Multiscale/3D Printing Cement Workshop

Combined Multiscale Modeling and Additive Manufacturing Enabling Tools for the Engineering of Novel Infrastructure Materials

Vanderbilt University, July 16-17, 2015

Workshop Organizers: F. Sanchez (Vanderbilt Univ.), Joe Biernacki (Tennessee Technological Univ.), Jan Olek (Purdue Univ.), and Pablo Zavattieri (Purdue Univ.)

Funding: National Science Foundation CMMI 1239979

Credit: Joe Biernacki

1. Workshop objectives and rationale

Following the US-Poland MCMoCM2012 workshop on multiscale modeling of cementitious materials and in view of the need for new approaches to integrated modeling and experimental strategies bridging length and time scales as well as new design paradigms and innovations in cements and concrete, the goal of the workshop was to **explore the promising potential of additive manufacturing** as (i) a **prototyping tool** in support of multiscale computational modeling for enhancing existing infrastructure materials, or even creating novel infrastructure materials with built-in multifunctional responses and resilience from the bottom-up as well as (ii) a **guiding tool** for the modeling efforts by offering insights to potential future required properties of materials.

The specific objectives of the *Multiscale/3D Printing workshop* were to:

1. Foster the exchange of ideas and knowledge between experts from different fields that use 3-D printing and computational modeling as tools for the creation of novel materials and interfaces;
2. Provide a forum for the world's leading experts on computational materials science of cement and concrete, computational mechanics, multiscale materials modeling, and experimentalists in cement chemistry, nano/microstructure, mechanical properties, and durability along with experts in additive manufacturing to identify opportunities and challenges for 3D printing of infrastructure materials; and,
3. Identify potential opportunities related to combining advanced material modeling with additive manufacturing in the area of infrastructure materials.

2. Workshop description and activities

The *Multiscale/3D Printing Cement* workshop was held on July 16-17, 2015 at Vanderbilt University, Nashville, TN. The workshop was a two-day meeting that engaged participants in discussions on key aspects of the integration of multiscale computational modeling and additive manufacturing as tools for creating and testing the next generation of infrastructure materials. The two-day activity included a day of invited talks on the workshop's four thematic areas: (i) Cement Microstructure Modeling, (ii) Additive Manufacturing Processes and Fabrication Strategies, (iii) Additive Manufacturing and Advanced Modeling as Tools for Engineering Materials and (iv) 3-D Printing of Cement-based materials, followed by a series of sessions designed to focus on key scientific hurdles in the path to widespread commercialization of additive manufacturing of cement-based materials.

Day 1 of the workshop consisted of eight (8) invited keynote presentations followed by technical discussions. The keynote presentations provided an overview and examples of the combined usage of additive manufacturing and multiscale modeling for creating novel materials and interfaces from different fields of research (e.g., biomedical, materials science, biomimetic, and aerospace). In addition, a state of the art review of multiscale modeling of cement-based materials was provided along with current status and challenges of 3D printing of concrete. The following is the list of the keynote presentations:

- ***Integrated Computational Materials Science and Engineering, Materials Genome, and Concrete*** (Edward Garboczi, National Institute of Standards and Technology)
- ***Coupling Manufacturing, Mechanics and Materials Design in Additive Manufacturing*** (Jian Cao, Northwestern University)
- ***CAD and 3D Printing of Patient-Specific Skeletal Implants, Fixation, and Surgical Tools*** (David Dean, Ohio State University)
- ***An Overview of Additive Manufacturing Activities at NASA Marshall Space Flight Center*** (Tracie Prater, NASA Marshall Space Flight Center)
- ***Modeling and Simulation Challenges in Materials Design for Additive Manufacturing Applications*** (Wing Kam Liu, Northwestern University)
- ***Combined 3D Printing and Multi-scale Modeling for the Development of Biomimetic Materials*** (Pablo Zavattieri, Purdue University)
- ***A Materials Science Approach to 3D Printing with Cementitious Materials*** (Henri Van Damme, MIT)
- ***ORNL's Experience with 3D Printing using Cementitious Materials*** (Catherine Mattus, Oak Ridge National Laboratory)

Day 2 of the workshop was focused on discussions of key scientific aspects for the development of additive manufacturing of cement-based materials and was organized around the following four (4) topics: (i) Topic 1: Cement Formulation, (ii) Topic 2: Microstructure/3D Printing Relationships, (iii) Topic 3: Modeling as tool for Engineering and Predicting the Material Properties, and (iv) Topic 4: 3D Printing Technology. The workshop participants were divided into four working groups that rotated through the four breakout session topics as shown in Figure 1.

Topic	8:50 - 9:35 am	9:45-10:30 am	10:50-11:35 am	11:45 am -12:30 pm
T1. Cement Formulation	Group 1	Group 4	Group 3	Group 2
T2. Microstructure/3D Printing Relationships	Group 2	Group 1	Group 4	Group 3
T3. Modeling as Tool for Engineering and Predicting the Material Properties	Group 3	Group 2	Group 1	Group 4
T4. 3D Printing Technology	Group 4	Group 3	Group 2	Group 1

Group 1 - Room FGH 136
T1 – Lead: K. Wang
T2 – Lead: E. Garboczi
T3 – Lead: S. Guelcher
T4 – Lead: R. Bohan

Group 2 - Room FGH 200
T1 – Lead: A. Daugherty
T2 – Lead: Z. Grasley
T3 – Lead: S. Rouzbeh
T4 – Lead: S. Shah

Group 3 - Room FGH 313
T1 – Lead: D. Kuehn
T2 – Lead: G. Cusatis
T3 – Lead: J. Nyman
T4 – Lead: T. Prater

Group 4 - Room JH 273
T1 – Lead: K. Sobolev
T2 – Lead: L. Wing
T3 – Lead: J. Dolado
T4 – Lead: G. Sant

Moderators
T1: Joe Biernacki
T2: Florence Sanchez
T3: Pablo Zavattieri
T4: Jan Olek

Figure 1. Breakout sessions.

3. Workshop participants

The workshop brought together 32 individuals from a broad range of disciplines and backgrounds including Biomedical, Civil, and Chemical Engineering; the Federal Highway Administration (FHWA); NASA; the National Institute of Standards and Technology (NIST); and industry (Table 1).

Table 1. List of 3D Printing Cement Workshop participants.

Name	Affiliation	Expertise	Role
Biernacki, Joe	Tennessee Technological University	Cement hydration	Co-organizer
Arango, David Restrepo	Purdue University	Graduate student	Participant
Ashraf, Warda	Purdue University	Graduate student	Participant
Betts, Jeremy	Essroc – Italcementi Group	Head of Technical Service Department for Essroc Italcementi Group	Participant
Bohan, Richard	Portland Cement Association	Director, Manufacturing Technology	Participant
Brown, Lesa	Vanderbilt University	Graduate student	Participant
Cao, Jian	Northwestern University	Manufacturing processes and systems	Keynote Speaker
Chaudhari, Ojas	Tennessee Technological University	Graduate student	
Cusatis, Gianluca	Northwestern University	Mechanics of infrastructure materials	Participant
Daugherty, Ann	ACI Foundation	Director	Participant
Dean, David	Ohio State University	Bone tissue engineering	Keynote Speaker
Dolado, Jorge	Labein-Technalia, Spain	Materials engineering	Participant
Garboczi Ed	NIST	Cement microstructure modeling	Keynote Speaker
Gonzalez, Raquel	Vanderbilt University	Post-doctoral researcher	

Grasley, Zach	Texas A&M	Mechanics and thermodynamics of concrete	Participant
Guelcher, Scott	Vanderbilt University	Polymeric biomaterials for bone tissue engineering	Participant
Kuehn, David	FHWA - Exploratory Advanced Research (EAR) Program	Program Manager	Participant
Liu, Wing	Northwestern University	Multiscale computational materials design for additive manufacturing	Keynote Speaker
Lu, Luna	Purdue University	High performance biocomposites for civil infrastructure applications	Participant
Mattus, Catherine	ORNL	Materials chemistry	Keynote Speaker
Nyman, Jeffry	Vanderbilt University	Bone biology	Participant
Olek, Jan	Purdue University	Concrete material and technology	Co-organizer
Prater, Tracie	NASA Marshall Space Flight Center	Materials and processes	Featured Speaker
Reches, Yonathan	Vanderbilt University	Graduate student	
Sanchez, Florence	Vanderbilt University	Chemo-mechanical behavior of cement-based materials	Co-organizer
Sant, Gaurav	Univ. of California, Los Angeles (UCLA),	Sustainable low-CO_2 foot-print materials for infrastructure construction applications	Participant
Surendra, Shah	Northwestern University	Connecting microscopic behavior to structural response of concrete	Participant
Shahsavari, Rouzbeh	Rice University	Atomistic modeling; Multi-scale modeling:	Participant
Sobolev, Konstantin	University of Wisconsin-Milwaukee	High-performance cement based composites, application of nanomaterials in construction	Participant
Van Damme, Henri	MIT	Physical chemistry and statistical physics of geomaterials	Keynote Speaker
Wang, Kejin	Iowa State University	Material properties and durability of portland cement concrete	Participant
Zavattieri, Pablo	Purdue University	Solid mechanics applied to the multiscale modeling of advanced and innovative engineering materials	Keynote Speaker

4. Results and key outcomes

Press releases on the workshop can be found at:
http://engineering.vanderbilt.edu/news/2015/experts-address-promises-and-problems-of-3d-printing-large-structures/
and,
http://ceramics.org/ceramic-tech-today/solid-processes-acers-members-lead-workshop-on-3-d-printing-of-cement-based-materials

The outcomes of the meeting include a list of technology advantages and research specific challenges that come along with additive manufacturing of cement-based materials. Among the most significant technology advantages (as compared to traditional portland cement concrete) identified are: (1) the additive approach enables the inclusion of all manner of co-printed reinforcements and control of reinforcement-matrix interfaces unimaginable with traditional casting or extrusion methods, thus, effectively redefining what a reinforcing element can be; (2) printing enables localized control of chemistry, process conditions (temperature and shear rate, etc.) and microstructure of the material; (3) highly localized control of shear could enable preferential alignment of inclusions (aggregate); (4) printing enables the designer to utilize a hierarchy of structures and patterns with much greater control and over a broader range of length-scales; and (5) the potential to eliminate the need for conventional formwork.

Along with these technological advantages, the workshop participants recognized key research challenges including: (1) vastly different liquid to solid transition (e.g. gelation) requirements; (2) a shift from a Bingham dominated rheology (traditional portland cement concrete) to a shear-thinning dominated domain; (3) deposition rate and filament scale dependent mix formulations; (4) introduction of vast numbers of inter-filament (between printed elements) interfaces; (5) the redefined nature of inclusions including reinforcing elements and aggregates and their associated interfaces (intra-filament boundaries); (6) the current knowledge about cement hydration, rheology and the linkage between the same and models of the same is very incomplete; and (7) printing machines and technology must be co-developed along with mix formulations and hierarchical design strategies since these factors are mutually dependent. While other technology advantages and technological hurdles were enumerated, these represent the broad, overarching outcomes of the workshop. Among these, the following items were ranked as high priority research topics to further the development and transformation of 3-D printed cement-based materials: (1) define cement system formulations with suitable properties (hydration rates, rheology, and gelation) for printing; and (2) understand the role of interfaces between elements within printed filaments and between printed filaments.
The following is a summary of the main discussion points and outcomes from each topical session.

Topic 1. Cement Formulation (Moderator: J. Biernacki, Tennessee Tech. Univ.)

1. What type of binder system do we imagine, e.g. polymer augmented, polymer loaded, ultra-fine aggregate, ultrafine cement particulate, existing or new chemical and mineral admixtures, etc.?
    - No longer confined to the Portland Cement (PC) paradigm – potential use of non-Portland (e.g. absence of gypsum), inorganic or mineral based (e.g. geopolymer), non-hydraulic - ALL BINDERS can be used. To be creative, need to shed the PC paradigm.
    - Binder system driven by application.
    - Role of time-scale in developing stiffness and strength will drive binder selection and composition.
    - Mineral-based, rather than polymer (volume demand, energy, sustainability, and cost).
2. What rheological properties must we achieve and how will we produce them?

- Depends on method of deposition.
  - Liquid deposition must control the liquid to solid transition (e.g. gelation)
  - May not pre-mix – use of multiple nozzles
- Rheology might not be a major challenge as pumpable concrete is already available.
- An important parameter of consideration is the set point of the cement. Flow behavior, especially thixotropy is also an important property for 3D printing (vs. yield stress and viscosity for traditional concrete).
- Clays, nano/microfibers, viscosity modifying admixtures (VMA) can be used to improve concrete thixotropy and shape-holding behavior.
- Highly reactive, ultrafine, and nano-sized materials can help control the rate of binder hydration and concrete setting.
- Cement chemistry can be engineered to remove the induction period.
- Rheology must control the dispersion of fibers, stabilization of the constituents in the microstructure.
- Particle packing, admixtures/polymers may play more important roles in rheology and hydration of 3D printing concrete.
- Removing the formwork is one of the greatest advantage of AM and is expected to provide design freedom.

3. What level of reactivity must we have or what relationship between rheological properties and reactivity must we achieve, i.e. how fast must the printed materials set relative to how fast they will flow and under what conditions?
   - Depends on method of deposition.
     - Liquid deposition must control the liquid to solid transition (e.g. gelation)
     - May not pre-mix – multiple nozzles
4. Can we (do we have a vision for how we might) alter the properties, e.g. chemical composition of cement, type of aggregate included, etc., as a function of printer location, i.e. continuously or in pulses?
   - 3D printing allows to blur the line between masonry and traditional concrete placement.
   - Printing of reinforcements (fibers, etc.).
   - Self-sustaining mineral structure that can be "fired" – vitrified by layers (laser, microwave); heat transfer between layers.
   - Alter bond between printed layers.
   - Addition of sensors and other smart materials for multifunctional concrete.
5. What has been achieved in terms of set and rheology with other high solids printing processes?
   - See literature on metals and ceramics.
6. What opportunities are there to draw upon the existing base of knowledge, e.g. reactive powder cements (RPC), geopolymer cement, macro-defect-free cements (MDF Cements), silica fume addition, use of fine limestone, etc.?
   - 3D printing allows use of these materials without previous process constraints.
   - Micro or nano deposition.
   - Modification with 3D printing for existing structure (printed, repair, etc.)
   - Control of interfaces (a subset of inhomogeneity).
7. How will aggregate requirements, size and shape, challenge printing technology and will the printing technology place constraints on the type of aggregates that can be used?

- Aggregate size is related to scale of what to print, depending upon the applications (floor boards, shear wall, building, etc.)
- Aggregate size will control the nozzle size.
- Solvable if we change the preconception of what an aggregate is and that it has to be pre-mixed.
- Robotically placed "aggregate" (think about century old dam structures)
- Printing aggregates? Printing binder free? (e.g. compacted fly ash, recycled concrete ground and pressed)

8. What role will multiscale modeling affect mix design/cementitious matrix?
   - Top down optimization of the bottom up constraints. Define constraints of materials properties, optimization model dictates what you need, then model the microstructure, then model the mix design.
   - Bottom up starting with the constituent materials, rheological modeling, constitutive modeling, structural design (Monte Carlo simulation).

Topic 2. Microstructure/3D Printing Relationships (Moderator: F. Sanchez, Vanderbilt Univ.)

1. What opportunities and challenges exist to control the microstructure of cement-based materials by 3D printing?

   Opportunities

   - Probably can use 3d printing technology to control milli-structure rather than microstructure. Perhaps new technology would allow control of microstructure in pastes.
   - Aligned fibers, controlled orientations, spatially varying.
   - Multiple nozzles, or time-variant deposition.
   - The temperature of the nozzles can be varied at different locations to have different microstructures.
   - Multiple nozzles can provide the benefit of mixing 10~12 ingredients with varying proportions in different layers.
   - Have varying w/c, mixture proportions, etc. with position.
   - Functionally graded structure.
   - Since we could mix at the nozzle, no need for dormant period. Could use flash set (no gypsum) for early structural stiffness.
   - Can use variable temperature at the nozzles that will change the hydration rate.
   - Ultra-fine cements, ultra-low w/c (low viscosity), high-heat of hydration.
   - Much higher degree of uniform dispersion for various additives (e.g., nanotubes, nanosilica, etc.).
   - Sequestering $C0_2$ by sequential spraying of layers.

   Challenges

   - Control of curing on surface (no forms).
   - Important factors of consideration are the surface chemistry between two layers of cement and maintaining proper bonding between the two layers.
   - Retaining the form and shape during printing.
   - Consistency of replicates.

- If the microstructure is varied between layers then real time sensing will be required for quality control purpose.

2. What reasonable resolution can be attained for cement-based materials using 3D printing?
    - Resolution of printing is related to particle sizes.
    - ~100 microns for fine cement paste
    - Mortar: mm
    - Concrete: cm
3. What type of internal microstructural features can be achieved for cement-based materials with 3D printing? For example, can patterned surface chemistry be realized?
    - Can use strong / dense microstructure at the bottom of the structure and less dense at the top of the structure.
    - A more uniform pore size distribution might be achievable.
    - Air entrainment could be controlled between different layers.
    - Bond control.
    - Coatings.
    - Multiple nozzles can be used to control the reactivity. With multiple nozzles it will also be possible to have variation between layers (i.e. w/c ratio).
4. How can 3D printing be used to alter and control the local microstructure of cement-based materials to meet desired local material properties?
    a. *What are the printing parameters during fabrication that should/can be altered?*
        - Rate, direction, different nozzles, nozzle size/geometry

    b. *What are the challenges related to the cement hydration process?*
        - Curing, but could use $C0_2$, other sprayed gases or sprayed/printed coatings

    c. *Can we manipulate the 3D printing process to precisely control the cement phase assemblage and structure on a nano/microscopic scale?*
        - Functionally graded chemistry (e.g., low CH at ITZ) and high pH cement at steel.

    d. *Can we specify location specific phase composition and structure?*
        - Can closely control interfaces for improved bond.

    e. *What are the challenges in controlling the microarchitecture (i.e., pore size)?*

    f. *What are the challenges in obtaining a high density packing microarchitecture?*
5. What are the opportunities and challenges in manufacturing pre-designed multifunctional microstructures where the material properties (e.g., mechanical, thermal, electrical) vary gradually?
    - Blurs line between masonry and conventional concrete by allowing robotic placement of large inclusions. Might reduce cement content.
    - Ability to print the reinforcement with the matrix. Perhaps long fibers deposited in real time by separate nozzle.
    - Printing embedded sensors.
    - Challenge: Unintended anisotropy (printing direction effects) or opportunity: intended anisotropy.
6. What dramatic changes could be made to pre-existing notions of how cement-based materials must be printed?
    - Print polymer skeleton that can serve as form/reinforcement, spray cementitious material.

    - Skeleton could be resorbable (pathways for plumbing, electrical, etc.).
  - Printing pavements?
    - Surface layers or through depth control of properties.
    - Embedded sensors.
  - Repair existing structures or pavements (e.g. potholes) by spraying – Could control thickness, embed sensors, fibers, etc. Could scan surface using imaging technology.

Topic 3. Modeling as Tool for Engineering and Predicting the Material Properties (Moderator: P. Zavattieri, Purdue Univ.)

1. What kind of modeling capabilities can we borrow from the existing body of knowledge in cement modeling? (in terms of multiscale, atomistic, nano-, micro- and mm-scale modeling)
   - In general, all can be utilized, including atomistic modeling for better interfacial interactions, and larger-scale modeling.
2. What are the more important gaps in current cement modeling that are still valid for 3D printing?
   - Microstructure modeling.
   - Rheological modeling.
   - Modeling of phase transition: liquid-to-solid transition.
   - Modeling of early stage aging.
   - Connection between scales.
   - Limited thermo-kinetic data for the setting reaction. Reaction mechanisms are not known in detail. Development of new design tool using thermo-kinetic data is required. Such model will be ultimately useful for designing the nozzle and overall printer design.
   - Current models cannot be used as design tools because fluid and solid (set) models cannot be connected. Not flexible to handle changes in materials or reaction mechanisms.
3. What are the main gaps that are only intrinsic of the 3D printing process?
   - Expanding current knowledge on rapid setting.
   - Modeling for new mixing processes at the nozzle.
   - Modeling residual stresses caused by printing.
   - Modeling spatial variation of ages. Large variations in the materials also need to be incorporated in the models.
   - Relating hydration kinetics to printing processes.
4. What new challenges do we face because of
   a. *The 3D printing process itself*
      - Need new collaboration with control, robotics community.
   b. *The curing process*
      - See question 2.
      - The chemistry is not well understood in detail for many systems. Models must be able to account for changes in the formulation (relative amounts of each component). Simulations need to address interactions between components. Large variety of materials used to formulate the cements. Simulations must address interactions between layers and bonding between each layer. Composite materials (cement with metal or other components)?
   c. *The fact that 3D printing will enable the fine control of geometrical features at very small scales*

- Need more consistent paste (lower cement size, smaller sand, narrower particle distribution, etc.)
- Fine control over the length scale of 0.5 mm, but in general resolutions required are about an order of magnitude greater than other applications.

d. *The fact that 3D printing will enable the new combination of cement with other materials to create novel microstructures*
   - Collaborating with the polymer and metal community.
   - Creating bio-inspired, multi-functional composites made of cement, polymers, metal, electronics, etc.

e. *Structural design requires new paradigms/methods*
   - Topology (vs. heterogeneity) optimization of the microstructure and structure at larger scales with the given loads.

f. *Modeling sustainability with 3D printing of materials*

5. Will the following aspects of 3D printing of cement be more critical now to motivate, accelerate and provide more resources for the development of better models?
   a. *Mixing* (Priority 1).
   b. *Rheology/flow of cement* (Priority 1).
   c. *Hydration process* (Priority 1).
   d. *Maturity* (Priority 1).
   e. *Shrinkage* (Priority 2).
   f. *Interfaces (e.g., between layers of cement of different ages, or between layers of different materials)* (Priority 1).
   g. *Microcracking* (Priority 2).

6. Can modeling be used to predict, design and optimize
   a. *Process control parameters*
   b. *Geometry*
   c. *Right combination of materials for given structural requirements*
   d. *Interfaces*
      - Rapid screening of range of process parameters and materials
   e. *Modeling totally new (non-hydraulic, non PC) cement*

7. Can we borrow from the existing body of knowledge on topology / microstructural optimization and/or biomimetics to design new materials with novel combination of properties that break the traditional material design paradigms?
   - Cement has the advantage of many different types of materials (many formulation options). There is no database of material properties that could be easily used in the models. Multi-component composition is an advantage – many parameters could be adjusted to optimize properties. Models as design tools could be used to identify formulations that optimize properties.

Topic 4. 3D Printing Technology (Moderator: J. Olek, Purdue Univ.)

1. What are the unique requirements for the 3D printing technology as applied to additive manufacturing of cement-based infrastructure materials?
   - Aging issue (evolving rheology), which is not seen for other materials used in AM.
   - Capability to provide reinforcement (directly from 3D printing or after).

- Mechanics of mixing (admixtures, additives, fibers, etc.) and the technology to mix and deliver the materials. Shotcrete uses a similar process.
- Printing of large size elements.

2. What amount of scaling-up (i.e. the size of the 3D printed object) will be required to verify (quantify) the design principles and modeled properties of the infrastructure materials?
    - Do staging study. Understanding from the smallest scale and build foundations until reaching the higher scale.
    - Scaling of fabrication methods. -> For higher structures it may be required larger speeds or larger nozzles. Have several printers at the construction site.
    - It may be necessary to model the construction process (like in CNC process but considering the entire structure).
    - Building up individual layers presents unique issues. Some layers will generate heat and evaporable water while others might absorb heat or evaporable water. This would depend on where the layer is located within the overall structure.

3. What are the specific research and technological directions that need to be undertaken with respect to development of economical and robust solutions for 3D printing of cement-based infrastructure materials? What are the technological limitations?
    - Modeling of the construction process.
    - Build-up from experience in extrusion process, shotcrete, Hatcheck process (composite cement boards).
    - Modeling of the structure system (looking for more economical solutions).
    - Ability to reduce or replace Portland cement.
    - Control inhomogeneity, e.g. different compositions can be printed (elimination of joints).
    - Real time control (feedback) for printing conditions (air, surface topography, humidity, etc.)
    - Integration of individual elements in building will be important. Individual layers may have different reaction rates depending on heat emission from adjacent layers. Thermal history of each layer will be important.
    - Hardware must be robust enough to handle the abrasive materials used in concrete formulations.

4. Are there any existing 3D printing solutions that can be adopted or expanded for applications to cement-based infrastructure materials?
    - Build-up from experience in extrusion process, shotcrete, Hatcheck process (composite cement boards).
    - Gypsum board.
    - Curing techniques from other technologies.
    - Integrate an intermittent finishing step.
    - Multiple nozzles attached to a single barrel allowing nozzles to be switched “on the fly.”

5. What type of 3D printing method will be most suitable for the additive manufacturing of cement-based novel infrastructure materials? (i.e. extrusion, layer by layer, co-extrusion, binder jetting)?
    - Multiple nozzle extrusion (co-extrusion. e.g. print fibers, others). Multiple head nozzles can be very useful for AM process of cement based materials. Different nozzles can also be used to add different types of admixtures.
    - Thin layer printing.

- Opposing nozzles.
- Vertical spraying.
- Internal formwork.

6. What are the potential barriers to application of additive manufacturing (AM) technologies toward development of novel infrastructure materials and how can these barriers be removed?
    - Construction industry resistance to change.
    - Uncertainty in the design process (i.e. design process is different, new standards are required).
    - Scaling issues (e.g. how to build high-rise structures?)
    - New testing standards and construction codes are necessary for 3D printing of concrete.
    - A strong educational aspect should be implemented to change paradigms towards a new technology in the construction community.
    - Learn or borrow from other industries (shotcrete, SCC, extrusion, petroleum, composite cement board, ceramic/electronics. (And Food).
7. What are the potential benefits of using the AM technologies in development of infrastructure materials (i.e. total customization, geometric freedom of design, reduced waste and increased material utilization, creation of materials with properties impossible to achieve via conventional methods, reduction of manufacturing time
    - Extreme control on material and structure.
    - Opening to new material formulations not possible before.
    - Rapid feedback in quality control.
    - Control inhomogeneity anisotropy.
    - No formwork, no formwork material or formwork labor costs.
    - No rebar (reinforcement will still be required but will not be conventional reinforcement).
    - Material savings (less waste).
    - Functionality of the building.
    - Active (smart) building elements vs. passive (dumb) building elements with attendant impact on building energy consumption.
8. What is the specific role of modeling and simulation tools as applied to AM manufacturing of infrastructure materials? (e.g. software tools that can simulate the object to be built and to determine whether it is printable)
    - Modeling of 3D printing construction process.
    - Guiding experimentation and material development.
    - Reduce number of design/test/build iteration.
    - System modeling that reflects the performance of printed elements within the overall building system.

Appendix A. Final program

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July 16-17, 2015
Vanderbilt University, Nashville, TN

Program

Organizing Committee
Florence Sanchez Vanderbilt University, USA
Jan Olek Purdue University, USA
Joseph J. Biernacki Tennessee Technological University, USA

THURSDAY, July 16, 2015

7:30 am – 9:00 am ♦ FGH Adams Atrium
Registration

7:30 am – 8:15 am ♦ FGH 136
Breakfast

8:15 am – 8:20 am ♦ FGH 136
Welcome

8:20 am – 8:45 am ♦ FGH 136
Introductions / Workshop Overview

8:45 am – 9:50 am ♦ FGH 136
Session 1: Overview of Cement Microstructure Modeling
Moderator: Florence Sanchez (Vanderbilt University)

8:45 am – 9:25 am
Integrated Computational Materials Science and Engineering, Materials Genome, and Concrete
Edward Garboczi, National Institute of Standards and Technology

9:25 am – 9:50 am
Discussions – Gaps / Challenges / Opportunities

9:50 am – 10:10 am ♦ FGH 136
Coffee Break

10:10 am – 12:20 pm ♦ FGH 136
Session 2: Additive Manufacturing Processes and Fabrication Strategies
Moderator: Pablo Zavattieri (Purdue University)

10:10 am – 10:50 am
Coupling Manufacturing, Mechanics and Materials Design in Additive Manufacturing
Jian Cao, Northwestern University

10:50 am – 11:15 am
Discussions – Gaps / Challenges / Opportunities

11:15 am – 11:55 am
CAD and 3D Printing of Patient-Specific Skeletal Implants, Fixation, and Surgical Tools
David Dean, Ohio State University

11:55 am – 12:20 pm
Discussions – Gaps / Challenges / Opportunities

12:20 pm – 1:15 pm ♦ FGH 110
Lunch Break (*Sponsored by the Civil and Environmental Engineering Department)*

> **12:45 pm –1:15 pm**
> **An Overview of Additive Manufacturing Activities at NASA Marshall Space Flight Center**
> Tracie Prater, NASA Marshall Space Flight Center

1:20 pm – 3:30 pm ♦ FGH 136
Session 3: Additive Manufacturing and Advanced Modeling as Tools for Engineering Materials
Moderator: Jan Olek (Purdue University)

1:20 pm – 2:00 pm
Modeling and Simulation Challenges in Materials Design for Additive Manufacturing Applications
Wing Kam Liu, Northwestern University

2:00 pm – 2:25 pm
Discussions – Gaps / Challenges / Opportunities

2:25 pm – 3:05 pm
Combined 3D Printing and Multi-scale Modeling for the Development of Biomimetic Materials
Pablo Zavattieri, Purdue University

3:05 pm – 3:30 pm
Discussions – Gaps / Challenges / Opportunities

3:30 pm – 3:50 pm ♦ FGH 136
Coffee Break

3:50 pm – 6:00 pm ♦ FGH 136
Session 4: 3D Printing of Cement-Based Materials
Moderator: Joe Biernacki (Tennessee Tech.)

3:50 pm – 4:30 pm
A Materials Science Approach to 3D Printing with Cementitious Materials
Henri Van Damme, MIT

4:30 pm – 4:55 pm
Discussions – Gaps / Challenges / Opportunities

4:55 pm – 5:35 pm
ORNL's Experience with 3D Printing using Cementitious Materials
Catherine Mattus, Oak Ridge National Laboratory

5:35 pm – 6:00 pm
Discussions – Gaps / Challenges / Opportunities

Dinner on Your Own
A group reservation will be made at a restaurant close to the hotel for those interested.

FRIDAY, July 17, 2015

8:00 am – 8:30 am ♦ FGH 136
Breakfast

8:30 am – 8:45 am ♦ FGH 136
Breakout Session Assignments

8:50 am – 12:30 pm
Breakout Sessions

Topic	8:50 - 9:35 am	9:45-10:30 am	10:50-11:35 am	11:45 am -12:30 pm
T1. Cement Formulation	Group 1	Group 4	Group 3	Group 2
T2. Microstructure/3D Printing Relationships	Group 2	Group 1	Group 4	Group 3
T3. Modeling as Tool for Engineering and Predicting the Material Properties	Group 3	Group 2	Group 1	Group 4
T4. 3D Printing Technology	Group 4	Group 3	Group 2	Group 1

Group 1 - Room FGH 136
T1 – Lead: K. Wang
T2 – Lead: E. Garboczi
T3 – Lead: S. Guelcher
T4 – Lead: R. Bohan

Group 2 - Room FGH 200
T1 – Lead: A. Daugherty
T2 – Lead: Z. Grasley
T3 – Lead: S. Rouzbeh
T4 – Lead: S. Shah

Group 3 - Room FGH 313
T1 – Lead: D. Kuehn
T2 – Lead: G. Cusatis
T3 – Lead: J. Nyman
T4 – Lead: T. Prater

Group 4 - Room JH 273
T1 – Lead: K. Sobolev
T2 – Lead: L. Wing
T3 – Lead: J. Dolado
T4 – Lead: G. Sant

Moderators
T1: Joe Biernacki
T2: Florence Sanchez
T3: Pablo Zavattieri
T4: Jan Olek

10:30 am – 10:50 am ♦ FGH 136
Coffee Break

12:30 pm – 1:00 pm ♦ FGH 110
Lunch Break (*Sponsored by the Civil and Environmental Engineering Department)*

1:00 pm – 1:30 pm
Writing of topic summaries
(T1: Room FGH 136, T2: Room FGH 200, T3: Room FGH 313, T4: Room JH 273)

1:40 pm – 2:35 pm ♦ FGH 136
Reports
1:40 – 1:50 pm: T1 - Cement Formulation
1:55 – 2:05 pm: T2 - Microstructure/3D Printing Relationships
2:10 – 2:20 pm: T3 - Modeling as Tool for Engineering and Predicting the Material Properties
2:25 – 2:35 pm: T4 - 3D Printing Technology

2:40 pm – 3:00 pm ♦ FGH 136
Conclusions / Next Steps / Adjourn

Workshop Venues:
Featheringill Hall, Room FGH 136
400 24th Ave S., Nashville
Vanderbilt University

Multiscale/3D Printing Cement Workshop

Combined Multiscale Modeling and Additive Manufacturing Enabling Tools for the Engineering of Novel Infrastructure Materials

July 16-17, 2015
Vanderbilt University, Nashville, TN

Abstracts

Organizing Committee
Florence Sanchez Vanderbilt University, USA
Jan Olek Purdue University, USA
Joseph J. Biernacki Tennessee Technological University, USA

SCHOOL OF ENGINEERING

PURDUE UNIVERSITY
Civil Engineering

TENNESSEE TECH UNIVERSITY

Session 1: Overview of Cement Microstructure Modeling

Integrated Computational Materials Science and Engineering, Materials Genome, and Concrete
Edward Garboczi, National Institute of Standards and Technology

The Materials Genome Initiative is a US-led initiative to enable the computational design, from appropriate fundamental elements, of materials for human manufacture. Another term for this effort is integrated computational materials science and engineering. The NIST focus at present is on metallic alloys and polymer nanocomposites. A combination of fundamental materials data and models are needed to make this approach work. This talk will briefly describe what NIST is doing for metals and polymers, including a brief review of additive manufacturing research, and then will mainly focus on what is still needed for cement and concrete manufacture and use to also operate at this high level.

Session 2: Additive Manufacturing Processes and Fabrication Strategies

Coupling Manufacturing, Mechanics and Materials Design in Additive Manufacturing
Jian Cao and Gianluca Cusatis, Northwestern University

Additive manufacturing (AM) methods for rapid 3D fabrication of materials have become increasingly popular over the past decade. For metallic materials, these processes typically involve an accumulation of cyclic phase changes, i.e., melting and solidification, of metallic particles during the built. The widespread interest in these methods is largely stimulated by their unique ability to create components of considerable complexity and their ability to create gradient materials. However, to fully utilize the potential of AM methods, predictability of properties of built-structure and optimization of process planning will be the keys. Modeling such processes is exceedingly difficult due to the highly localized and drastic material evolution which occurs over the course of the manufacture time of each component. Final product characterization and validation are currently driven primarily by time consuming and costly experimental means as a result of the lack of robust modeling procedures. The primary purpose of this talk is to discuss the major detrimental aspects of AM process modeling and also some of the latest techniques being used to predict material (metal) evolution through the process by combining the fields of manufacturing, mechanics, and materials science. Extending the theme of combined materials and process design, the recent study of a novel material made of sulfur and Mars soil simulants will be presented.

CAD and 3D Printing of Patient-Specific Skeletal Implants, Fixation, and Surgical Tools
David Dean, Ohio State University

Additive manufacturing, also known as 3D printing, has only recently become a mainstream industrial fabrication strategy. However, almost from its inception in the mid-1980's 3D printing has been part of the medical device field. It did not take long for 3D printers to be used to render anatomic models based on shapes derived from medical images. These models were used in planning patient-specific surgical interventions and to guide the manual fabrication of implants and surgical guides. Manual fabrication of medical implants, fixation devices, and surgical guides gave way to direct 3D printing of these devices for use in the operating room. Where they have been demonstrated to perform better than off-the-shelf devices, 3D printed medical devices are now standard of care. However, there is much more room for growth in this field, especially in the areas of Computer Aided Design (CAD) software and new 3D printable materials. Medical CAD software is currently used to design the shape of patient-specific implants, fixation devices, and surgical guides. The next phase in the development of this software is likely to be the incorporation of anatomical templates and material properties in order to design, restore, and regenerate final function. In order to bring about more appropriate and reliable final function, new 3D printable materials are needed. Most of these materials fall into the categories of polymer (solid cured or hydrogel), ceramic, or metal. The next generation of regenerative and restorative implants and fixation devices will likely include inert materials that match the biomechanical characteristics of the tissues they attach to; 3D printable resorbable materials which resorb so as not to prevent the ingrowth, remodeling, and homeostasis of new tissue; and, biological components such as cells and growth factors. The 3D printing of medical implants containing live cells has been termed Bioprinting. All of these applications fall under the rubric of Biofabrication. Much of what has and is being learned about Biofabrication may translate to other fields as they attempt to develop their own specialized CAD software and 3D printable materials.

An Overview of Additive Manufacturing Activities at NASA Marshall Space Flight Center

Tracie Prater, NASA Marshall Space Flight Center

NASA Marshall Space Flight Center in Huntsville, Alabama has been engaged in additive manufacturing research activities since 1991, when the Additive Manufacturing Laboratory was established with two primary purposes: 1) to provide a rapid prototyping capability for spaceflight hardware and 2) develop methods to build parts in-space using material extrusion techniques such as fused deposition modeling (FDM). In recent years, the laboratory has focused on maturing metallic AM techniques to produce rocket propulsion hardware, specifically the qualification of electron beam and powder bed fusion processes for these application. The laboratory's in-space manufacturing activities to date culminated in 2014 with the launch of a 3D printer built by Made in Space to the International Space Station (ISS) as part of the 3D Printing in Zero G technology demonstration mission. This hardware represents the first manufacturing capability on board the ISS. The first phase of Acrylonitrile butadiene styrene (ABS) produced on ISS are currently undergoing testing at NASA MSFC to characterize the effect of microgravity on the FDM process. The 3D printing technology demonstration mission represents the first step in a portfolio of projects with the goal of reducing reliance on earth based platforms, enhancing crew safety, and developing a capability that is critical for long duration spaceflight.

Session 3: Additive Manufacturing and Advanced Modeling as Tools for Engineering Materials

Modeling and Simulation Challenges in Materials Design for Additive Manufacturing Applications

Wing Kam Liu, Northwestern University

The report from the National Academy of Engineering titled "Making a World of Difference: Engineering Ideas into Reality" covers the engineering inventions that have transformed lives in the last 50 years, and the breakthroughs that may evolve in the next half century. One of the future trends identified is the development of new materials, which is an integral part in the advancement of the world of design and manufacturing. Additive Manufacturing (AM) enables the printing of 3D complex geometries that are otherwise impossible to manufacture, such as a part within a part. AM comes in many different varieties for numerous material systems including polymeric, biological, cement-based, and metallic materials. These processes typically involve an accumulation of cyclic phase changes, e.g., melting and solidification of metallic particles, until the desired 3D geometry is achieved. This has major implications for concurrent material and product design as it is quite simple using AM to adjust material composition for bulk property improvement or functional grading within the material.

Patient-specific implants and prosthetics are perhaps the most obvious of applications of AM for medical purposes. Extending the life of existing products and engineering systems is of particular importance for many applications. Digital manufacturing is a digital framework for concurrent virtual design of materials, components, materials systems, and manufacturing process chains simultaneously. One can imagine a situation in which a patient-specific implant is needed which includes specific design constraints. The biological feature can be scanned and imported as a CAD file, then sent into a simulation-based analysis preprocessor, followed by topological optimization, and finally a virtual design loop which iteratively develops a robust and practical set of process parameters and material composition for the desired application. The process is flexible enough that once the topology, material composition, and process have been successfully designed, the part can be produced with minimal to no human interaction. This also improves the viability of AM in distributed manufacturing networks and cloud manufacturing.

While the benefits and impact of using AM to create products is quite clear, the governing physics which drive materials design for additive manufacturing applications to be versatile also greatly complicate our ability to fully characterize the effect of the process on final product performance. This indicates that there is a strong need for robust and efficient modeling and computational approaches which can improve predictive capabilities in these processes. In this talk, I will discuss primary detrimental hurdles that have plagued effective modeling of additive manufacturing methods for metallic materials while also providing logical speculation into preferable research directions for overcoming these hurdles. The primary focus of this talk encompasses the specific areas of high-performance computing, multiscale modeling, materials characterization, and process modeling for final product performance of additively manufactured metallic components. The proposed approaches are applicable to other material systems with the appropriate amendment of materials physics and manufacturing processes.

References
[1] KI Elkhodary; MS Greene; S. Tang; T. Belytschko; WK Liu, "Archetype-blending continuum theory," Comput. Methods Appl. Mech. Engrg. 254 (2013) 309–333.
[2] MS Greene, Y. Li, W. Chen, WK Liu, "The archetype-genome exemplar in molecular dynamics and continuum mechanics," Computational Mechanics, Volume 53, Issue 4 (2014), Page 687-737.
[3] Wentao Yan, Jacob Smith, Wenjun Ge, Feng Lin, Wing Kam Liu, "Multiscale modeling of electron beam and substrate interaction: a new heat source model," Computational Mechanics, pp. 1-12 (2015).
[4] Jacob Smith, Wei Xiong, Wentao Yan, Jian Cao, WK Liu, "Computational Challenges in Final Product Performance Prediction of Additively Manufactured Components," Computational Mechanics.

Combined 3D Printing and Multi-scale Modeling for the Development of Biomimetic Materials

Pablo Zavattieri - Purdue University

There is a strong demand for new paradigms of design and development of advanced high-performance structural materials with high strength and durability that are low-cost and renewable with novel combinations of properties. Yet, most of these applications require high-performance materials that are not only stiff and strong for structural purposes, but also they need to be tough and capable of absorbing energy to avoid catastrophic failure under extreme events. Unfortunately, most engineering materials have an inverse relation between these desired properties. By natural selection, Nature has evolved, through millions of years, efficient strategies to synthesize materials that often exhibit exceptional mechanical properties that significantly break the trade-offs often achieved by man-made materials. In fact, most biological composite materials achieve higher toughness without sacrificing stiffness and strength comparing to typical engineering material. Interrogating how Nature employs these strategies and decoding the structure-function relationship of these materials is a challenging task that requires knowledge about the actual loading and environmental conditions of the material in their natural habitat, as well as a complete characterization of their constituents and hierarchical ultrastructure through the use of modern tools such as in-situ electron microscopy, small-scale mechanical testing capabilities, additive manufacturing, and advanced multiscale numerical models. In turn, this provides the necessary tools for the design and fabrication of biomimetic materials with remarkable properties. I will particularly focus my talk on how 3D printing, analytical/computational modeling and mechanical testing can successfully be combined to evaluate some important hypotheses about the key morphological features of the microstructure and most important toughening mechanisms that are unique in these naturally-occurring hierarchical materials.

Session 4: 3D Printing of Cement-Based Materials

A Materials Science Approach to 3D Printing with Cementitious Materials

Henri Van Damme, Roland J.-M. Pellenq, Franz-Josef Ulm - MIT

Very few industrial sectors are more traditional than the building construction sector. This is true not only for masonry construction, it is also largely true for large buildings in concrete and/or steel. On one hand, there has been tremendous progress in the way buildings are designed and in the way construction sites are managed, thanks to the generalized use of computer-assisted methods. On the other hand, concrete itself has made equally remarkable progress with the development of ultra-high strength concrete, almost as strong as steel in compression, and several other forms of functionalized concrete such as self-compacting, self-leveling, self-healing, or self-cleaning concrete. But in the very core of the construction process itself, only limited progress has been made. All attempts to introduce robotic methods or any other radical change have so far failed. Construction with concrete is still based on a step-by-step formwork-filling process. The introduction of geolocalization, drones and/or additive manufacturing (3D-printing) methods has the potential to introduce a technological leap in this picture. As far as 3D-printing is concerned the benefits could be both faster and more flexible, tailormade, construction. However, in order to meet these promises, the rheological behavior and the setting kinetics of the cementitious material has to be adapted to the printing process. Ideally, one would wish to have a system in which the transition from a readily flowing state to a high yield stress state with rapid hardening would spontaneously occur immediately after deposition. Alternatively, the transition could be triggered by an external stimulus such as light, heat or ultrasound for instance. Both routes will most probably require new polymer admixtures. This will be illustrated in the presentation.

ORNL's experience with 3D printing using cementitious materials

Catherine Mattus - Oak Ridge National Laboratory

In 2008 ORNL financed an internally funded project to demonstrate that 3D printing could be a possible future for the construction of low rising commercial and residential building. At the time, 3D printing was just starting to emerge as a new technology and plastic was the material commonly used. The ORNL's team was composed of engineers and scientists from four different divisions with expertise in different technical areas and materials. Cementitious material was selected for the project. At the end of the two years project it was successfully demonstrated that:

- Novel cementitious materials suitable for AFC using admixtures for plasticity and cohesiveness control, accelerators for gel and set time and strength control, fibers for increased strength, PCMs for increased thermal mass, and replacement of part of Portland cement by secondary materials to show the feasibility of path for greater sustainability was achievable.
- Rapid 3D deposition of layers (< 1 min successive layers) to create various shapes with cementitious materials was realized
- Multi-purpose (e.g., structural + insulating) layered concept for the construction of the wall of a house with automated freeforming of the external wall's "bondaries" using a cement mortar, followed by pouring structural concrete in half of the wall's thickness and insulating material in the second half could be a concept to produce a zero energy building type of construction.