Computational modeling of molecular discrete systems: the role of nonlocality on flaw-tolerance

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Outline

- **Motivations**
  - Analyze an equivalent discrete system with long range interactions to detect nonlocal behaviour at the continuum level
- **Computational Model**
  - Nonlocal effect in discrete systems
  - Nonbonded interaction generalized potential
  - FE model based on large displacement formulation
  - MD model based on potential energy formulation
- **Numerical examples**
  - Monodimensional Case study
  - Bidimensional Case Study
    - ✓ Flaw-tolerance and Force-distribution
- **Conclusions**
- **Coming progresses**

Scenario

<u>Nonlocal</u> *continuum* theories to describe long-range interactions

Gradient models

Integral formulations

Fractional calculus

•Z. Bazant, J. Eng. Mech., 120(3), 593–617
•A.C. Eringen, Springer Verlag, 2002
•M. Di Paola, M. Zingales, Int J Solids Struct, 45: 5642-5659, 2008
•A. Carpinteri, P. Cornetti, A. Sapora, M. Di Paola, M. Zingales, Phys Scripta, T136: 014003-014010, 2009

<u>Discrete</u> systems of particles or molecules to describe long-range interactions

Lattice beam models

Born models

Spherical elements models

Molecular Dynamics

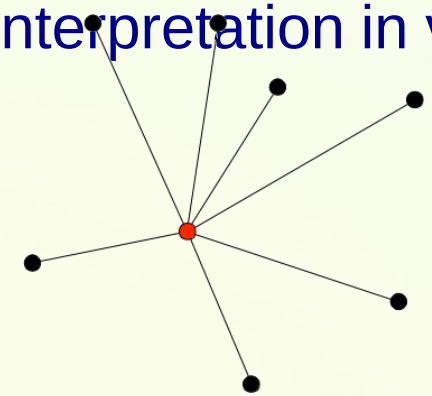
- J.G.M. van Mier, E. Schlangen, A. Vervuurt, Continuum Models for Materials with Microstructure: 341-377, 1995
- J.G.M. van Mier, Int J Fracture, 143: 41-78, 2007
- A. Parisi, G. Caldarelli, L. Pietronero, EPL, 52 (3): 304-310, 2000
- V.E. Tarasov, Journal of Physics A 39: 14895-14910, 2006

New model proposal

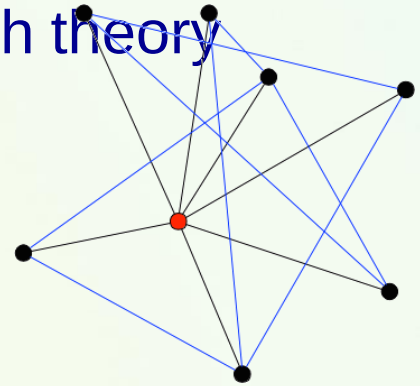
Objectives:

1)Nonlocal behaviour prediction for continua by upscaling the mechanical behaviour of discrete nonlocal structures

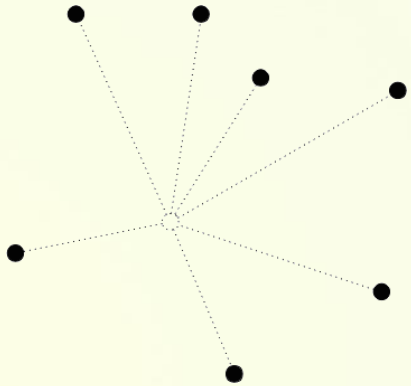
2)Interpretation in view of network and graph theory

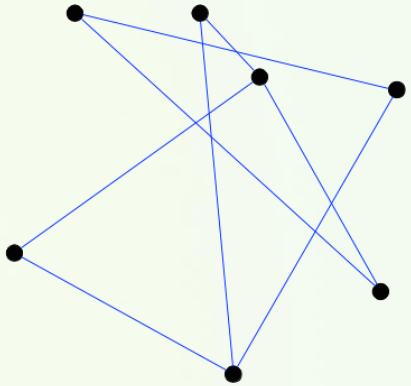


Node Removal *Nonlocal effects*



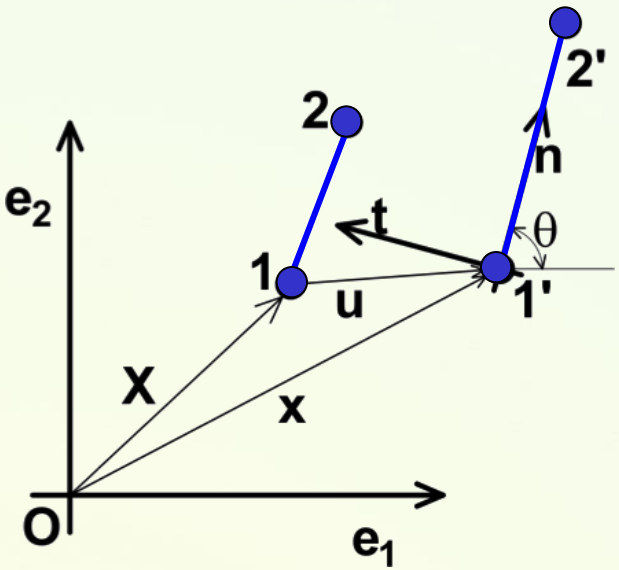
Redundancy





Numerical method

Discrete system of atoms or molecules



$\mathbf{X} = (X_1, Y_1, X_2, Y_2)^T$ Initial coord. in global system

$\mathbf{u} = (u_1, v_1, u_2, v_2)^T$ Element displ. vector

$\mathbf{x} = \mathbf{X} + \mathbf{u}$ Coord. in updated config. (large displ. theory)

$\mathbf{g}_{loc} = \mathbf{RLx}$ Gap vector in local ref. system

R = rotation matrix

L = operator matrix

Force vector in local system $\mathbf{F}_{loc} = (F_{LJ}, 0)^T$

P. of V.W. linearization to apply Newton-Raphson procedure

Residual vector $\mathbf{p} = \left(\mathbf{RL} + \frac{\partial \mathbf{R}}{\partial \mathbf{u}} \mathbf{Lu} \right)^T \mathbf{F}_{loc}$

Third order tensor

Stiffness matrix $\mathbf{K} = \mathbf{K}_{mat} + \mathbf{K}_{geom}$

FEAP

Finite Elements Analysis Program

M. Paggi, P. Wriggers (2011) Comp. Mat. Sci., 50:1634-1643

Constitutive law: L-J potential

$$E_{tot} = \cancel{E_b} + E_{nb}$$

$$P_{LJ} = 4e\left[\left(\frac{r_0}{g_n}\right)^a - \left(\frac{r_0}{g_n}\right)^b\right]$$

e = depth of potential well

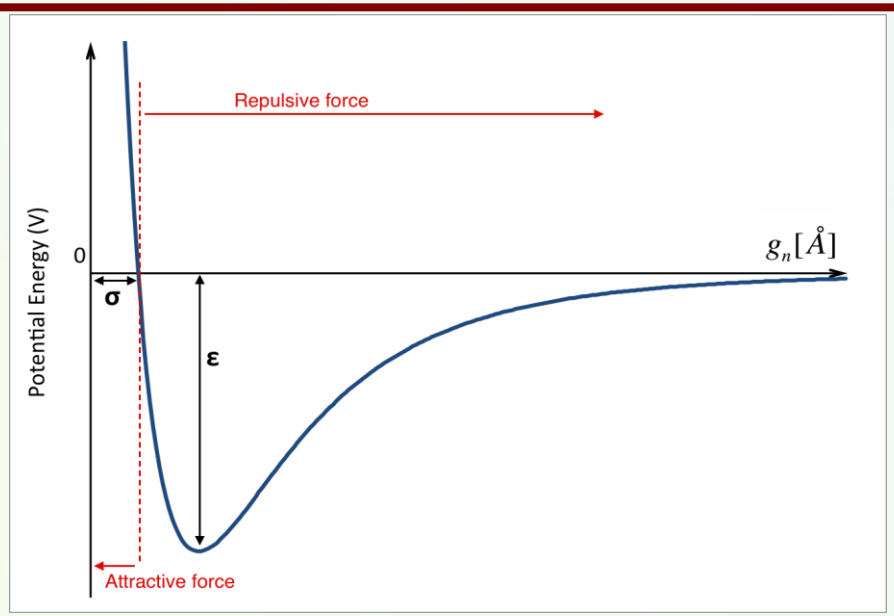
r_0 = equilibrium distance

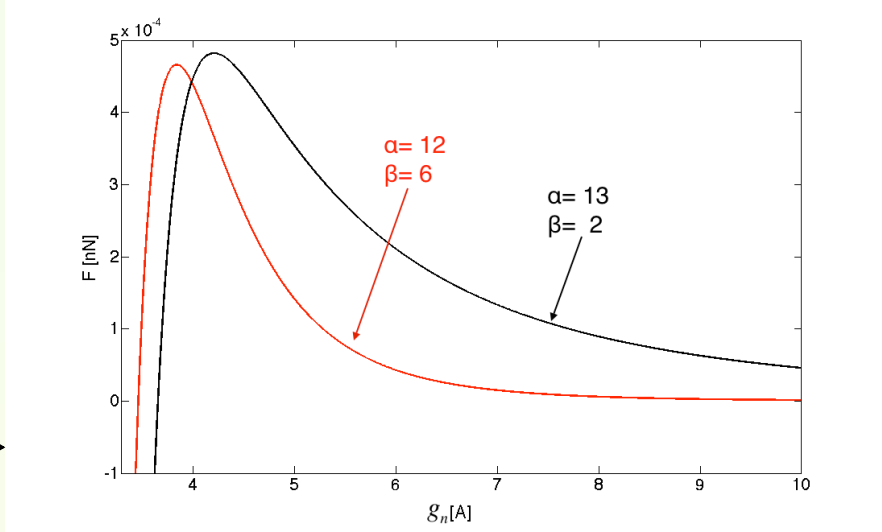
$$F_{LJ}(g_n) = -\nabla P_{LJ}(g_n) = -\frac{dP_{LJ}(g_n)}{d(g_n)}$$

$$= -4e\left[a\left(\frac{s^a}{g_n^{a+1}}\right) - b\left(\frac{s^b}{g_n^{b+1}}\right)\right]$$

Generalized formulation

a = 13 b = 2





L.Y. Jiang et al. (2006) J. Mech. Phys. Solids 54: 2436-2452

Monodimensional Model

NLI = NonLocality Index

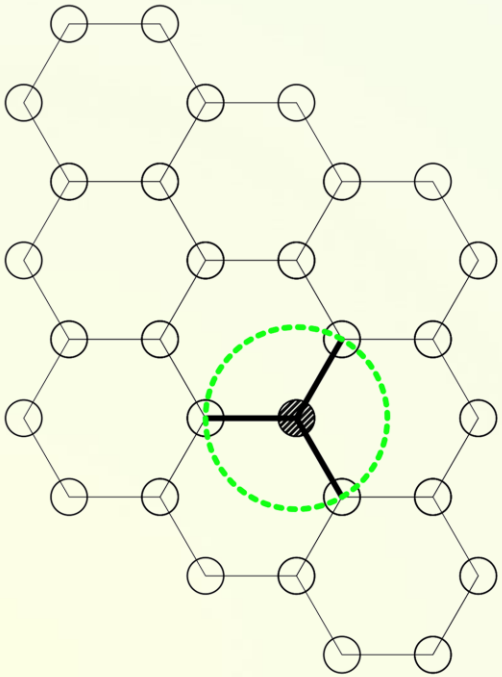
$$NLI = \frac{max(l_i)}{l_0}$$

l_i = length of the i-th link

l_0 = local link length

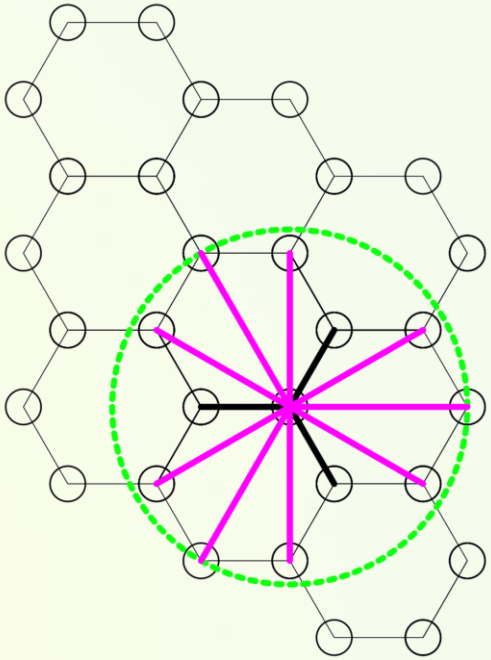
Local system

NLI = 1

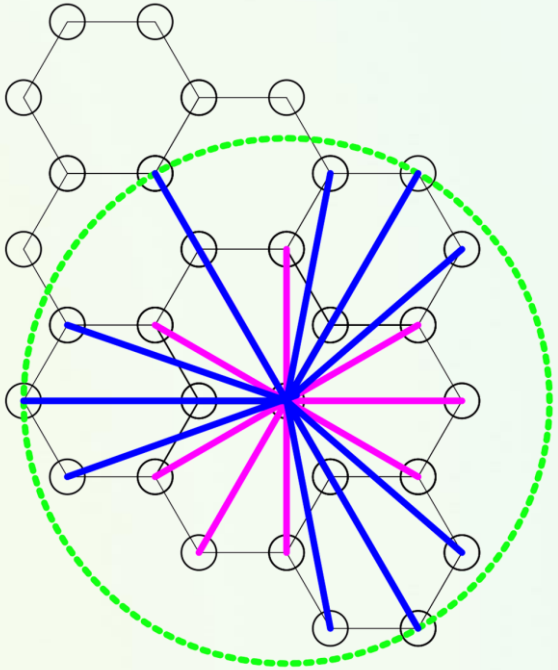


Nonlocal systems

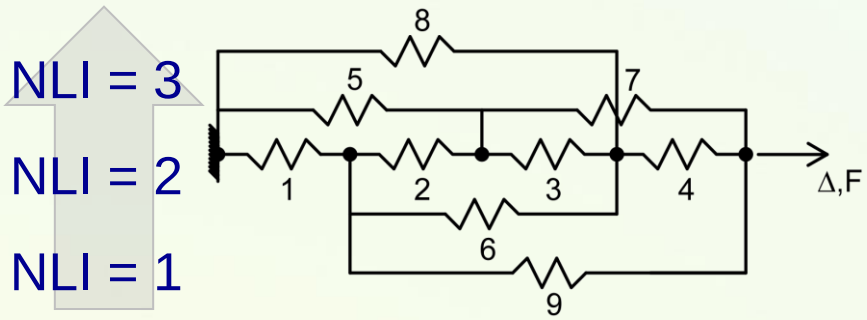
NLI = 2



NLI =3

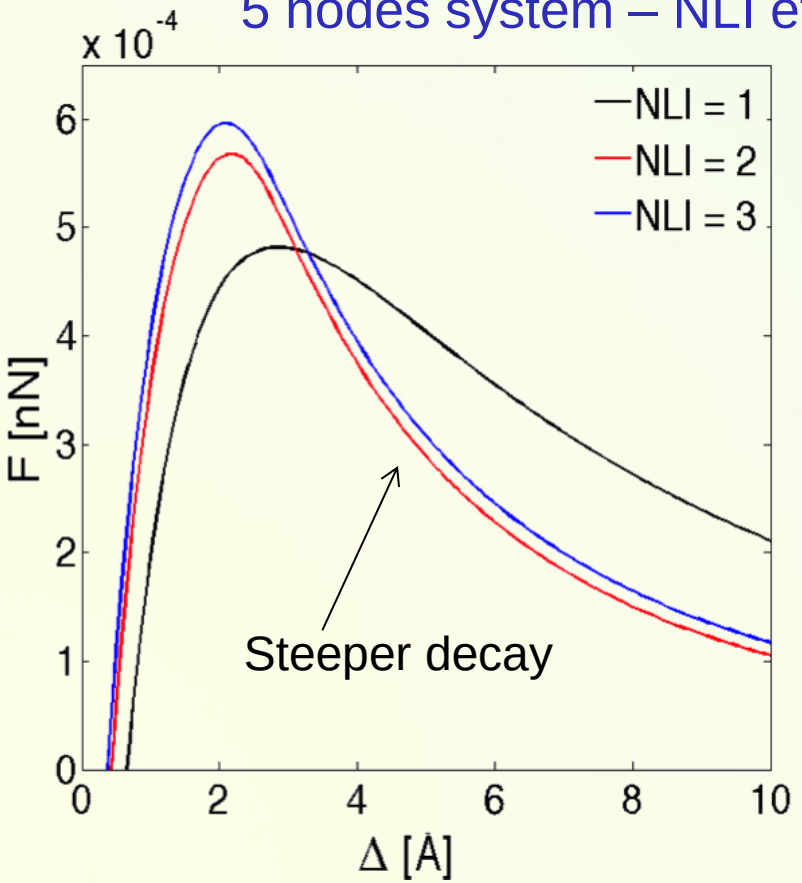


Monodimensional Model

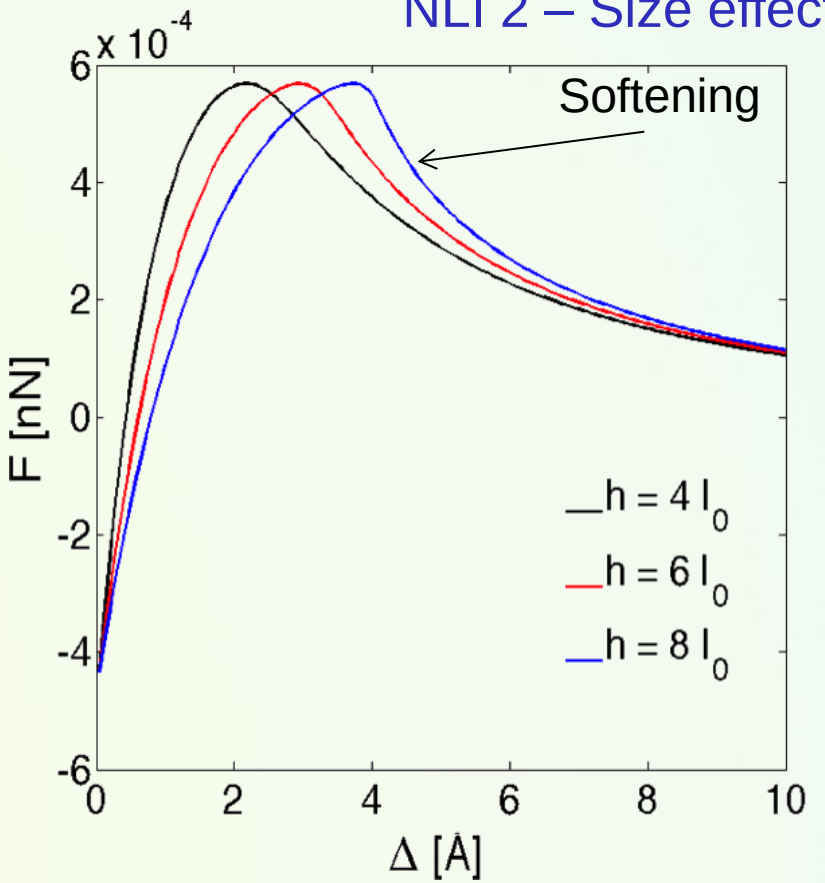


Global force vs. global displacement

5 nodes system – NLI effect



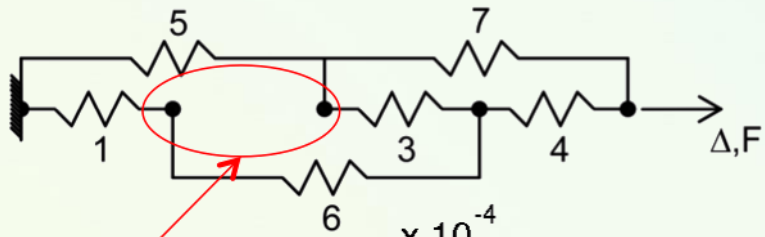
NLI 2 – Size effect



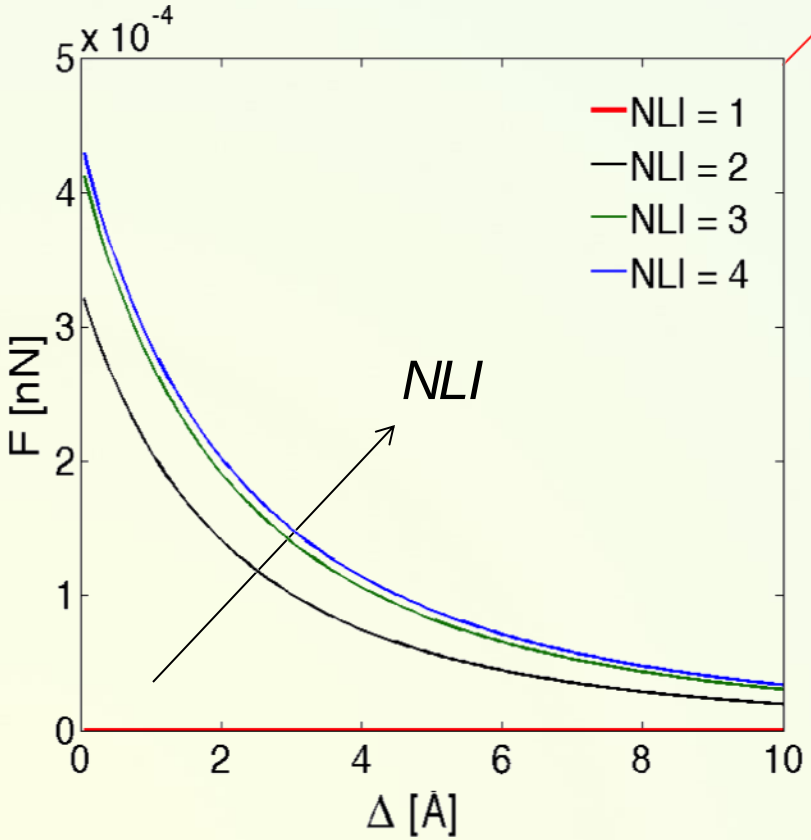
Monodimensional Model - with defects

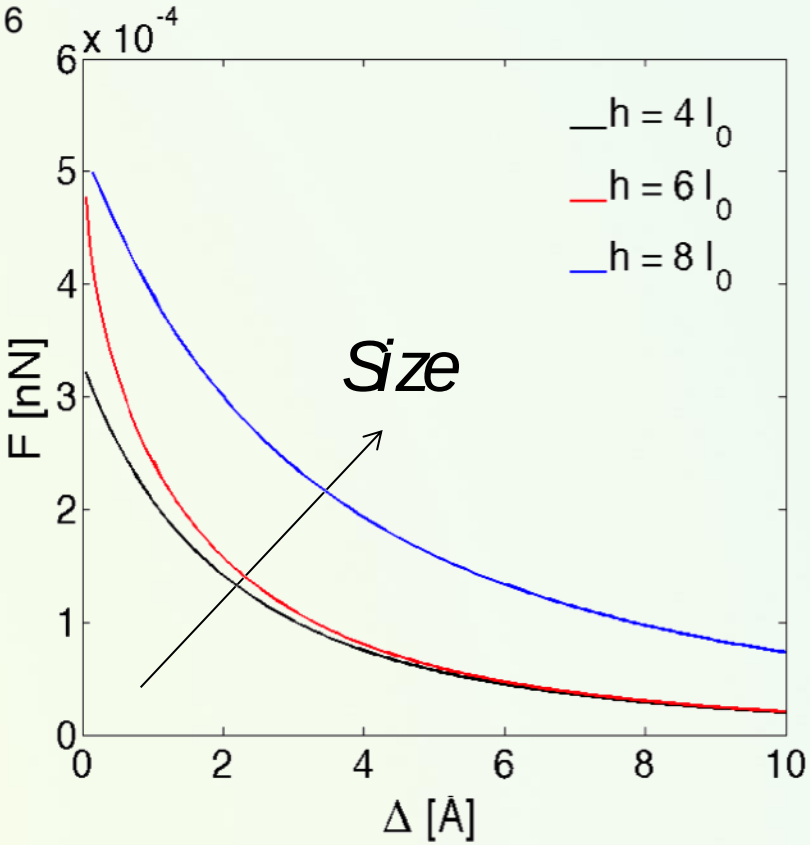
Global force vs. global displacement

5 nodes system
NLI effect



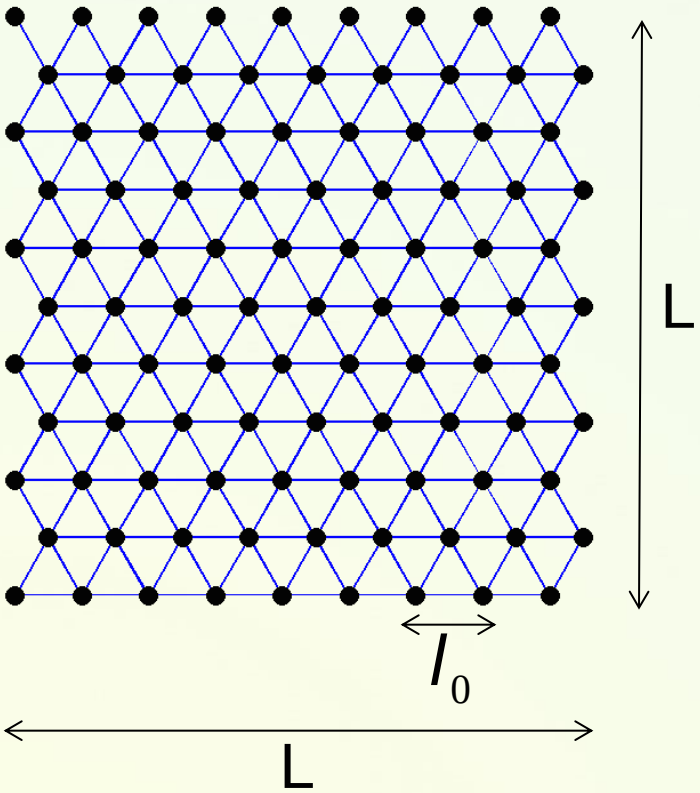
NLI=2
Size effect





Defect better tolerated with increasing NLI and system size

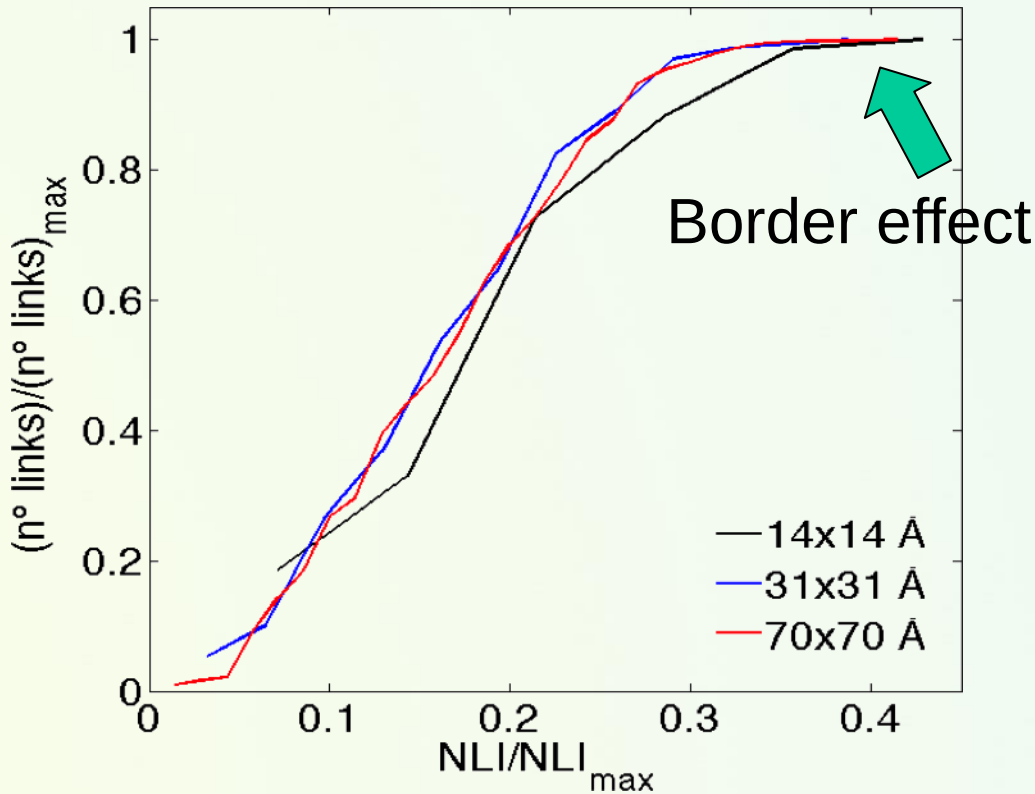
Bidimensional Model



Hexagonal mesh

$l_0 = 3.5\text{Å}$ $\quad NLI = 1 \longrightarrow NLI_{max}$

Relation between NLI and n° links

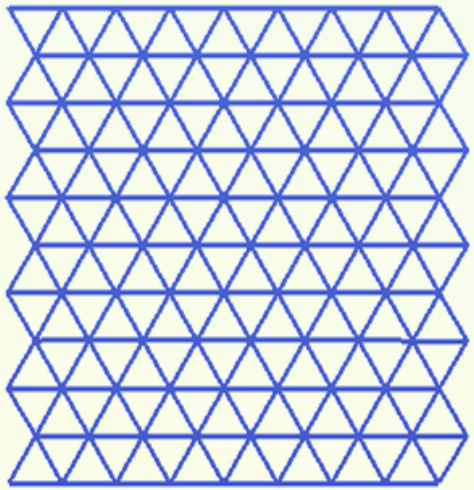


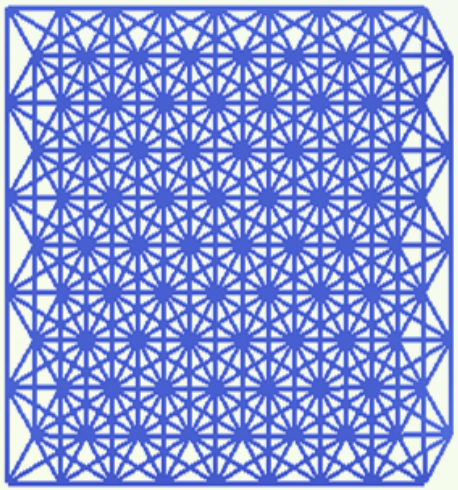
L [Å]	NLI_{max}	n. links
14	6	600
31	12	4.851
70	29	126.756

Bidimensional Model

ParaView
Parallel Visualization Application

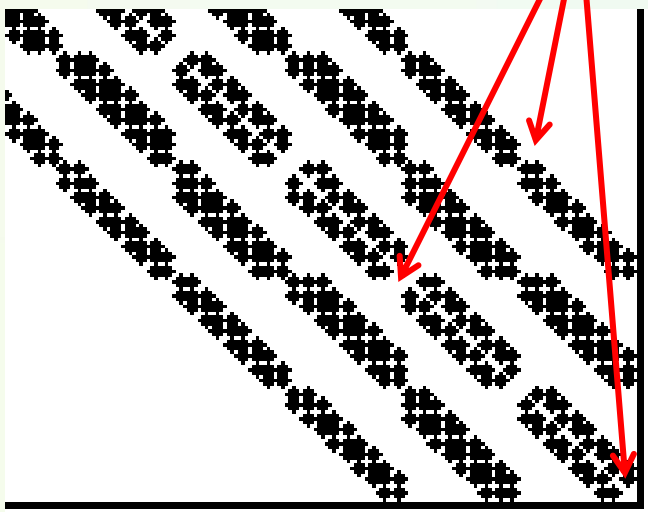
Connectivity Matrix: links increase with NLI

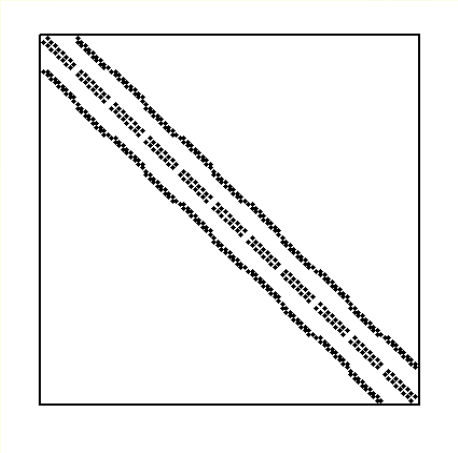


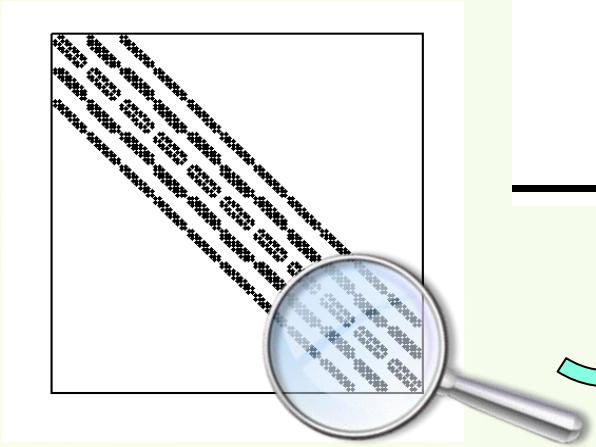


NLI=1 → NLI=3

Border effects due to finite size of the system





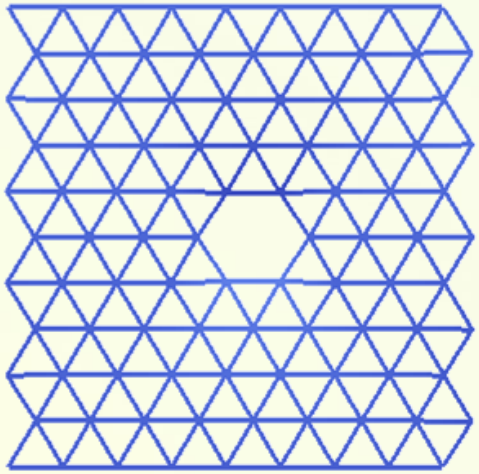


Bidimensional Model - with defects

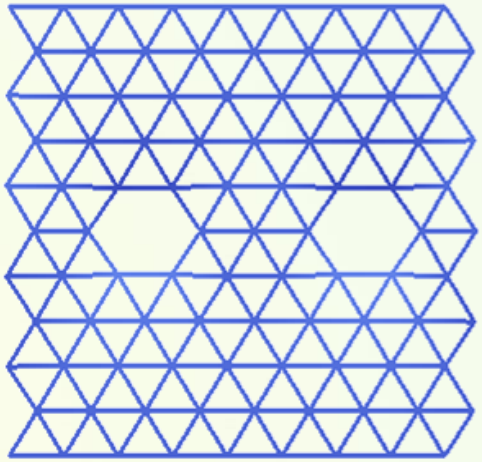
Flaw-tolerance study

Evaluation of the influence of NLI and defect position

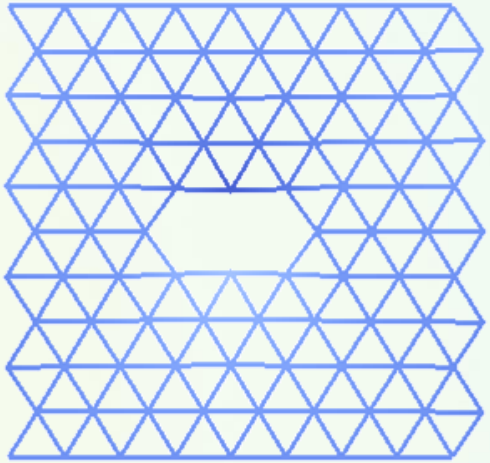
Case 1
One node removal



Case 2
Two non adjacent nodes removal

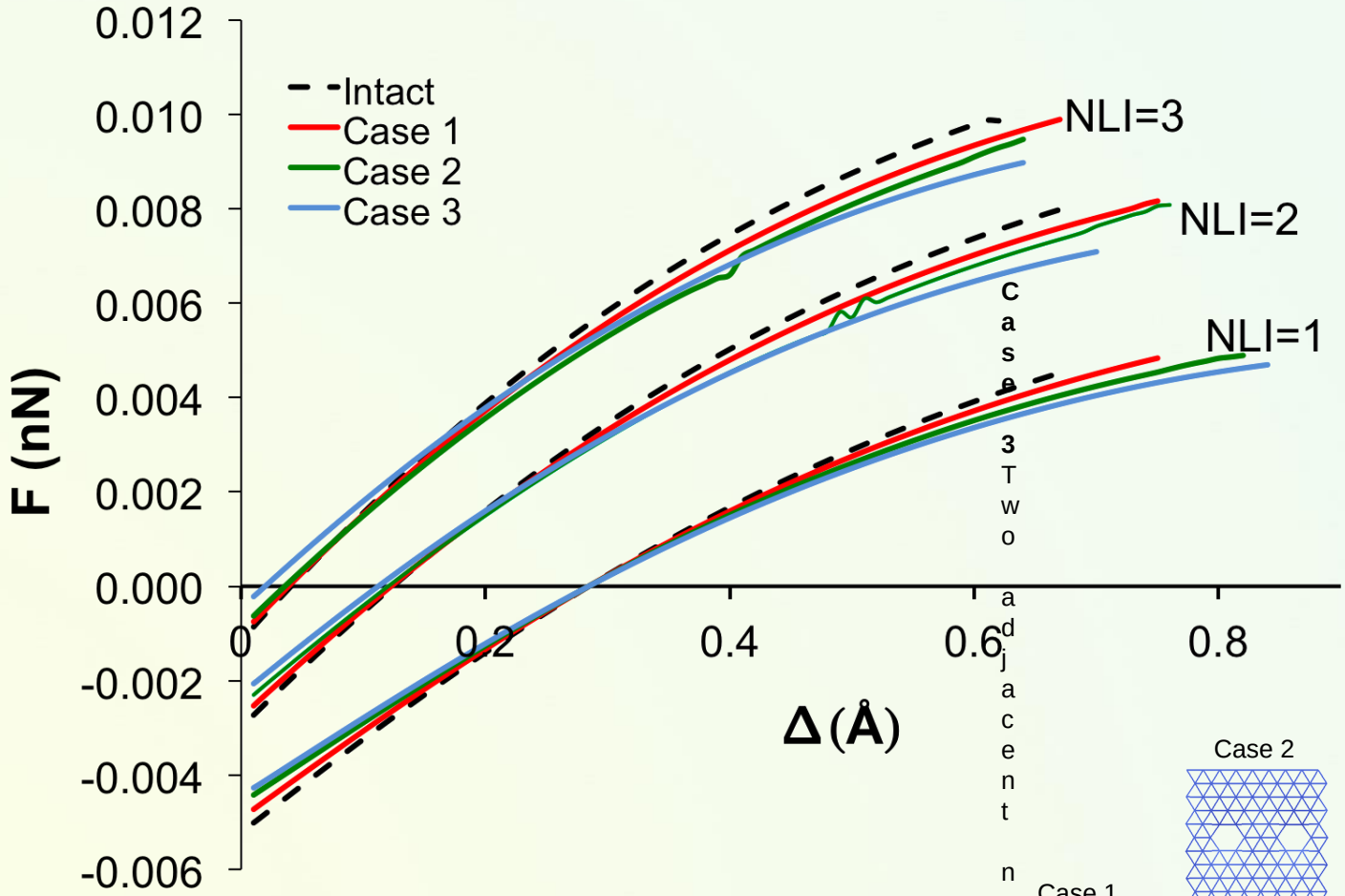


Case 3
Two adjacent nodes removal

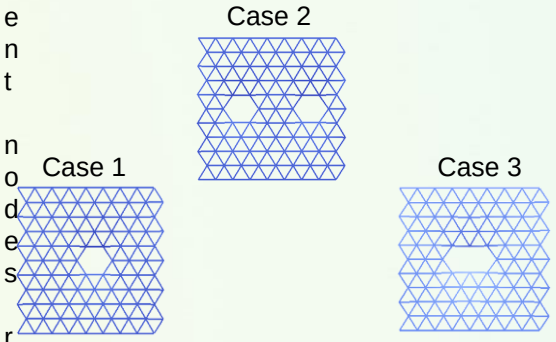


Bidimensional Model - with defects

Flaw-tolerance study



Case 3 Two adjacent nodes rem



For all given NLI: case 3 is the worst, it is due to:

- *position of removed node (respect to case 2)*
- *number of removed links (respect to case 1)*

Remarks

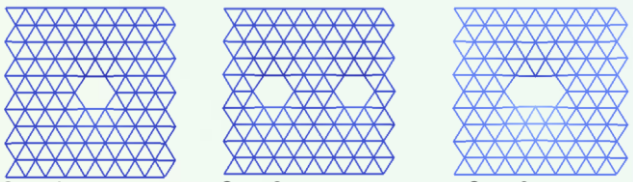
- **The role of NLI is important to characterize the network and has a considerable influence on the load carrying capacity of the system**

- **In discrete systems with nonlocal links have been observed strain localization phenomena**

Study of force level and distribution across the elements of the discrete system

Bidimensional Model - with defects

Forces distribution in a defective 31 x 31 Å sample

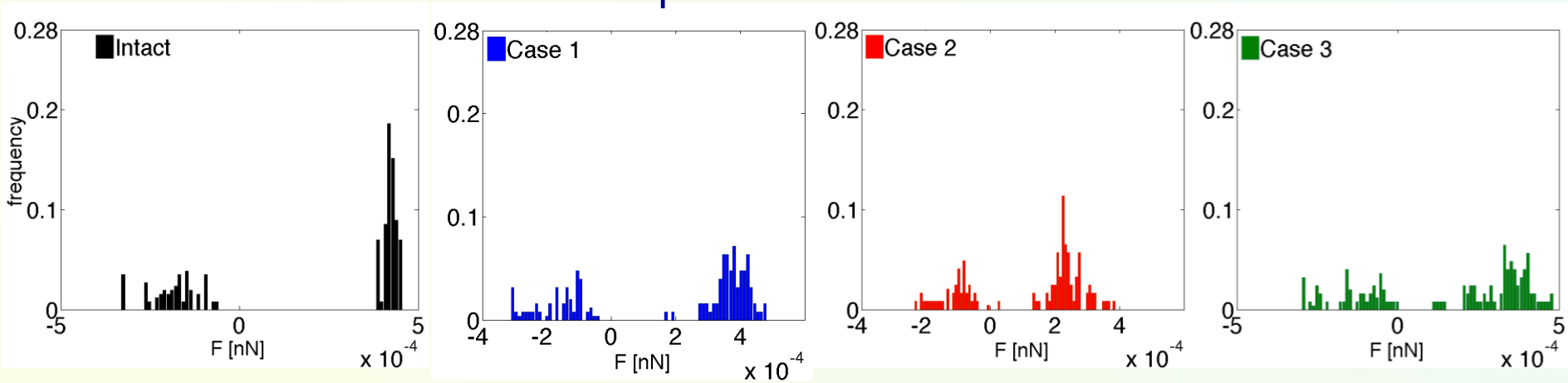


Case 1 One node removal

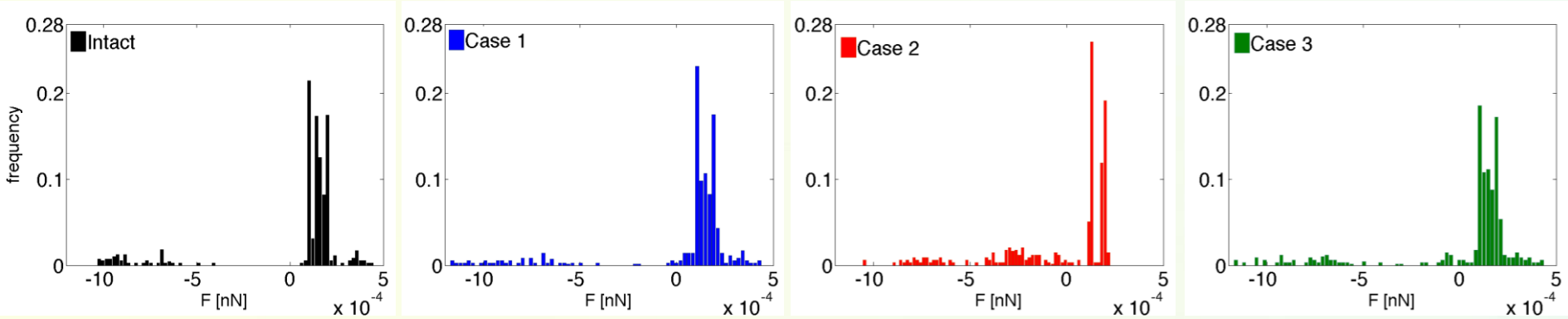
Case 2 Two non adjacent nodes removal

Case 3 Two adjacent nodes removal

NLI = 1 Widespread distribution



NLI = 3 Lower values of forces



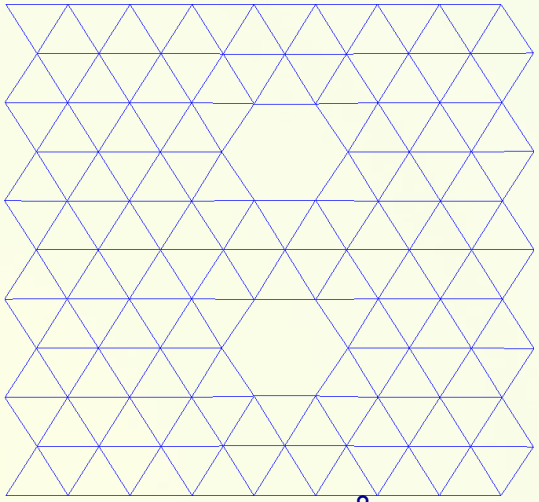
Bidimensional Model - with defects

Forces distribution for different sample dimensions

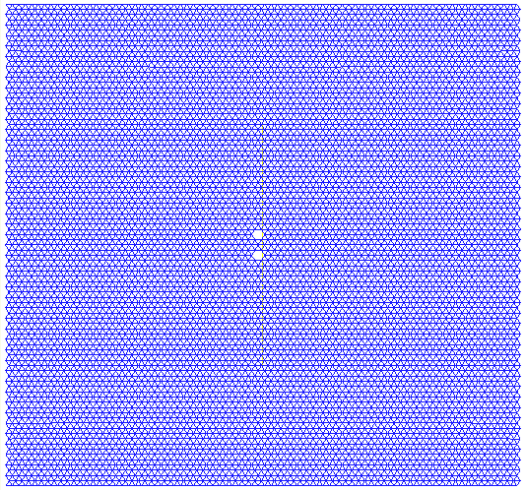
	NLI=3	
L [Å]	n. links	F_{max} [nN]
31	1216	0.776E-04
93	13568	3.849E-04
297	129316	117.57E-04

Results:

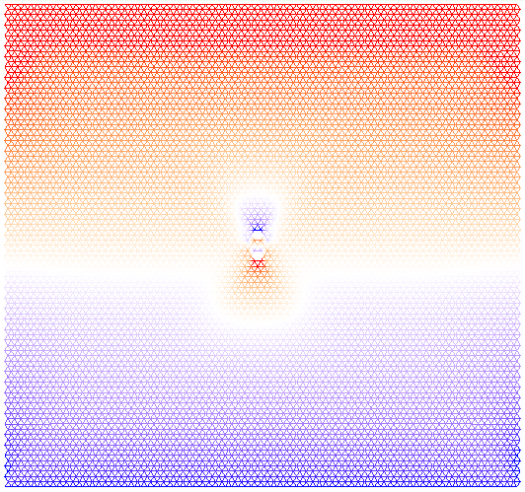
- Peak frequency is reached for lower force values
- More broad force distribution with the increase of dimensions



31 x 31 Å

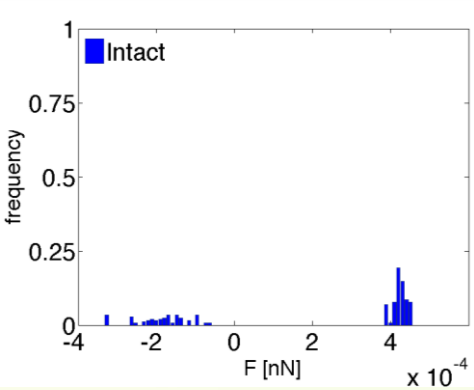


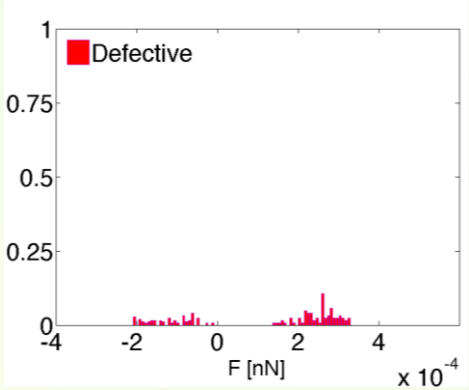
279 x 279 Å



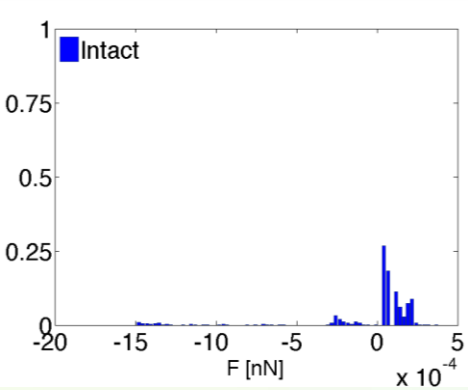
Bidimensional Model - with defects

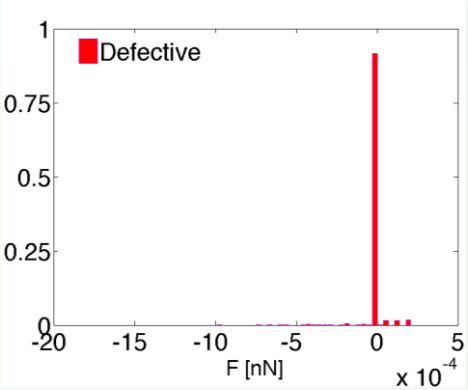
31 x 31 Å – NLI=1





31 x 31 Å – NLI=3

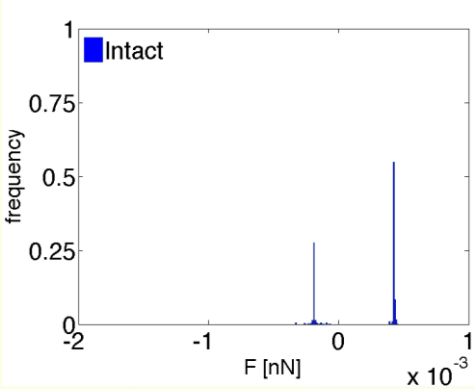


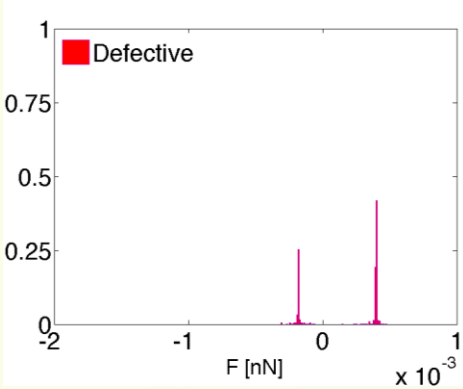


dim. increase = less boundary effects (force more concentrated)

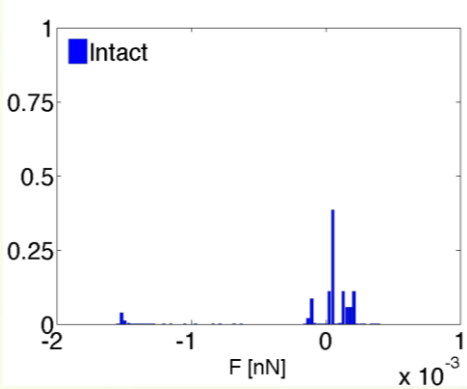
bigger sample is more flaw-tolerant

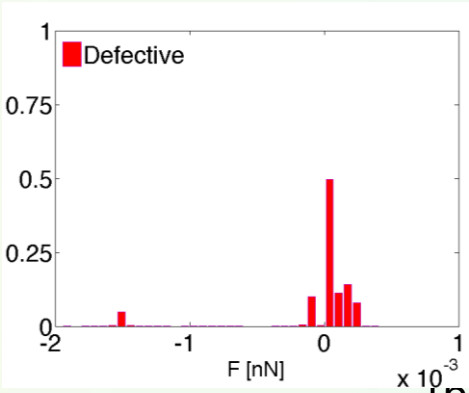
279 x 279 Å – NLI=1





279 x 279 Å – NLI=3

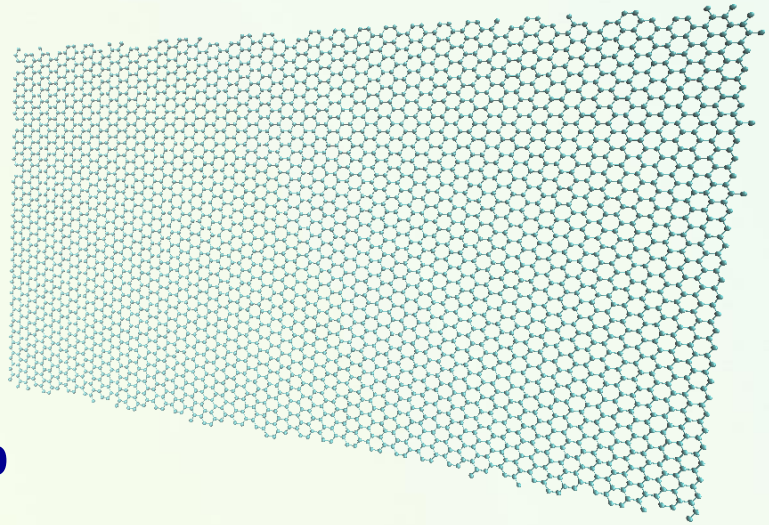




MD model

- ✓ **Pure MD simulation with LAMMPS Molecular Simulator***
- ✓ **AIREBO** (complete) potential considering pairing energy between -C- atoms**

31x31 Å
931 atoms } **sample box**
9528 links
'f f f' boundary conditions
1.1E+06 total steps @ 1 fs timestep

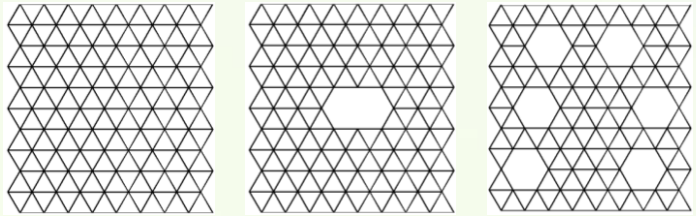


* S. J. Plimpton (1995), J Comp Phys, 117: 1-19

** D.W. Brenner (2002) J. Phys. Condens. Matter 14:783–802

In collaboration with:
Laboratoire Modélisation et Simulation Multi Echelle
Université Paris-Est, Marne-la-Vallée, France

MD model



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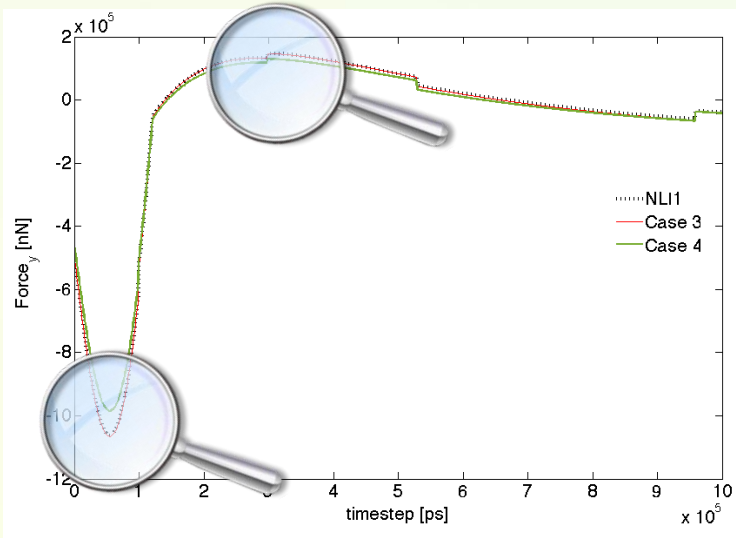
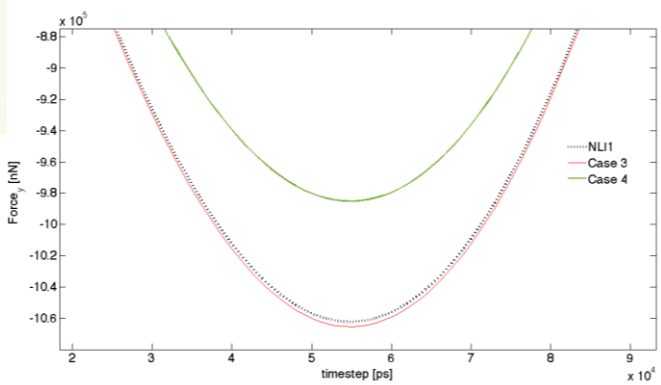
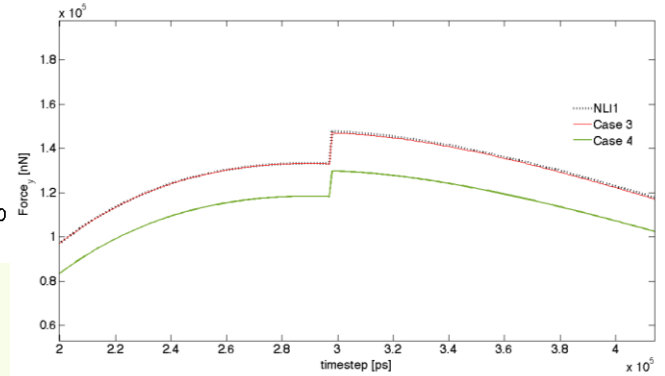
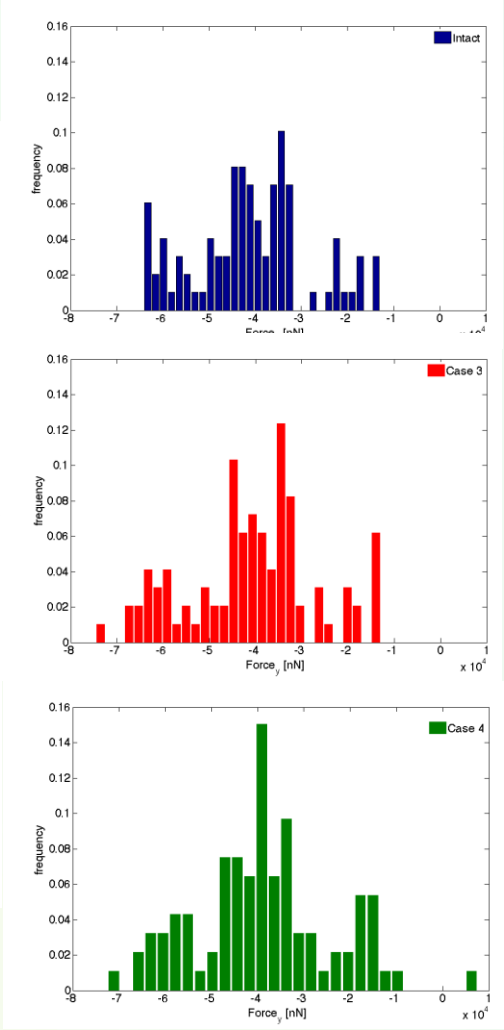








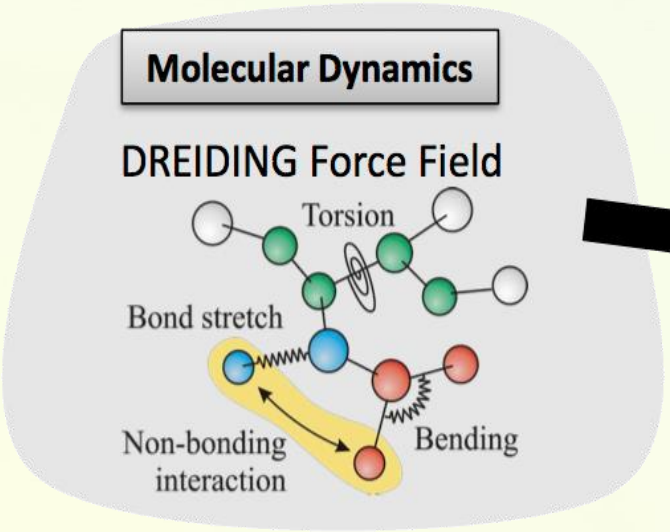
Due to strong bonded interactions the system is well tolerant but it is less evident the redistribution of forces

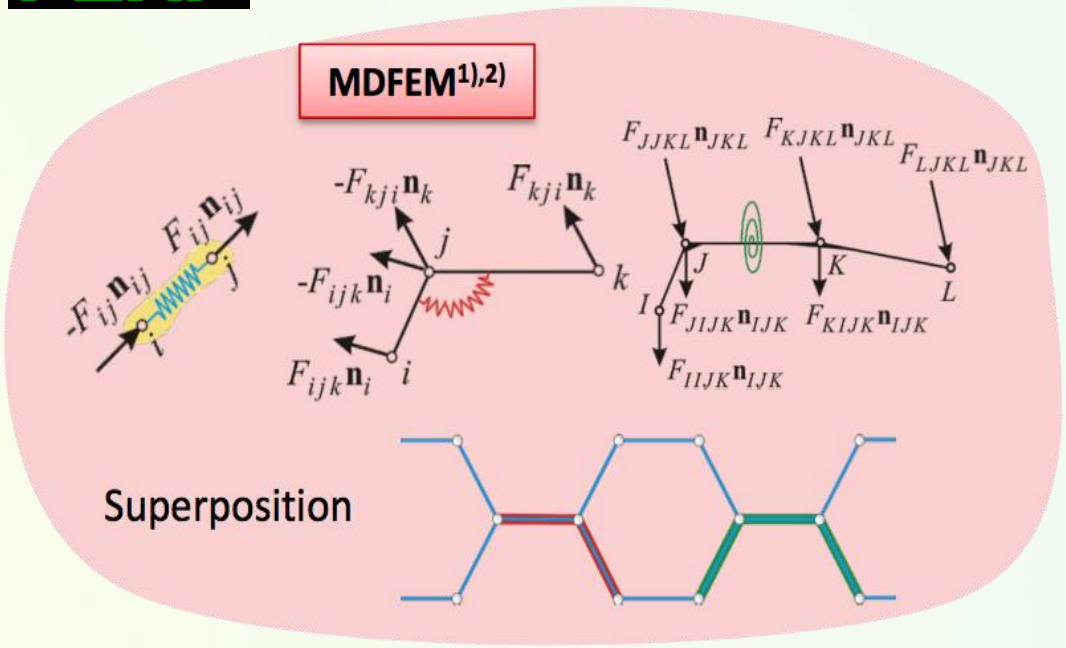
Work in progress – model enrichment

Model completion introducing potential for <u>bonded interactions</u> due to physical links between molecules.

4 nodes element DREIDING (b) + vdW (nb)

MDFEM simulation using FEAP





L. Nasdala et al. (2005) Comp. Mat. Sci. 33: 443-458

Acknowledgements

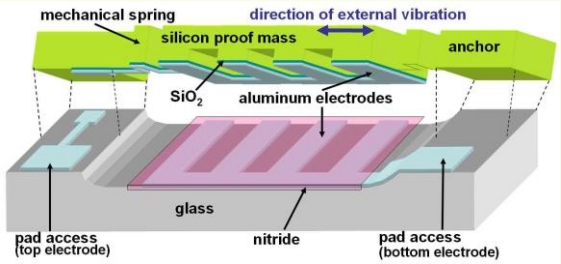
Thank you

(…Merci beaucoup!)

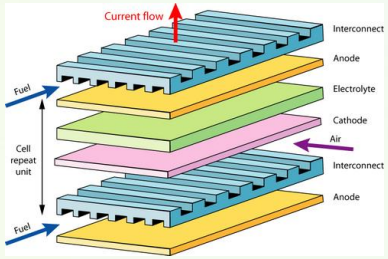
FIRB Future in Research 2010

Structural mechanics models for renewable energy applications

Photovoltaics (POLITO)



MEMS for wind energy harvesting (UNISAL)



Solid oxide fuel cells (UNITN)