Historical, Philosophical, and Ontological Roots of the Computational Materials Science of Concrete as Related to Early Collective Thought in Post-Modern Reductive Analysis of the Paradigm Shift in the Physical Sciences: Part I – An Introduction to the Establishment and Definition of Pertinent Jargon Parameters

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The Computational Materials Science of Concrete: Past – Present - Future

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Outline

- Where the computational materials science of concrete came from
  - **With some bias from my personal point of view**
- Current trends
- The future of the computational materials science of concrete

An historical note

- At a special ACBM conference in 2000 to honor Francis Young at his retirement I used a similar title:
  - **The past hasn't changed, but the present and the future look a bit different to me 12 years later**


PAST

My background

- 1985 – Ph.D. in condensed matter physics from Michigan State (thesis on simulation models of amorphous semiconductors)
- 1985-1988 at Armstrong World Industries working on calcium phosphate cements – phosphoric acid plus wollastonite, for inorganic ceiling boards (chemically-bonded ceramics)
- Went to MDF-type twin-roll process, so I had to study up on MDF, DSP, famous issue of Proc. Roy. Soc.
- I became interested in cement and concrete in general and moved to NIST in 1988

Phil. Trans. R. Soc. Lond. A **310**, 1–207 (1983) [1]
Printed in Great Britain

TECHNOLOGY IN THE 1990s: DEVELOPMENTS IN THE SCIENCE AND TECHNOLOGY OF HYDRAULIC CEMENTS

A Discussion organized and edited by Sir Peter Hirsch, F.R.S., J. D. Birchall, F.R.S., D. D. Double, A. Kelly, F.R.S., G. K. Moir and C. D. Pomeroy

(*Discussion held* 16 *and* 17 *February* 1983 – *Typescripts received* 28 *April* 1983)

[Nine plates]

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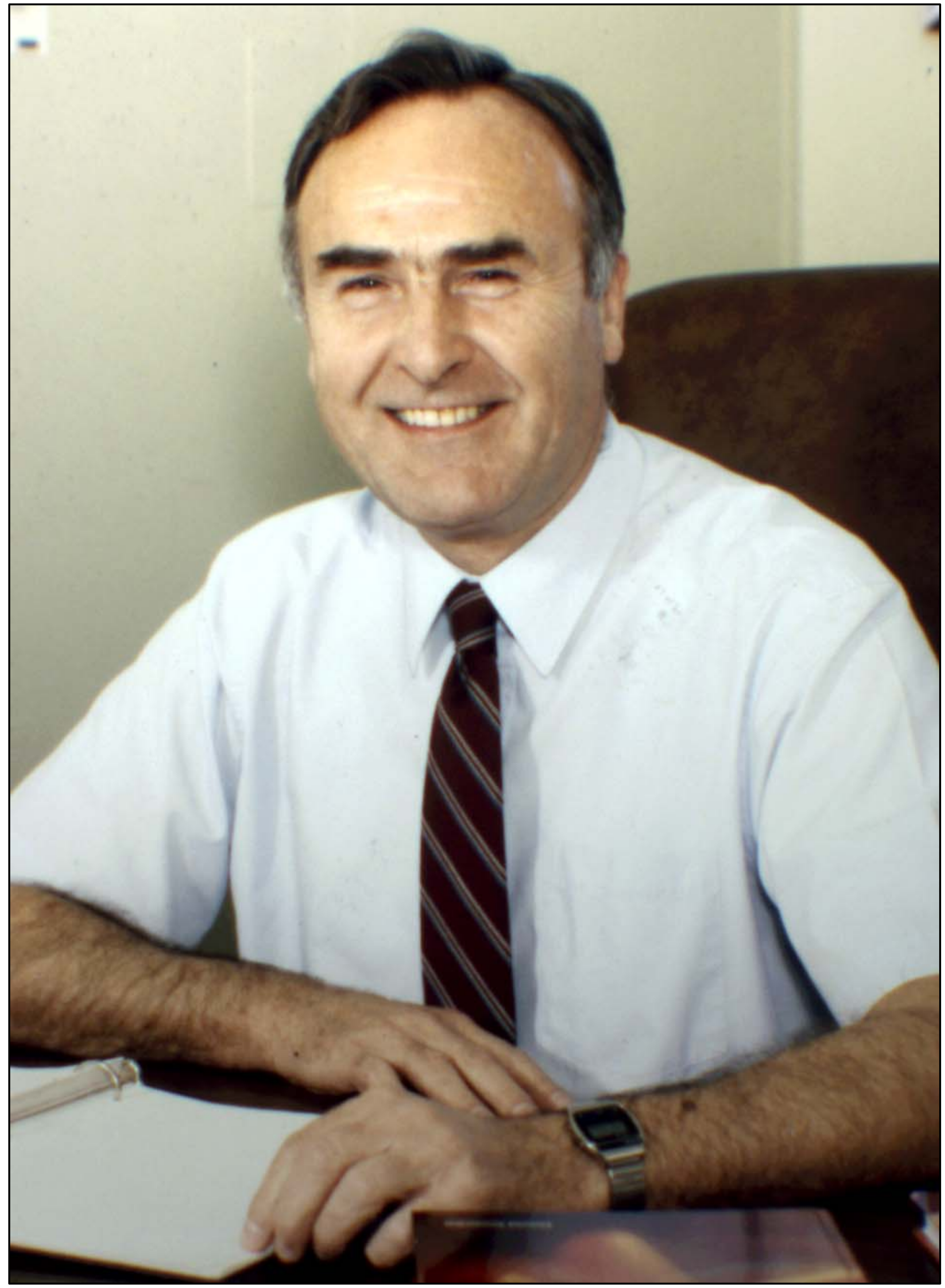
A visionary scientist
and leader:
Dr. Geoffrey
Frohnsdorff
(1928-2006)



"…two or three good ideas…"

- **"The Mathematical Simulation of Chemical, Physical, and Mechanical Changes Accompanying the Hydration of Cement" – G.J.C. Frohnsdorff et al**
  - 5th Inter. Symp. Chem. Cement (Tokyo, 1968)
  - first computer model of hydration

My motivation

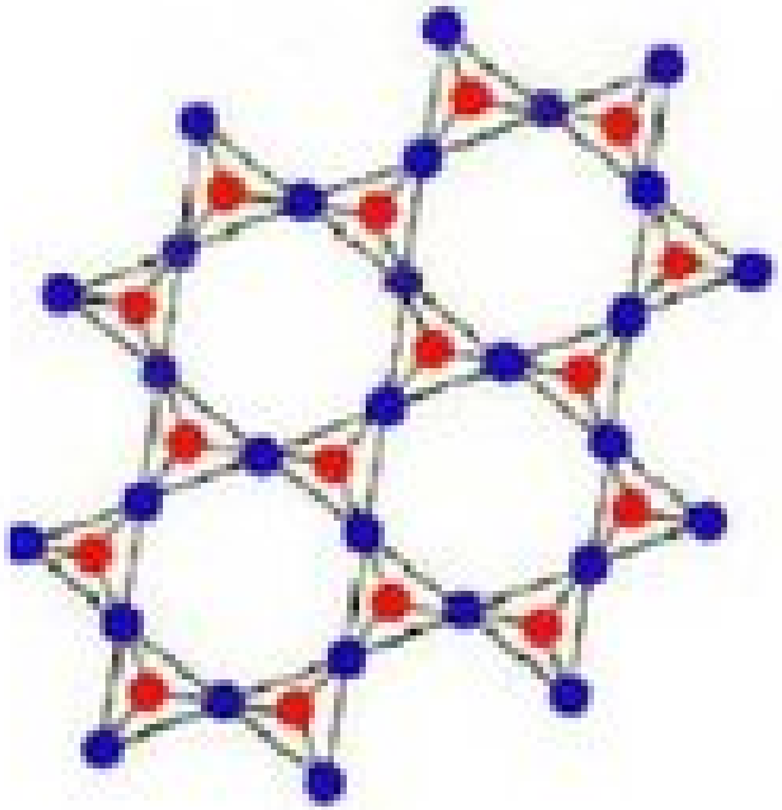
- I wanted to make the computational materials science of concrete a viable discipline that could work with experiment as an equal partner in order to solve the hard problems of this complex, random, multi-scale material

- “Physicists don’t work on messy problems like concrete…”
- “Just look at the average concrete worker…”
- "Common sense is the collection of prejudices acquired by age eighteen." (Albert Einstein)

My Intellectual Sources

- Amorphous semiconductors like silicon, germanium arsenide
  - **No good way to make predictions to accompany experiment**
- Challenges
  - **Establishing amorphous structure in some systematic way**
  - **Using numerical structure to calculate properties that could be directly compared to experiment**
- Use results to give a "theory" to work with, guide, and interpret experiments
  - **Computational materials science of amorphous semiconductors**
- 1960s – computers were just powerful enough to have simulations of a few 100 atoms with amorphous structure (no quantum mechanics, just spring connections)

Periodic to Amorphous



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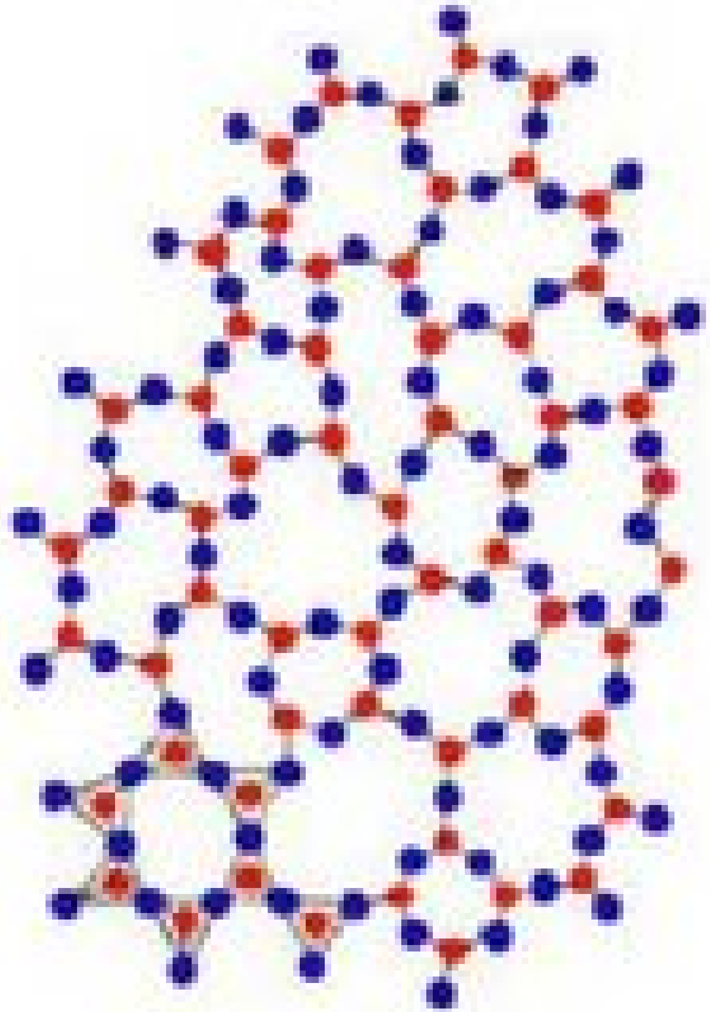
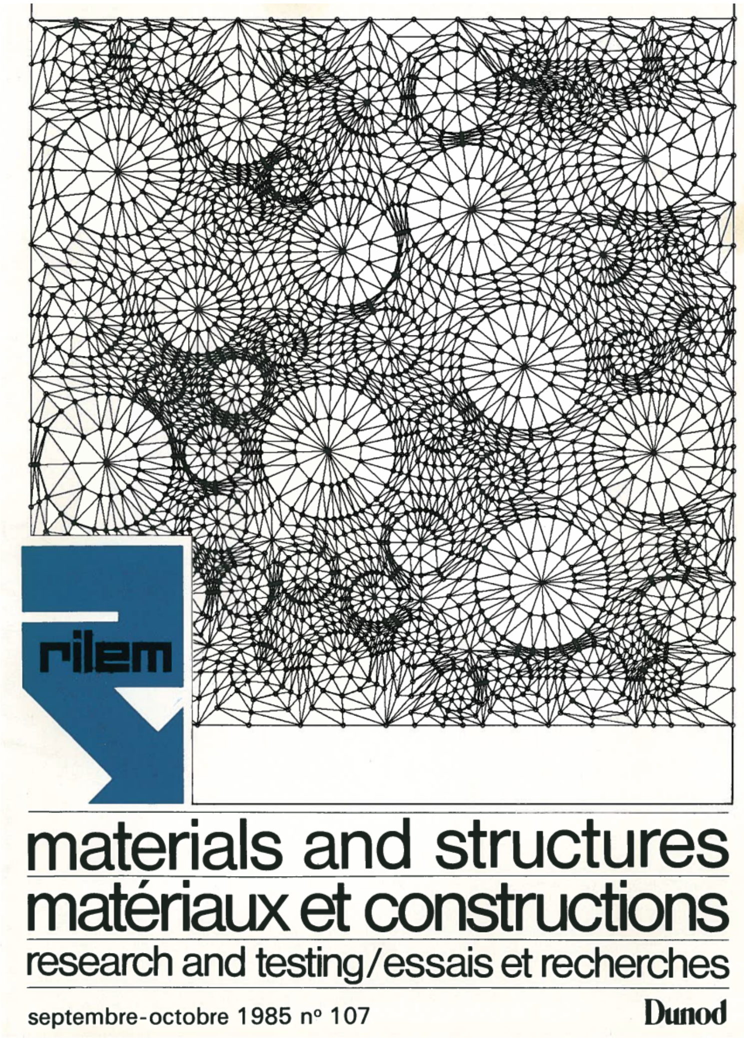


(b)

Intellectual Sources - Wittmann

- **Le béton numerique**
  Roelfstra, Sadouki, Wittmann, September, 1985

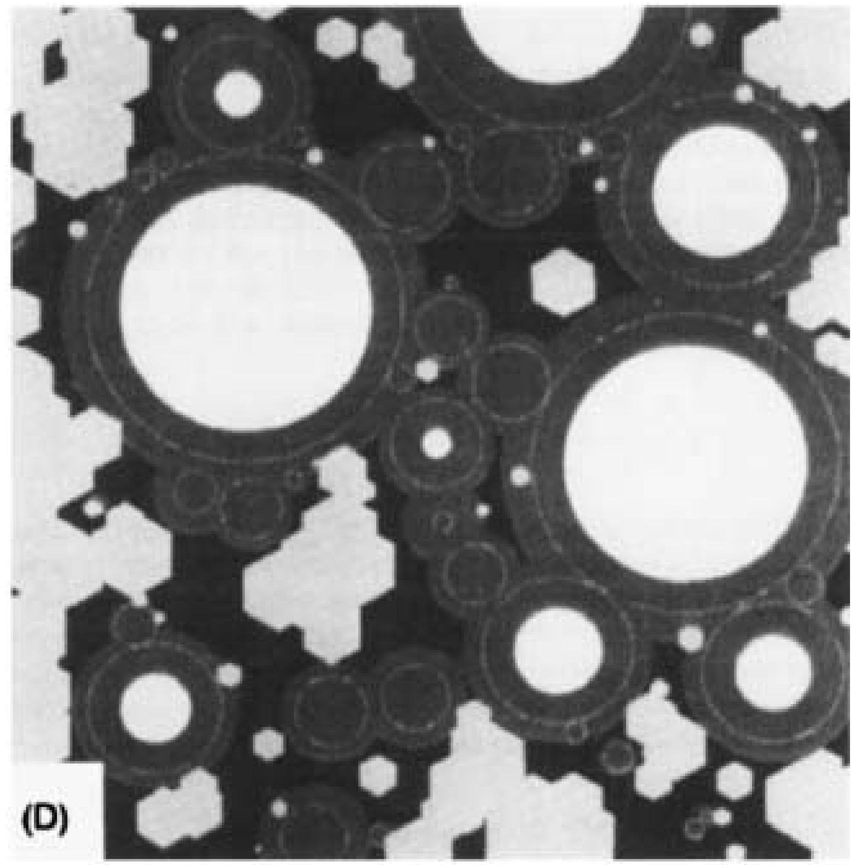
- Same idea - to provide a numerical framework upon which computations could be made and then compared to experiment



- Concrete structure in (2-D), later non-circular shape 2-D aggregates

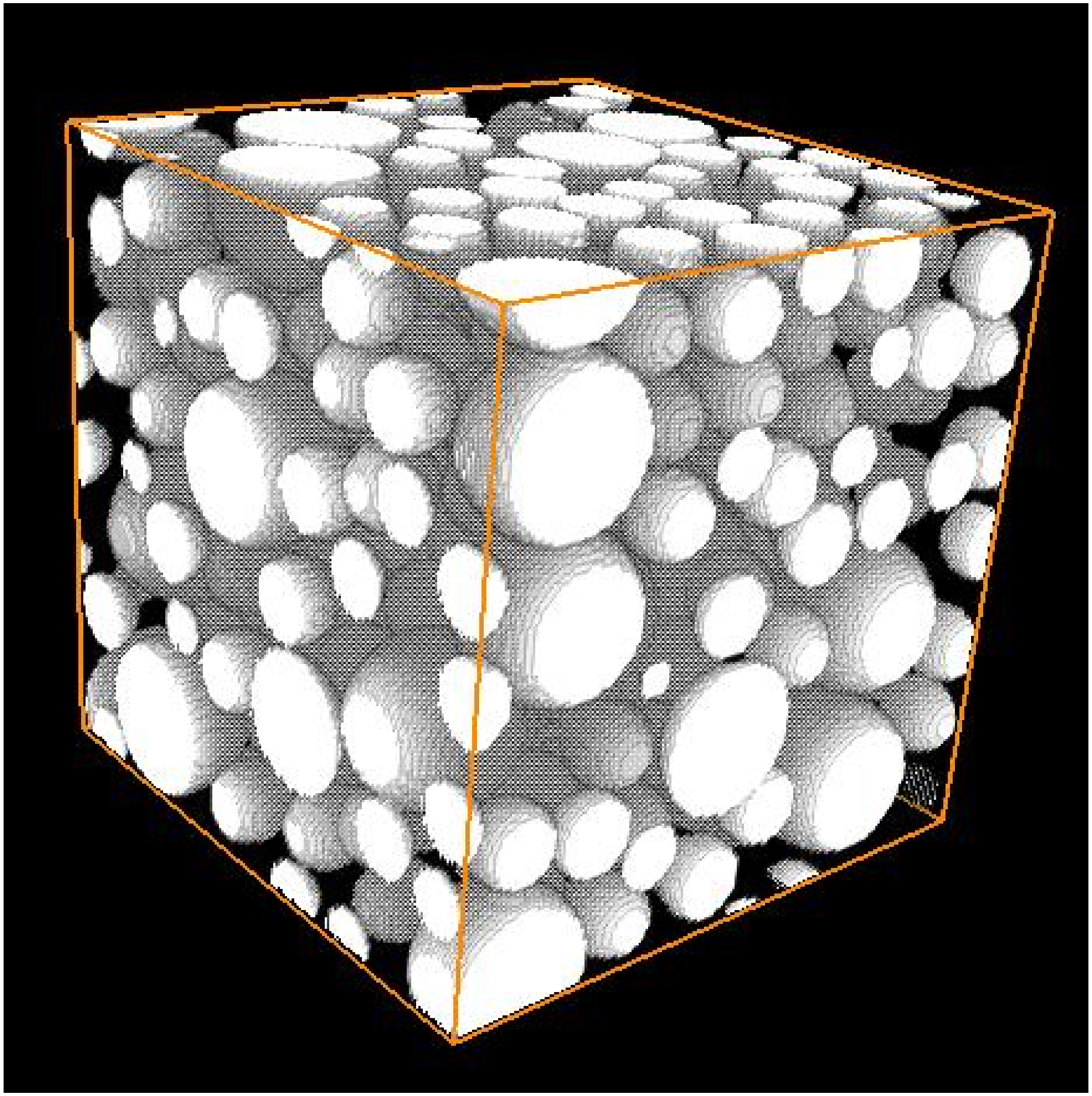
Intellectual Sources - Jennings

- Hamlin Jennings and Steve Johnson, 1986, American Ceramic Society Journal
- Formation of 3-D cement paste model, with hydration geometry



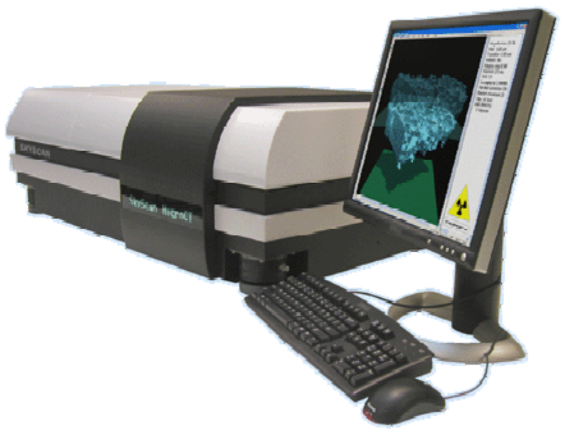
Continuing the story…

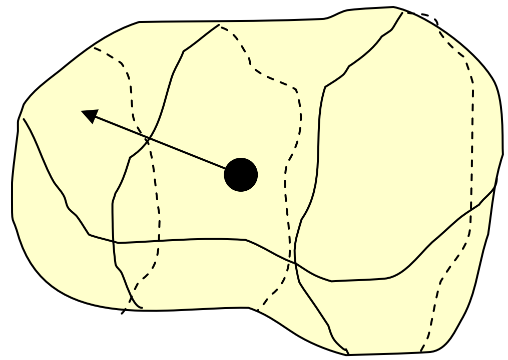
- I came to NIST in 1988, took over work on this model.
  - **major limitation was that no properties could be calculated**
- Random-walk algorithm to compute diffusivity of porous material was re-discovered by my friend Larry Schwartz at Schlumberger
- While at NIST, I learned digital images from Dale Bentz
- Combination of random walks and digital images led Dale and I to a new kind of digital image cement paste model whose random structure was built up by random walks
- Digital image format allowed the computation of any property, though with some restrictions on microstructure length scales
  - **Many new algorithms written for property computation**
  - **Realistic clinker mineralogy (Dale Bentz and Paul Stutzman)**



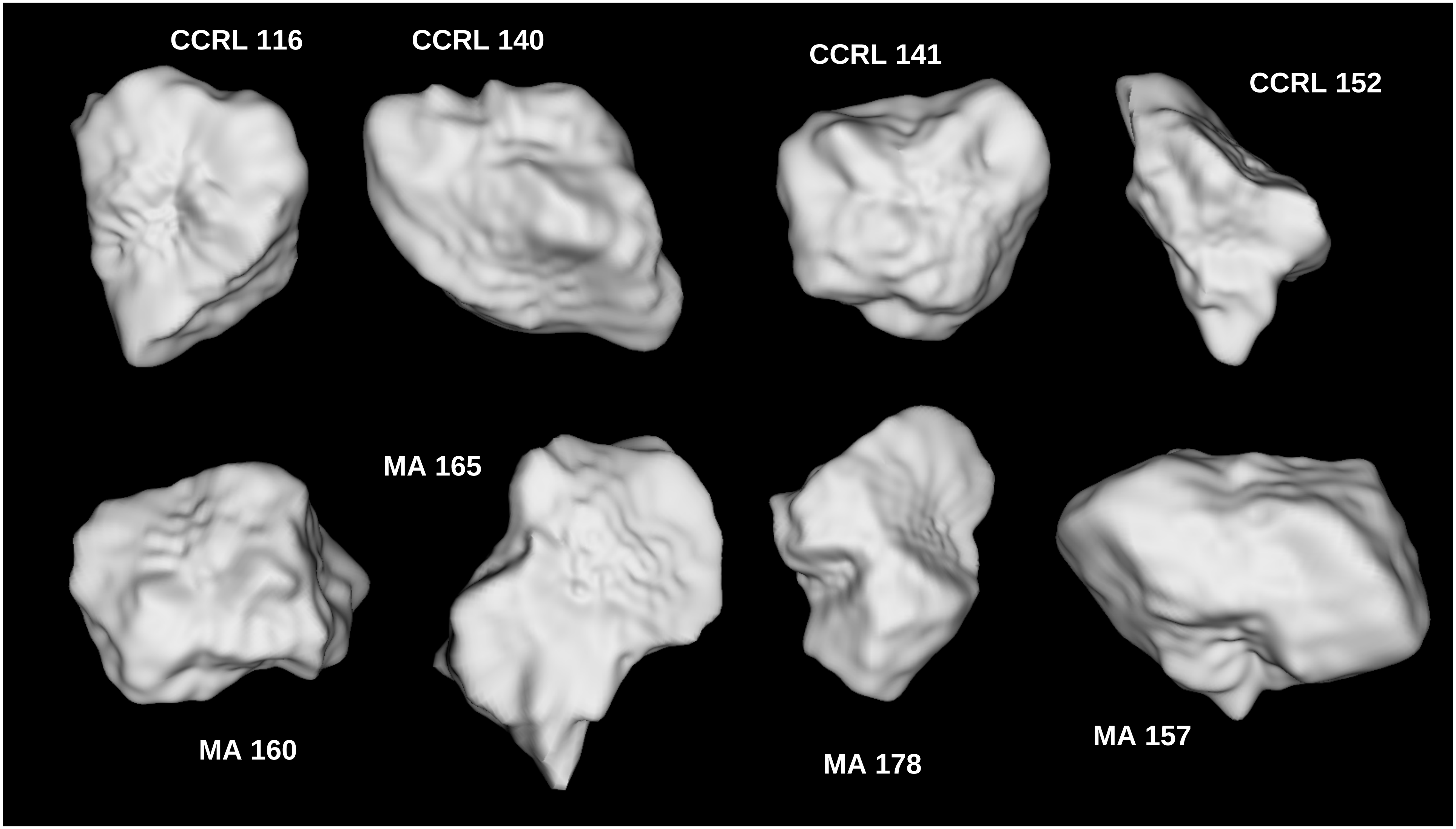
Spherical harmonic analysis and X-ray CT

- Define $r(\theta, \phi)$ from center of mass to surface





- Compute $r(\theta, \phi) = \Sigma_{n,m}\, a_{nm}\, Y_n^m(\theta, \phi)$
- Y_n^m = spherical harmonic function
- Comprehensive mathematical characterization of shape, n = 0 –20 or 30, $-n < m < n$
- *All shape and size information for particle is in the $(n+1)^2$ coefficients*


CCRL 116
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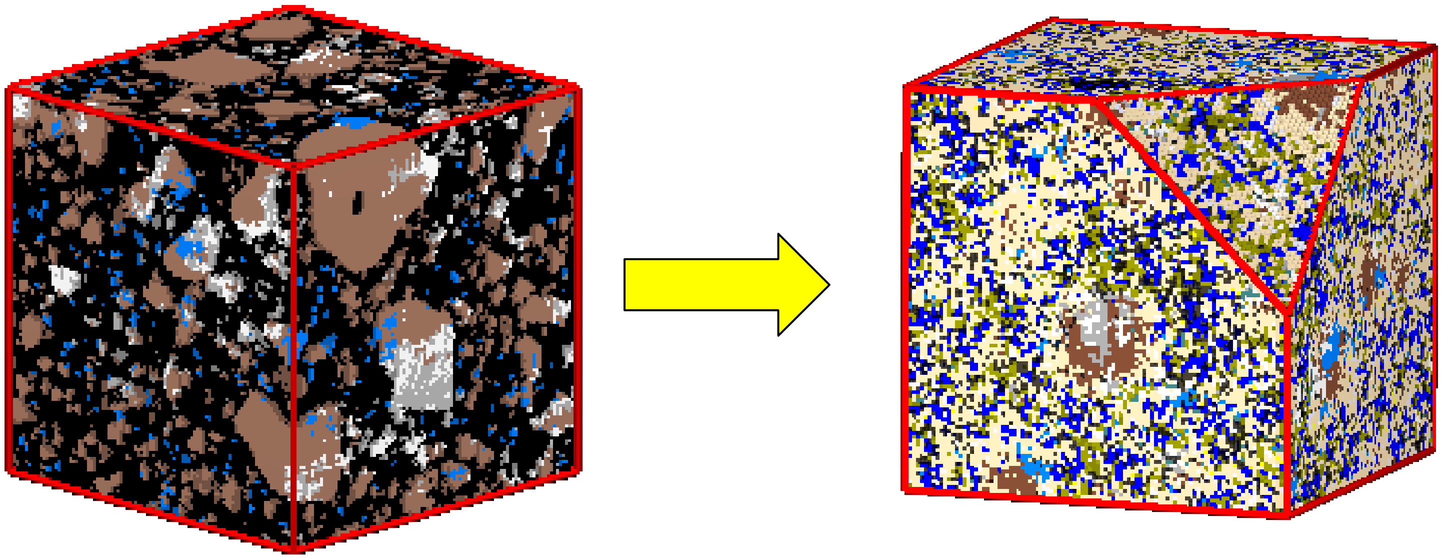
Cement Hydration (CEMHYD3D)

- Simulation of cement hydration, using realistic cement particles (chemistry and shape), producing a 3-D microstructure



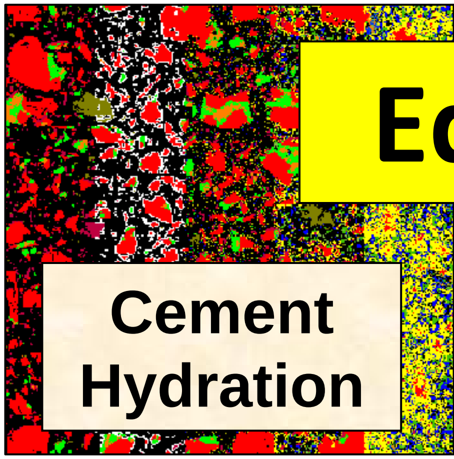
VCCTL

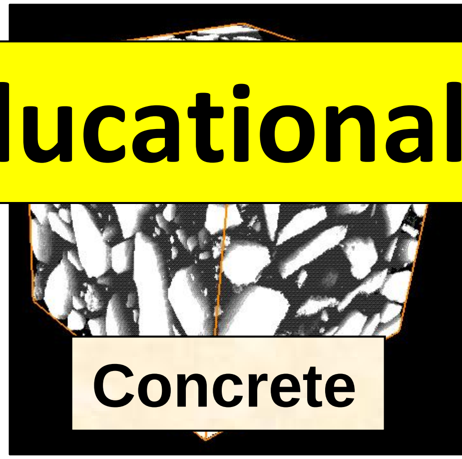
- Virtual Cement and Concrete Testing Laboratory
  - **Put many models together in integrated package**
  - **Micrometer to millimeter scale**
- SCG example of success
- “Desktop computing”
- But VCCTL becomes more effective with more computing power
  - **Multi-cores, more memory, etc.**

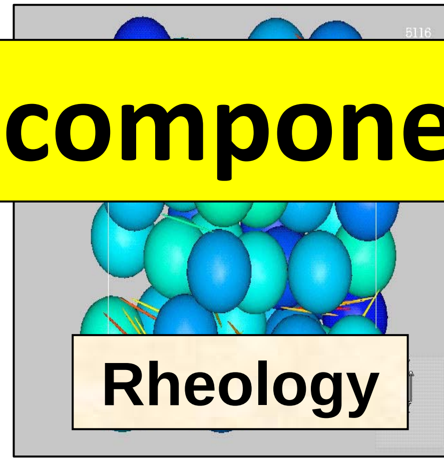
Simple vs. complex models

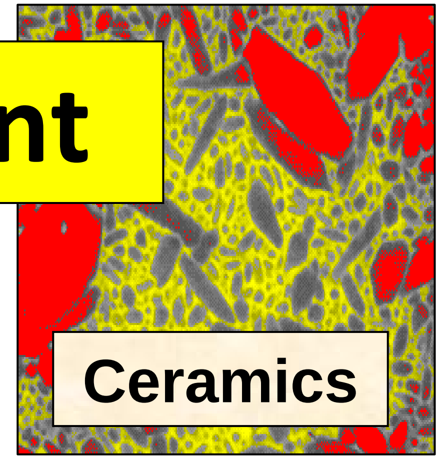
- Desktop computer vs. supercomputer models
  - **Don’t disparage the one by insisting that the other is the only valid approach**
  - **Difference between models that daily help industry, and models that help us understand complex, fundamental issues**
- Build simple, valid, non-fitting models by abstraction from validated, realistic, complex models
  - **"Everything should be made as simple as possible, but not simpler.“ (Einstein)**

Educational component

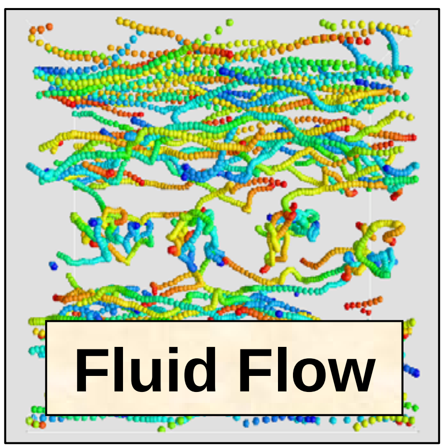


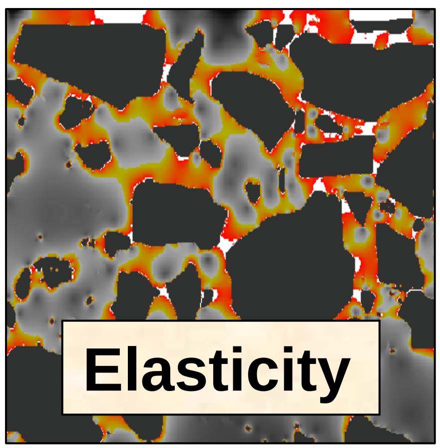


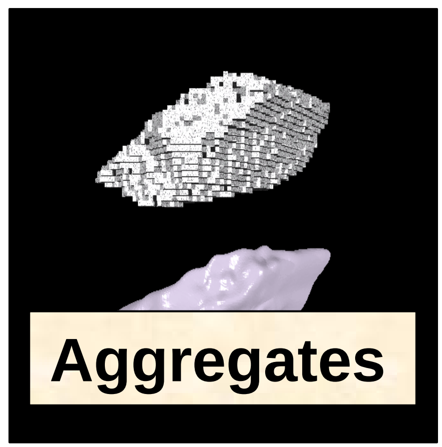


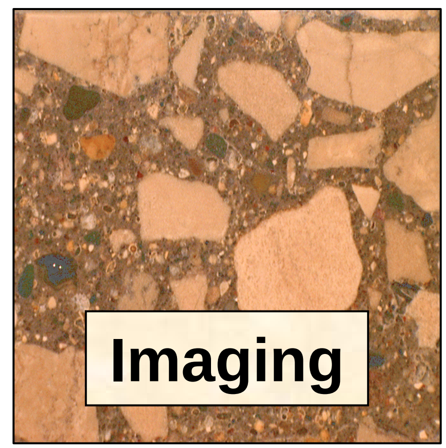


13th ACBM/NIST Computer Modelling Workshop June 10-13, 2002



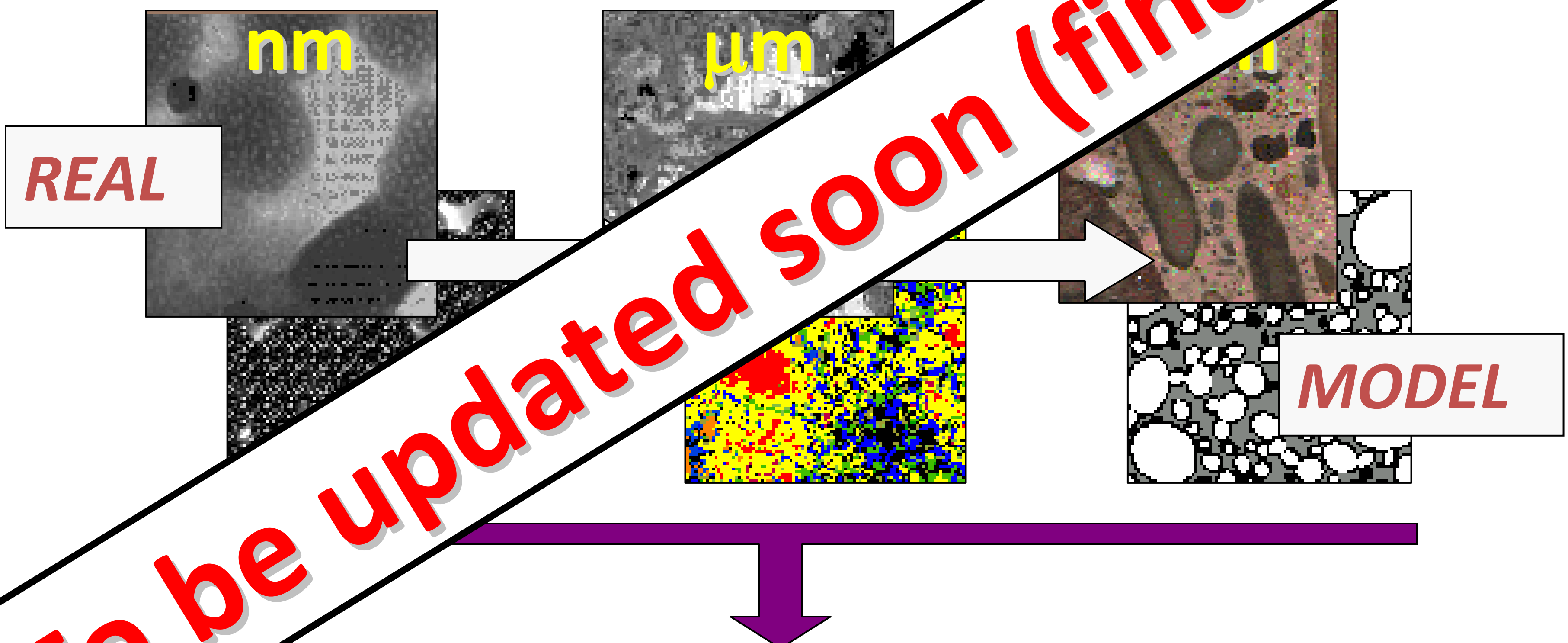






Modeling and Measuring the Structure and Properties of Cement-Based Materials

http://concrete.nist.gov/mono



To be updated soon (finally) !!!!

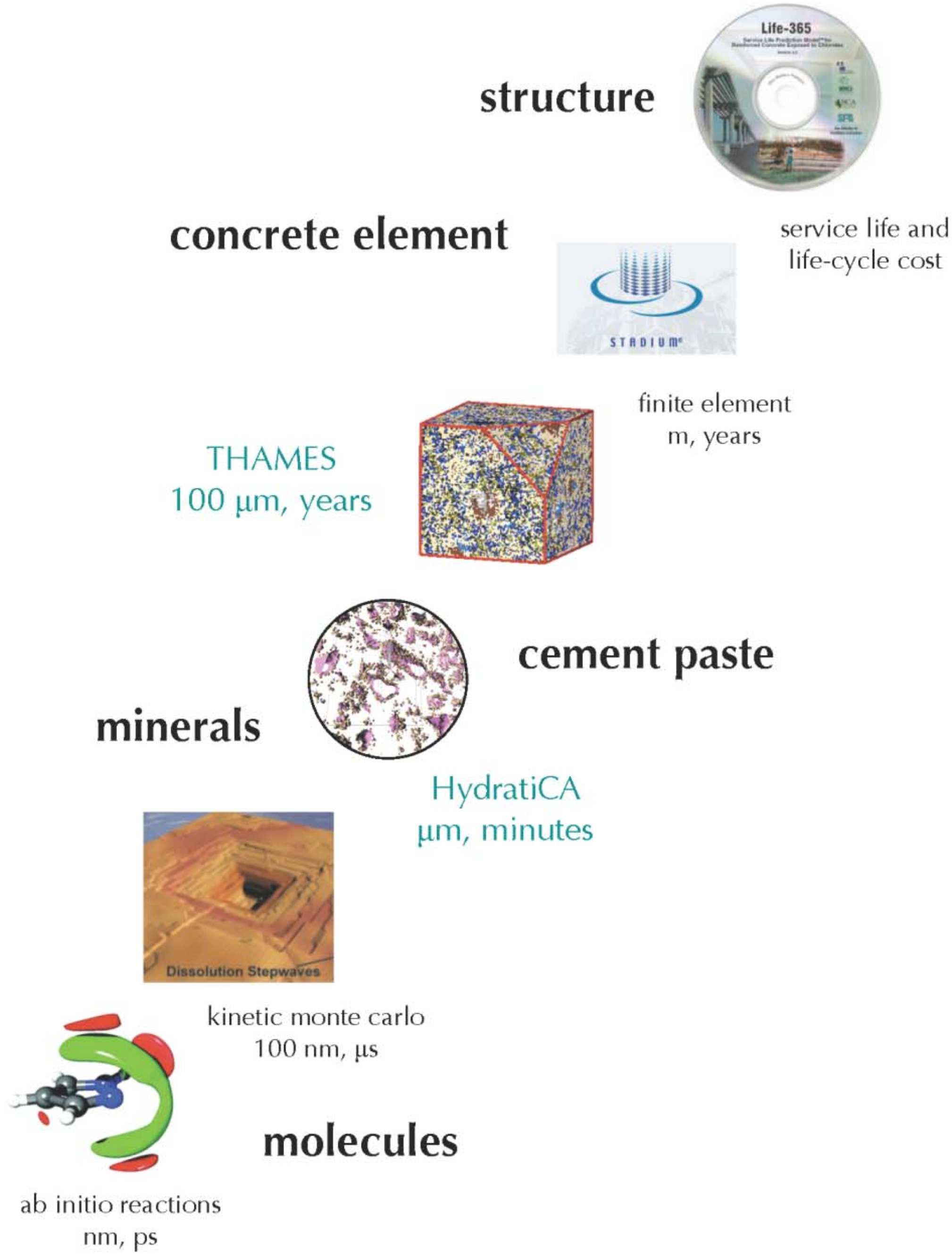
,000+ users from 90+ countries per month

Encouraging signs

- Much more computational work now than in the past, both US and Europe
- Civil engineers are doing molecular dynamics!
- Computer power is still increasing with parallel processing and GPUs
  - **The progress of this field goes hand in hand with progress in computer hardware and software**
- NSF likes to see combined experimental and computational approaches for cement-based materials
  - **Joint experimental-theoretical approach is best for fundamental advances in physics (e.g. Kepler-Newton)**

Encouraging signs

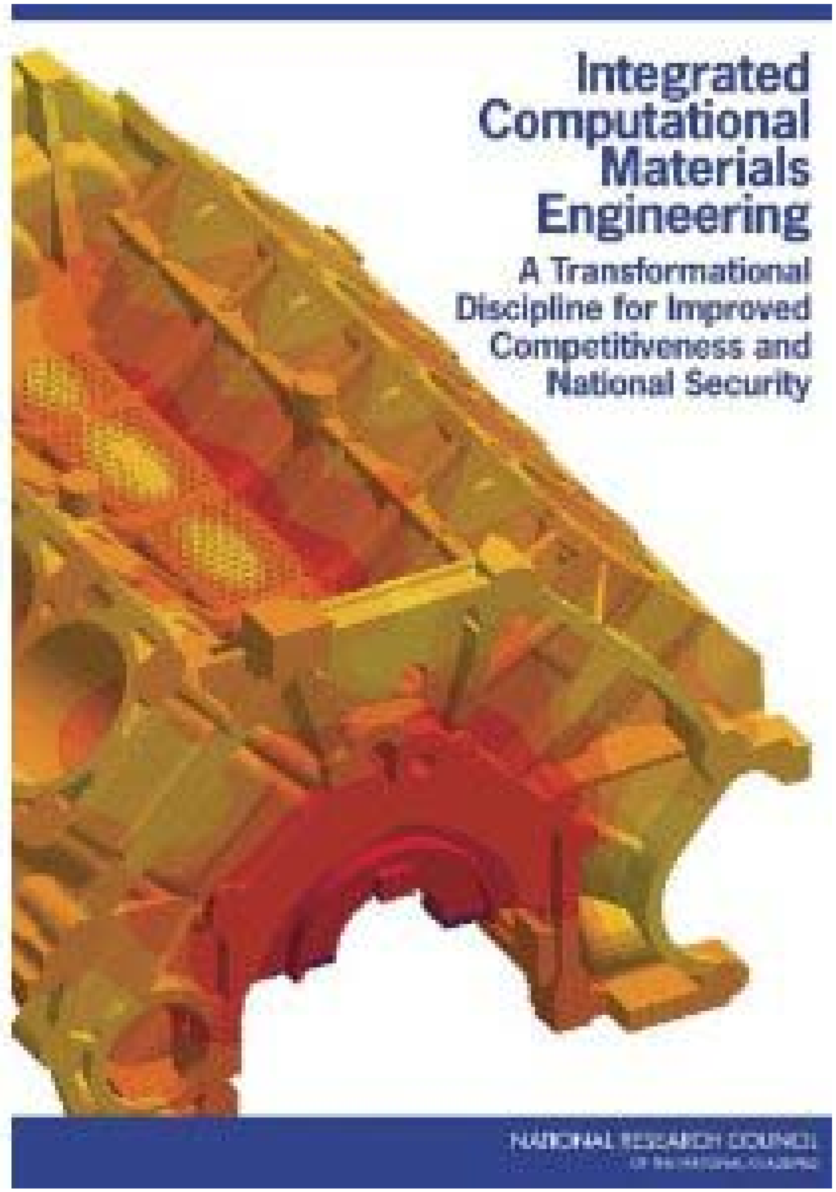
- Molecular and nanometer-scale models are starting to be generated at a number of institutions
  - **MIT work is funded by industry, which is very encouraging - e.g, PCA, RMC, Schlumberger**
- For the first time, we have the opportunity to start assembling a multi-scale suite of models, version 1.0
  - **There will be many gaps, but it is good to identify the gaps so we know where to focus attention**



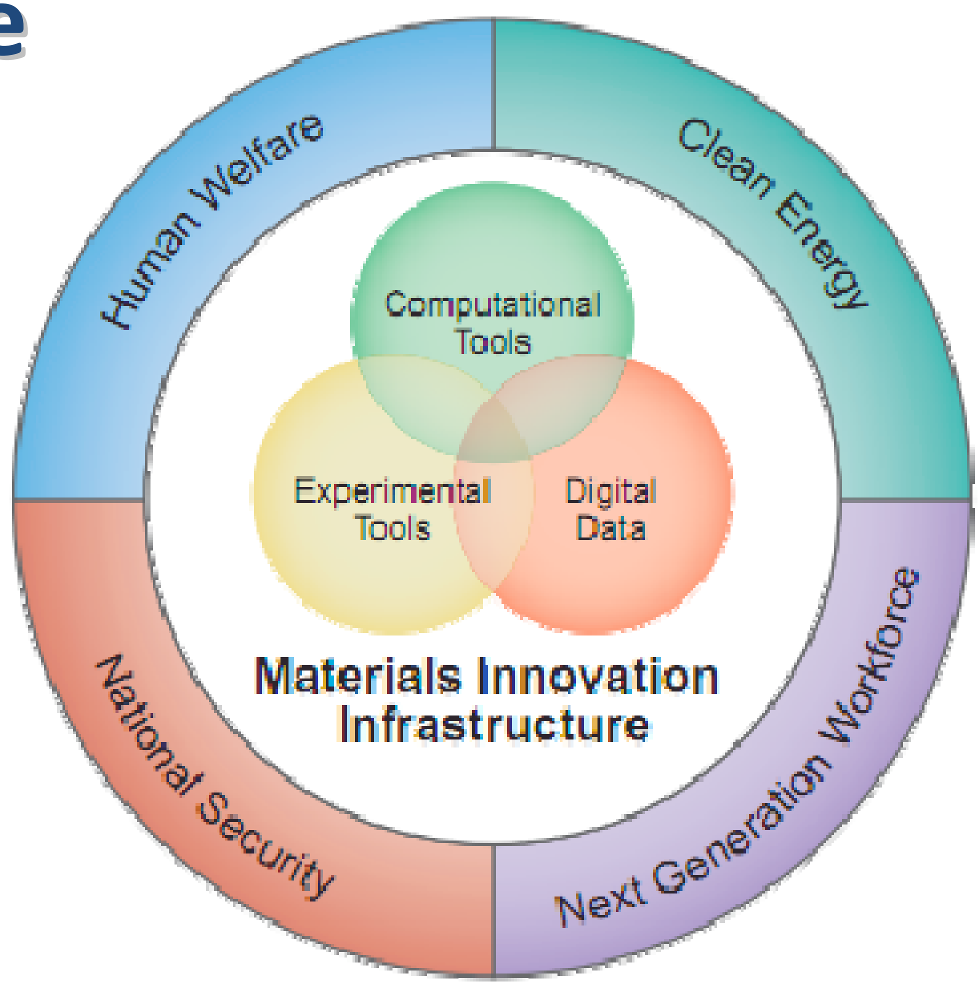
structure
Life-365
service life and
life-cycle cost
concrete element
STADIUM
finite element
m, years
THAMES
100 μm, years
cement paste
minerals
HydratiCA
μm, minutes
Dissolution Stepwaves
kinetic monte carlo
100 nm, μs
molecules
ab initio reactions
nm, ps

Integrated Computational Materials Engineering

- ICME
  - **US National Academy of Science**
- Idea that experiments must be performed together with computational models
- We have been doing that for 20 years!
  --**physics for 400 years**

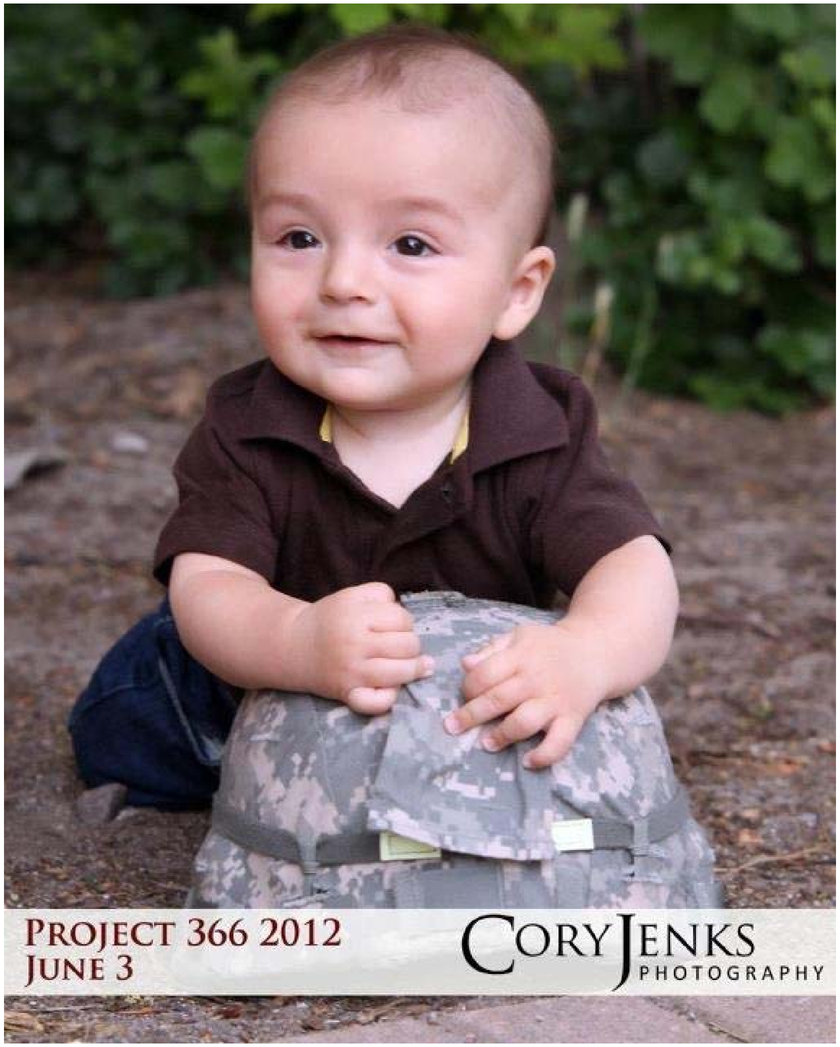


Materials Genome Initiative



- MGI
- Current focus, at least at NIST, is on alloys, polymer composites, **databases**, and information transfer
- Related to manufacturing
- Large opportunity for concrete, if we can take the models to the next step (details later)

Future materials scientist



Bruce Christian Garboczi Evans

Trends that are needed

- More trained people, more application of techniques (workshop, university courses)
- Processing power will grow without our help
- Need new algorithms to take advantage
  - **Parallel processing, GPU**
- Experiments and computations must be planned to work together from the start

Living off our seed corn…

- The heart of the computational materials science of concrete is building cement paste microstructure (and C-S-H nanostructure) by simultaneously modeling chemistry and the growth of structure
- But what measurements is this effort founded on?
- I would argue that the current amount of success is largely based on the measurements of the past
- But we have used up our seed corn – our models are still living off the past and can’t progress further without a new influx of experiments
- What new measurements must we do to progress and play at the ICME, MGI, and multi-scale level?

Experimental measurements needed

- **Basic hydration reactions**
  – Only broad form is known
  – Details of what phases form in solution not known
  – Rate constants are not known nor what are the rate-controlling mechanisms that determine the rate constants
- **Thermodynamics**
  – Solubility products of pure clinker phases and hydration products
  – Solubility limits of known impurities in clinker minerals and hydration products
  – Models of the activity of solute components at high ionic strengths

Experimental measurements needed

- **Dissolution of EACH cement mineral**
  - Rate of pure dissolution in isolation as a function of composition and temperature; undersaturation
  - Adsorption isotherm and rate for all common solution components on each clinker mineral surface
  - Influence of sorbed species on rate of dissolution in electrolytes as a function of surface absorbate concentration

Experimental measurements needed

- **Nucleation of EACH hydration product**
  - Nucleation rates for hydration products as function of solution composition and temperature
  - Nucleation mode in the presence of different surfaces
  - For heterogeneous nucleation, strength of adhesion of product to surface and ability of product to affect further dissolution of covered surface

Experimental measurements needed

- **Growth of EACH hydration product**
  - Rate of pure growth in supersaturated solution as function of temperature and supersaturation degree
  - Rate of uptake of various solution impurities in hydration products
  - How modification of composition via impurity uptake affects growth rate

Elastic properties analogy

- Task – calculate effective elastic moduli of concrete
- For each possible phase, you don't know
  - **Form of Hooke's law – linear or not?**
  - **Are its elastic properties time dependent or not?**
- When phases are assembled in the composite, important interphases form whose elastic properties are unknown
- AND, assume we know that the effective elastic moduli were very sensitive to these kinds of details
- Could YOU calculate the effective elastic moduli of concrete?
  - **Most powerful finite element solver in the world would be worthless**

Database

- Put all this information into a cement materials thermokinetic database
  - **NIST would be happy to host it**
- Validated experimental data from all over the world could feed into it – also molecular scale models
- To make effective use of this database, one will need to have good material characterization
- Who will pay for this?
  - **Need long-term, sustained, coordinated support**
  - **But once it is done, it is DONE!**
  - **Will be incredibly useful…**

What can you get?

- Confident predictions of time dependent properties, effect of new chemistries
  - **e.g. oil well cements, calcium sulfo-aluminate cements**
- Predict influence of chemical admixtures
  - **e.g. limiting volume beyond which is little additional effect**
- Inspire (not design) new chemical admixtures by running models to show possible effects of changes in mechanisms

What can you get?

- If SCM introduces the same kinds of phases/chemistry, then models will handle this accurately as well
  - **Still need to characterize SCM, along with any physical nucleation effects**
- Degradation reactions and time-dependent early-age rheology can be predicted
  - **Service life prediction**
  - **Need to combine mechanical/flow models with chemical models**
- And the list goes on…

Prospectus

- If we can develop this database:
- Concrete modeling will have the basis to reach the next level, be truly multi-scale, and be a paradigm of the ICME and the Materials Genome Initiative approach
- Someone will earn a lot of money as concrete will be able to be engineered to any application and make effective use of a wide range of component materials
- But the funding sources will have to be patient…
  - **“People love chopping wood. In this activity one immediately sees results.” (Albert Einstein)**

Future (from 2000 Francis Young retirement conference)

- Viscoelasticity, rheology
- Nanostructure of C-S-H
- Blended cement hydration and microstructure development
- Transport properties
- Simulation of long-term degradation processes
- Effect of degradation processes on concrete properties (effect of cracking)
- Prediction of tensile and compressive strength

Future (from 2000 Francis Young retirement conference)

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- Blended cement hydration and microstructure development
- Transport properties
- Simulation of long-term degradation processes
- Effect of degradation processes on concrete properties (effect of cracking)
- Direct prediction of tensile/compressive strength

Acknowledgments

- NIST colleagues
  - **Jeff Bullard, Dale Bentz, Paul Stutzman, Clarissa Ferraris, Nick Martys, Ken Snyder, Jack Douglas, Geoff Frohnsdorff, Jim Clifton**
- ACBM: Suru Shah, Francis Young, Tom Mason, Hamlin Jennings
  - **ACBM played a big role in starting my career in cement and concrete**
- Plus many, many other colleagues in academia and industry, in the US and abroad

Final personal thoughts

- “The most incomprehensible thing about the world is that it is comprehensible.” (Albert Einstein)
- I have enjoyed trying to bring comprehension to my own little part of concrete research, which itself is a very little part of the entire scientific endeavor

- Einstein was a far, far better physicist than I’ll ever be, but I do believe one thing about comprehensibility that he didn’t:
- “In the beginning, God created the heavens and the earth”
  - **we were created in His image, so the universe, also His creation, is in general comprehensible to us**
- I think that makes science ultimately worth pursuing…and a lot more interesting…