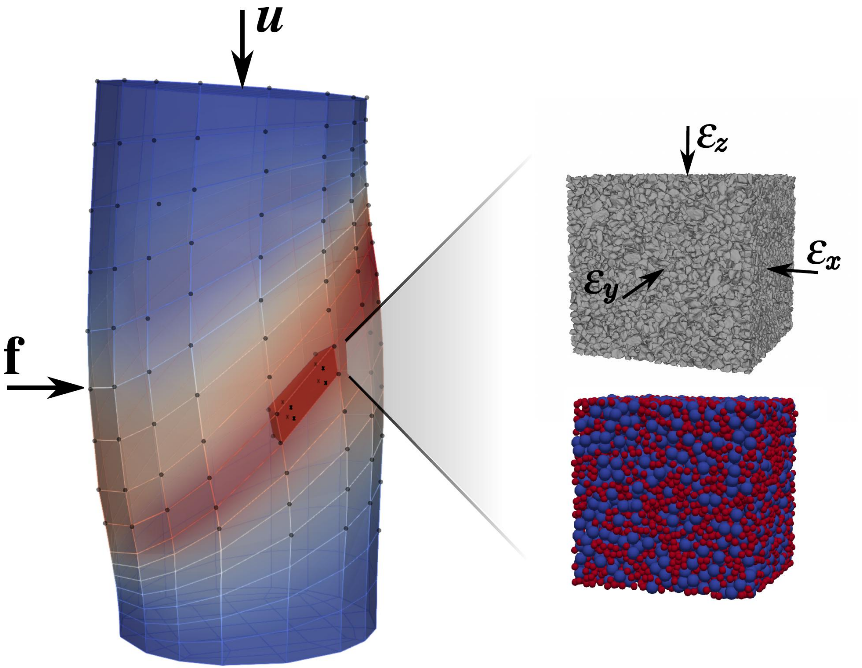


CIVIL-408 Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

Week 9

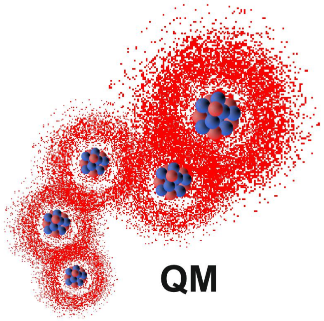
Brief recap of atomistics

Atomic **positions**: $\boldsymbol{q}(t) = \{\boldsymbol{q}_1(t), \ldots, \boldsymbol{q}_N(t)\}$

Atomic **momenta**: $\boldsymbol{p}(t) = \{\boldsymbol{p}_1(t), \ldots, \boldsymbol{p}_N(t)\}$

Total **Hamiltonian** of the system: $$\mathcal{H}(\boldsymbol{q}, \boldsymbol{p}) = \sum_{i=1}^{N} \frac{|\boldsymbol{p}_i|^2}{2m_i} + V(\boldsymbol{q})$$

- either empirical potential
- or by electronic structure calculation

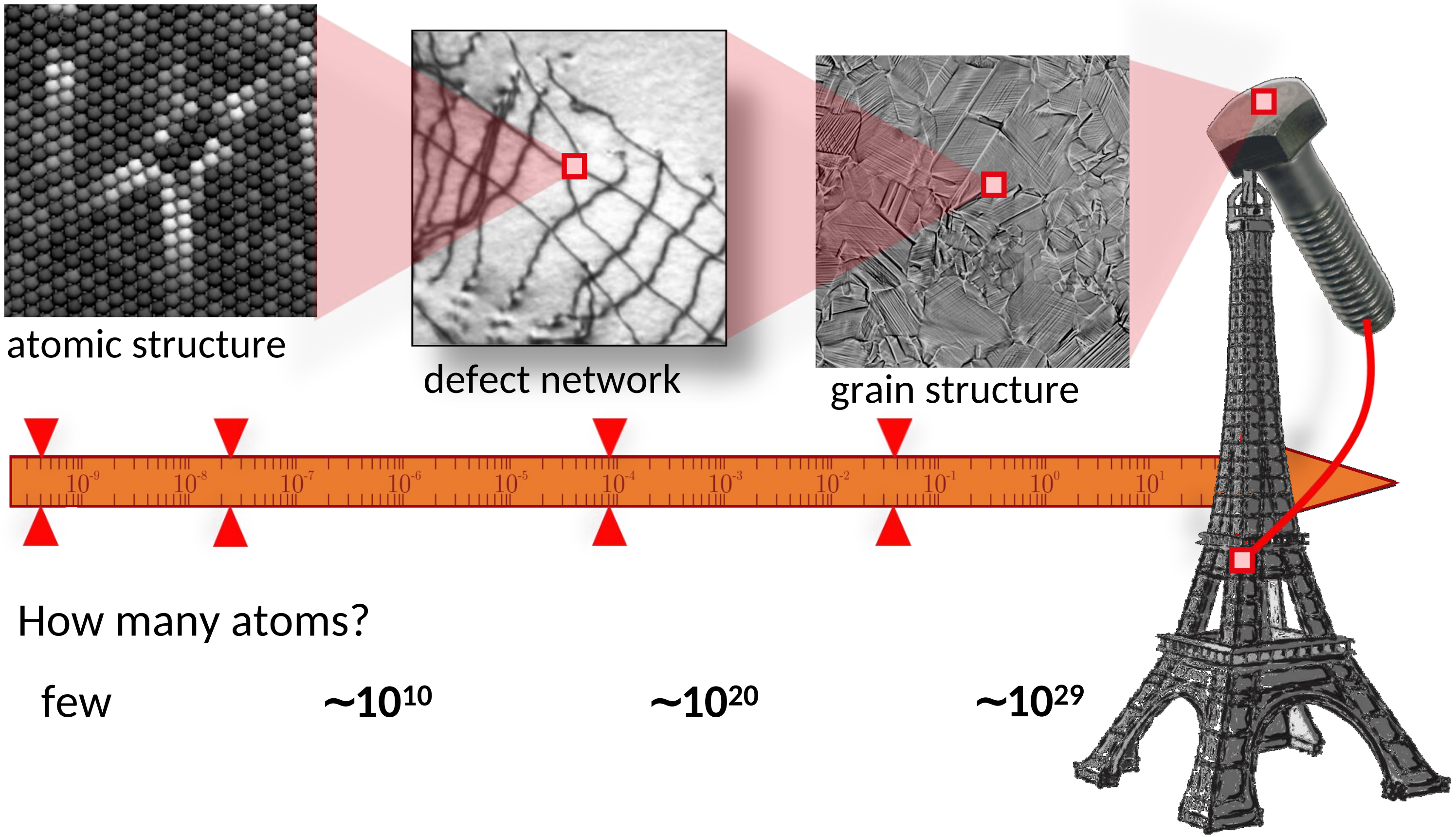


Equations of motion: $$m_i \ddot{\boldsymbol{q}}_i = \boldsymbol{f}_i(\boldsymbol{q}) = -\frac{\partial V}{\partial \boldsymbol{q}_i}(\boldsymbol{q})$$

+ constraints from atomistic ensembles $\longrightarrow$ Thermostat, barostat

How big of a system can we simulate?

How many atoms in a structure?



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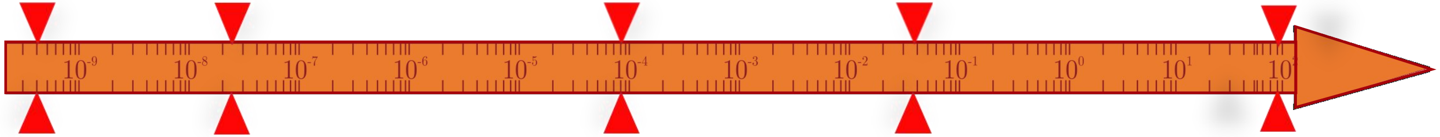
How big of a system can we simulate?

How many atoms can we handle in a computer?

laptop computer:
~1,000,000

computer cluster:
~300,000,000

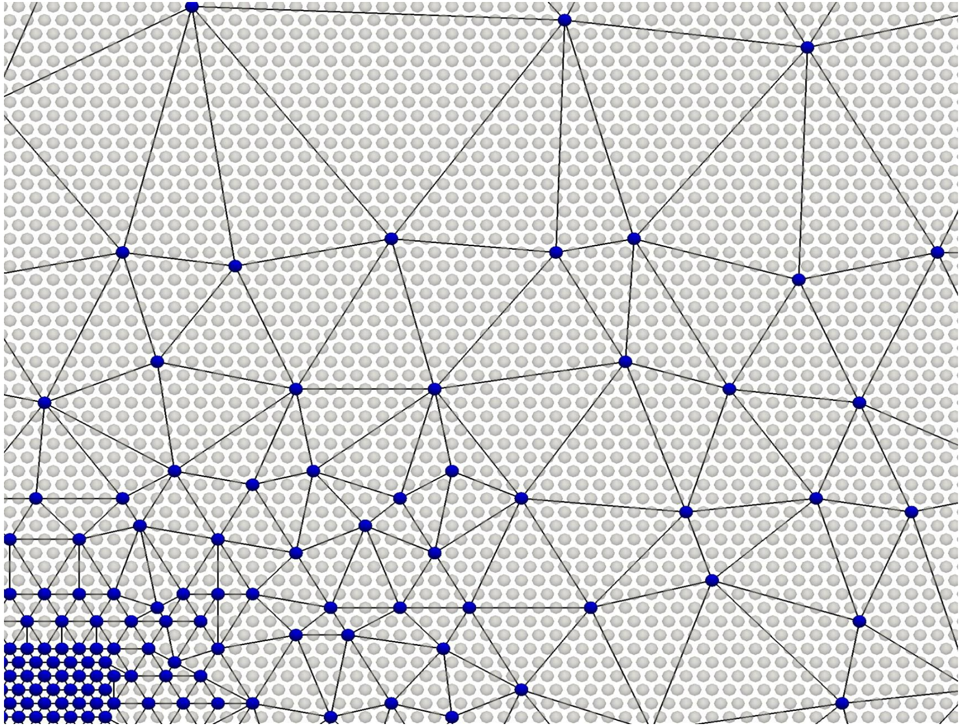
supercomputer:
~10^{12}



Even modern supercomputers can only simulate μm-scale volumes…

Concurrent techniques

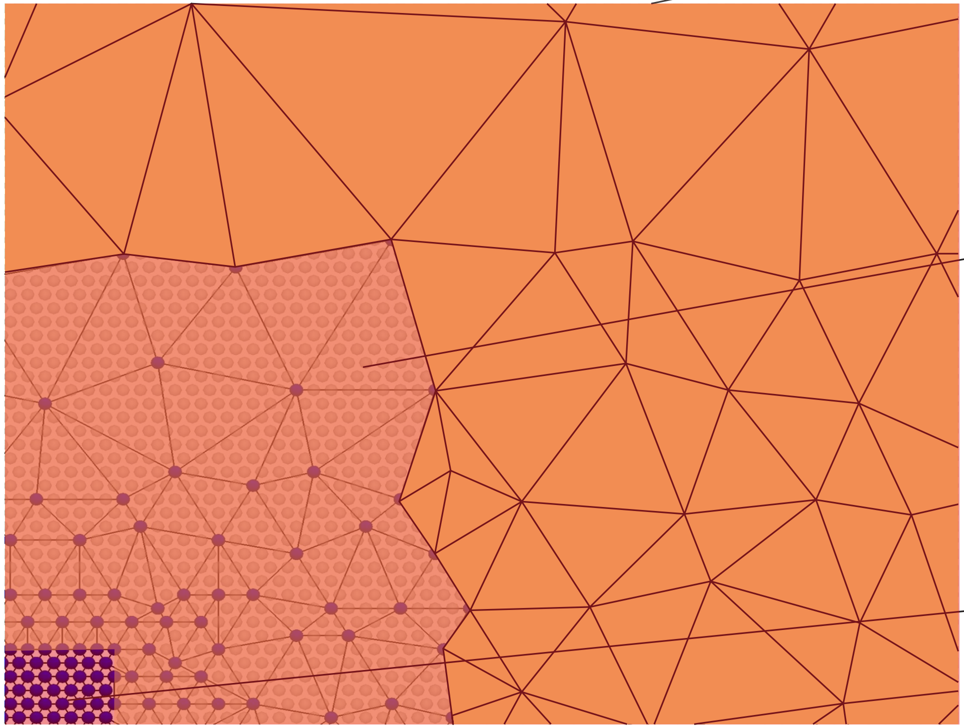
Handshake method



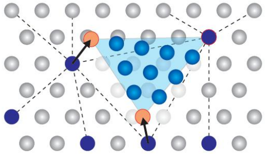
Concurrent techniques

Handshake method

finite element description
(which constitutive model?)



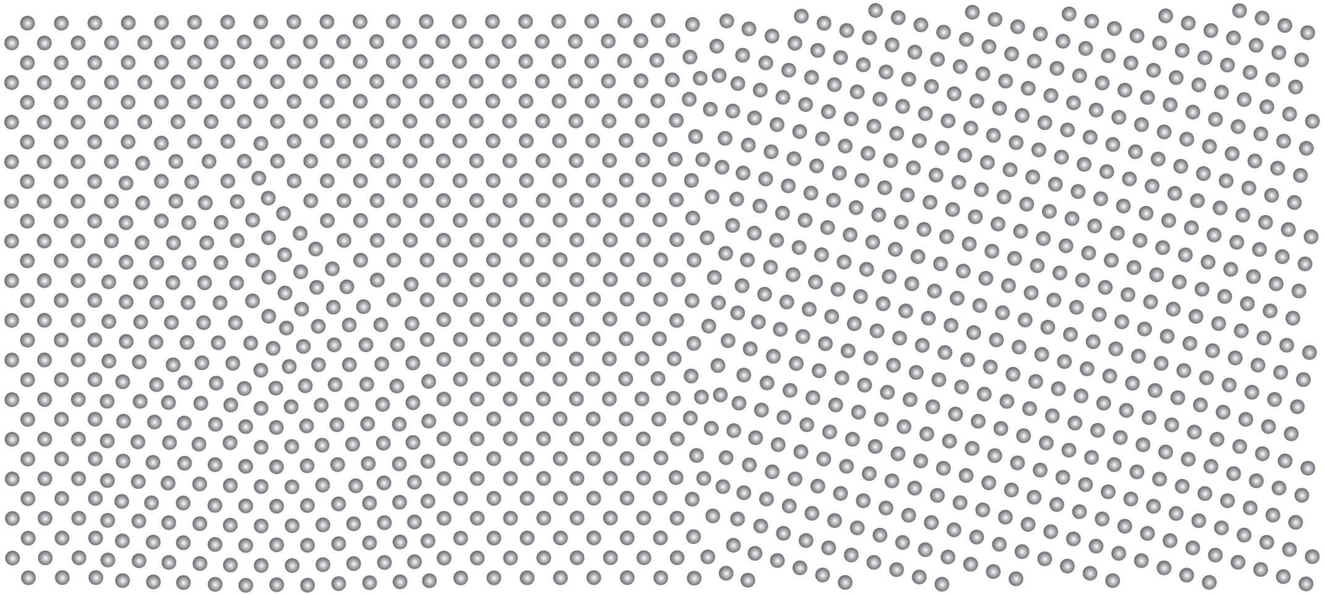
transition region, e.g.



geometric constraint

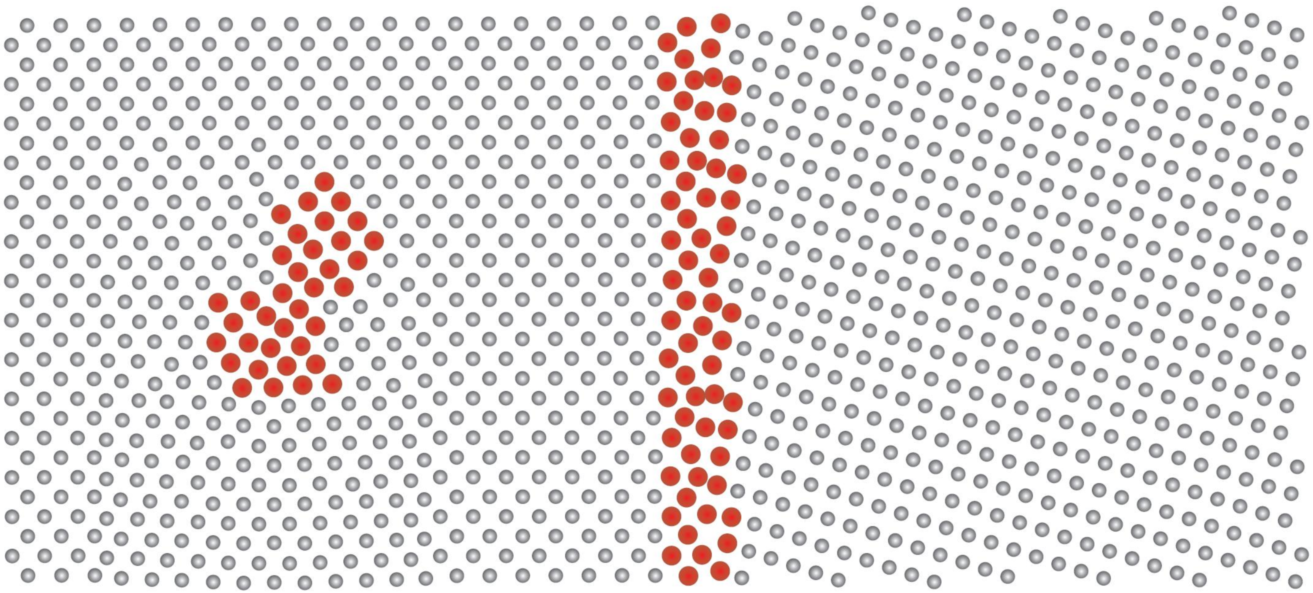
atomistics
(e.g. MS)

Coarse-graining in a nutshell



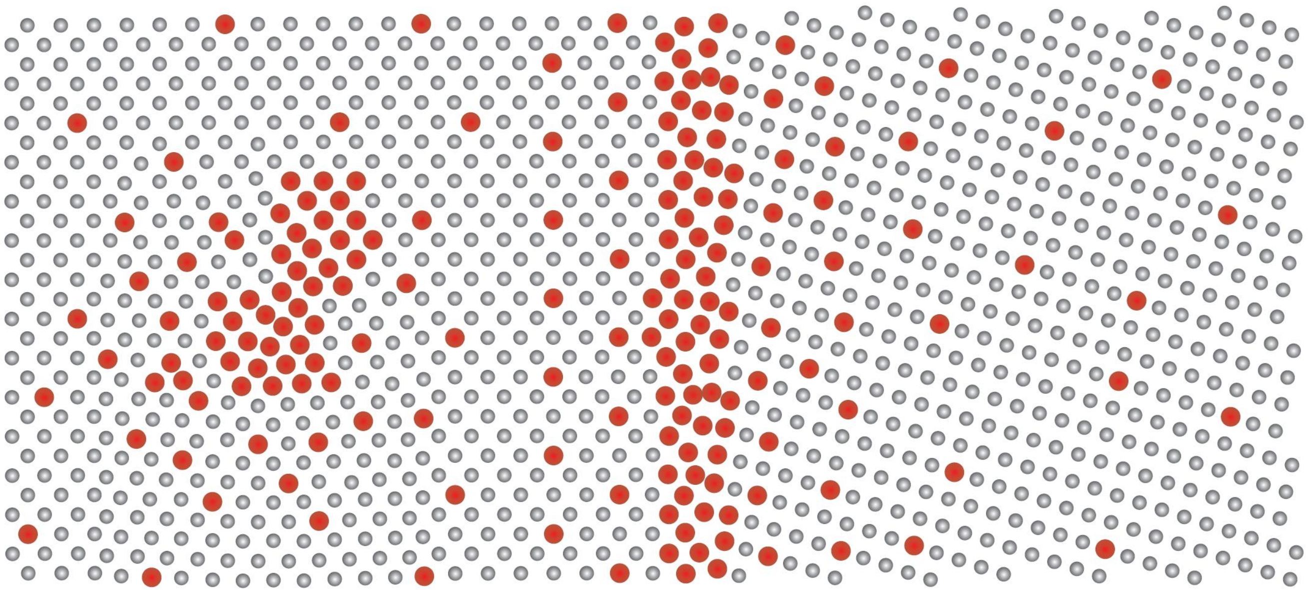
atomic crystal

Coarse-graining in a nutshell



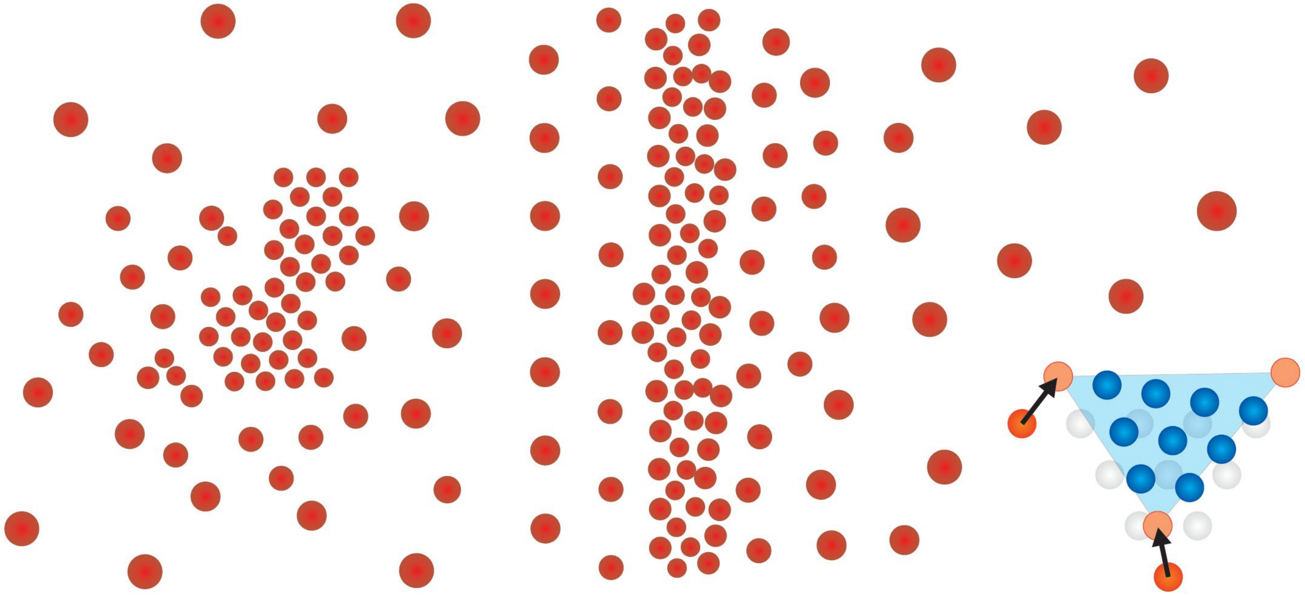
atomic crystal with lattice defects

Coarse-graining in a nutshell



selection of representative atoms

Coarse-graining in a nutshell



representative atoms + weights + interpolation = the QC method

The Quasicontinuum Method

Geometric constraint (the QC approximation):

$$\boldsymbol{q}_i \approx \boldsymbol{q}_i^h = \sum_{a=1}^{N_h} N_a(\boldsymbol{X}_i)\,\boldsymbol{x}_a$$

$$\boldsymbol{p}_i \approx \boldsymbol{p}_i^h = m_i\,\dot{\boldsymbol{q}}_i^h = m_i \sum_{a=1}^{N_h} N_a(\boldsymbol{X}_i)\,\dot{\boldsymbol{x}}_a$$

Resulting Hamiltonian and repatom forces:

$$\mathcal{H}^h(\boldsymbol{x},\dot{\boldsymbol{x}}) = \sum_{i=1}^{N} \frac{|\boldsymbol{p}_i^h|^2}{2m_i} + V(\boldsymbol{q}^h)$$

$$\boldsymbol{F}_k(\boldsymbol{x}) = -\frac{\partial V(\boldsymbol{q}^h)}{\partial \boldsymbol{x}_k} = \sum_{j=1}^{N} \boldsymbol{f}_j^h(\boldsymbol{q}^h)\,N_k(\boldsymbol{X}_j)$$

with $$\boldsymbol{f}_j^h(\boldsymbol{q}^h) = -\frac{\partial V(\boldsymbol{q}^h)}{\partial \boldsymbol{q}_j^h} = -\sum_{i=1}^{N} \frac{\partial E_i(\boldsymbol{q}^h)}{\partial \boldsymbol{q}_j^h}$$

Summation/sampling rules:

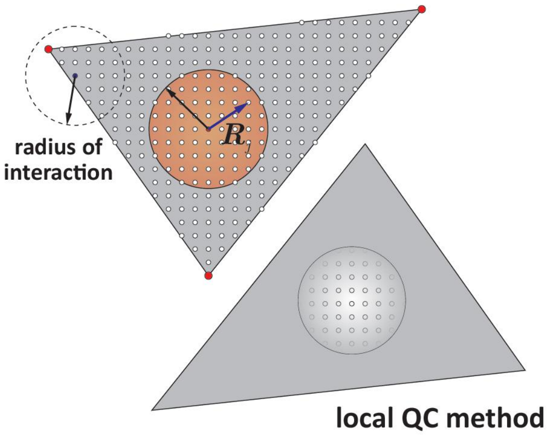
$$V(\boldsymbol{q}^h) = \sum_{i=1}^{N} E_i(\boldsymbol{q}^h) \quad \approx \quad \widetilde{V}(\boldsymbol{q}^h) = \sum_{\alpha=1}^{N_s} w_\alpha\,E_\alpha(\boldsymbol{q}^h)$$

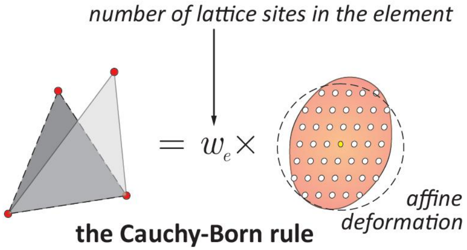
Resulting force approximation:

$$\widetilde{\boldsymbol{F}}_k(\boldsymbol{x}) = -\frac{\partial \widetilde{V}(\boldsymbol{q}^h)}{\partial \boldsymbol{x}_k} = -\sum_{\alpha=1}^{N_s} w_\alpha \sum_{j=1}^{N} \frac{\partial E_\alpha(\boldsymbol{q}^h)}{\partial \boldsymbol{q}_j^h}\,N_k(\boldsymbol{X}_j)$$

EPFL

The Quasicontinuum Method





dilemma:

$$H(\overline{\boldsymbol{q}}, \overline{\boldsymbol{p}}) = \sum_{i=1}^{N} \frac{m_i}{2} |\dot{\boldsymbol{x}}_i|^2 + V_i(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$$

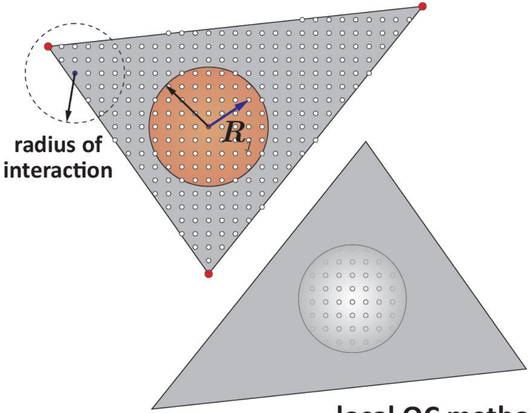
local QC: approximation per element

$$H(\overline{\boldsymbol{q}}, \overline{\boldsymbol{p}}) \approx \sum_{e} H_e(\overline{\boldsymbol{q}}, \overline{\boldsymbol{p}})$$

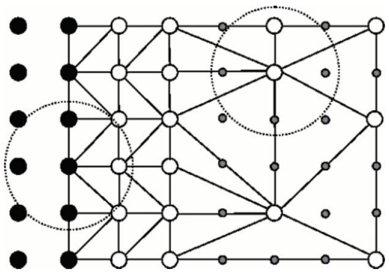
$$H_e = w_e \, H(\boldsymbol{x}_1^e, \ldots, \boldsymbol{x}_N^e)$$

$$\boldsymbol{x}_i^e = \boldsymbol{F}_e \boldsymbol{X}_i^e$$

The Quasicontinuum Method



local QC method



local-nonlocal QC method

dilemma:

$$H(\overline{\boldsymbol{q}}, \overline{\boldsymbol{p}}) = \sum_{i=1}^{N} \frac{m_i}{2} |\dot{\boldsymbol{x}}_i|^2 + V_i(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$$

local QC: approximation per element

$$H(\overline{\boldsymbol{q}}, \overline{\boldsymbol{p}}) \approx \sum_{e} H_e(\overline{\boldsymbol{q}}, \overline{\boldsymbol{p}})$$

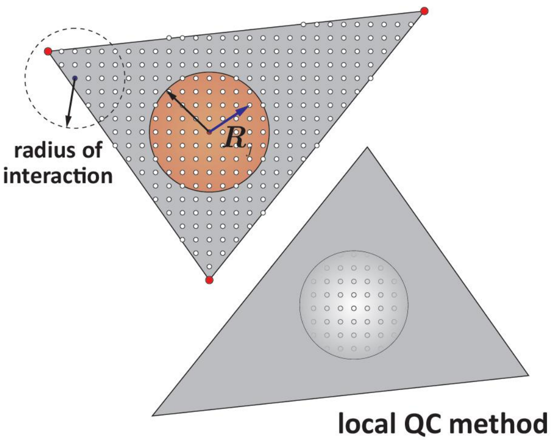
$$H_e = w_e \, H(\boldsymbol{x}_1^e, \ldots, \boldsymbol{x}_N^e)$$

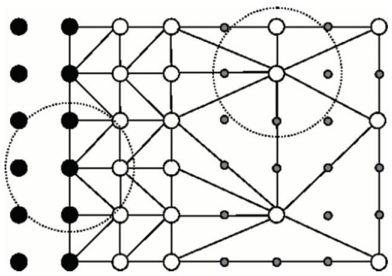
$$\boldsymbol{x}_i^e = \boldsymbol{F}_e \boldsymbol{X}_i^e$$

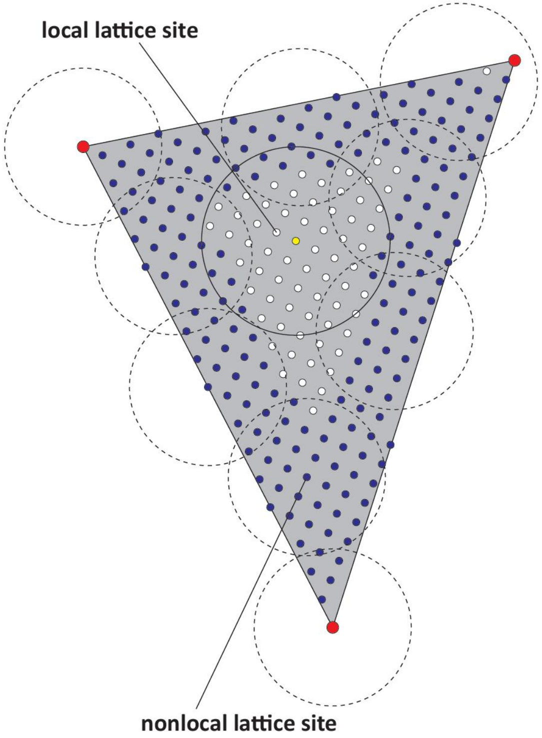
local-nonlocal QC:

use local QC where possible and
exact summation in transition regions
(reconstructing neighbors by interpolation)

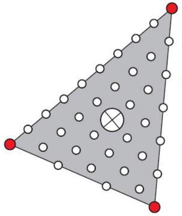
The Quasicontinuum Method





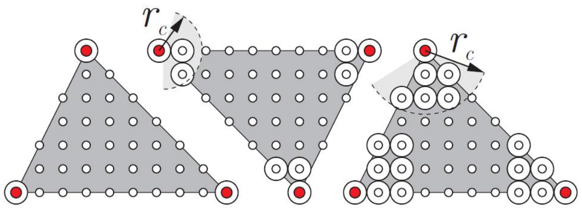


The Quasicontinuum Method



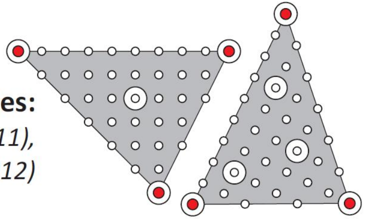
local QC:

Tadmor et al. (1996), Shennoy et al. (1998)
Miller et al. (1998), Tadmor et al. (2013)



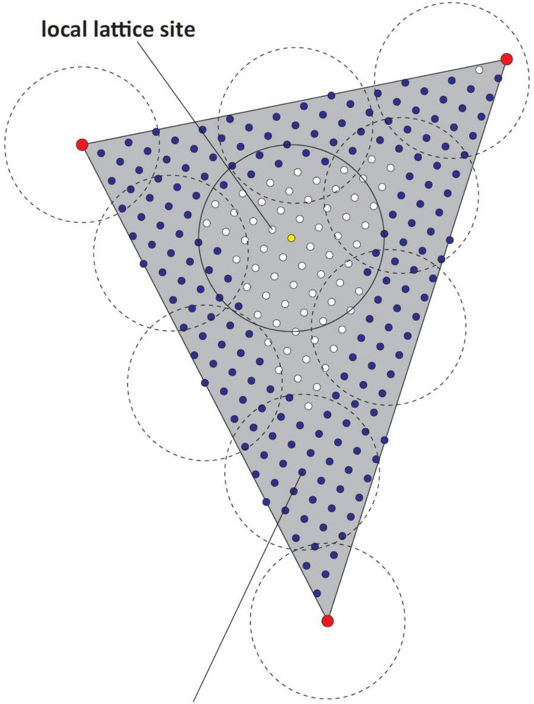
nodal cluster rules:

Knap & Ortiz (2001), Eidel & Stukowski (2009)

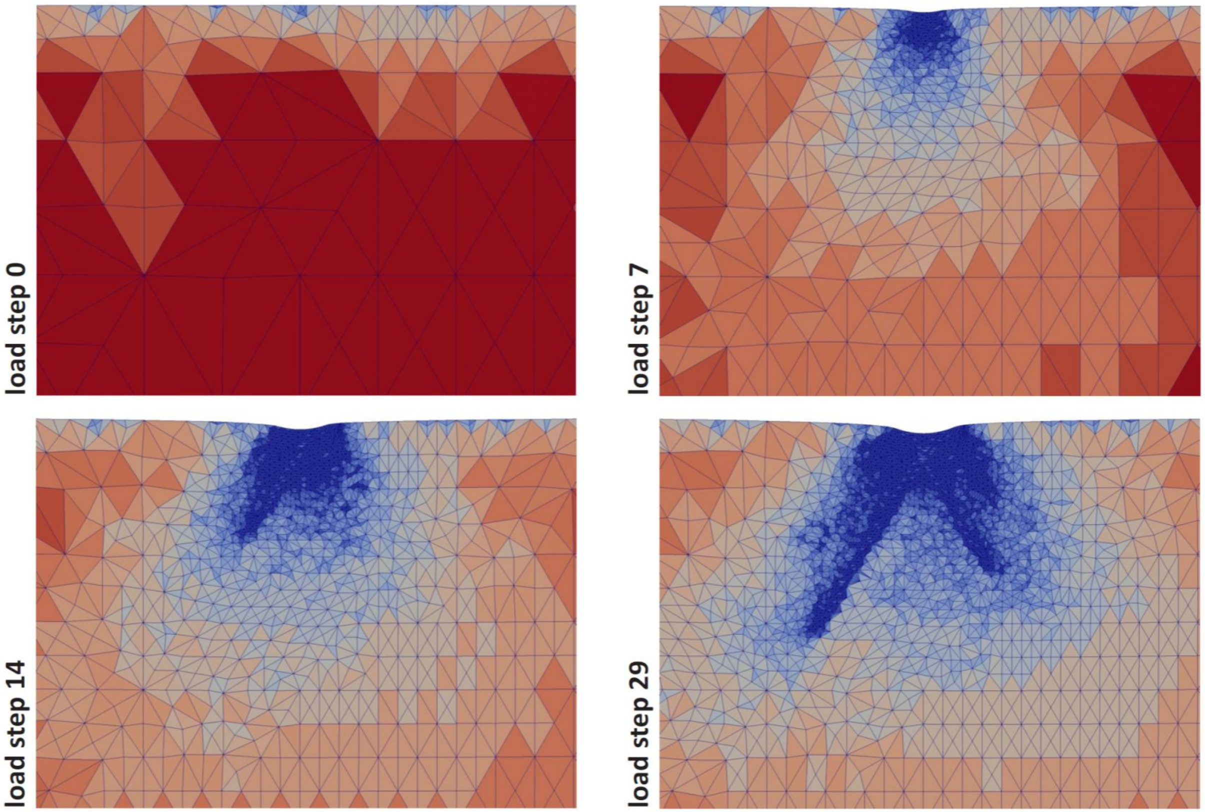


quadrature rules:

Gunzburger & Zhang (2010,2011),
Chen et al. (2012)



Adaptive refinement

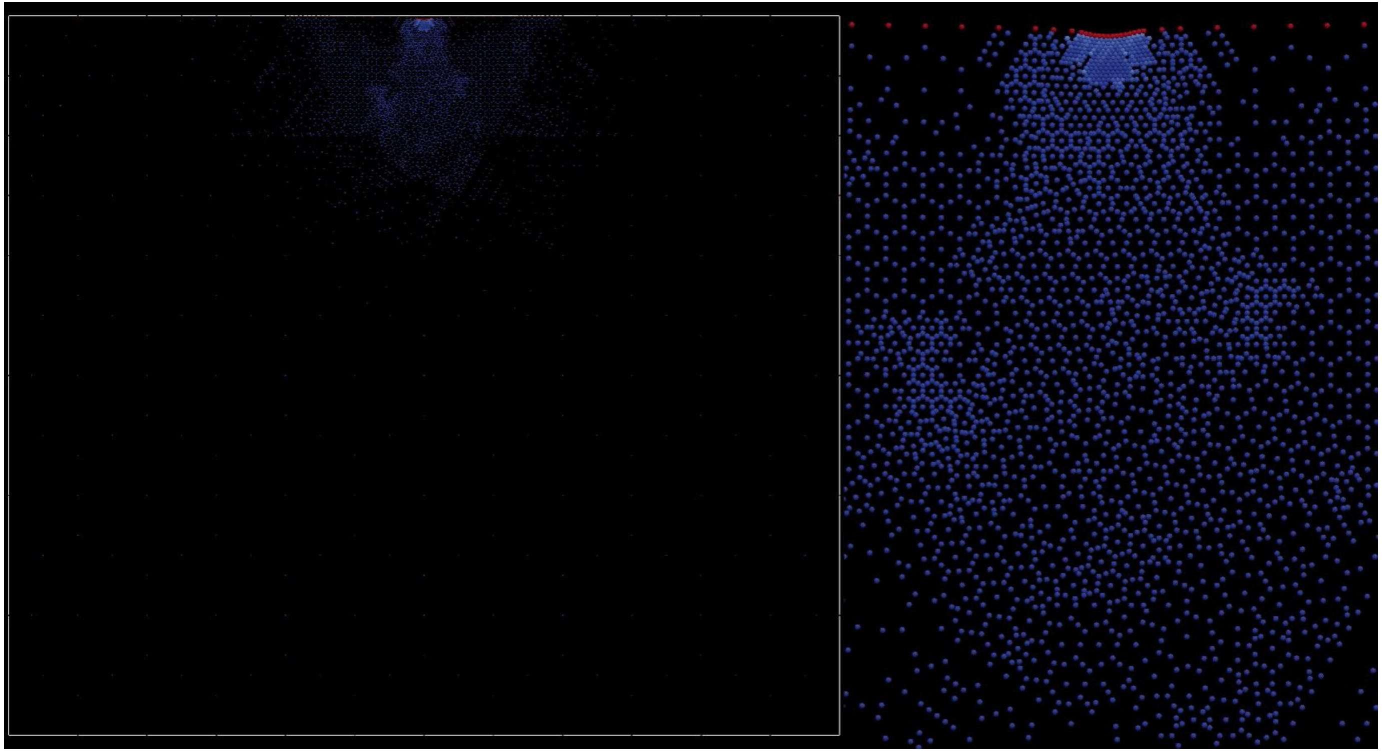


refinement criterion, e.g.

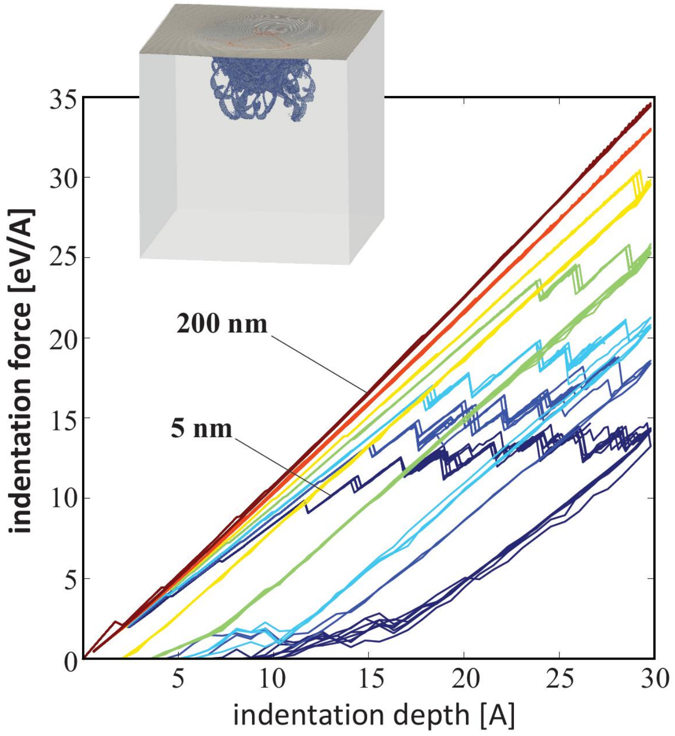
$$\text{if } I_2(\boldsymbol{F}_e) > \text{tol.} \;\Rightarrow\; \text{refine}$$

refinement algorithm, e.g. longest-edge bisection

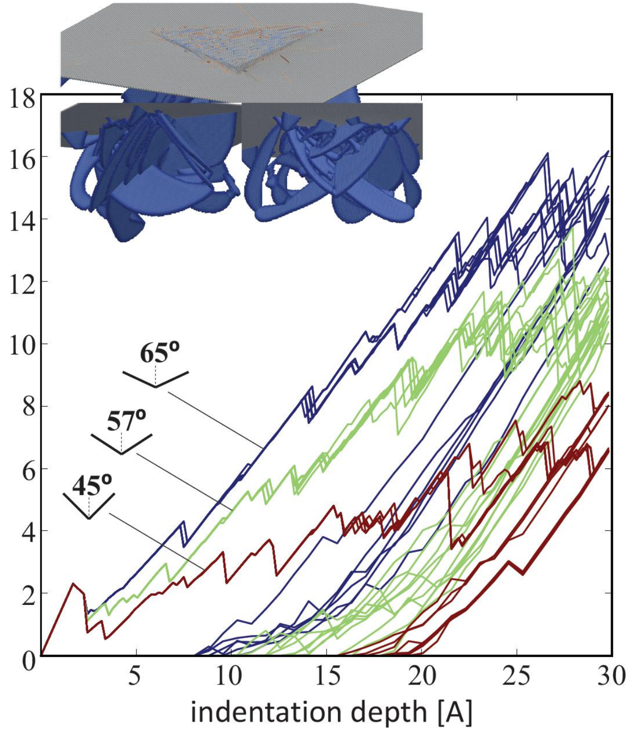
Application: Nanoindentation



Application: Nanoindentation



(a) spherical indenter



(b) pyramidal indenter

Application: Fracture Mechanics

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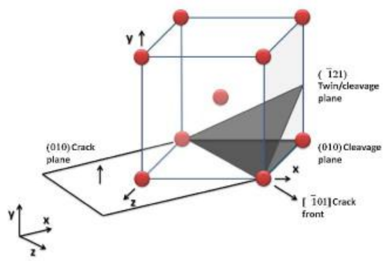
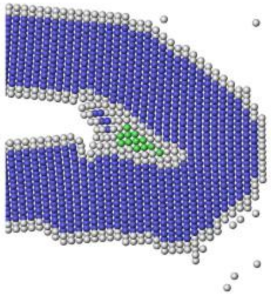
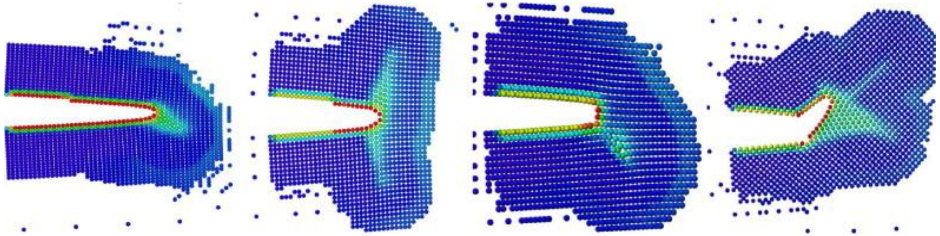


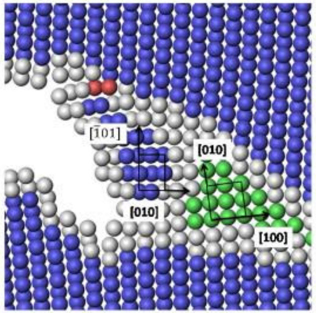
(a) Unit cell with possible cleavage and slip/twin planes.



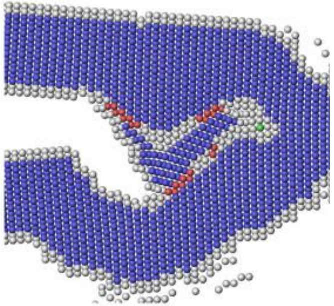
(b) Start of fracture.



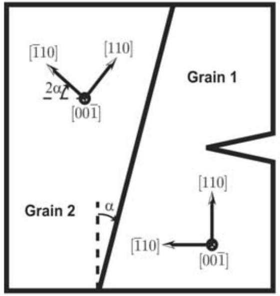
(a) Orientation 1 (b) Orientation 2 (c) Orientation 3 (d) Orientation 4

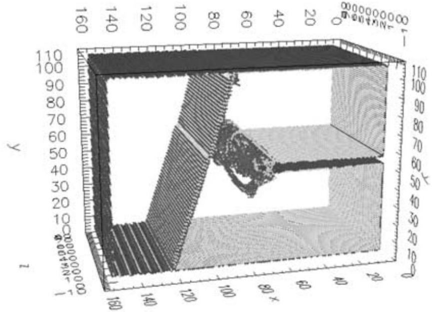


(c) After some growth two grains are observed at the crack tip, one bcc and one fcc.



(d) As the crack grows further twinning is observed.





(Miller & Tadmor, 2002; Ringdalen Vatne et al., 2011)

QC vs Molecular Statics

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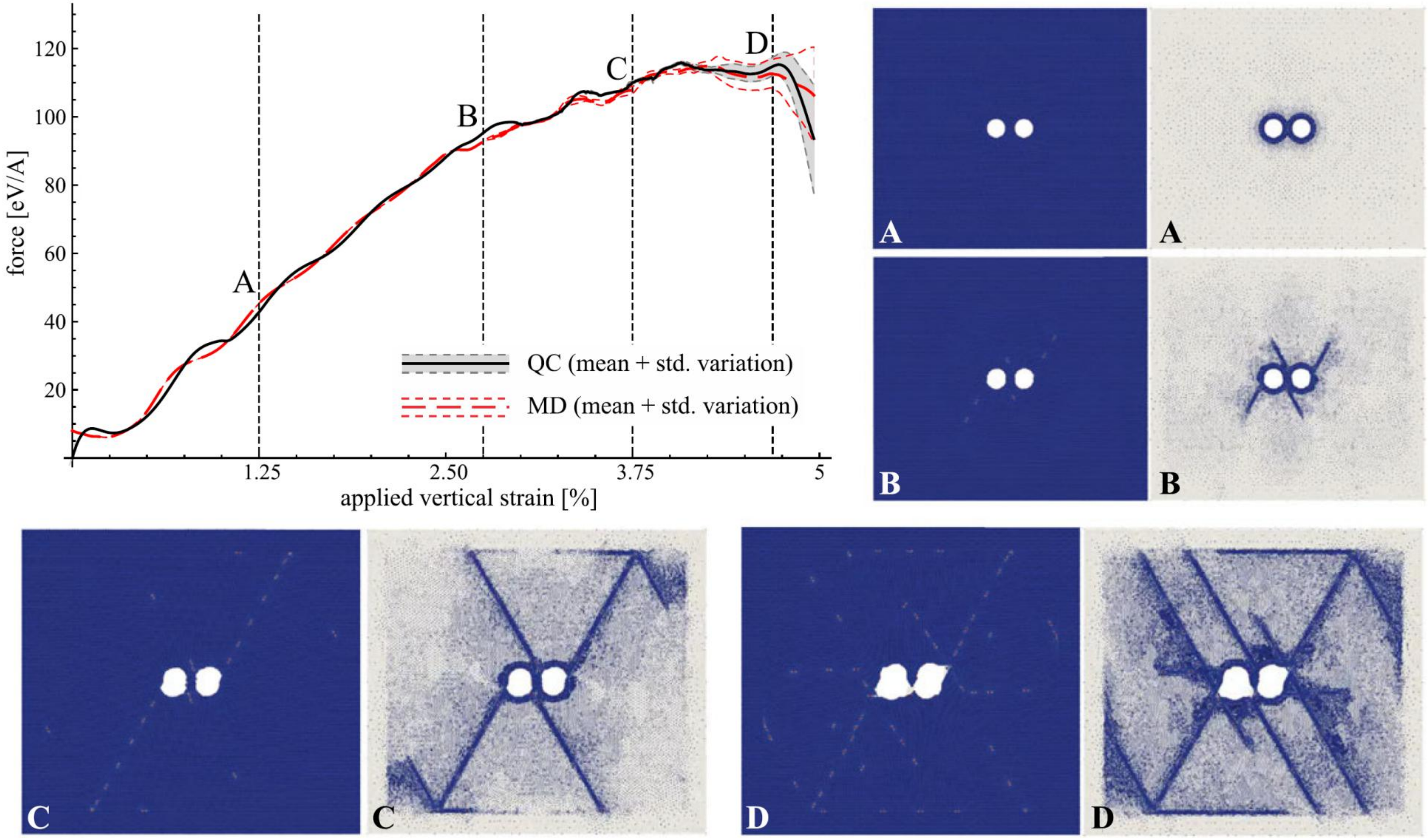
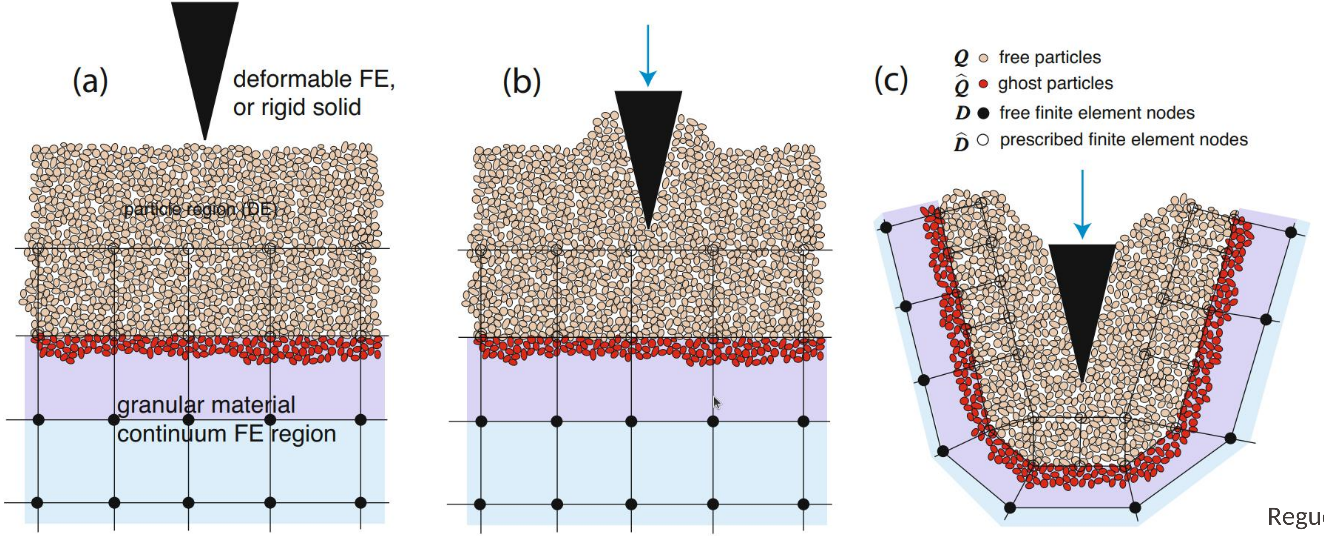


(Tembhekar et al., IJNME 2017)

Concurrent techniques in granular media

Handshake method



Regueiro et al., 2011

Q: Why would it be challenging to develop QC approaches for granular media?

Discussion

That's what I prepared for you today.

What would you like to discuss?

Reading for next class:

Data-Driven Modeling ALERT Doctoral School

- Chapter 5

- Chapter 9