COMPUTATIONAL MANUFACTURING AND MATERIALS LABORATORY GROUP RESEARCH THEMES

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February 4, 2019





- INDUSTRIAL GOAL: RAPID SIMULTANEOUS CONTROL OF DEPOSITION, LASERS/HEAT AND MATERIALS
- 2 3DP COMBINES: POSITIONING \leftrightarrow DEPOSITION \leftrightarrow HEATING \leftrightarrow FUNCTIONALIZED MATERIALS
- 3 MULTISTAGE PROCESSES: NEXT-GENERATION MACHINES NEED COMPUTATIONAL GUIDANCE!
- NEXT-GEN MACHINE (DMG MORI): https://www.youtube.com/watch?v=g8sT8ESfjrg
- RESEARCH COLLABORATORS: AHPCRC, APPLE, ARAMCO, ARL, AUTODESK, BASF, BOEING, DOE, FAA, LAWRENCE BERKELEY, LAWRENCE LIVERMORE, LOCKHEED-MARTIN, DMG-MORI, PEER, POWLEY FOUNDATION, SAMSUNG, SANDIA, SIEMENS, TOYOTA

DRIVER: LARGE-SCALE ADDITIVE MANUFACTURING AND FINE-SCALE 3D PRINTING WITH SPECIALIZED MATERIALS



MICRO-ELECTRONIC DEVICE













- DESIRED PROPERTIES: (1) ELASTIC (2) THERMAL (3) ELECTRICAL (4) MAGNETIC (5) OPTICAL ETC.
- KEY MOTIVATION: STRATEGIC/RARE MATERIAL REPLACEMENT WITH MICRO-DESIGNED MIXTURES
- KEY INGREDIENT: SPECIALIZED PROPERTY DESIGN-BY USE OF FINE-SCALE PARTICLES
- ULTIMATE OBJECTIVE: REDUCE PRODUCT DEVELOPMENT TIME AND COSTS THROUGH SIMULATION

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- KEY COMPONENTS:
- PART 1: DETAILED MODELING OF DYNAMIC DEPOSITION OF COMPLEX MIXTURES (DEM)
- PART 2: DETAILED MODELING OF LASER PROCESSING OF DEPOSITION (COMPUTIONAL OPTICS)
- PART 3: DETAILED MODELING OF CONTINUUM BEHAVIOR (DIGITAL/VOXEL-IMAGE COMPUTATION)
- PART 4: MACHINE-LEARNING EXTENSIONS (ARTIFICIAL NEURAL NETWORKS)
- INDUSTRIAL GOAL: RAPID SIMULTANEOUS CONTROL OF DEPOSITION, LASERS AND MATERIALS

PART 1: PLACEMENT OF PARTICLES: MANY APPROACHES TO GET THE PARTICLES INTO THE CORRECT LOCATION



- REGARDLESS OF POST-PROCESSING: CRITICAL FIRST STEP IS TO PLACE PARTICLES ACCURATELY
- METHOD 1: DOCTOR BLADE TO SMEAR PARTICLES-THEN HEAT/LASER (COMMON)
- METHOD 2: POUR FLUIDIZED/INK PARTICLES-THEN HEAT/LASER (COMMON)
- METHOD 3: SPRAY AEROSOLIZED/ATOMIZED PARTICLES-THEN HEAT/LASER (COMMON)
- METHOD 4: ELECTRICALLY GUIDE PARTICLES (MIXTURES)-THEN HEAT/LASER ACCURATE=FUTURE
- PROVIDES EXTREME FAULT-TOLERANCE (ROBOTIC ERROR COMPENSATION)
- ELECTRIFICATION AND CHARGING PRODUCES CONTROLLABLE FLUID-LIKE BEHAVIOR
- SECONDARY (BLUE) PARTICLES FUNCTIONALIZED THE MIXTURE FOR DESIRED PROPERTIES

COMPARISON: WITH AND WITHOUT TARGETED ELECTRIFICATION



INDUSTRIAL GOAL: RAPID SIMULTANEOUS CONTROL OF DEPOSITION, LASERS/HEAT AND MATERIALS
 3DP COMBINES: POSITIONING ↔ DEPOSITION↔ HEATING ↔ FUNCTIONALIZED MATERIALS
 MULTISTAGE PROCESSES: NEXT-GENERATION MACHINES NEED COMPUTATIONAL GUIDANCE!
 CRITICAL FIRST STEP IS TO PLACE PARTICLES ACCURATELY-THEN THERMALLY PROCESS

EXAMPLE: DETAILED DEM MODELING OF MULTIPHASE IONIZED MIXTURE DEPOSITION WITH ELECTRIC FIELD





- REPEATED, ACCURATE, CONSISTENT DEPOSITION IS POSSIBLE-LIKE ELECTROSTATIC COPIERS!
- DESPITE PLATEAU-RAYLEIGH-LIKE INSTABILITY
- CHARGE-INDUCED PSEUDO-SURFACE TENSION LEADS TO SURFACE-AREA MINIMIZATION



CONSISTENT TARGETED DEPOSITION IS ACHIEVABLE-ELECTRICALLY (AND ELECTROMAGNETICALLY)!





• Features are added by sintering, melting, vaporizing the materials.

LASER-BASED POST PROCESSING/FINISHING-MANY POSSIBILITIES





PART 3: CONTINUUM ANALYSIS OF DEPOSITED MATERIAL: DIGITAL/VOXEL-IMAGE VOXEL-BASED COMPUTATION



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 $\mathsf{DIGITAL/VOXEL}\ \mathsf{CONVERGENCE:}\ 41 \times 41 \times 41(206763DOF) \Rightarrow 61 \times 61 \times 61(680943DOF) \Rightarrow 81 \times 81 \times 81(1594323DOF)$



- DIGITAL/VOXEL-BASED COMPUTATION CAN BE INTERPRETED AS A VARIANT OF:
- FDTD-FINITE DIFFERENCE TIME DOMAIN METHOD:

https://en.wikipedia.org/wiki/Finite-difference_time-domain_method

IBM-IMMERSED BOUNDARY METHOD: https://en.wikipedia.org/wiki/Immersed_boundary_method

$\mathsf{DIGITAL/VOXEL}\ \mathsf{CONVERGENCE:}\ 41\times41\times41(206763DOF) \Rightarrow 61\times61\times61(680943DOF) \Rightarrow 81\times81\times81(1594323DOF)$



PDE-SOLUTION CONVERGENCE CLOSELY CORRELATES TO DIGITAL/VOXEL CONVERGENCE

RESIDUAL STRESS EVOLUTION DURING COOLING: DIGITAL/VOXEL-BASED COMPUTATION



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PART 4-MACHINE LEARNING EXTENSIONS: SYSTEM-WIDE ULTRAFAST SEARCH-ARTIFICIAL NEURAL NETS (ANN)



- FUNDAMENTAL: $OUTPUT = B(INPUT, W_1, W_2, ..., W_N)$ WHERE B IS "MIMICED" WITH AN ANN
- SYNAPSES: MULTIPLY INPUT BY A WEIGHT WHICH REPRESENTS INPUT'S RELEVANCE TO OUTPUT
- NEURONS: ADD OUTPUTS FROM ALL OF THE SYNAPSES AND APPLY AN "ACTIVATION" FUNCTION
- TRAINING: RECALIBRATE WEIGHTS FOR DESIRED OUTPUT \Rightarrow OUTPUT = $\mathcal{B}(INPUT, W_1, W_2, ..., W_N)$
- ULTIMATELY, ONE CONSTRUCTS A SYSTEM WITH OPTIMIZED WEIGHTS TO MIMIC A "BRAIN" (B)



MODELING AND SIMULATION INGREDIENTS:

- STAGE 1: DYNAMIC DEPOSITION PROCESSING SIMULATION: DISCRETE ELEMENT METHODS
- STAGE 2: RAPID LASER PROCESSING SIMULATION: COMPUTATIONAL OPTICS
- STAGE 3: CONTINUUM ANALYSIS OF DEPOSITED MATERIAL: DIGITAL/VOXEL-IMAGE COMPUTATION
- STAGE 4: MACHINE-LEARNING "WRAPPER": DEEP-LEARNING AND ARTIFICIAL NEURAL NETWORKS
- RESEARCH COLLABORATORS: AHPCRC, APPLE, ARAMCO, ARL, AUTODESK, BASF, BOEING, DOE, FAA, LAWRENCE BERKELEY, LAWRENCE LIVERMORE, LOCKHEED-MARTIN, DMG-MORI, PEER, POWLEY FOUNDATION, SAMSUNG, SANDIA, SIEMENS, TOYOTA



- Zohdi, T. I. and Wriggers, P. (Book, 2008) Introduction to computational micromechanics. Second Reprinting. Springer-Verlag.
- Zohdi, T. I. (Book, 2012) Electromagnetic properties of multiphase dielectrics. A primer on modeling, theory and computation. Springer-Verlag.
- Zohdi, T. I. (Book, 2017). Modeling and simulation of functionalized materials for additive manufacturing and 3D printing: continuous and discrete media. Springer-Verlag.
- **POSTED PAPERS**: http://www.me.berkeley.edu/faculty/zohdi/







EM-COMPOSITES

CHARGED SPRAYS



OPTICS



CELL GROUPS

SWARMS(BBC PHOTO)

EM-FABRIC

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LEFT: NASA'S EARTH OBSERVATORY (LANDSAT/MODIS/J. STEVENS)
RIGHT: NASA'S TERRA SATELLITE





- DYNAMICS: $m_i \frac{d\boldsymbol{v}_i}{dt} = m_i \boldsymbol{g} + \frac{1}{2} \rho_a C_D || \boldsymbol{v}_s \boldsymbol{v}_i || (\boldsymbol{v}_s \boldsymbol{v}_i) A_i$
- **THERMO:** $m_i C_i \frac{d\theta_i}{dt} = hA_i^s(\theta_s \theta_i) + \epsilon\beta A_i^s(\theta_s^4 \theta_i^4) + \gamma \frac{1}{2}\rho_a C_D ||\mathbf{v}_s \mathbf{v}_i||^3 A_i$

MANUFACTURING SAFETY: SPATIO-TEMPORAL FOOTPRINTS OF INCANDESCENT EJECTA



EXTENSIONS TO MULTIPLE ZONES-PROPAGATION OF EMBERS" "SPOTTING"









- THE ALGORITHM RAPIDLY HUNTS DOWN THE BEST MODEL "ON THE FLY"
- THE KEY: EACH SCENARIO-SIMULATION TAKES A FRACTION OF A SECOND
- CAN RAPIDLY TEST THOUSANDS OF SCENARIOS/PARAMETER SETS QUICKLY!



THE RISE OF QUADCOPTERS AND MAPPING STRATEGIES





EASE OF USE OF DRONES HAS LED TO DEVELOPMENT OF MULTIDRONE STRATEGIES FOR MAPPING

MODELING SWARMS: LARGE-SCALE BIOMIMICRY



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SWARM MODELING: TYPES OF INTERACTION



• DYNAMICS :
$$m_i \ddot{r}_i = \Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_i, ..., \mathbf{r}_n) = \Psi_i^{M-M} + \Psi_i^{M-T} + \Psi_i^{M-O}$$

• MEMBER : $\Psi_i^{M-M} = \sum_{k \neq i}^{n} \left(\left(\underbrace{\alpha_1^{M-M} || \mathbf{r}_i - \mathbf{r}_k ||^{\beta_1^{M-M}}}_{\text{attraction}} - \underbrace{\alpha_2^{M-M} || \mathbf{r}_i - \mathbf{r}_k ||^{-\beta_2^{M-M}}}_{\text{repulsion}} \right) \frac{\mathbf{r}_k - \mathbf{r}_i}{|| \mathbf{r}_k - \mathbf{r}_i ||} \right)$
• TARGET : $\Psi_i^{M-T} = \left(\alpha^{M-T} || \mathbf{r}_* - \mathbf{r}_i ||^{\beta^{M-T}} \right) \frac{\mathbf{r}_* - \mathbf{r}_i}{|| \mathbf{r}_* - \mathbf{r}_i ||}$
• OBSTACLE : $\Psi_i^{M-O} = -\sum_{j=1}^{q} \left(\left(\alpha^{M-O} || \mathbf{r}_{oj} - \mathbf{r}_i ||^{-\beta^{M-O}} \right) \frac{\mathbf{r}_{oj} - \mathbf{r}_i}{|| \mathbf{r}_{oj} - \mathbf{r}_i ||} \right)$

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1 USE CASES: Well-suited for nonconvex, nonsmooth, multicomponent, multistage systems

- **2 POPULATION:** Generate system population: $\Lambda^i \stackrel{\text{def}}{=} \{\Lambda^i_1, \Lambda^j_2, \Lambda^i_3, ..., \Lambda^i_N\} \stackrel{\text{def}}{=} \{\alpha_i, \beta_i ...\}$
- **3 PERFORMANCE:** Compute fitness/performance of each genetic string: $\Pi(\Lambda^i)$ and rank them (i = 1, ...)

4 MATING: Mate pairs/produce offspring:
$$\lambda^{i} \stackrel{\text{def}}{=} \Phi^{(l)} \Lambda^{i} + (1 - \Phi^{(l)}) \Lambda^{i+1}$$
 where $0 \leq \Phi \leq 1$

- 6 ELIMINATION: Eliminate poorly performing genetic strings, keep top parents, top offspring
- **6** NEXT GENERATION: Repeat the process with the new gene pool and new random genetic strings
- POST-PROCESSING: Employ gradient-based methods afterwards in the local "valleys"-if smooth enough













MORE SOPHISTICATED CONTROL: SWARM SELF-ORGANIZATION-SEARCHING MULTIPLE SITES



- EXAMPLE-DESIGN VARIABLES: INTERACTION PARAMETERS= α_i , β_i , i = 1, ..., N
- STARLINGS (STURNUS VULGARIS): INTERACT WITH SPECIFIC MEMBERS
- ANOTHER CASE: INTERACTION WITH EVERY OTHER SWARM MEMBER
- ANOTHER CASE: INTERACTION WITHIN A COMMUNICATION RADIUS
- ANOTHER CASE: INTERACTION WITHIN A VISUAL FIELD
- THE KEY IS TO TRANSLATE BEHAVIOR INTO EQUATIONS

MODEL PROBLEM: CHASING A MOVING TARGET



• $T_x = x_0 + a_1 \cos(a_2 t) + a_3 t$, $T_y = y_0 + b_1 \sin(b_2 t) + b_3 t$, $T_z = z_0 + c_1 \cos(c_2 t) + c_3 t$

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AGENT-BASED COMPUTATION: POPULATION DYNAMICS



- BASIC GROWTH: $P(t + \Delta t) = \lambda P(t) \rightarrow P(t + \Delta t) P(t) = (\lambda 1)P(t) \rightarrow P(t) = P(0)e^{(\lambda 1)t} = P(0)e^{(b-d)t}$
- **PARAMETERS:** $\lambda = 1 + b d$ WHERE BIRTHRATE=b DEATH RATE=d
- COUPLED: $\dot{P}_1 = rP_2 \tau P_1$ AND $\dot{P}_2 = aP_1 \gamma P_2$
- OUTCOMES: $\dot{P}_1 = rP_2 \tau P_1 > 0$ AND $\dot{P}_2 = aP_1 \gamma P_2 > 0$
- LIKELY SCENARIO: (1) MASS FATALITIES (2) ENCLAVES (3) BOUNDARY EVOLUTION
- CHARACTERISTICS: (1) REPORODUCTIVE RATES (2) LIFESPANS (3) COMBAT SKILLS (4) MOBILITY



• CONFLICT RADIUS:
$$||r_i^{(1)} - r_j^{(2)}|| \le d_{ij}^{(1-2)}$$

• SUPPORT-1: $||r_i^{(1)} - r_j^{(1)}|| \le s_{ij}^{(1-1)}$ and support-2: $||r_i^{(2)} - r_j^{(2)}|| \le s_{ij}^{(2-2)}$

• **PROPORTIONS:**
$$\phi_1 = \frac{p_1}{p_1 + p_2}$$
 AND $\phi_2 = \frac{p_2}{p_1 + p_2}$

- STEP 1: SET POPULATION PARAMETERS
- STEP 2: GENERATE INITIAL LOCATIONS
- STEP 3: CHECK FOR CONFLICTS
- STEP 4: COMPUTE SURVIVORS
- STEP 5: COMPUTE BIRTHS AND DEATHS
- STEP 6: UPDATE AGES
- STEP 7: REPEAT STEPS 2-6

AGENT-BASED COMPUTATION: POPULATION DYNAMICS-GLOBALLY-DISPERSED



AGENT-BASED COMPUTATION: POPULATION DYNAMICS-INITIALLY ISOLATED



MODELING DISEASED RED BLOOD CELL (RBC) DETECTION



- GOAL: RAPID NON-INVASIVE TESTING
- COLLABORATOR: F. KUYPERS (OAKLAND CHILDREN'S HOSPITAL)

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DISEASED RED BLOOD CELL GALLERY



- SHAPE-RELATED R-B CELL DISORDERS/IMPAIRED FUNCTION
- EXCESSIVE RED CELL DESTRUCTION OCCURS
- Cells removed prematurely by the spleen \Rightarrow anemia

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- RED BLOOD CELLS TRANSPORT OXYGEN AND CARBON DIOXIDE
- SICKLE-CELL ANEMIA IS PREVALENT IN 0.03 0.05% OF POPULATION
- HIGHER IN AFRICAN, MEDITERRANEAN AND ASIAN ANCESTRY POP.
- GOAL: RAPID NON-INVASIVE TEST TO DETERMINE DISEASED CELLS

HIGH-FREQUENCY OPTICAL APPROACHES FOR LIGHT PROPAGATION



- COMPUTE RAY REFLECTIONS (FRESNEL RELATIONS)
- 2 COMPUTE ABSORPTION BY CELLS
- INCREMENT RAY POSITIONS FORWARD

EXPERIMENTAL RESULTS FOR ENERGY PERCENTAGE



CELLS	6 ENERGY: # 1	ENERGY: # 2	ENERGY: # 3	ENERGY: # 4
1650	0.97390	0.96450	0.96700	0.96760
4090	0.88700	0.85700	0.88230	0.87580
6510	0.85700	0.86390	0.83370	0.86710
8100	0.75300	0.70050	0.77650	0.70900



CELLS	ENERGY
1000	0.97501
2000	0.92201
4000	0.87046
8000	0.76656

MODELING BALLISTIC FABRIC SHIELDING





• Applications: ballistic fabric such as KEVLAR, ZYLON and biological tissue

EXPERIMENTAL FACILITIES AT UC BERKELEY









• Pneumatic (nitrogen) gun, breech and barrel set up. ZYLON samples.

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- The yarn remain straight, undergoing a homogeneous stress state
- The forces only act along the length of the yarn
- The joint connections produce no bending or moments
- The yarn do not buckle
- The yarn do not slide relative to one another ("combing")





- SECOND PIOLA-KIRCHHOFF STRESS: $S = \mathcal{F}(U = \frac{L}{L_{\alpha}}) = \alpha I E^{\gamma} E$
- GREEN-LAGRANGE STRAIN: $E = \frac{1}{2}(U^2 1)$

• FORCE:
$$\Psi = USA_o = \frac{L}{L_o}SA_o$$

• DAMAGE:
$$\alpha(t) = \min\left(1, \alpha(0 \le t^* < t), \frac{(exp(-\lambda(U(t) - U_{crit})) - exp(-0.03\lambda))}{(1 - exp(-0.03\lambda))}\right)$$

• DAMAGE PARAMETER RESTRICTION: $0 \le \alpha(t) \le 1$



- Move the fabric node to the closest point on the projectile's surface (there are a variety of algorithms to perform this operation).
- Compute contact forces from the interpenetrated (predictor) position and the corrected position (the difference is denoted the "gap").
- If there is friction, then a stick condition is assumed, then the friction force is checked against the static limit which, if violated, enacts a sliding friction force.



- NODAL DYNAMICS: $m_i \dot{v}_i = \Psi_i^{tot} = INTRA-YARN + EXTERNAL FORCES$
- COUPLED SYSTEM: $v_i(t + \Delta t) = v_i(t) + \frac{\Delta t}{m_i} \left(\phi \Psi_i^{tot}(t + \Delta t) + (1 \phi) \Psi_i^{tot}(t) \right)$

• \Rightarrow $\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t + \phi \Delta t) \Delta t = \mathbf{r}_i(t) + (\phi \mathbf{v}_i(t + \Delta t) + (1 - \phi) \mathbf{v}_i(t)) \Delta t$

• SOLVED ITERATIVELY (IMPLICITLY) WITH TIME-STEP ADAPTATION

AN IMPACT SEQUENCE FOR A SHEET-CONTACTOR PAIR



- COMPUTE DISPLACEMENTS/CONTACT
- COMPUTE YARN STRETCH
- COMPUTE FIBRIL RUPTURE
- COMPUTE CONTACTOR POSITION
- IF TOL MET, INCREMENT TIME
- IF TOL NOT MET, REDUCE TIME STEP





- $m\dot{v} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$
- COMPONENT FORM:

$$\dot{v}_1 = rac{q}{m}(E_1 + (v_2B_3 - v_3B_2))$$

$$\dot{v}_2 = rac{q}{m}(E_2 - (v_1B_3 - v_3B_1))$$

$$\dot{v}_3 = rac{q}{m}(E_3 + (v_1B_2 - v_2B_1))$$

- CHOOSE THE COMPONENTS OF B FOR THE DESIRED EFFECT
- INDUCES HELICAL MOTION ⇒ HARNESSED FOR TUMBLING
- MAGNETIC EFFECTS \Rightarrow TURNING RADIUS = R = $\frac{m||\mathbf{v}||}{|q|||\mathbf{B}||}$
- *KEY EFFECT: ROTATION TIME= $\frac{R\theta}{||\mathbf{v}||} = \frac{m\theta}{|q|||\mathbf{B}||} = \underline{VELOCITY-INDEPENDENT}$



ELECTROMAGNETIC FABRIC SHIELDS: HARNESSING LORENTZ FORCES



- PROJECTILE PUSHES CHARGED FABRIC INTO MAGNETIC FIELD
- THIS INDUCING ROTATION VIA THE CONTACT FORCES
- FABRIC DYNAMICS: $m\ddot{r}_i = \underbrace{\Psi_i^{tot}}_{i} = \underbrace{\Psi_i^{nn}}_{i} + \underbrace{\Psi_i^{con}}_{i} + \underbrace{\Psi_i^{fric}}_{i} + \underbrace{q_i(E_i + v_i \times B_i)}_{i}$

total yarn contact friction electromagnetic forces

COMPARISON: REGULAR AND "ELECTROMAGNETIC" FABRIC SHIELDS





• PATENT: T. I. Zohdi. US Application No. 61/313,058

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