TOPOLOGICAL DATA ANALYSIS APPLIED TO INTERACTION NETWORKS IN PARTICULATE SYSTEMS

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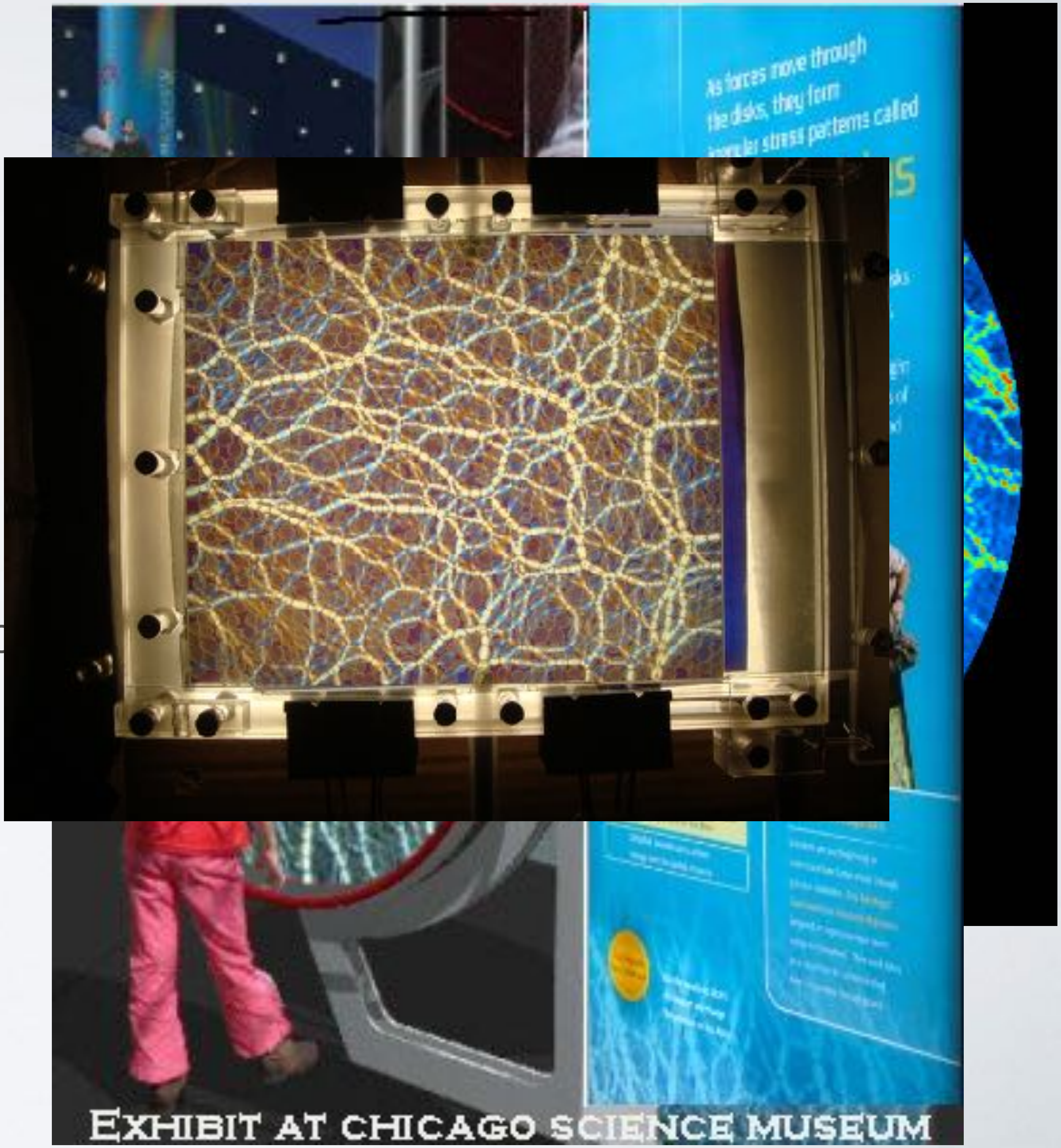
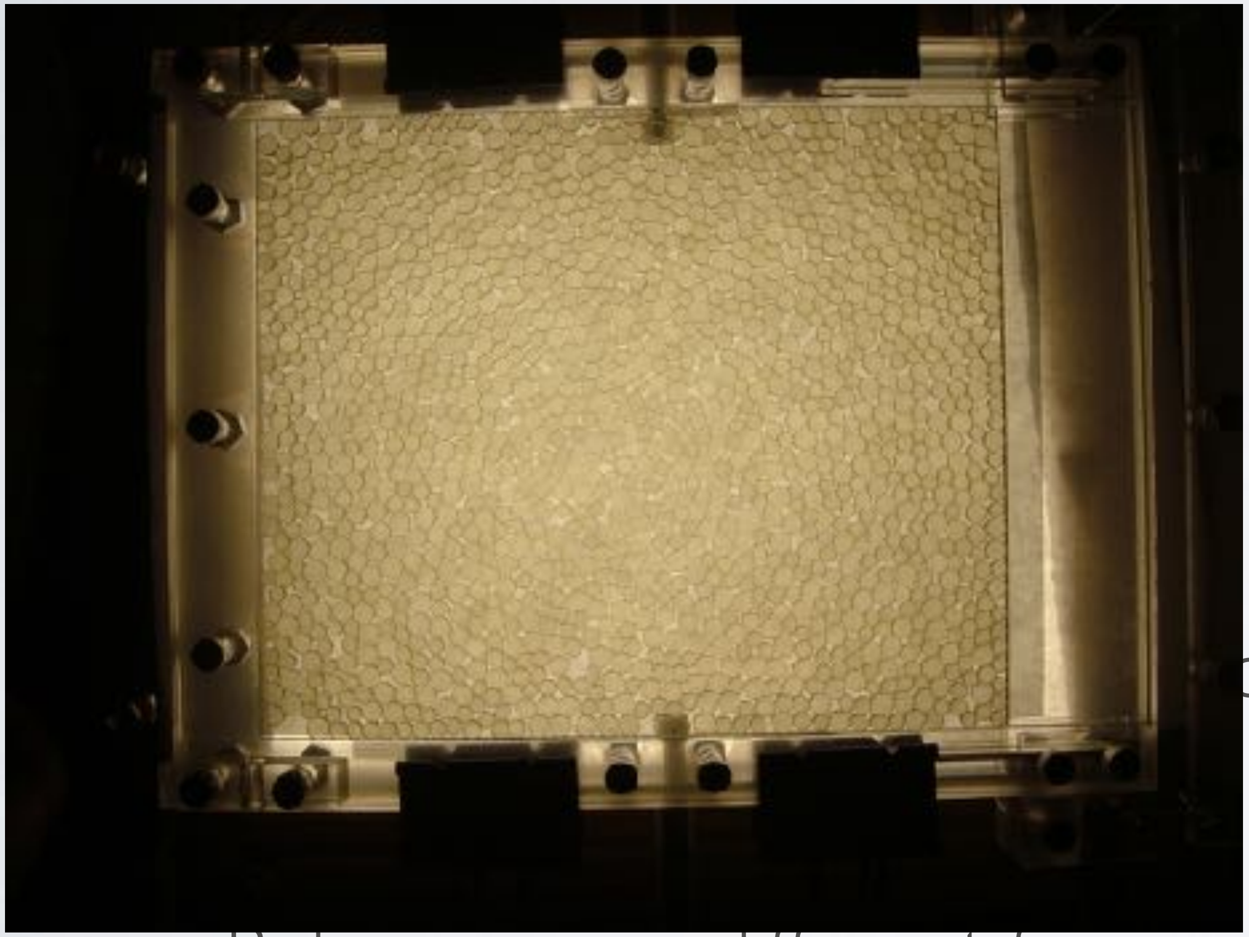
WHAT IS SPECIAL ABOUT PARTICULATE SYSTEMS?

re

- To understand bett
stresses develop c
systems and simple

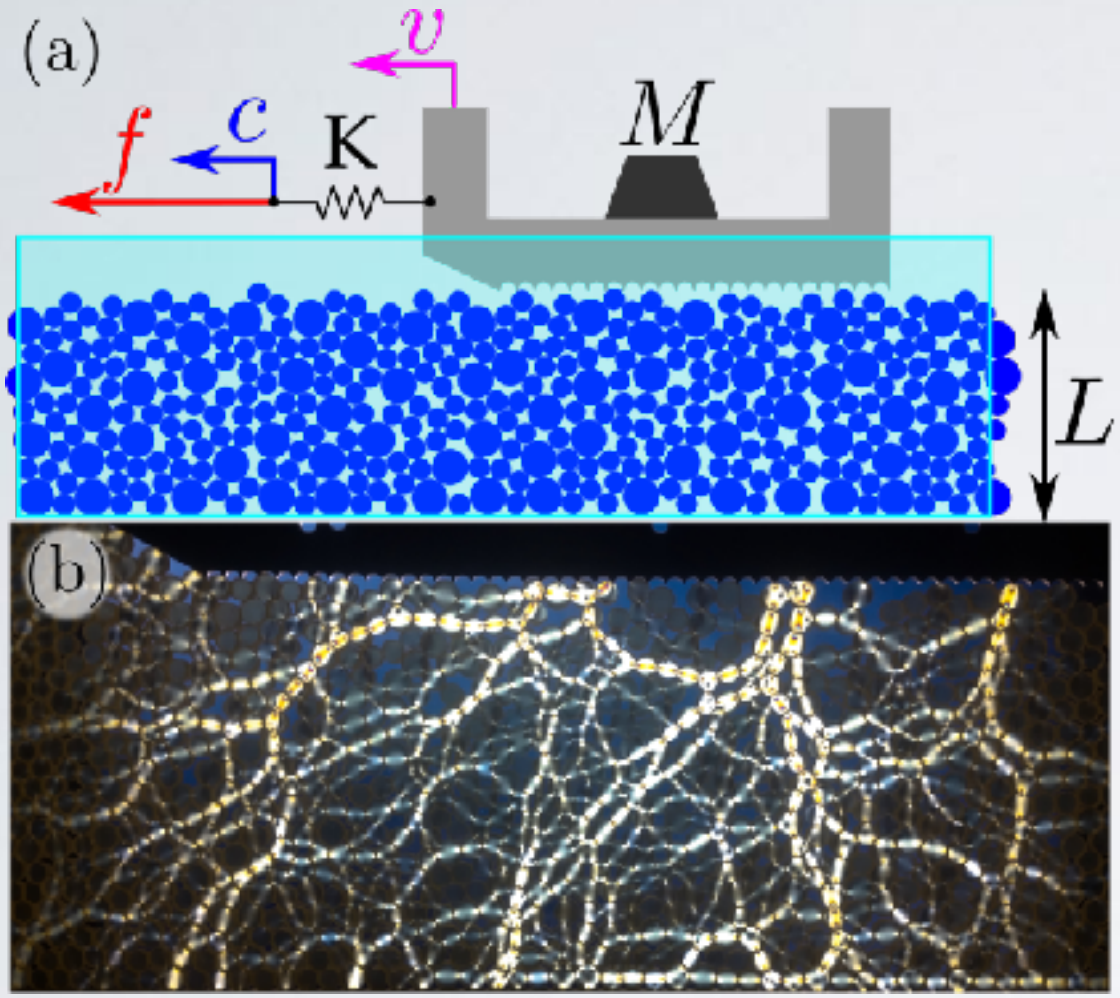
INTERACTION NETWORKS: EXPERIMENTS

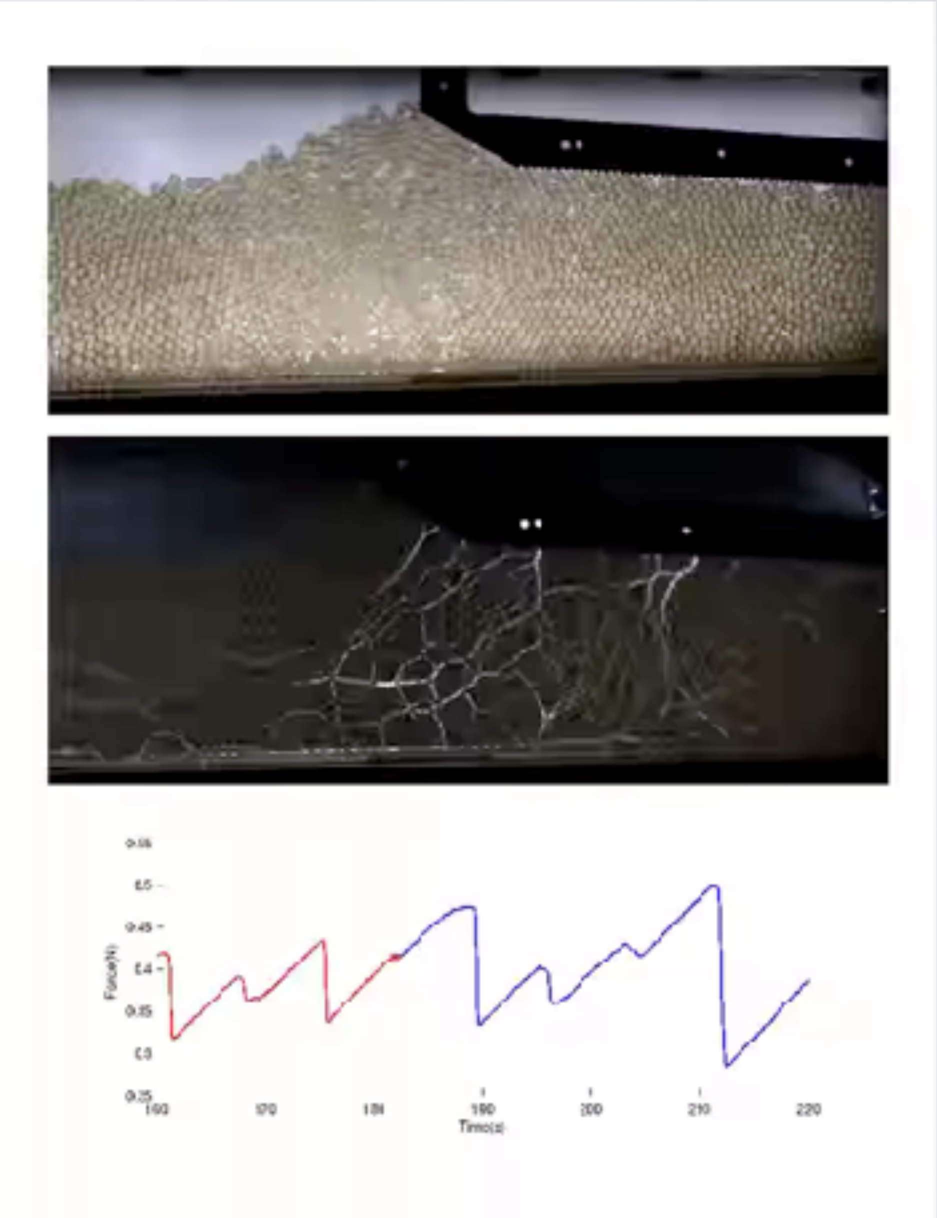




- Behavior very different from `usual' materials

EXPERIMENT

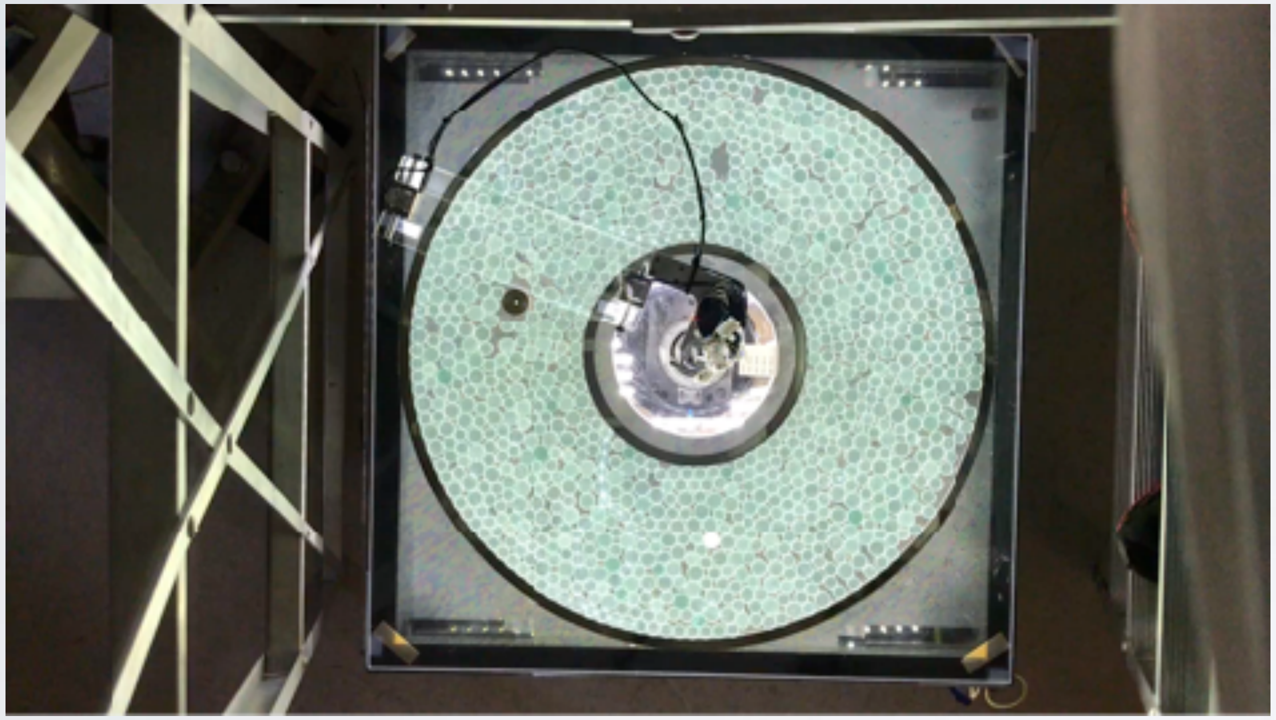


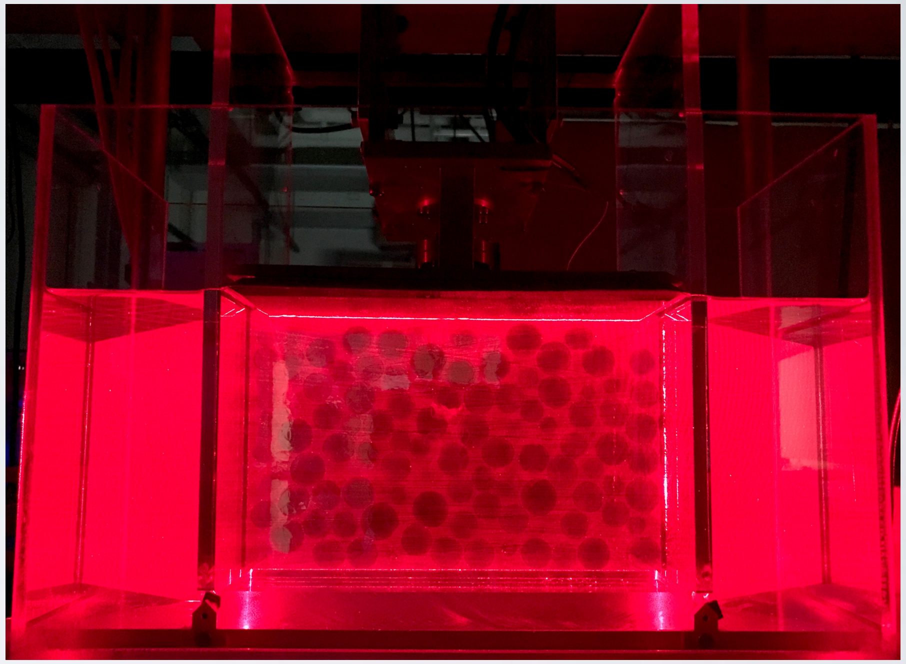


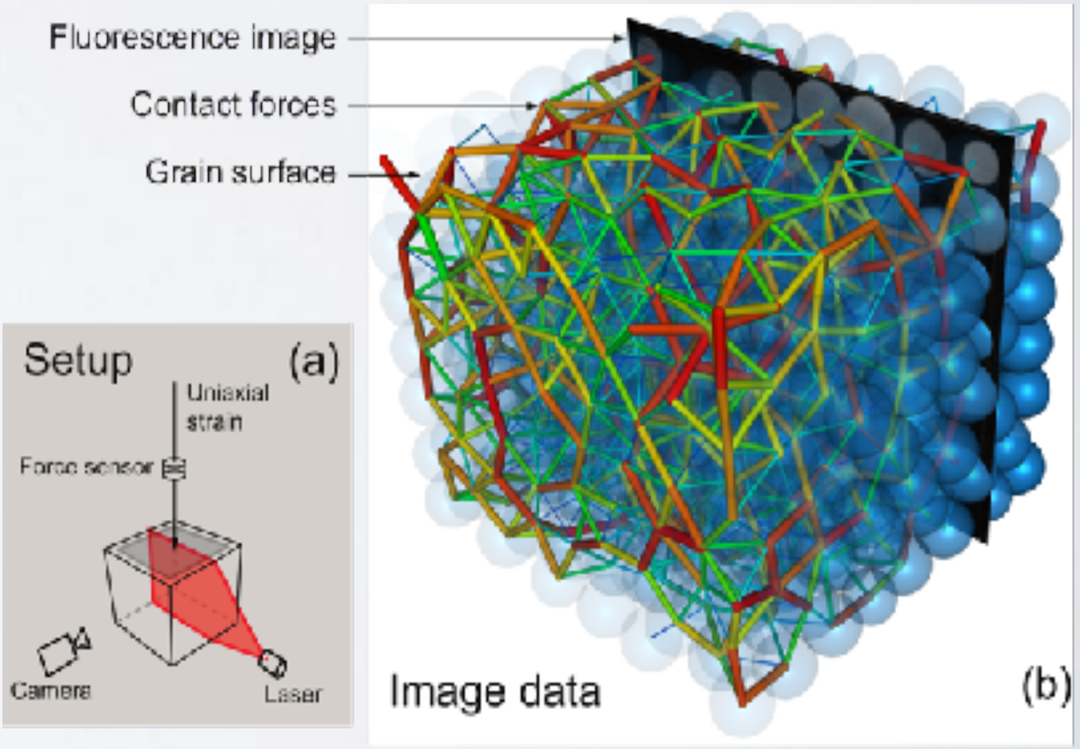
(from Zadeh, Bares, Behringer, PRE 2019)

- Is there a connection /between force networks and slider dynamics?

INTERACTION NETWORKS: EXPERIMENTS

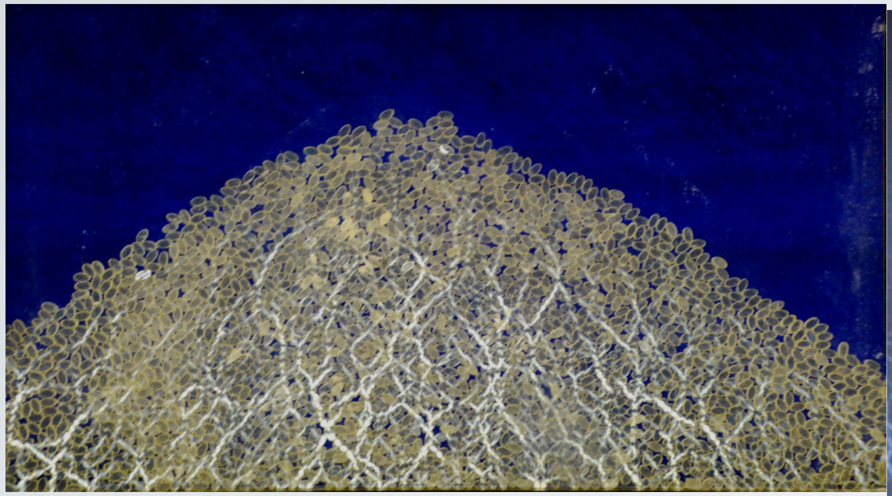


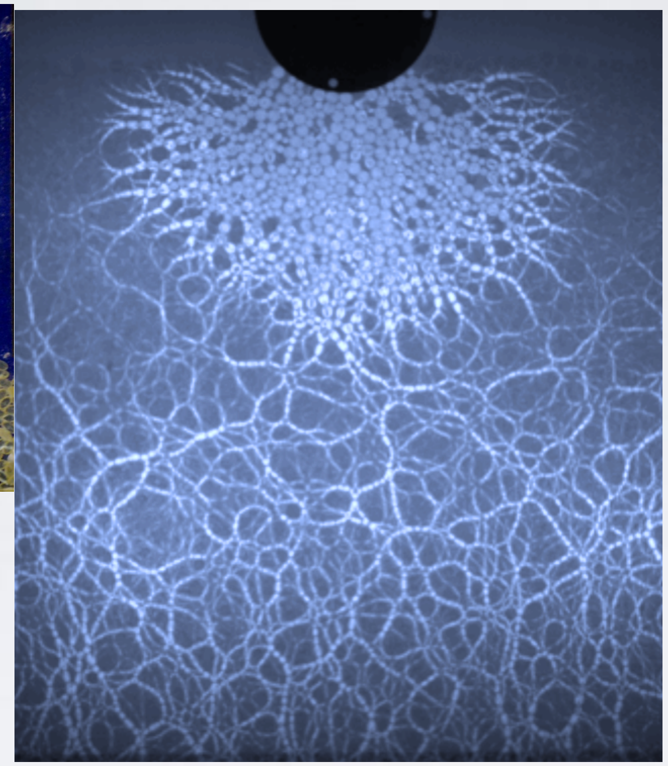


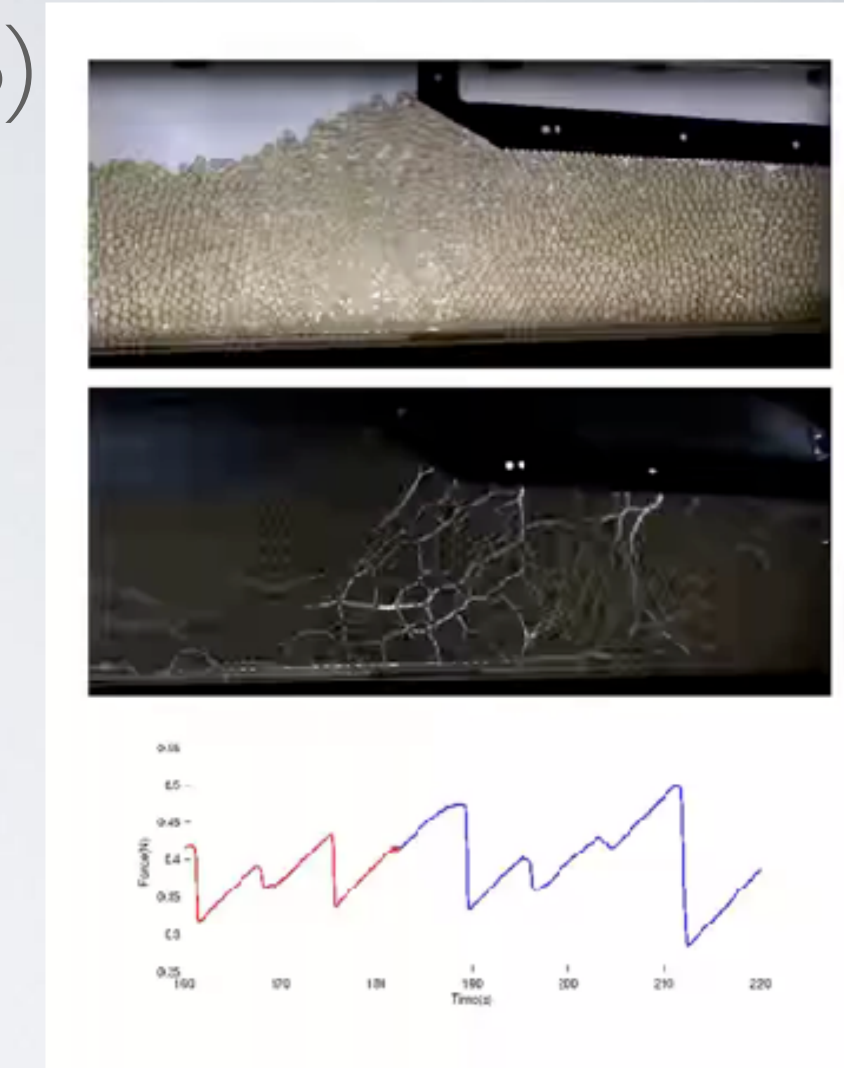


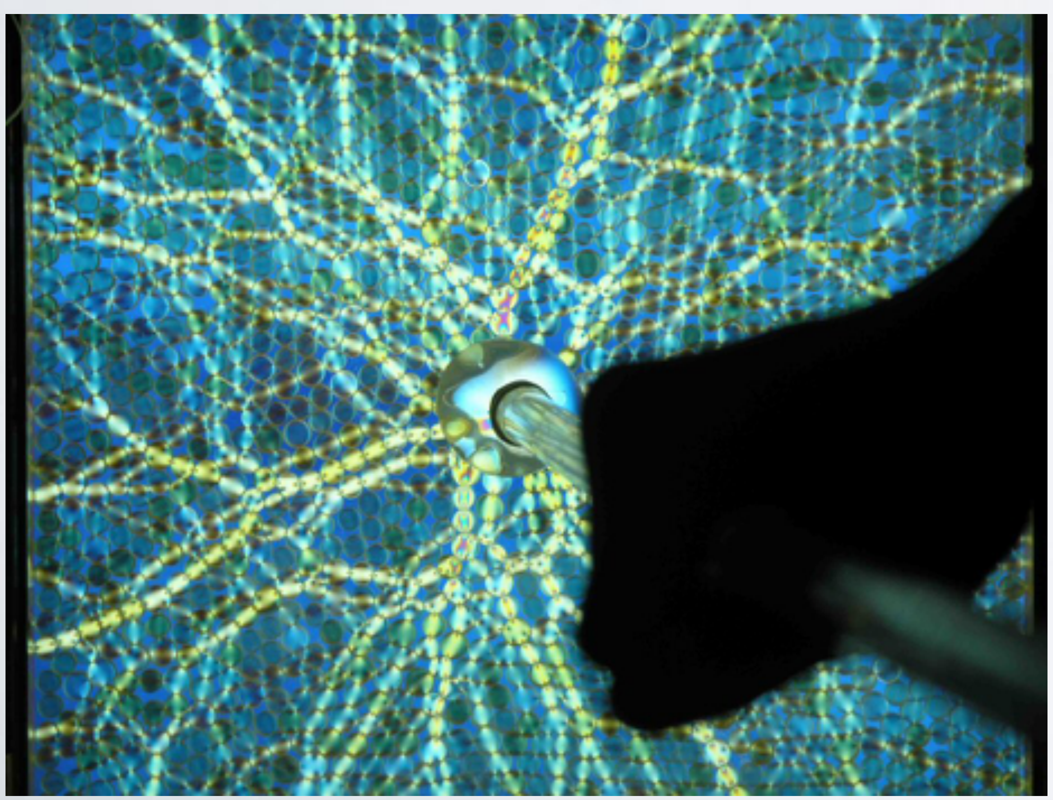
(Kozlowski etal, PRE 2019)

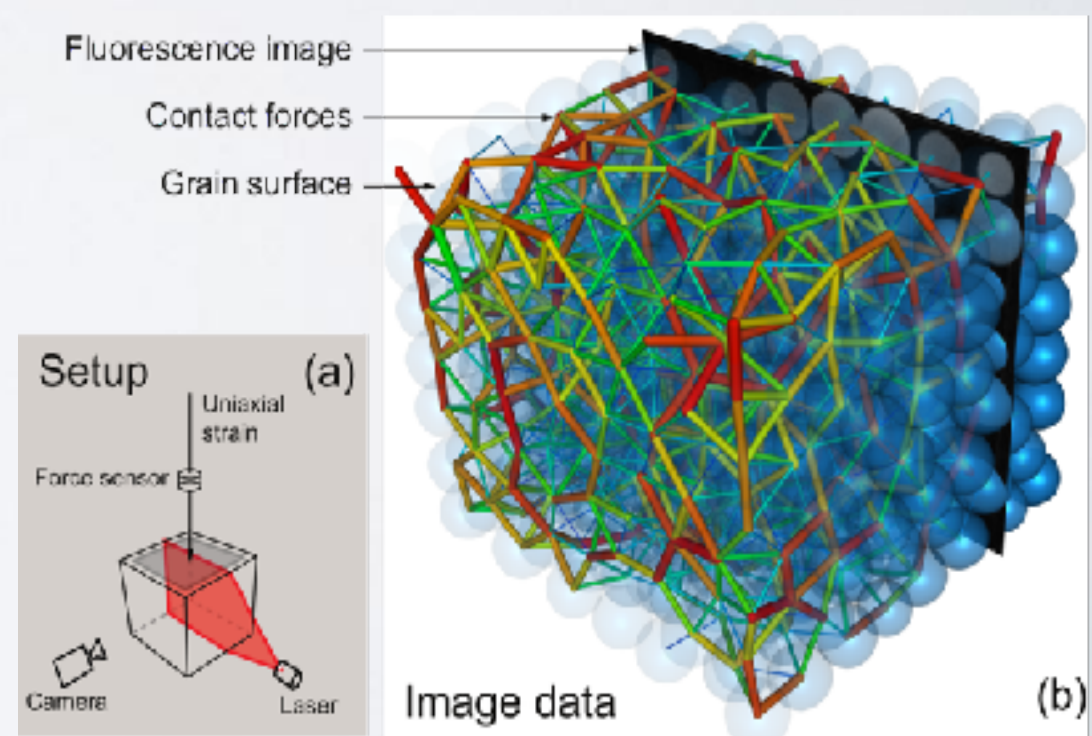
FORCE NETWORKS IN EXPERIMENTS (BEHRINGER'S LAB)



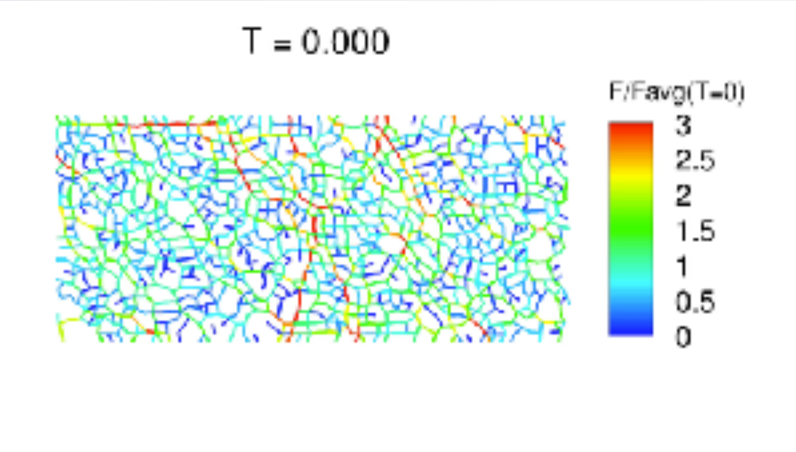


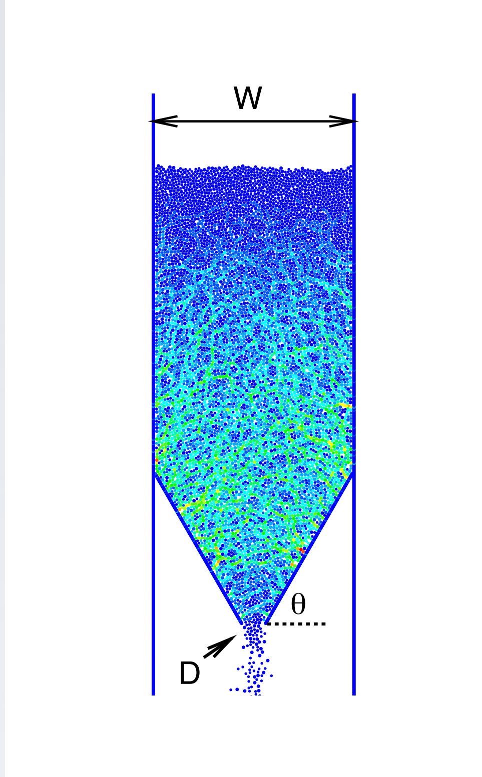




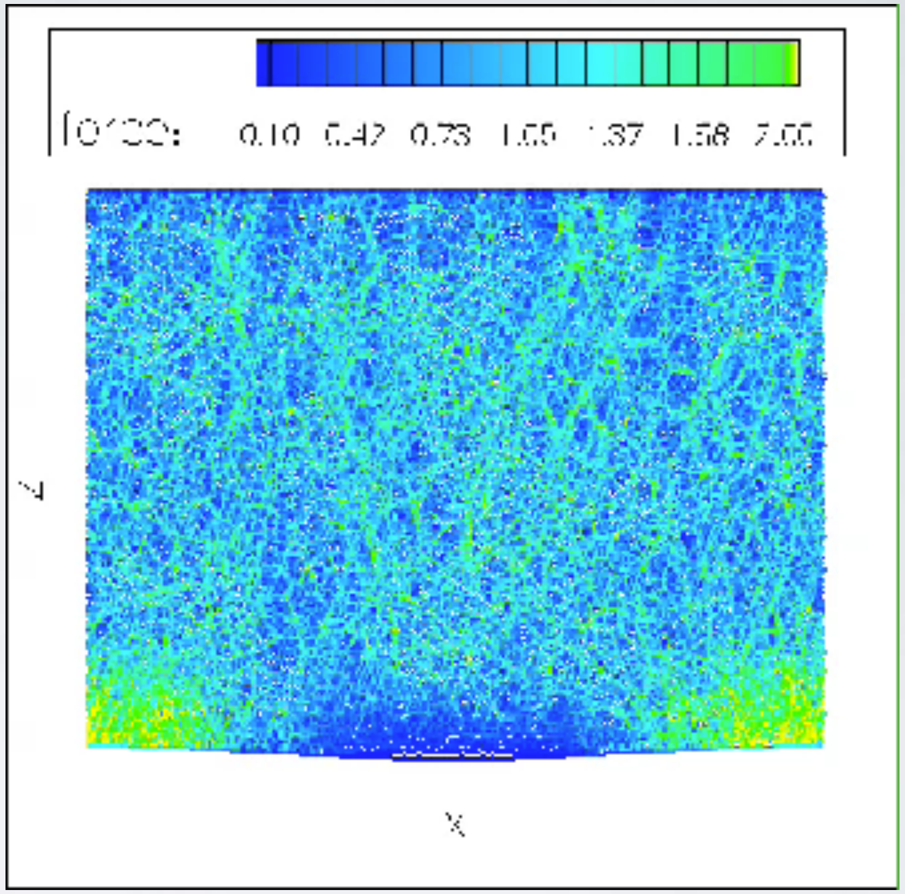


FORCE NETWORKS IN SIMULATIONS

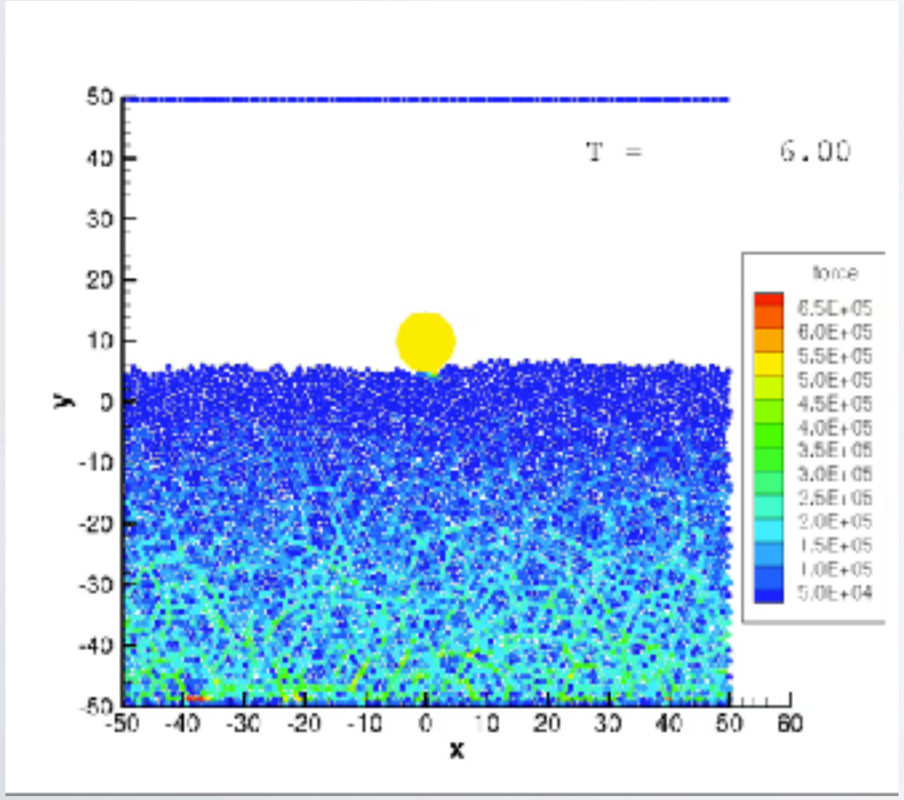


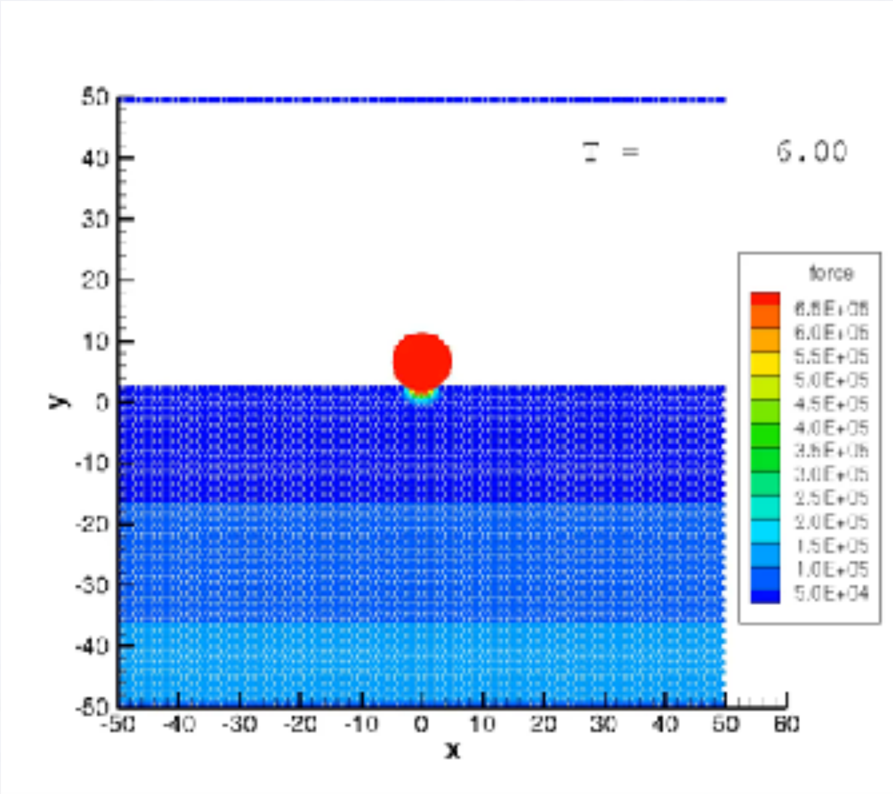


LK, Granular Matter '14

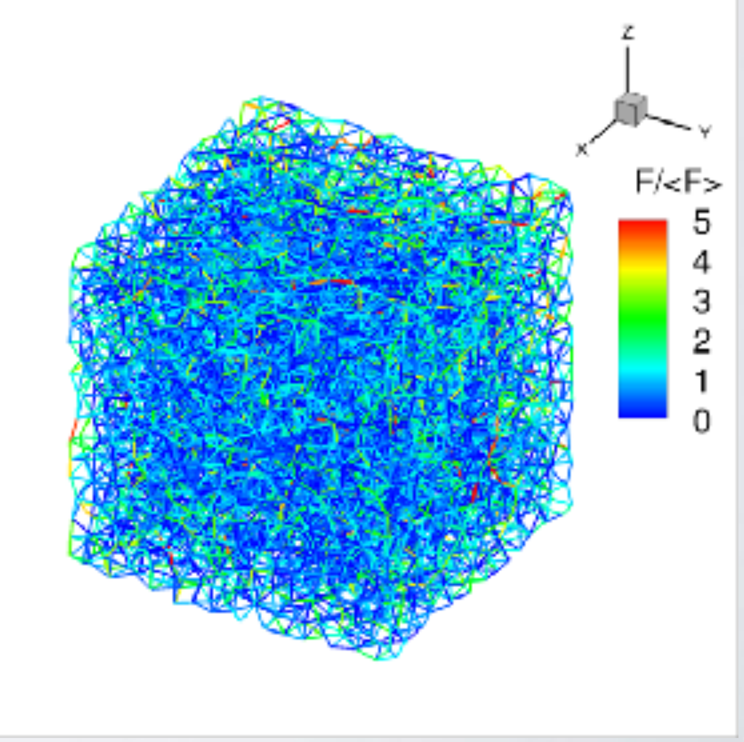


LK, Dybenko, Behringer, PRE '09

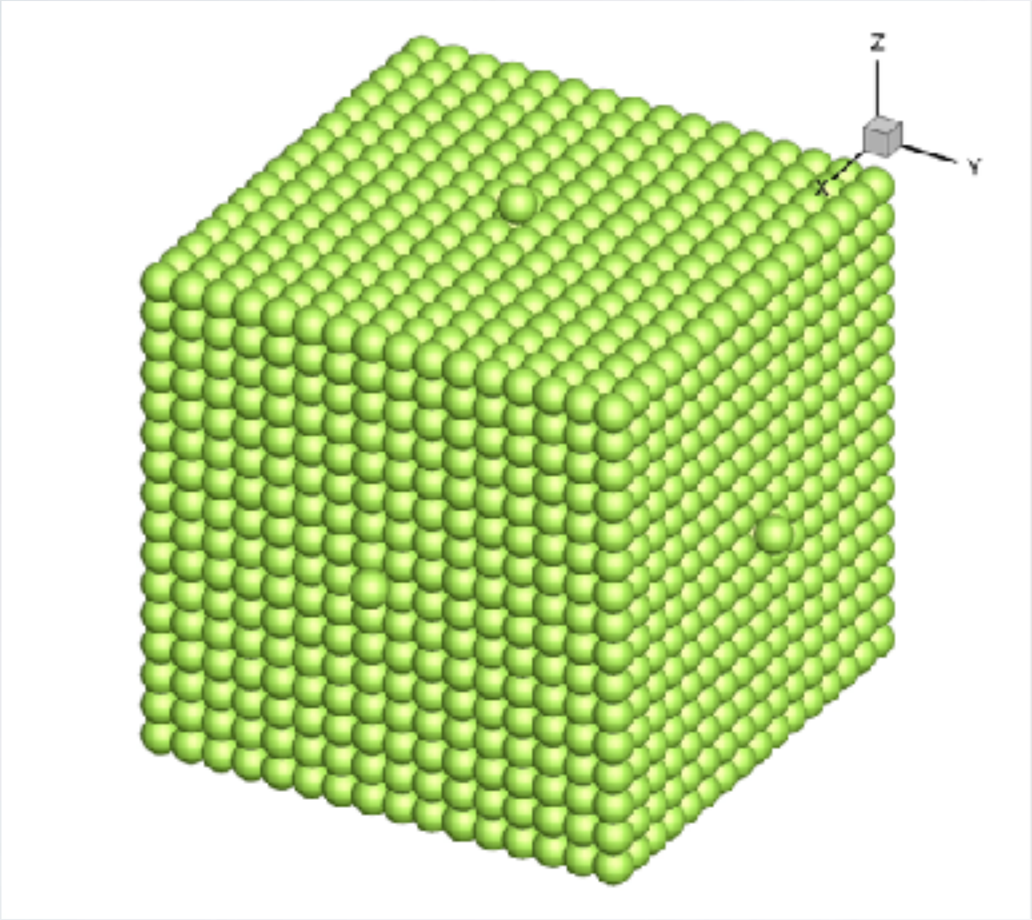


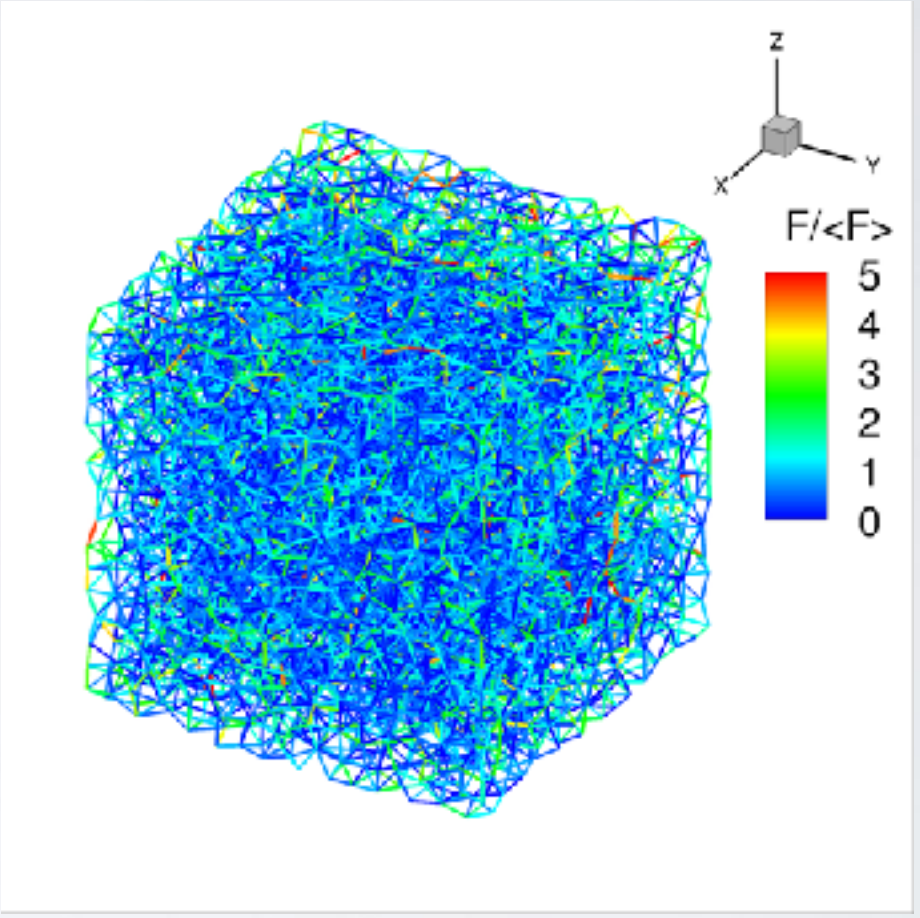


LK, Fang, Losert, O'Hern, Behringer, PRE '12



INTERACTION NETWORKS IN 3D





QUESTIONS

- How to quantify (and simplify) the information contained in the interaction networks?
- How to correlate the evolution of force networks (mesoscale) to the evolution of the system as a whole (macro scale)?
- And in general: How to characterize temporal evolution of complex networks in materials systems? [Note similar structures existing in a number of other systems such as: suspensions, gells, glassy systems, soft solids]

OVERVIEW I

- *General approach:* use the computational topology to help understand complex spatio-temporal dynamics of particulate based systems
- *Outcome*: data reduction, inspired by physics of the considered systems, allowing to proceed from huge amount of data to tractable data sets
- *Methods*: discrete element/MD simulations coordinated with analysis based on computational topology; extraction of quantities that could be used as input to machine learning algorithms

PERSISTENT HOMOLOGY: OVERVIEW

- Use topology based approach to carry out data reduction: from large time dependent data sets to simpler well-defined mathematical structures
- Important point: the resulting mathematical structures still contain the most important physics of the considered systems and therefore their analysis allows to reach new insights into the physical properties of the considered systems

- Kramar, Goullet, LK, Mischaikow, PRE 2013; PRE 2014; Physica D 2014

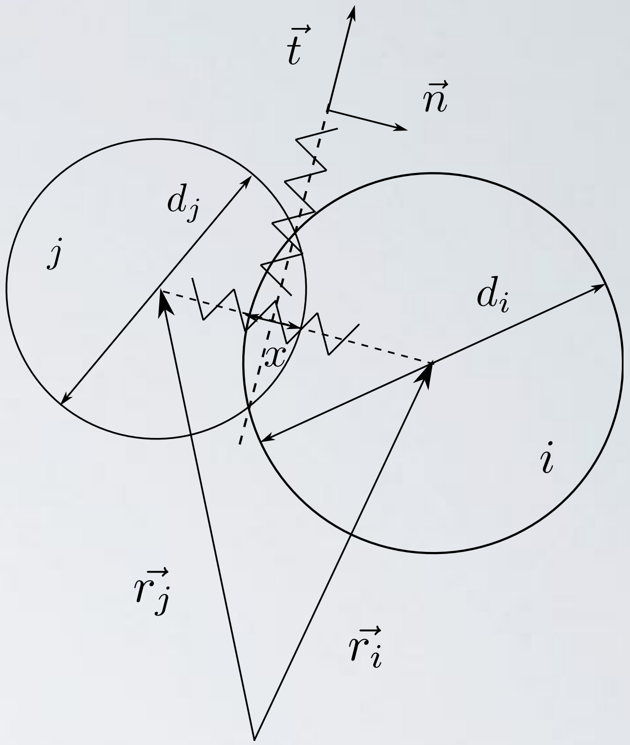
PERSISTENT HOMOLOGY: FEATURES

- Force threshold independent: provides information about all thresholds at once
- Applicable equally well in 2D and 3D
- It can be applied to systems containing particles of arbitrary shapes
- Works for both experimental and simulation data
- Basic idea: strength of the interaction between particles is crucial: filtering force networks by varying force thresholding provides
  - important information about the system across all thresholds
  - the means for analysis of spatial and temporal properties of the force networks

DISCRETE ELEMENT MODELS

- Level of complexity of interaction models
  - spherical, elastic, frictionless particles interacting infinitely fast only when in contact
    - relatively easy to implement, can be connected to continuum fluid-mechanics like theories
    - certain part of physics is lost...
  - spherical particles with inelasticity and friction interacting with repulsive or attractive interactions when in contact
    - relatively easy to implement
    - typically use relatively simple force interaction laws
  - More complex approaches:
    - resolving details of individual contacts (linear/nonlinear elasticity theory) (see Johnson, Contact Mechanics)
    - aspherical particles
    - long range interactions
    - ...

MD/DISCRETE ELEMENT SIMULATIONS



- soft spheres/disks interacting via normal and tangential forces
- the method allows for realistic simulations of a number of different systems

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = m_i \mathbf{g} + \mathbf{F}_{i,j}^{n}$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = -\frac{1}{2} d_i \mathbf{n}_i \times \mathbf{F}_{i,j}^{t}$$

$\mathbf{F}^n \propto x$ linear, 2D

$\mathbf{F}^n \propto x^{3/2}$ nonlinear, 2D and 3D

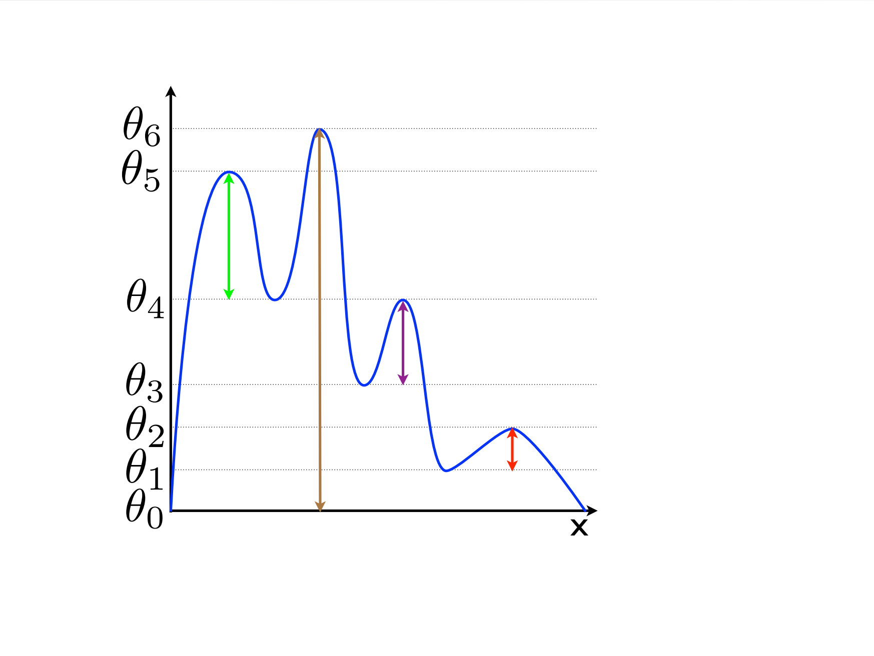
$$\mathbf{n}_i = \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$F_{i,j}^t = -min(\gamma_s \bar{m} |v_{vel}^t|, \mu_s |F_{i,j}^n|)$$

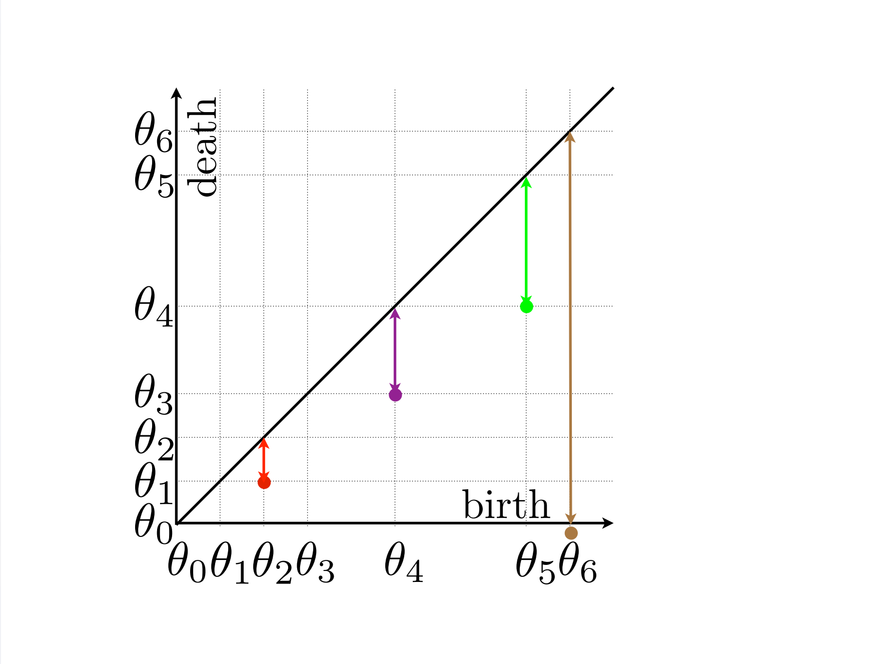
PERSISTENT HOMOLOGY: 1D TOY EXAMPLE

- Homology: way to associate algebraic objects to topological spaces
- Persistent homology: a method of computing topological features at different spatial scales; in the context of granular matter, the word `persistence' is meant in terms of inter-particle forces: over which range of forces certain topological feature (chain, loop) persists?

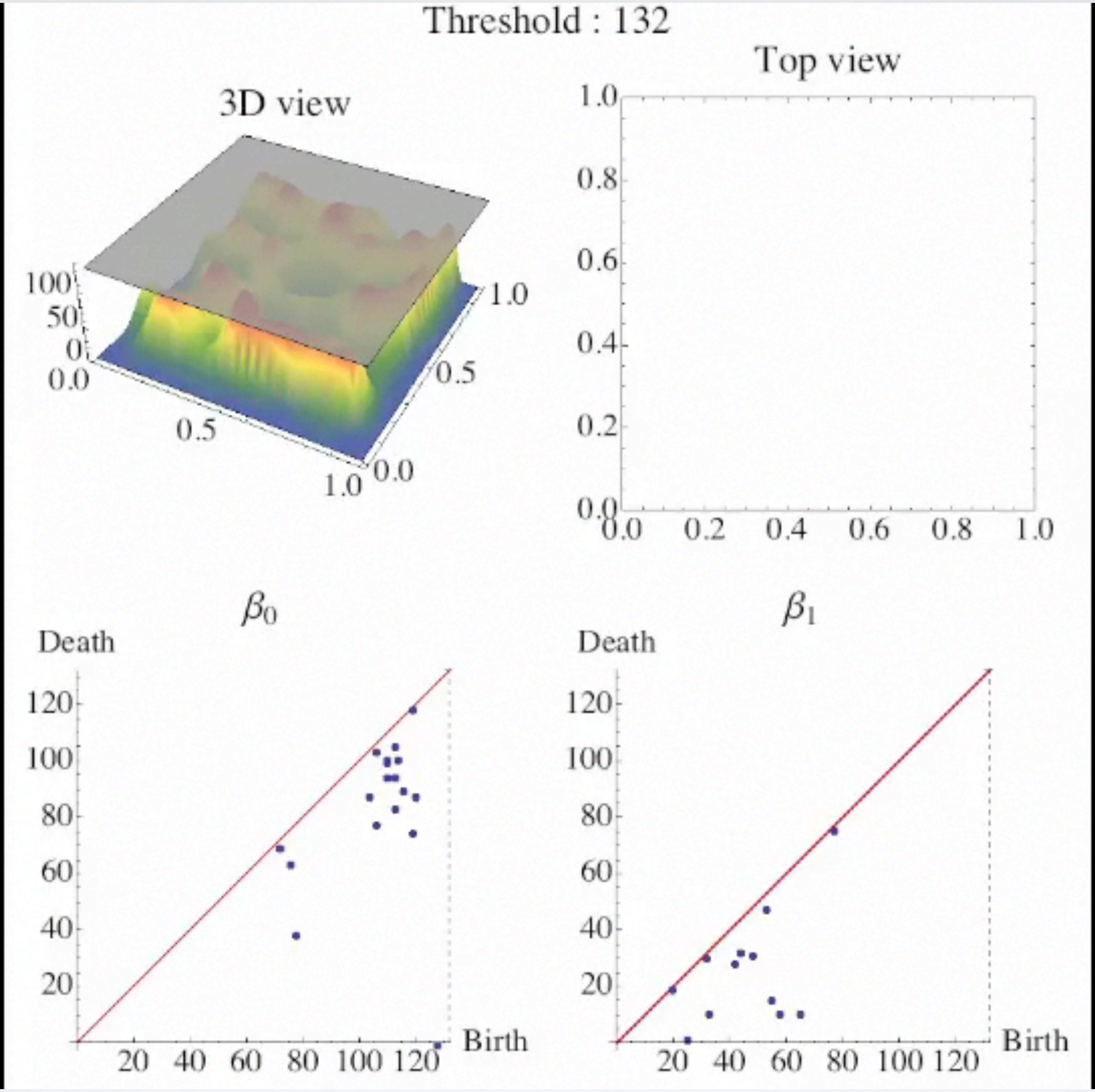
Toy example in 1D
f(x)
x: space
f: contact force



Persistence diagram (PD) describing main features of f(x)



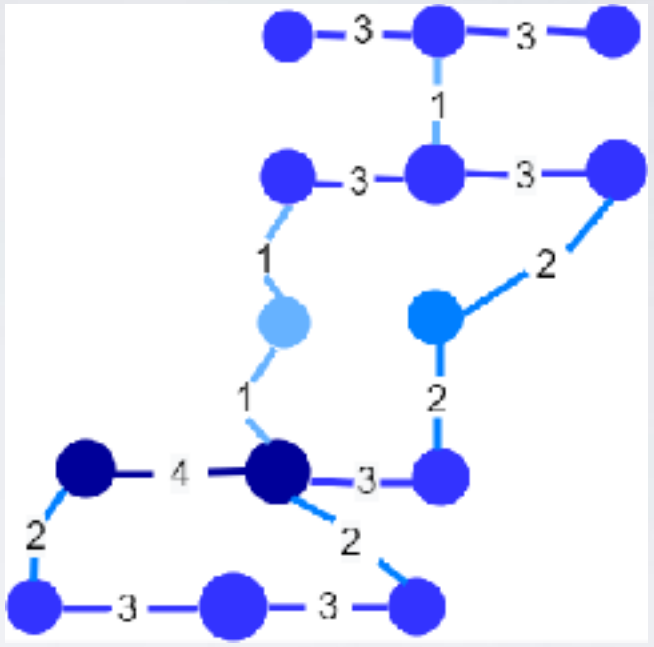
PERSISTENCE DIAGRAMS: 2D TOY EXAMPLE

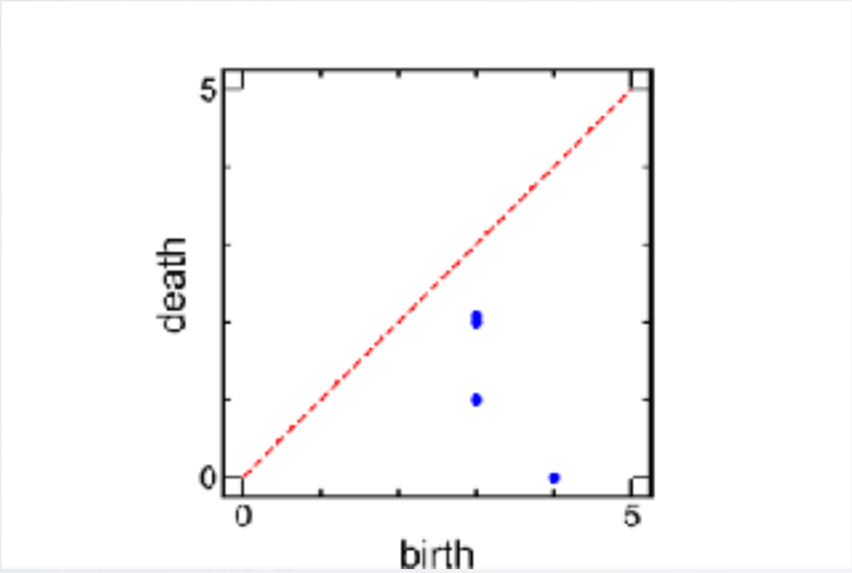


From a complicated function to point clouds

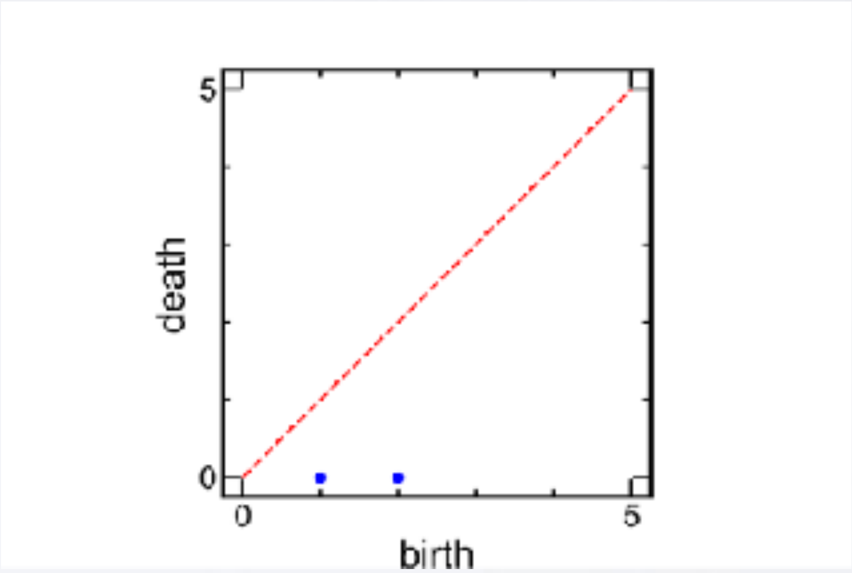
PARTICLE TOY EXAMPLE

simple force network with force strength illustrated by numerical values





PD 0 (`chains')



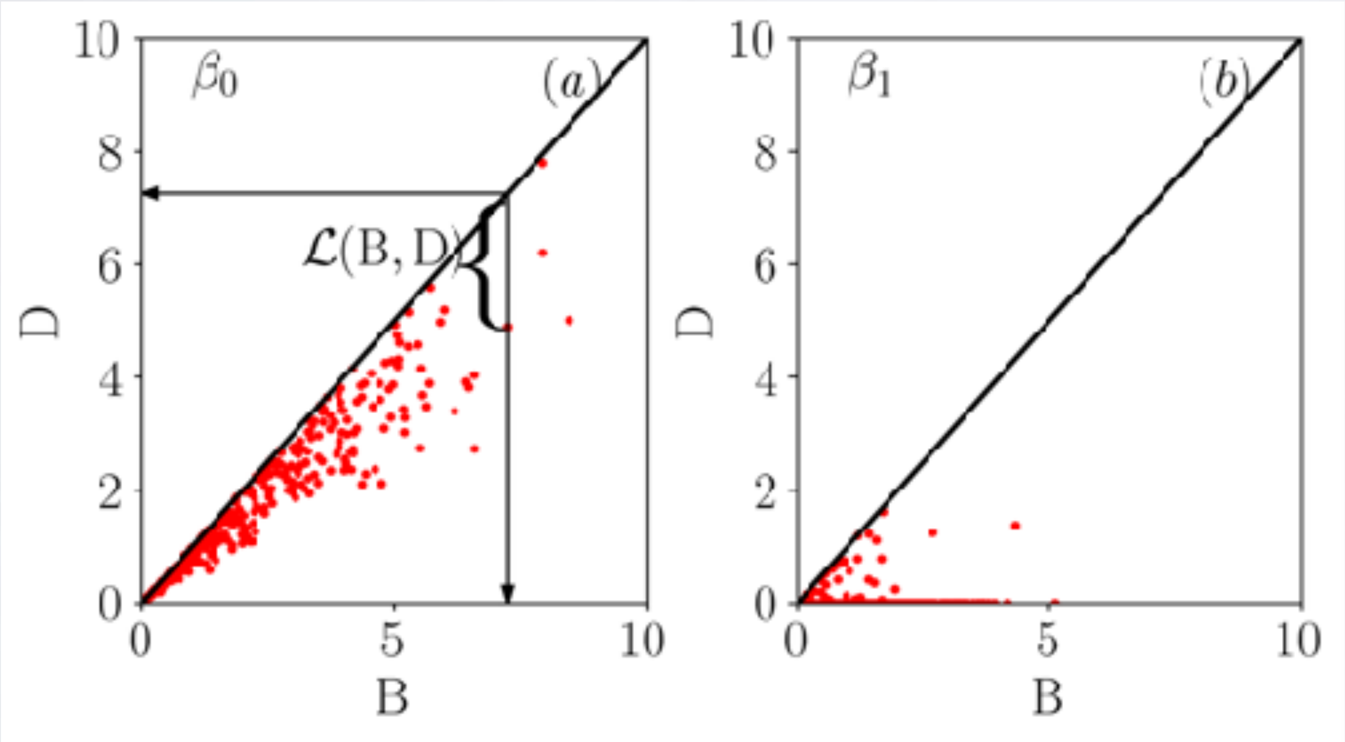
PD 1 (loops)

From weighted network to point clouds

PERSISTENT HOMOLOGY: MEASURES

- PDs describe complex weighted network in terms of point clouds
- Further data reduction:
  - Static information: compress point cloud to one number: Total Persistence, sum of all lifespans
  - Dynamic information: compare PDs by defining difference between them (Wasserstein distance, W2) [describes the minimal rearrangement required to map one PD to another one; extra points mapped to the diagonal; W2 uses L2 norm]

death



$$\mathrm{TP} = \sum \mathcal{L}$$

birth

components/chains

TP0

loops/cycles

TP1

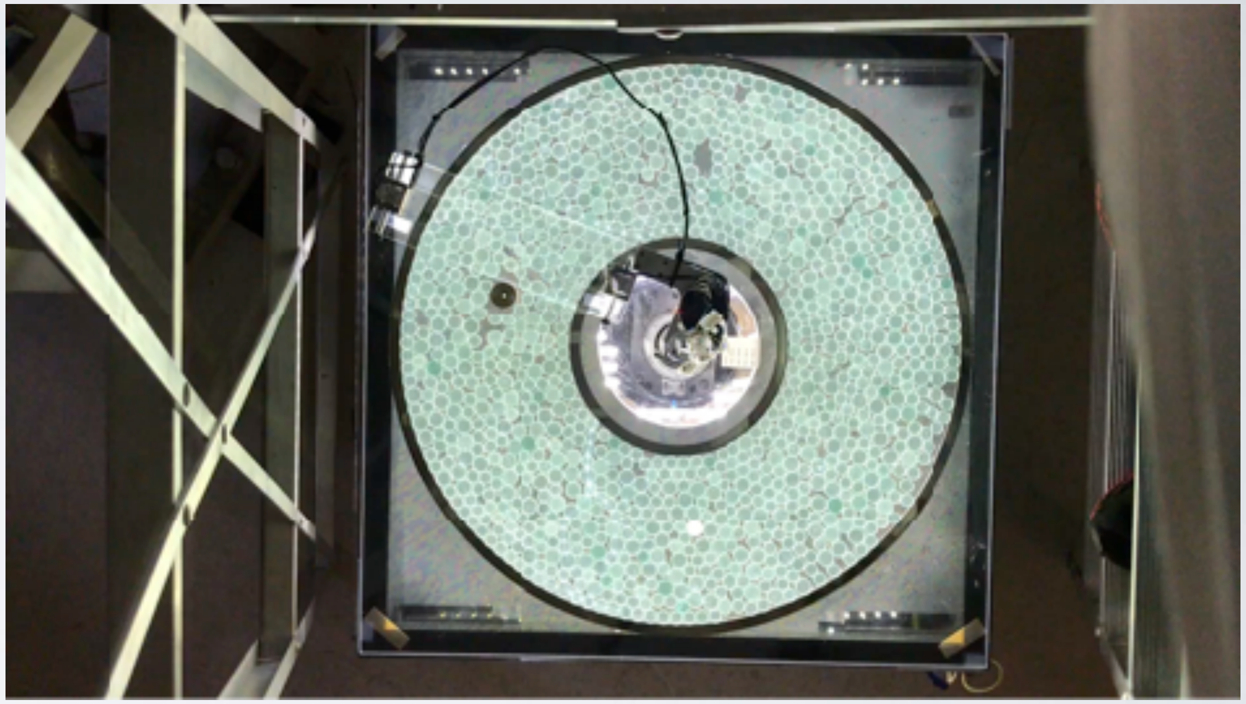
COUETTE SHEAR: EXPERIMENTS AND SIMULATIONS

- Idea: understand intermittent dynamics of a particle size intruder in a Couette shear cell

- Motivation: Couette geometry allows for continuous shear and therefore a large amount of data could be collected

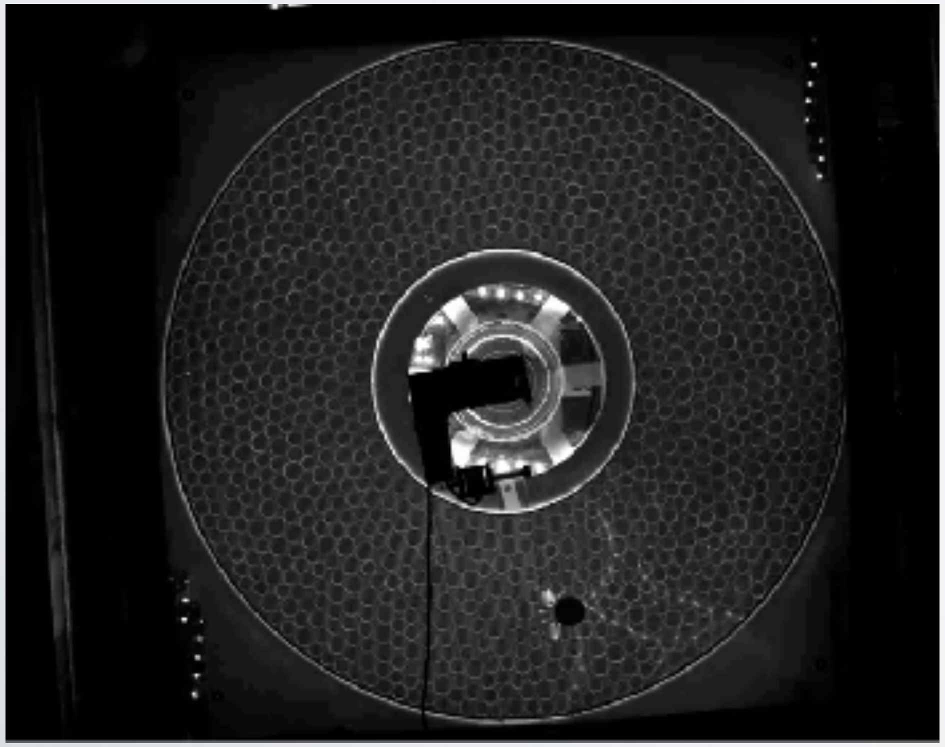
- Ongoing project: so far, detailed analysis of intruder dynamics has been carried out

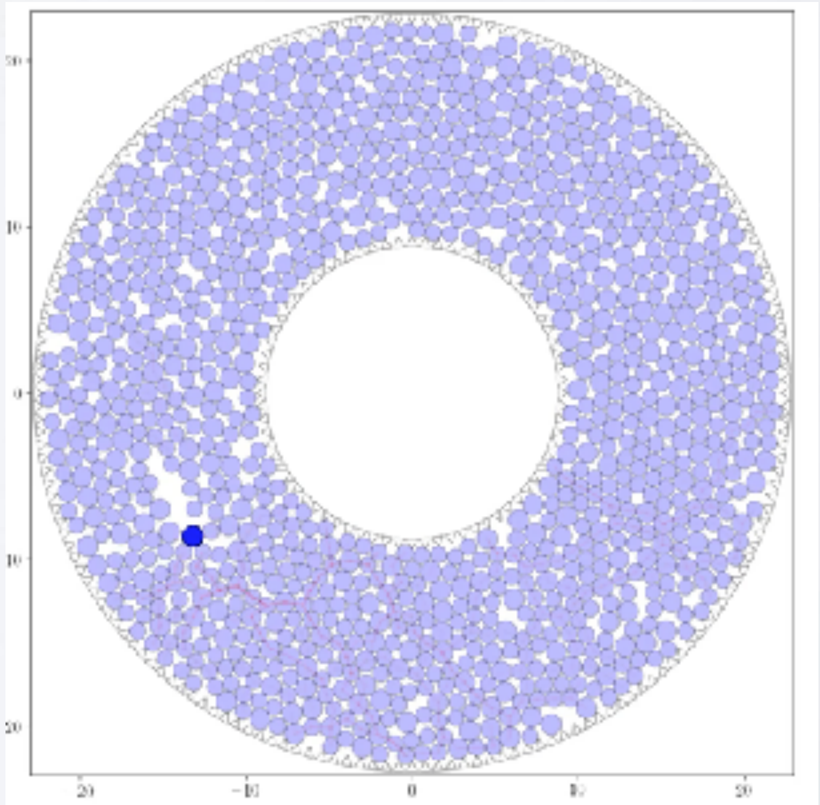
- Next steps: analysis of interaction networks in both experiments and simulations



ANALYSIS OF STICK-SLIP DYNAMICS, PART I

- Experiments: careful study of the intruder dynamics
  - Kozlowski, Carlevaro, Daniels, LK, Pugnaloni, Socolar, Zheng, Behringer, Phys. Rev. E 100, 032905 (2019)
- Simulations: direct comparison to experiments
  - Carlevaro, Kozlowski, Pugnaloni, Zheng, Socolar, LK, Phys. Rev. E 101, 012909 (2020)
- both experiments and simulations carried out with disks and pentagons





ANALYSIS OF STICK-SLIP DYNAMICS, PART II

- Challenge: quantify statics and dynamics of force networks
- Use TDA: description of force networks via `persistence diagrams (PDs)'
  - point clouds that quantify connectivity of a weighted network
- PDs computed using the methods emerging from persistent homology, well established discipline of computational topology

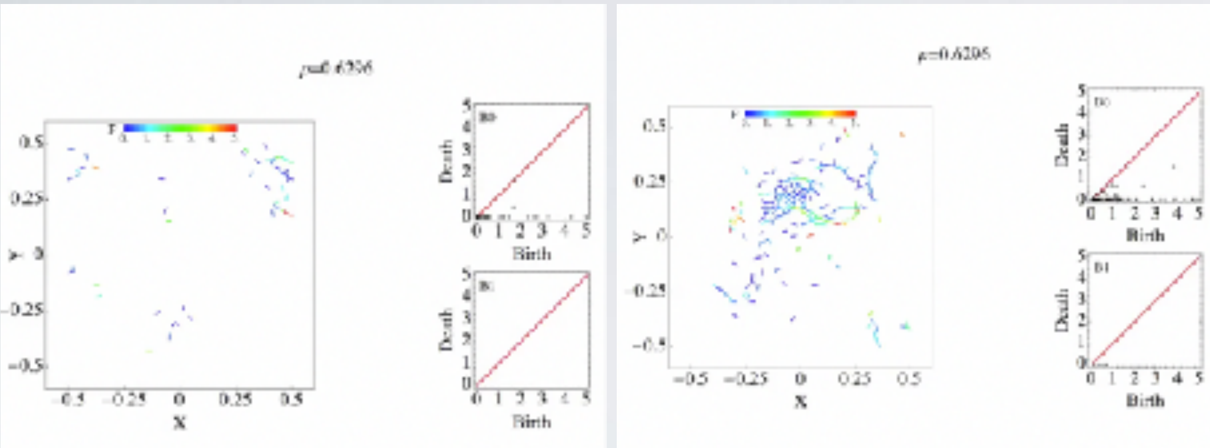
PERSISTENT DIAGRAMS

- PDs: a method of computing topological features at different spatial scales; in the context of granular matter, the word `persistence' is meant in terms of inter-particle forces: over which range of forces certain topological feature (chain, loop) persists?
- Important features of PDs
  - *significant data reduction*: from terabytes to megabytes
  - keep important information about connectivity of force networks
  - computed using the same techniques and codes in *2D and 3D*
  - uses as input experimental images (obtained using photoelasticity or some other method) or simulation data
  - live in a metric space, meaning they could be compared: *dynamics can be extracted*
  - applicable to any weighted network

PERSISTENT HOMOLOGY: APPLICATIONS TO GRANULAR SYSTEMS

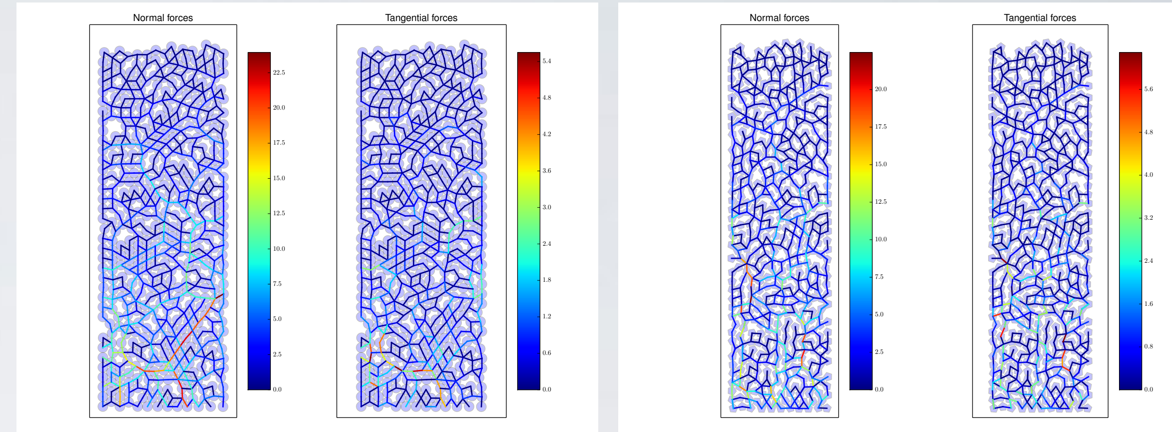
compression - monodisperse frictionless

compression -polydisperse frictional



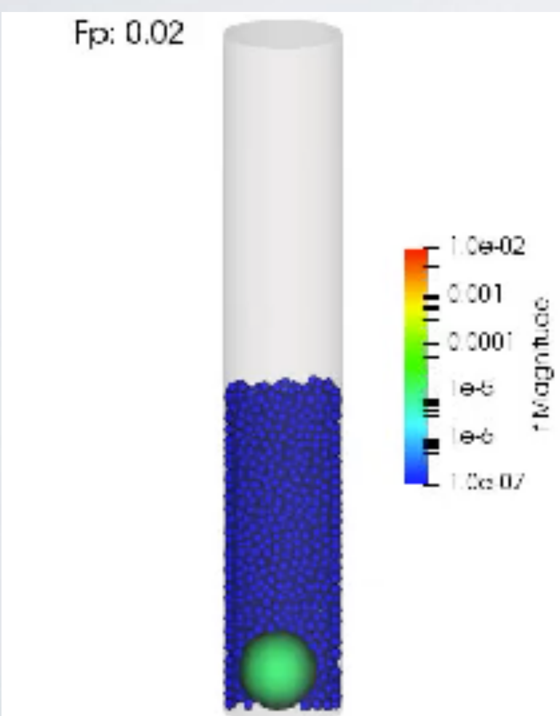
Kramar, Goullet, LK, Mischaikow, Physica D 2014

disks vs. pentagons: tapping



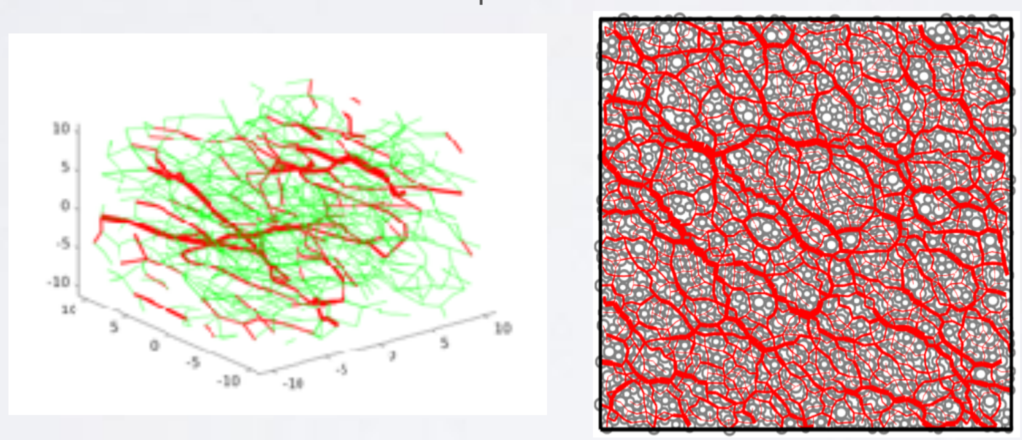
Pugnaloni etal, LK etal PRE 2016

pulling out an intruder



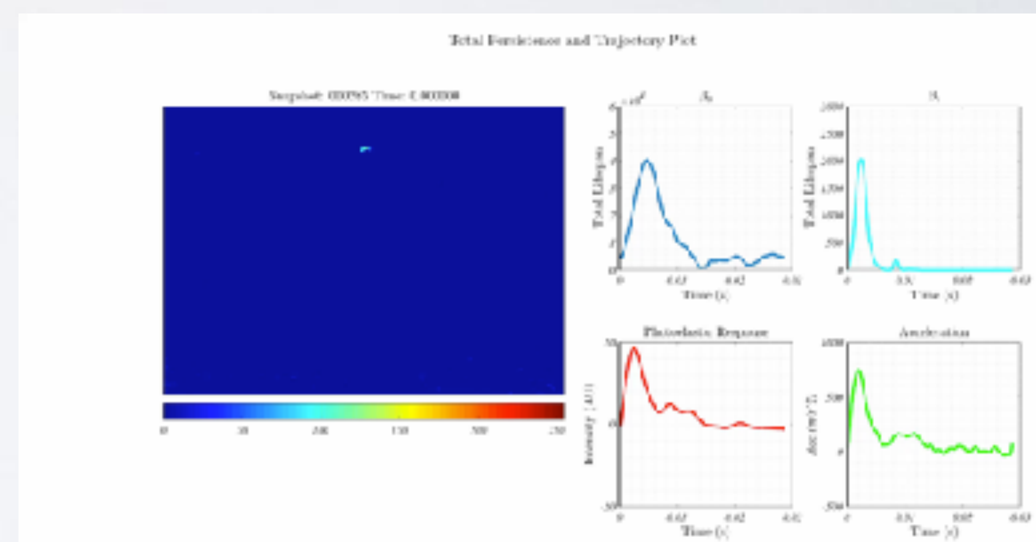
Shah, Cheng, Jalali, LK, Soft Matter 2020

suspensions



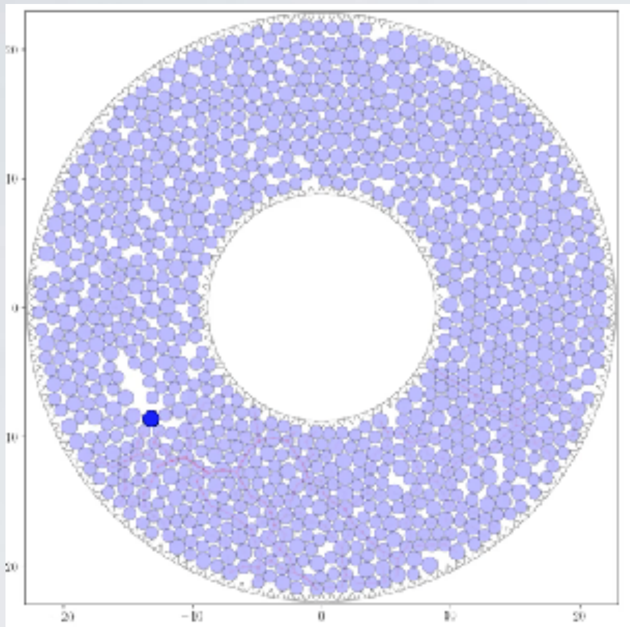
Singh, Gameiro, LK Mischaikow, Morris, PR Fluids 2020

impact (experiment)

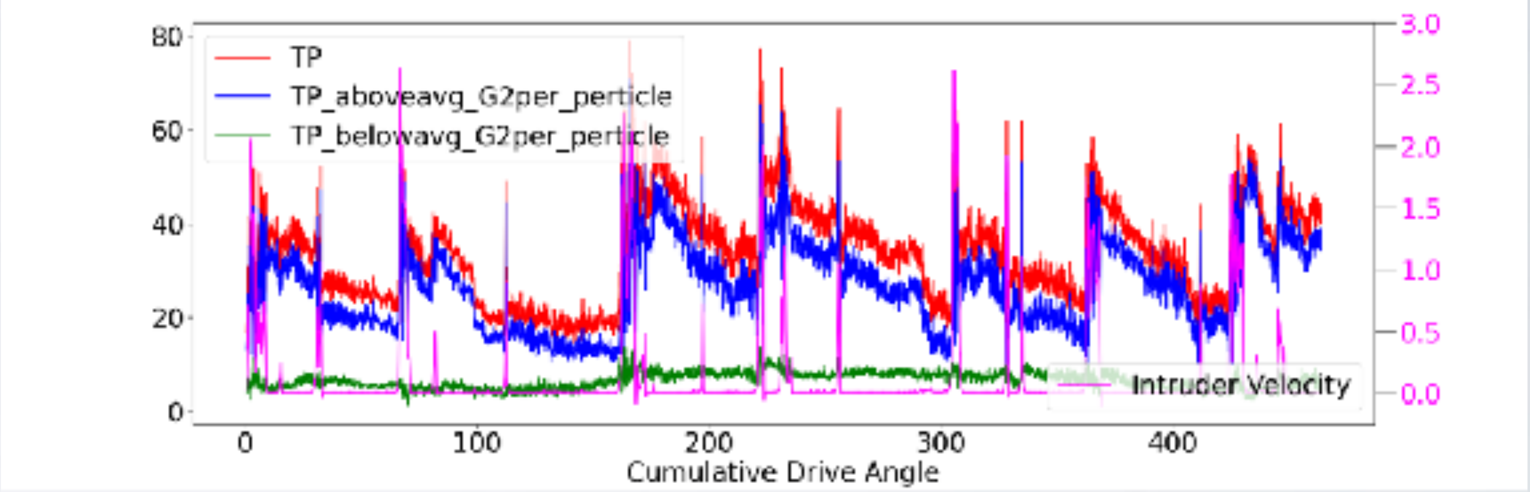


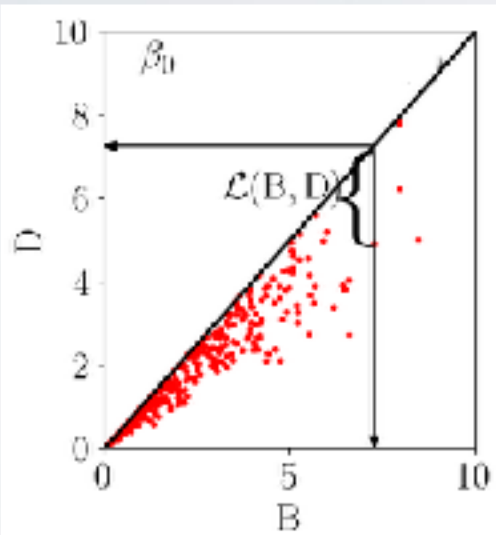
Tadanaga, Clark, Majmudar, LK PRE 2018

INTERACTION NETWORKS IN SIMULATIONS: TOTAL PERSISTENCE



chains

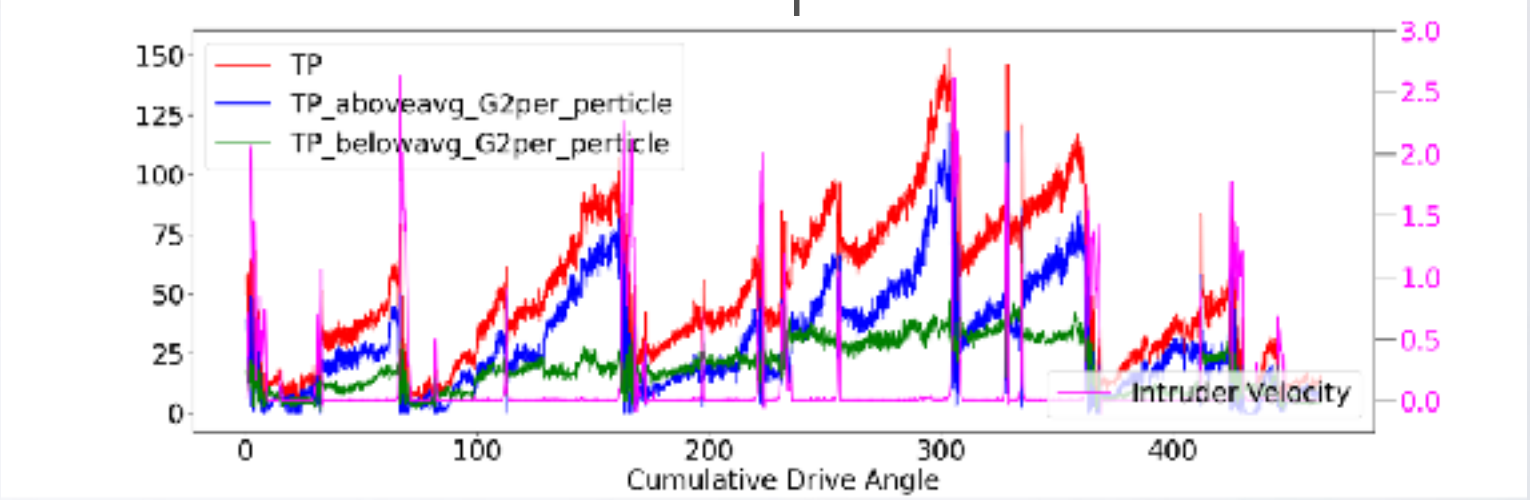




$$\text{TP} = \sum \mathcal{L}$$

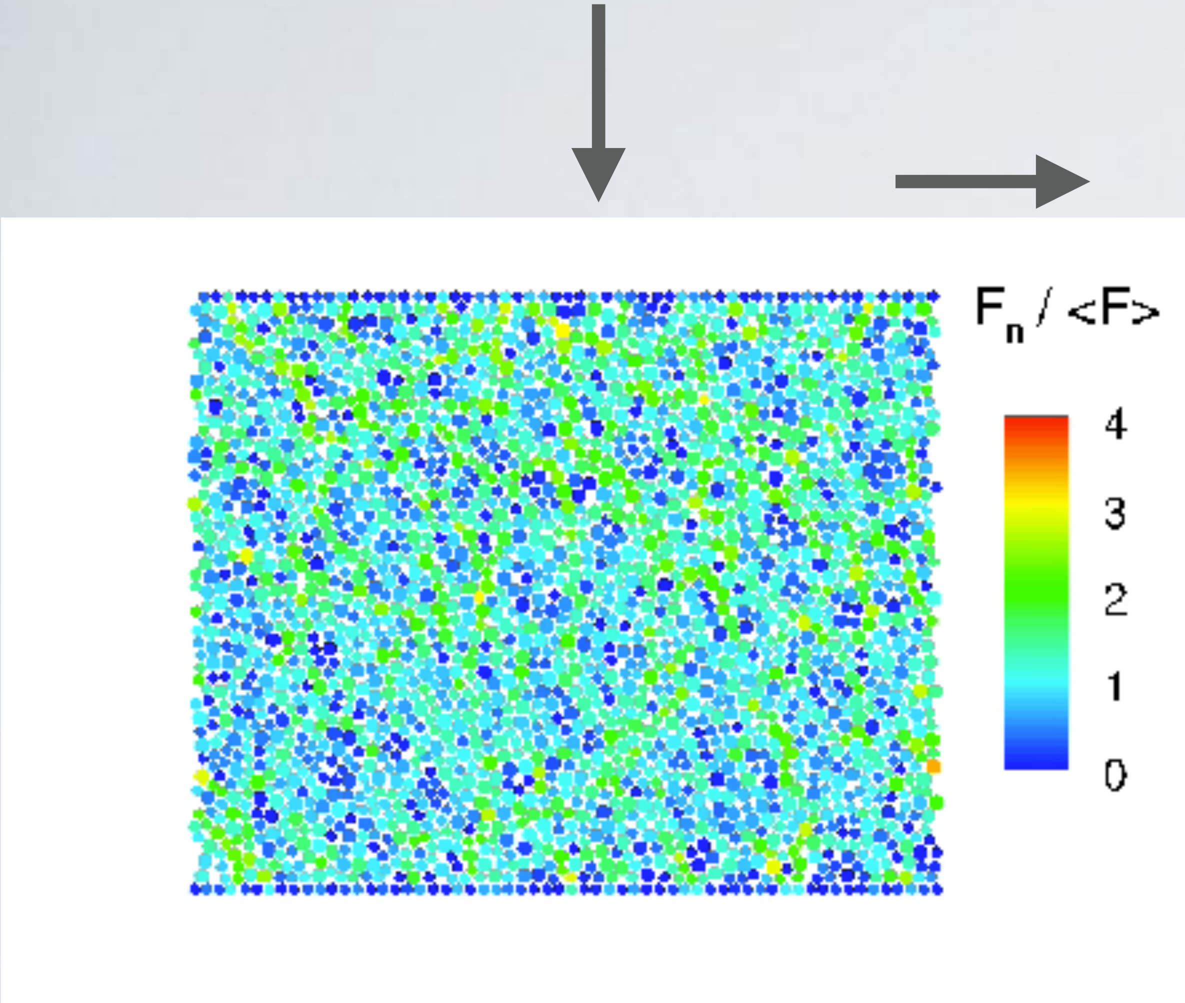
B : birth
D : death

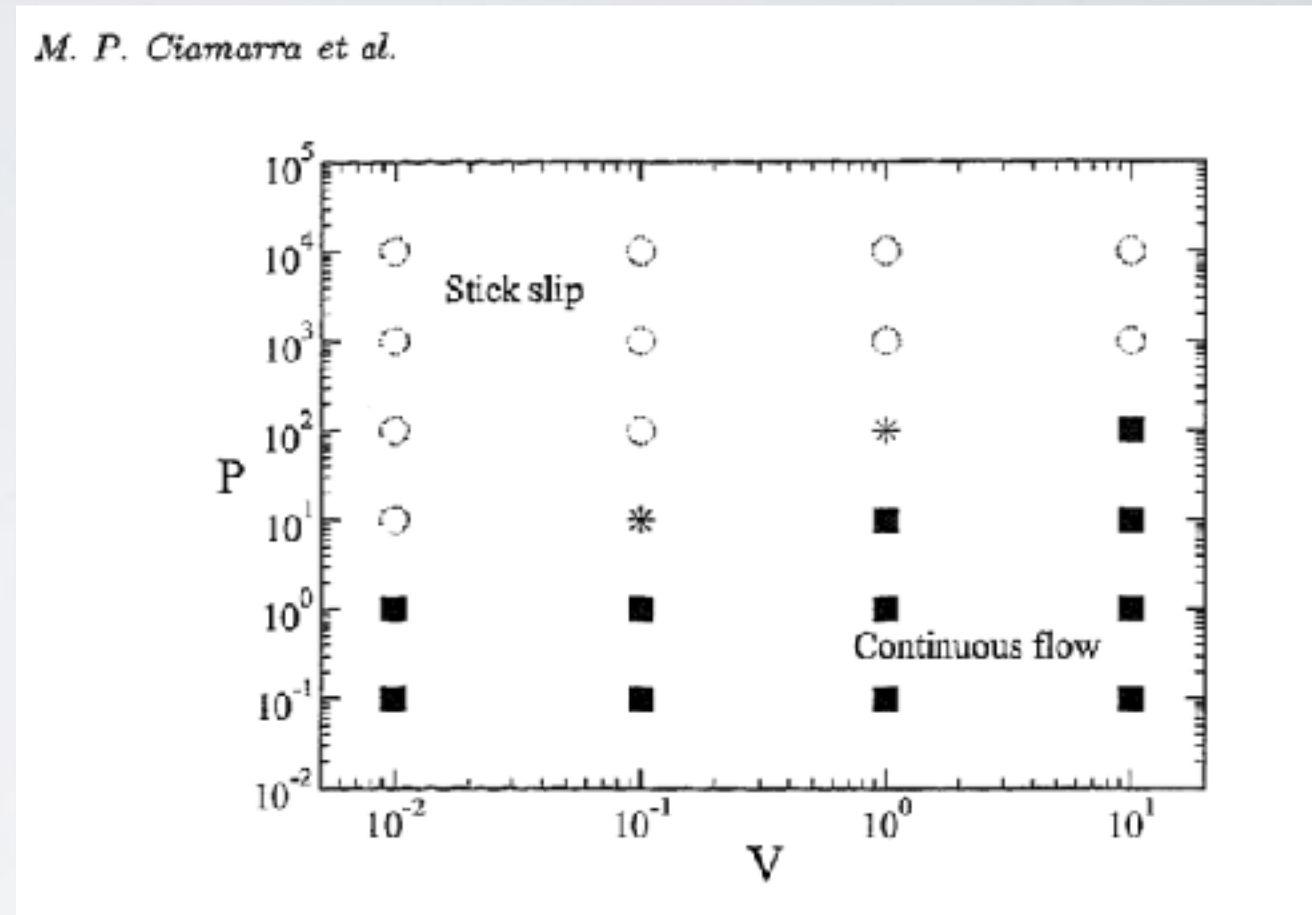
loops



- TP (total persistence) captures well the changes of force networks due to intruder's dynamics, and shows significant difference between components (`chains') and loops (`cycles')

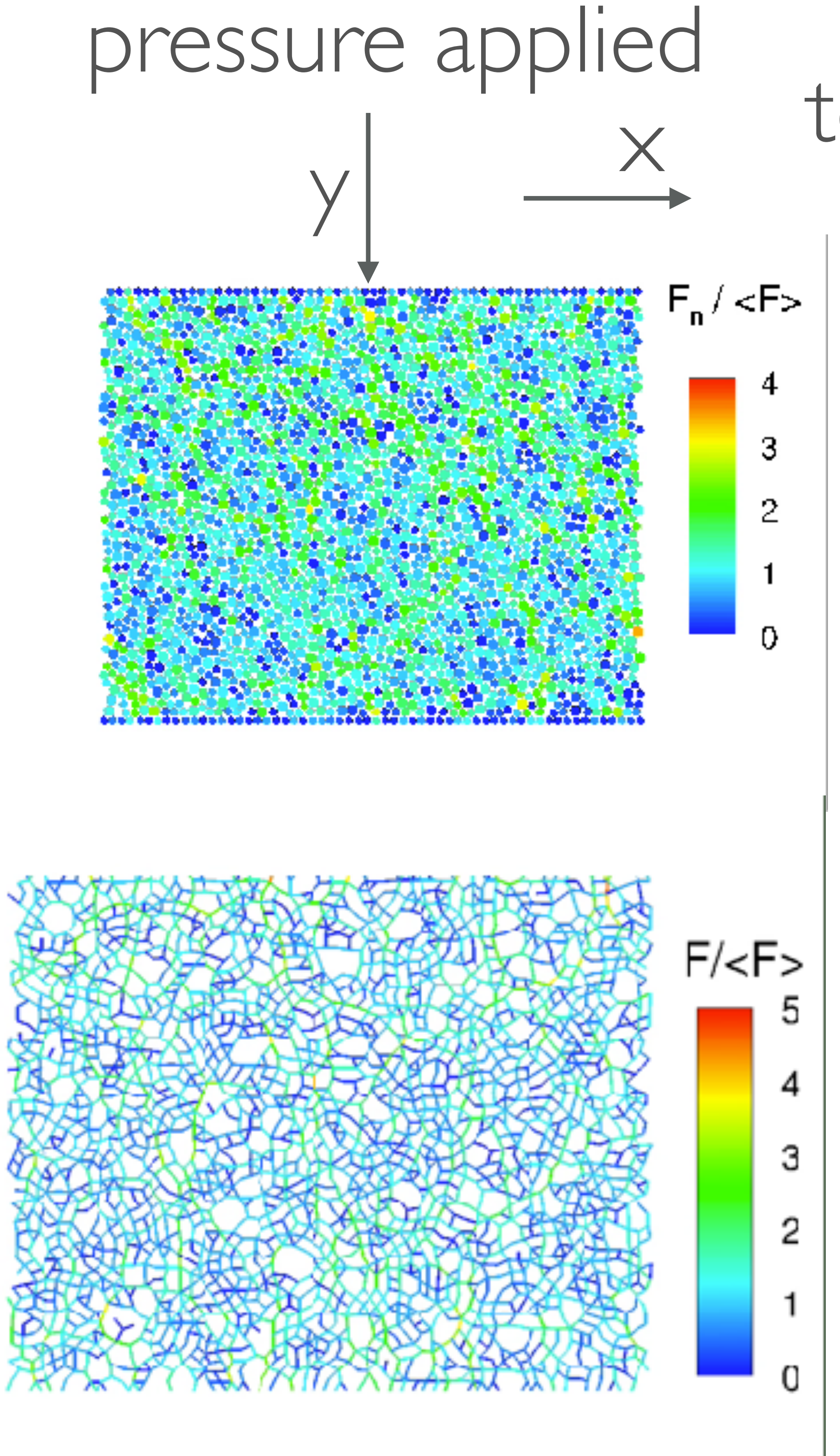
CASE STUDY: STICK SLIP DYNAMICS



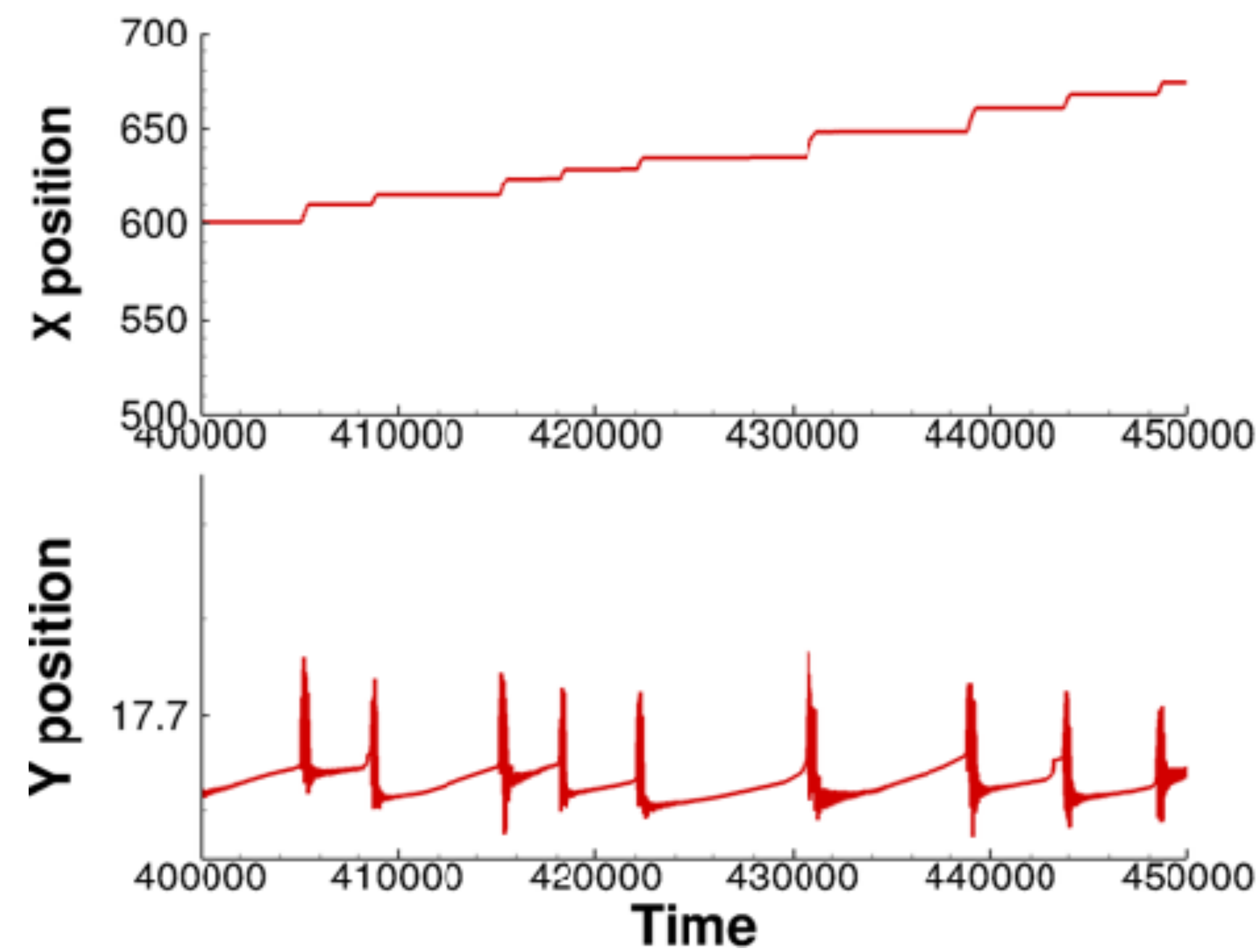


soft bidisperse frictional particles (2D disks)
shear imposed by a spring attached to the top wall
no gravity

USE PERSISTENCE TO ANALYZE AVALANCHES: STICK - SLIP DYNAMICS

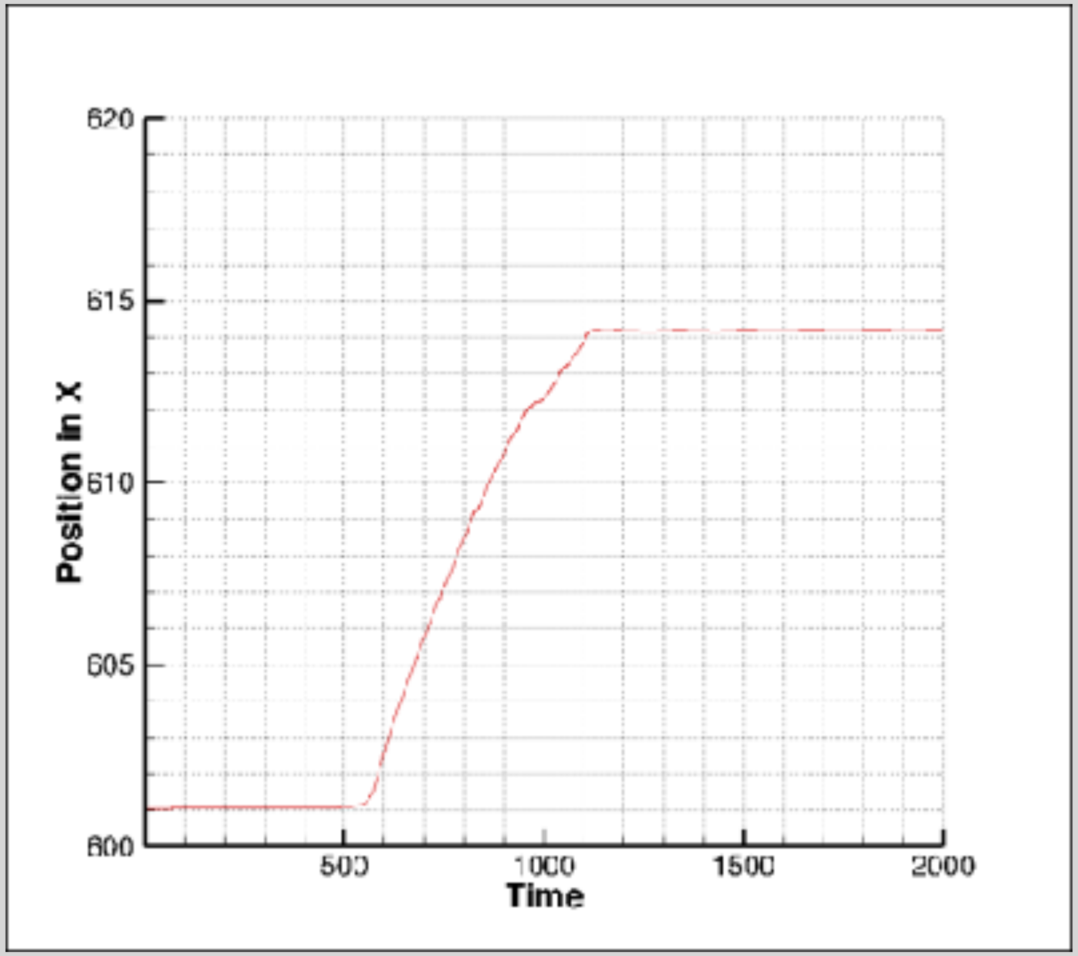


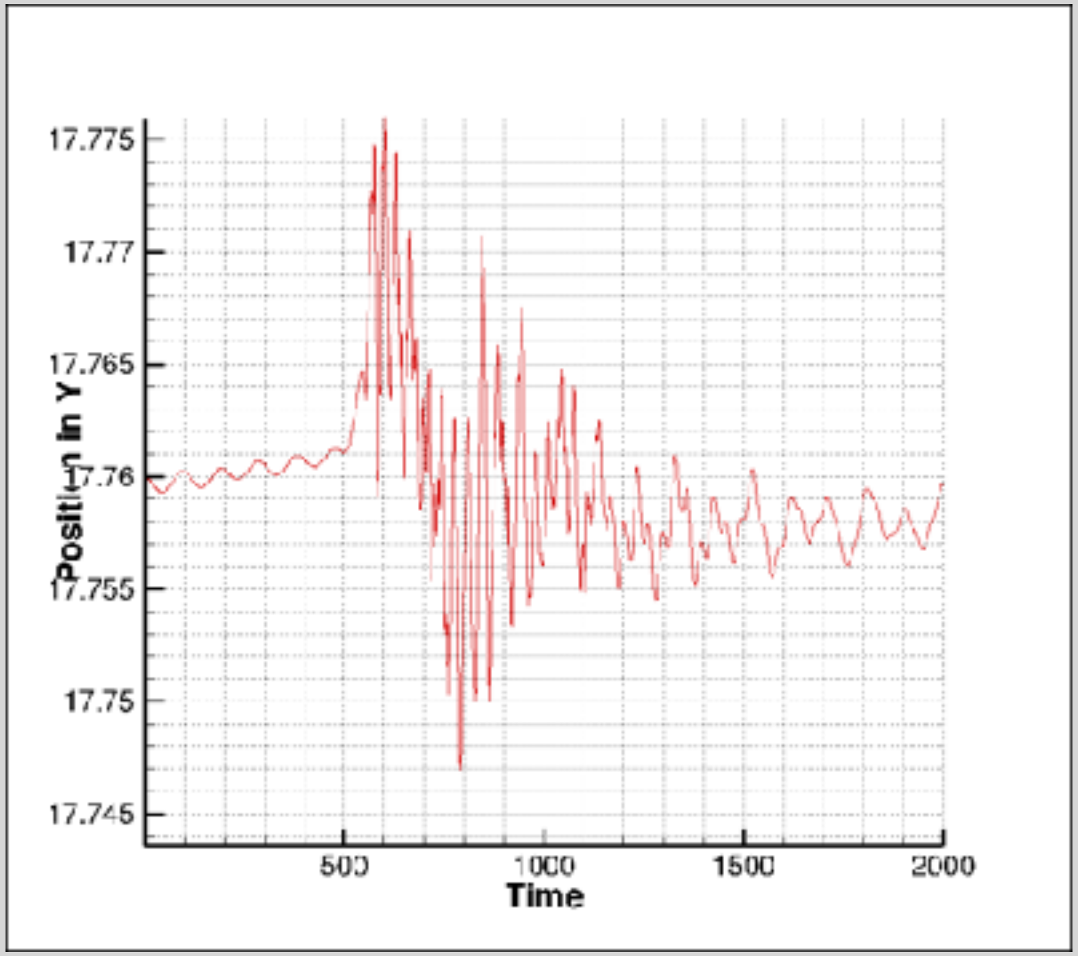
top wall pulled by a spring



Is there a signature of upcoming slip event?

Single Slip Event - Wall Movement



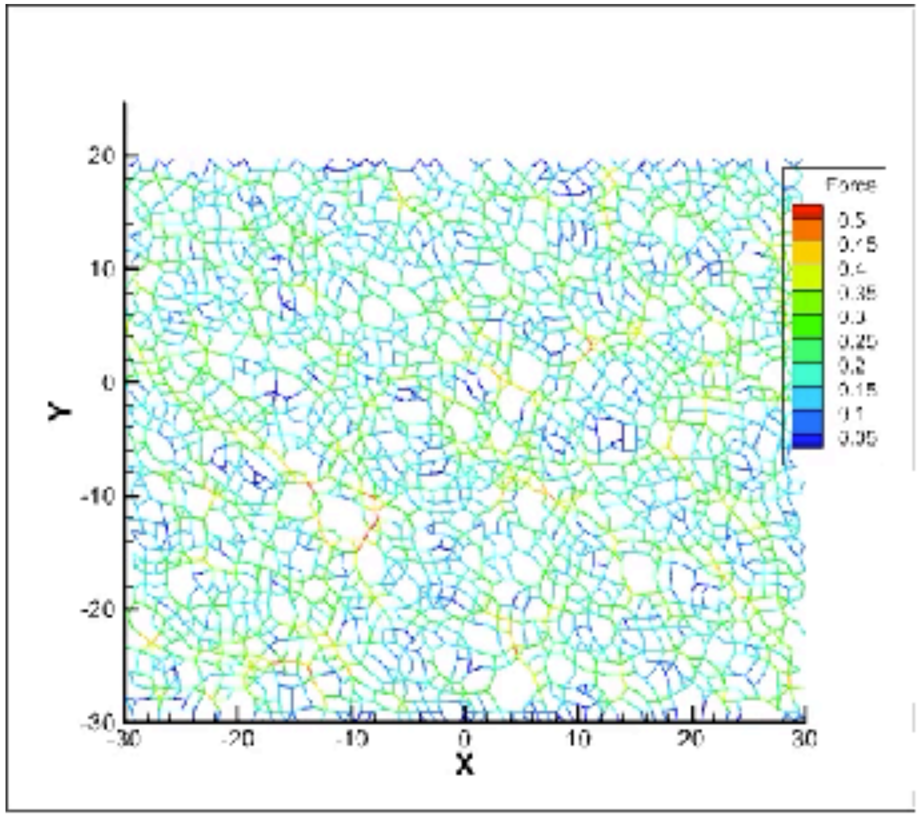


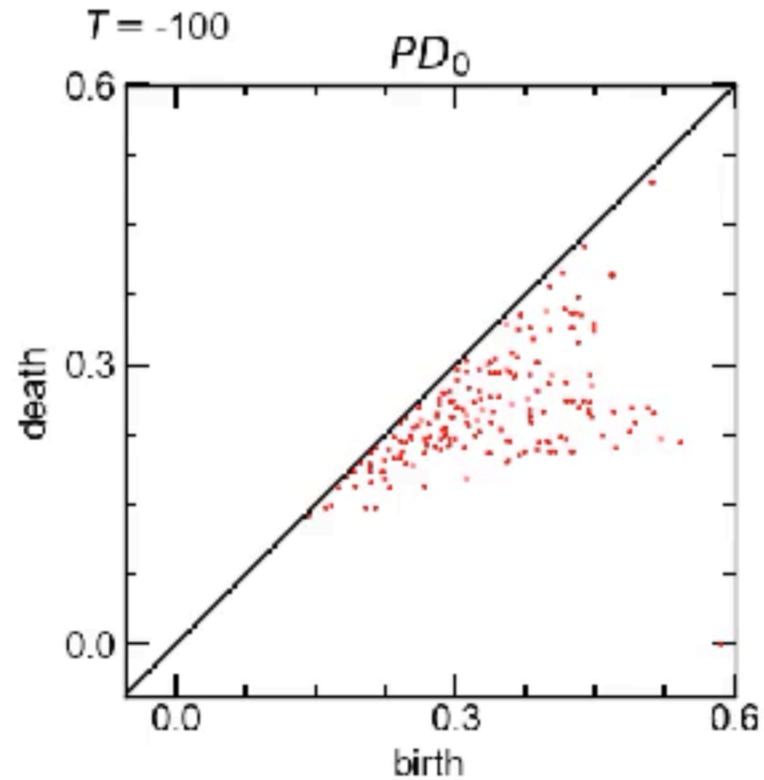
DISTANCE BETWEEN PERSISTENCE DIAGRAMS

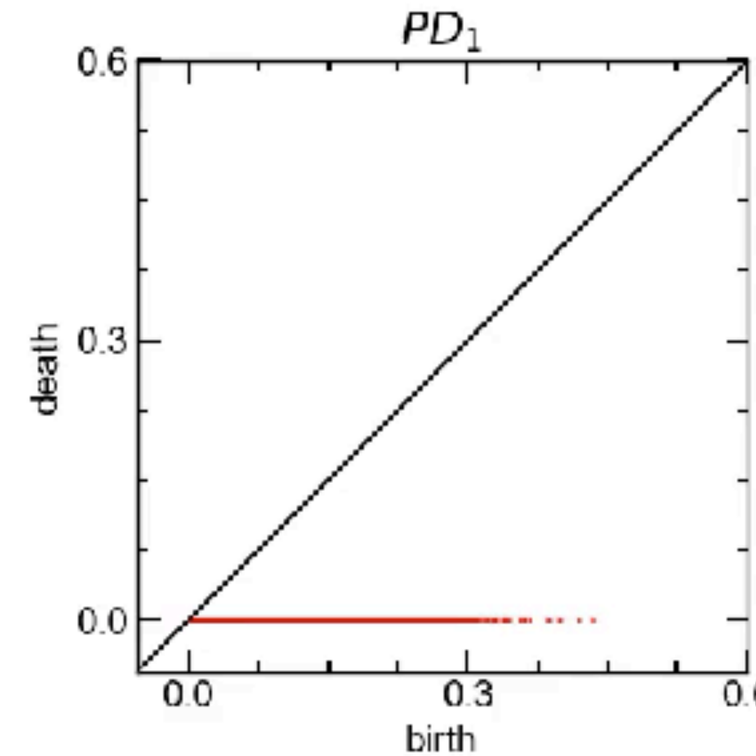
- persistence diagrams live in a metric space and therefore can be compared
- approach: compute the distance between all points in a diagram, and match the points so that this distance is minimized
  - (if the number of points is different, match the extra points to the diagonal)
  - use appropriate norm to put desired weight on small or large differences

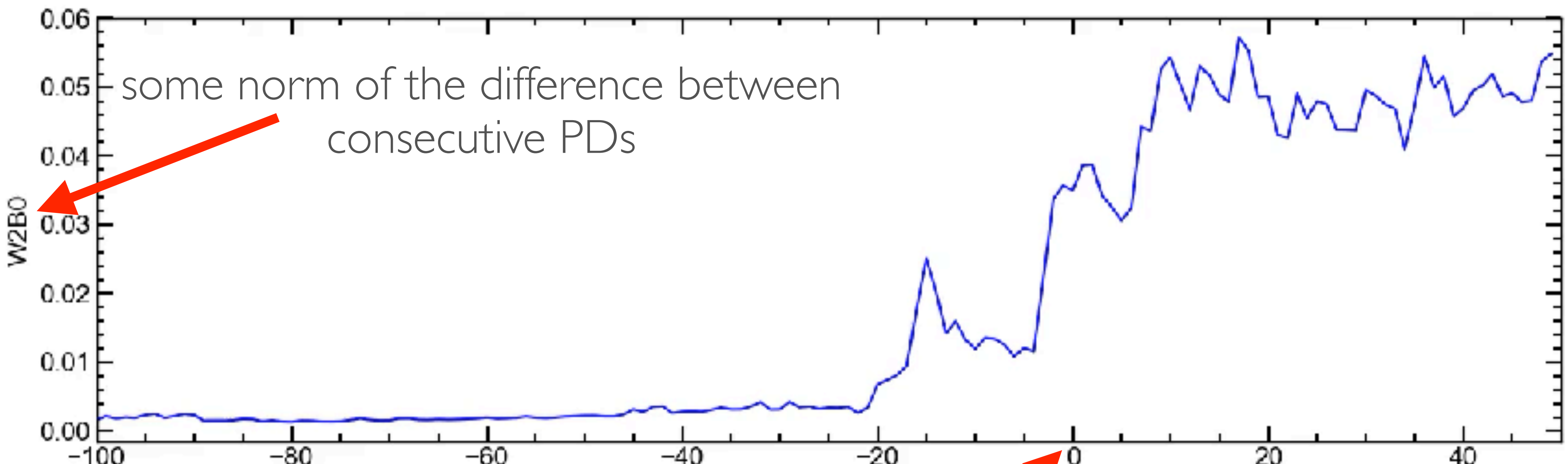
$$d_{W^q}(PD, PD') = \left[\sum_{i=0}^{n} \inf_{\gamma, PD_n \rightarrow PD'_n} \sum_{p \in PD_n} \|p - \gamma(p)\|_\infty^q \right]^{1/q}$$

Single Slip event Force Network



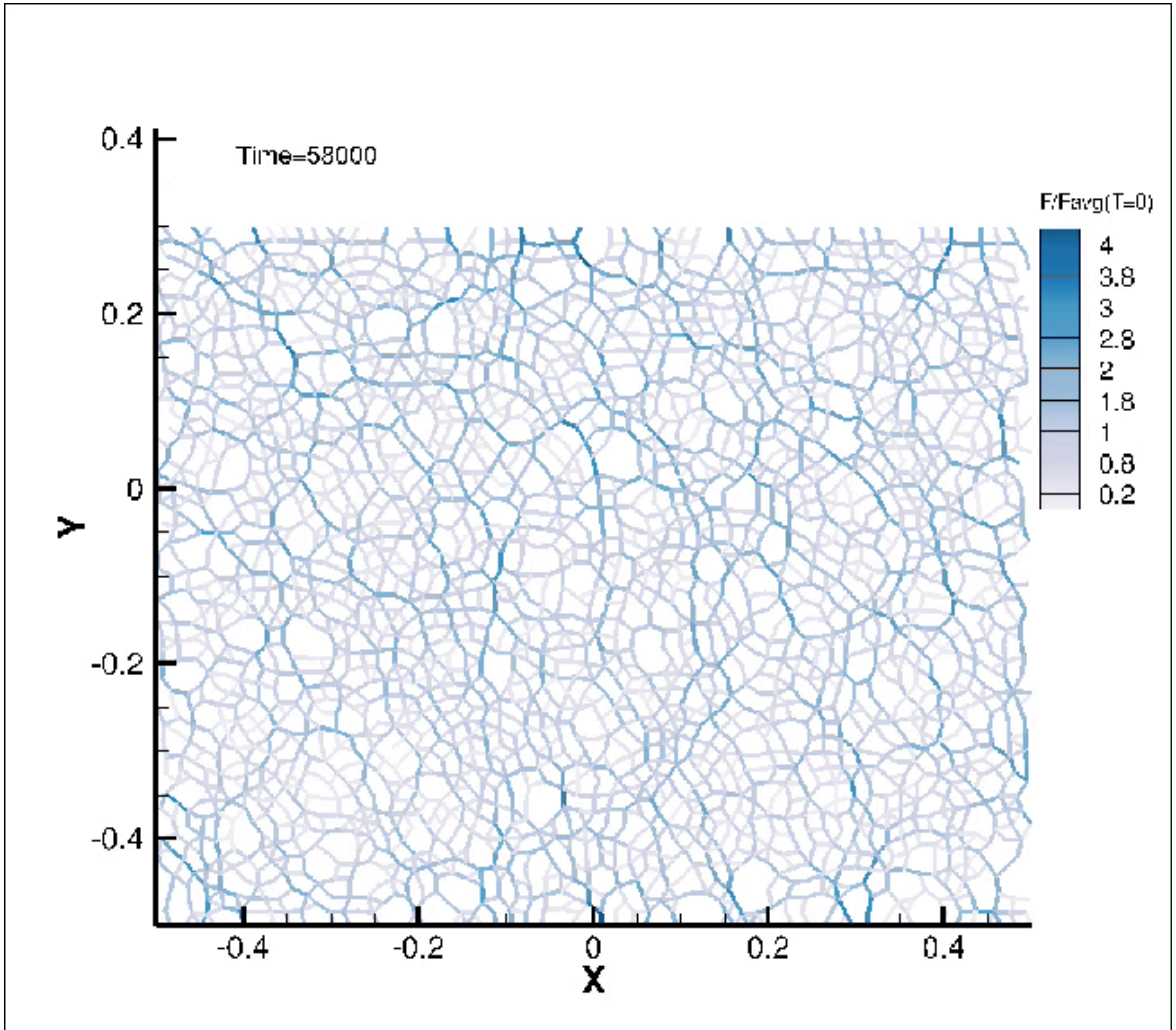




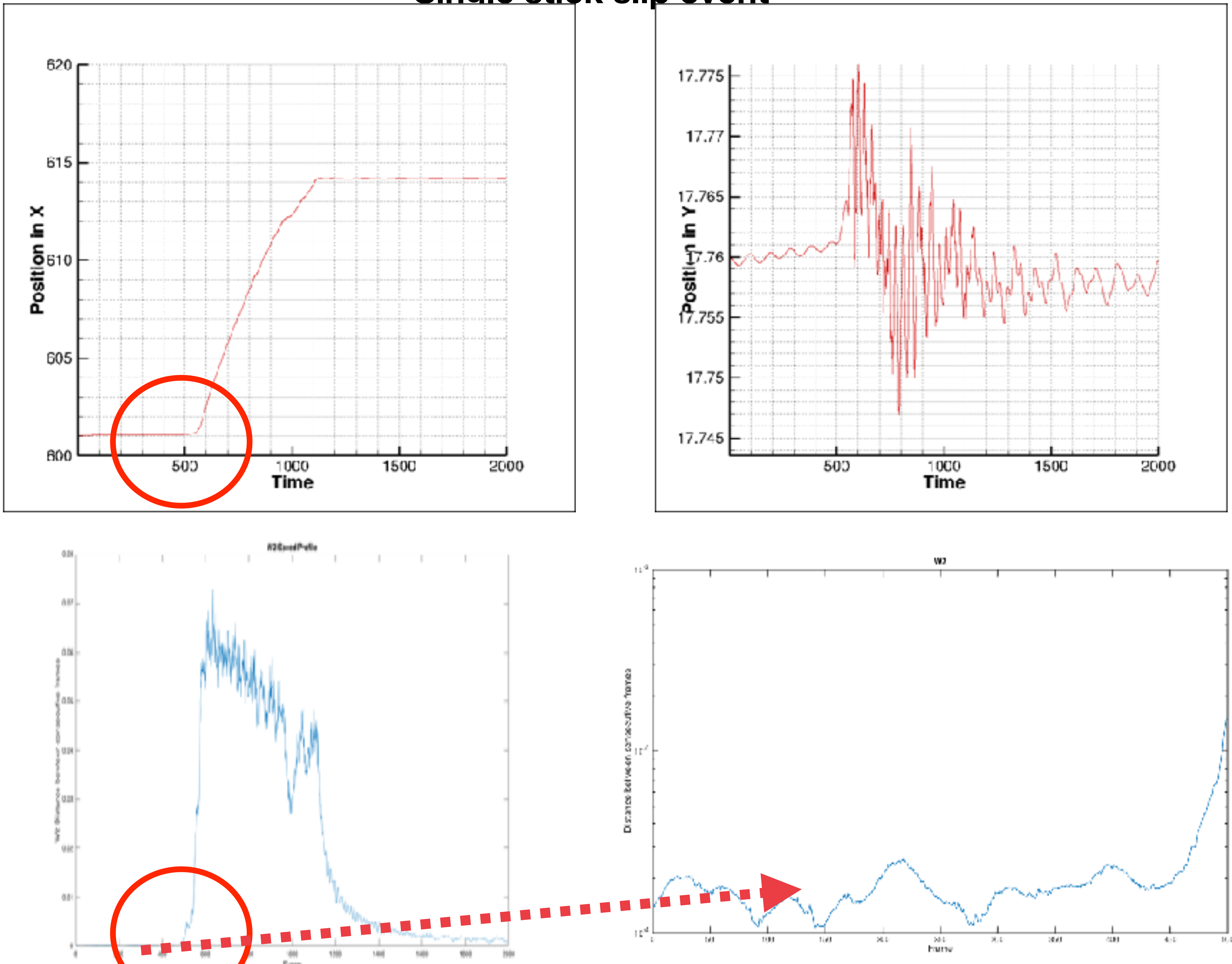


start of the slip event

Single Slip event Force Network

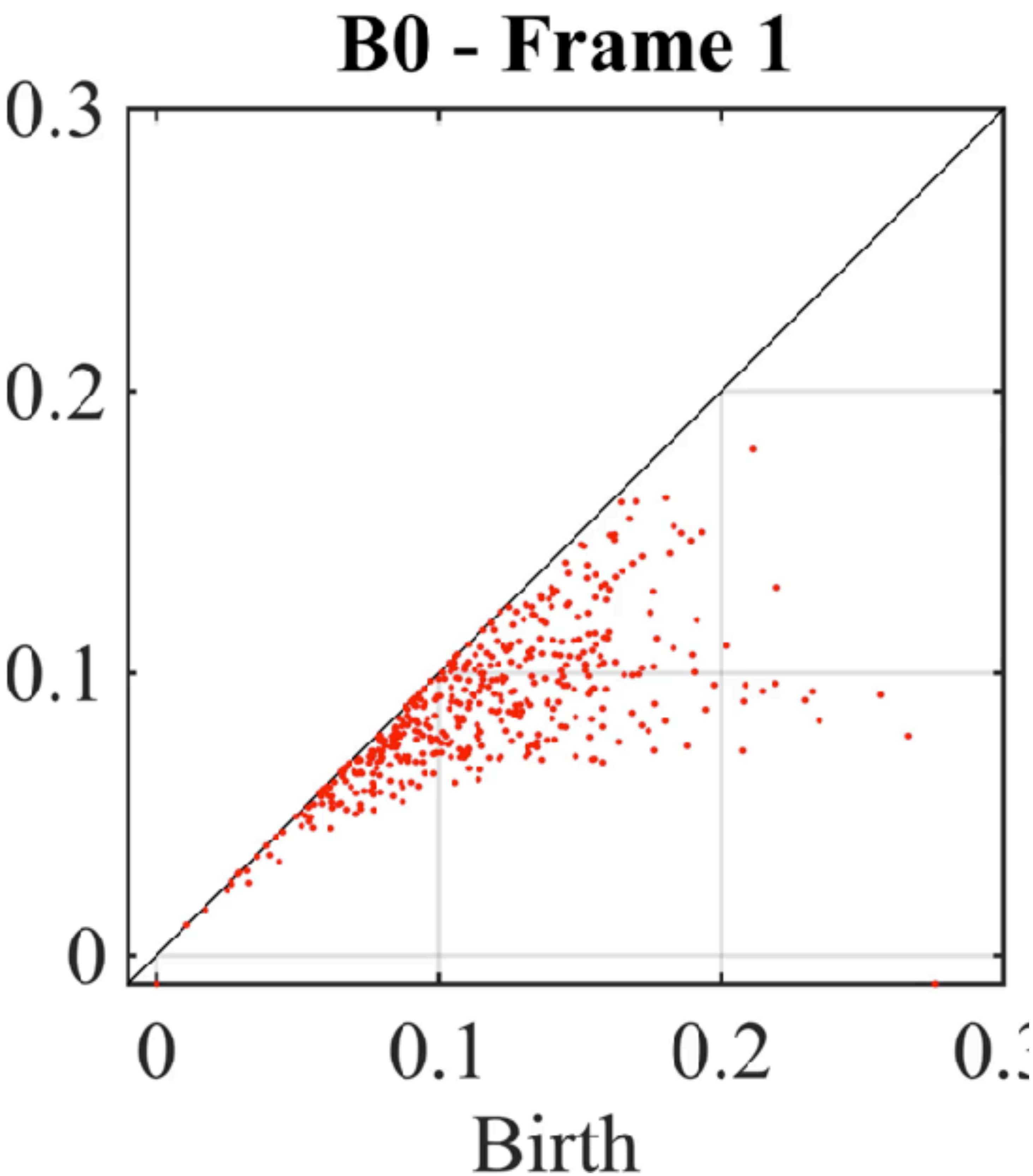


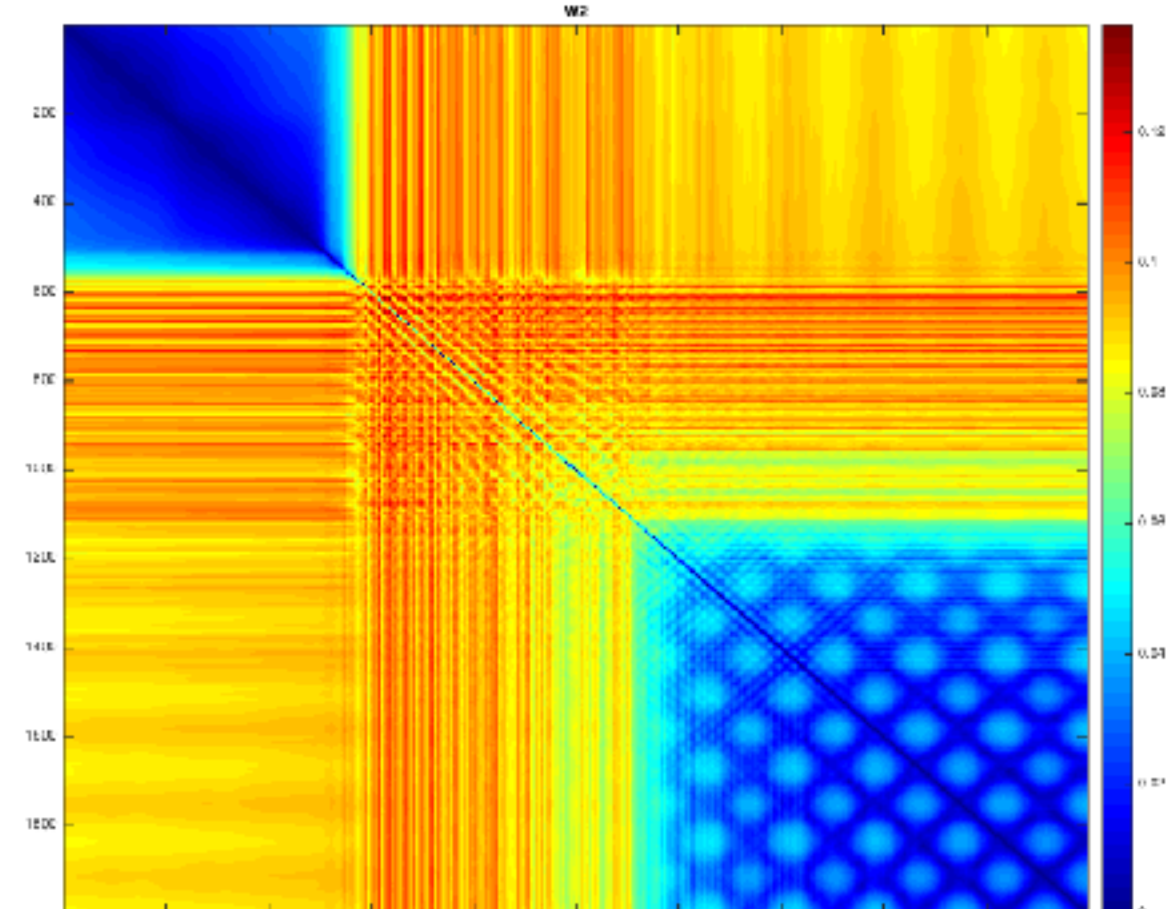
Single stick slip event

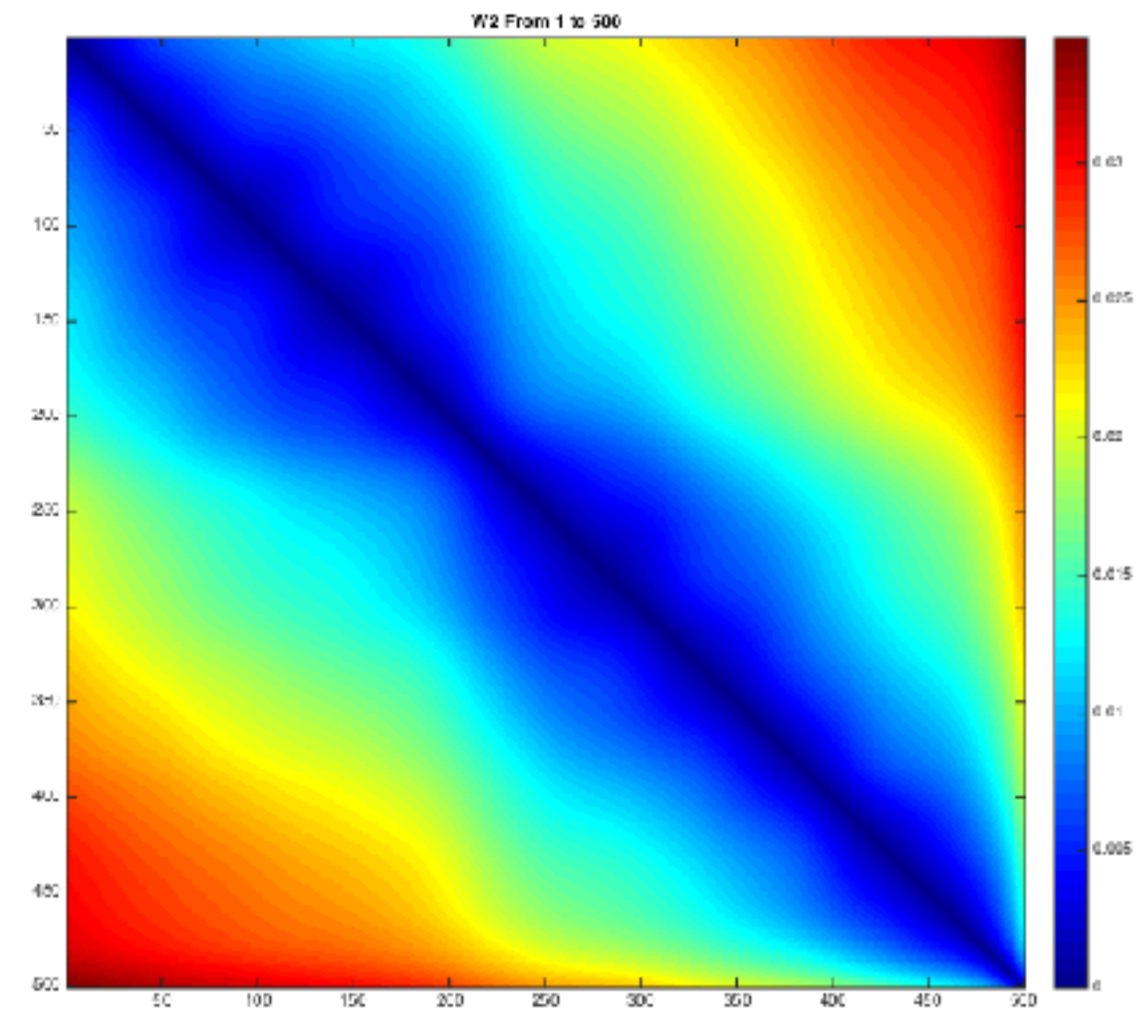


W2-distances between consecutive frames

Single Slip Event







STICK-SLIP: WHAT HAVE WE LEARNED

- Topology based methods provide a way to simplify considerably quantitative description of interaction networks in sheared granular systems
- Based on the simplified description, we are able to quantify the connection between mesoscale information (interaction networks) and macroscopic system response (slip)
- Interaction networks analysis suggests existence of precursors to slip events
- Current work:
  - carry out analysis of a large number of slip events
  - describe more precisely the slip precursors and their properties
  - explore the use of machine learning to predict future events

MACHINE LEARNING (ML)

- Can we learn when a system is going to yield based on the state of the system while it is static?
- Relevance: huge!
- Idea: feed the data from simulations to ML software and ask what kind of information is needed to be able to develop predictions
- Ongoing project with the group led by Kramar at OU, using the 2D data produced here
- Future projects: use our data in 3D, as well as the experimental and simulation data produced by our collaborators

SUMMARY

- We are attempting to describe systems for which there is no continuum theory in terms of partial differential equations: this is not an easy task
- The methods based on analysis of force networks provide a path from micro to macro scale, allowing to connect particle properties to macroscopic system response (rheology, yielding, avalanching)
- Our results suggest that the force networks evolve even while the system is stuck: quantifying this evolution may be a key in developing predictive capabilities
- Preliminary results suggest that predicting upcoming slip events should be possible: the question is what type of information is needed for this purpose? subject of our current work

RECENT WORKS ON TDA, STICK-SLIP AND INTERMITTENT DYNAMICS

- Kozlowski, Carlevaro, Daniels, LK, Pugnaloni, Socolar, Zheng, Behringer, Phys. Rev. E 100, 032905 (2019)
- Cheng, Jalali, LK, Soft Matter 16, 7685 (2020)
- Gameiro, Singh, LK, Mischaikow, Morris, Phys. Rev. Fluids 5, 034307 (2020)
- Carlevaro, Kozlowski, Pugnaloni, Zheng, Socolar, LK, Phys. Rev. E 101, 012909 (2020)
- Kramar, Kovalcinova, Mischaikow, LK, Chaos 31, 033126 (2021)
- Cheng, Zadeh, LK, EPJ Web of Conferences, 249, 02007 (2021)
- Jalali, Zhao, Socolar, Soft Matter 17, 2832 (2021)
- Basak, Carlevaro, Kozlowski, Cheng, Pugnaloni, Kramar, Zheng, Socolar, LK, J. Eng. Mech. 147, 04021100 (2021)

Thank you for your attention!

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