \frac{\delta}{R} \right)^3$$



Current list of equipment

- N-Tact precision slot die coater (1-10 micron patch coatings over wide range of viscosity)
- RG gravure printer – 20 micron feature size
- GtK Superproofer gravure/flexographic printer with 5 micron resolution and 10 micron overlay
- Direct write machines
- Ink characterization: Rheometers, goniometers, DWS, zetasizers, etc.
- Film characterization: multispectral ellipsometer, SAW,
- Two-photon Lithography tool (100 nm)
- NanoScribe Multiphoton lithography tool
- Solidification tools: drying, UV curing, etc.





Commercial Licenses

- Grants rights for SNL-developed IP for commercialization and/or private use
- “Up-front” fees, annual minimums, & running royalties are negotiable
- Field of use and commercialization requirements also negotiable

Funds-in (NFE)

- Provides access to SNL's unique facilities and personnel
- R&D and unique technical services are sponsored
- Not collaborative
- 100% sponsor funded
- DOE approval required
- Partner IP rights are dependent upon circumstances

Designated Capability (DC)

- SNL creates a DC, DOE “pre-approves” for generic umbrella SOW
- Agreements written within SOW
- Can be with many different sponsors
- Sponsor provides 100% funding



User Facility Agreement

- Allows sponsors to use Sandia's unique facilities for research, testing, and developing prototypes
- 100% sponsor funded
- Sponsor employees at SNL facilities
- Not intended for use when IP would be generated