Plan of the rest of this talk ..

- ❑ What Mechanics tells us about length scales of observed patterns in granular materials
- ❑ Pattern recognition from Complex Systems Theory and what patterns teach us about the nature of complex systems

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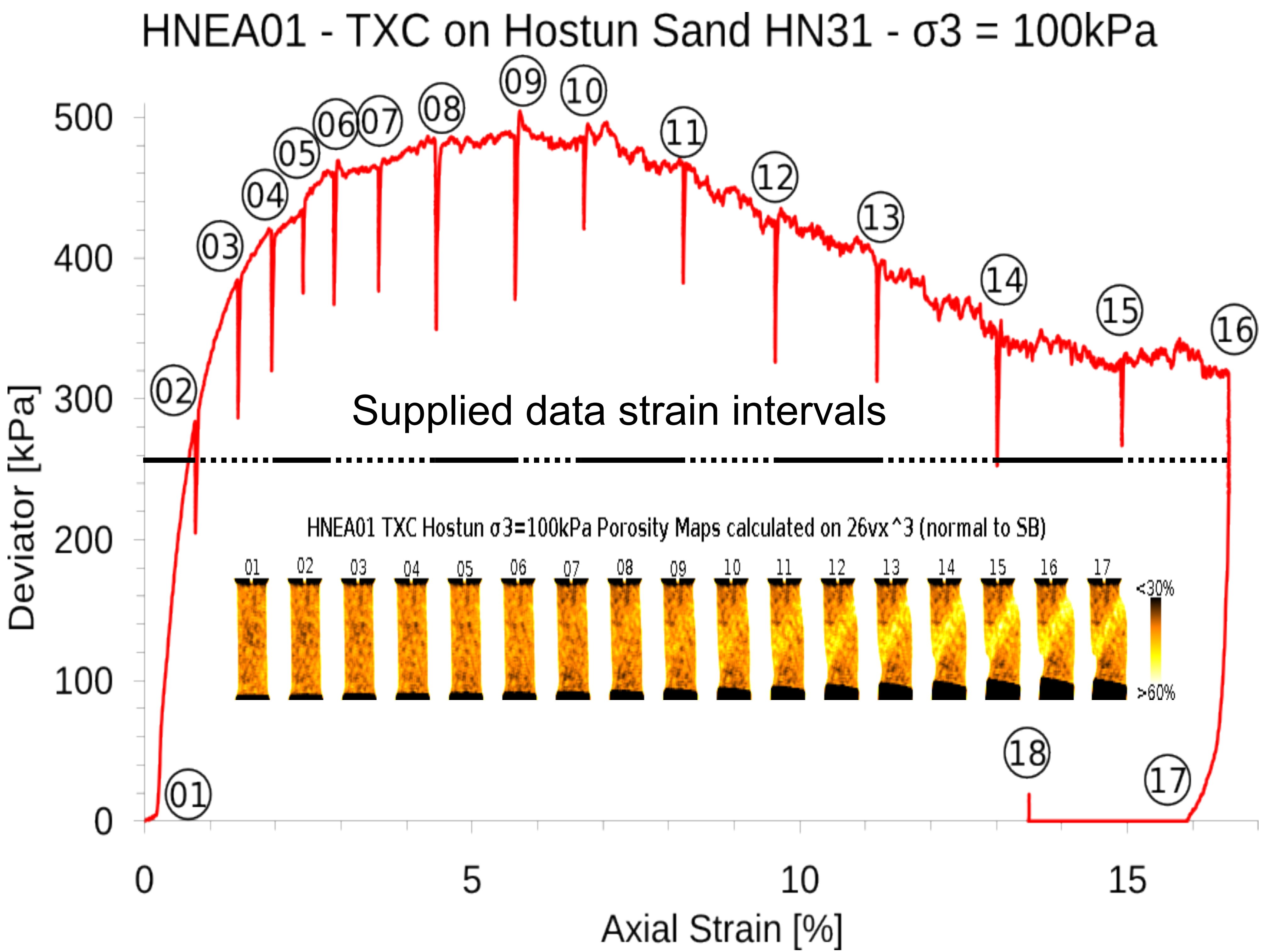
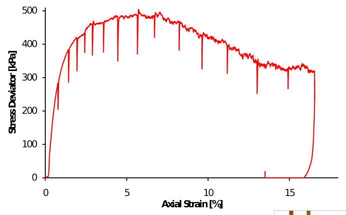
- ❑ **Extraction of length scales from Grenoble data on Hostun sand**
- ❑ Results from extraction
- ❑ Inception of Hostun sand and the null hypothesis to test length scales are robust, meaningful and **real**
- ❑ Results from inception
- ❑ Lessons learned and where to next …


HNEA01 - TXC on Hostun Sand HN31 - σ3 = 100kPa
Deviator [kPa]
Axial Strain [%]
0
100
200
300
400
500
0
5
10
15
01
02
03
04
05
06
07
08
09
10
11
12
13
14
15
16
17
18
Supplied data strain intervals
HNEA01 TXC Hostun σ3=100kPa Porosity Maps calculated on 26vx^3 (normal to SB)
<30%
>60%



ID-Track on Triaxial μ-Tomography Test
On Hostun Sand at σ3=100kPa

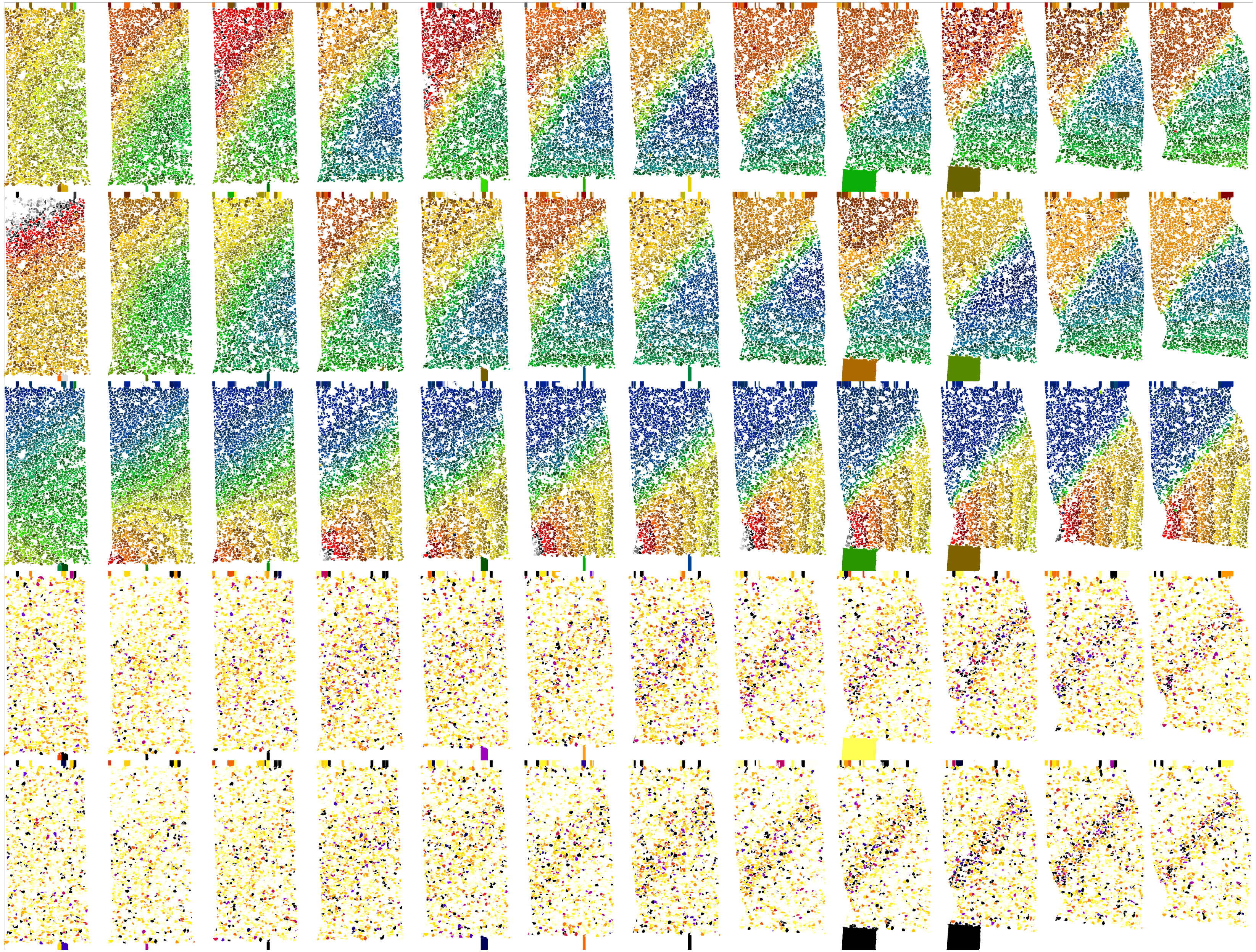
X Displacement
(Normalised by axial strain increment)

Y Displacement
(Normalised by axial strain increment)

Z Displacement
(Normalised by axial strain increment)

Grain Rotations
(Normalised by axial strain increment)

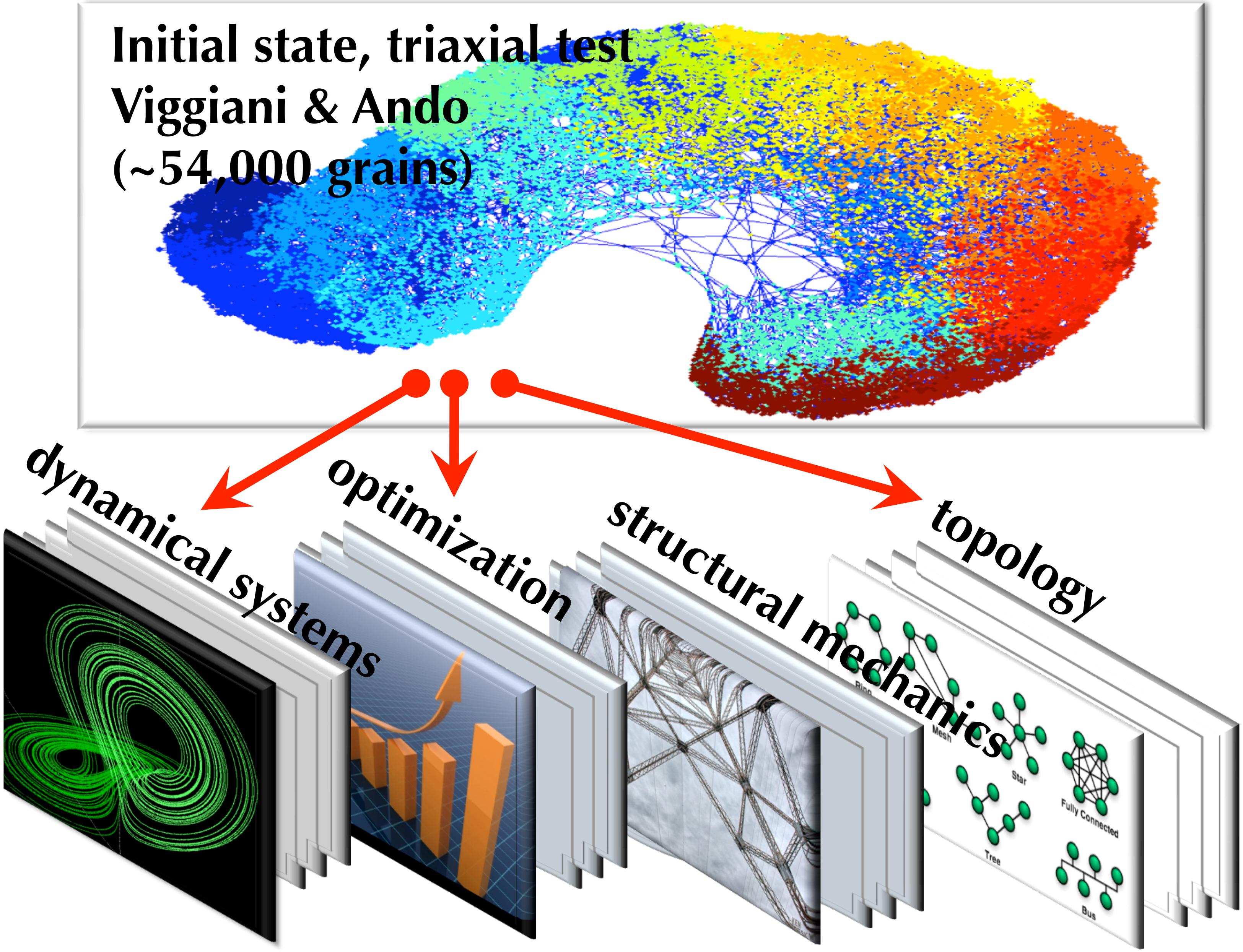
Grain Rotations Component in Plane
(Normalised by axial strain increment)



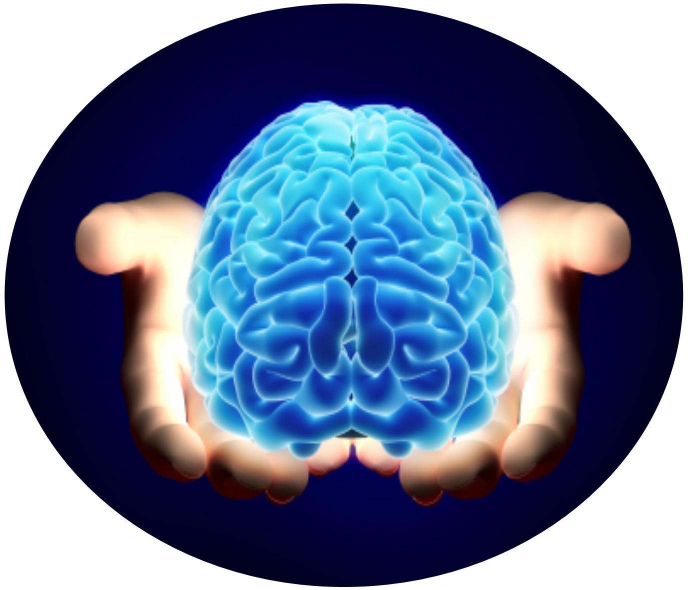
Complex Systems: Our Approach

Stage 1

Stage 2

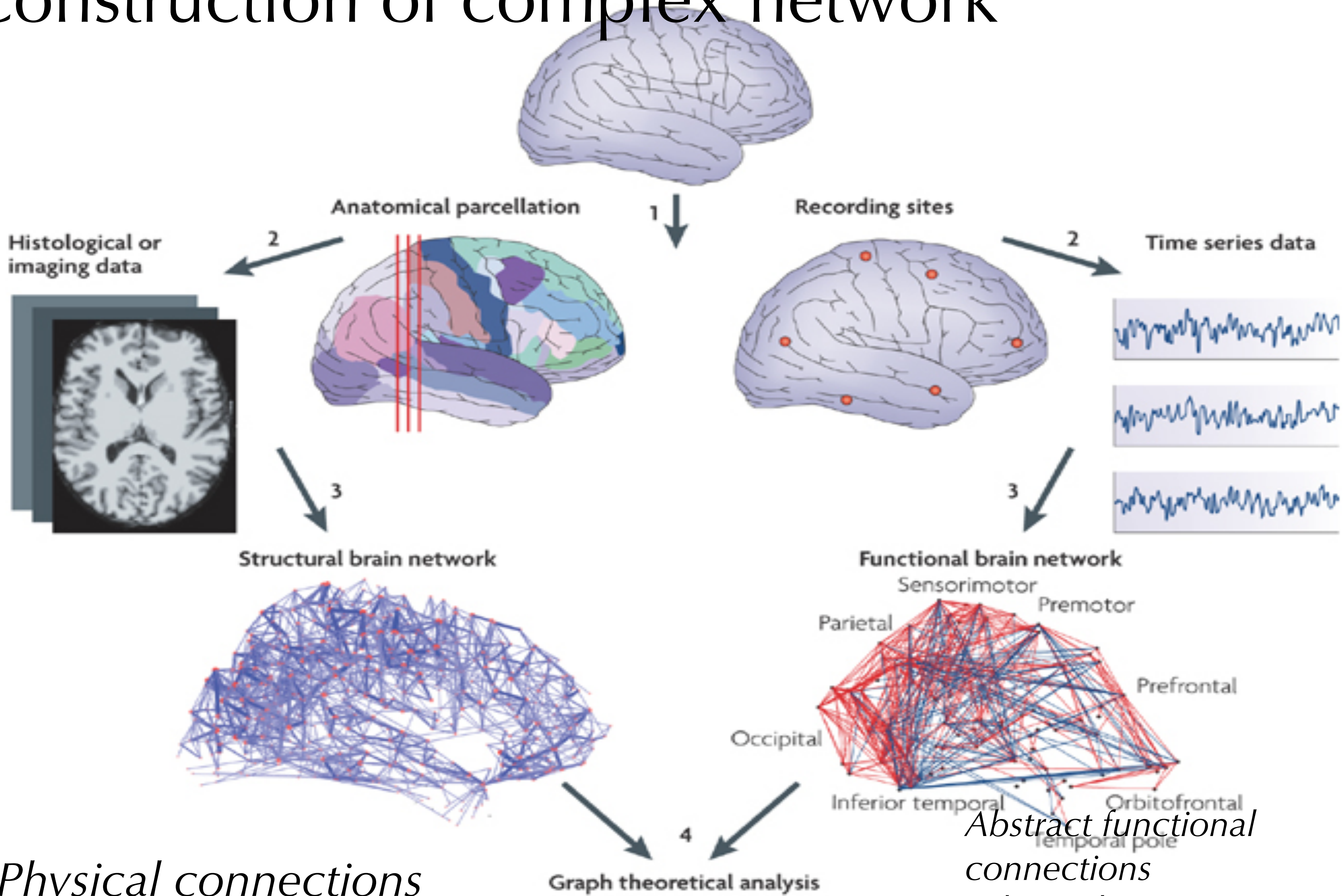


From brains to grains



- ❑ massively parallel information processing
- ❑ 10 billion neurons, each connected to other neurons through ~10,000 synapses
- ❑ adapts, 'learns' by self-organization
- ❑ fault-tolerant & capable of partial recovery from damage

Construction of complex network



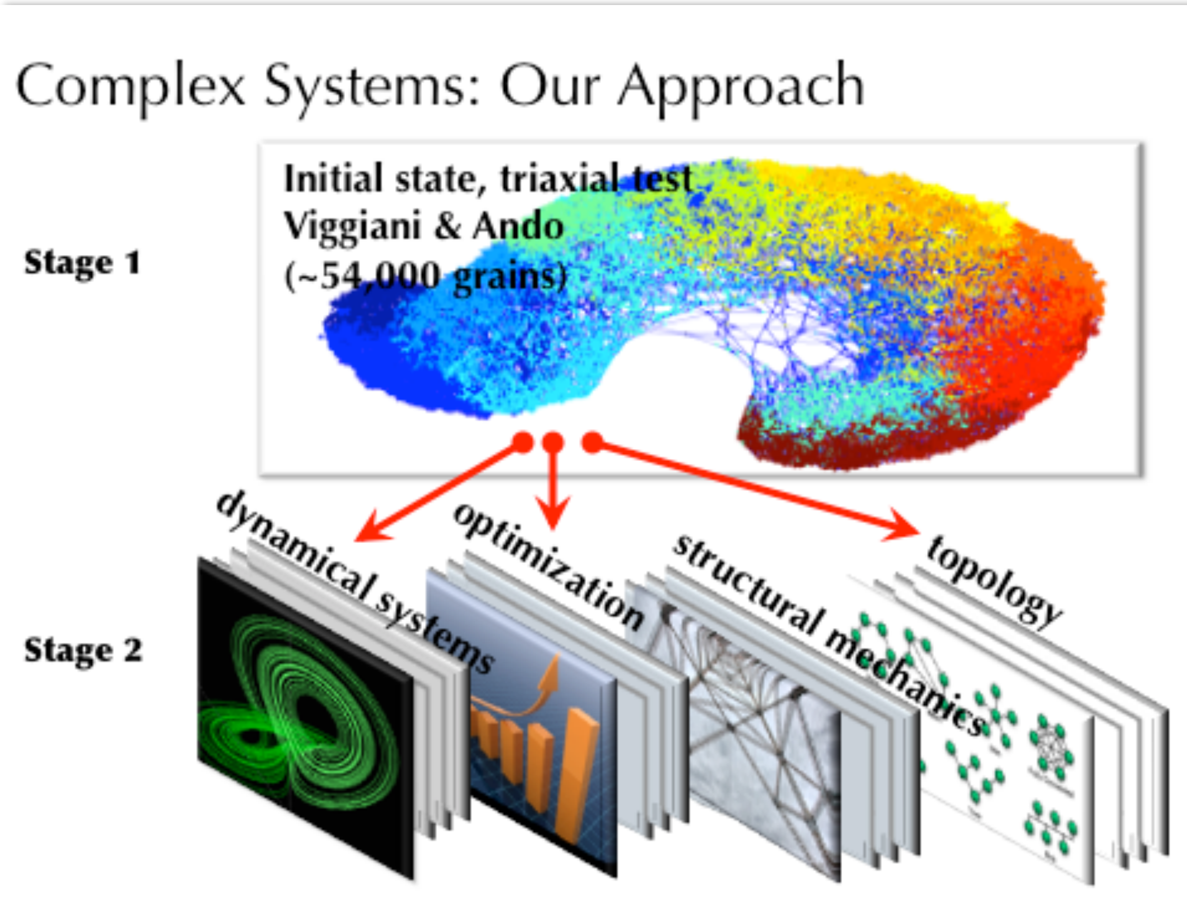
Physical connections

Abstract functional connections (physical connection not necessary)

Nature Reviews Neuroscience **10**, 186-198 (2009)

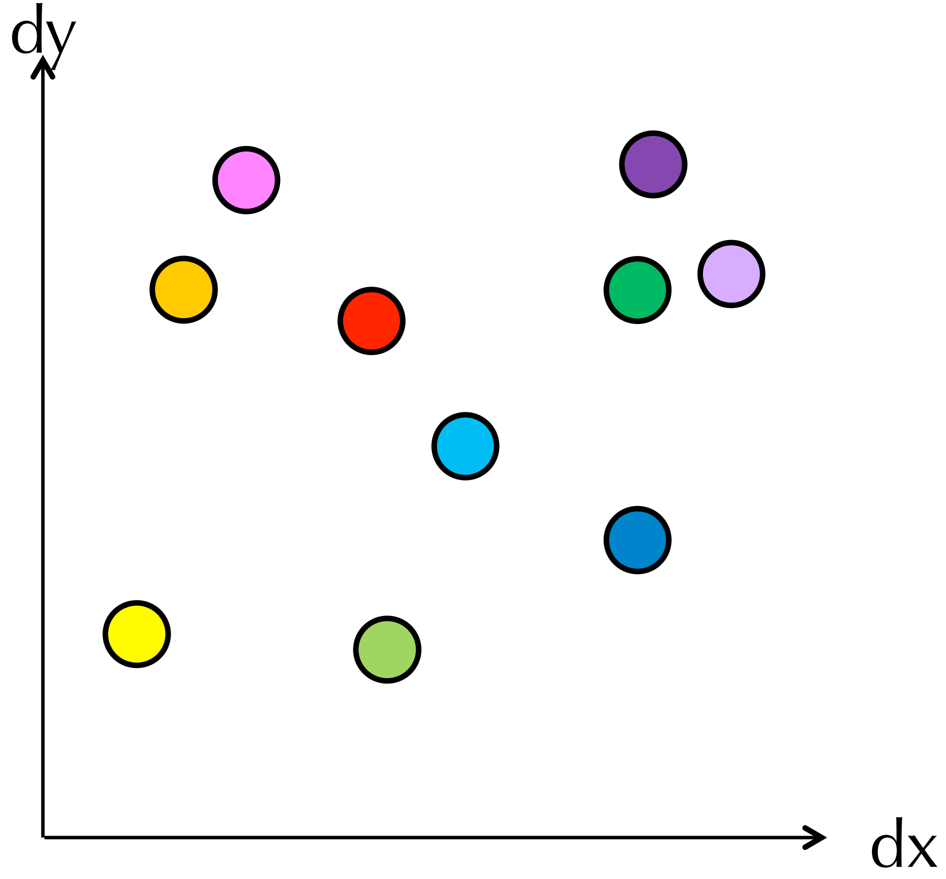
Hostun data:

- ❑ Currently no information on physical connections
- ❑ Time series not possible as only 12 states
- ❑ *Need to manufacture many clones of Ed to achieve both the above!*



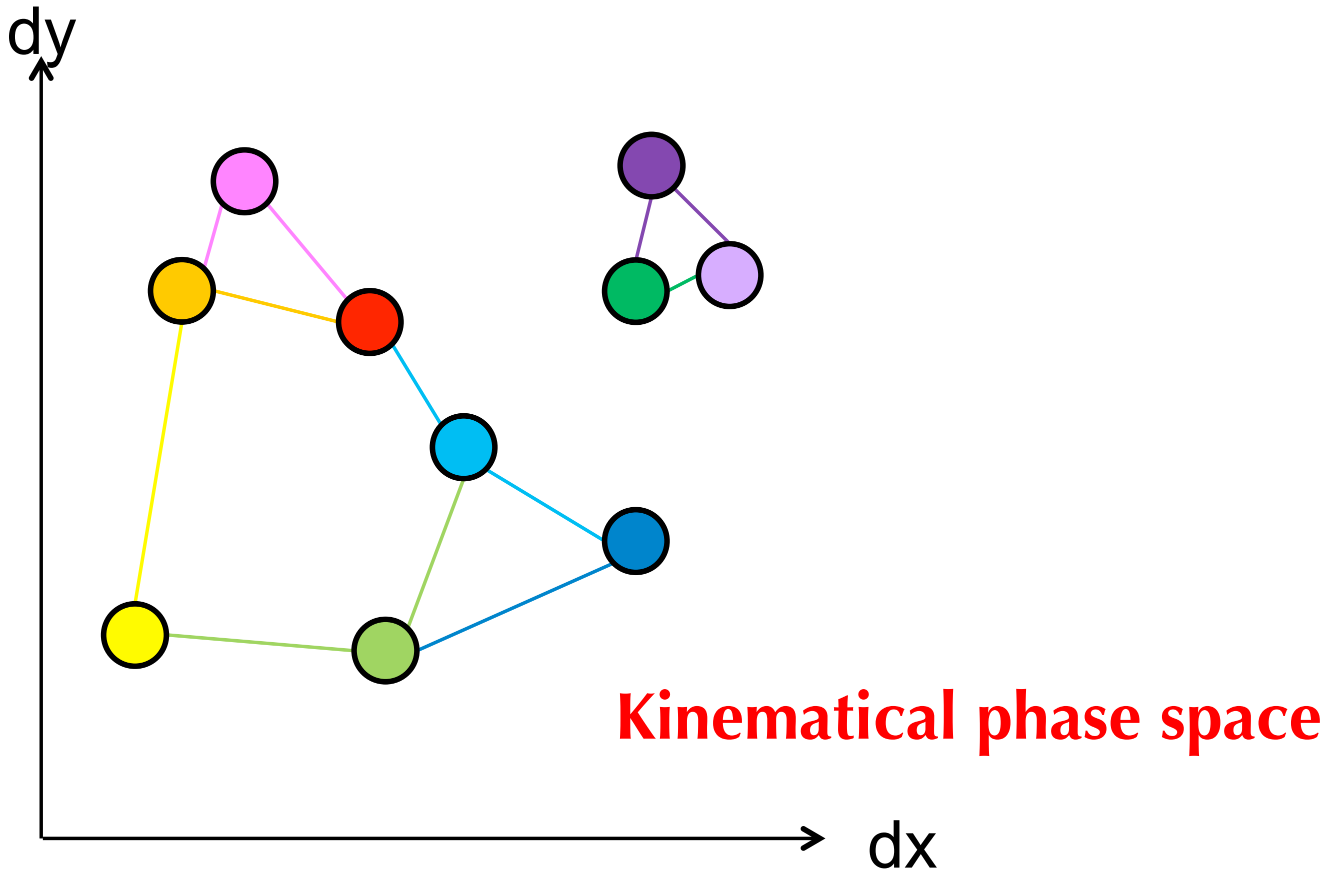
Construction of a functional network: k-Net

- ❑ Consider simpler data set: displacements of 10 particles in 2D
- ❑ Iteratively connect each node to its closest *k* neighbours
- ❑ Choose *k* to be the minimum *k* needed to connect all nodes into a single-connected network, i.e. one component



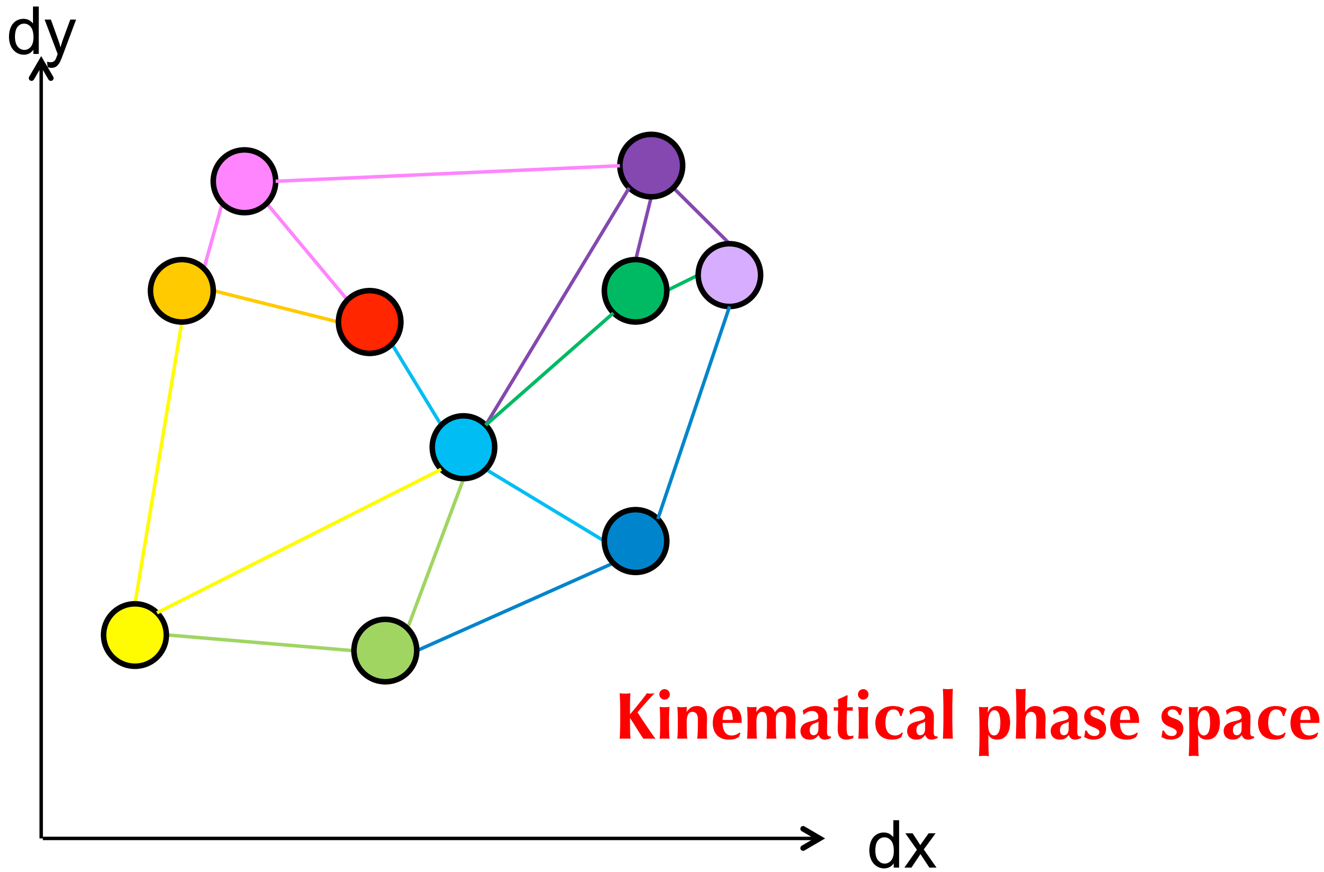
Kinematical phase space

Construction of a functional network: k-Net



- ❑ Try k= 2: connect each node to its two closest neighbours.
- ❑ Check number of components: 2
- ❑ Try k=3

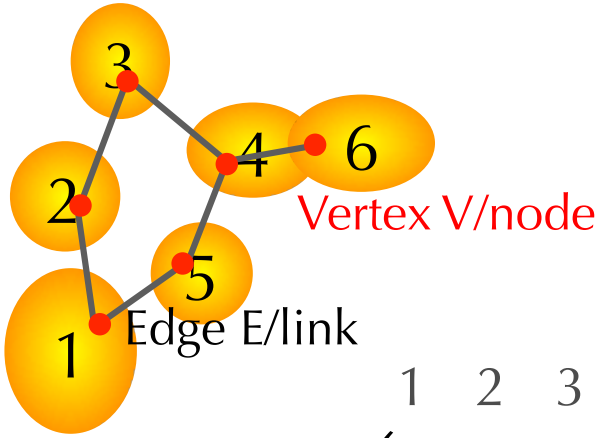
Construction of a functional network: k-Net



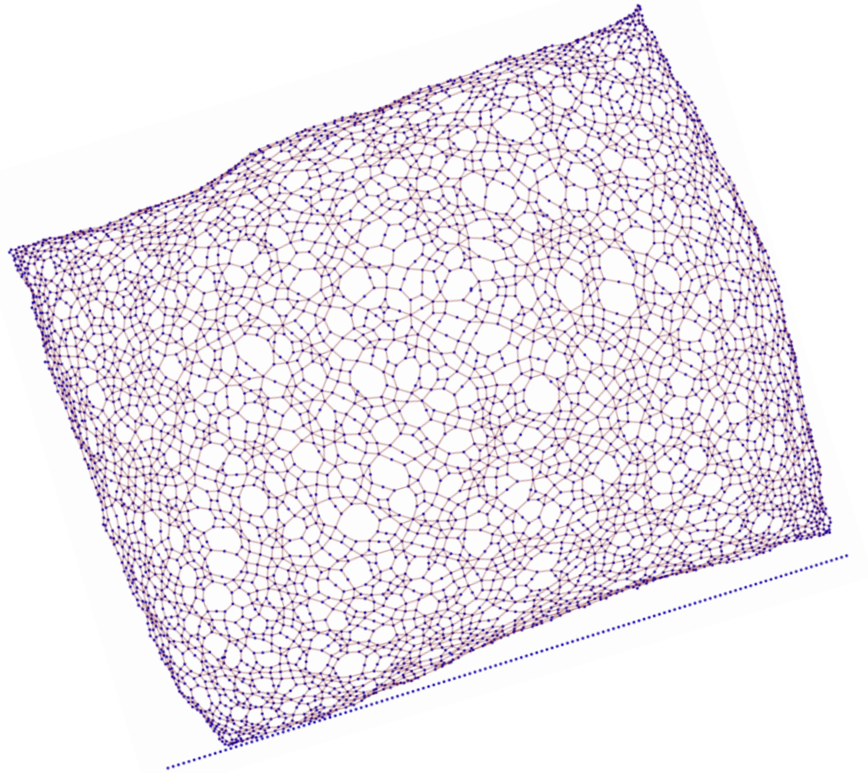
- ❑ One component: hence the final network is 3-Net.

Complex Networks

Connectivity: graph G(V,E)



$$A = \begin{array}{c c} & \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} & \begin{pmatrix} \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} \\ \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \end{pmatrix} \end{array}$$



- ❑ Example for contact network (Walker & Tordesillas IJSS 10; Tordesillas PRE 10)

Questions about Hostun sand .....

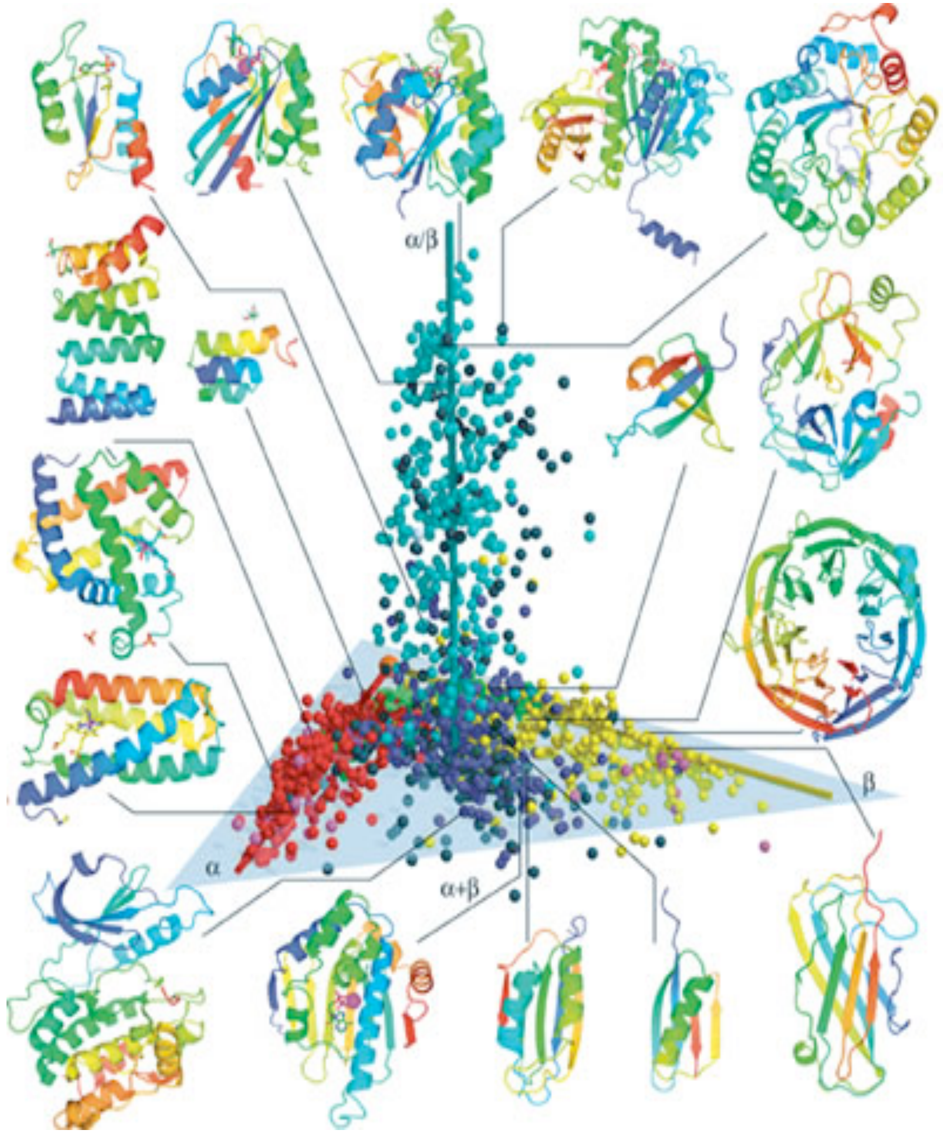
1. Is there a community structure to the functional networks from kinematic fields?

2. What are the length scales (spatial), if any, from such communities?

3. Which are in the best position to spread information (nodes of highest efficiency) to all the other nodes in the network?

Community structures

- ❑ 54,000 grains! Can we organize this system into groups of grains – each with a common attribute and possibly serving a similar function?
- ❑ Community structure: "natural fault lines" dividing a network into communities, i.e. groups of nodes in which connections are dense within each group and relatively sparse between groups
- ❑ Helps to understand structural organization
- ❑ ***First 3D map of protein architecture, identifying ~10,000 groups of structural motifs serving similar function from trillions of proteins (Kim et al UC Berkeley, PNAS 11)***

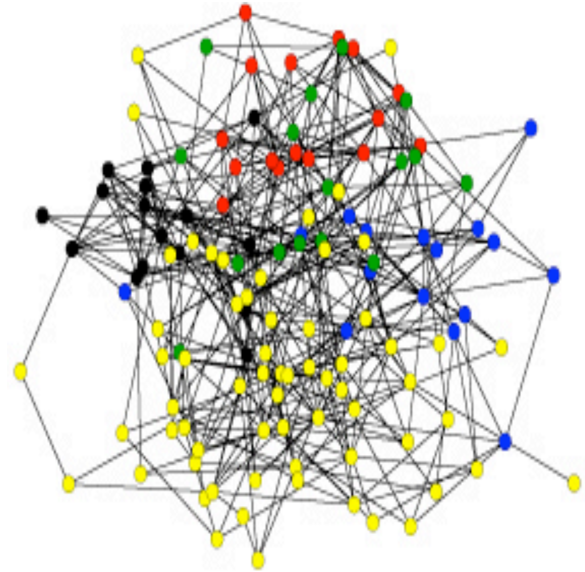


Community detection

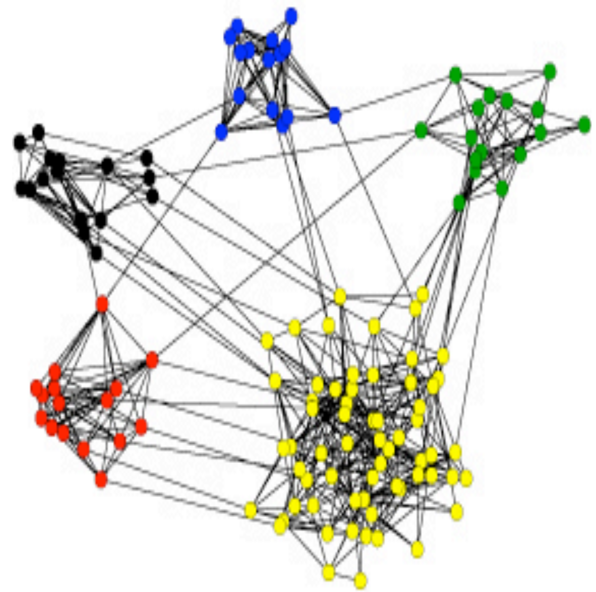
❑ The human eye: poor detector of community structures or "natural fault lines" of a network. Need an algorithm & computer to execute!

❑ Active research; existing methods are state-of-the-art. One method: maximize community modularity *Q*

❑ Q is a cost function maximized by a partitioning of nodes with higher density ***intra***-connections compared to ***inter***-connections



(a)



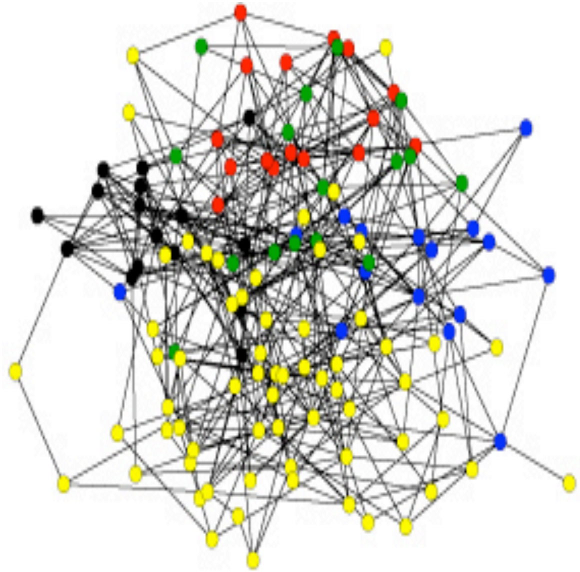
(b)

Community modularity

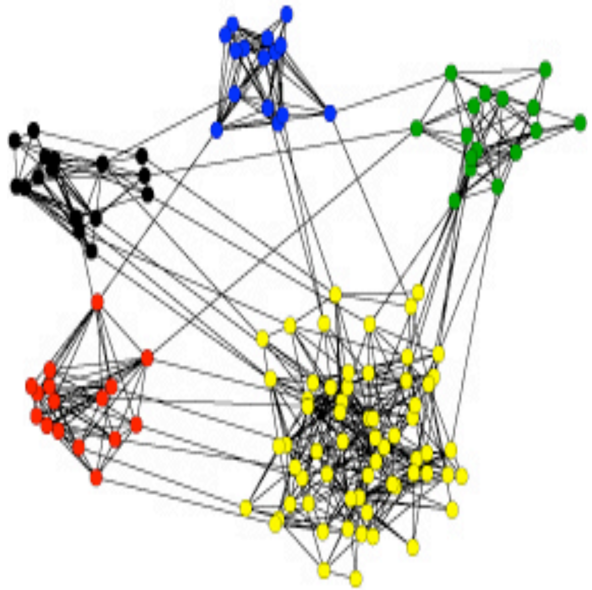
❑ Given a graph/network let the set of nodes be partitioned into k subsets where each belongs to one community. The community modularity Q of this partition is

$$Q = \sum_{i=1}^{k} q_i \quad \mapsto \quad q_i = e_{ii} - a_i^2$$

❑ e_{ii} is the percentage of number of links that has both ends in a community V_i (e.g. blue-blue), and a_i is the percentage of links that start from a community V_i (blue-black, blue-green, blue-red, etc.)



(a)

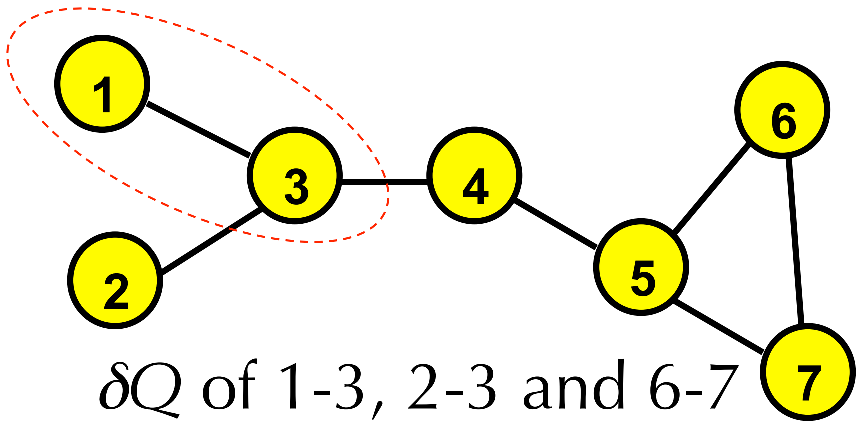


(b)

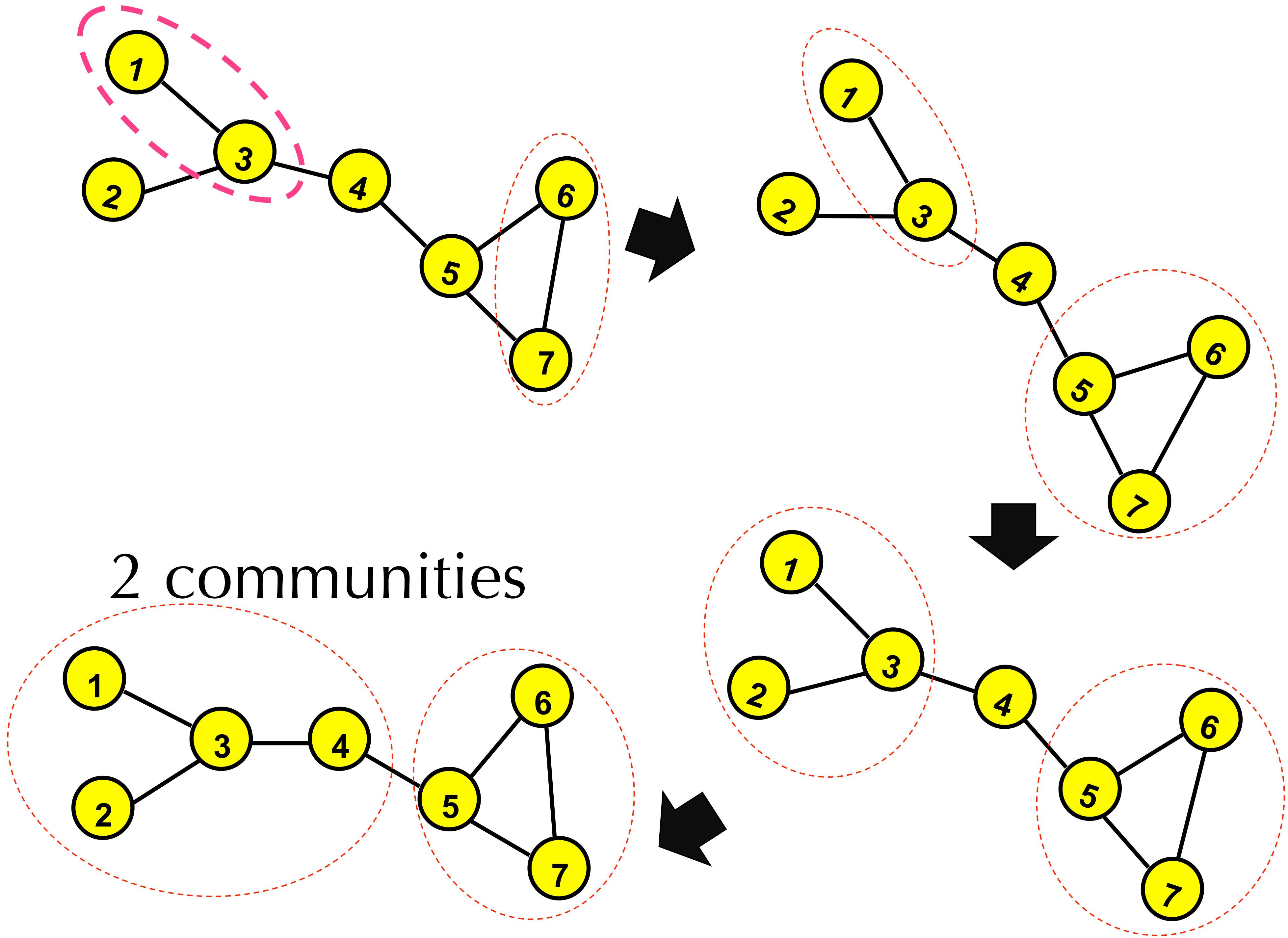
Algorithm

- ❑ Initially, treat each node as a community.
- ❑ Successively amalgamate groups in pairs, choosing at each step the pair which leads to highest increase in Q.
- ❑ Terminate if highest change in Q is negative.

$1-3$	$\mapsto$	$\delta Q = 17/9$
$2-3$	$\mapsto$	$\delta Q = 17/9$
$3-4$	$\mapsto$	$\delta Q = 27/16$
$4-5$	$\mapsto$	$\delta Q = 27/16$
$5-6$	$\mapsto$	$\delta Q = 27/16$
$5-7$	$\mapsto$	$\delta Q = 27/16$
$6-7$	$\mapsto$	$\delta Q = 17/9$



δQ of 1-3, 2-3 and 6-7 are identically maximum: any of these connections can be chosen



1
2
3
4
5
6
7
2 communities

Plan of the rest of this talk ..

- ❑ What theory tells us about length scales of observed patterns in granular materials
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---

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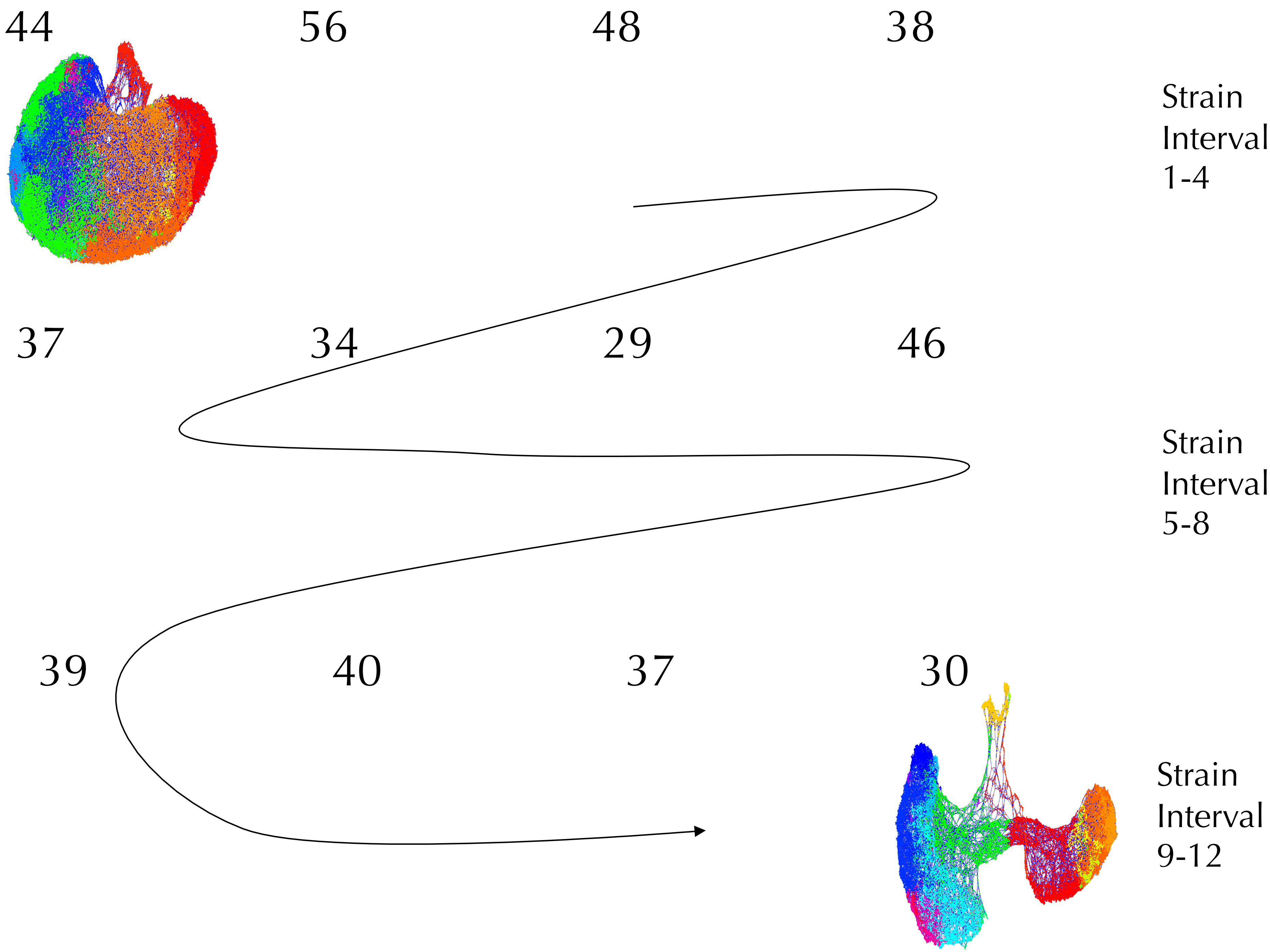
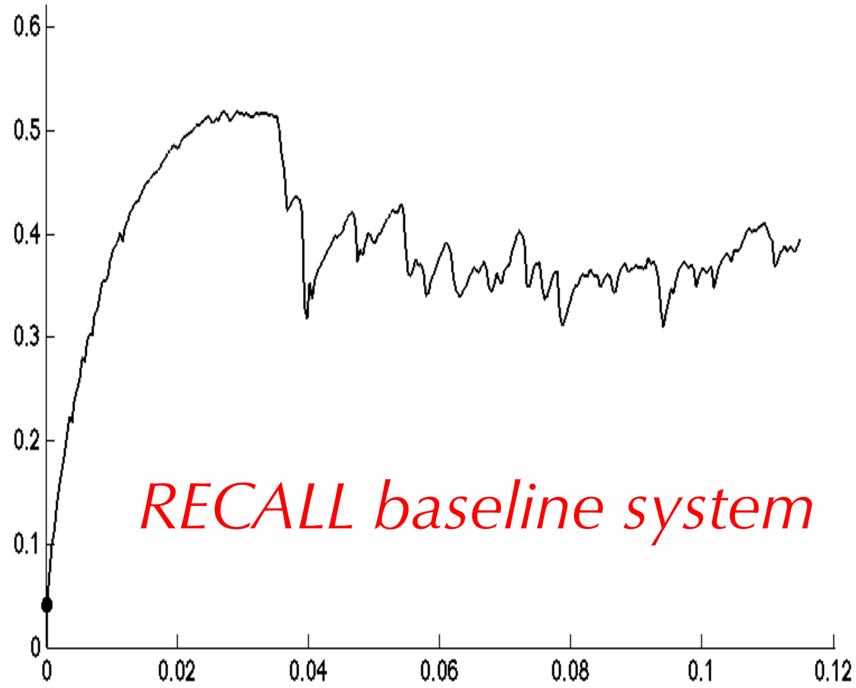
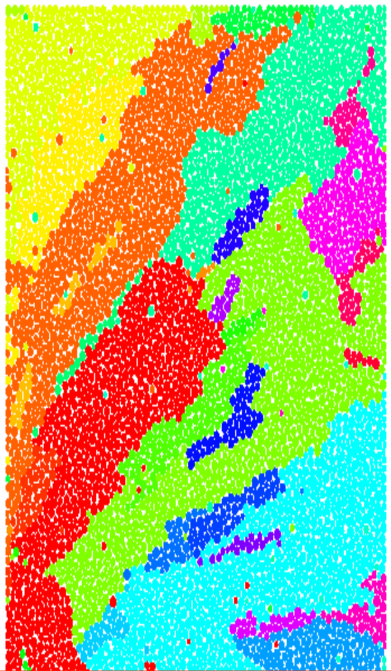

44
56
48
38
Strain
Interval
1-4
37
34
29
46
Strain
Interval
5-8
39
40
37
30
Strain
Interval
9-12

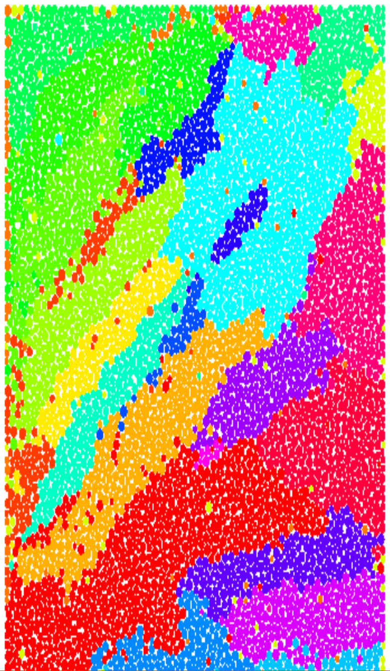
Community boundaries

❑ Boundaries described *figuratively speaking* – as 'natural faultlines' in a network….

❑ But can this ***actually*** capture the natural faultlines in geomaterials?



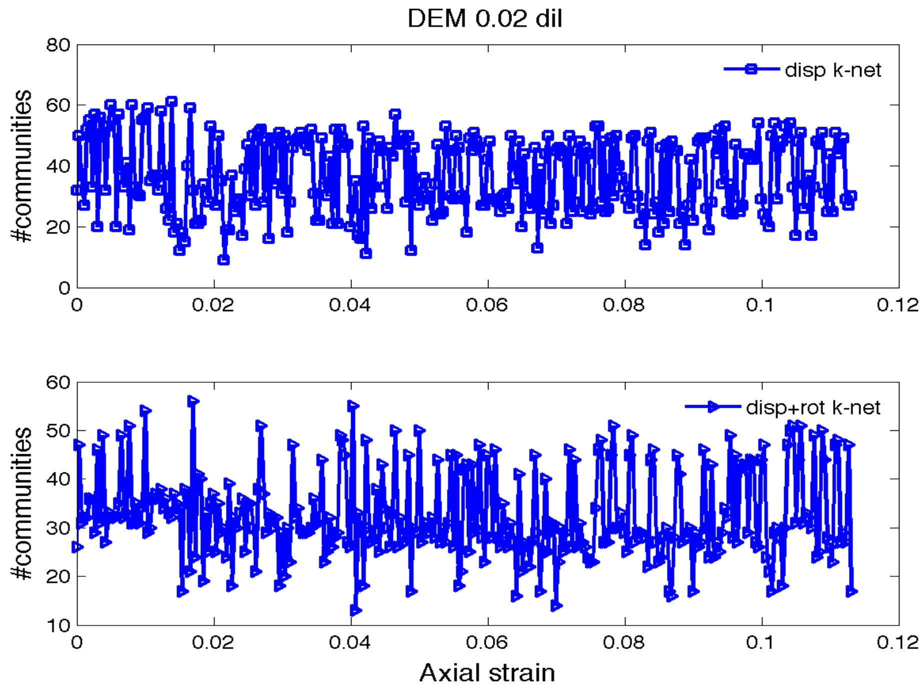


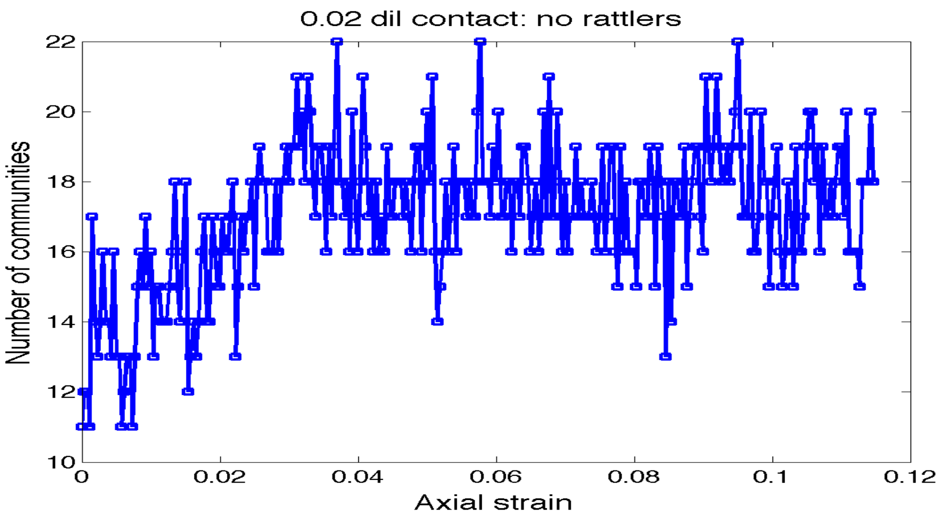


Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

Number of communities

- ❑ k-nets: fluctuations about a near constant value throughout loading
- ❑ similar range to Hostun
- ❑ C-net has much less number of partitions but tracks evolution to failure well





Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

Questions about Hostun sand …..

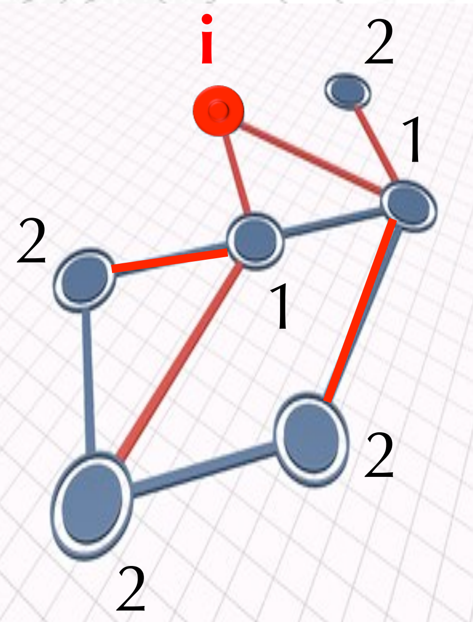
1. Is there a community structure to the functional networks from kinematic fields? YES: partitions into 29-48 communities

2. What are the length scales (spatial), if any, from such communities?

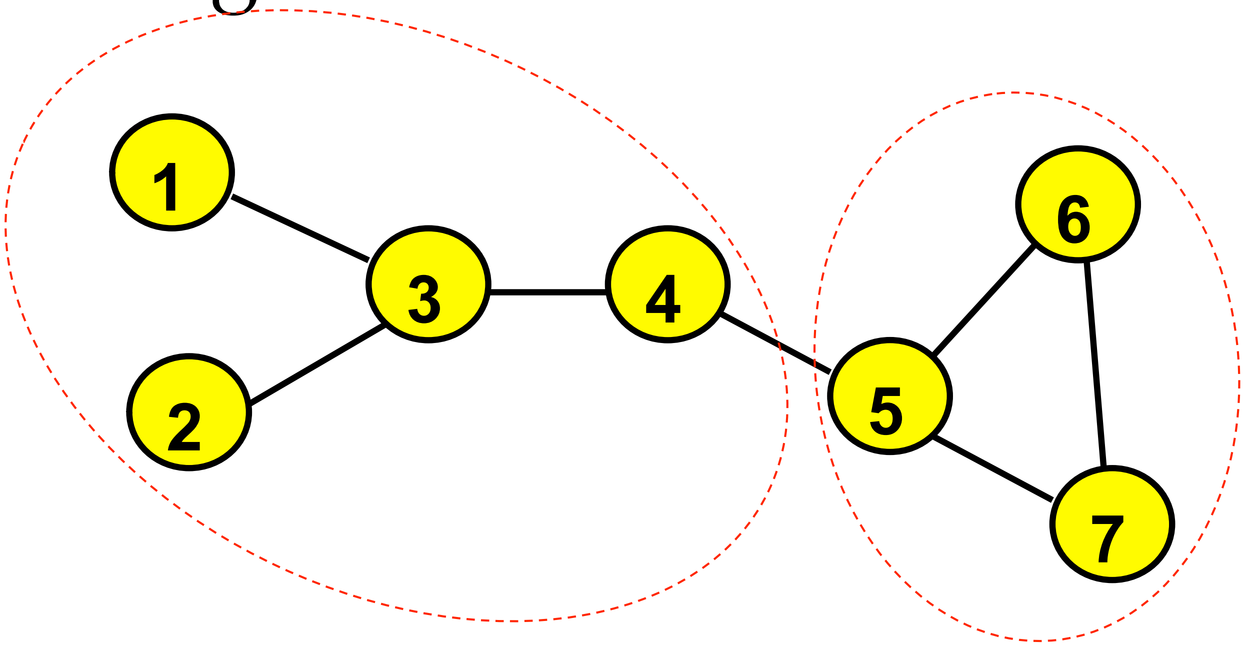
3. Which are in the best position to spread information (nodes of highest efficiency) to all the other nodes in the network?

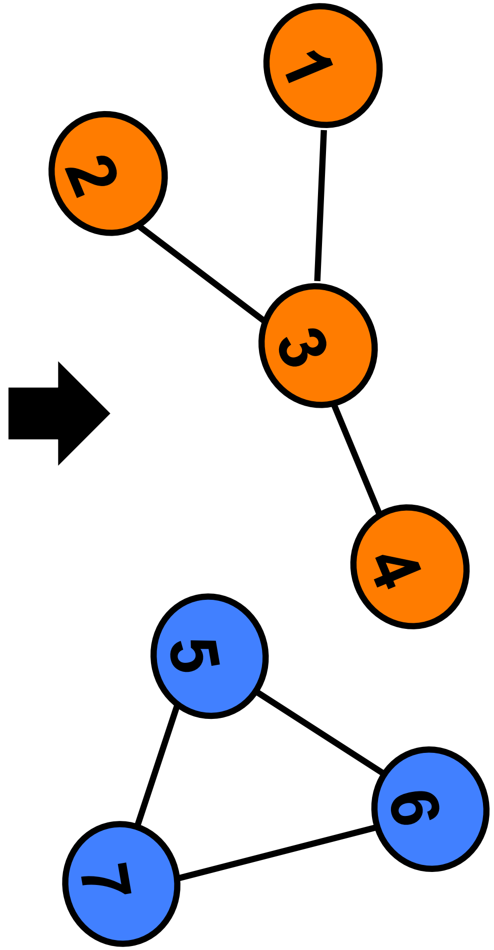
The long and short of “shortest paths”

- Length scales in networks typically come from **shortest path**, i.e. path between two nodes with **minimum number of links**
- Various network measures of dynamics and flow in networks are based on shortest paths
- **Average path length** of a network: the average number of links along shortest paths for all pairs of nodes.
  - Also known as ‘size of network’
  - The smaller the better: i.e. more easily negotiable hence more efficient flow of information through network.
  - Key measure in traffic, road and communication networks



Length scale from individual communities



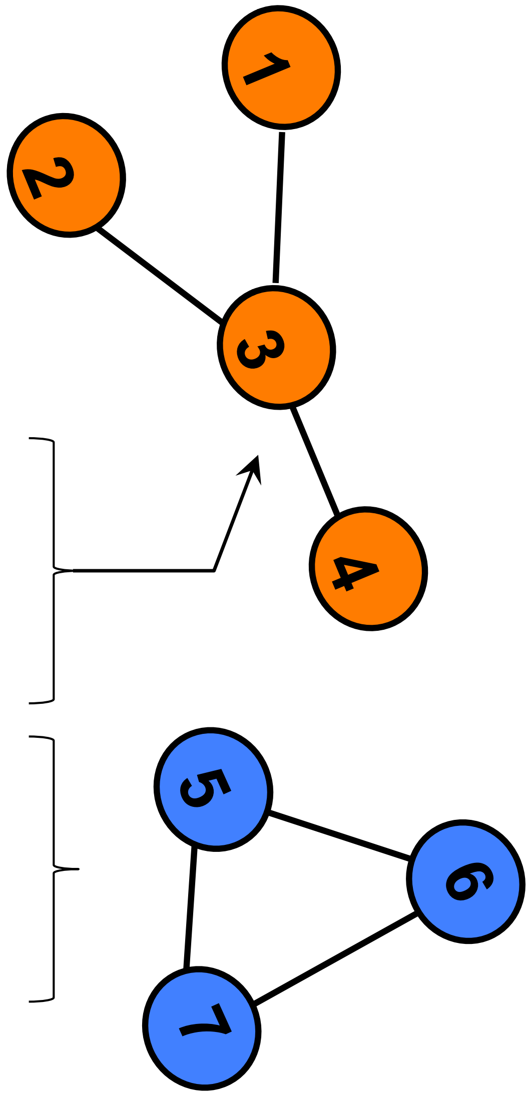


$$A = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

Length scales from communities

- For each community i, extract subgraph (eg adjacency matrix $A_{i\ (i=1,2)}$)
- Compute average shortest path length for each community i,

1-2	1-3	1-4	2-3	2-4	3-4	Tot	Ave
2	1	2	1	2	1	9	3/2
5-6	5-7	6-7				Tot	Ave
1	1	1				3	1

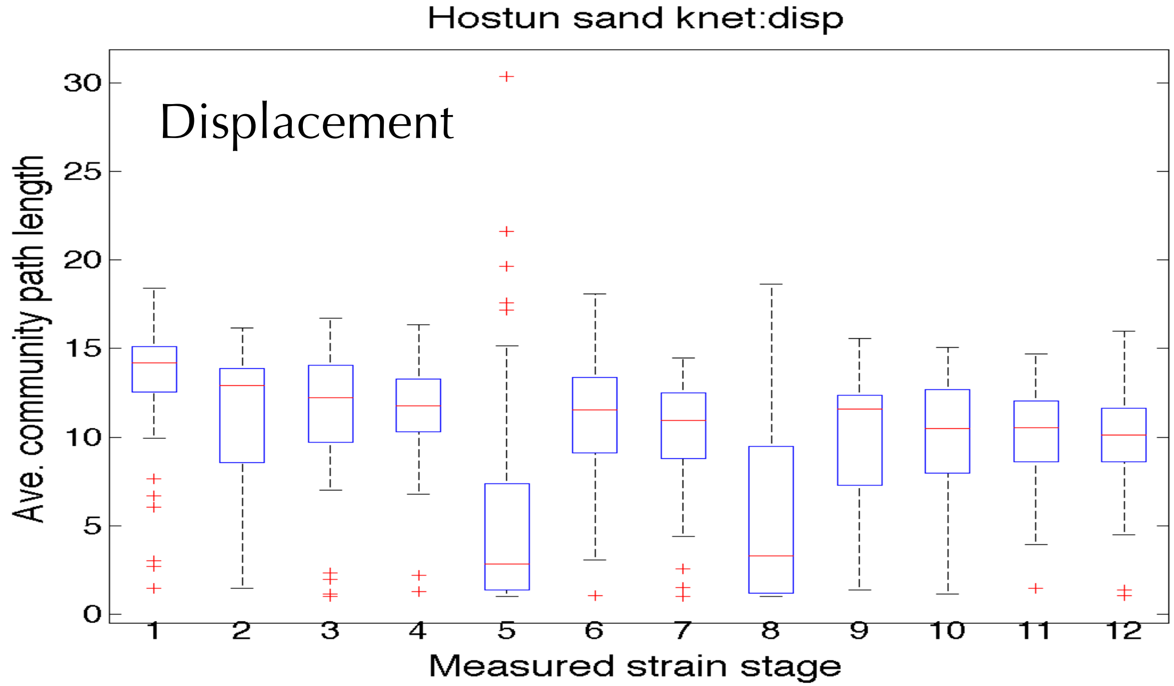


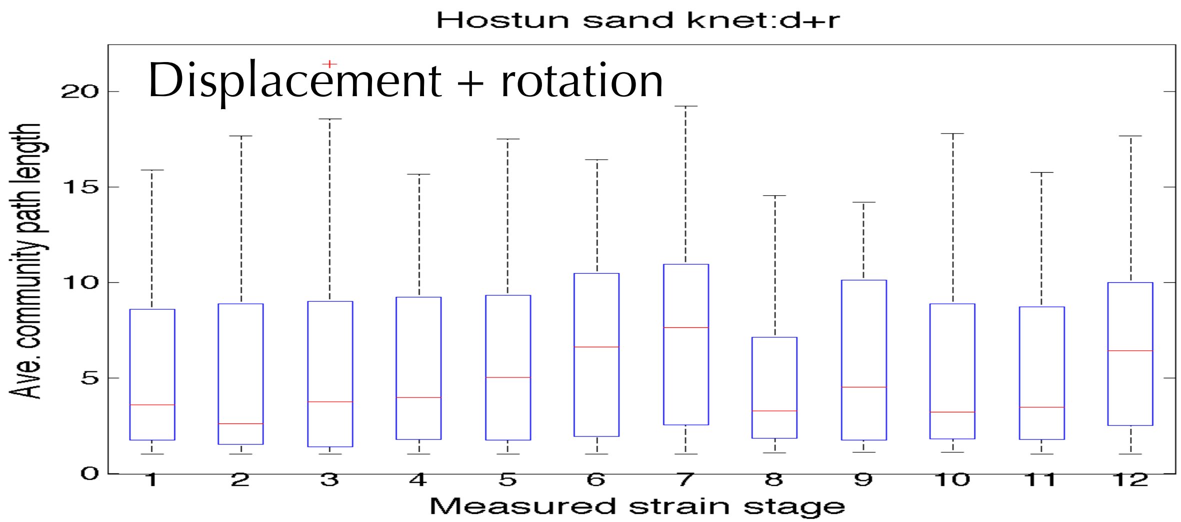
Average across communities: (3/2 + 1)/2 = 5/4

Average shortest paths (efficiency)

- ❑ Narrow range of shortest paths with mean ~10D-15D for displacement k-Net (5D-6D for disp+rot)

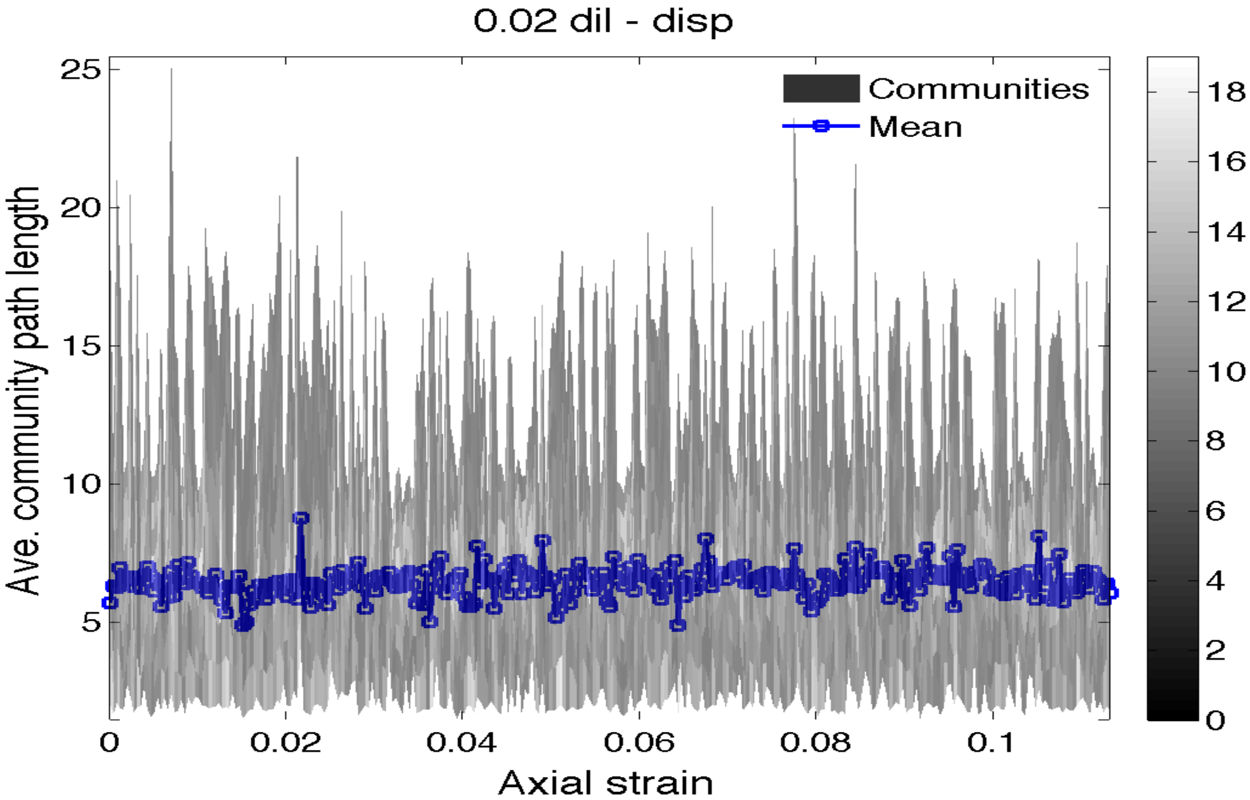
- ❑ Measure tied to efficiency or how fast information flows through the network

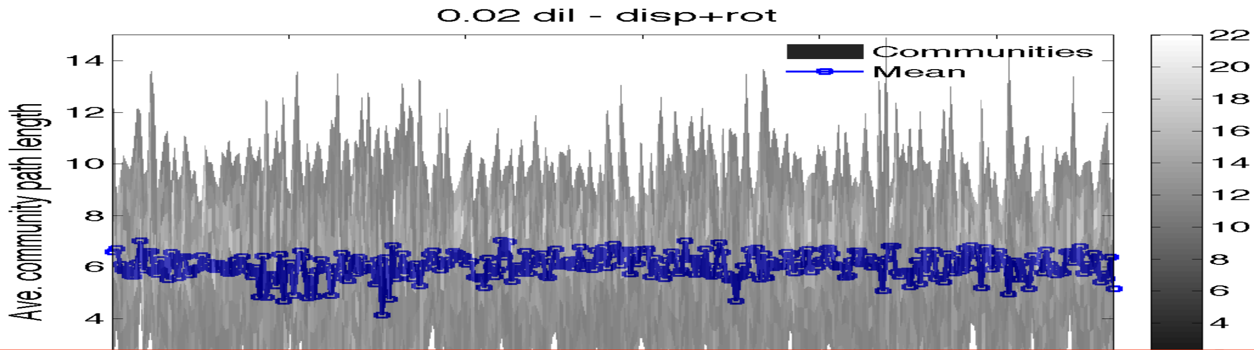




Average shortest paths (efficiency)

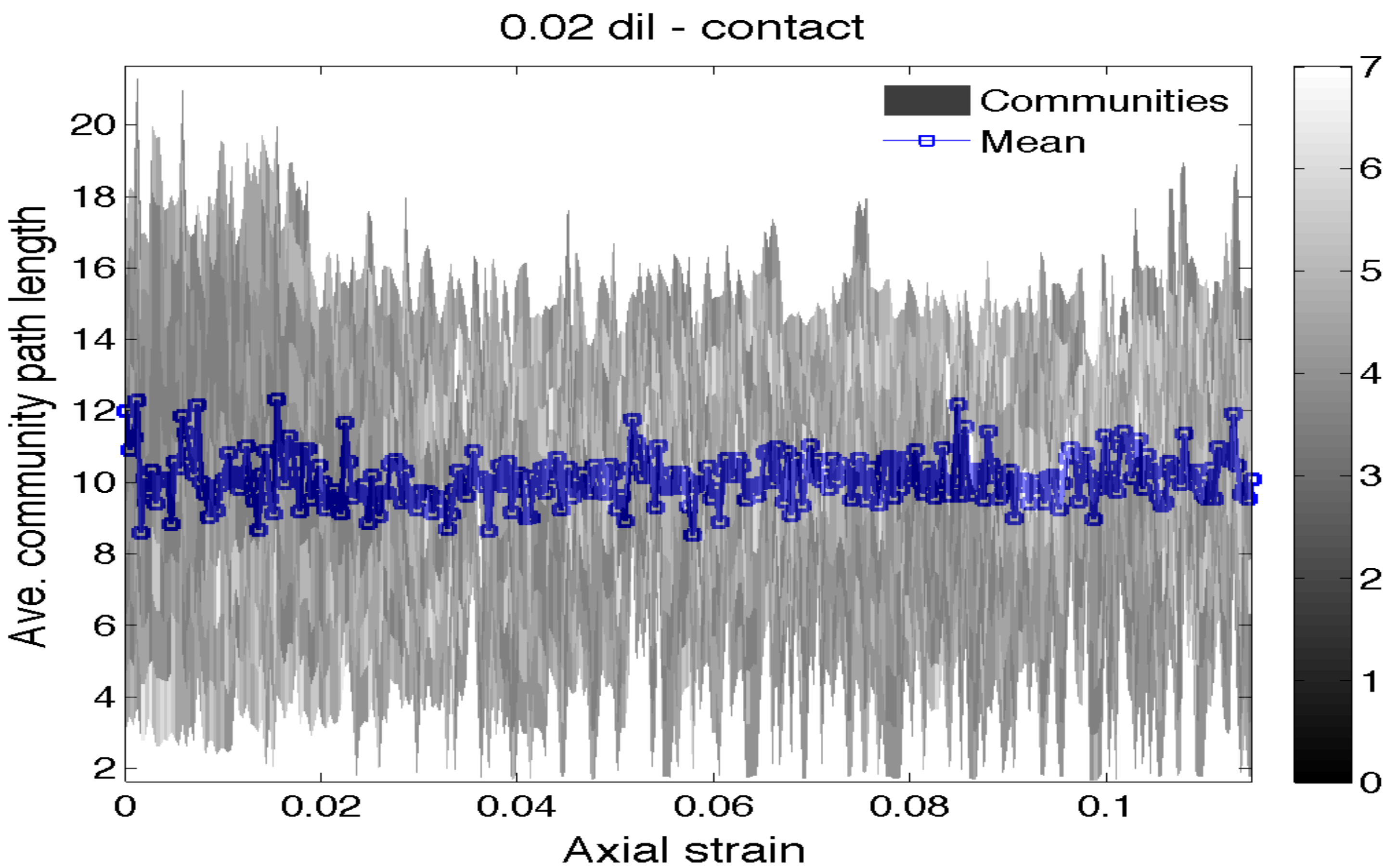
- ❑ Like Hostun sand, relatively narrow range of shortest paths and displacement k-net has (slightly)larger length scale





Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

Length scales from communities: C-Net



❑ mean shortest path length scale from contact network C-Net ~ 10D throughout loading history (larger than k-nets)

Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

Questions about Hostun sand .....

1. *Is there a community structure to the functional networks from kinematic fields? YES: partitions down to 29-48 communities*

2. *What are the length scales (spatial), if any, from such communities? 10D-15D displacements; 5D-6D displacement+rotation*

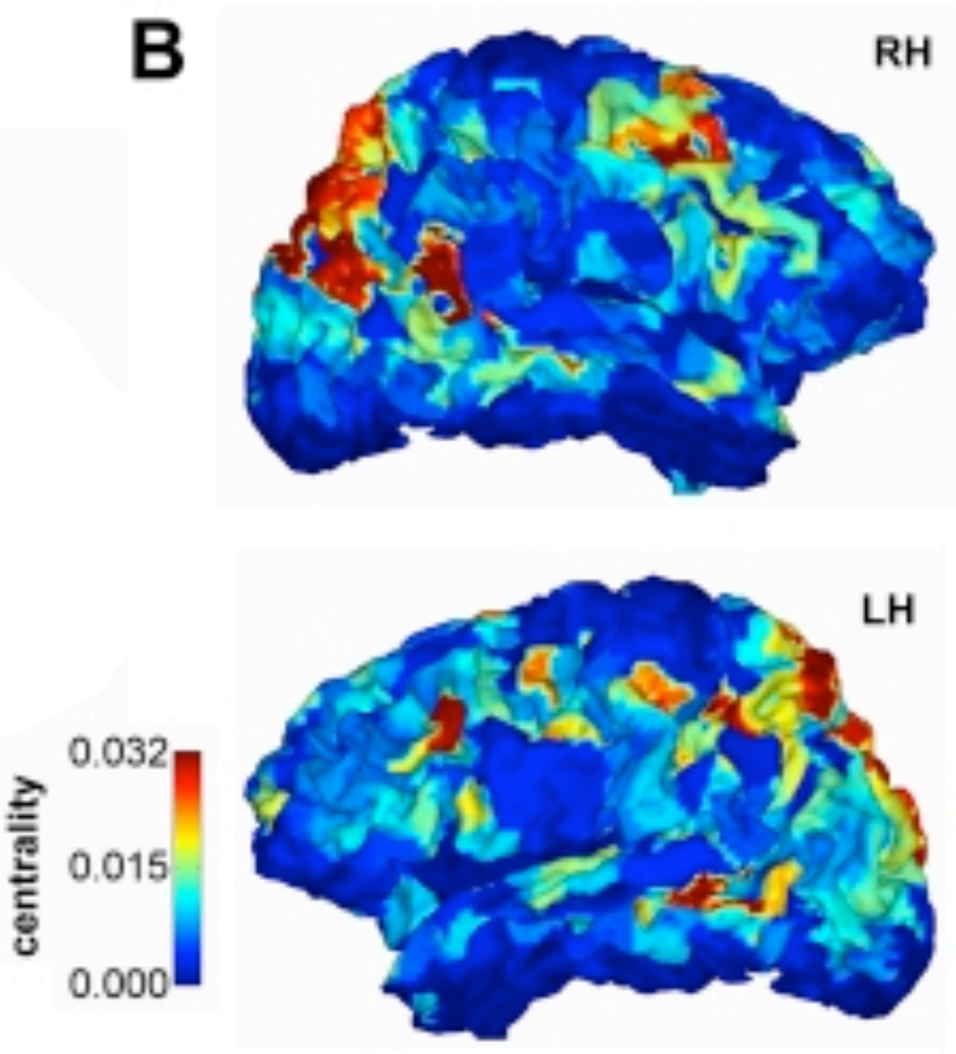
3. *Which are in the best position to spread information (nodes of highest efficiency) to all the other nodes in the network?*

Closeness Centrality

❑ Measures inverse mean shortest path from a node to all other nodes in network

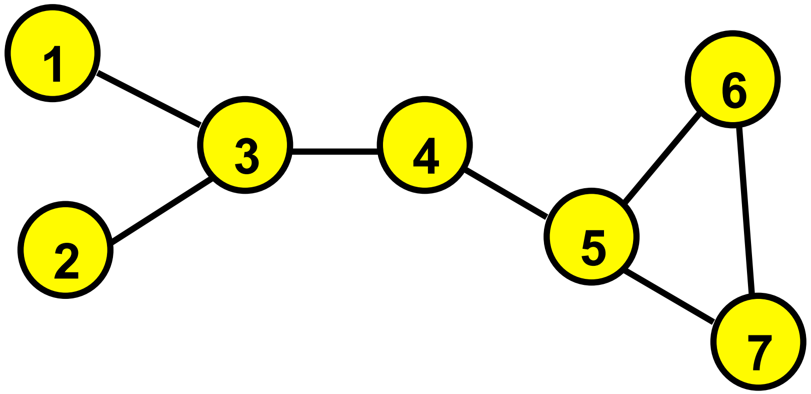
❑ High closeness centrality means high efficiency (small average shortest path lengths) – **fastest spread of information** – from vertex to all others

❑ Recall Fornito's findings, i.e. coincides with regions where genetics has most influence. ***So is our ultimate fate determined from birth?***



Hagmann et al. 08

Closeness Centrality



$$C_i = \frac{1}{l_i} = \frac{n}{\sum_j d_{ij}}, \quad l_i > 0; \;\; C_i > 0$$

$$\sum_j d_{1j} = 16 \;\Rightarrow\; C_1 = 7/16$$

$$\sum_j d_{2j} = 16 \;\Rightarrow\; C_2 = 7/16$$

$$\sum_j d_{3j} = 11 \;\Rightarrow\; C_3 = 7/11$$

$$\sum_j d_{4j} = 10 \;\Rightarrow\; C_4 = 7/10$$

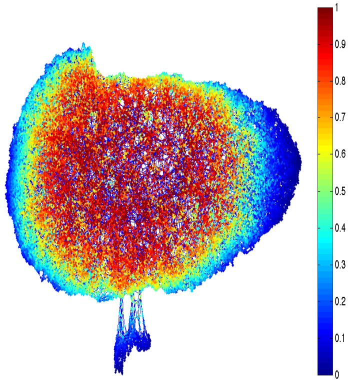
$$\sum_j d_{5j} = 11 \;\Rightarrow\; C_5 = 7/11$$

$$\sum_j d_{6j} = 15 \;\Rightarrow\; C_6 = 7/15$$

$$\sum_j d_{7j} = 15 \;\Rightarrow\; C_7 = 7/15$$

- ❑ Inverse mean shortest path from a node to all other nodes in network
- ❑ Nodes with high (relative) closeness centrality are close/ **central** to other nodes (low d_{ij}) so crucial to **efficient flow of information** in the network
- ❑ Node 4 is the “closest” to any other node

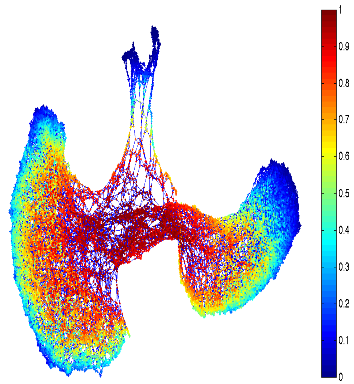
Closeness centrality (k-net)



Strain Interval 2-4

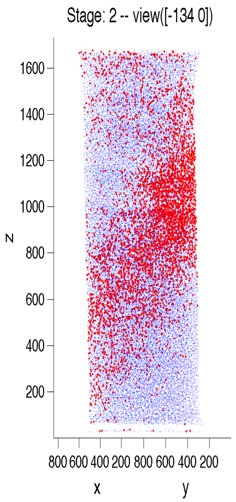
Strain Interval 5-8

Red nodes: shortest paths to/from all the other nodes to the node under consideration



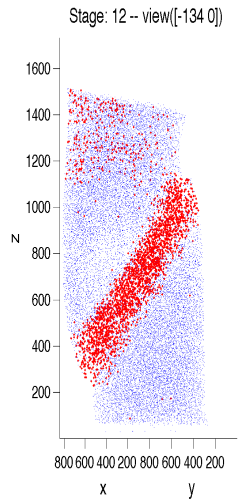
Strain Interval 9-12 (peak-)

High closeness centrality



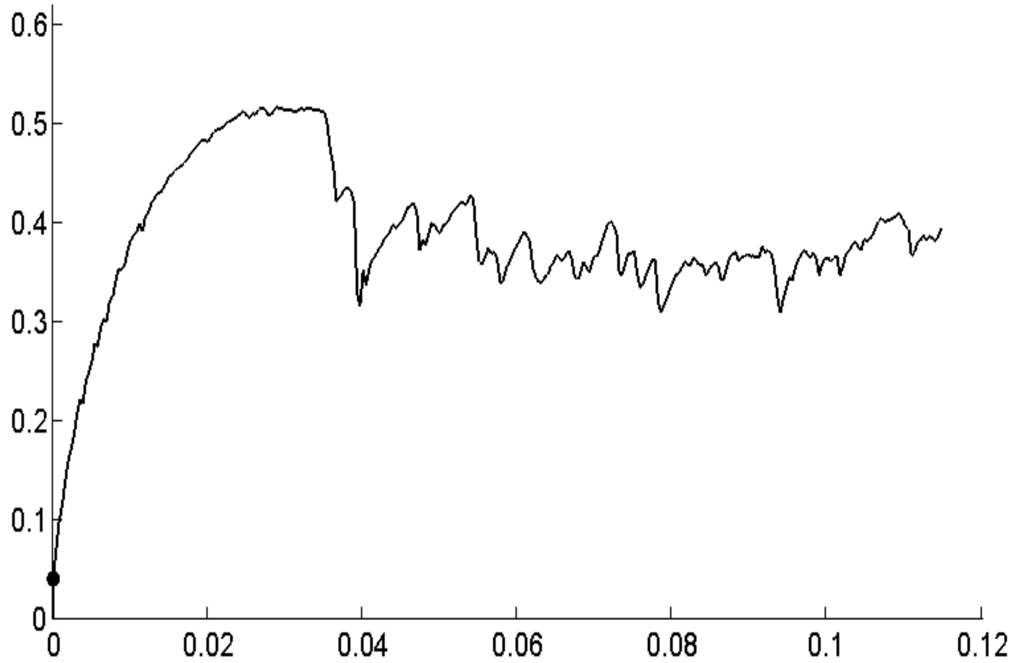
Strain Interval 2-4

Strain Interval 5-8



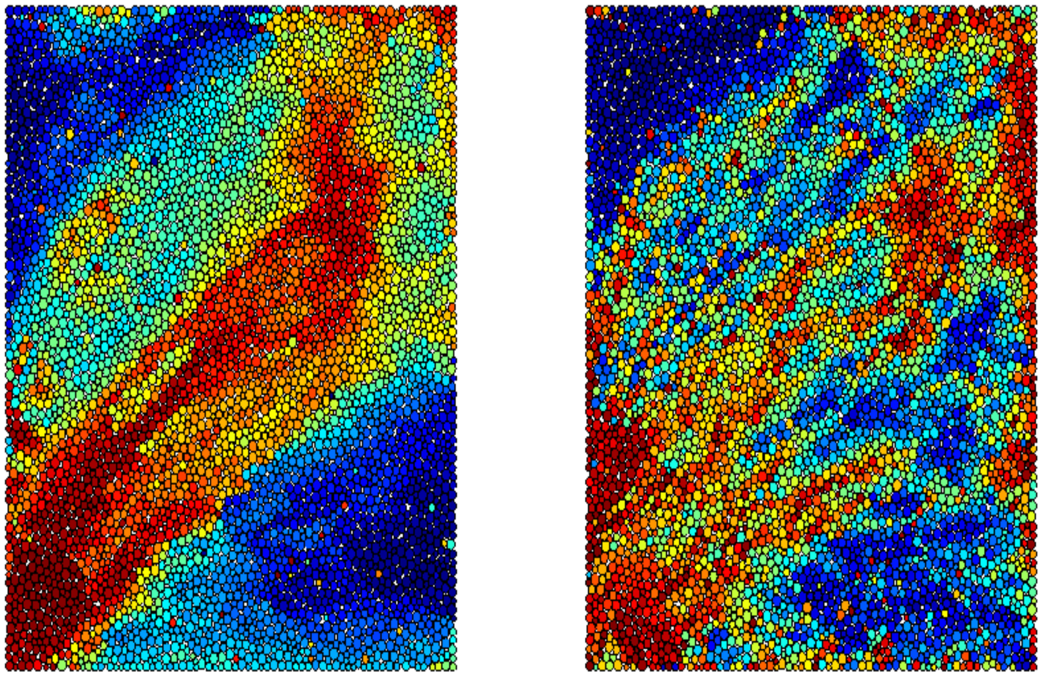
Strain Interval 9-12

How do we know this isnt just a happy coincidence?



❑ Recall baseline system and check result is reproduced in DEM

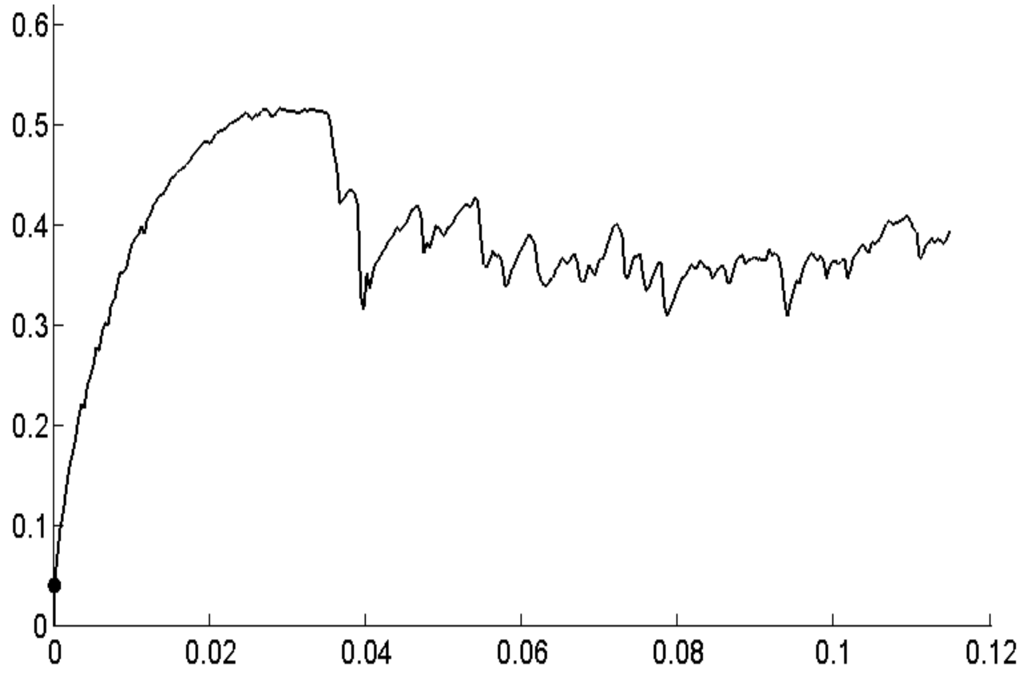
❑ Compare to contact network. Region of high relative closeness centrality lies in middle of sample (red core): next slide

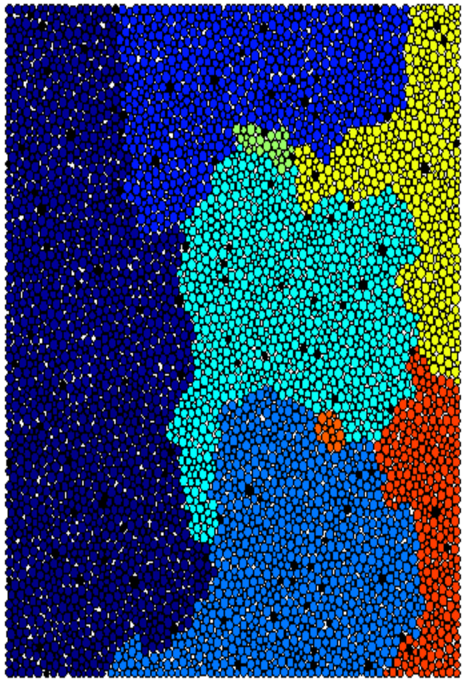


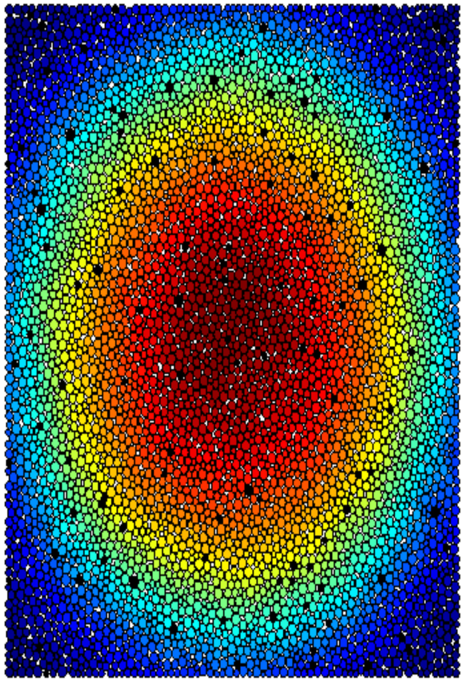
Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

Baseline system

❑ Closeness centrality (right) from contact network







Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

Questions about Hostun sand …..

1. *Is there a community structure to the functional networks from kinematic fields? YES: partitions down to 29-48 communities*

2. *What are the length scales (spatial), if any, from such communities? 10D-15D displacements; 5D-6D displacement+rotation*

3. *Which are in the best position to spread information (nodes of highest efficiency) to all the other nodes in the network? Nodes in the region of the shear band. Trend prevails from ONSET of loading.*

Plan of the rest of this talk ..

- ❑ What theory tells us about length scales of observed patterns in granular materials
- ❑ Pattern recognition from complex networks and what patterns teach us about the nature of complex systems

---

- ❑ **Extraction of length scales from Grenoble data on Hostun sand**
- ❑ **Results from extraction**
- ❑ **Inception of Hostun sand and the null hypothesis to test length scales are robust, meaningful and real**
- ❑ Results from inception
- ❑ Lessons learned and where to next …

‘Inception’

- Randomize wiring inside Hostun: repeat many times (surrogates)

- **Null Hypothesis H_0**: results on Hostun are a product of chance

- Verdict from statistics of Hostun vs surrogates:

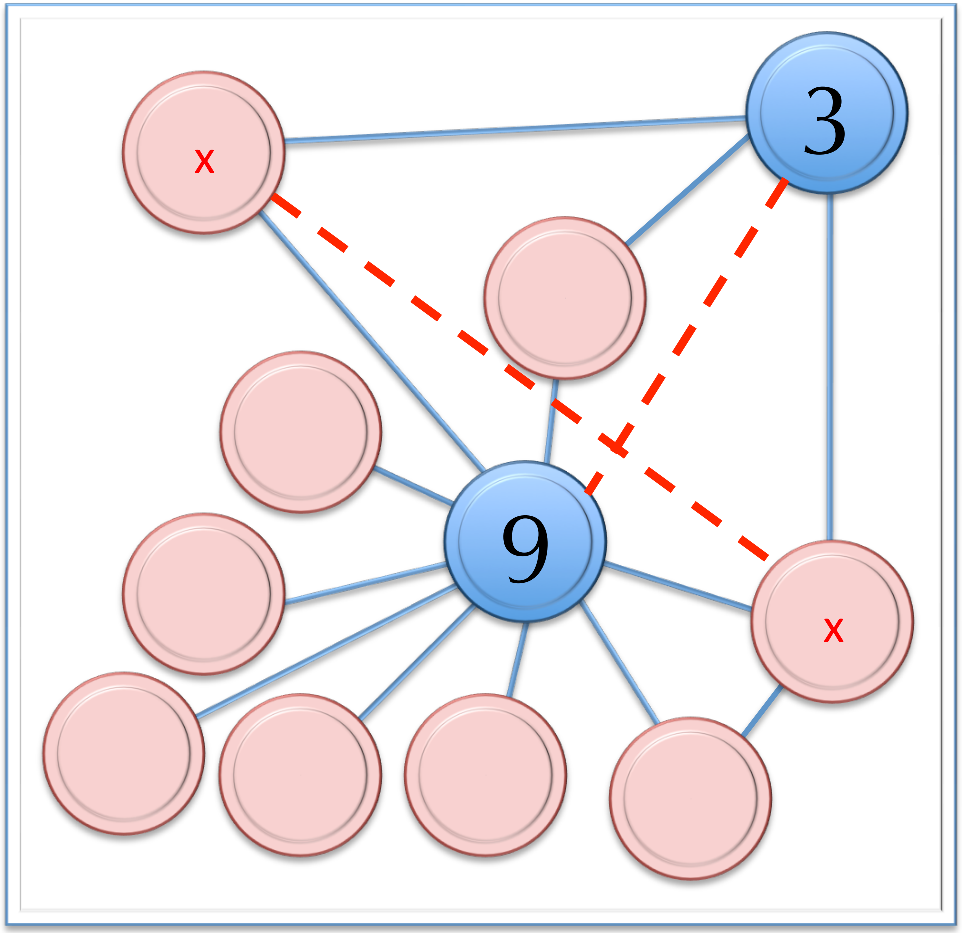
Reject H_0 <u>or</u> Fail to reject H_0

Rewiring Algorithm I : preserve degree

- Can conceive many rewiring strategies ..

- One strategy:
  - Randomly select Y nodes (e.g. Y=4)
  - Shuffle one neighbour of each node (also selected randomly), while preserving degree of each node

- Repeat above until X% of the nodes in the system are rewired



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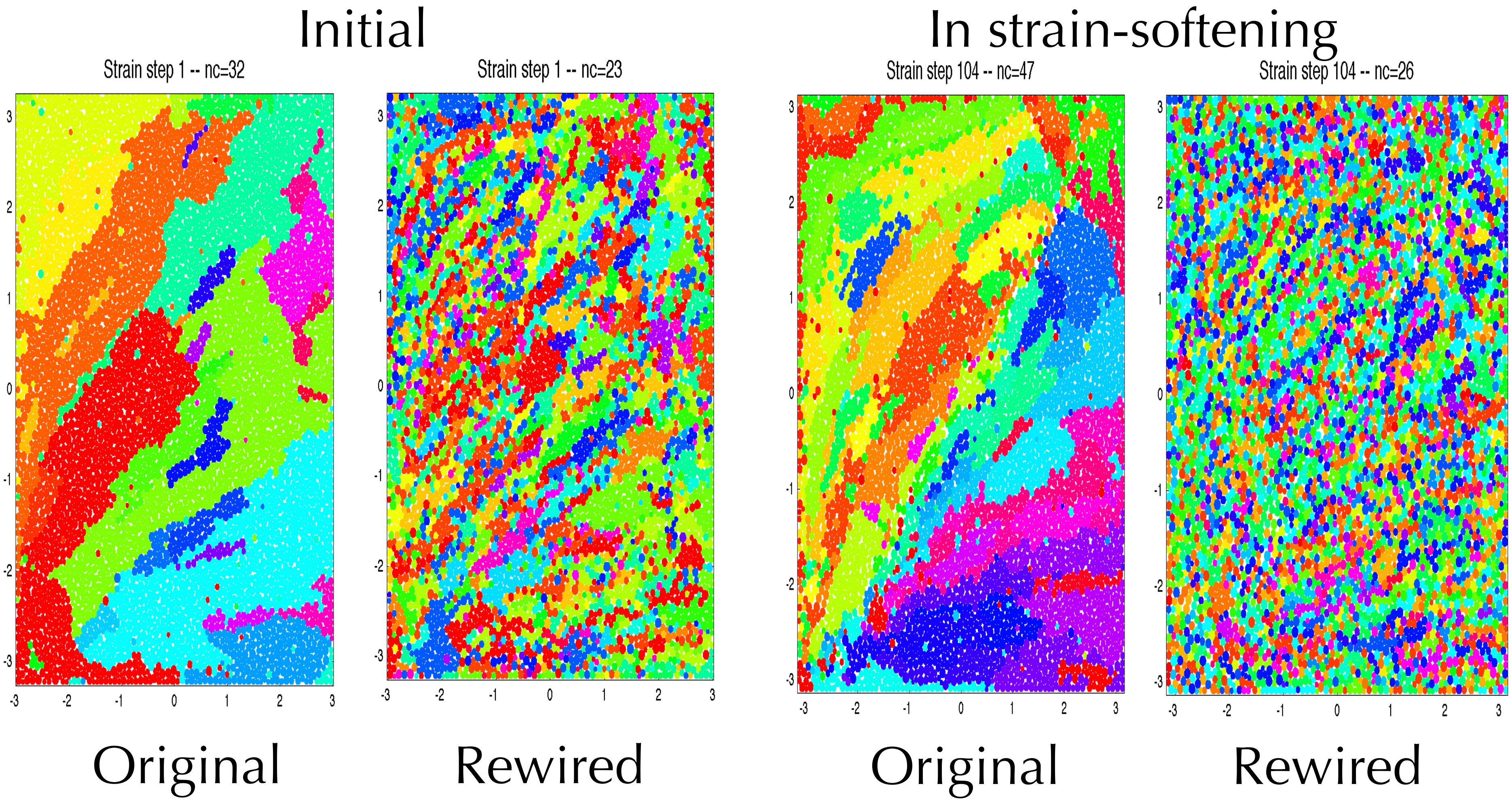
- ❑ **Results from inception**
- ❑ Lessons learned and where to next …

TEST 1: Rewire DEM, check community structure of k-Net from adjacency matrix

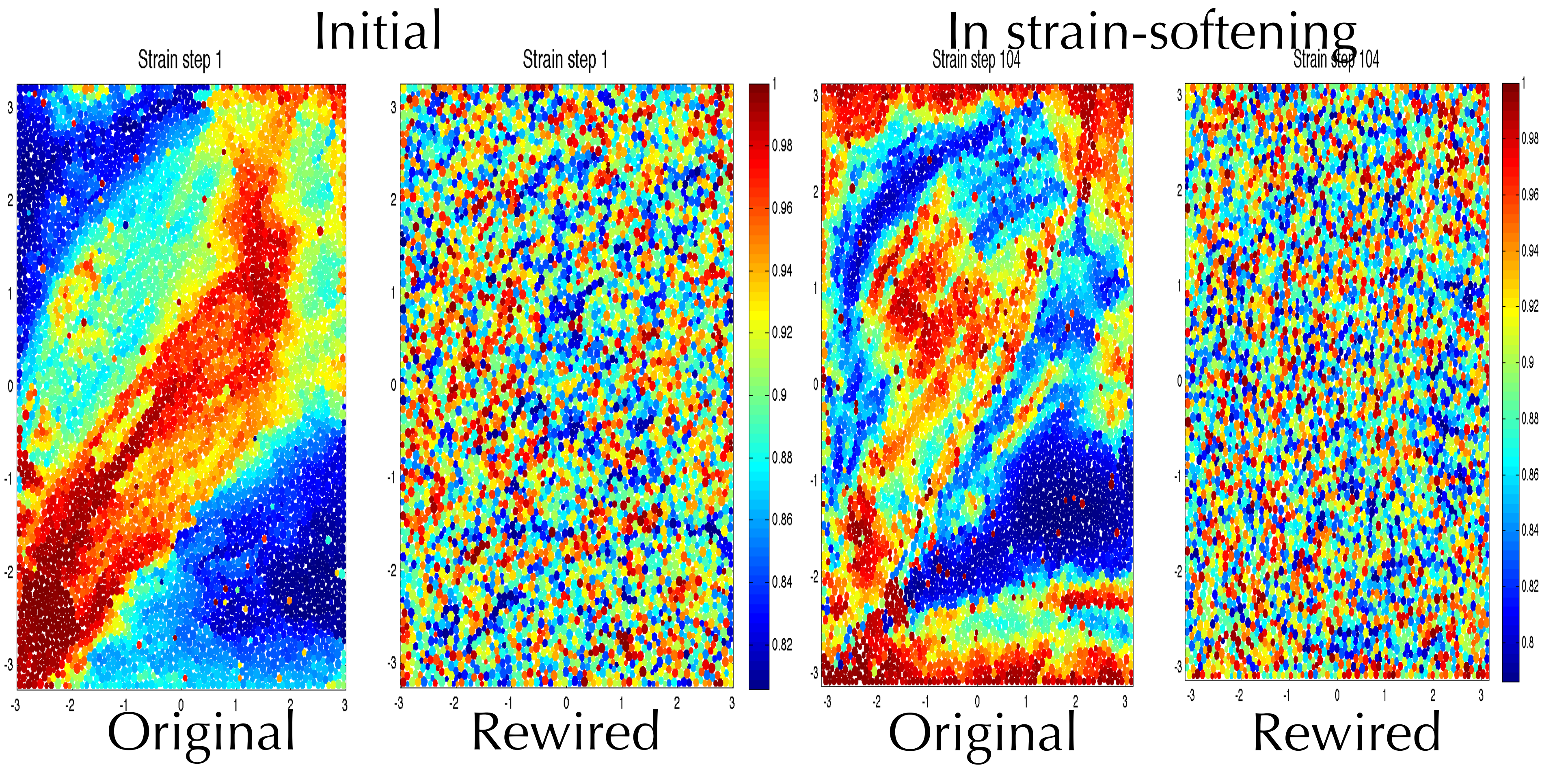
Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

TEST 2: For rewired DEM, check community structure & boundaries from k-Net



Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

TEST 3: For rewired DEM, check closeness centrality of k-Net

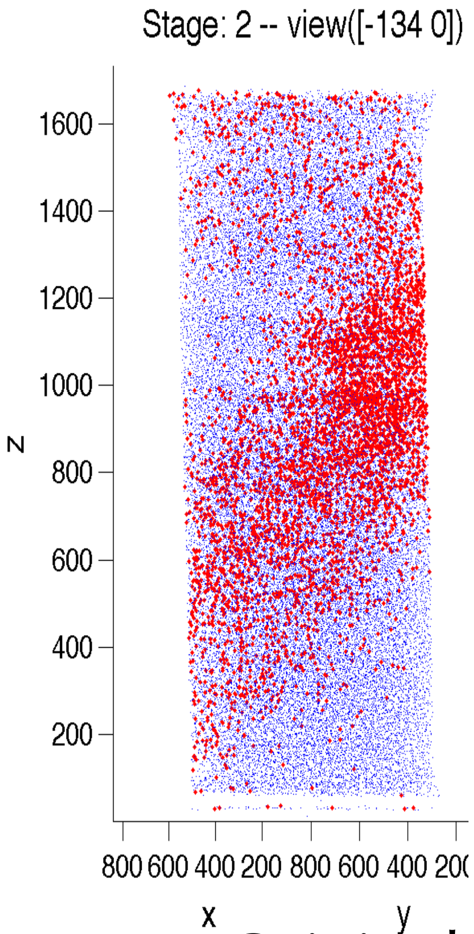


Baseline system: 2D DEM, Biaxial test with constant confining pressure, 5098 particles

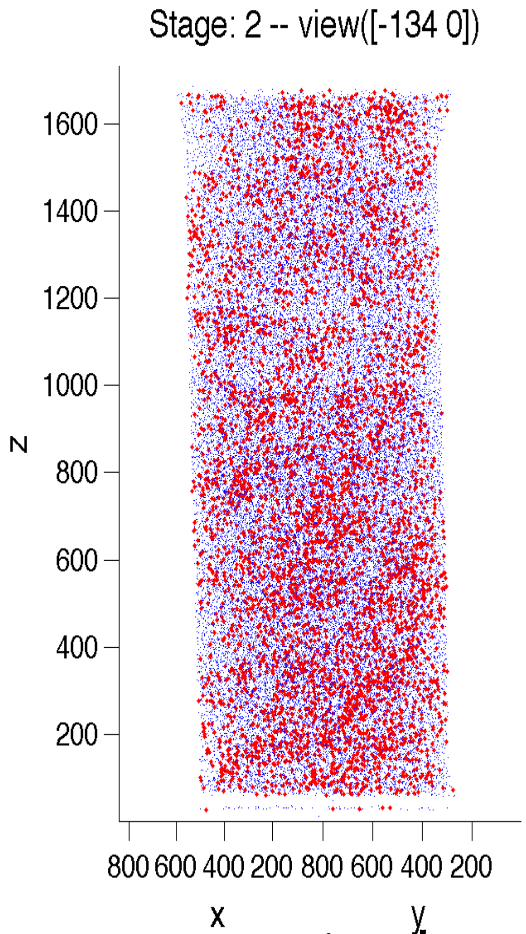
TEST 4: Rewire Hostun, check community structure of k-Net from adjacency matrix

TEST 5: For rewired Hostun, check closeness centrality

Initial

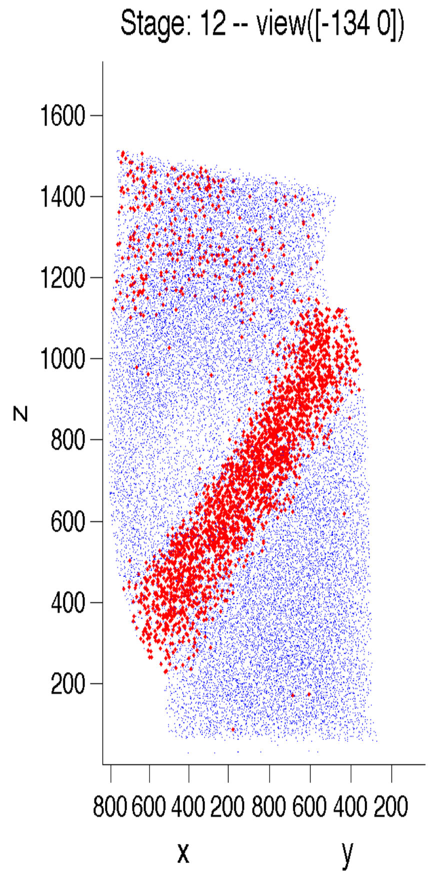


Original

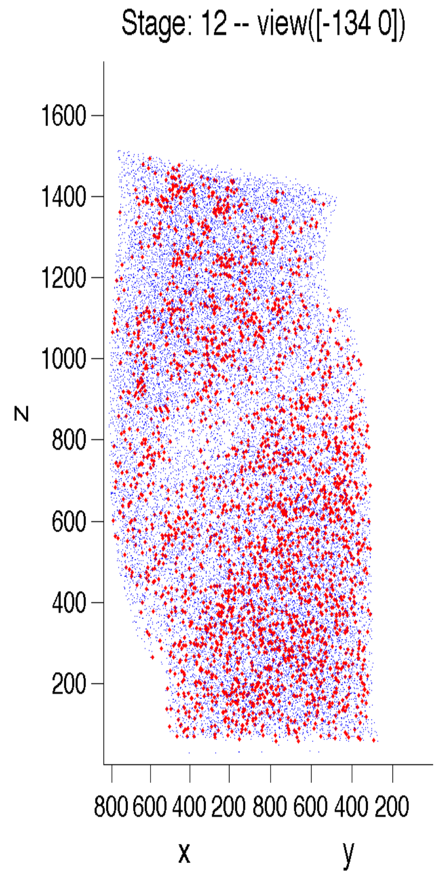


Rewired

Final



Original



Rewired

Plan of the rest of this talk ..

- ❑ What theory tells us about length scales of observed patterns in granular materials
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On Hostun rheology

- ❑ Intelligent design or a product of chance?

- ❑ Not a product of chance. But still continuing to check statistics for sensitivity. How many realizations do we need to do? Also more than 101 ways to rewire a network? …. At what point do we stop?

- ❑ This is just the first steps toward the first complete map of the evolution of functional and structural connectivities in a deforming sand…. …..
there is much to do..

Image from Andò et al

On Micromechanics

We are awashed with data! As grain scale data accumulate – from DEM and high resolution experiments:

- ❑ **Where is micromechanics headed in material characterization?**

- ❑ **Where is micromechanics headed in constitutive modelling?**

- ❑ **How do we tie developments in these two strands together?**

Pesky particles pacified in pixels?

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