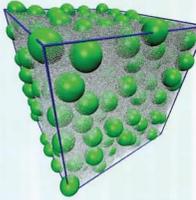


Nanoparticle Flow, Ordering and Self-Assembly

Sandia National Laboratories

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- Nanoparticles can have a profound effect on thermo-physical, mechanical and optical properties
- Processing particles into products through fluidization is a promising approach
- Suspensions exhibit complex rheological and dispersion stability behavior prior to or during processing

NANOPARTICLE FLOW, ORDERING AND SELF-ASSEMBLY

Project Purpose and Approach

Achieve a stronger scientific understanding of dispersion/suspension rheology, dispersion stability, phase behavior, and surface modification using numerical simulation and experimental validation for implementing nanocomposite manufacturing processes.

R&D Goals & Milestones

- Develop a Navier-Stokes/discrete element method for nanoparticle suspensions
- Perform molecular dynamics simulations including solvent explicitly to establish the necessary "subgrid" physics
- Perform rheological experiments of model systems to support and validate modeling

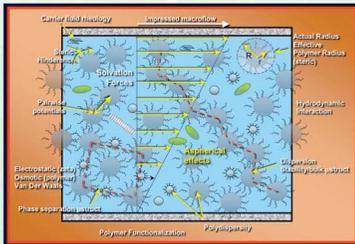
Key Accomplishments

- Coupled Navier-Stokes solver and discrete-element method code
- Implemented coarse-grained, particle-based approach
- Molecular dynamics simulations with nanoparticles and explicit solvent
- Rheological and acoustic measurements of model silica particles

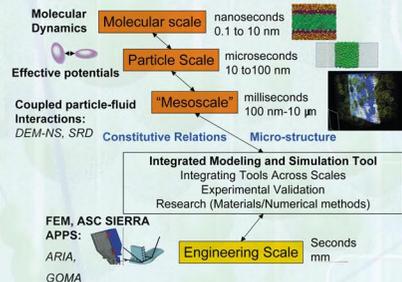
Significance of Results

Develop a new capability that can be used as a technical basis for designing manufacturing processes of nanocomposite materials

TECHNICAL CHALLENGES: RICH PHYSICAL PHENOMENA

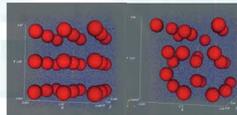
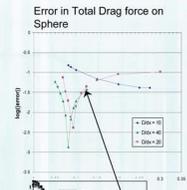


TECHNICAL APPROACH: INTEGRATED CAPABILITY



RESULTS - I

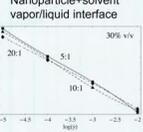
- Coupled Navier-Stokes (NS) solver and discrete-element method (DEM) code
 - PS/7D BM: convergence non-uniform, pressure field degenerates
 - Proto-hybrid efficient fractional stepping and explicit FE schemes in ARIA
- Coarse-grained, particle based approach
 - Implemented stochastic rotational dynamics (SRD) method in LAMMPS
 - SRD bulk fluid equilibrium properties and momentum transport
 - SRD fluid coupling to colloids



Pressure distribution on sphere

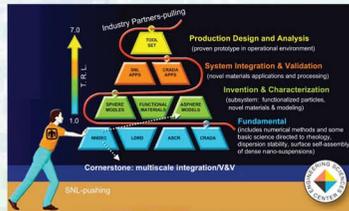
RESULTS - II

- Multi-million atom simulations with nanoparticles and explicit solvent
 - Nanoparticle phase diagram
 - Bulk properties, diffusion of nanoparticles in solvent
 - Non-equilibrium simulations to model rheology
- Significant improvements to LAMMPS
 - Multi-region neighbor lists
 - Improved communications
 - ~100-200 times faster for 20:1 size ratio of nanoparticle to solvent
- Model system - PDMS-Functionalized silica spheres in silicon oil
 - Rheological and acoustic measurements



Shear thinning for nanoparticle suspensions

GOAL: PREDICTIVE MANUFACTURING CAPABILITY



FOLLOW-ON FUNDING/ACTIVITIES

- Industrial partnership (CRADA) formed to develop production-level computational capability aimed at designing nanoparticle flow processing strategies
 - Multi-party CRADA participants (signed in May 2007): P&G, 3M, Corning, BASF and ICI
- Synergism with the National Institute for Manufacturing (NIM) and Center for Integrated Nanotechnology (CINT) in modeling suspensions of spherical nanoparticles and self-assembly
- Development of improved functionalized nano-particle dispersions for implementation into production manufacturing