The Virtual Cement and Concrete Testing Laboratory

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Materials and Construction Research Division Seminar
16 June 2005

Virtual Testing in a Nutshell

- Physical tests on concrete require large amounts of material and long times (~ 28 days)

- **Idea**: Provide computer models with a virtual representation of the material and simulate the results of physical tests

- **Applications**:
  1. Design of new materials
  2. Supplant QA testing
  3. Understanding

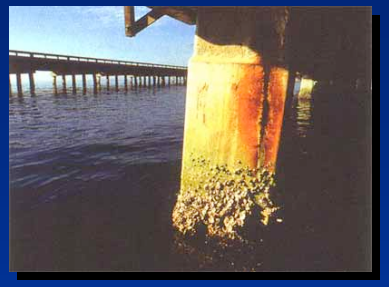
Why Concrete?

- Concrete is fairly inexpensive on a mass basis (compared to metals, ceramics), BUT
- It is produced in huge quantities:
  - 6 billion metric tons produced globally
  - 1 billion metric tons cement produced globally
  - U.S. production of $8.3 billion/year in 2000

Concrete is the **2nd** most widely consumed resource on the *planet* (on a mass basis)

- Trimming production costs by pennies per ton is a big benefit ⇒ **streamline testing**

What Needs To Be Tested ?



Mix → **Place** → **Cure** → **Service Life**

Mix proportions

Mineralogical composition

Chemical admixtures
- retarders
- accelerators
- dispersants

Rheological properties of dense suspensions on different scales
- pumping and flow
- surface finishing
- formwork pressure

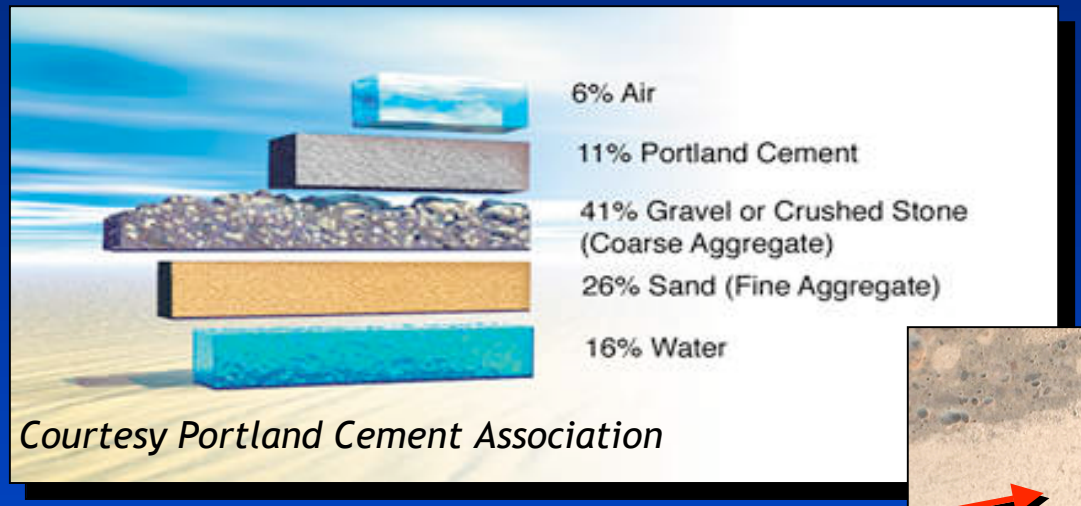
Suspension of solids due to chemical reactions and physical changes
- setting and hardening
- self-dessication

Mechanical properties:
- (visco)elastic behavior
- Strength

Durability:
- Leaching of solids
- Attack by sulfates/chlorides
- Freeze/thaw damage

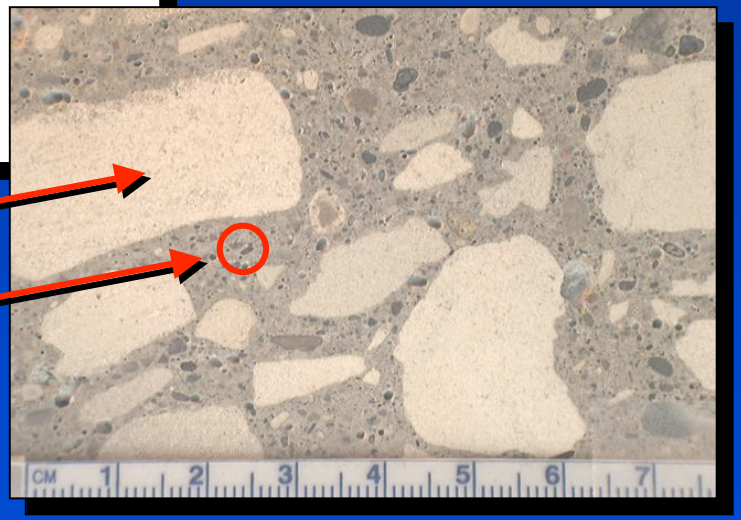
What IS Concrete ?

Macro-scale



Courtesy Portland Cement Association

Mix to form a 3D random composite with time-dependent chemical and physical properties



Coarse Aggregate

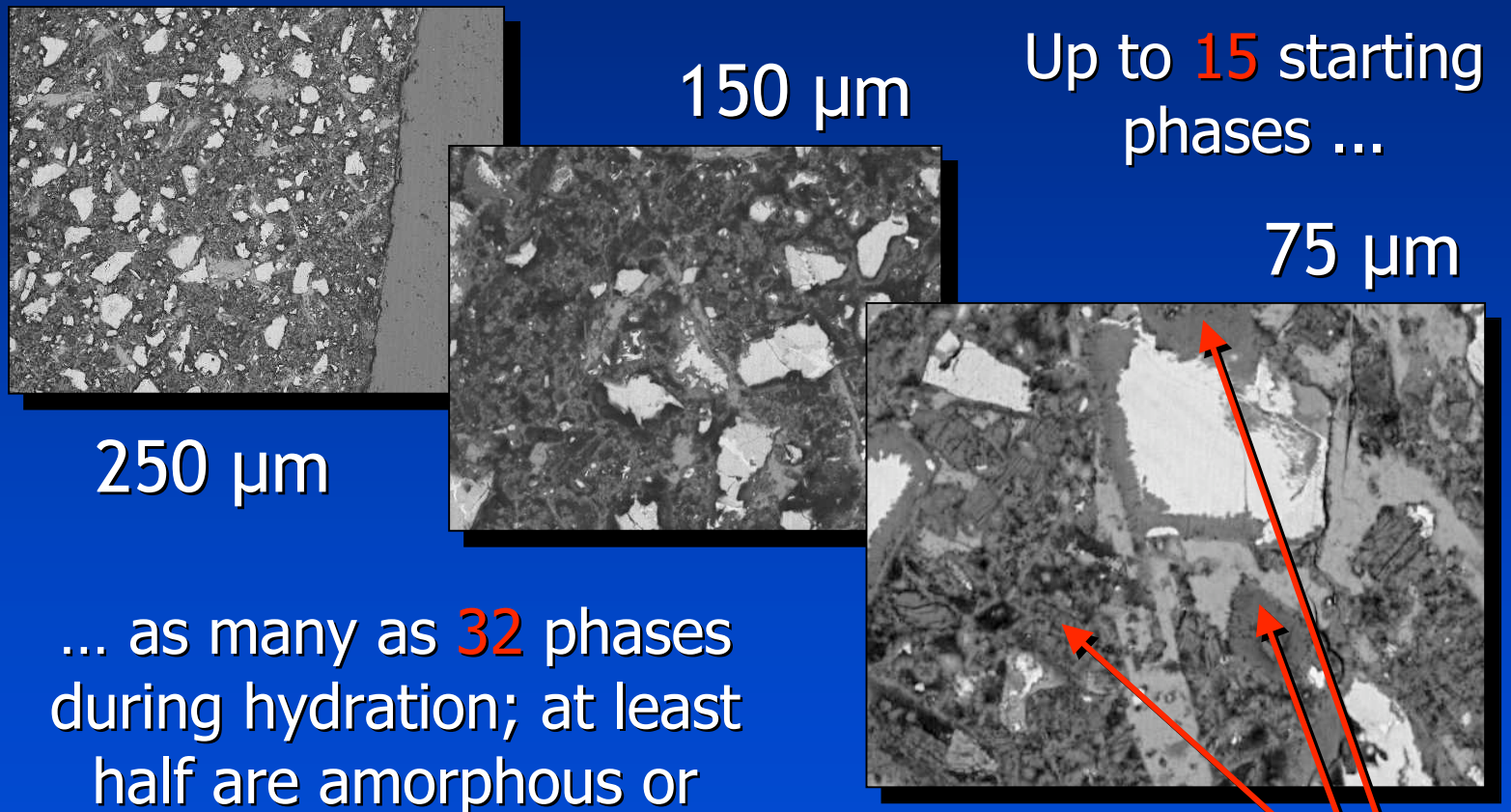
Binder

- Sand
- Cement Paste

The clue is the glue **(F. Ulm, MIT)**

What IS Concrete ?

Micro-scale: Cement Paste



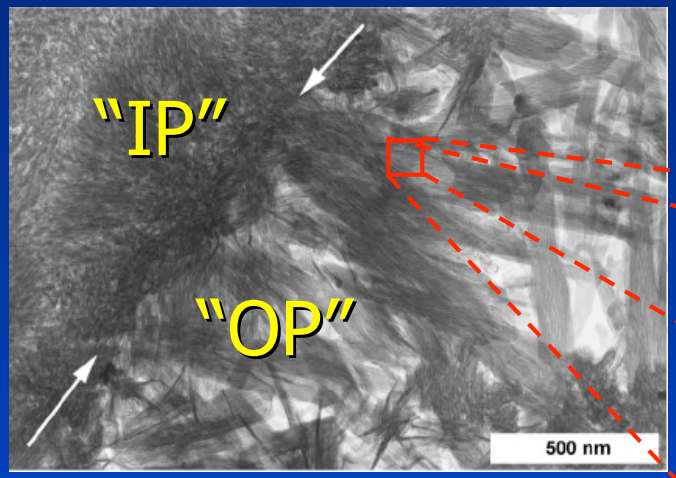
Up to 15 starting phases ...

... as many as 32 phases during hydration; at least half are amorphous or poorly crystalline

Calcium silicate hydrate (C-S-H)

What IS Concrete ?

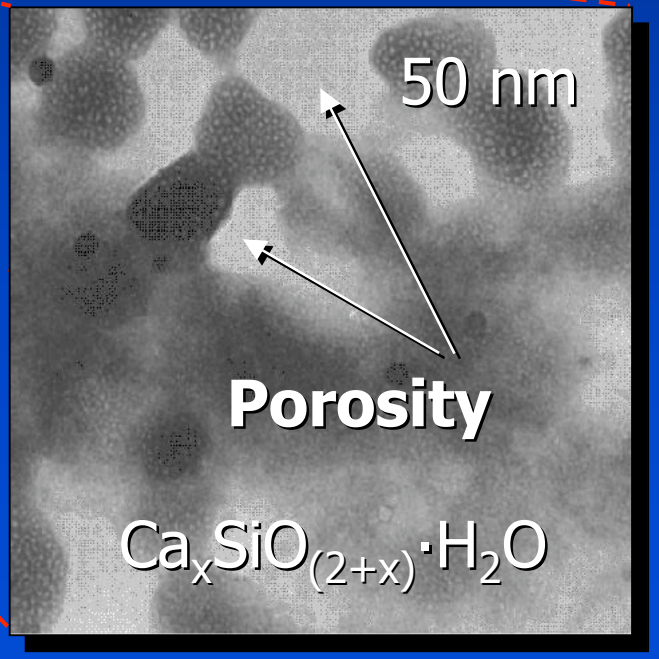
Nano-scale: C-S-H



Micrograph courtesy of I.G. Richardson, University of Leeds

Silicate chemistry

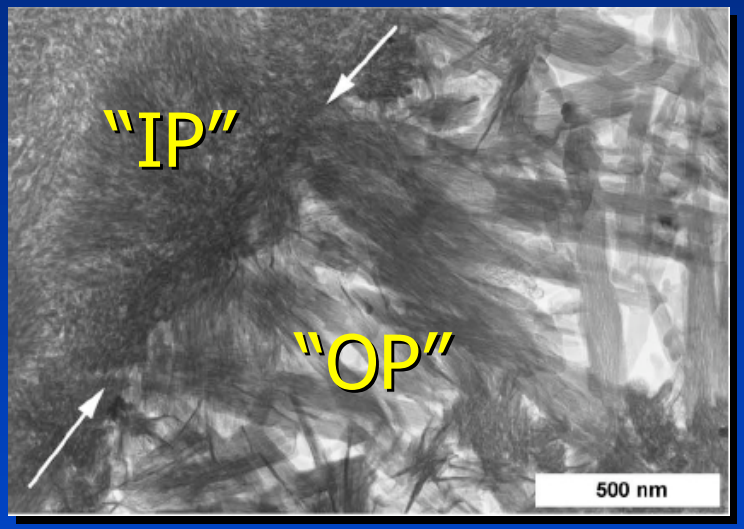
- Only organic is more complicated
- Wide range of compositions and structural variants



Growth by condensation of hydroxylated silicate mers in solution. Morphology depends on temperature and composition

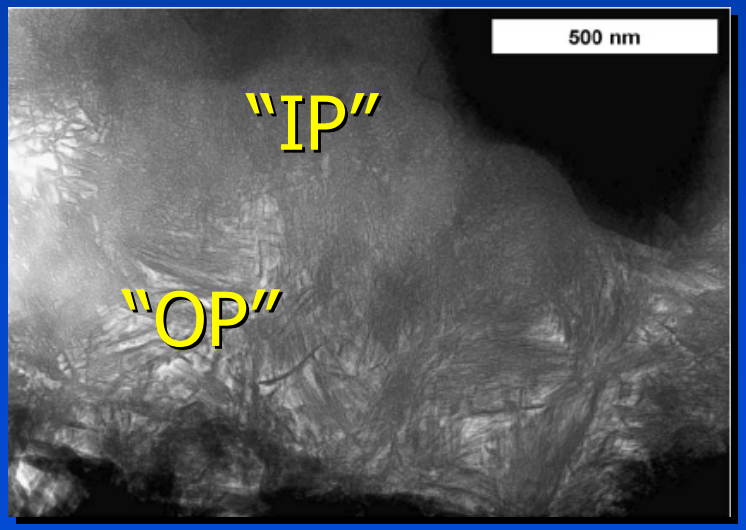
What IS Concrete ?

Nano-scale: C-S-H



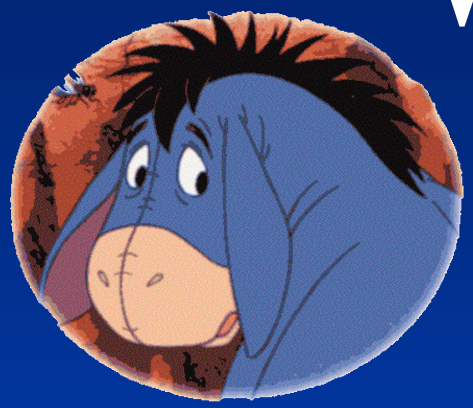
Ca_3SiO_5 paste, 20°C, 8 yr

Micrographs courtesy of I.G. Richardson, University of Leeds



Ca_3SiO_5 paste, 80°C, 8 d

What Hope Is There ?

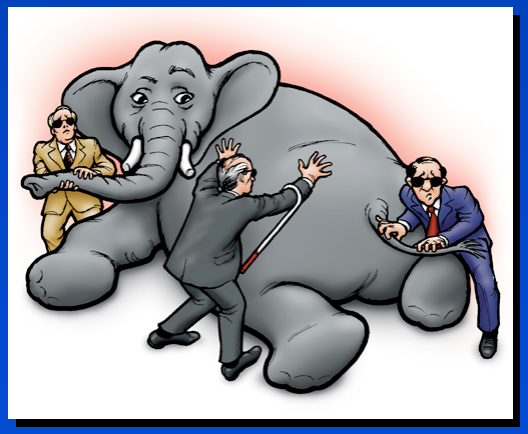


Materials scientists usually target **MUCH** simpler materials for predictive modeling (Cu, MgO, etc)

Added complexity built into models only after simpler systems are understood (e.g. metal alloy models built from models of single component metals)

With **concrete**:

- Interdependent, multiscale phenomena
- Experiments are difficult to design and often ambiguous



What is the Goal of Modeling ?

Science

Understand

- Idealized systems
- Based on physics / chemistry
- Few adjustable parameters

Test

- Idealized experiments
- Direct test of model

Increase complexity; repeat

Engineering

Empirical
Reliance on fitting
Interpolative

VCCTL

Predict Behavior of Complex Materials

Extrapolative
Solid foundation
Costly

Virtual Cement and Concrete Testing Laboratory

- **1982** – Development at NIST, under Geoff Frohnsdorff's leadership, by Hamlin Jennings of first simple cement hydration model (continuum based)
- **1989**
  - NIST starts developing first (primitive) pixel-based simulation of cement hydration (Bentz & Garboczi)
  - NIST starts developing finite difference methods for computing properties of pixel-based systems (Garboczi)
- **January 1, 2001** – Start of **VCCTL Consortium**
  - Led by NIST (BFRL and ITL)
  - Charter membership of six industrial partners
  - Organization and further development of user-friendly software based on 20+ years of NIST research
  - Software product = VCCTL

VCCTL Models

Philosophy

Develop predictive models of real concrete by building in as much materials science, physics, and chemistry as we know:

Hydration **Rheology** **Mechanical Properties**

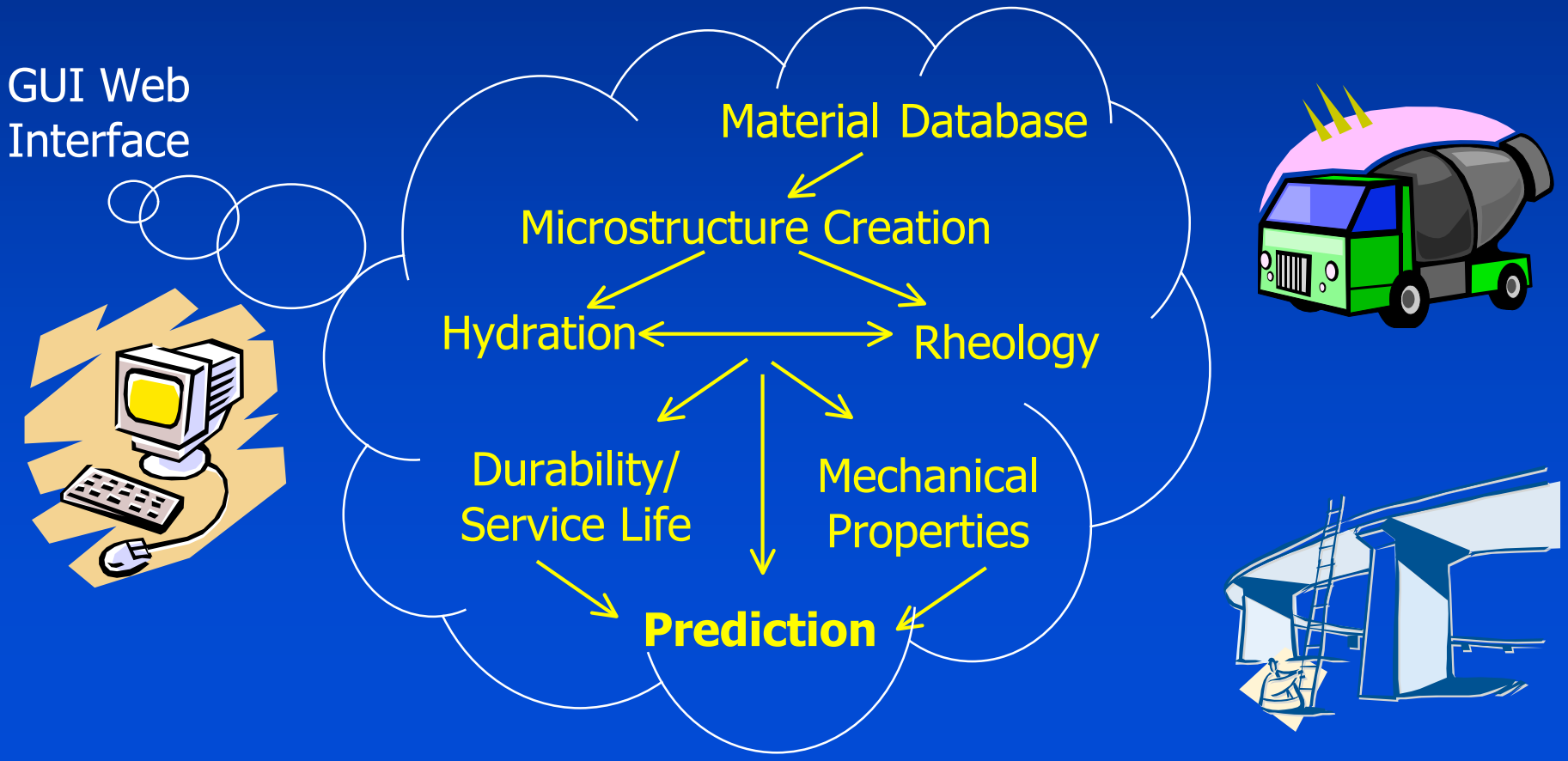
Leverage computational power to apply these principles to complex chemistry and physics of concrete

Check predictions against experiment

- Agreement: GOOD!
- Disagreement: Build in better science or use fitting parameters/empiricism to make predictions better

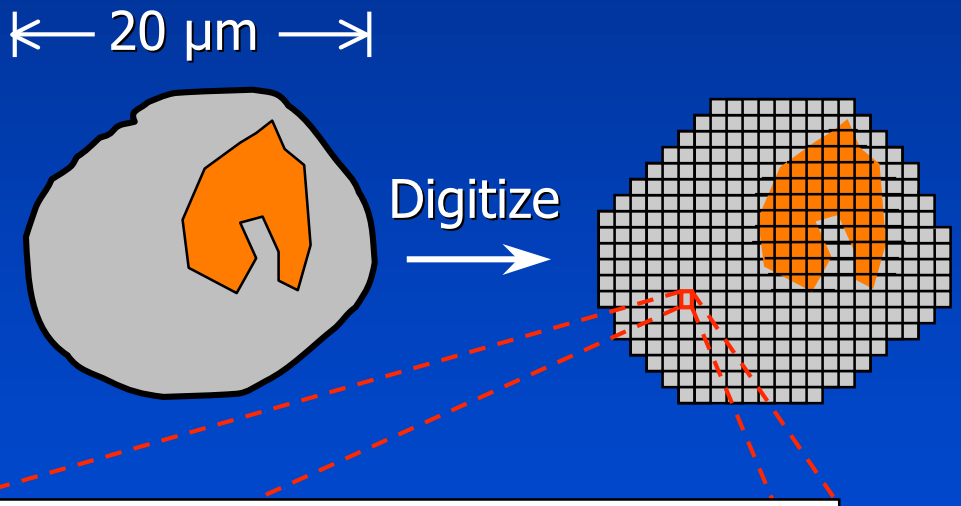
Virtual Cement and Concrete Testing Laboratory

VISION: Integrate and enhance NIST' s state-of-the art computational materials science models into a tool that is relevant and useful to industry.



Integrated Modeling Approach

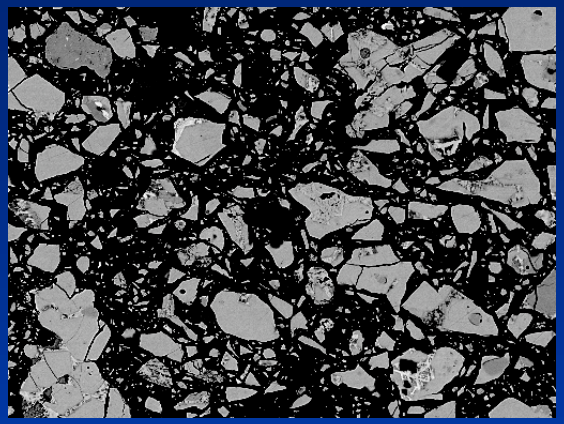
- 3-D Microstructure-Based
  - Spatial resolution at the sub-particle level using small volume elements (1 μm cubes)

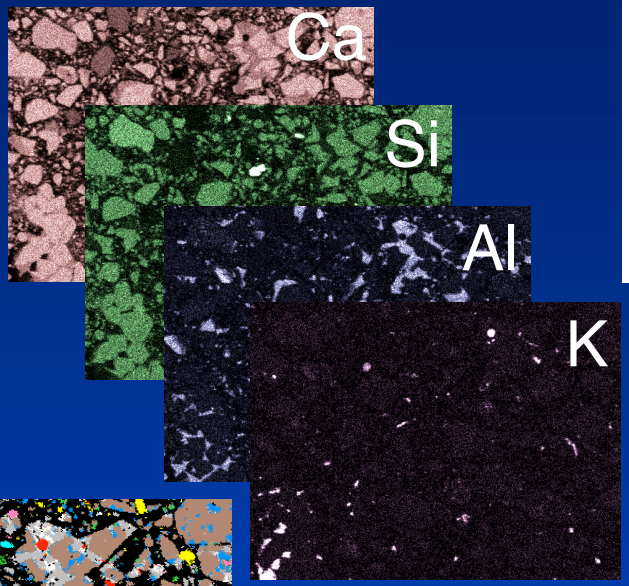


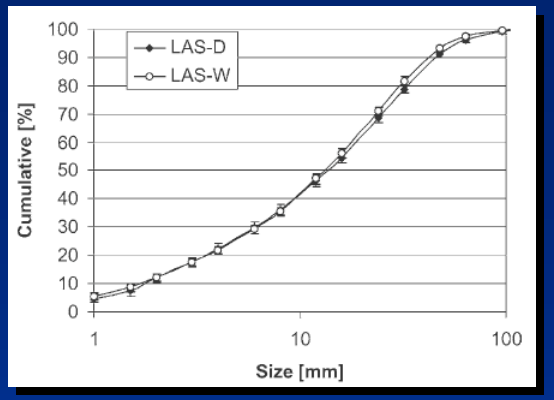
Each volume element has properties of the phase at that location in space

input μ-structure
↓
model hydration of μ-structure
↓
predict properties
↓
compare w/ experiment

SEM/BSE Image…

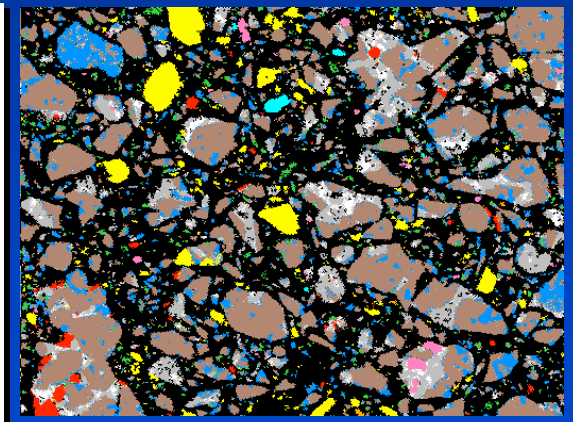






… Particle Size Distribution …

- C3S
- C2S
- C3A
- C4AF
- Gypsum
- CaCO3
- K2SO4
- Mg/Ca Oxide
- Aluminosilicate
- Slag
- Silica



… X-ray element maps …

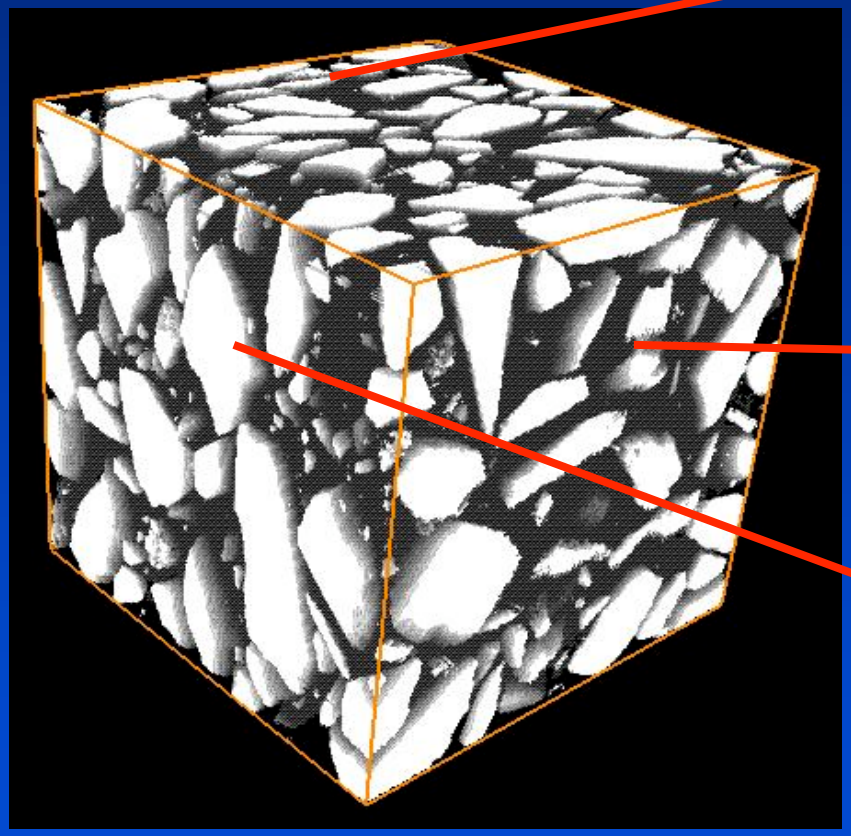
… segment image into **phases** …

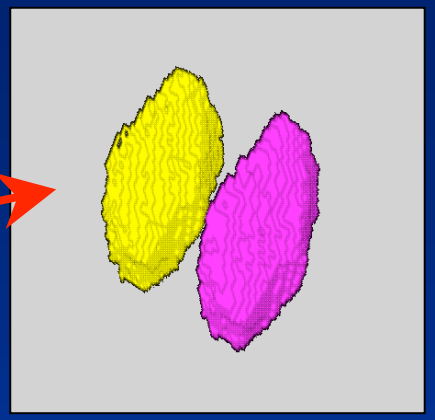
Measure autocorrelation fns on majority phases

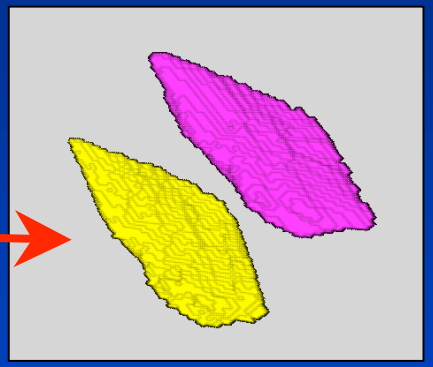
Reconstruct 3D Image

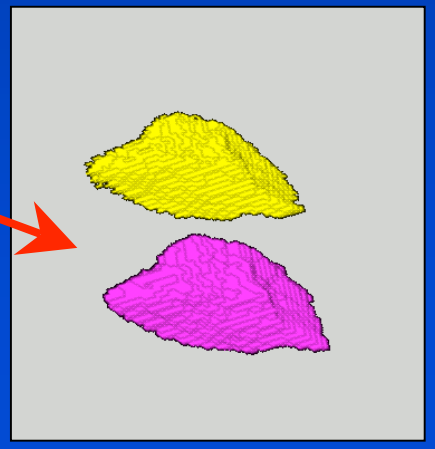
Contributors: D. Bentz and P. Stutzman

"Extract" particle/aggregate shapes, then mathematically analyze and store them

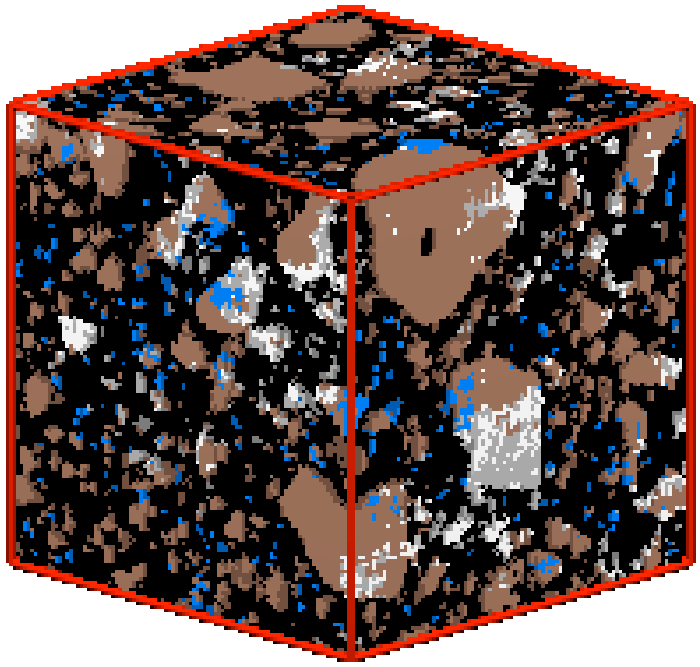








Contributor: E. Garboczi



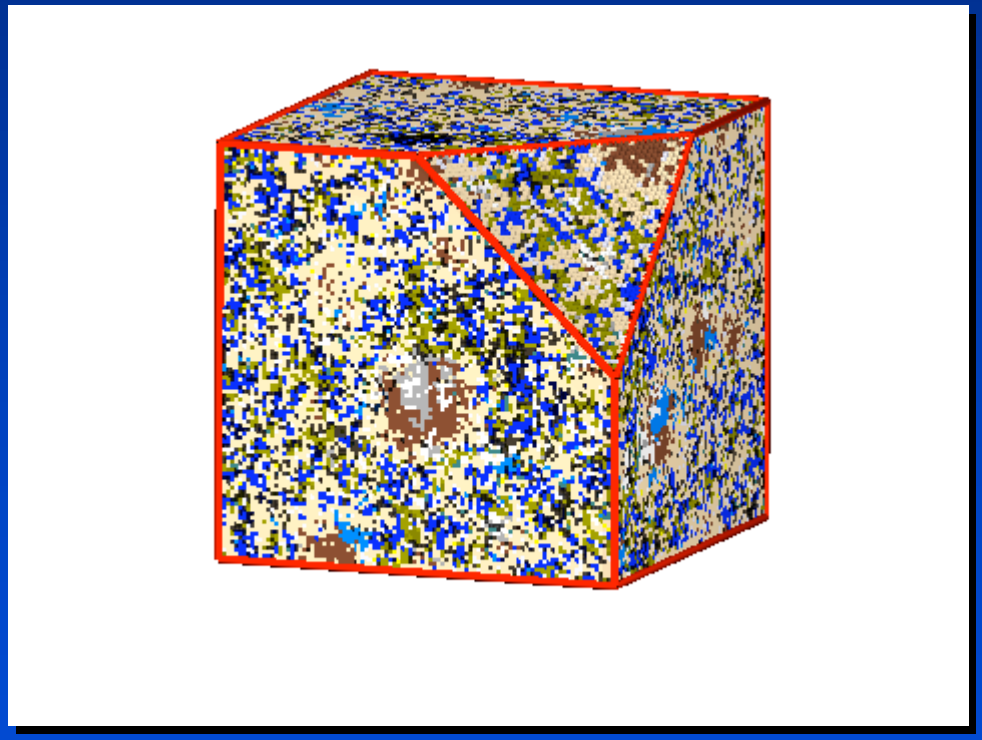
3-D image of model cement particles

Captures

- Volume fractions
- Surface fractions
- PSD
- w/s ratio

Module for
Cement Paste Hydration

Contributor: D. Bentz



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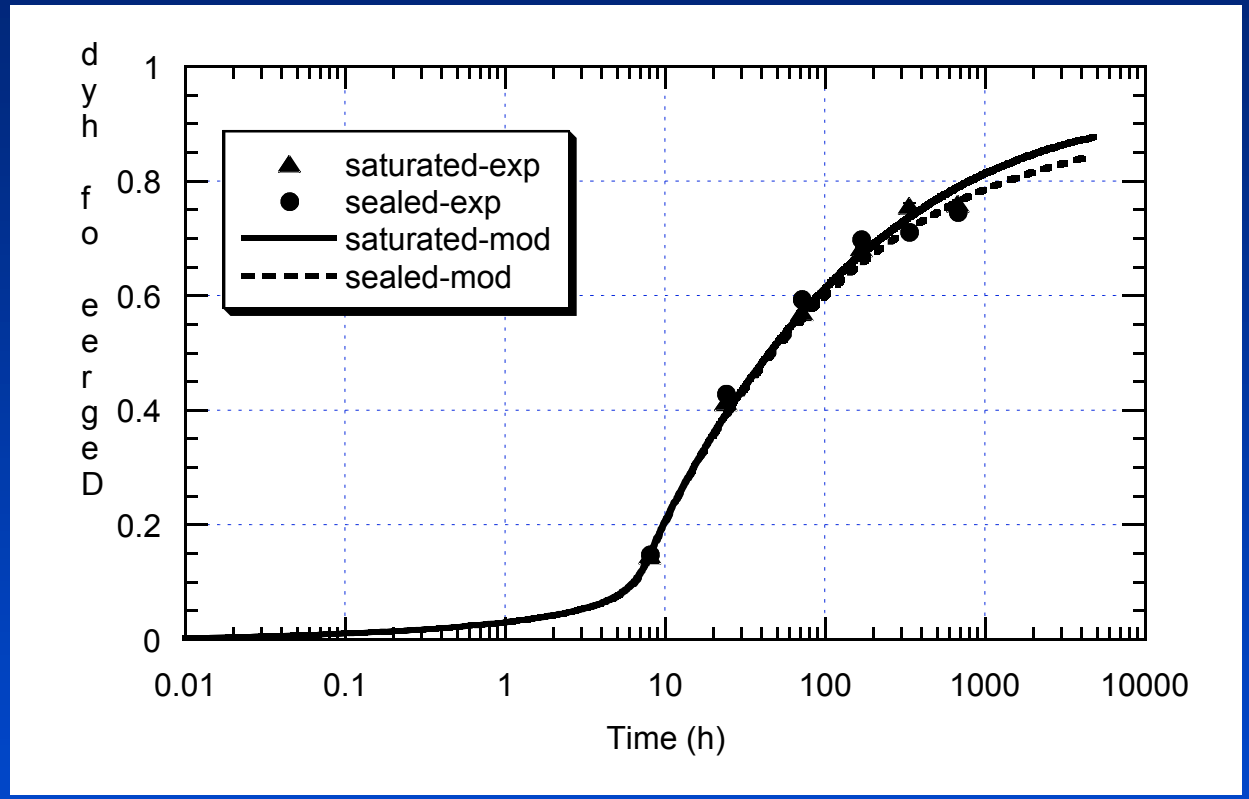
Degree of Hydration



CCRL Proficiency Sample 135
w/c = 0.4, T = 25° C

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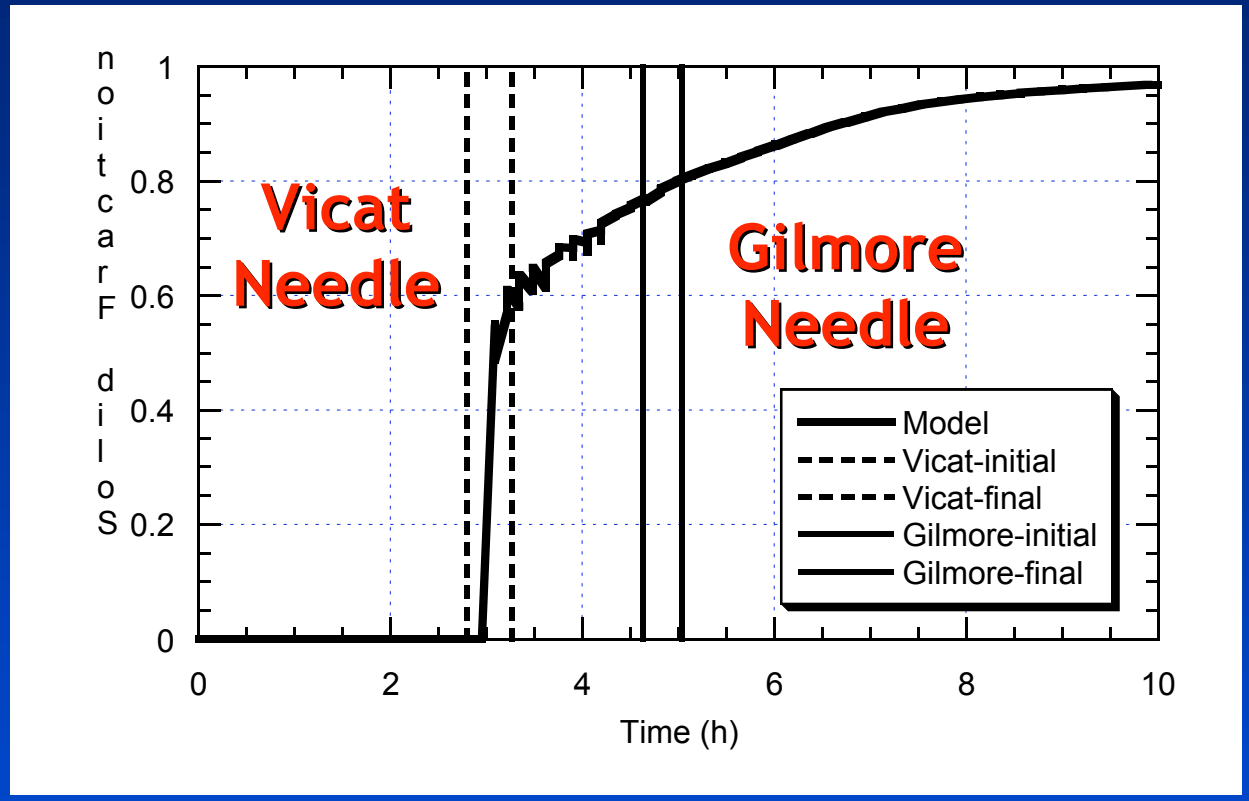
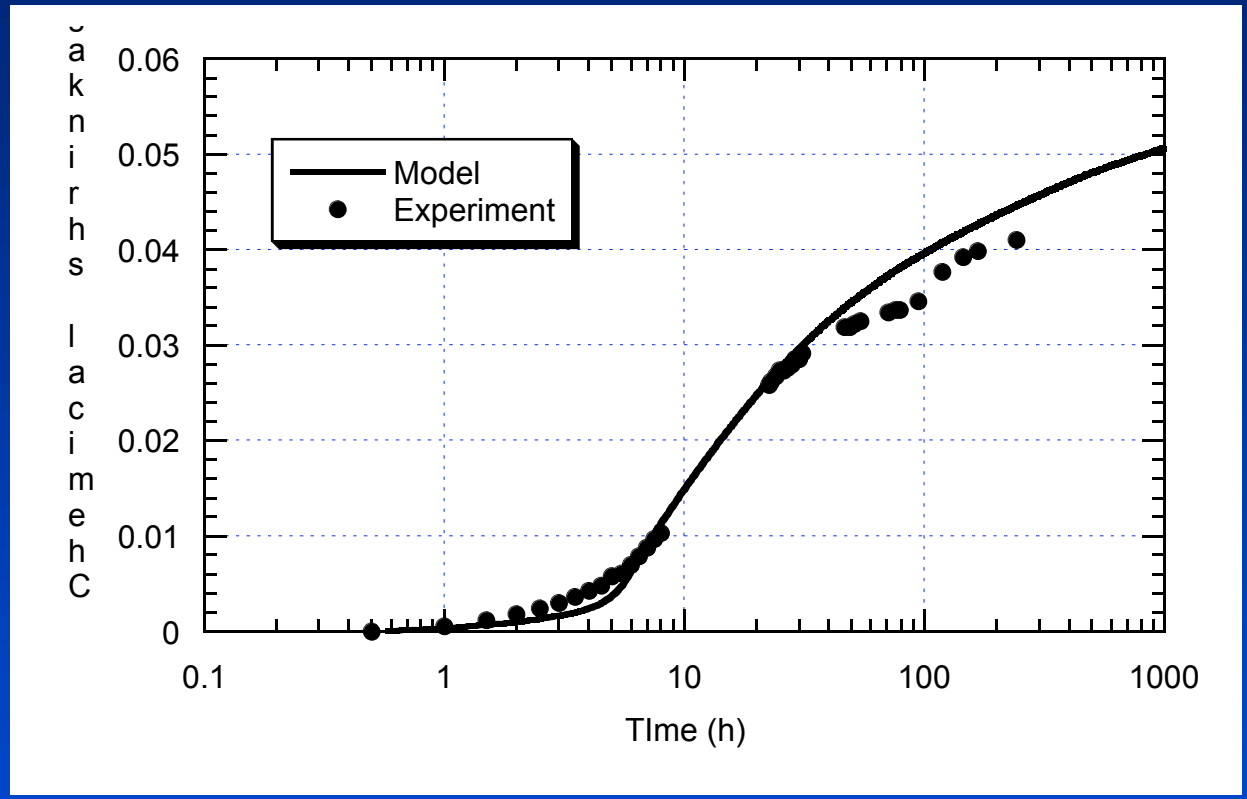
Setting Time



CCRL Proficiency Sample 135
w/c = 0.25, T = 25° C

Chemical Shrinkage



CCRL Proficiency Sample 135
w/c = 0.3, T = 25° C

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Module for
Rheological Properties of Fresh Concrete

Contributors: N. Martys, C. Ferraris

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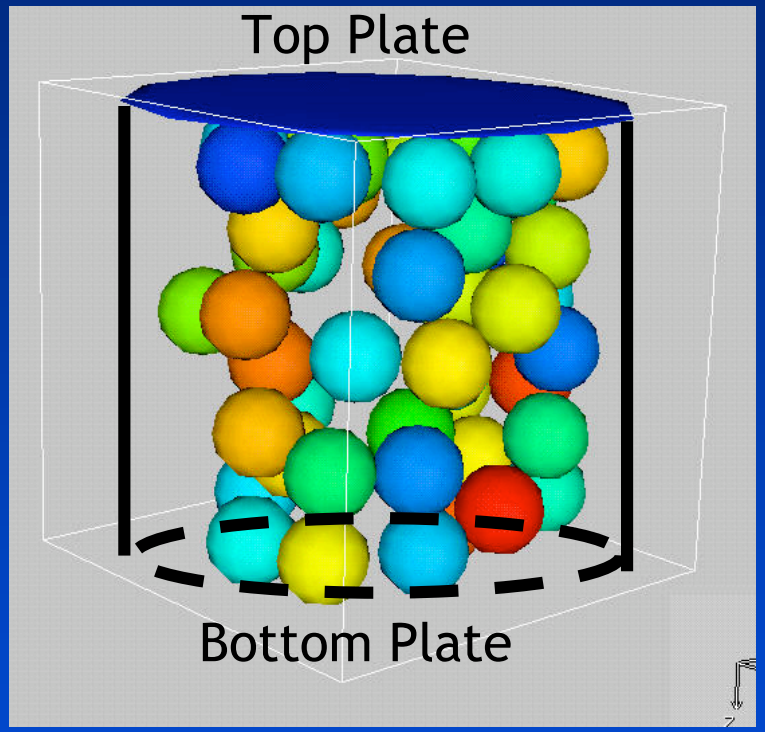
Concrete Rheology is a Multiscale Problem

- **Micro**: cement in water (Cement Paste)
- **Milli**: sand in cement paste (Mortar)
- **Macro**: coarse aggregates (Concrete)

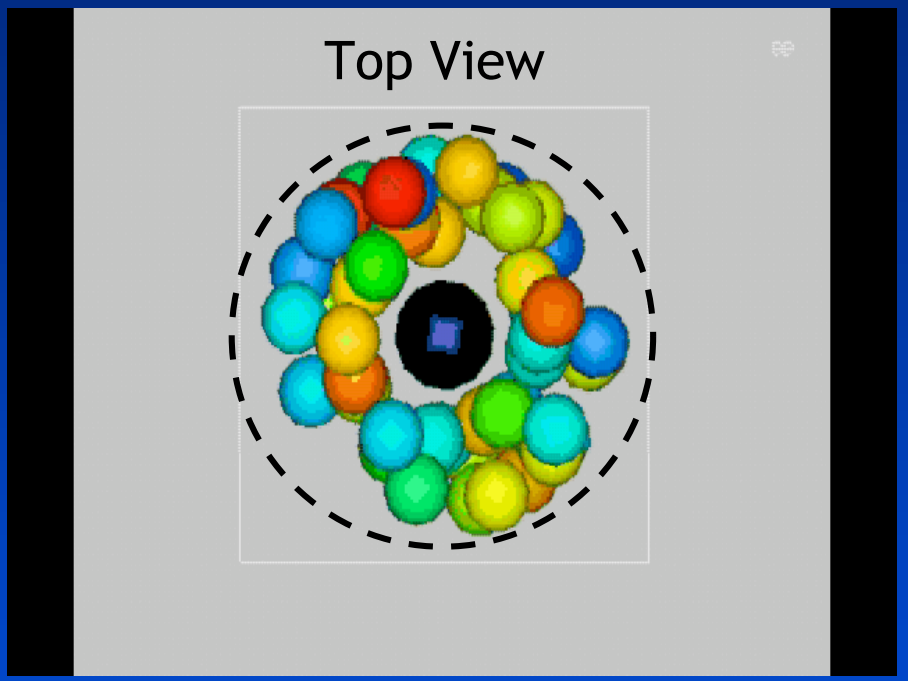
Approach:

- Experiments on simplified, model systems
- Simulations based on Dissipative Particle Dynamics

DPD Simulation of Concrete Rheometers

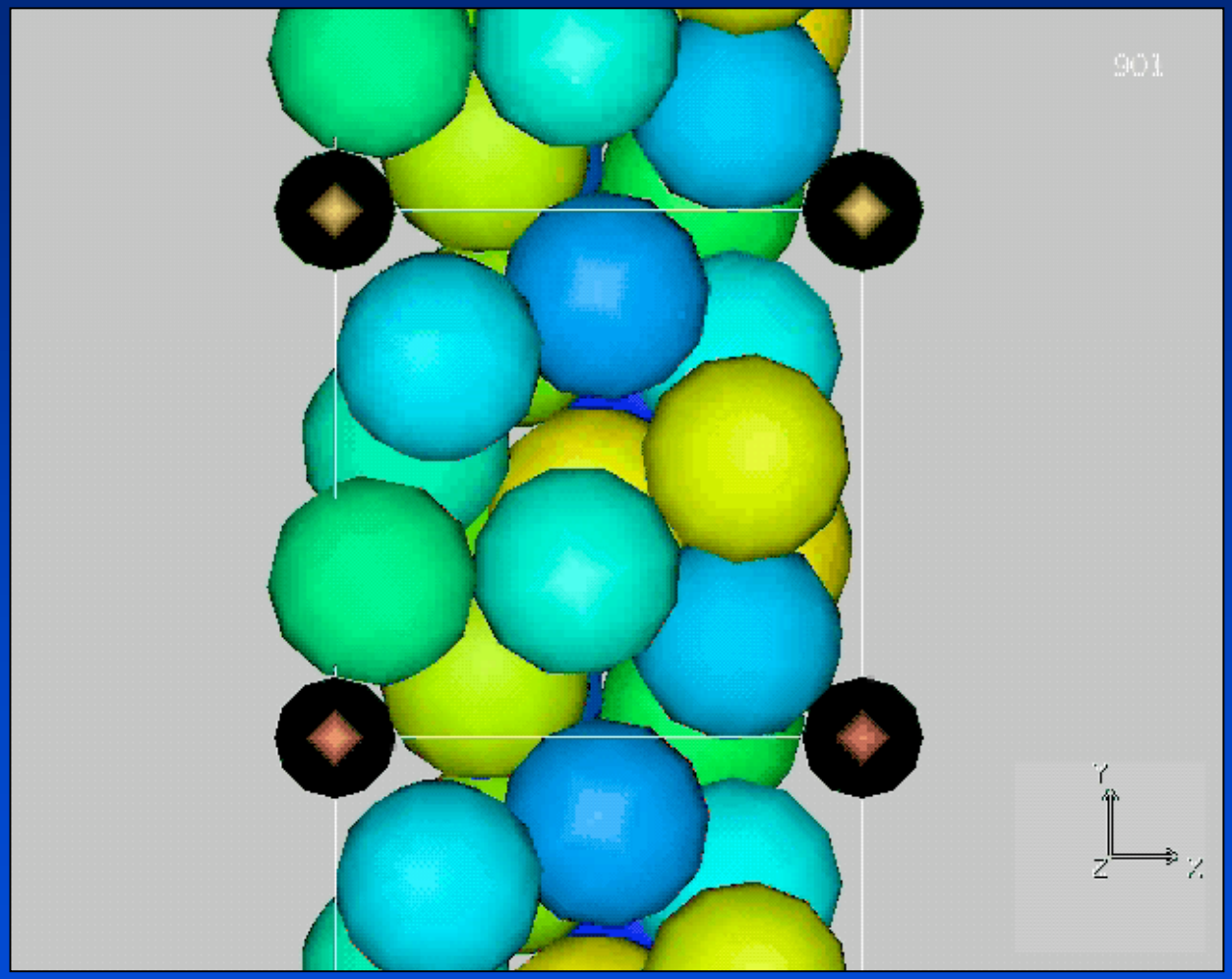


Parallel Plate



Coaxial

Self-consolidating Concrete



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Module for
Mechanical Properties of Concrete

Contributor: E. Garboczi

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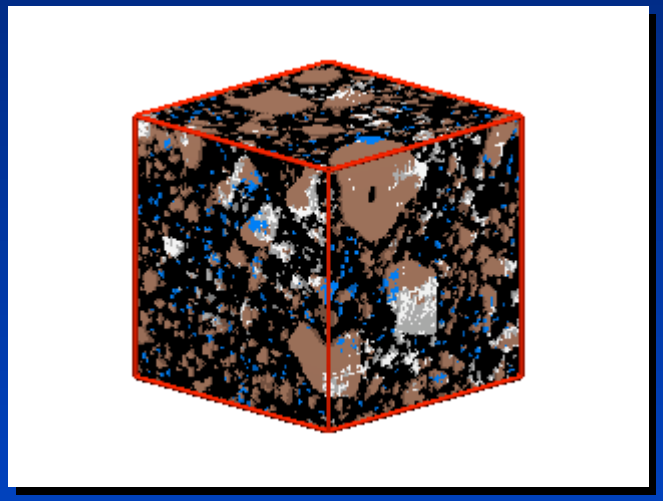
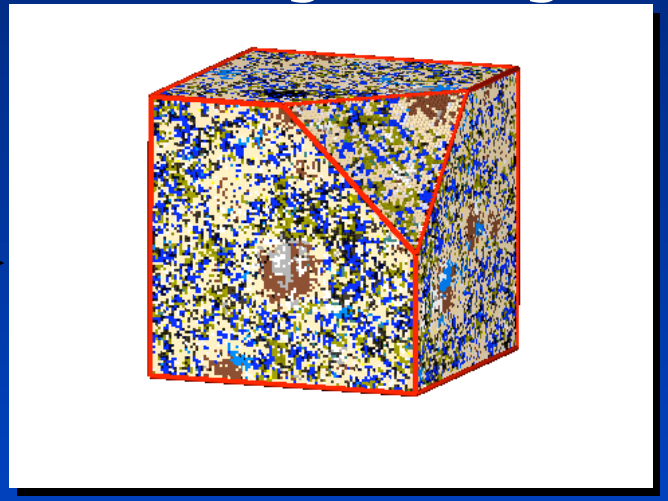
Elastic Properties of Cement Paste

Virtual Cement



Cure to given age

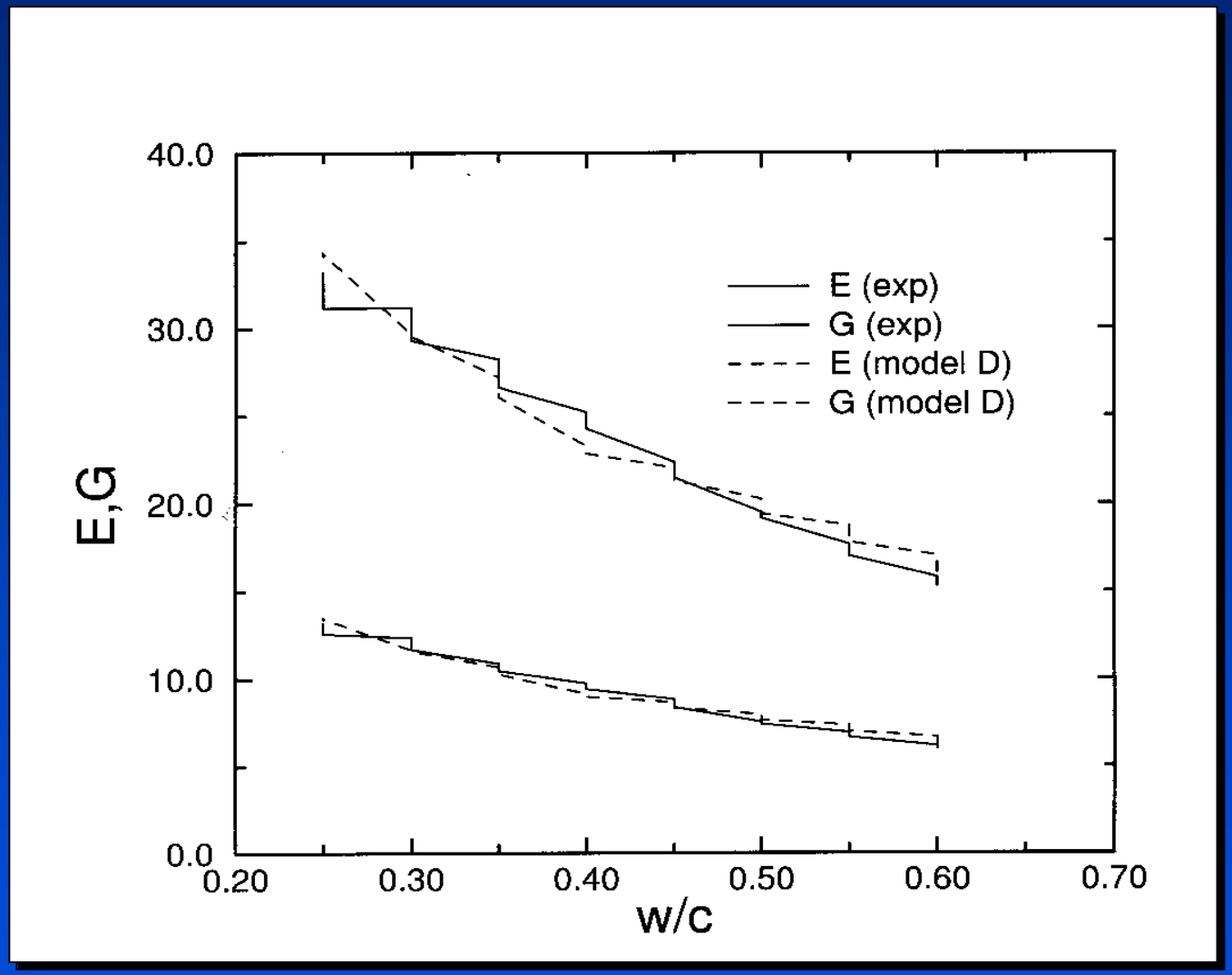


Finite Element Model:

- input phase moduli
- input microstructure

Output Paste Elastic Moduli

Cement Paste Elastic Moduli



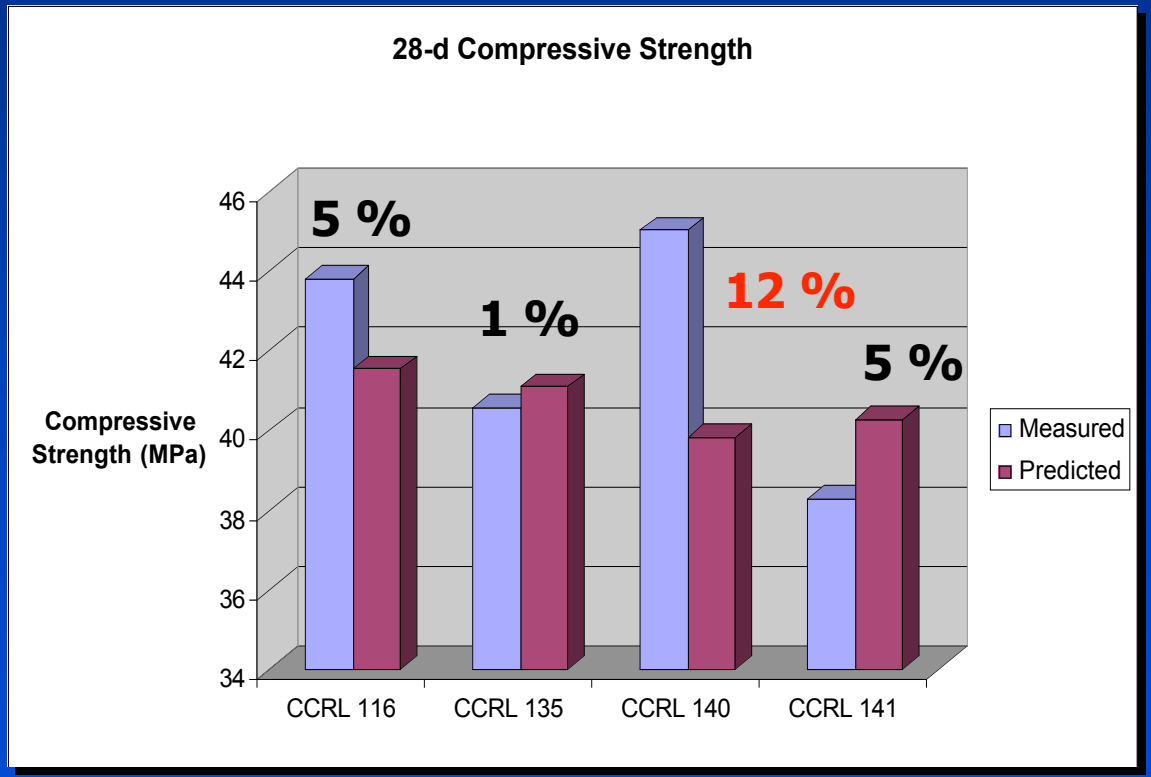
Moduli and Strength of Concrete

- **Effective Medium Theory (EMT)**
  - Provides estimate of **elastic moduli** of mortar and concrete

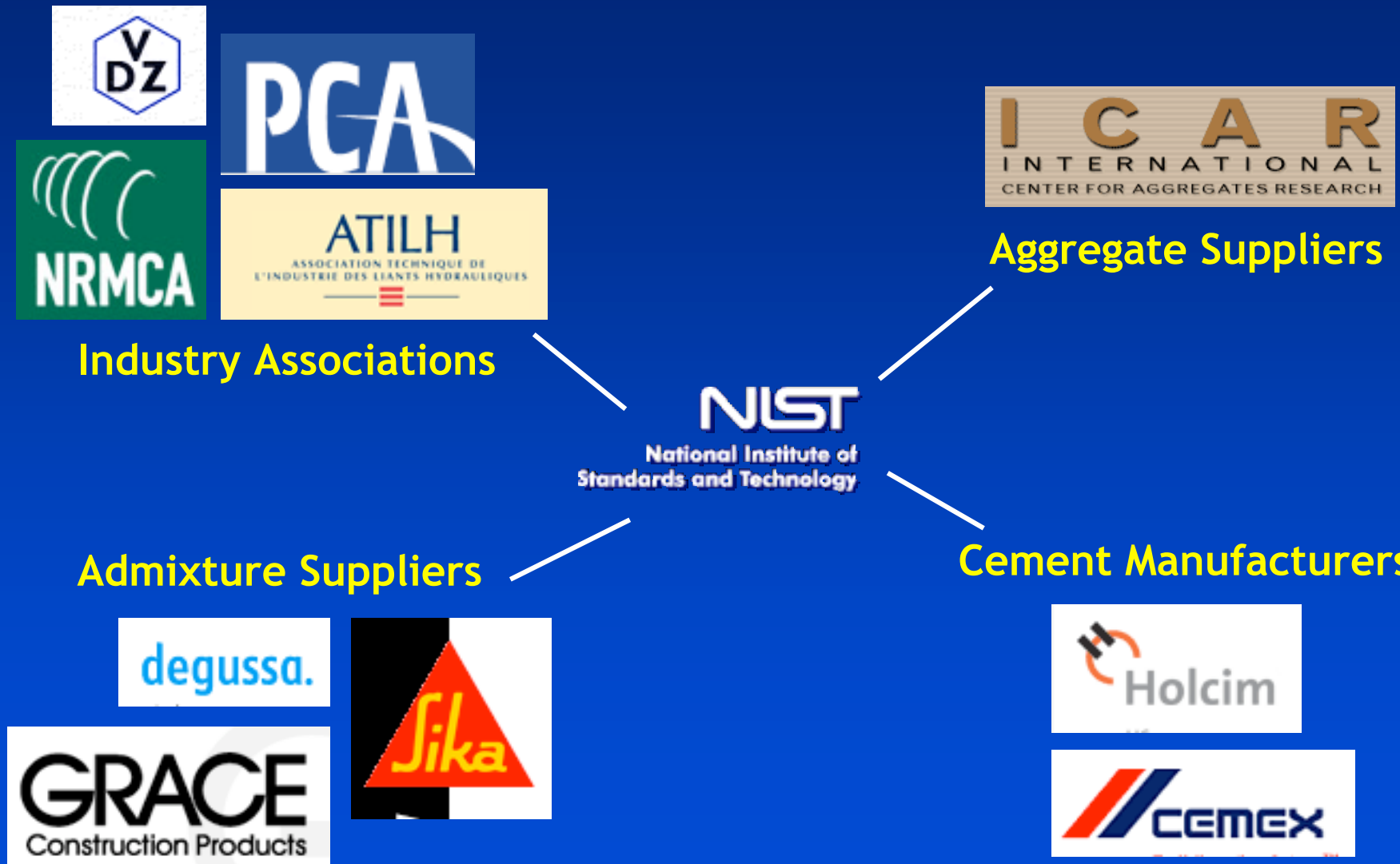
Input:

- volume fractions of air, aggregate
- elastic properties of paste and aggregate
- thickness and elastic properties of ITZ

Compressive strength estimated from empirical relation (Neville)



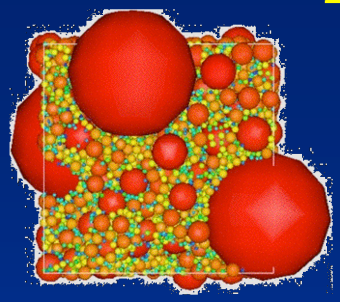
VCCTL Consortium: 5th Year



VCCTL Consortium: Year 5

- Restructured for better administration and communication
  - ✎ Industrial Advisory Board
  - ✎ Focused working groups
- Narrower scope to accelerate research in two key areas
  - ✎ Hydration modeling
  - ✎ Rheology modeling

Rheology



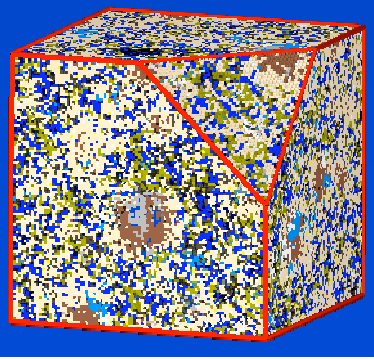
Influence of aggregate size distribution on viscosity

Real-shape aggregate effects
Influence of lubrication and inter-particle forces on rheology of fresh concrete

Hydration

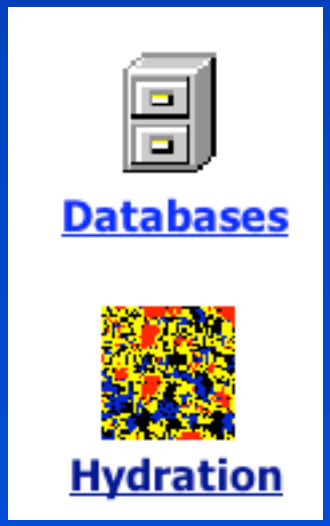
HydratiCA: Next-generation hydration model

Thermodynamic and kinetic framework for microstructure development



Systematic validation effort underway

Version 5.0:



Menu driven
Graphical output
Rebuild for v6.0, enable better session management & database interactivity

User Interface

Final Remarks

- VCCTL software can be used to
  - Streamline testing and save $$
    - Two industry projects which realized cost savings
      - ~ **$1M** in one month (Dyckerhoff)
      - ~ **$700K** in several weeks (Cemex)
  - Expedite design of new materials and admixtures
  - Help educate students and professionals
  - Drive changes in standard test methods