08/16/2011

GOMA 6.0: Computational Mechanics Capabilities for Manufacturing: Thin-film Coating and Drying, Imprinting/ Embossing, Dispersion casting

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Nanoscale and Reactive Processes Department
Sandia National Laboratories

Title

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.
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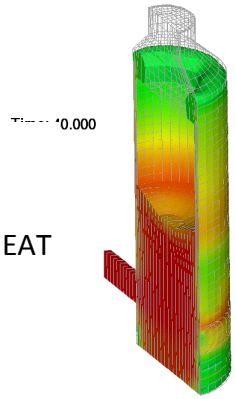
NNSA National Nuclear Security Administration

COMPUTER SIMULATIONS IN MANUFACTURING AT SANDIA – *GOMA 6.0, A Multiphysics Finite Element Code*

MOLD FILLING

-POLYMERS

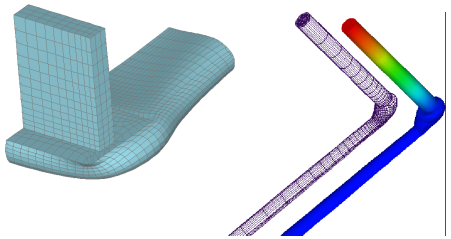
-METALS



--FLUID FLOW, HEAT

PHASE CHANGE,

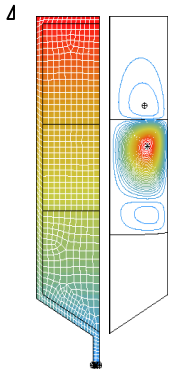
FREE SURFACES



EXTRUSION AND COATING

3D FLUID FLOW, FREE SURF

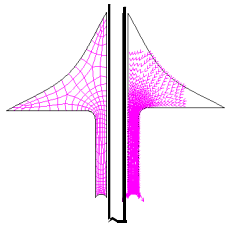
DP

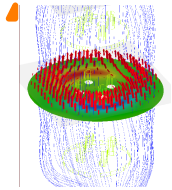


SOLDERING

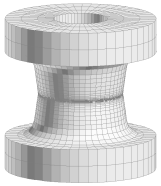
-HEAT, MOMENTUM,

FREE SURFACE,
SOLIDIFCATION





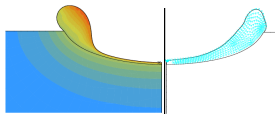
BRAZING, FURNACE
MODELING

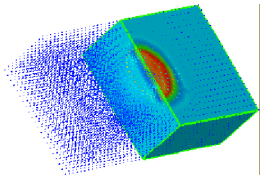


ALLOY
PROCESSING

WELDING

-HEAT, MOMENTUM,
SOLIDIFICATION,



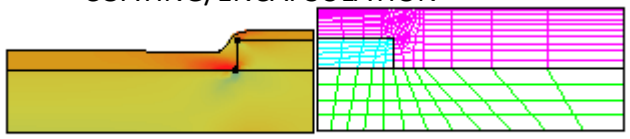


- COUPLED OR SEPARATE HEAT, N-SPECIES, MOMENTUM (SOLID AND FLUID) TRANSPORT
- FULLY-COUPLED FREE AND MOVING BOUNDARY PARAMETERIZATION
- SOLIDIFCATION, PHASE-CHANGE, CONSOLIDATION, REACTION OF PURE AND BLENDED MATERIALS
- HOST OF MATERIAL MODELS FOR COMPLEX RHEOLOGICAL FLUIDS AND SOLIDS

UNIQUE FEATURES

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

COATING/ENCAPSULATION



CRMPC CRADA/DP

GOMA'S CAPABILITY BASED ON CUSTOMER NEED -- INVOLVES MANY TECHNOLOGIES

1) MECHANICS – *INCLUDES ALL MAJOR BRANCHES OF MECHANICS, AND MORE. CONJUGATE CAPABILITY*

2) MATERIALS MODELS AND CONSTITUTIVE EQUATIONS -- *INCLUDES GENERALIZED NEWTONIAN AND VE FOR FLUIDS, ELASTIC AND ELASTOVISCOPLASTIC FOR SOLIDS, FICKIAN, MULTICOMPONENT, AND NON-FICKIAN FLUXES, AND MORE*

3) FREE SURFACE/FREE BOUNDARY TRACKING -- *SOLIDIFICATION SURFACES, CAPILLARY FREE SURFACES, CONSOLIDATION FRONTS, MOLD FILLING FRONTS, SATURATION FRONTS, USER-PRESCRIBED KINEMATICS/ GEOMETRY, ABLATION FRONTS, AND MORE*

4) MULTIDIMENSIONAL WITH 2.5D CAPABILITY. FULL SHELL CAPABILITY.

5) PLATFORM GENERALITY. *HIGH-END, HIGH-PERFORMANCE, AND COMMODITY HARDWARE*

GOMA'S CAPABILITY BASED ON CUSTOMER NEED -- INVOLVES MANY TECHNOLOGIES

6) USER-PRESCRIBED/USER-DEFINED CAPABILITY

7)FLUID-STRUCTURAL INTERACTIONS. *COMPUTATIONAL LAGRANGIAN SOLIDS AND ALE IN BOTH SOLIDS AND FLUIDS WITH EULERIAN-EULERIAN METHODS AN ACTIVE RESEARCH AREA*

8) SATURATED AND UNSATURATED, DEFORMABLE, POROUS MEDIA - PORO-ELASTIC/PORO-PLASTIC

9) FULL-NEWTON COUPLED ALGORITHMS/AUTOMATED CONTINUATION, AUGMENTING CONDITIONS, STABILITY ANALYSIS - *ALL IN A PRODUCTION SETTING*

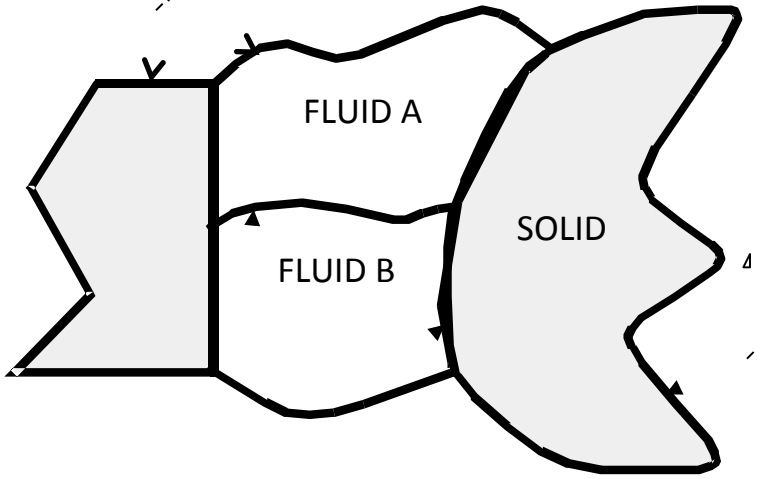
10) OTHER ADVANCED FEATURES- SHELL REDUCED ORDER MODELS, SOLID-MODEL-BASED GEOMETRY SUPPORT; ADVANCED POST PROCESSING FEATURES

11) PIXEL/VOXEL-TO-MESH CAPABILITY

GOMA - BASIC FOUNDATION FOR COUPLED MECHANICS – ALE/LAGRANGIAN

- *TREAT MESH EVERYWHERE AS A DEFORMABLE SOLID BODY*
- *INVOKE LAGRANGIAN AND/OR ALE FORMULATIONS AS REQUIRED BY REGION*
- *APPLY IMPLICIT DISTINGUISHING CONDITIONS FOR USER-PRESCRIBED, KINEMATIC, OR DYNAMIC BOUNDARY MOTION*

EXTERNAL FLUID (MATERIAL) BOUNDARIES LAGRANGIAN AND SHEAR FREE



FLUID - ALE

SOLID - LANGRANGIAN OR ALE

EXTERNAL PRESCRIBED PSEUDO-SOLID/REAL-SOLID BOUNDARIES EULERIAN/STRESS SPEC

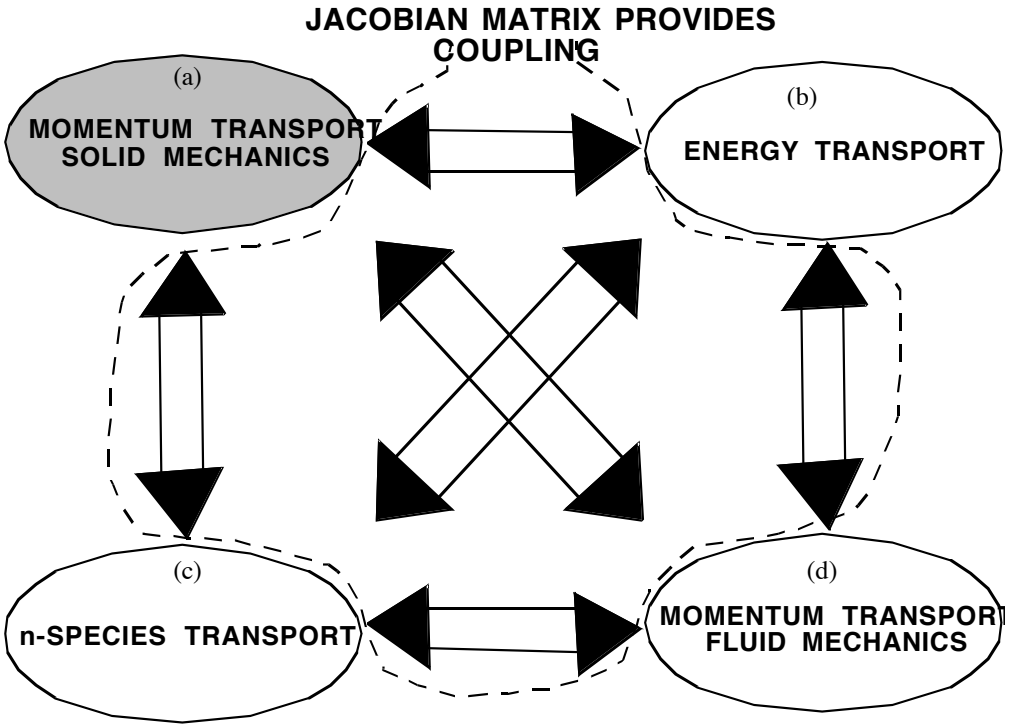
INTERNAL LIQUID/MATERIAL BOUNDARIES LAGRANGIAN OR EULERIAN/BALANCED FORCES/ CONTINUOUS DISPLACEMENT

NATURAL CAPABILITY

-BOUNDARY PARAMETERIZATION BASED ON ANY KINEMATIC OR DYNAMIC CONDITION

...INCLUDING FLUID-SOLID CONTACT LINE MOTION

GOMA 6.0 - CLOSE, COMPREHENSIVE MECHANICS COUPLING



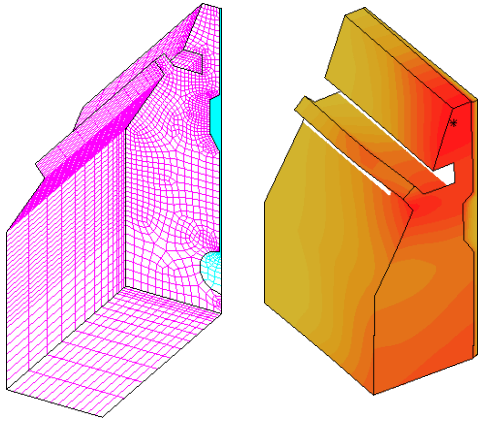
NEWTON'S METHOD

EVERY MAJOR BRANCH OF MECHANICS CLOSELY COUPLED!

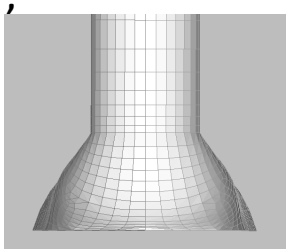
- MINIMAL TUNING REQUIRED OF ALGORITHMS
- FASTER, QUADRATIC CONVERGENCE
- OPTIMAL ALGORITHM FOR VISCOUS AND CAPILLARY-DOMINATED PROBLEMS
- MACHINERY FOR INCORPORATING ADVANCED ALGORITHMS, E.G., AUGMENTING CONDITION CAPABILITY, LINEAR STABILITY, AUTOMATED, HIGHER-ORDER CONTINUATION...

GOMA - HIGHLIGHTS/FEATURES...

MATERIAL MODELS - FLUIDS

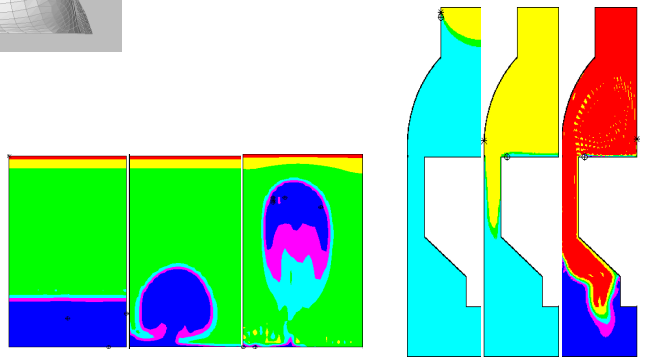


•GENERALIZED NEWTONIAN (CONCENTRATION, TEMPERATURE AND SHEAR-RATE DEPENDENCE). CARREAU, CARREAU-WLF, MOLTEN GLASS, EPOXY, EPOXY CURE, BINGHAM-PLASTIC)



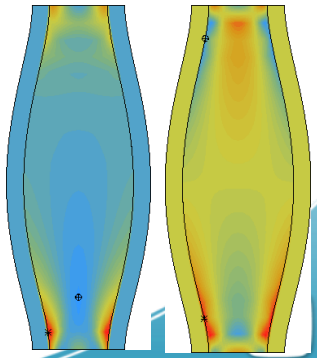
INDUSTRY APPS: EXTRUSION, POLYMER PROCESSING, COATING

•SUSPENSION BALANCE MODELS (PHILLIPS MODEL FOR PARTICLE CONCENTRATION, KRIEGER FOR VISCOSITY)



INDUSTRY APPS: MULTIPHASE MANUFACTURING FLOWS

•SINGLE OR MULTIMODE VISCOELASTIC WITH EVSS SPLIT STRESS APPROACH



INDUSTRY APPS: EXTRUSION, POLYMER PROCESSING, COATING

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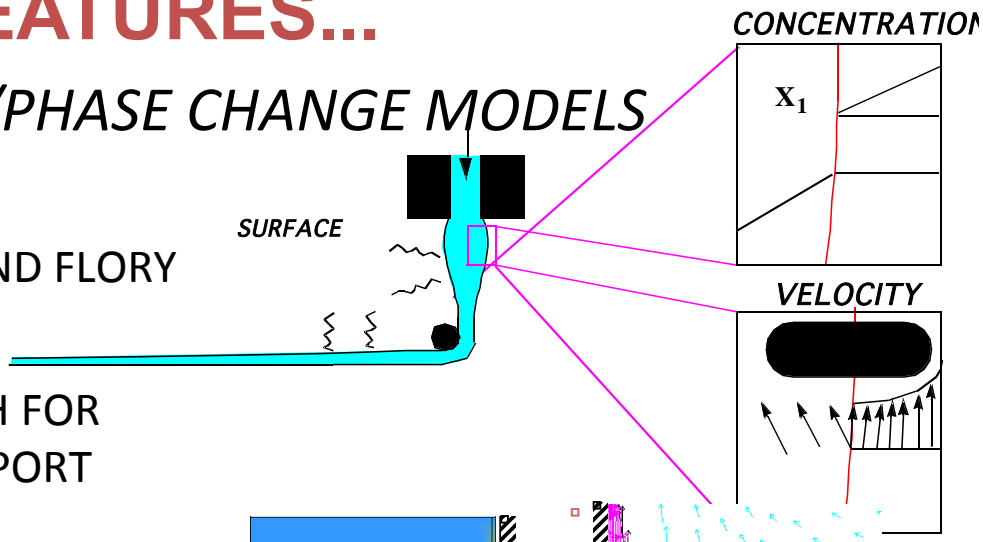
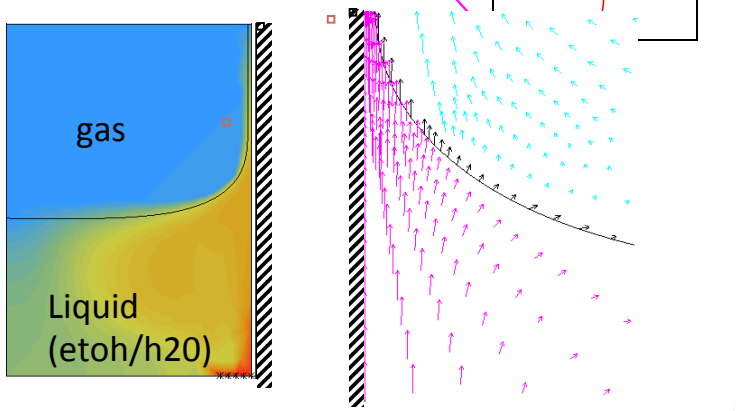
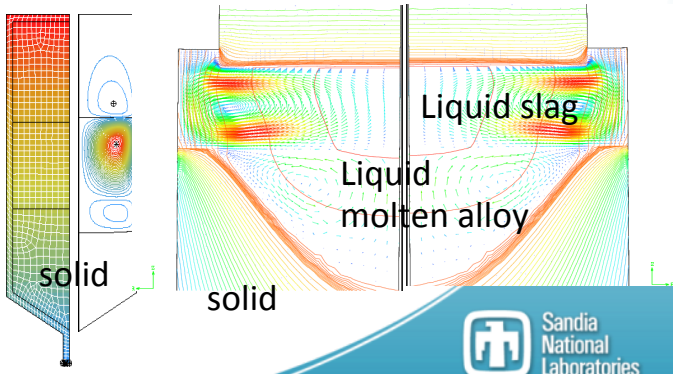
GOMA - HIGHLIGHTS/FEATURES...

THERMO-PHYSICAL PROPERTY/PHASE CHANGE MODELS

- VAPOR/LIQUID EQUILIBRIUM - IDEAL AND FLORY HUGGINS
- DISCONTINUOUS VARIABLES APPROACH FOR INTERPHASE MASS-MOMENTUM TRANSPORT (SCHUNK AND RAO, IJNMF 1994)
- VAPOR-PRESSURE VS (T, C, K) MODELS, VIZ. KELVIN EQUATION, RIEDEL, ANTOINE, ETC.
- LIQUID/SOLID EQUILIBRIUM - SCHEIL OR SOLUTE DEPENDENT SOLIDIFICATION (LATENT HEAT RELEASE WITH ENTHALPY OR INTEFACIAL STEPHAN CONDITION)
- LIQUID/SOLID MACROSEGREGATION WITH FLEMINGS-MEHRABIAN MODEL
- POLYMER THERMOSET AND CONDENSATION CURING







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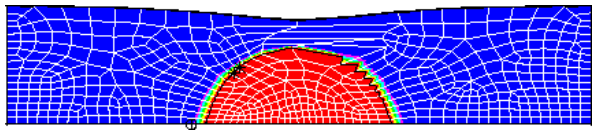
GOMA - ADDITIONAL UNIQUE FEATURES...

FOR DRYING, CURING, ELECTROLYTIC PROCESSES

MATERIAL MODELS - SPECIES TRANSPORT

- FICKIAN OR NON-FICKIAN WITH CONSTANT, USER-DEFINED, OR FREE-VOLUME THEORY DIFFUSIVITIES

POLYMER-SOLVENT, SOLVENT-SOLVENT SYSTEMS, ELECTROCHEMICAL SYSTEMS.

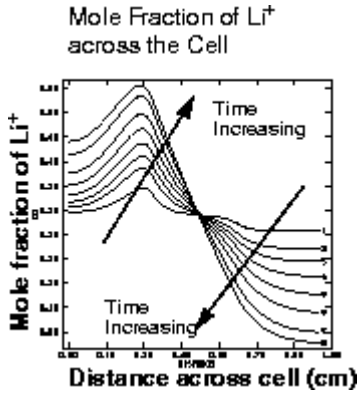


SOLVENT SYSTEM AND GAS BUBBLE

- MULTICOMPONENT DIFFUSION

STEFAN-MAXWELL FORMULATION

COMPANION ELECTROSTATICS FOR CHARGED SPECIES

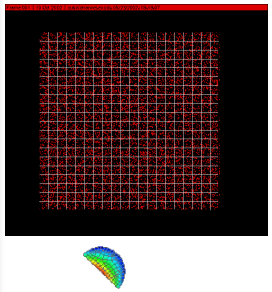


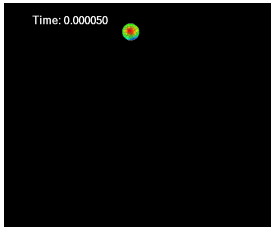
- CHEMISTRY: SURFACE CHEMKIN/ LIQUID PHASE CHEMKIN (IN PROGRESS FOR CORROSION AND ELECTROCHEMICAL APPS.)

CONDENSATION CHEMISTRY FOR EPOXIES

GOMA FREE AND MOVING BOUNDARY TECHNOLOGY:
MECHANICS AND FRAME OF REFERENCE GENERALITY

Large Kinematic/Small Mechanical



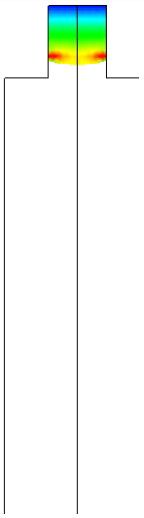


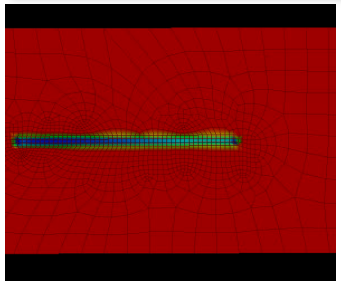
2, 6, 8, 4

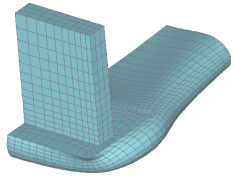
1. **ALE SOLID**
2. **ALE FLUID**
3. **ALE SOLID & FLUID (TALE)**
4. **LAGRANGIAN SOLID (DYNAMIC)**
5. **ALE FLUID/LAGRANGIAN SOLID**
6. ***EULERIAN SOLID***
7. **EULERIAN FLUID(LEVEL SET)**
8. ***EULERIAN SOLID/FLUID***
9. ***EULERIAN FLUID/LAGRANGIAN SOLID (OVERSET GRID)***

Large Kinematic/ Large Mechanical Fluid

2, 7



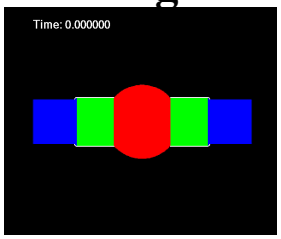




Small Kinematic/ Large Mechanical

1, 2, 3, 4

Large Kinematic/Large Mechanical Solid



6, 7, 8

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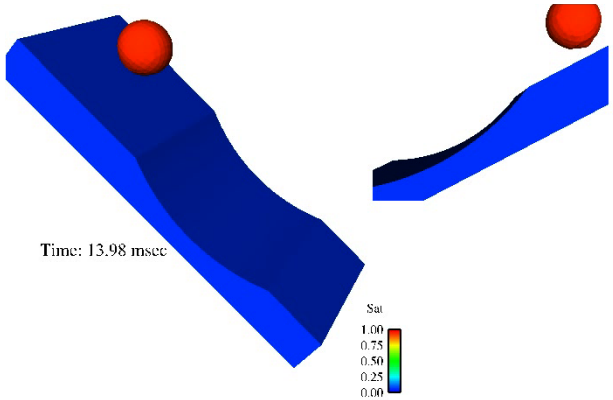
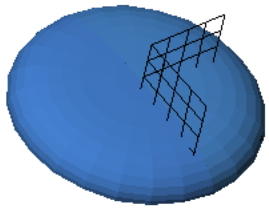
General Free Surface Capability for Continuum and Shell Regions.

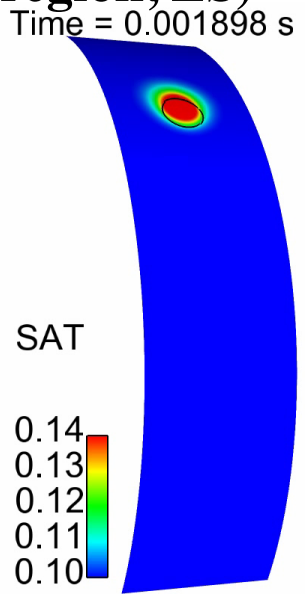
Drop Impact on Porous Substrate (Porous, Wetting, 3D free surface)



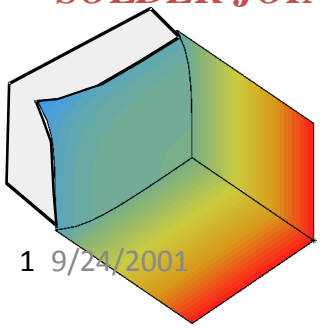
Drop Running Down a Hydrophobic Surface (Wetting, free Surface)



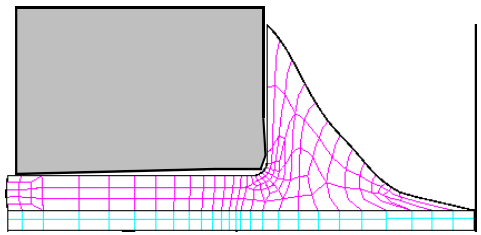
Drop Running between a impermeable and porous shell (shell thin region, LS)

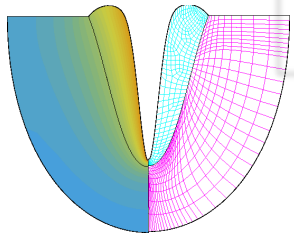


SOLDER JOINTS



LEADLESS CHIP SOLDER JOINTS





LASER WELDING

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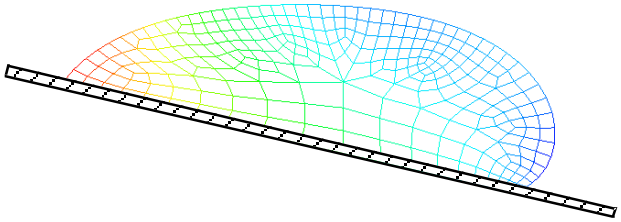
GOMA 6.0 - GENERAL FEM/SOLVER FEATURES...

FINITE ELEMENT INFRASTRUCTURE/SOLVER TECHNOLOGY

- 4/9 NODE QUADS, 9/27 NODE HEXES (MIXED Q2/P1 OR NO CONTRAINTS ON Q2, Q1, OR DISCONTINUOUS ON ANY DOF). TRI-3, TET-4, SHELL-4, SHELL-9 PRESSURE STABIIZED SCHEMES, MASS LUMPING.
- FULLY INTEGRATED ELEMENTS - GAUSSIAN QUADRATURE
- STEADY/TRANSIENT (1ST OR 2ND ORDER, NEWMARK-BETA)
- NEWTON'S AND RELAXED NEWTON'S METHOD, MODIFIED NEWTON
- DIRECT (SPARSE, UMF, FRONT, SUPERLU_DIST), ITERATIVE (TRILINOS 10.2) SOLVERS
- DISCONTINUOUS GALERKIN FOR STRESS, SPECIES, ETC.
- LBB ELEMENTS DEFAULT, PSPG/SUPG OPTIONS AVAILABLE
- DECOUPLED MARCHING LOOP FOR HYPERBOLIC EQUATIONS
- ANALYTICAL JACOBIAN FOR ALL BUT EVP AND AUGMENTING CONDITIONS
- GENERALIZED COORDINATE SYSTEMS (2D, CYLINDRICAL, SWIRLING, SPHERICAL, 3D)
- ~100 DIFFERENT DIFF EQS, ~200 DIFFERENT BOUNDARY CONDITIONS
- HIGHER-ORDER QUANTITY POST-CALC., INTEGRATED FLUX OUTPUT, ...
- EXTENSION SHELL-ELEMENT AND REDUCED ORDER ELEMENT TECHNOLOGY (LUBRICATION, STRUCTURAL, SPECIES, HEAT-TRANSFER)
- FULLY PARALLEL PASS-OFF TIME

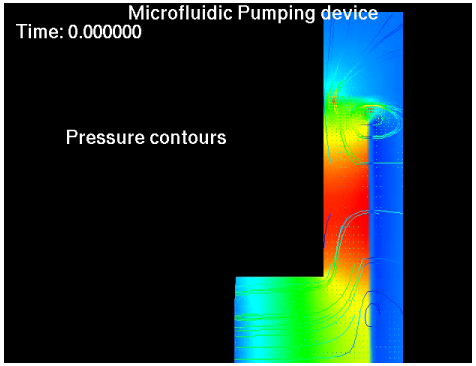
GOMA - ADDITIONAL UNIQUE FEATURES…

ADVANCED ANALYSIS CAPABILITIES



•AUGMENTING CONDITIONS (E.G. VOLUME & MESH CONSTRAINTS, OPTIMIZATION)

BORDERED ALGORITHM, NUMERICAL & ANALYTICAL JACOBIAN

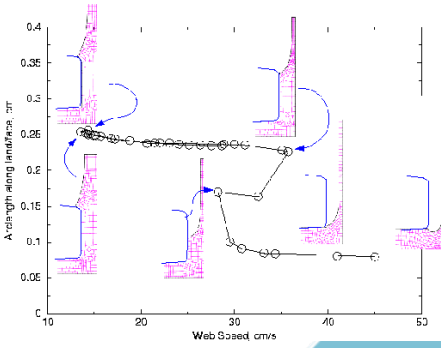


•AUTOMATED ZEROTH, FIRST, ARCLENGTH AND MULTIPARAMETER CONTINUATION

NONLINEAR PARAMETER OPERATING SPACE PREDICTION FOR MANUFACTURING

•LINEAR STABILITY ANALYSIS USING (ARPACK AND ANAZAZI)

2D AND 3D LINEAR STABILITY OF DYNAMIC SYSTEMS. 3D STABILITY OF 2D BASE FLOW.



SUPPORT OF THESE IS "HIGH MAINTENANCE" AND REQUIRES GOOD INTERFACE FOR USER TO DEFINE CONDITIONS

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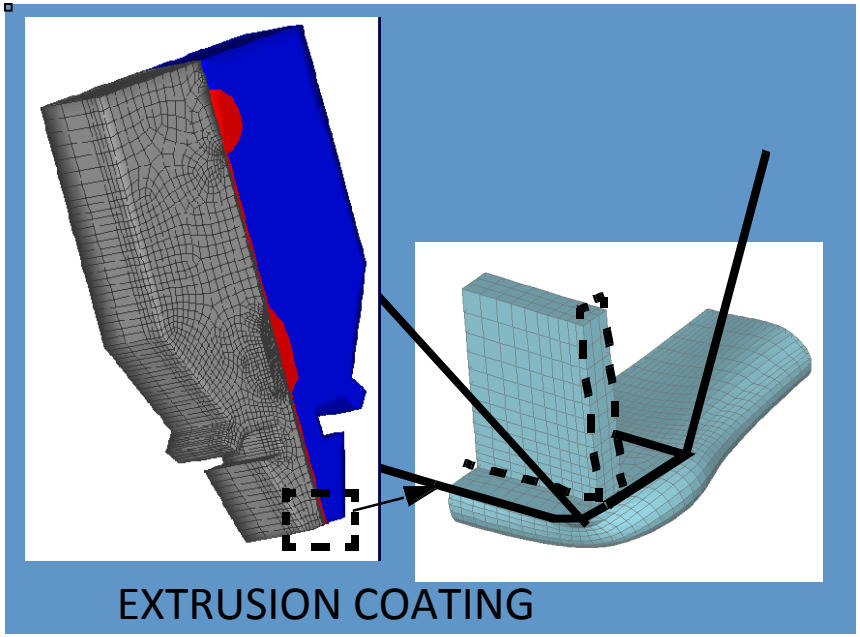
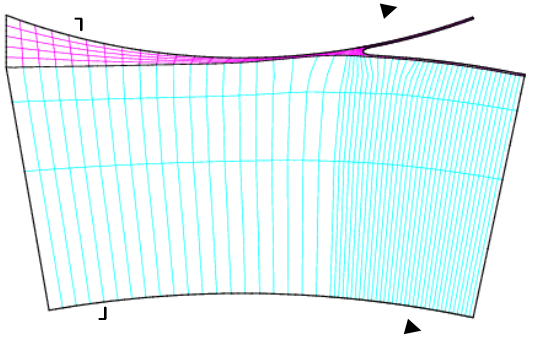
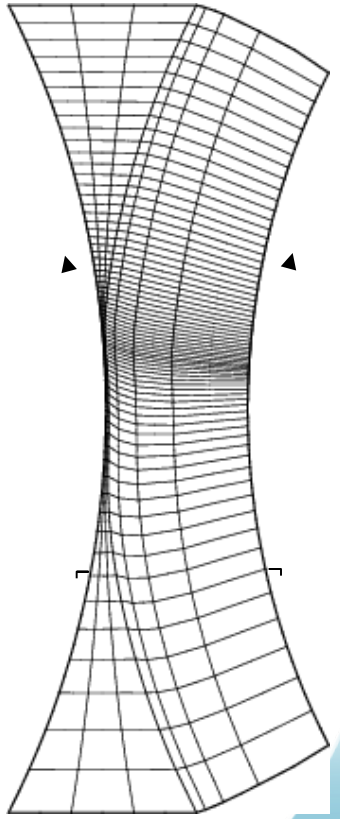
THIN-CONTINUOUS LIQUID FILM COATINGS AND STRUCTURES

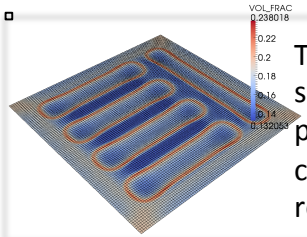




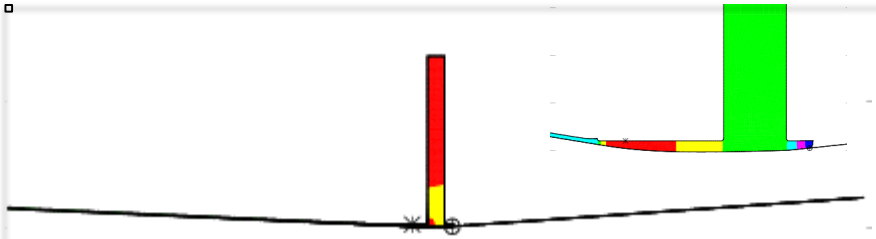
Deformable roll liquid metering and laminating.



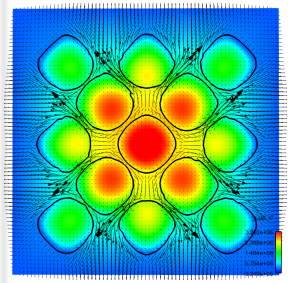
Current State-of-the-Art Capabilities: Thin film manufacturing flows.

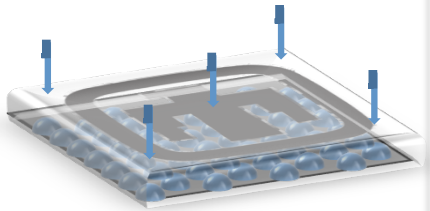


Thin-film Drying and surface energy patterning (full continuum and reduced order models)



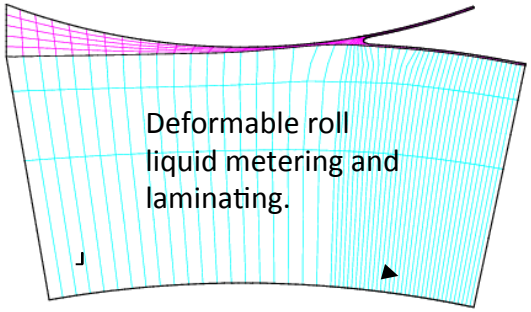
Elastohydrodynamics in coating: Reduced-order shells for webs. Coupled Cap-Hydro continuum



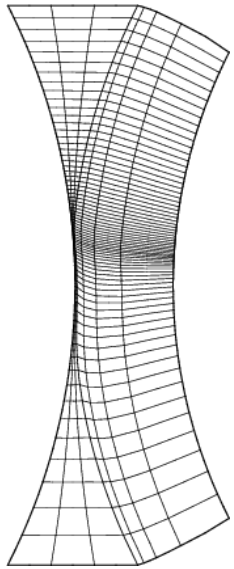


Reduced-order lubrication-shells, porous shells, Multiphase/cap-hydro -- (e.g. S-FIL process)

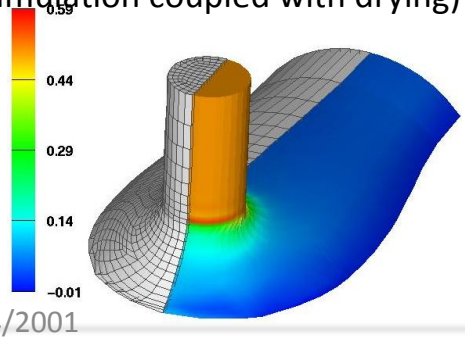
General FSI: Coupled Lagrangian or ALE solid (TALE) with full-up Navier-Stokes and ALE free-surface. Porous Solids.

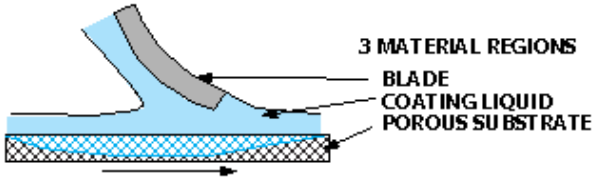


Deformable roll liquid metering and laminating.

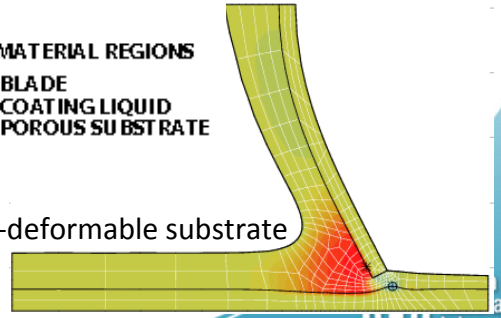


General ALE Capillary Free Surface Capability (micro-dip-pen simulation coupled with drying)



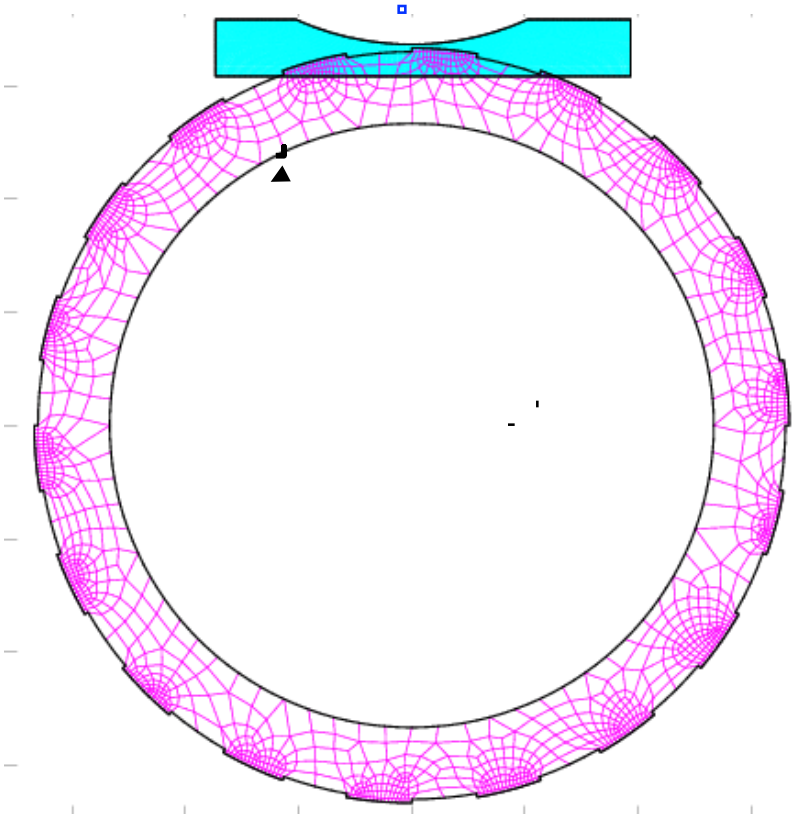


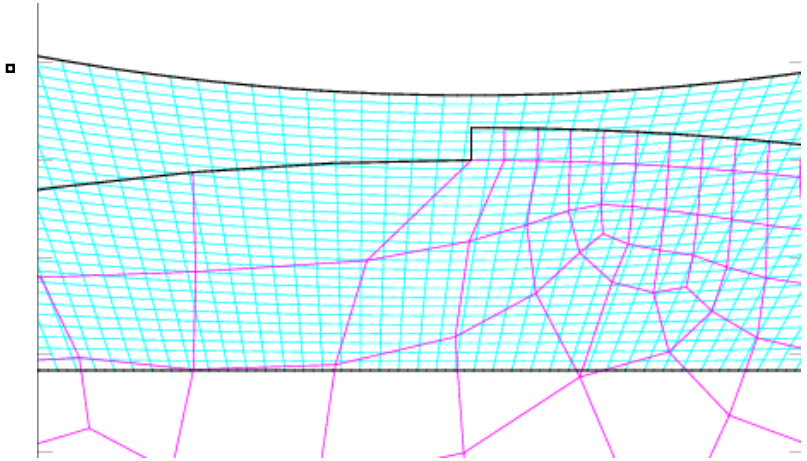
Deformable blade/porous-deformable substrate

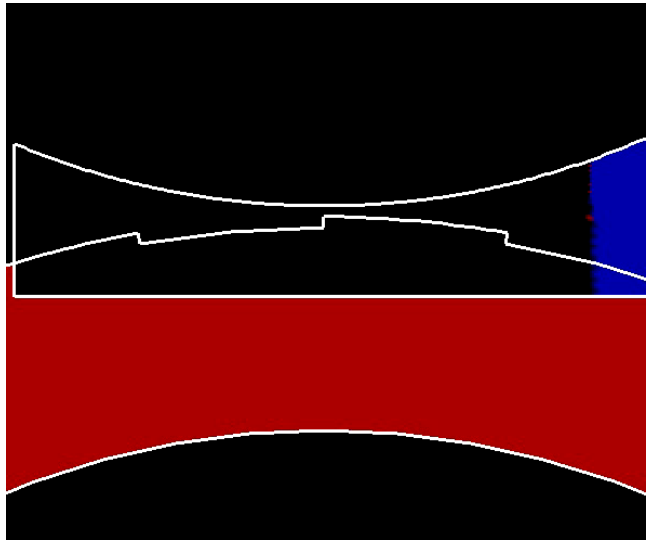


Gravure Roll Coating (Overlap Grid Method – 2D only)

Viscosity – 10 P
Roll Speed – 100 cm/s (ID)
Density – 1 gm/cm^3

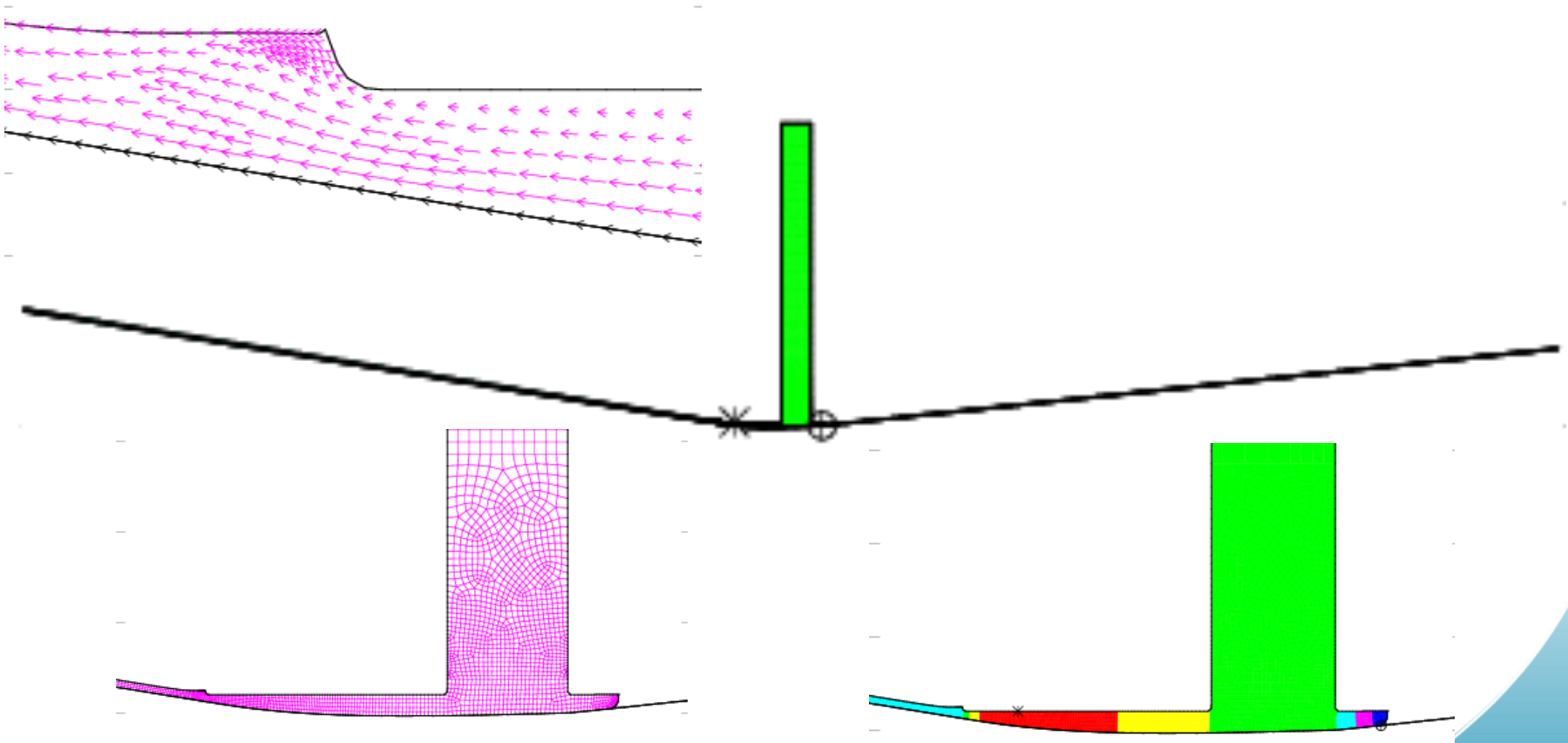






Tensioned-Web Slot Coating

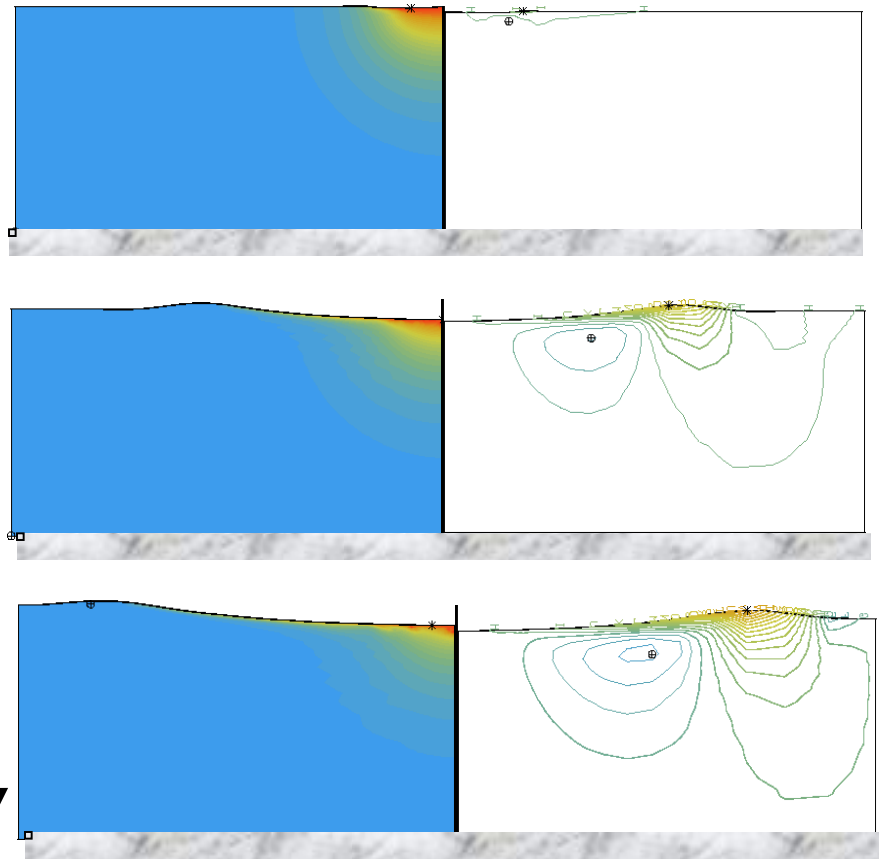
Viscosity = 2 g/mm-s; Web_tension = 1.e8 Web_angle_U = 6 deg
Web_angle_D = 10.7, Webspeed = 1 m/s, ST = 60 dyn/cm



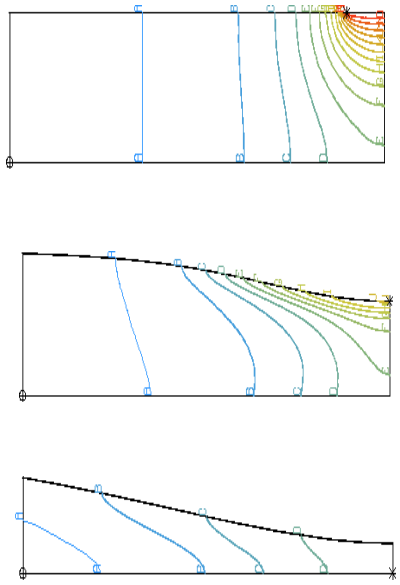
DRYING AND CURING OF THIN FILMS

TIME

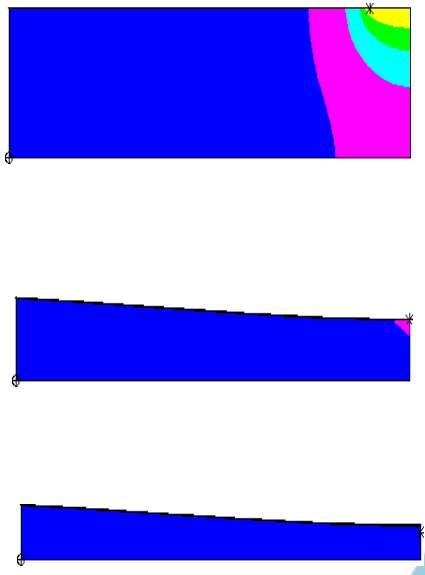
Contaminant



Fast drying/ curing



Slow drying/ curing



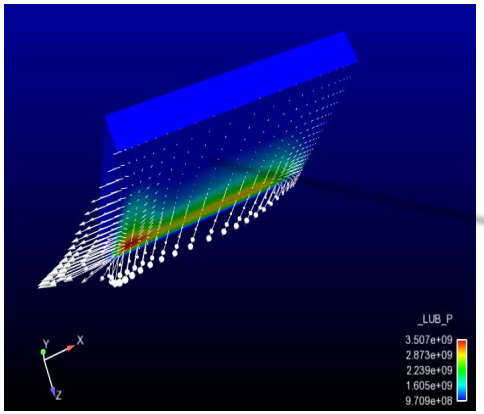
Solidified Defect

Self Healing/ Leveling

Finite Elements and thin regions calls for Shell Elements!

- **Shell Element Technology Ideal when large-aspect-ratio regions (structures) prevail.**
  - Shell-Element: reduced-order continuum element (integrated with presumed mechanical response in one direction – membrane, inextensible shell, lubrication, porous) – *Three dimensional coordinates but only two integration coordinates*
  - We have developed and integrated true curvilinear shell capability for *lubrication* (first of its kind to our knowledge integrated with continuum codes), *porous penetration*, and *integrated structure*.

Lubricated Slider Bearing, Melt Lubrication

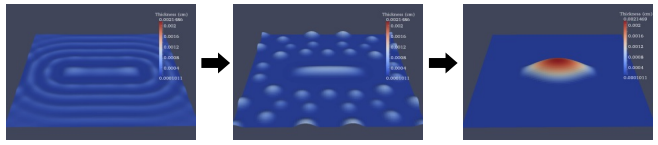


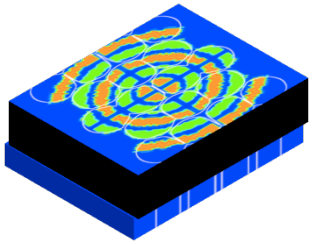
Layer thickness < 5 microns, slider dimension ~10 cm

"Shell elements are also thought of as a way (data-structure, mechanism) to apply overloaded, fancy BCs"

Motivation is Application Driven

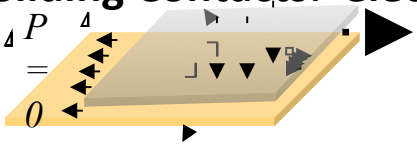
Top-down nano-manufacturing: fluid distribution, printing, mold filling in large-aspect ratio regions

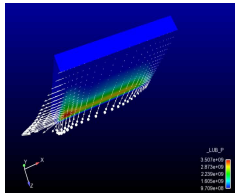


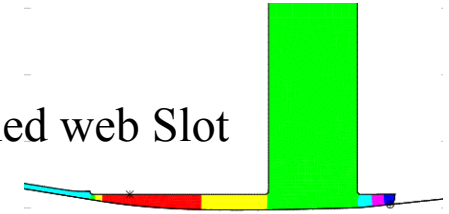


Thin-liquid film coating: film flow, metering flows, thin metering structures

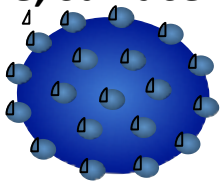
Sliding Contacts: electrical brush

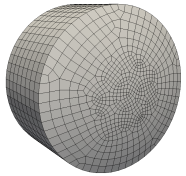






Capillary surface microstructure, surface rheology: emulsions, surface rheometry, oil recovery





Miscellaneous: surface microprobes (Moore et al., "Hydrophilicity and the Viscosity of Interfacial Water", submitted to Langmuir)*, tire hydro-plane etc.*

GOMA 6.0: DOCUMENTATION PROJECT
TRAINING, VERIFICATION, VALIDATION, ADVANCED USE

-GOMA 6.0 USER'S MANUAL – Unlimited release

-GOMA SUPPLEMENTAL MANUAL FOR ADVANCED TOOLS (Automated Continuation, Stability, Augmenting conditions)

-MEMOS/TUTORIALS/RELATED DOCUMENTATION - *3 VOLUMES, ~1000 PAGES*

-GT-001.pdf – Introduction and Beginner's Training – Unlimited release

-GT-002 -> GT-043 – Various and sundry tutorials and training templates covering many examples including: Premetered coating flows, roll coating flows, viscoelasticity, parallel processing, drying and solidification, overset grid method, and much more…

-DEVELOPERS' MANUAL ~200 PAGES

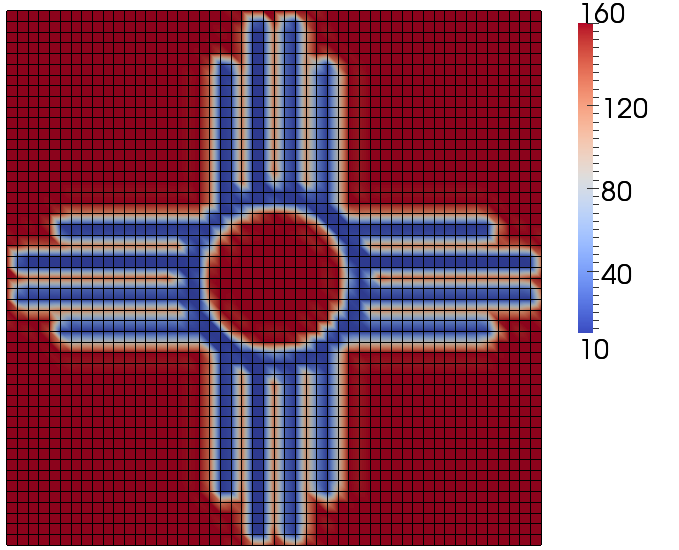
-Technical memos (validation studies, etc.) – 20-30. C

PATTERN REPRESENTATION
COARSE – GRAINING METHOD

ORIGINAL PATTERN IMAGE

IMAGE PROCESSING
+
LEAST SQUARES FIT TO MESH

PATTERN OVERLAID MESH



- ***NO NEED TO GRID THE PATTERN INTO THE MESH → REDUCE MESH REQUIREMENTS TO RESOLVE THE PATTERN***

- ***CAN BE GENERALIZED TO OTHER FIELD PARAMETERS SUCH AS PORES HEIGHT, PILLAR HEIGHT, …***

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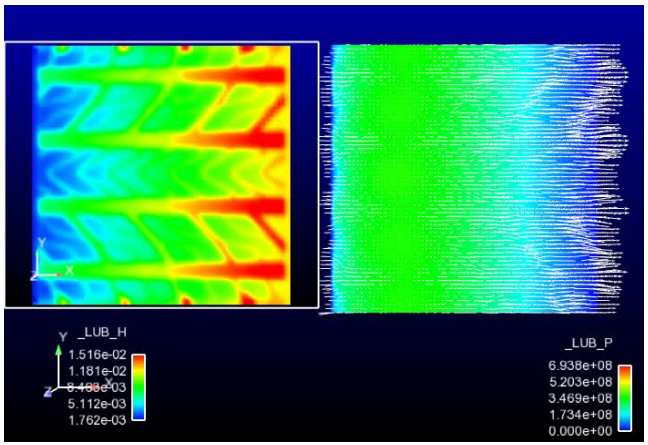
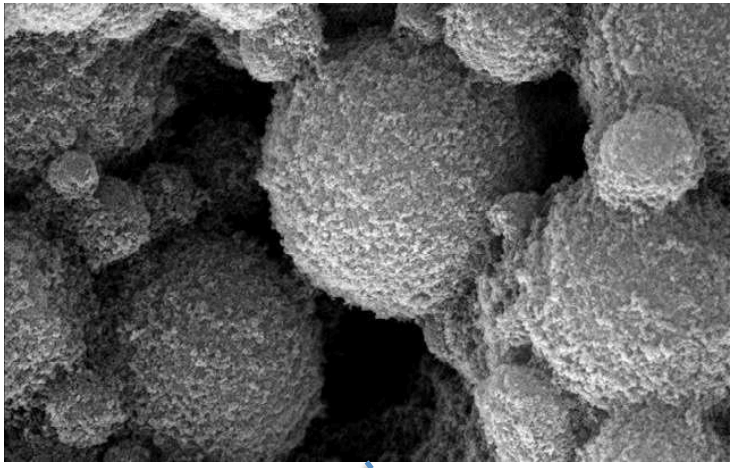
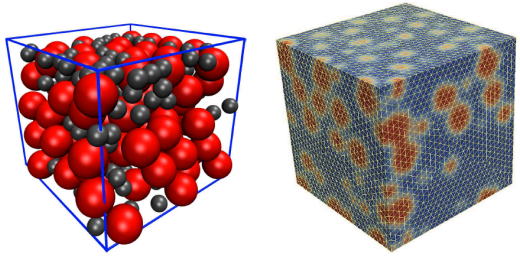
Examples: Application of Pattern-to-Mesh Tool: Rolling tire hydroplaning, Microstructure/property calculation



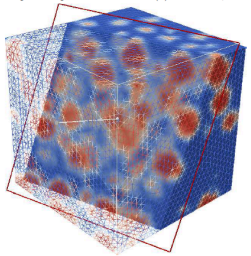


DEM-To Background Structured Mesh



(a) Disordered spherical particle pack

(b) FEM field, new voxel-to-mesh algorithm

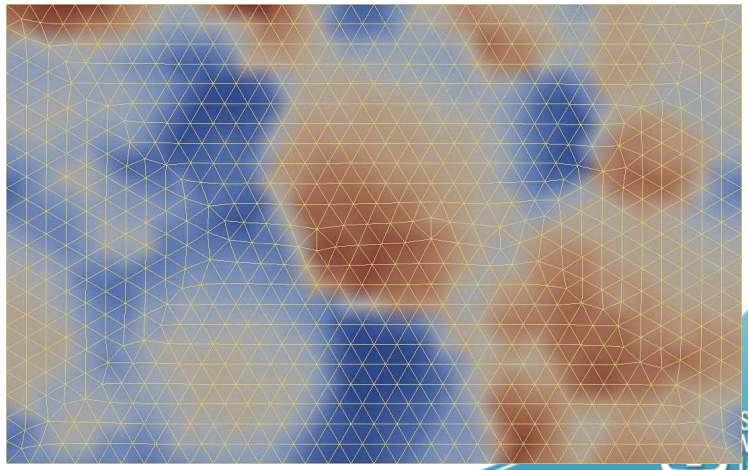


(c) FEM field, new voxel-to-mesh algorithm, view showing internal structure

Figure 2: 3-D pixel-to-mesh capability

BB

Tomographic Data-To-Mesh



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GOMA 6.0 Wrap-Up and Outlook

- GOMA 6.0 released under the GNU public license
- Third party library requirements: Trilinos 10.0 or higher, Sparse 1.3, SEAMS, other.
- State-of-the-Art Mod/Sim technology for a variety of manufacturing processes (liquid-based with solidification) exists within Sandia (GOMA)
- Support and training available

INFRASTRUCTURE STATUS—GOMA 6.0

ONGOING TRANSLATOR DEVELOPMENT

Post Processing

-PARAVIEW (available freely on web)

-ENSIGHT

-SEAMS and SEACAS

-Tecplot ? (translator available)

Pre-Processing

-ANSYS Workbench

-MSC Software-PATRAN (PATEXO)

-CSIMSOFT - CUBIT/Trelis (C

-I-DEAS ?? Bought out by someone.

-SOLIDWORKS/PRO-E geometries. Read these into CUBIT/Trelis

Platforms

LINUX/UNIX (Preferred flavor RedHat 6.0) –