Computational Modeling of Concrete Structures

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Lecture # 2: The Lattice Discrete Particle Model (LDPM)

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1. The Lattice Discrete Particle Model (LDPM)
LDPM in a Nutshell

- LDPM simulates concrete at the meso-scale.
- LDPM is formulated in the framework of discrete models for which the unknown displacement field is not continuous but only defined at a finite number of point.
- Size and distribution of the particles are obtained according to the actual aggregate size distribution of concrete.
- Discrete compatibility and equilibrium equations are used to formulate the governing equations.
- Particle contact behavior represents the mechanical interaction among adjacent aggregate particles through the embedding mortar.
- Such interaction is governed by meso-scale constitutive equations simulating meso-scale tensile fracturing with strain-softening, cohesive and frictional shearing, and nonlinear compressive behavior with strain-hardening.
Summary

1. Particle generation
2. Particle placement
3. Topology definition
4. Domain tessellation
Particle size distribution (psd):

\[ f(d) = \frac{qd^q}{[1 - (d_0/d_a)^q]d^{q+1}} \]

Cumulative distribution function (cdf):

\[ P(d) = \int_{d_0}^{d} f(d)dd = \frac{1 - (d_0/d)^q}{1 - (d_0/d_a)^q} \]

Sieve curve:

\[ F(d) = \left(\frac{d}{d_a}\right)^{n_F} \]

where \( n_F = 3 - q \). For \( q = 2.5 \), \( n_F = 0.5 \), \( F(d) = \) Fuller curve.
For given cement content $c$, water-to-cement ratio $w/c$, specimen volume $V$, maximum aggregate size $d_a$, and minimum particle size $d_0$:

- Compute aggregate volume fraction as
  $$v_a = 1 - c/\rho_c - w/\rho_w - v_{air},$$
  where $w = (w/c)c$ is the water mass content per unit volume of concrete, $\rho_c = 3150 \, \text{kg/m}^3$ is the mass density of cement, $\rho_w = 1000 \, \text{kg/m}^3$ is the mass density of water, and $v_{air}$ is the volume fraction of entrapped or entrained air (typically 3-4%).

- Compute the volume fraction of simulated aggregate as
  $$v_{a0} = [1 - F(d_0)]v_a = [1 - (d_0/d_a)^{nF}]v_a$$

- Compute the total volume of simulated aggregate as $V_{a0} = v_{a0}V$
Particle Generation, Cont.

- Compute particle diameters by sampling the cdf by a random number generator:
  \[ d_i = d_0 \left[ 1 - P_i \left(1 - \frac{d_0^q}{d_a^q}\right) \right]^{-1/q}, \]
  where \( P_i \) is a sequence of random numbers between 0 and 1.

- For each newly generated particle in the sequence, check that the total volume of generated particles
  \( \tilde{V}_{a0} = \sum_i \left(\frac{\pi d_i^3}{6}\right) \)
  does not exceed \( V_{a0} \).

![Diagram a](image1.png)  ![Diagram b](image2.png)
In order to simulate the external surfaces of the specimen volume, the generated particles are augmented with zero-diameter particles (nodes).

One node for each vertex is first added to the particle list.

\[ N_e = \text{INT}(L_e/h_s) \] and \[ N_p = \text{INT}(A_p/h_s^2) \] nodes are associated with each edge \( e \) and polyhedral face \( p \), respectively.

The average surface mesh size \( h_s \) is chosen such that the resolution of the discretization on the surface is comparable to the one inside the specimen.

Numerical experiments show that this can be achieved by setting \( h_s = \xi_s d_0 \) with \( \xi_s = 1.5 \).
- Vertex nodes are placed first.
- Nodes are distributed over the edges and surfaces by allowing a minimum distance of $\delta_s d_0$, $\delta_s = 1.1$.
- Particles are placed throughout the volume one by one from the largest to the smallest.
- A check is made for possible overlaps of this particle with previously placed particles and with the surface nodes.
- During this phase, the surface nodes are assigned a fictitious diameter of $\tilde{\delta}_s d_0$.
- A minimum distance of $d_i/2 + d_j/2 + \zeta d_0$, $\zeta = 0.2$, between the centers of particles with diameters $d_i$ and $d_j$ is enforced.
- Delaunay tetrahedralization of particle centers.
Figure: c) Particle distribution; d) Delaunay triangulation.
Figure: e) Tessellation of a typical LDPM tetrahedron connecting four adjacent particles. f) Edge-point definition.
Figure: g) Face-point definition. h) Tet-point definition.
Figure: i) LDPM cells for two adjacent aggregate particle.
The tetrahedron is subdivided into four subdomains $V_i$ ($i = 1, \ldots, 4$). In each subdomain, the displacement field is defined through rigid-body kinematics: $u(x) = u_i + \theta_i \times (x - x_i) = A_i(x)Q_i$

$$A_i(x) = \begin{bmatrix} 1 & 0 & 0 & 0 & x_3 - x_{3i} & x_{2i} - x_2 \\ 0 & 1 & 0 & x_{3i} - x_3 & 0 & x_1 - x_{1i} \\ 0 & 0 & 1 & x_2 - x_{2i} & x_{1i} - x_1 & 0 \end{bmatrix}$$

$$Q_i^T = [u_i^T \theta_i^T]$$

$$u_i^T = [u_{1i} \ u_{2i} \ u_{3i}]$$

$$\theta_i^T = [\theta_{1i} \ \theta_{2i} \ \theta_{3i}]$$

**Figure:** a) Portion of a tetrahedron associated to one particle
Facet strains

\[
\varepsilon_N = \frac{n^T[u_C]}{\ell_e} = B_N^2 Q_2 - B_N^1 Q_1
\]

\[
\varepsilon_M = \frac{m^T[u_C]}{\ell_e} = B_M^2 Q_2 - B_M^1 Q_1
\]

\[
\varepsilon_L = \frac{l^T[u_C]}{\ell_e} = B_L^2 Q_2 - B_L^1 Q_1
\]

\[
B_P^N = \frac{1}{\ell_e} n^T A_p(x_C)
\]

\[
B_P^M = \frac{1}{\ell_e} m^T A_p(x_C)
\]

\[
B_P^L = \frac{1}{\ell_e} l^T A_p(x_{Ck})
\]

Figure: b) Original and projected LDPM facets; c) Effect of meso-scale pure shear loading
The elastic behavior is formulated by assuming that normal and shear stresses are proportional to the corresponding strains:

\[
\sigma_N = E_N \varepsilon_N; \quad \sigma_M = E_T \varepsilon_M; \quad \sigma_L = E_T \varepsilon_L
\]

where \( E_N = E_0, \quad E_T = \alpha E_0 \). \( E_0 \) and \( \alpha \) are assumed to be material properties.

Approximated relationships with Young’s modulus and Poisson ratio:

\[
E_0 = \frac{1}{1 - 2\nu} E \quad \iff \quad E = \frac{2 + 3\alpha}{4 + \alpha} E_0
\]

and

\[
\alpha = \frac{1 - 4\nu}{1 + \nu} \quad \iff \quad \nu = \frac{1 - \alpha}{4 + \alpha}
\]
Theoretical  Numerical

\( E / E_0 \) [-]

\( \alpha \) [-]

The Lattice Discrete Particle Model (LDPM)

\( \nu \) [-]

\( \alpha \) [-]

**Figure:** a) Young’s modulus. b) Poisson’s ratio.
Fracturing behavior is characterized by tensile normal strains, $\varepsilon_N > 0$.

Effective strain, $\varepsilon = \sqrt{\varepsilon_N^2 + \alpha(\varepsilon_M^2 + \varepsilon_L^2)}$

Effective stress, $\sigma = \sqrt{\sigma_N^2 + (\sigma_M^2 + \sigma_L^2)/\alpha}$

$\dot{\sigma} = E_0\dot{\varepsilon}$ and $0 \leq \sigma \leq \sigma_{bt}(\varepsilon, \omega)$

Damage-like Relationships

$$\sigma_N = \sigma \frac{\varepsilon_N}{\varepsilon}; \quad \sigma_M = \sigma \frac{\alpha\varepsilon_M}{\varepsilon}; \quad \sigma_L = \sigma \frac{\alpha\varepsilon_L}{\varepsilon}$$

Derived through the PVW
Strain-dependent boundary

\[ \sigma_{bt}(\varepsilon, \omega) = \sigma_0(\omega) \exp \left[ -H_0(\omega) \frac{\langle \varepsilon_{\max} - \varepsilon_0(\omega) \rangle}{\sigma_0(\omega)} \right] \]

The coupling variable \( \omega \) represents the degree of interaction between shear and normal loading

\[ \tan \omega = \frac{\varepsilon_N}{\sqrt{\alpha \varepsilon_T}} = \frac{\sigma_N \sqrt{\alpha}}{\sigma_T} \]

Maximum effective strain:

\[ \varepsilon_{\max} = \sqrt{\varepsilon_{N,\max}^2 + \alpha \varepsilon_{T,\max}^2} \]

where

\[ \varepsilon_{N,\max}(t) = \max_{\tau<t} [ \varepsilon_N(\tau) ] \quad \text{and} \quad \varepsilon_{T,\max}(t) = \max_{\tau<t} [ \varepsilon_T(\tau) ] \]
Effective strength

\[ \sigma_0(\omega) = \sigma_t \frac{-\sin(\omega) + \sqrt{\sin^2(\omega) + 4\alpha \cos^2(\omega) / r_{st}^2}}{2\alpha \cos^2(\omega) / r_{st}^2} \]

Effective Softening Modulus

\[ H_0(\omega) = H_t \left( \frac{2\omega}{\pi} \right)^{n_t} \]

\[ H_0(\pi/2) = H_t \]

\[ H_0(0) = 0. \]

\[ H_t = \frac{2E_0}{(\ell_t/\ell-1)} \]

\[ \ell_t = 2E_0G_t/\sigma_t^2 \]

**Figure:** a) Failure domain and its evolution
Constitutive Equations :: Fracturing Behavior, Cont.

Figure: b) Typical stress versus strain curves at the LDPM facet level. c) Unloading-reloading model.
The Lattice Discrete Particle Model (LDPM)

**Constitutive Equations :: Pore Collapse and Compaction**

**Strain-dependent Normal Boundary**

\[
\sigma_{bc}(\varepsilon_D, \varepsilon_V) = \begin{cases} 
\sigma_{c0} \\
\sigma_{c0} + \langle -\varepsilon_V - \varepsilon_{c0} \rangle H_c(r_{DV}) \\
\sigma_{c1}(r_{DV}) \exp\left[(-\varepsilon_V - \varepsilon_{c1})H_c(r_{DV})/\sigma_{c1}(r_{DV})\right] 
\end{cases}
\]

where \( r_{DV} = \varepsilon_D/\varepsilon_V \), \( \varepsilon_D = \varepsilon_N - \varepsilon_V \), \( \varepsilon_V = (V - V_0)/V_0 \)

**Figure:** d) Compressive behavior

\[
H_c(r_{DV}) = \frac{H_{c0}}{1 + \kappa_{c2} \langle r_{DV} - \kappa_{c1} \rangle}
\]

\( \varepsilon_{c0} = \sigma_{c0}/E_0 \), \( \varepsilon_{c1} = \kappa_{c0} \varepsilon_{c0} \)

\( \sigma_{c1} = \sigma_{c0} + (\varepsilon_{c1} - \varepsilon_{c0})H_c(r_{DV}) \)
Plasticity Formulation

\[ \dot{\sigma}_M = E_T (\dot{\varepsilon}_M - \dot{\varepsilon}_M^p), \quad \dot{\sigma}_L = E_T (\dot{\varepsilon}_L - \dot{\varepsilon}_L^p) \]
\[ \dot{\varepsilon}_M^p = \lambda \partial \varphi / \partial \sigma_M, \quad \dot{\varepsilon}_L^p = \lambda \partial \varphi / \partial \sigma_L, \quad \varphi = \sqrt{\sigma_M^2 + \sigma_L^2 - \sigma_{bs} (\sigma_N)} \]

\[ \sigma_{bs} (\sigma_N) = \sigma_s + (\mu_0 - \mu_\infty) \sigma_{N0} - \mu_\infty \sigma_N - (\mu_0 - \mu_\infty) \sigma_{N0} \exp \left( \frac{\sigma_N}{\sigma_{N0}} \right) \]

**Figure:**

e) Shear strength as a function of negative normal stresses (frictional behavior).

f) Typical shear stress versus shear strain curve.
Translational and rotational equilibrium equation of each particle

\[ M_u^I \ddot{U}^I - V^I b^0 = \sum_{F_I} A t^{IJ}; \quad M_\theta^I \ddot{\Theta}^I = \sum_{F_I} A c^I \times t^{IJ} \]
Calibration Procedure

### LDPM Parameters

**StaticParameters**

- **NormalModulus** 67000 MPa // nmo
- **Alpha** 0.25 // this is another comment
- **CompressiveYieldingStress** 500 MPa // fcm ⇒ Hydrostatic compression test
- **InitialHardeningModulusRatio** .36 // IHm ⇒ Hydrostatic compression test
- **TransitionalStrainRatio** 2 // hts ⇒ Hydrostatic compression test
- **DensificationRatio** 2.5 // dnm ⇒ Hydrostatic compression test, unloading
- **TensileStrength** 4 MPa ftm ⇒ Fracture test
- **TensileCharacteristicLength** 150 mm // tcl ⇒ Fracture test
- **TensileUnloadingParameter** 0.2 // ⇒ Fracture test, unloading
- **ShearStrengthRatio** 17 // fsm ⇒ Unconfined/Low-confinement comp. test
- **InitialFriction** .5 // μ0 ⇒ Unconfined/Low-confinement comp. test
- **SofteningExponent** 0.2 // ncm ⇒ Unconfined/Low-confinement comp. test
- **TransitionalStress** 300 MPa // fts // ⇒ High-confinement comp. test
- **DeviatoricStrainThresholdRatio** 2 // dk1 // ⇒ High-confinement comp. test
- **DeviatoricDamageParameter** 1 // dk2 // ⇒ High-confinement comp. test

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\[a\] Values reported here are for COR-TUF, a ultra-high performance concrete
### Some Reference Values for Standard Concrete

<table>
<thead>
<tr>
<th>Symbol [Units]</th>
<th>Set 1</th>
<th>Set 2</th>
<th>Set 3</th>
<th>Set 4</th>
<th>Set 5</th>
<th>Set 6</th>
<th>Set 7</th>
<th>Set 8</th>
<th>Set 9</th>
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<td>$d_0$ [mm]</td>
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<td>4</td>
<td>4</td>
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<td>6</td>
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<tr>
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<td>2.65</td>
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<td>100</td>
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<td>200</td>
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<td>100</td>
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<tr>
<td>$(G_t^1$ [N/m])</td>
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<td>(10)</td>
<td>(22.4)</td>
<td>(49)</td>
<td>(24.6)</td>
<td>(15.1)</td>
<td>(10.7)</td>
<td>(49.1)</td>
<td>(19.4)</td>
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\[ G_t = \ell_t \sigma_t^2 / (2E_0) \]
http://mars.es3inc.com/
Unconfined Compression

- Defining the model

1. Generating the LDPM specimens: Prism or Cylinder
2. Generated specimens: Prism or Cylinder
3. Running the simulation
Unconfined Compression, Cont.

**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.
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.
Postprocessing :: Paraview, Quasar, and jHist

1. Plotting curves
2. Visualize geometry
3. Visualize facet state variables (crack opening, facet stress and strain, etc)
4. Visualize nodal state variables (velocities, displacement, stress tensor, etc)
Biaxial tests are carried out imposing a constant stress ratio \( \kappa = \sigma_2/\sigma_1 \) but in displacement control because of softening:

1. Apply velocity \( \dot{u}_1^{n+1/2} \)
2. Compute force \( P_1^n \) and stress \( \sigma_1^n \)
3. Compute \( P_2^n = A_2\sigma_1^n \)
4. Compute \( \dot{u}_2^{n+1/2} \)
Figure: Biaxial Behavior. Macroscopic stress-strain curves for a) uniaxial compression; b) uniaxial tension; c) equibiaxial compression; d) biaxial compression; e) biaxial tension. f) Biaxial failure envelope.
Figure: Biaxial Behavior. g) Contours of meso-scale crack opening at failure for different biaxial loading paths.
Simulation is performed in two stages

In stage 1 pressure is applied everywhere up to the reference value $p_0$ and velocity of the top rigid plate is recorded.

In stage 2 pressure is applied on the lateral surface and velocity is applied to the top plate.
Figure: Macroscopic stress-strain curves for a) hydrostatic compression; b) uniaxial unconfined compression; c) triaxial compression; d) uniaxial strain compression; e) hydrostatic and uniaxial strain response; f) uniaxial strain compression with lateral expansion.
Figure: g) Contours of meso-scale crack opening at failure for different confinement level.
Combining LDPM with regular Finite Elements

Figure: Geometry of three point bending test specimens.
For example to simulate notches, a hexahedral supporting mesh with 3 elements is used to generate the LDPM particles.
Fracture Tests :: Load vs Displacement Curves

Load-displacement curves for three-point bending tests on a) medium size specimens; b) large size specimens; c) small size specimens. d) Load-displacement curves for direct tension tests on dogbone specimens. e) Contours of meso-scale crack opening at failure.
Figure: Geometry of the splitting (Brazilian) size effect tests specimens.
Figure: Splitting size-effect tests. a) Nominal macroscopic stress versus displacement. b) Size effect on splitting tensile strength. c) Contours of meso-scale crack opening at failure.