Nanoscale Modeling and Simulation: Impact on NanoEngineering

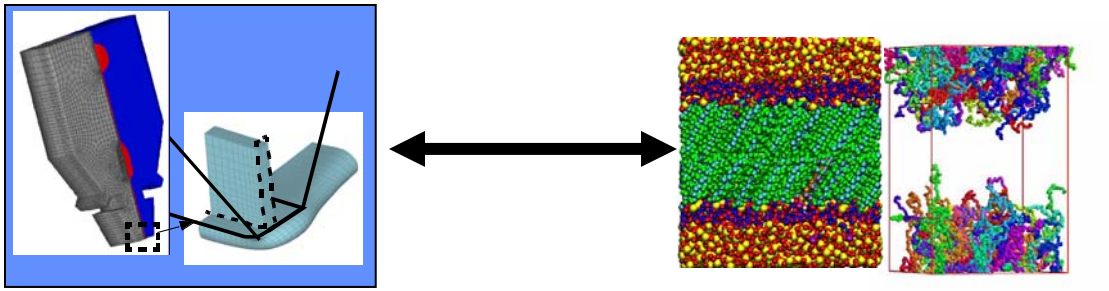
NINE Technical Workshop

28-29 July 2008

P. Randall Schunk

Distinguished Member Technical Staff

Nanoscale and Reactive Processes Department



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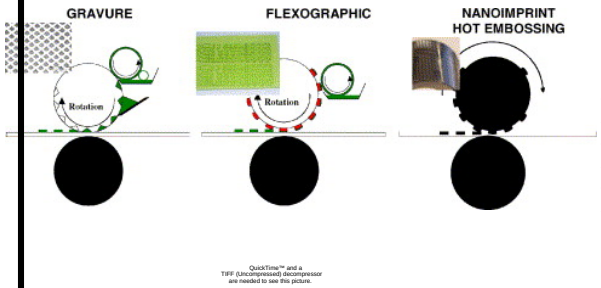
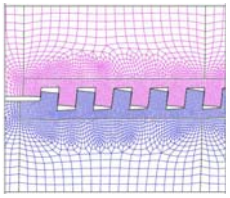
NanoEngineering: Modeling and Simulation at Sandia

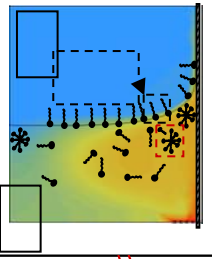
"Nanotechnology" refers to a field of applied science and technology whose theme is the control of matter on the atomic and molecular scale, generally 100 nanometers or smaller, and the fabrication of devices or materials that lie within that size range (Wikipedia 2008).

NanoEngineering ⟷ NanoTechnology



"Macro"
Nanomanufacturing
Nanomaterials
Nanodevices

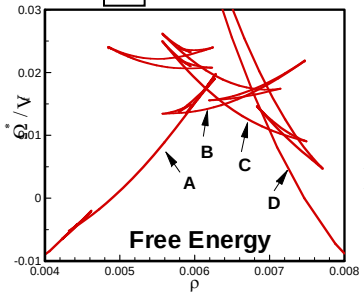




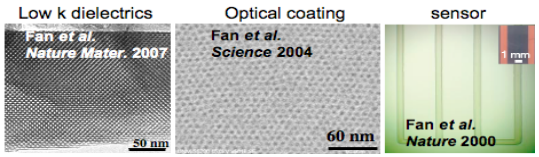
Sierra Mechanics
Goma, Aria, JAS, Adagio

"meso"

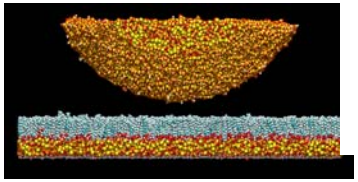
Bridging



Coarse-grained
MD/DFT
LAMMPS, Tramonto



"atomistic"



MD/DFT
LAMMPS, Tramonto

Quantum DFT
QUEST, SOCORRO

SNL's state-of-art self-assembly and nanomanufacturing capability

Length
Time scale

Nanoscience (material science)

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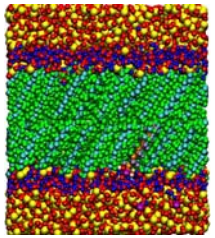
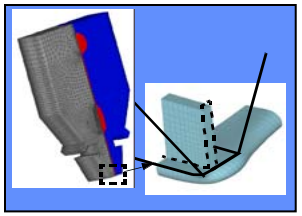
Nano-Scale Modeling and Simulation:
Envisoned Role In NanoEngineering

Understanding at the Nano-Scale (material science)





9-10 orders of magnitude in scale

Controlling at the Nanoscale (NanoTechnology and Nano Engineering)

- **Nanotechnology requires macro-knobs.**
- **Mod/Sim in NanoEngineering epitomizes multiscale analysis (true backing to the current hype in mod/sim)**

- **Sandia Strengths: HPC, atomistics and classical MD, Computational Continuum Mechanics, Multiscale methods/analysis . Many activities ongoing at "mesoscale"**
- **Killer-Apps: Manufacturing (NIMS, NPFC)**
- **Core Production Codes: LAMMPS, GOMA/ARIA, Tramonto**

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Essential Mod/Sim technology for reaching down into the "micro/nano-world"

From an "engineering" viewpoint.
Controlling at the Nanoscale requires understanding and capabilities in

•Bulk and surface mechanics of solids and fluids (gases and liquids) on microscale. This is our carrier of nanobuilding blocks or the mechanics which controls the device/machine!

•Interaction of materials at interfaces (mechanical, chemical). Liquid and solid surfaces (Wetting and spreading) and solid-solid interfaces (adhesion).

•Species transport and phase change. (Neutral or charged, multicomponent transport, continuous and meso-phase change)

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Impact of M/S on Nanotechnology: Capability Requirements

Large Length/Long Time End: Mechanics (continuum) modeling capability at device/machine scale (fluids, solids, thermal, chemical species, and possible electromagnetic)

Specialized capability for continuum: capillary free surfaces, three-phase contact, fluid-structure interaction, multiphase flow (suspension, porous medium)

Small length/Short Time End: Materials modeling at atomistic/molecular scale (with necessary links to quantum scales)

These extremes can be linked with "mesoscale connections" or by brute force:

- mesoscale capability (coarsed grained from atomic scale)
- constitutive equations ("subgrid" physics from continuum scale),
- integrated models (spinning a molecular scale model in the "subgrid" of a continuum.
- Brute force DNS (achieve macro- time and length scales from a MD capability)

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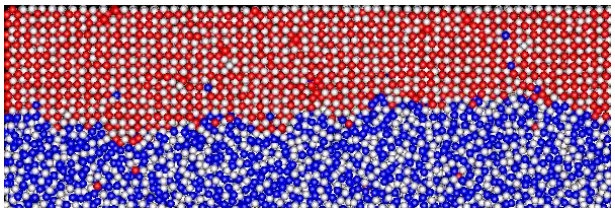
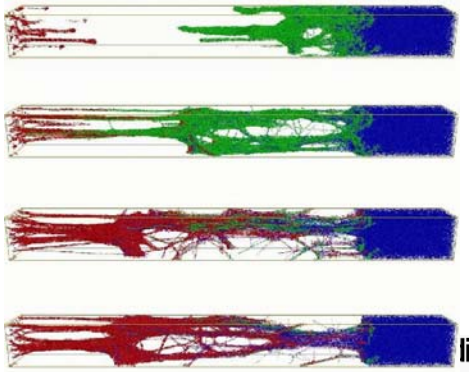
LAMMPS Overview and Upgrades

Contact: Steve Plimpton (sjplimp@sandia.gov)

- Classical molecular dynamics (MD) code:
  - serial: fast on one processor
  - parallel: scalable to billions of particles on big machines
- One foot in biomolecules and polymers
- One foot in materials science
- One foot in mesoscale to continuum
  - *Part of that foot in nanoparticles and colloids, and coupled to bulk hydrodynamics! Another part in granular flow*

QuickTime™ and a
Cinepak decompressor
are needed to see this picture.

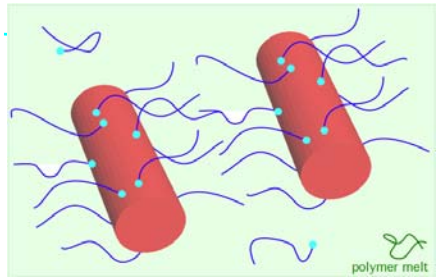


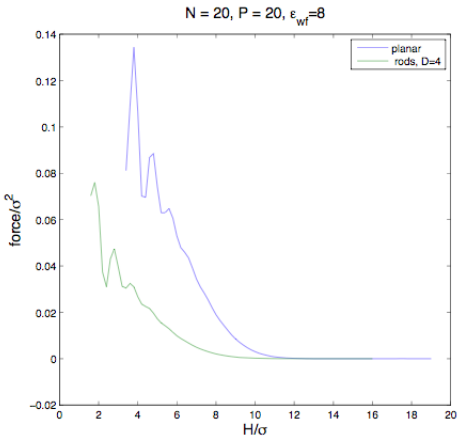


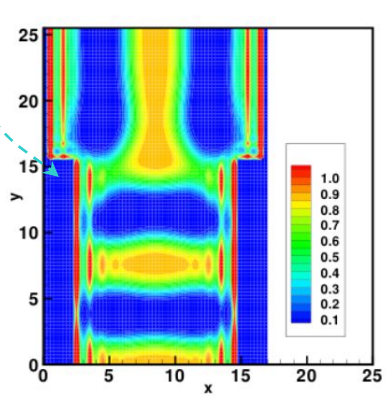
Tramonto

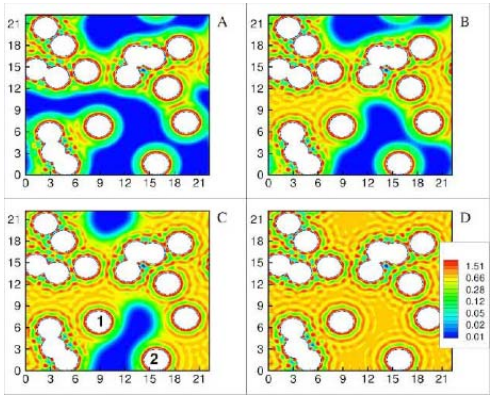
DFT Capability

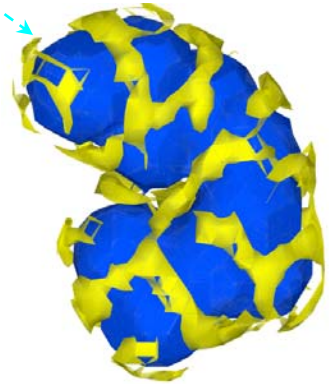
- -forces between particles
- -phase behavior
- -solvation free energies
- implicit solvent
- -complex geometries
- -complex chain architectures
- -compare to simulation (MD)

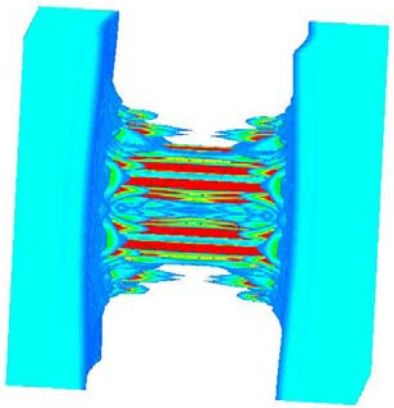












"Frischknecht, Amalie L" <alfrisc@sandia.gov>, PI

http://software.sandia.gov/tramonto/index.html

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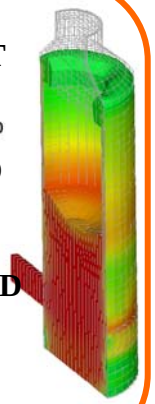
GOMA MULTIPHYSICS CODE

Contact: P. R. Schunk (prschun@sandia.gov)

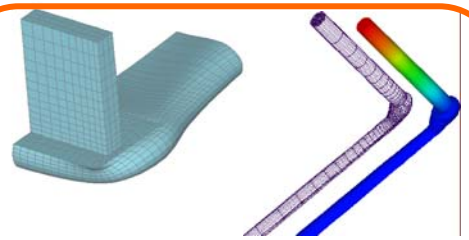
A MP FINITE ELEMENT CODE FOR MULTIPHYSICS FREE AND MOVING BOUNDARY PROBLEMS

DELIVERY OF POLYMER/CERMET ENCAPSULANTS FOR MICRO ELECTRONICS AND NEUTRON GENERATOR PERFORMANCE AND RELIABILITY



DP NG/NG TUBE FEED THROUGH

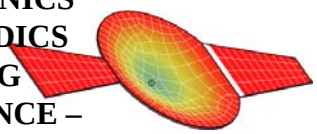
DP

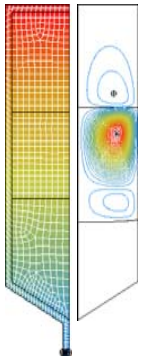


CERAMIC SLURRY EXTRUSION/RAPID PROTO FOR NG/ PZT APPS

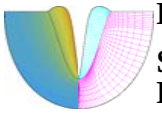
- COUPLED OR SEPARATE HEAT, N-SPECIES, MOMENTUM (SOLID AND FLUID) TRANSPORT
- FULLY-COUPLED FREE AND MOVING BOUNDARY PARAMETERIZATION
- SOLIDIFCATION, PHASE-CHANGE, CONSOLIDATION, REACTION OF PURE AND BLENDED MATERIALS
- HOST OF MATERIAL MODELS FOR COMPLEX RHEOLOGICAL FLUIDS AND SOLIDS

MICROELECTRONICS AND MEMS-FLUIDICS MANUFACTURING AND PERFORMANCE – DP/ASCI

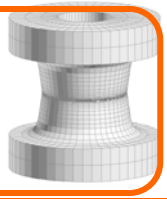




ALLOY PROCESSING CRADA

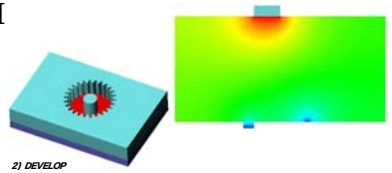


BRAZE/WELD/ SOLDER JOINT FORMATION - DP



CORROSION/ELECTROCHEMICAL APPLICATIONS

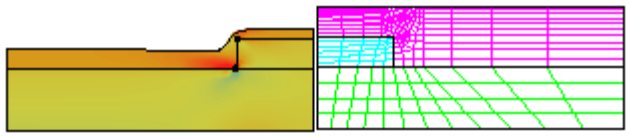
PERFORMANCE, AGING AND RELIABILITY, LIGA



UNIQUE FEATURES MAKE GOMA IDEAL FOR MANUFACTURING PROCESSES IN WHICH

- FREE SURFACES ARE UBIQUITOUS
- COUPLED FLUID-SOLID MECHANICS
- COMPLEX MATERIAL RHEOLOGY/LOW SPEED
- MULTIPHASE FLOW/POROELASTICITY

COATING/ENCAPSULATION



CRMPC CRADA/DP

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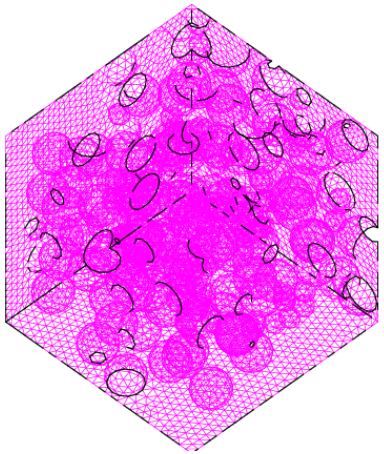
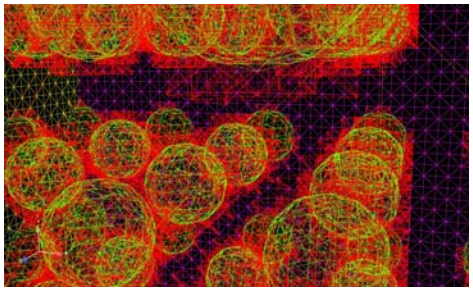
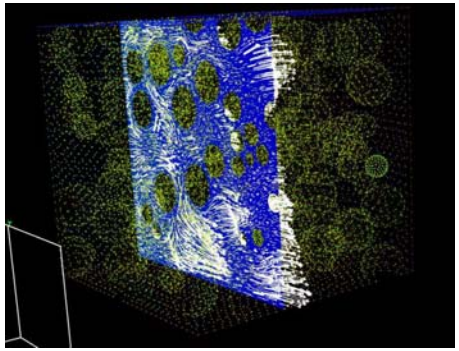
SIERRA Mechanics and Legacy Mechanics Codes

E.G. ARIA/Goma ASC Code as Flow Solver for nanoparticle suspension dynamics and Adagio/JAS nano-embossing

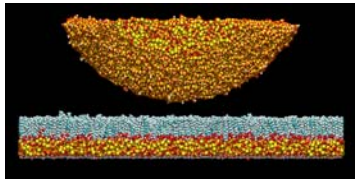
- 600-particle case, moving structures in fluids (with Colloidal forces)

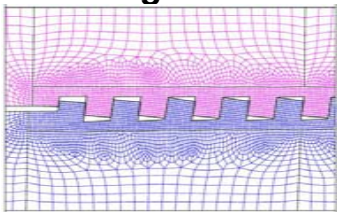






- Nanoscale release model of nano-indentation process (including fracture toughness)





- Other examples include constitutive equations for phonon transport (thermal)

Coupled with Coarse-grained LAMMPS we will achieve a bridge between atomistics and continuum (meso and not quite engineering) scale.

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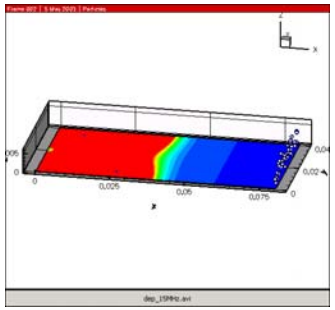
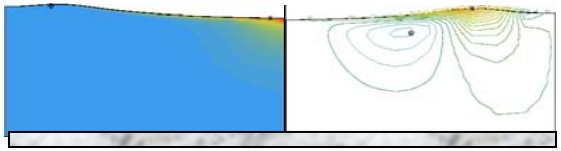
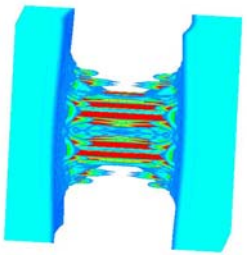
Mod/Sim in NanoEngineering: Validation best achieved with numbers!

FEM-Based Continuum Codes (GOMA/ARIA): Currently installed and active at more than 10 sites, including 3M, P&G, Corning. Has been active in the past at as many as 30 companies.

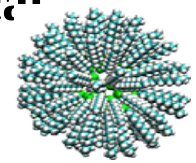


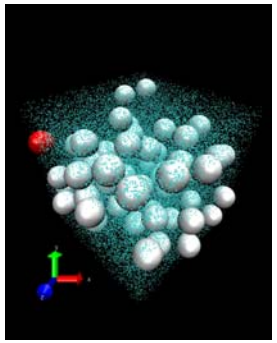




Tramonto is open source software. 201 downloads since 3/15/2007. Approx. 5-10 serious users.

LAMMPS/Colloid package active at 5 sites (including Corning and 3M) for nanoparticle suspension modeling through the NPFC. Validation ongoing with rheological testing.





LAMMPS/MD is open source with 25 downloads/day, 365 days per year.

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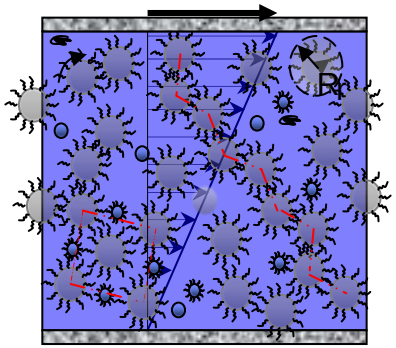
Nanoparticle Flow Consortium (NPFC) CRADA

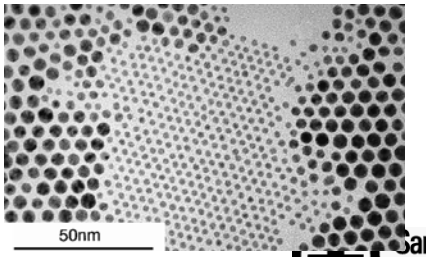
"nanoparticle" is colloidal in nature with characteristic size of 10 nm - 500 nm.

- **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



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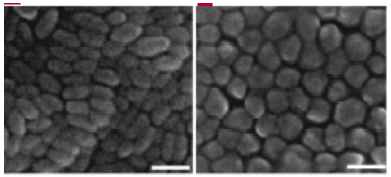
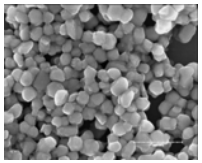
Imbedding Nanoparticles in Functional Materials : *Technology Horizon*

ceramic



polymer

silica



Nanoparticle Manufacture
- Solution, HighT, etc.

Size/ shape

Nanoparticle batch characterization
- Microscopy…

Distribution

Dispersion Chemistry
- Polymer functionalization

Rheology, stability

Fluidization/Processing - e.g. coating, casting…
- Rheology, Microstructure, self-assembly

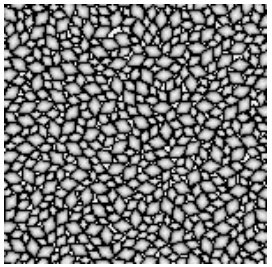
μstruct

Solidification
- Drying, curing, sintering

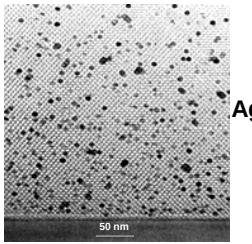
μstruct/residual stress

Product properties
-Thermophysical, mechanical characterization/prediction

(other means of processing into product do exist)



SNL Apps: energy (fuel cells, solid state lighting, solar); high strength, lightweight composites; thermal interface materials, etc.



Ag-Silica nanocomposite

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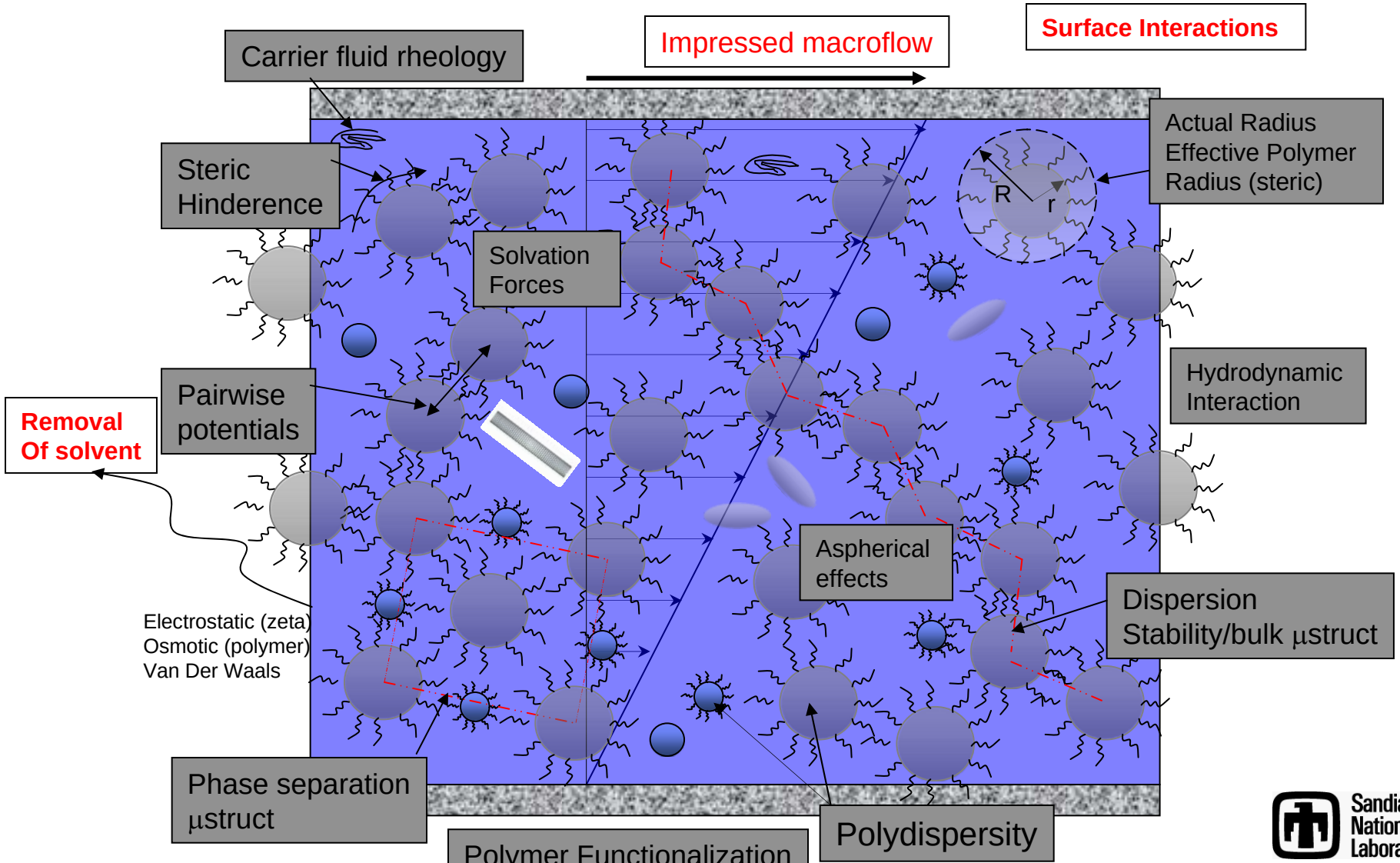
The Problem--Predictive Rheology, Microstructure (bulk and surface)



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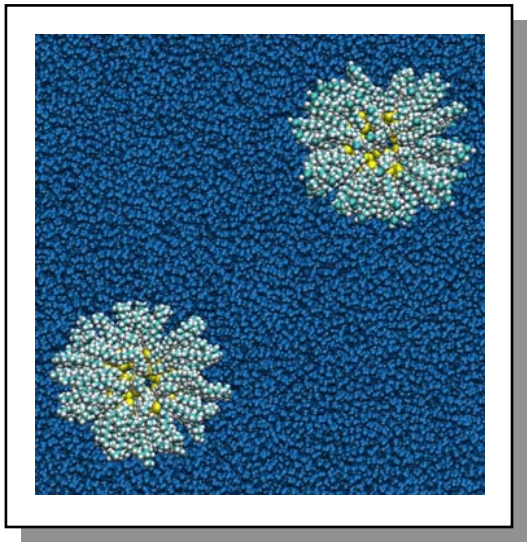
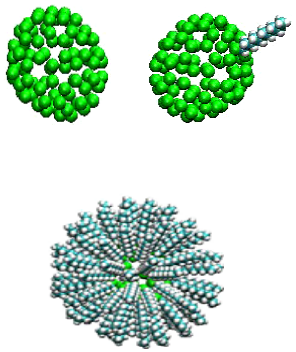
Effective Potential Development

- **Molecular dynamics. Determining interparticle potentials for mesoscale?**
  - **Velocity dependent and independent parts**
  - **Various formulations**
- **Direct force measurement (IFM, Optical Trapping)**



MD of actual Gold/Thiol/Water System (Dynamic and Equilibrium)



Lane et al. (2008)

QuickTime™ and a TIFF (Uncompressed) decompress are needed to see this picture.

- approx. 120,000 water molecules
- approx. 400,000 total atoms
- 128 processors for 16 days
- Less than 2% of T-Bird machine

Silica/PEO in Water

Accurate effective pair potentials required for simulations of nanoparticles in suspension

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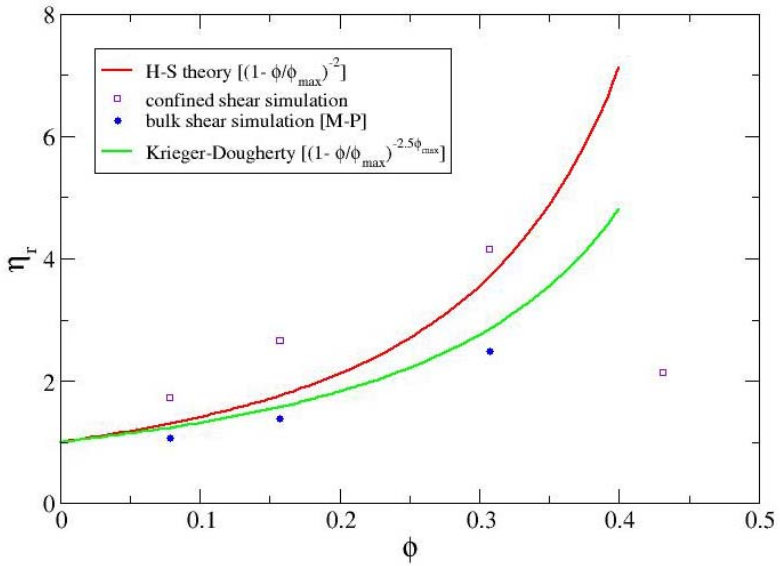
SAMPLE CAPABILITY: COARSE-GRAINED LAMMPS+HYDRODYNAMICS OF SOLVENT



QuickTime™ and a YUV420 codec decompressor are needed to see this picture.

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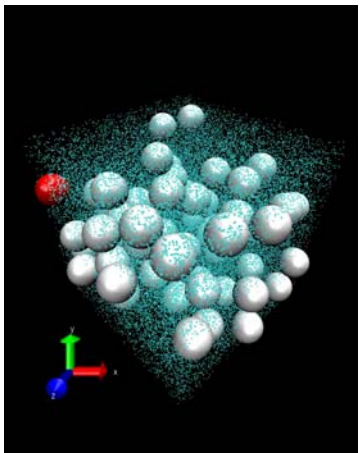

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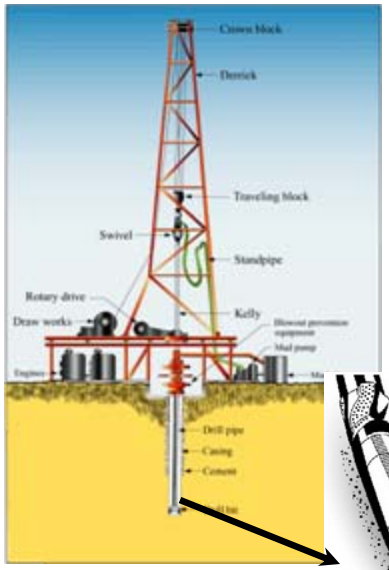
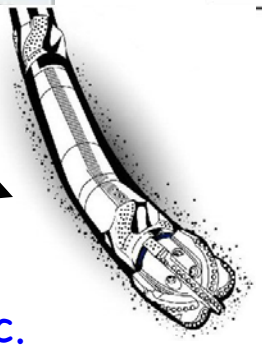
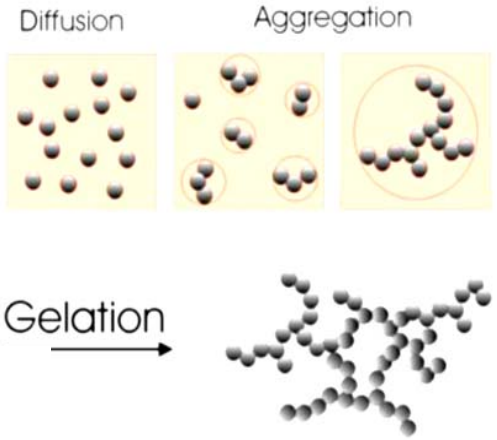
NINE Partnership with UT. Anisotropic Particle Potentials. App: Characterization of aging in drilling fluids. Contact Roger Bonnecaze, ChE.

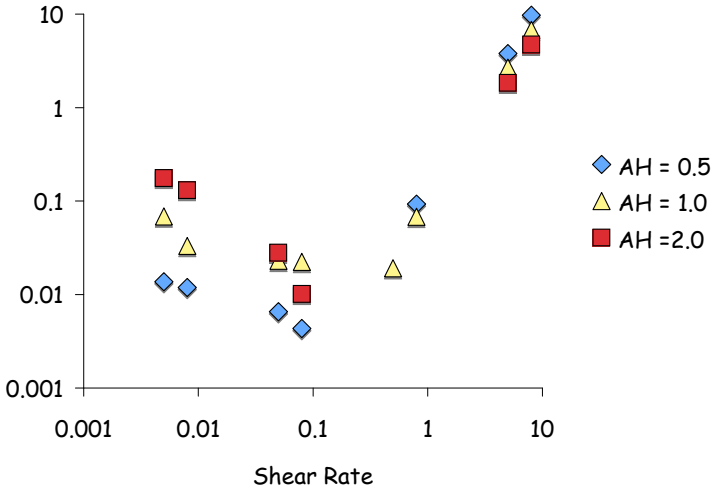
- Dispersions of colloidal particles and other additives in water or oil.





- Cooling drill string, bits etc.





- Ramified clusters because of strong attractive interactions.
- Stress bearing capacity of network quantified by the **GEL STRENGTH** of drilling fluid.
- Rock fragment bearing capacity.
- Pump pressure requirement for re-circulation.

QuickTime™ and a YUV420 codec decompressor are needed to see this picture.

Aspherical particle Potential development

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UIUC Collaboration - *Microstructure and Rheology of Anisotropic Colloidal Suspensions. Contact Prof. Jonathon Higdon, ChE*

- **Large Scale Flow/Discrete Element coupling using Stokesian Dynamics.**

Department of Chemical & Biomolecular Engineering
THE UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

Anisotropic Particles : Fused Dumbbells 42%

Pe = 0.01 : End View

- *New Accelerated CAPABILITY Now Available in LAMMPS through NPFC. Ongoing joint research in algorithms for HPC.*

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NanoManufacturing: Nanostructured Materials Created Layer-by-Layer

Sandia PI: Randy Schunk UT PI: Roger Bonnecaze

Goal: "NanoManufacturing" => "Practical" => High-througput and Large-Area/Volume.

Concept: Produce nanostructured films layer-by-layer by two feasible approaches. 1) Proximity patterning by molding/ forming/imprinting 2) Coating dispersions of nanoparticles.

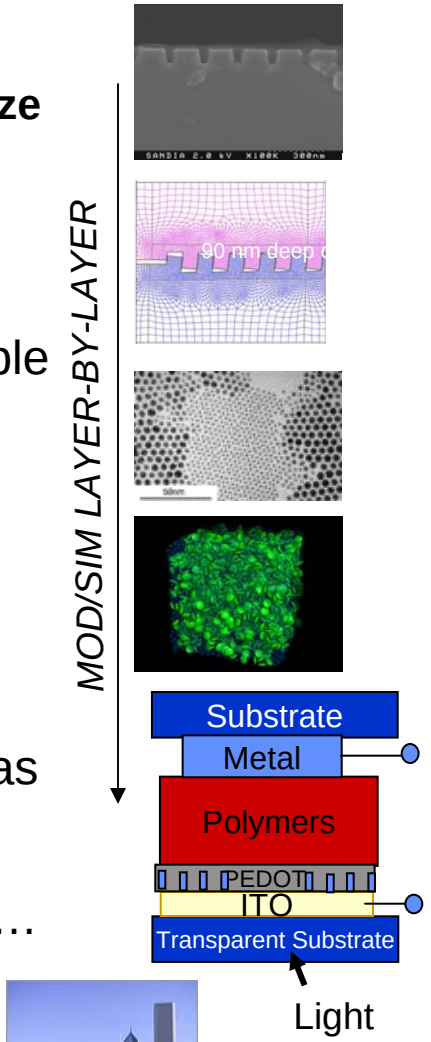
Approach: Integrated computational toolset for underpinning mechancis. Multiscale algorithms to connect nano/atomistic scales to machine design!

Challenges: Multiscale algorithms to predict defects over large areas (large aspect ratios, fluctuating fluids, code integration).

Applications: Photovoltaics, photosynthesis membranes, sensors, …

Collaborators and Partners: University of Texas at Austin. Looking for more.

E.G. Multilayered-Films For Photovoltaics →



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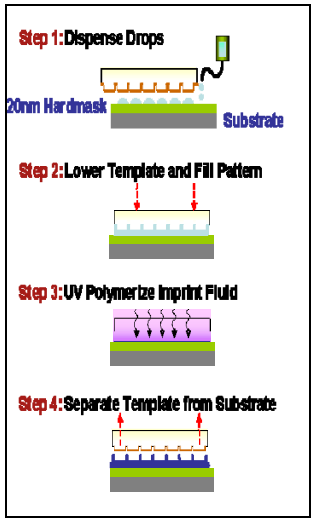
Integrated Computer-Aided Engineering for Nanopatterning Processes - Funded partnership with UT

Nanopatterning

Surface

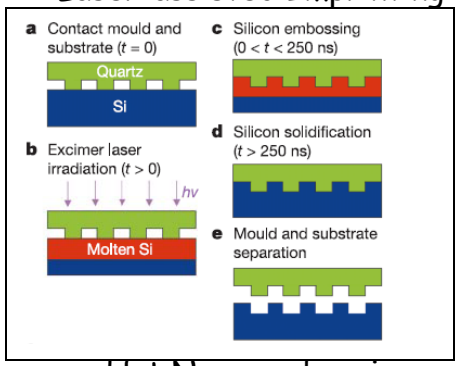
Surface/bulk

Proximity Nanoprinting

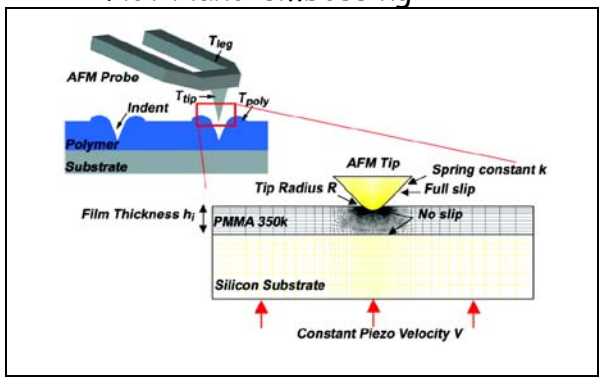


Flash Imprint Lithograph

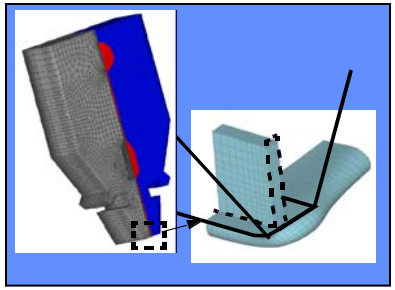
Laser-assisted Imprinting



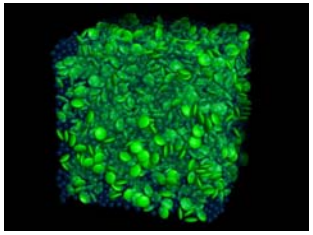
Hot Nano-embossing



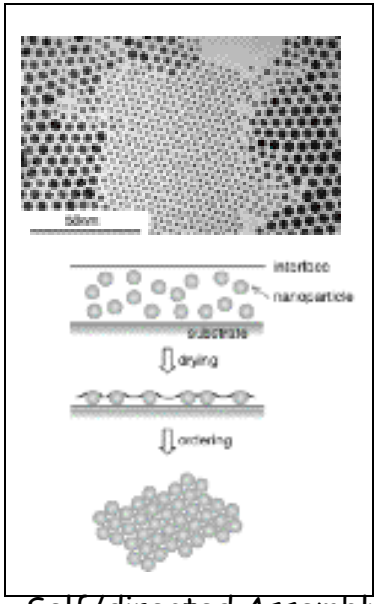
Nanoparticle dispersions Directed and Self Assembly



Coating/Extrusion



Dispersion rheology



Self/directed Assembly

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SNL's Mod/Sim Capabilities and Activities in NanoEngineering - Retrospective and Opportunities

- **Production code platforms and multiscale activities which span all relevant scales (10 orders of magnitude) EXIST TODAY!**
- **SNL has experience with industry needs in computing**
- **Active programs in nanomanufacturing (NPFC and NIMS activity) are soliciting new partners - *Opportunity***
- **NINE University research in critical path**
- **Software engineering which takes advantage of unique HPC environment.**
- **List of contacts:**
  - **Randy Schunk (NIMS, NPFC, Goma, Sierra) - prschun@sandia.gov**
  - **Steve Plimpton. LAMMPS. Sjplimp@sandia.gov**
  - **Amalie Frischknecht. Tramonto alfrisc@sandia.gov**

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