Multiscale Modeling of Alkali Silica Reaction Deterioration of Concrete Structures

Gianluca Cusatis

1st Zdeněk P. Bažant (ZPB) FraMCoS Workshop
Berkeley, CA (USA)

May 29, 2016
Acknowledgments

Collaborators

- Mohammed Alnaggar, RPI, Troy (NY), USA.
- Jianmin Qu, Tufts University, Boston (MA), USA.
- Roozbeh Rezakhani, Northwestern University, Evanston (IL), USA.
- Daniele Pelessone, Xinwei Zhou, ES3, San Diego (CA), USA.
- Giovanni Di Luzio, Politecnico di Milano, Milan, Italy.

Financial Support

- National Science Foundation (NSF)
- Department of Homeland Security
- Nuclear Regulatory Commission
Introduction

Alkali Silica Reaction (ASR) Model

The Lattice Discrete Particle Model (LDPM)

Numerical Simulations

Interpretation of Nonlinear Ultrasound Measurements

Mathematical Homogenization

Conclusions
Example of Deterioration: Alkali Silica Reaction (ASR)

Dams

Bridges

Nuclear Power Plants

Townsend Lake Dam, North Carolina
USA 1967

Cracking noticed, Repairs done in the late 1970s

Guess What?
 Didn’t work!!!
Replacement Started 2009
Example of Deterioration: Alkali Silica Reaction (ASR)

Dams

Townsend Lake Dam, North Carolina, USA 1967
Cracking noticed, Repairs done in the late 1970s

Bridges

1 of 9 Bridges in US is STRUCTURALLY DEFICIENT

Historic 6th Street viaduct, Los Angeles, CA, USA built in 1932
Guess What? Didn’t work!!! Replacement Started 2009
Repairs? … Did’t work, rebuilding in 2015

Nuclear Power Plants
Example of Deterioration: Alkali Silica Reaction (ASR)

Dams
- Townsend Lake Dam, North Carolina, USA 1967
- Cracking noticed, Repairs done in the late 1970s

Bridges
- 1 of 9 Bridges in US is STRUCTURALLY DEFICIENT
- Historic 6th Street viaduct, Los Angeles, CA, USA built in 1932
- Repairs? ..... Didn’t work, rebuilding in 2015

Nuclear Power Plants
- Seabrook Nuclear Power Plant, New Hampshire, USA, 1986
- In 2009 Concrete Foundation Walls lost 22% of its original Strength due to ASR

FraMCoS ZPB 2016 :: G Cusatis
Alkali Silica Reaction (ASR) in a Nutshell

- Chemical Reaction (Very simplistic description)

- Mechanical Deterioration
Concrete is a Multiscale Material

---

**Material Science**

**Mechanics**

**Structural Engineering**

---

**I: Full Structure Scale**

**II: Structural Element Scale**

**III: Plain Concrete Scale**

**IV: Concrete Mesoscale**

**V: Mortar Scale**

**VI: Cement Paste Scale**

**VII: C-S-H Scale**

---

< $10^{-5}$ $10^{-4}$ $10^{-3}$ $10^{-2}$ $10^{-1}$ $10^{0}$ $10^{1}$ $10^{2}$ $L$ [m]

---

FraMCoS ZPB 2016 :: G Cusatis
Concrete is a Multiscale Material

**Material Science**

**Mechanics**

**Structural Engineering**
Concrete is a Multiscale Material

- **VII:** C-S-H Scale
- **VI:** Cement Paste Scale
- **V:** Mortar Scale
- **IV:** Concrete Mesoscale
- **III:** Plain Concrete Scale
- **II:** Structural Element Scale
- **I:** Full Structure Scale

Scale:
- $< 10^{-5}$
- $10^{-4}$
- $10^{-3}$
- $10^{-2}$
- $10^{-1}$
- $10^0$
- $10^1$
- $10^2$

- **Material Science**
- **Mechanics**
- **Structural Engineering**
Concrete is a Multiscale Material

**Material Science**

**Mechanics**

**Structural Engineering**

**Scale**

- **I:** Full Structure Scale
- **II:** Structural Element Scale
- **III:** Plain Concrete Scale
- **IV:** Concrete Mesoscale
- **V:** Mortar Scale
- **VI:** Cement Paste Scale
- **VII:** C-S-H Scale

**Dimensions**

\[ L [m] \]

- \(< 10^{-5} \]
- \(10^{-4} \]
- \(10^{-3} \]
- \(10^{-2} \]
- \(10^{-1} \]
- \(10^{0} \]
- \(10^{1} \]
- \(10^{2} \]

**Scales**

- **I:** Full Structure Scale
- **II:** Structural Element Scale
- **III:** Plain Concrete Scale
- **IV:** Concrete Mesoscale
- **V:** Mortar Scale
- **VI:** Cement Paste Scale
- **VII:** C-S-H Scale

**Introduction**

FraMCoS ZPB 2016 :: G Cusatis

Northwestern ENGINEERING

6 / 52
Definition of Multiscale Modeling

Given

1. A specific engineering problem and
2. A fine-scale model of reference

A multiscale model is

an approximation of the fine-scale solution characterized by the max accuracy for a given acceptable cost or the min cost for a given required accuracy

- Accuracy must evaluated against a Calibrated and Validated fine scale model of reference to avoid “Garbage-down, Garbage-up”
- Cost is application and resource dependent.
Available Multiscale Methods

- **Information Passing** - Discretized subscale material element is embedded into a point of the macro-scale continuum (an integration point of a finite element (e.g. Computational homogenization, mathematical homogenization, microplane model, etc.))

- **Concurrent** - A finite region of the macro-continuum coarse mesh is overlapped or replaced by a fine mesh or discrete sub-structure (meso-structure) model representing the subscale (e.g. Variational multiscale method, bridging scale method, multigrid methods).

- **Coarse-graining**  Coarse and fine scale models are both discrete and one particle of the coarse scale simulate the behavior of a certain number of fine-scale particles.
## Multiscale Computational Framework

<table>
<thead>
<tr>
<th>Miniscale</th>
<th>Mesoscale</th>
<th>Macroscale</th>
</tr>
</thead>
<tbody>
<tr>
<td>- ASR gel formation&lt;br&gt;- Water imbibition&lt;br&gt;- ASR Gel expansion&lt;br&gt;- Length scale from $\mu$m to mm</td>
<td>- Cracking&lt;br&gt;- Creep and Shrinkage&lt;br&gt;- Length scale of mm to cm</td>
<td>- Strength and Stiffness&lt;br&gt;- Degradation&lt;br&gt;- Length scale of cm to m</td>
</tr>
</tbody>
</table>
Presentation Outline

1. Introduction
2. Alkali Silica Reaction (ASR) Model
3. The Lattice Discrete Particle Model (LDPM)
4. Numerical Simulations
5. Interpretation of Nonlinear Ultrasound Measurements
6. Mathematical Homogenization
7. Conclusions
ASR Model :: Assumptions

Simplifying a very complex phenomenon

- The aggregate particles are assumed to have spherical shape.
- Silica is assumed to be smeared uniformly over the aggregate volume.
- The dissolution of silica is assumed to progress in a uniform manner in the radial direction inward from the surface towards the particle center.
- The expansion of ASR gel is mostly due to water imbibition.
- Continuous supply of water is needed for the swelling to continue over time.
**Reaction front:**

\[
\dot{z} = -a_s(h, T)w_e(h, \alpha_c)/[r_w c_s \dot{z} (1 - \frac{2z}{D})]
\]

**ASR Gel permeability:**

\[
a_s = e^{\left(\frac{E_{aq}}{RT_0} - \frac{E_{aq}}{RT}\right)} a_s^1 \left[1 + \left(\frac{a_s^1}{a_s^0} - 1\right) (1 - h)^n_z\right]^{-1}
\]

**ASR Gel Mass:**

\[
M_g = \kappa_a \frac{\pi}{6} (D^3 - 8z^3) c_s \frac{m_g}{m_s}
\]

**Effect of Alkali Content:**

\[
\kappa_a = \min\left(\langle c_a - c_a^0 \rangle / (c_a^1 - c_a^0), 1\right)
\]
Reactor front:
\[
\dot{z} = -a_s(h, T)w_e(h, \alpha_c) \left[ r_w c_s z \left( 1 - \frac{2z}{D} \right) \right]
\]

ASR Gel permeability:
\[
a_s = e^{\left( \frac{E_{a_g}}{R T_0} - \frac{E_{a_g}}{R T} \right)} a_s^1 \left[ 1 + \left( \frac{a_s^1}{a_s^0} - 1 \right) (1 - h)^n z \right]^{-1}
\]

ASR Gel Mass:
\[
M_g = \kappa_a \pi \frac{m_g}{m_s} \left( D^3 - 8z^3 \right)
\]

Effect of Alkali Content:
\[
\kappa_a = \min \left( \frac{\langle c_a - c_a^0 \rangle}{(c_a^1 - c_a^0)}, 1 \right)
\]
Reaction front:

\[ \dot{z} = -a_s(h, T)w_e(h, \alpha_c)/[r_w c_s z (1 - \frac{2z}{D})] \]

ASR Gel permeability:

\[ a_s = e^{\left( \frac{E_{ag}}{RT_0} - \frac{E_{ag}}{RT} \right)} a_s^1 \left[ 1 + \left( \frac{a_s^1}{a_s^0} - 1 \right) (1 - h)^n Z \right]^{-1} \]

ASR Gel Mass:

\[ M_g = \kappa_a \pi \frac{D^3}{6} (D^3 - 8z^3) c_s m_g/m_s \]

Effect of Alkali Content:

\[ \kappa_a = \min(\langle c_a - c_a^0 \rangle/(c_a^1 - c_a^0), 1) \]
**ASR Model :: Gel Formation**

**Reaction front:**
\[
\dot{z} = -a_s(h, T)w_e(h, \alpha_c)/\left[r_w c_s z \left(1 - \frac{2z}{D}\right)\right]
\]

**ASR Gel permeability:**
\[
a_s = e^{\left(\frac{E_{ag}}{RT_0} - \frac{E_{ag}}{RT}\right)}a_1^s \left[1 + \left(\frac{a_1^s}{a_0^s} - 1\right)(1 - h)^{nnz}\right]^{-1}
\]

**ASR Gel Mass:**
\[
M_g = \kappa_a \frac{\pi}{6} \left(D^3 - 8z^3\right) c_s \frac{m_g}{m_s}
\]

**Effect of Alkali Content:**
\[
\kappa_a = \min\left(\frac{\langle c_a - c_{a0}^0 \rangle}{(c_a^1 - c_{a0}^0)}, 1\right)
\]
Driving force (Thermodynamic Affinity) :

\[ A_i = \kappa_i^0 \exp\left(\frac{E_{ai}}{RT_0} - \frac{E_{ai}}{RT}\right) M_g - M_i \]

Imbibition Characteristic time :

\[ \tau_i = \delta^2 / C_i \]

Water Imbibition Coefficient :

\[ C_i = C_i^1 \exp(-\eta M_i) (1 + (C_i^1 / C_i^0 - 1)(1 - h)^n_M)^{-1} \]

Water Imbibition Rate :

\[ \dot{M}_i = A_i / \tau_i \]
### Driving force (Thermodynamic Affinity):

\[
A_i = \kappa_i^0 \exp \left( \frac{E_{ai}}{RT_0} - \frac{E_{ai}}{RT} \right) M_g - M_i
\]

### Imbibition Characteristic time:

\[
\tau_i = \frac{\delta^2}{C_i}
\]

### Water Imbibition Coefficient:

\[
C_i = C_i^1 \exp(-\eta M_i)(1 + (C_i^1/C_i^0 - 1)(1 - h)^n_M)^{-1}
\]

### Water Imbibition Rate:

\[
\dot{M}_i = \frac{A_i}{\tau_i}
\]
Driving force (Thermodynamic Affinity):

\[ A_i = \kappa_i^0 \exp \left( \frac{E_{a_i}}{RT_0} - \frac{E_{a_i}}{RT} \right) M_g - M_i \]

Imbibition Characteristic time:

\[ \tau_i = \delta^2 / C_i \]

Water Imbibition Coefficient:

\[ C_i = C_i^1 \exp(-\eta M_i)(1 + (C_i^1 / C_i^0 - 1)(1 - h)^{n_M})^{-1} \]

Water Imbibition Rate:

\[ \dot{M}_i = \frac{A_i}{\tau_i} \]
Driving force (Thermodynamic Affinity):

$$A_i = \kappa_i^0 \exp \left( \frac{E_{ai}}{RT_0} - \frac{E_{ai}}{RT} \right) M_g - M_i$$

Imbibition Characteristic time:

$$\tau_i = \delta^2 / C_i$$

Water Imbibition Coefficient:

$$C_i = C_i^1 \exp(-\eta M_i)(1 + (C_i^1 / C_i^0 - 1)(1 - h)^{n_M})^{-1}$$

Water Imbibition Rate:

$$\dot{M}_i = \frac{A_i}{\tau_i}$$
Introduction

Alkali Silica Reaction (ASR) Model

The Lattice Discrete Particle Model (LDPM)

Numerical Simulations

Interpretation of Nonlinear Ultrasound Measurements

Mathematical Homogenization

Conclusions
Facet Strains

\[ \epsilon_\alpha = \frac{1}{r} [\mathbf{u}_C] \cdot \mathbf{e}_\alpha; \quad [\mathbf{u}_C] = \frac{1}{r} \left( \mathbf{U}^J + \Theta^J \times \mathbf{c}^J - \mathbf{U}^I - \Theta^I \times \mathbf{c}^I \right) \]
Constitutive Laws

- Fracture and cohesion due to tension and tension-shear
  \[ \varepsilon = \sqrt{\varepsilon_N^2 + \alpha (\varepsilon_M^2 + \varepsilon_L^2)} \]
  \[ t = \sqrt{t_N^2 + (t_M + t_L)^2} / \alpha \]
  \[ t_N = (t/\varepsilon) \varepsilon_N; \quad t_M = \alpha (t/\varepsilon) \varepsilon_M; \quad t_L = \alpha (t/\varepsilon) \varepsilon_L. \]
  \[ \sigma_{bt} = \sigma_0(\omega) \exp \left[ -H_0(\omega) \langle \varepsilon - \varepsilon_0(\omega) \rangle / \sigma_0(\omega) \right]; \]

- Compaction and pore collapse from compression
  \[ -\sigma_{bc}(\varepsilon_D, \varepsilon_V) \leq t_N \leq 0; \quad \sigma_{bc} = \sigma_c + \langle -\varepsilon_V - \varepsilon_{c0} \rangle H_c(r_{DV}); \]

- Frictional Behavior
  \[ \dot{t}_M = E_T(\dot{\varepsilon}_M - \dot{\varepsilon}_p^M); \quad \dot{t}_L = E_T(\dot{\varepsilon}_L - \dot{\varepsilon}_p^L); \]
  \[ \varphi = \sqrt{t_M^2 + t_L^2} - \sigma_{bs}(t_N) \]
  \[ \sigma_{bs} = \sigma_s + (\mu_0 - \mu_\infty) \sigma_{N0} [1 - \exp(t_N / \sigma_{N0})] - \mu_\infty t_N \]

Translational and rotational equilibrium equations of each particle

\[ M_u^I \ddot{U}^I - V^I b^0 = \sum_{\mathcal{F}_I} A t^{IJ} \]
\[ M_\theta^I \ddot{\Theta}^I = \sum_{\mathcal{F}_I} A (c^I \times t^{IJ} + m^{IJ}) \]
LDPM :: Some Results

Tensile Fracture

Unconfined Compression

Biaxial Loading

Triaxial Compression

The Lattice Discrete Particle Model (LDPM)
Unconfined Compression, Cont.

**Figure:** Unconfined compressive behavior. a) Contours of meso-scale crack opening at failure for low friction boundary conditions; b) Contours of meso-scale crack opening at failure for high friction boundary conditions.
Figure: a) Low friction coefficient \( \mu(s) = \mu_d + (\mu_s - \mu_d)s_0/(s_0 + s) \), \( \mu_s = 0.03 \), \( \mu_d = 0.0084 \), and \( s_0 = 0.0195 \) mm; b) Stress-strain curves for cubes; c) Lateral expansion for cubes; d) Stress-strain curves for very short prisms; e) Stress-strain curves for short prisms; f) Stress-strain curves for long prisms.
LDPM :: Even More Results

Over Reinforced Beam

Deep Beam in Shear
Amalgamation of ASR Model with LDPM

- Radius increase of each aggregate particle:
  \[ r_i = \left( \frac{3M_i}{4\pi \rho_w} + r^3 \right)^{1/3} - r \]

- Normal meso-scale eigenstrain:
  \[ e_{N}^{a} = \langle (r_{i1} + r_{i2})/2 - \delta_c \rangle / \ell \]
  for \( \zeta = 0 \) and \( \dot{e}_{N}^{a} = 0 \)

- Incremental LDPM strain:
  \[ \Delta \epsilon^{*} = \Delta \epsilon - \Delta \epsilon_{a}^{a} \]

Limitations. The formulation does not account explicitly for:
- ... the actual chemistry of gel formation.
- ... multi ion transport.
- ... gel expansion into pores and cracks.
- ... non-uniform silica distribution within the aggregate.
- ... local water diffusion through (a) pores, (b) cracks; and (c) gel.
Radius increase of each aggregate particle $r_i = \left( \frac{3M_i}{4\pi \rho_w} + r^3 \right)^{1/3} - r$

Normal meso-scale eigenstrain
$$e_{N}^a = \langle (r_{i1} + r_{i2})/2 - \delta_c \rangle/\ell$$ and $\dot{e}_{N}^a = 0$ for $\zeta = 0$

$$e_{M}^a = e_{L}^a = 0 \rightarrow \epsilon^a = [e_{N}^a \ 0 \ 0]^T$$

Incremental LDPM strain
$$\Delta \epsilon^* = \Delta \epsilon - \Delta \epsilon^a$$

Limitations. The formulation does not account explicitly for ...

- the actual chemistry of gel formation.
- multi ion transport.
- gel expansion into pores and cracks.
- non-uniform silica distribution within the aggregate.
- local water diffusion through (a) pores, (b) cracks; and (c) gel.
Model Calibration


Simulated 1: No Creep nor Shrinkage

![Graph showing volumetric strain over time for experimental and simulated cases.]

- Experimental
- Simulated 1
- Simulated 2
- Simulated 3

Sealed

240 mm

130 mm
Model Calibration


Simulated 1: No Creep nor Shrinkage

Simulated 2: Creep + Experimental Shrinkage

Sealed

240 mm

130 mm
Model Calibration


Simulated 1: No Creep nor Shrinkage

Simulated 2: Creep + Experimental Shrinkage

Simulated 3: Creep + Code Shrinkage

Volumetric Strain [%]

Time [days]

Experimental

Simulated 1

Simulated 2

Simulated 3

Sealed

240 mm

130 mm
Validation :: Stress Effect - Axial Stresses

Vertical applied stress: 0, 10, 20 MPa

Unrestrained
Validation :: Stress Effect - Axial Stresses

Vertical applied stress:
0, 10, 20 MPa

Unrestrained

Vertical applied stress:
0, 10, 20 MPa

Confined by 3mm steel rings

Experimental
Simulated 1
Simulated 2
Simulated 3
Validation :: Stress Effect - Axial Stresses

Vertical applied stress: 0, 10, 20 MPa
Unrestrained

Vertical applied stress: 0, 10, 20 MPa
Confined by 3mm steel rings

Vertical applied stress: 0, 10, 20 MPa
Confined by 5mm steel rings

Numerical Simulations
FraMCoS ZPB 2016 :: G Cusatis
Animation of Damage Evolution

- Free Expansion
- 20 MPa / Unrest.
- 00 MPa / Rest.
Presentation Outline

1. Introduction
2. Alkali Silica Reaction (ASR) Model
3. The Lattice Discrete Particle Model (LDPM)
4. Numerical Simulations
5. Interpretation of Nonlinear Ultrasound Measurements
6. Mathematical Homogenization
7. Conclusions
1D nonlinear wave propagation
\[ \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial X^2} \left( 1 + \beta \frac{\partial u}{\partial X} \right) \]

Solution with perturbation analysis
\[ u = -\frac{1}{8} \beta k^2 A_1^2 X + A_1 \cos(kX - \omega t) + \frac{1}{8} \beta k^2 A_1^2 X \cos[2(kX - \omega t)] + \ldots \]
\[ = A_0 + A_1 \cos(kX - \omega t) + A_2 \cos[2(kX - \omega t)] + \ldots \]

Acoustic Nonlinearity Parameter (ANLP)
\[ \beta = \frac{8 A_2}{k^2 L A_1^2} \propto \frac{A_2}{A_1^2} \]

How does it relate to damage?
Accelerated Mortar Bar Test with ANLP testing

1”x1”x10”

4”x4”x10”

Pie charts and graphs showing expansion and normalized amplitude over exposure time.
Alkali Ion Macro Diffusion

Nonlinear Alkali ion diffusion model

\[
\frac{dc_i}{dt} = \nabla \cdot \left( D_i(c_i) \nabla c_i \right) \quad \text{With} \quad D_i(c_i) = D_i^1 \left[ 1 + \left( \frac{D_i^1}{D_i^0} - 1 \right) \left( 1 - \frac{c_i}{c_{i,\text{max}}} \right)^{n_i} \right]^{-1}
\]

- Modification of ASR-LDPM for Variable Alkali Content

Reaction Front:

\[
\dot{z}_\kappa = - \frac{a_s(T) w_s 3^{3/2} \sqrt{\kappa_a}}{r_w c_s z_\kappa \left( 1 - \frac{2z_\kappa}{D} \right)} \quad \text{,} \quad z_\kappa = z 3^{3/2} \sqrt{\kappa_a}
\]

Total Mass of Gel per Aggregate:

\[
M_g = \frac{\pi D^3}{6} \left( \kappa_a - \left( \frac{2z_\kappa}{D} \right)^3 \right) c_s m_g m_s
\]
Separation of Scales

\[ x = \eta y \]

\[ 0 < \eta << 1 \]

- Separation of scales
- \( x \) is the coarse scale coordinate system
- \( y \) is the fine scale coordinate system

RVE problem at each macroscopic Gauss point

Periodicity of particle distribution

FE representation of Macro domain
Asymptotic expansion of particle displacement

\[ \mathbf{u}(x, y) \approx \mathbf{u}^0(x, y) + \eta \mathbf{u}^1(x, y) \]

Asymptotic expansion of particle rotation

\[ \theta(x, y) \approx \eta^{-1} \omega^0(x, y) + \varphi^0(x, y) + \omega^1(x, y) + \eta \varphi^1(x, y) \]
Length type variable change \( x = \eta y \)

Taylor expansion of \( U^J \) and \( \Theta^J \) around \( x^I \)

Asymptotic expansion of displacement and rotation fields

Facet strain \( \epsilon^{IJ}_\alpha \) and curvature \( \chi^{IJ}_\alpha \) definition

Reordering terms of different orders

Multiple scale definition of facet strain and curvature

\[
\begin{align*}
\epsilon_\alpha &= \eta^{-1}\epsilon^{-1}_\alpha + \epsilon^0_\alpha + \eta\epsilon^1_\alpha \\
\eta\chi_\alpha &= \eta^{-1}\psi^{-1}_\alpha + \psi^0_\alpha + \eta\psi^1_\alpha
\end{align*}
\]
\[ \eta^{-2} \sum_{F_I} \tilde{A} t_{\alpha}^{-1} e_{\alpha}^{IJ} + \eta^{-1} \sum_{F_I} \tilde{A} t_{\alpha}^{0} e_{\alpha}^{IJ} + \sum_{F_I} \tilde{A} t_{\alpha}^{1} e_{\alpha}^{IJ} - \tilde{M}_u \ddot{u}^{0I} + \tilde{V}^{I} b^{0} + \mathcal{O}(\eta) = 0 \]

\[ \mathcal{O}(\eta^{-2}) \]

\[ \eta^{-2} \sum_{F_I} \bar{A} (p_{\alpha}^{-1} e_{\alpha}^{IJ} + q_{\alpha}^{-1} e_{\alpha}^{IJ}) + \eta^{-1} \sum_{F_I} \bar{A} (p_{\alpha}^{0} e_{\alpha}^{IJ} + q_{\alpha}^{0} e_{\alpha}^{IJ}) - \tilde{M}_\theta \ddot{\omega}^{0I} + \sum_{F_I} \bar{A} (p_{\alpha}^{1} e_{\alpha}^{IJ} + q_{\alpha}^{1} e_{\alpha}^{IJ}) + \mathcal{O}(\eta) = 0 \]

\[ \text{Macroscopic governing Eqs.} \]
Rigid Body Motion

- Considering facet level elastic constitutive law along with $O(\eta^{-2})$
- $u^0$ and $\omega^0$ are rigid body motion and rotation of the RVE
- $w_i^0(x, y) = v_i^0(x) + \varepsilon_{ijk} y_k \omega_j^0(x)$
- revise facet strain and curvature definition $\epsilon_\alpha = \epsilon_\alpha^0 + \eta \epsilon_\alpha^1$; $\eta \chi_\alpha = \psi_\alpha^0 + \eta \psi_\alpha^1$

Fine-scale displacement jump

$$
\epsilon_\alpha^0 = \bar{r}^{-1} \left( u_i^{1J} - u_i^{1I} + \varepsilon_{ijk} \omega_j^{1J} \bar{c}_k^J - \varepsilon_{ijk} \omega_j^{1I} \bar{c}_k^I \right) e_{\alpha i}^{IJ} + P_{ij}^\alpha (\gamma_{ij} + \varepsilon_{jmn} \kappa_{im} y_n^c)
$$

$$
\psi_\alpha^0 = \bar{r}^{-1} \left( \omega_i^{1J} - \omega_i^{1I} \right) e_{\alpha i}^{IJ} + P_{ij}^\alpha \kappa_{ij}
$$

Fine-scale rotation jump

$$
P_{ij}^\alpha = n_i^{IJ} e_{\alpha j}^{IJ} \text{ is the projection operator}
$$
 Terms of $\mathcal{O}(\eta^{-1})$ state RVE equilibrium equations

- Force equilibrium equation
  \[ \sum_{\mathcal{F}_I} A t^0_\alpha e^{IJ}_\alpha = 0 \]

- Moment equilibrium equation
  \[ \sum_{\mathcal{F}_I} A (c^{I} \times t^0_\alpha e^{IJ}_\alpha + m^0_\alpha e^{IJ}_\alpha) = 0 \]
Terms of $O(\eta^0)$ state macroscopic equilibrium equations

- Macroscopic translational equation of motion

$$M^I_u \ddot{u}^0_i = \eta \sum_{J} F^I_A \frac{\partial t^I_J}{\partial \epsilon^1_\alpha} \epsilon^1_\alpha + V^I b^0_i$$

Sum over all particles and divide by the RVE volume and some mathematical work

$$\rho_u \ddot{v}^0_i = \sigma^0_{ji,j} + b_i \quad ; \quad \sigma^0_{ij} = \frac{1}{2V_0} \sum_{I} \sum_{F} A r^0_{\alpha} P^\alpha_{ij}$$

$$\rho_u = \sum_{I} M^I_u / V_0$$ mass density of the macroscopic continuum
Macrosopic Governing Equations

- Terms of $O(\eta^0)$ state macroscopic equilibrium equations
  
  Macroscopic rotational equation of motion
  \[
  M^I_{\alpha j} \varepsilon_{ijk} X^I_j \left( \dot{v}^0_k + \varepsilon_{kmn} \eta^{-1} \dot{\omega}^0_m x^I_n \right) + \eta^{-1} M^I_{\alpha} \dot{\omega}^0_i = \eta \sum_{\mathcal{F}_I} A \left( \frac{\partial w^I_{ij}}{\partial \epsilon^1_0} \epsilon^1_0 + \frac{\partial m^I_{ij}}{\partial \psi^1_0} \psi^1_0 \right) + V^I \varepsilon_{ijk} X^I_j b^0_k
  \]

  Sum over all particles and divide by the RVE volume and some mathematical work

  \[
  \rho_{\theta ij} (\eta^{-1} \dot{\omega}^0_j) = \epsilon_{ijk} \sigma^0_{ij} + \frac{\partial \mu^0_{ij}}{\partial x_j} ; \quad \mu^0_{ij} = \frac{1}{2V_0} \sum_I \sum_{\mathcal{F}_I} A r (m^0_{\alpha} P^\alpha_{ij} + t^0_{\alpha} Q^\alpha_{ij})
  \]

  \[
  \rho^\theta_{im} = \sum_I \left[ M^I_{\theta} \delta_{im} + M^I_{\alpha j} \varepsilon_{ijk} \varepsilon_{kmn} x^I_j x^I_n \right] / V_0 : \text{the inertia tensor of the unit cell}
  \]

  \[
  Q^\alpha_{ij} = n^I_{ik} \varepsilon_{jkl} x^C_k e^I_l : \text{projection tensor}
  \]
(Left) Two-scale homogenization problem. (Right) Full mesoscale prism model.
Volumetric expansion of concrete prism for different alkali contents by experiment and full fine-scale analysis.
Volumetric expansion using RVE size of (left) 35 mm (center) 50 mm, and (right) 75 mm.
Comparison of the homogenization results using different RVE sizes with the full fine-scale ones.
Comparison of the compressive strength obtained by the full fine-scale simulation and the homogenization framework.
Crack opening contour of the concrete prism and RVEs of different sizes under (a) free expansion due to ASR effect with $C_a = 3.9 \text{ kg/m}^3$ and (b) uniaxial compression after ASR expansion.
Computational cost in full fine-scale analysis and homogenization framework with different RVE sizes.
Full scale dam analysis ...
**MARS** (Modeling and Analysis of the Response of Structures) is a multipurpose object-oriented computational software for simulating the mechanical response of structural systems subjected to short duration events.

It is based on dynamic explicit algorithms and it implements all the capabilities and versatility of a general finite element code.

Presentation Outline

1. Introduction
2. Alkali Silica Reaction (ASR) Model
3. The Lattice Discrete Particle Model (LDPM)
4. Numerical Simulations
5. Interpretation of Nonlinear Ultrasound Measurements
6. Mathematical Homogenization
7. Conclusions
Alkali Silica Reaction is a complex multiscale-multiphysics phenomenon affecting the deterioration of concrete structures worldwide.

Predictive computational models are needed to evaluate existing deteriorated structures.

A multi scale framework was proposed to simulate ASR deterioration within the LDPM framework.

LDPM can be extended effectively to account for various aging and deterioration phenomena.

Classical mathematical homogenization can be used to upscale LDPM response for durability related structural analysis.

All LDPM-based algorithms are currently implemented in the commercially available MARS software – www.mars.es3inc.com
Free time with my students