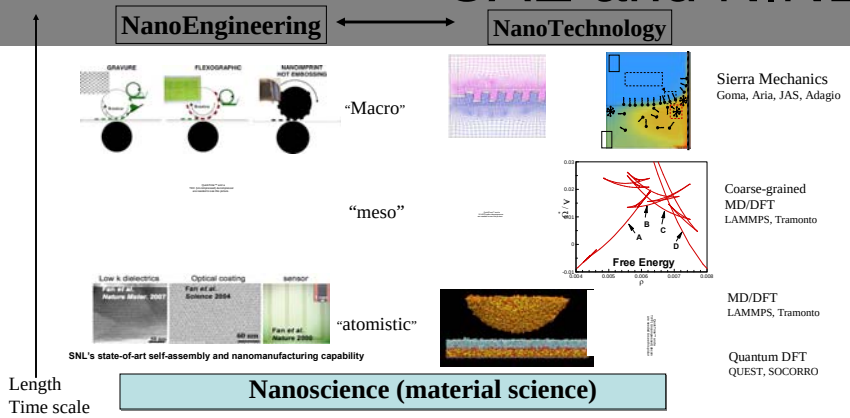
National Institute for Nano Engineering

Nanoscale Modeling and Simulation

CAE and NINE

NanoEngineering: Modeling and Simulation at Sandia



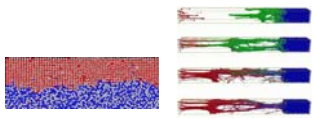
"Nanotechnology": field of applied science and technology aimed at controlling matter at a 10-100 nm scale

"Modeling and Simulation": discipline for developing a level of understanding of the interaction of the parts of a system, and of the system as a whole.

SNL UNIQUE CAPABILITIES AND TOOLS

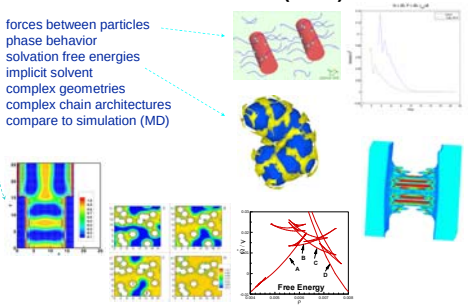
LAMMPS (MD and Coarse-grained DEM)

Classical molecular dynamics (MD) code:
open source (GPL), large user community (12K downloads in 2.5 years)
serial: fast on one processor
parallel: scalable to billions of particles on big machines
reasonably efficient if 100s to 1000s particles/processor
One foot in biomolecules and polymers
One foot in materials science
One foot in mesoscale to continuum
One foot now in nanoparticles and colloids, and coupled to bulk hydrodynamics!

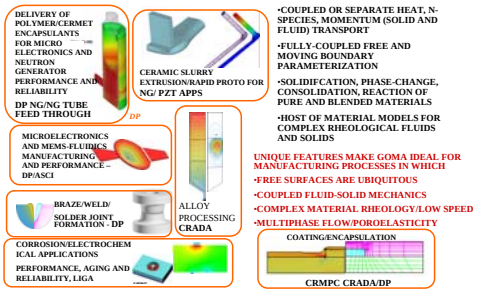


TRAMONTO (DFT)

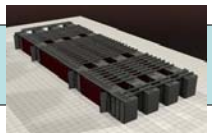
forces between particles
phase behavior
solvation free energies
implicit solvent
complex geometries
complex chain architectures
compare to simulation (MD)



GOMA/ARIA (FEM MULTIPHYSICS)



HPC



Computing Capacity/Capability

EXAMPLE APPLICATIONS

Goal: Predictive Manufacturing Capability

NanoManufacturing: Nanostructured Materials Created Layer-by-Layer

Sandia PI: Randy Schunk UT PI: Roger Bonnecaze

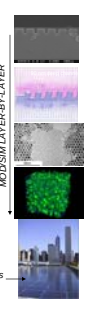
Goal: "Manufacturing" => "Practical" => High-througput and Large-Area/Volume.

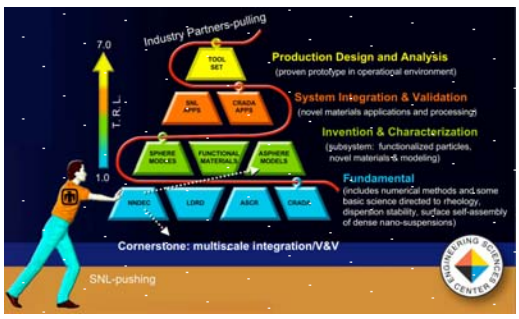
Concept: Produce nanostructured films layer-by-layer by two feasible approaches. 1) Proximity patterning by molding/ forming/imprinting 2) Coating dispersions of nanoparticles.

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, …





Nanoparticle Flow Consortium (NPFC) CRADA

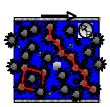
ÑanoparticleÓis colloidal in nature with characteristic size of 10 nm - 500 nm.

Project Description - NCAE Tools For NanoManufacturingÓ

- 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.

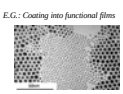
Partners: 3M, Corning, Procter and Gamble, BASF, ICI (Materials Manufacturing Industry)

Arrangement: Consortium bound by NArticles of CollaborationÓcame to us and requested a partnership (3-year CRADA). Born out of the CRMPC (Coatings and Related Manufacturing Process Consortium) which partnered with Sandia for 12+ years (1996-2008).



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

E.G.: Coating into functional films



NINE

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Sandia National Laboratories