NETWORK MODELING OF FLUID FLOW THROUGH MEMBRANES

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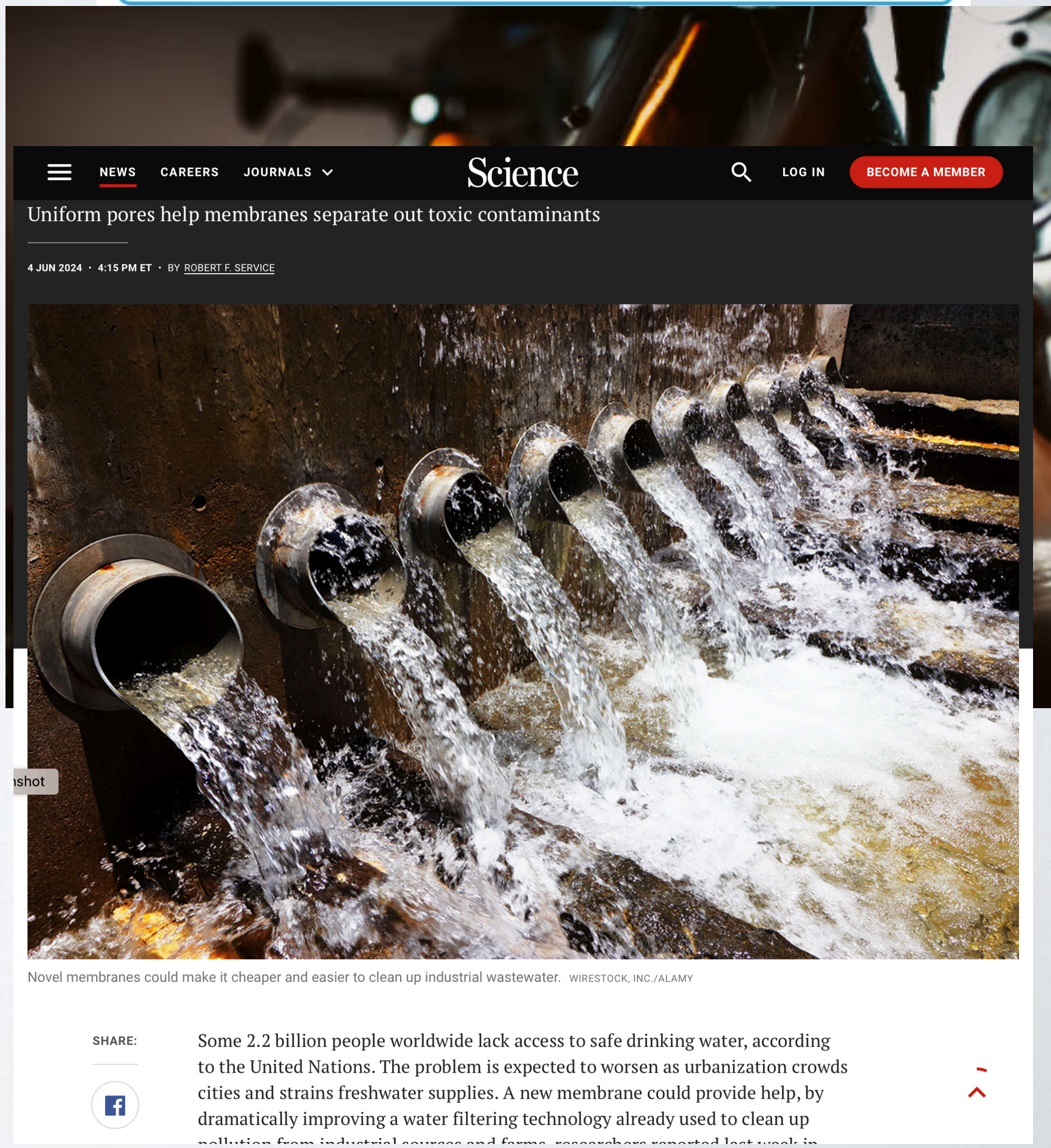
WHAT MAKES A GOOD FILTER?

- It depends
  - do we want good espresso or filter coffee?
  - do we want clean water?
  - huge number of applications
- Present approach: consider generic scenarios, and discuss how morphology of filter influences:
  - throughput: how much liquid goes through
  - concentration: how many particles from the liquid go through



NEWS CAREERS JOURNALS Science LOG IN BECOME A MEMBER

Uniform pores help membranes separate out toxic contaminants

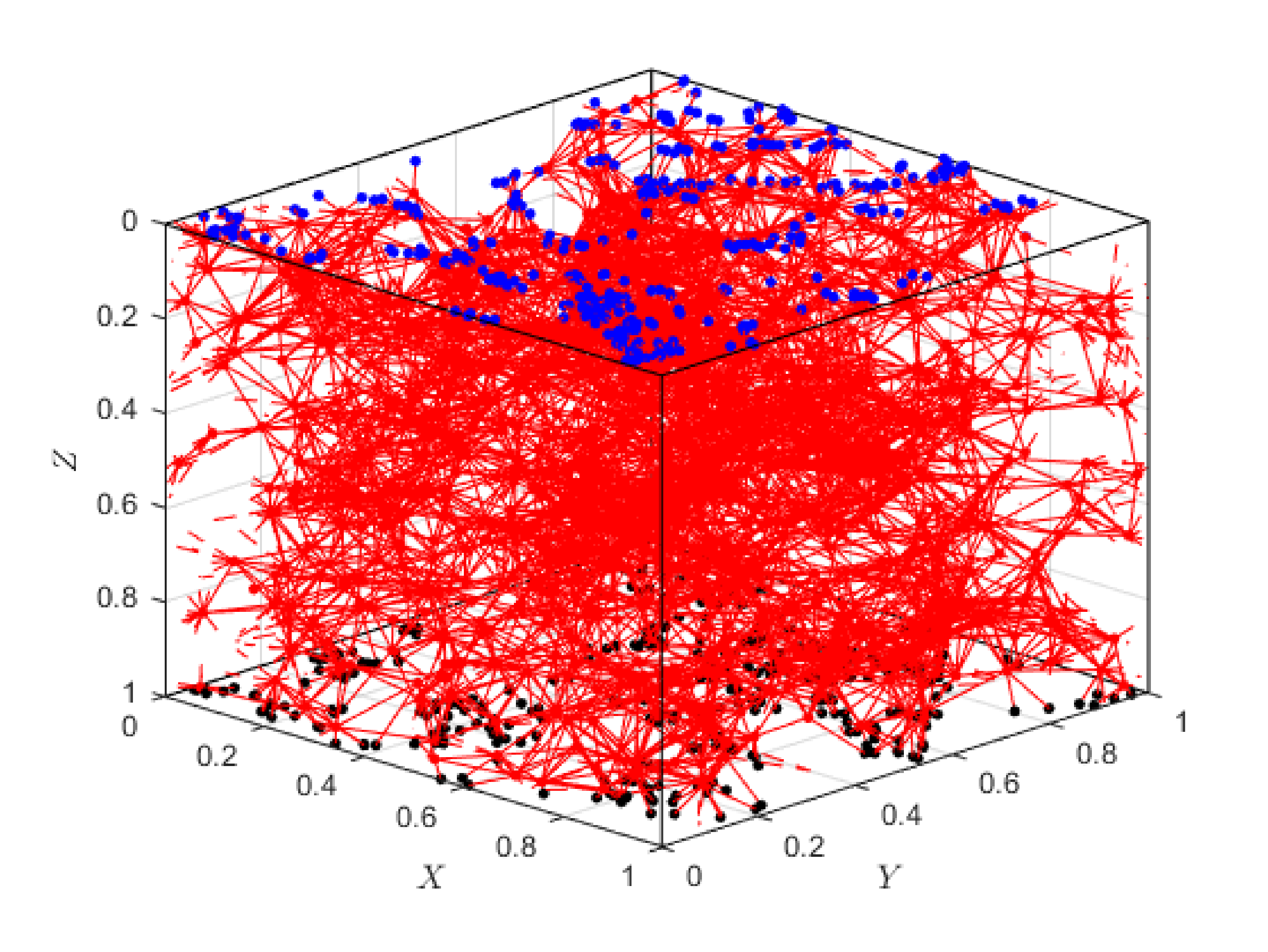
4 JUN 2024 · 4:15 PM ET · BY ROBERT F. SERVICE

Novel membranes could make it cheaper and easier to clean up industrial wastewater. WIRESTOCK, INC./ALAMY

SHARE:

Some 2.2 billion people worldwide lack access to safe drinking water, according to the United Nations. The problem is expected to worsen as urbanization crowds cities and strains freshwater supplies. A new membrane could provide help, by dramatically improving a water filtering technology already used to clean up

MODELING FILTRATION: MAIN IDEA

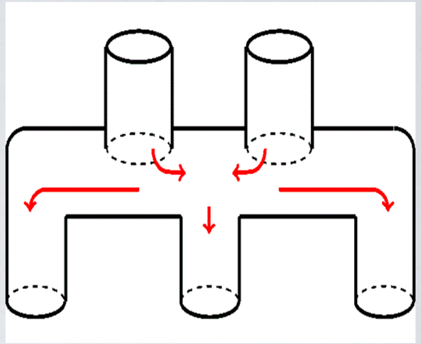


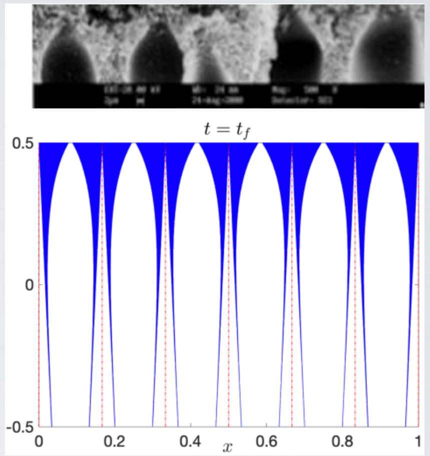
- Network model of a filter: set of connecting pores
- Fluid + particles flow in from the top, out through the bottom
- Flow governed by simplified fluid dynamics based approach
- Particles from the fluid absorbed by the pores whose size decrease in the process
- Flow stops when there is no open part from top to bottom

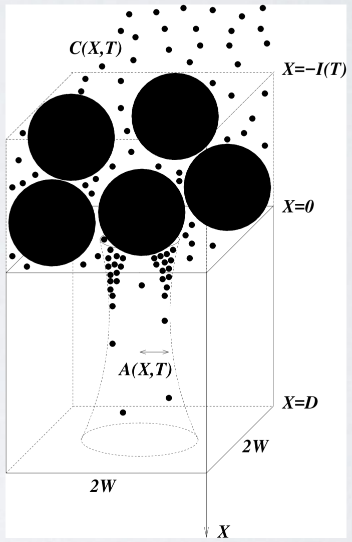
  - Important: Efficiency: can simulate 1000's of realization with modest computing resources
  - Main question: how do properties of the network influence filtration performance such as throughput and output particle concentration

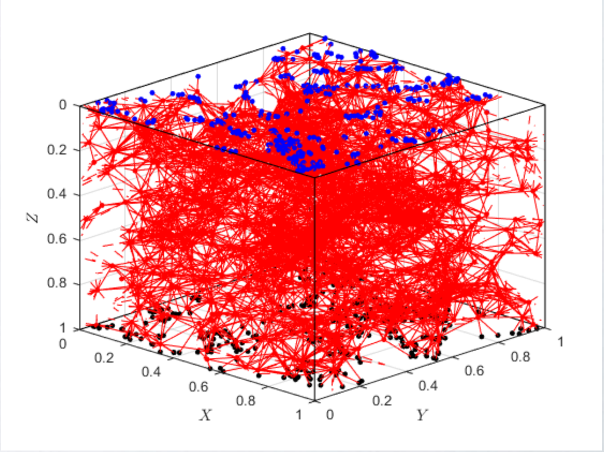
RECENT WORKS

- Influence of pore connectivity on filter performance: *J. Fluid Mech. (2020)*
- Modeling and design of pleated membrane filters: *Phys. Rev. Fluids (2020)*
- Membrane filtration with multiple fouling mechanisms: *Phys. Rev. Fluids (2019)*
- Network-based modeling of filtration: uniform pores: *SIAM Journal of Applied Mathematics (2022)*
- Network-based modeling of filtration: non-uniform pores: *J. Membrane Science (2022)*
- Network-based modeling of filtration: layered filters: *Phys. Rev. Fluids (2023)*
- Topology versus geometry in the context of filtration: *Phys. Rev. E (2026)*
  - Review: *ARFM (2026)*









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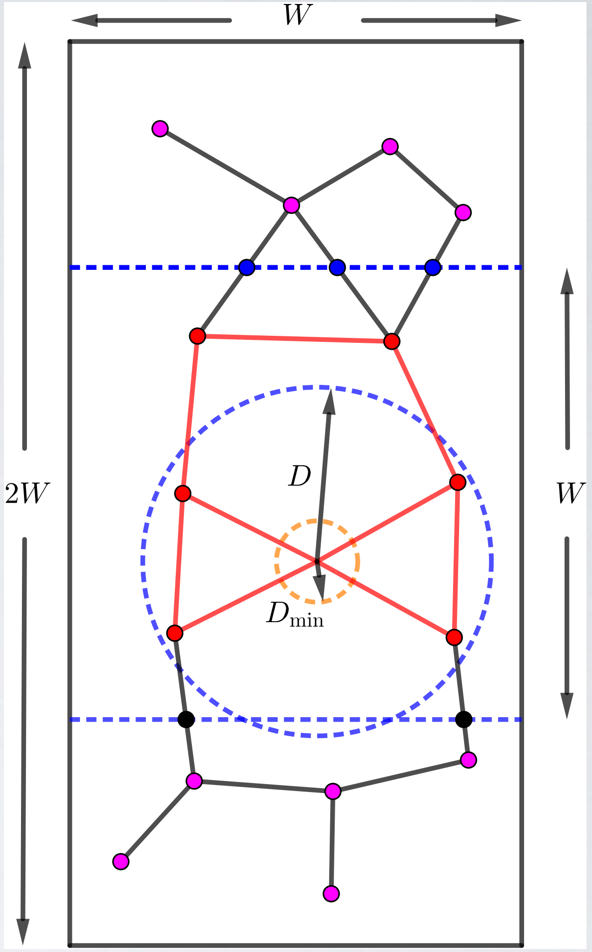
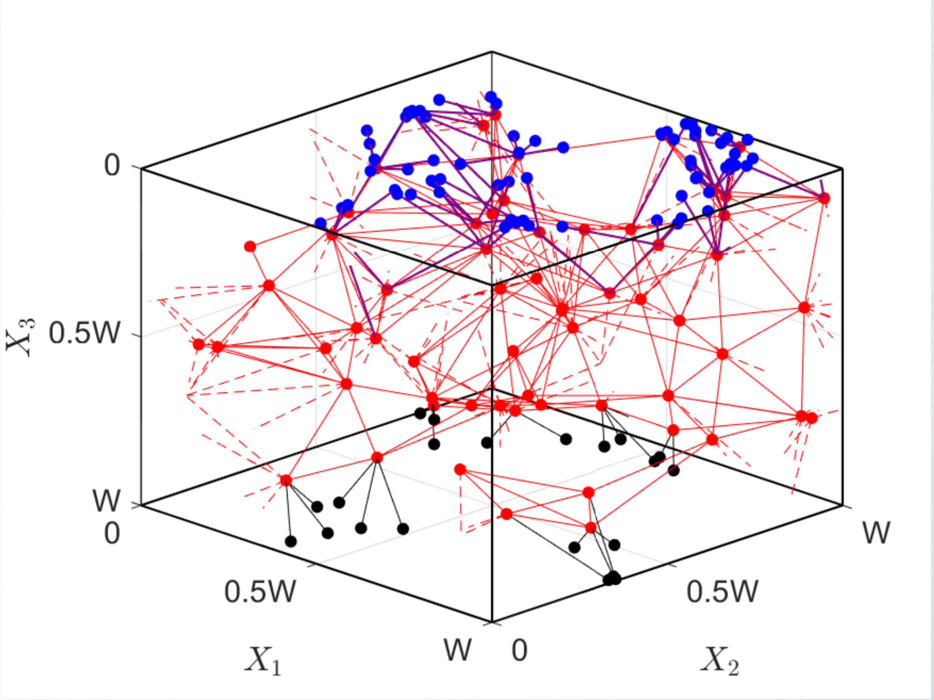
SETUP OF A FILTER: NETWORK

- Network: randomly distributed nodes
- Nodes at the distance less than a search distance D (parameter in the problem) connected by pores of radius R
- To simplify fluid flow modeling, the pore length has to be larger than some minimum distance, D_{min} such that $R \ll D_{min}$
- Domain cut at top and bottom to leave cubic domain of length size W
- Inlets and outlets defined as intersection of the pores with the top/bottom cuts
- The domain boundaries (left/right) usually considered as periodic
- Number of nodes and search distance D determine the porosity of the filter





SETUP OF A FILTER: FLUID FLOW

- Hagen - Poiseuille model, connecting flux Q and the pressure drop ΔP via conductance K

$$Q = K \Delta P, \quad K = \frac{\pi R^4}{8 \mu A}$$

- The pressures at the top and bottom are prescribed, and at the interior nodes solved using flux conservation at each node
    - done by formulating adjacency matrix and corresponding graph Laplacian leading to system of linear algebraic equations for pressure at each node *(Gu, LK, Cummings, SIAM Journal of Applied Mathematics (2022))*
- Once pressures are found, fluid fluxes can be calculated
- Note that each network configuration needs to be solved separately
- Efficient calculations allow for computing flow though many (thousands) of networks using very reasonable computational resources

SETUP OF A FILTER: FOULANT ADSORPTION

- Fluid is assumed to carry particles of a specified concentration
- Concentration satisfies (steady state) advection equation with specified value at the inlet nodes
- Pore radii decrease due to foulant adsoption
- Filter lifetime is reached when outflow flux drops to zero (no open path from top to bottom of the filter)

$$Q\frac{\partial C}{\partial Y} = -\Lambda R C, \quad 0 \le Y \le A,$$

$$C\left(0, T\right) := C_{\mathrm{up}}\left(T\right)$$

$$\frac{dR}{dT} = -\Lambda \alpha C_{\mathrm{up}}\left(T\right), R\left(0\right) = R_0$$

$\alpha \sim$ particle volume

ANALYSIS OF THE RESULTS: SCALING

- To simplify interpretation, use nondimensional quantities

$$A_{ij} = W a_{ij}, \quad (R_{ij}, R_{ij,0}) = W\,(r_{ij}, r_{ij,0})\,,$$

$$P_i = P_0 p_i, \quad (C_i, C_{ij}) = C_{\text{top}}\,(c_i, c_{ij})\,,$$

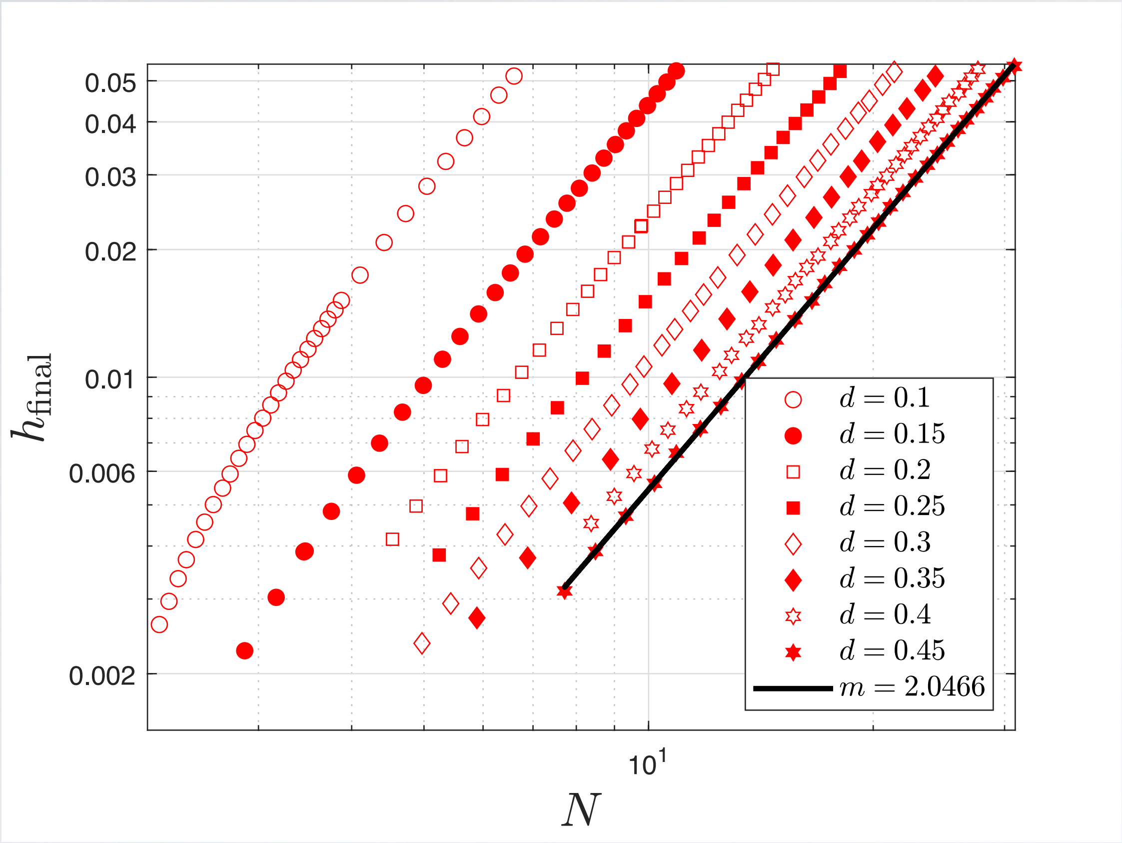
$$\Lambda = \frac{\pi W P_0}{8\mu}\lambda, \quad T = \frac{W}{\Lambda \alpha C_{\text{top}}} t$$

ANALYSIS OF THE RESULTS: PERFORMANCE METRICS

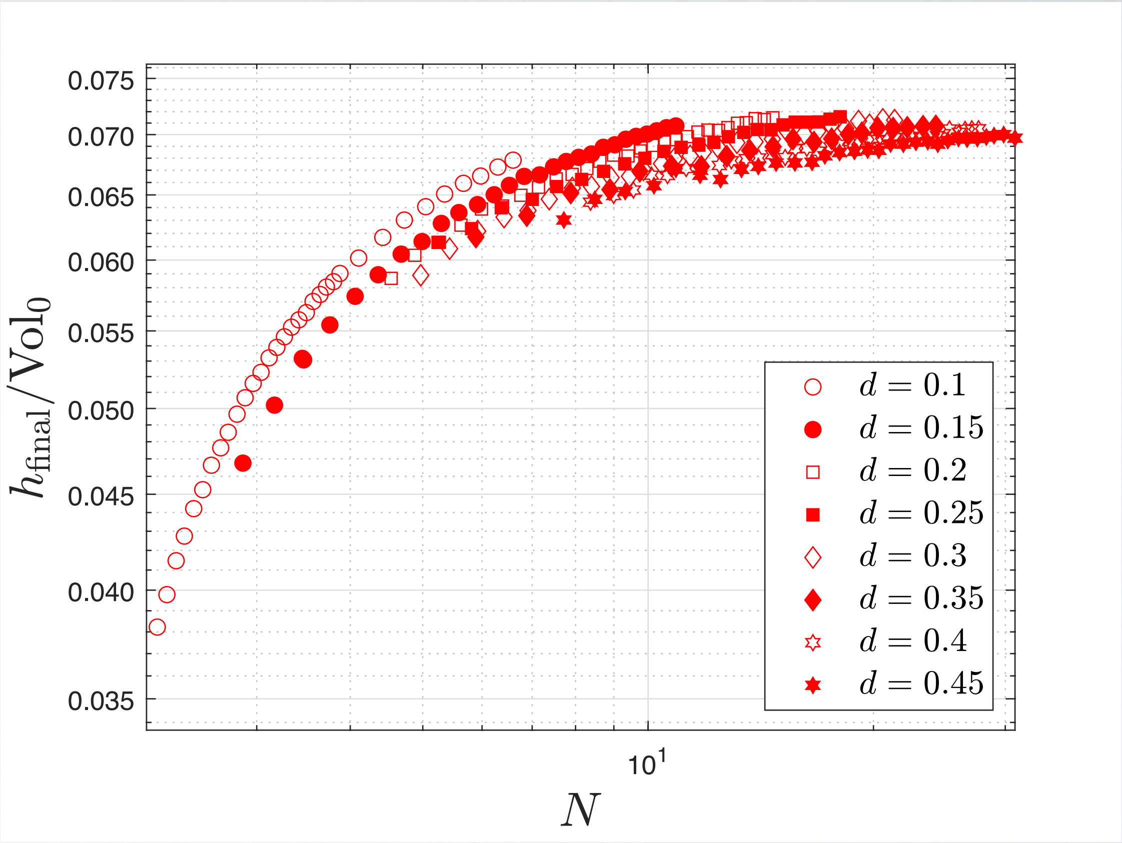
- We will consider the following quantities
  - throughput: the amount of fluid passing through the filter before it clogs h
  - (total) concentration of the foulant concentration at the outlet C
  - initial membrane porosity Vol_0
  - tortuosity: typical path length that particles take from top to bottom of the filter τ

RESULTS I: UNIFORM PORES (I)

throughput



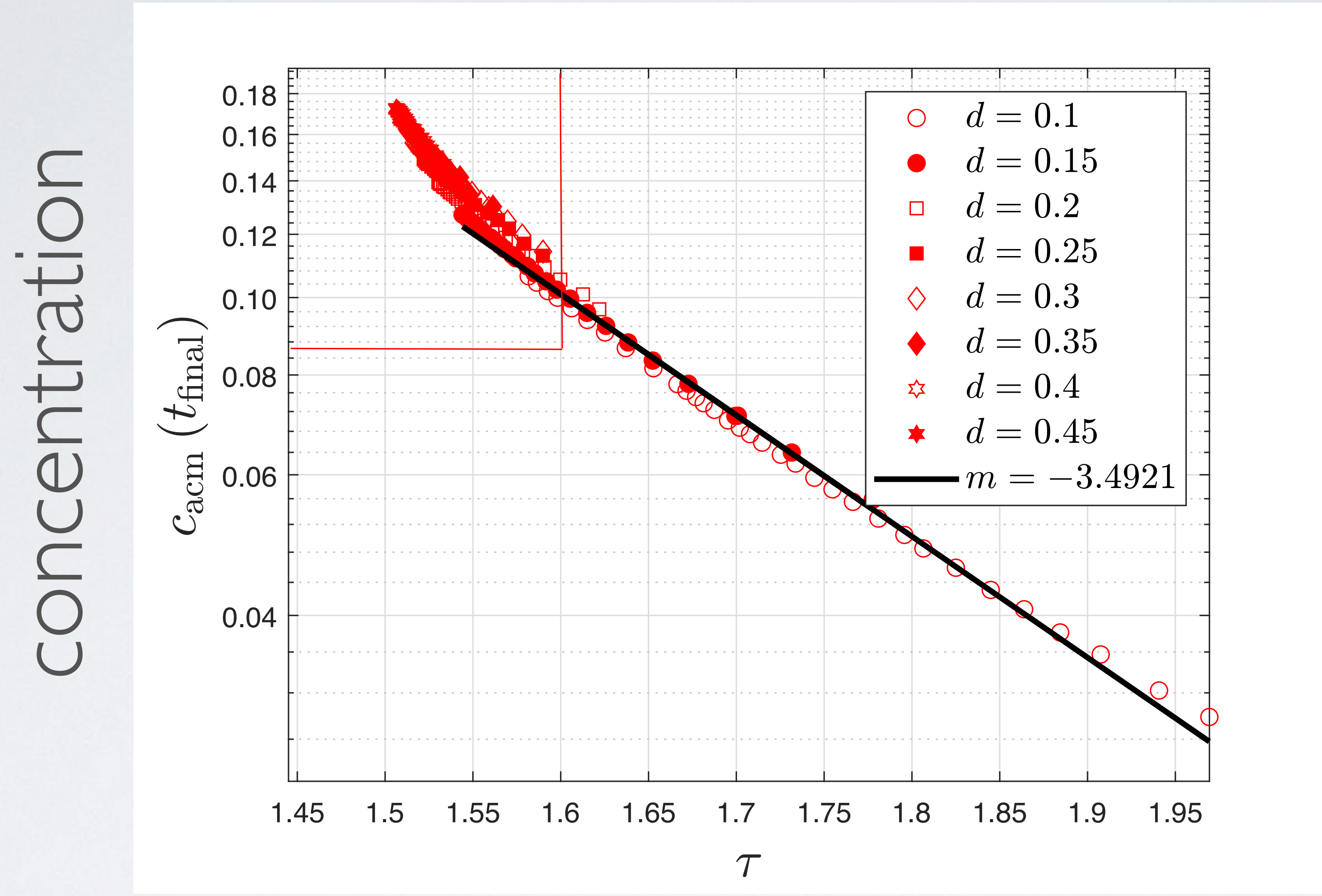
throughput/porosity



N : number of neighbors

- Given N, shorter pores lead to larger throughput
- When normalized by porosity, the dependence on pore length almost disappears

RESULTS I: UNIFORM PORES (4)



Note: porosity varies

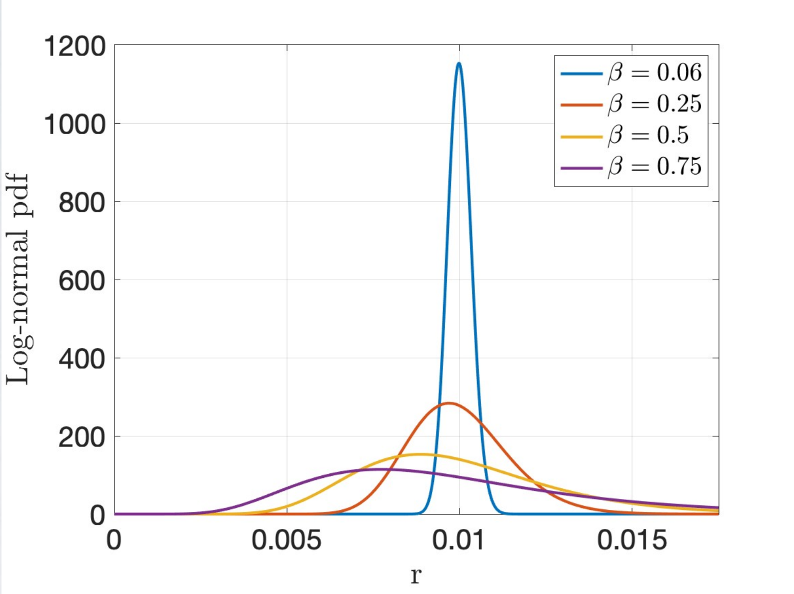
τ : tortuosity

- When considering concentration as a function of τ the results nicely collapse (it turns out that porosity plays a crucial role here since it influences strongly both tortuosity and concentration)

RESULTS II: NON-UNIFORM PORES

- Now, allow the pore size to vary randomly using a given distribution (log-normal and uniform distribution explored)
  - ask the following questions:
    - which stochastic component is more relevant: variation of networks (pore connectivity) or of noise (pore radii)?
    - Is variability of the pore size beneficial to filtration performance?
    - For answers obtained using similar measures as the ones implemented for uniform pores see *Gu, LK, Cummings, J. Memb. Sci. (2022)*
    - Here: focus on the discussion of topology based measures

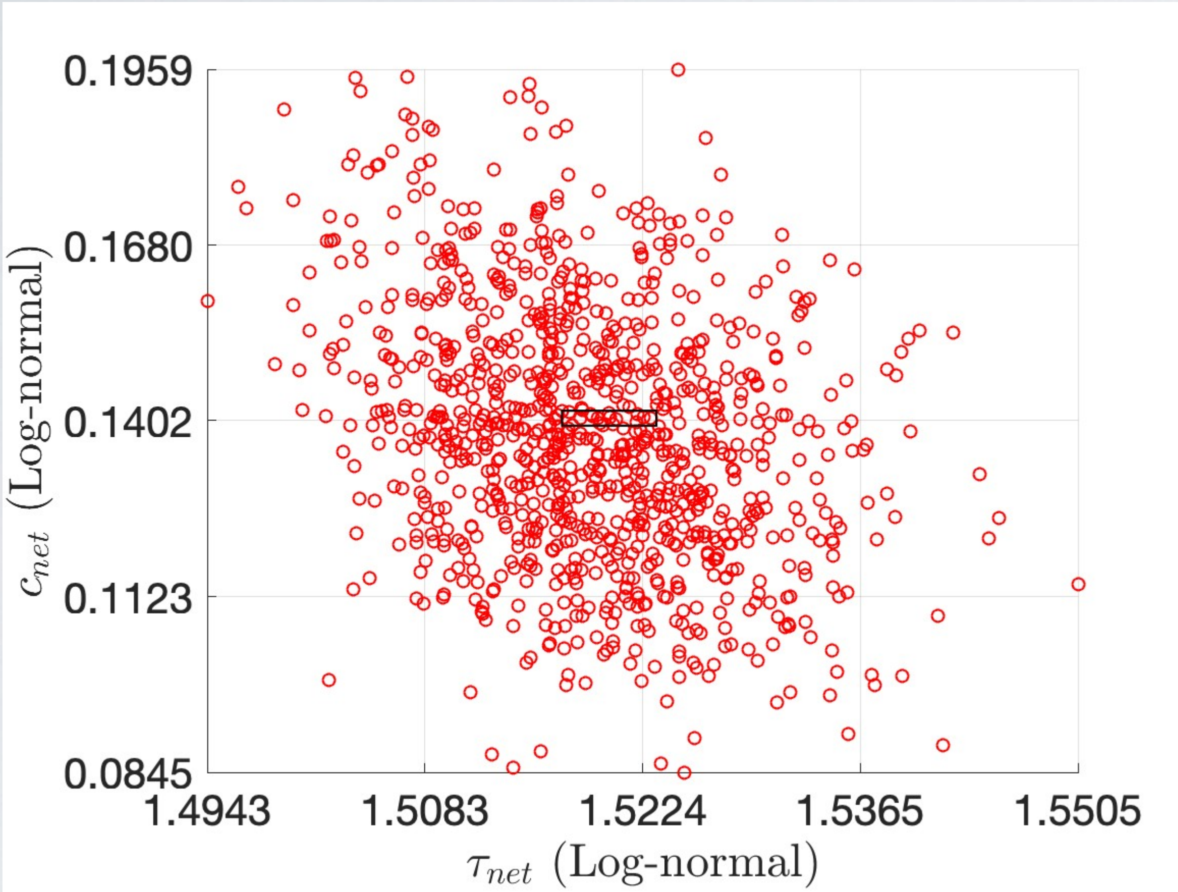
FOCUS:



- Consider fixed porosity of 0.6
- Consider the log-normal distribution of pore thicknesses
- *Main questions*:
  - is tortuosity still a useful variable describing filter performance?
  - does the networks' topology correlate with the filtration properties, such as particle concentration?
  - To be able to answer the second question, we need to be able to *quantify the topology of the pore networks*: for this purpose we use the measures discussed next and applied to the pores at their initial state (before starting the flow and absorption)

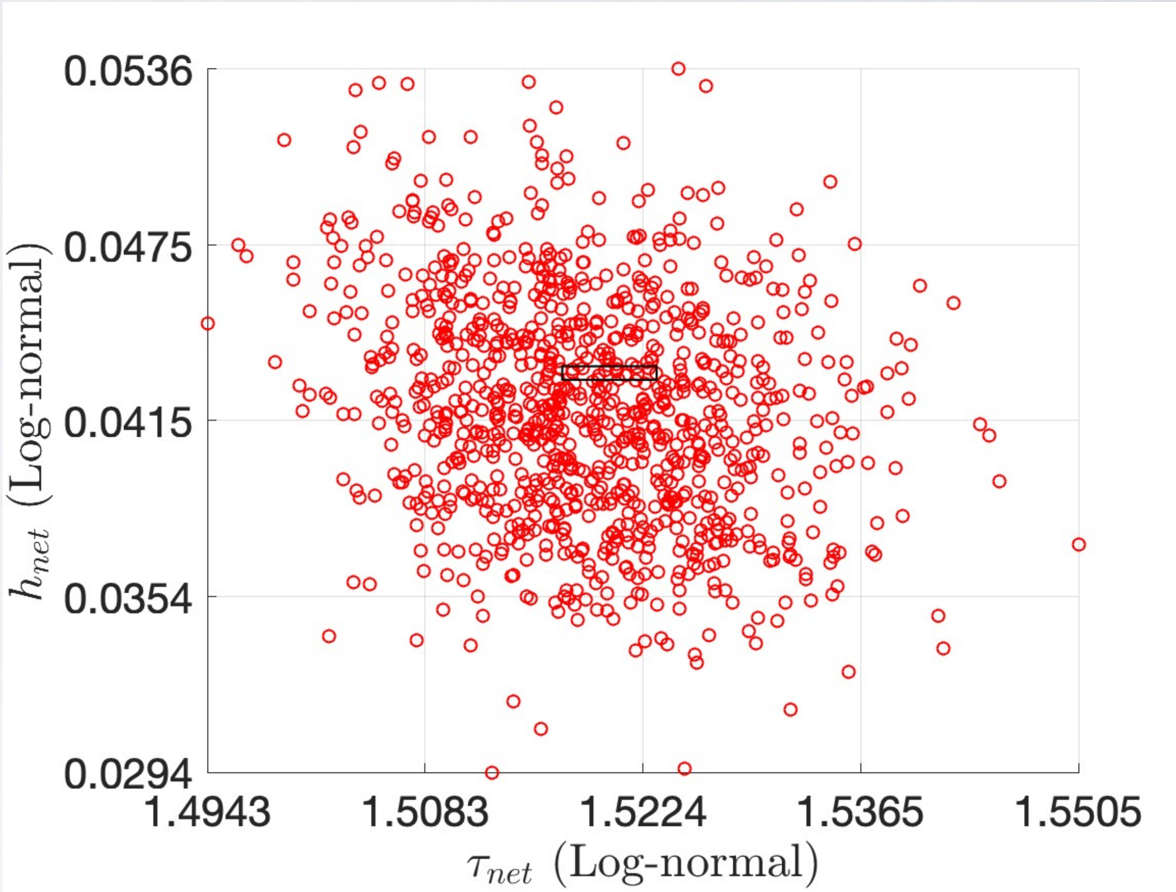
RESULTS: CONCENTRATION AND THROUGHPUT VERSUS TORTUOSITY

concentration



tortuosity

throughput



tortuosity

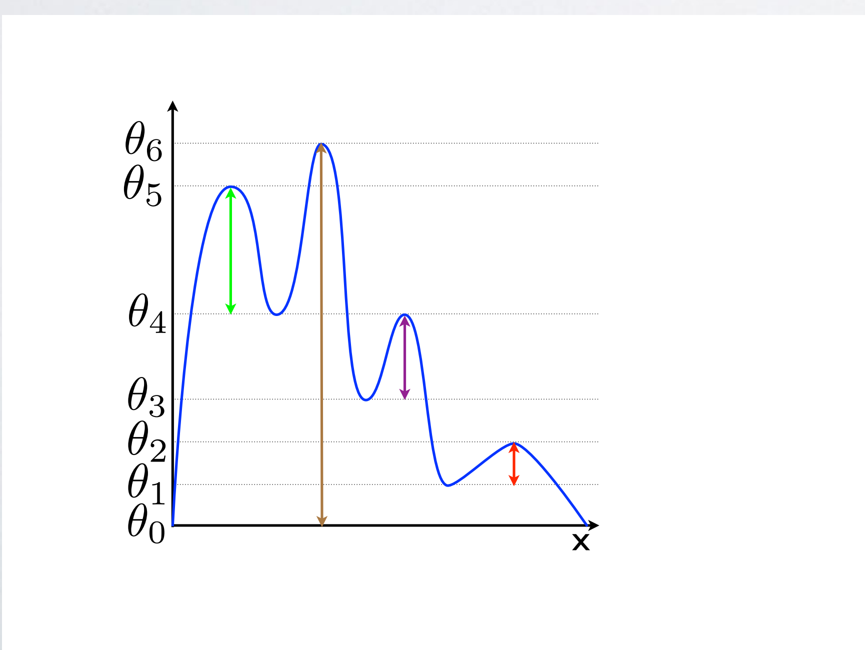
- Tortuosity is not a good measure for the considered networks (recall different results for variable porosity; for fixed porosity (0.6 for this and following slides), these results show that *tortuosity does not provide good insight regarding filter performance*)

Illingworth, Gu, Cummings, LK, PRE 2026

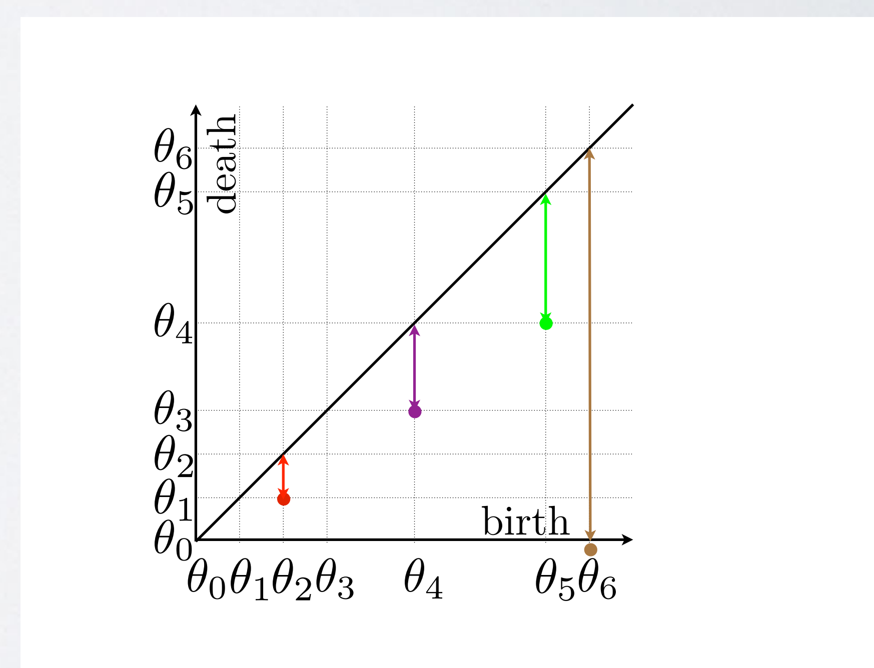
TOPOLOGICAL DATA ANALYSIS & PERSISTENT HOMOLOGY: 1D TOY EXAMPLE

- 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 pores the word `persistence' is meant in terms of pore thicknesses: over which range of thicknesses a certain topological feature (chain, loop) persists?

Toy example in 1D
f(x)
x: space
f: pore thickness

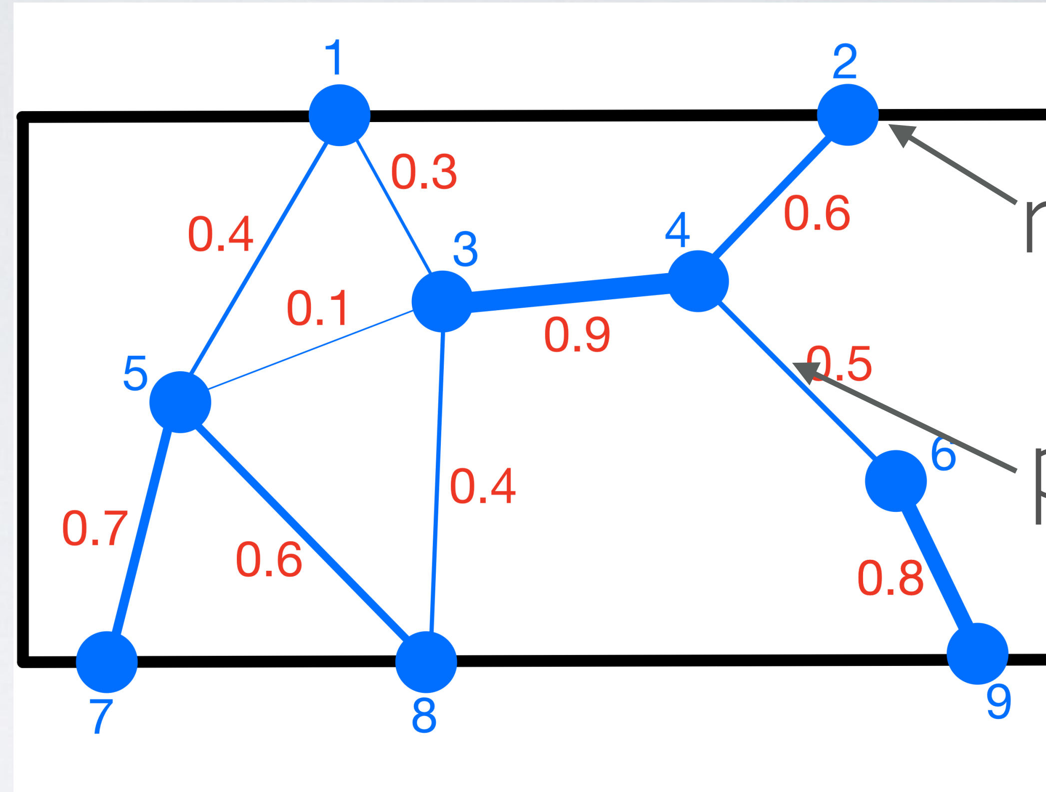


Persistence diagram (PD) describing main features of f(x)



TOPOLOGICAL DATA ANALYSIS APPLIED TO NETWORKS

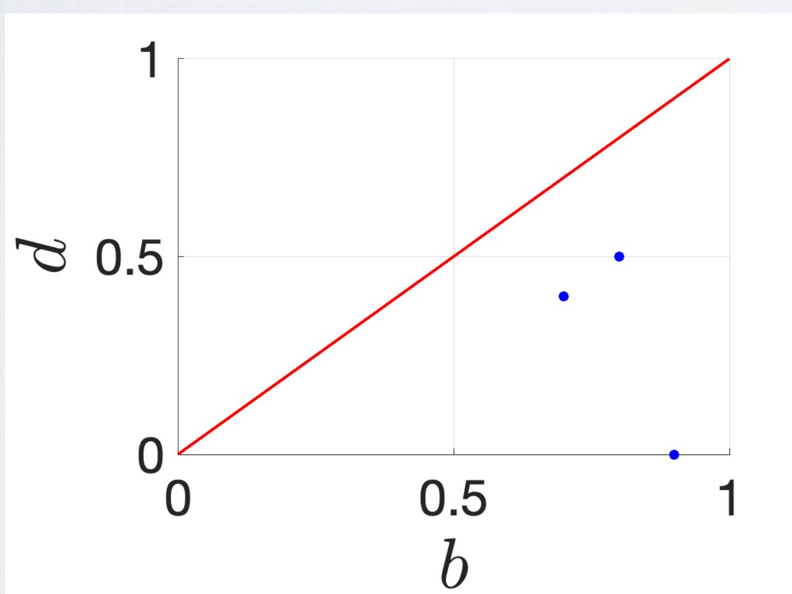
example: weighed network with pore width illustrated by numerical values



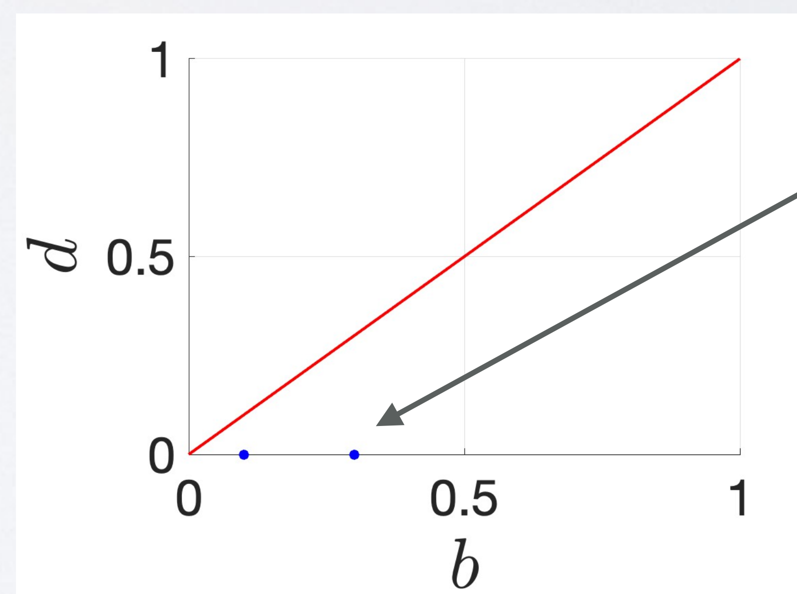
nodes

pores

Persistence diagrams:



PD 0 (open components)



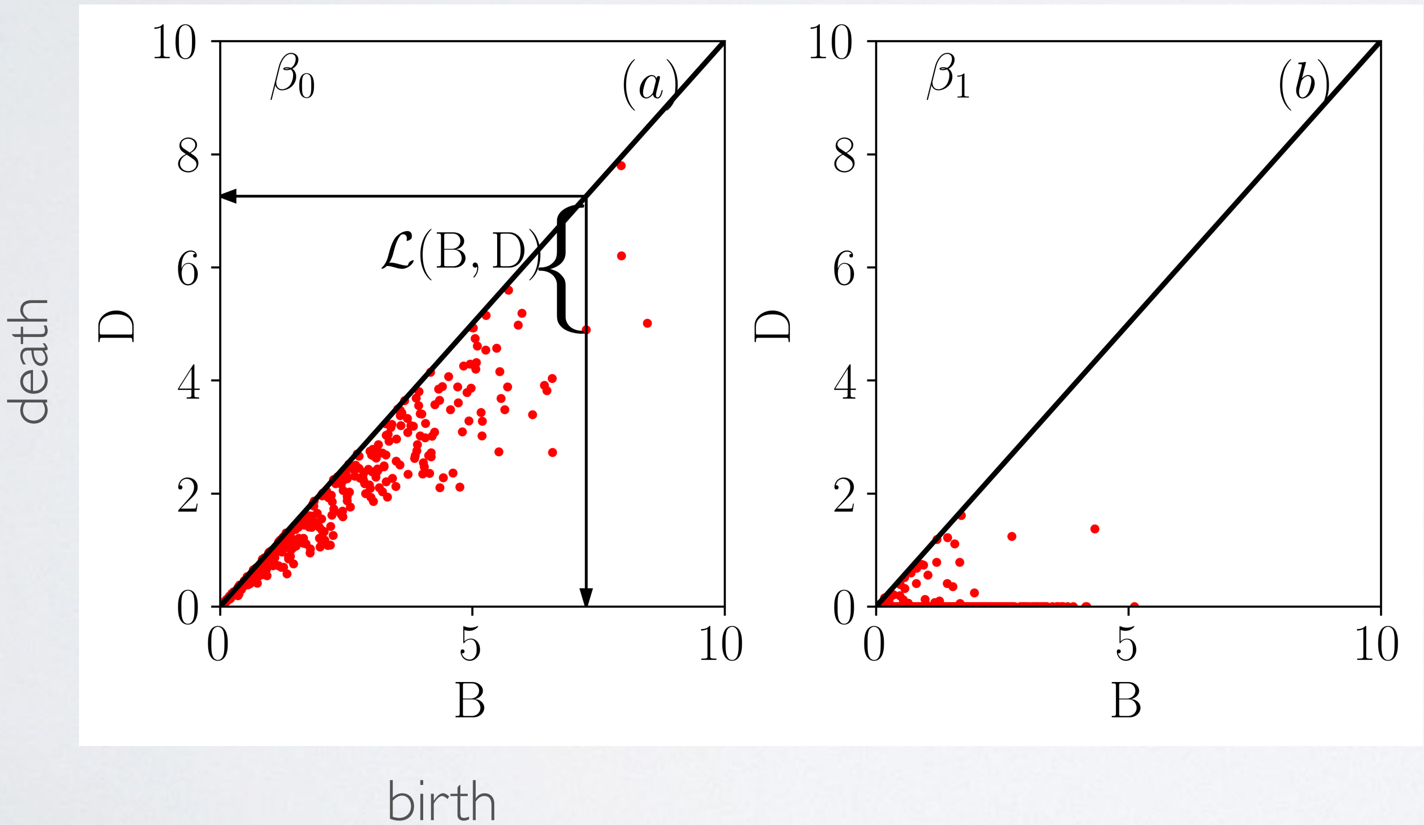
`generators'

PD 1 (loops/cycles)

From weighted network to point clouds

PERSISTENT HOMOLOGY: MEASURES

- Persistence diagrams (PDs) describe complex weighted network in terms of point clouds
- Further data reduction:
  - Compress point cloud to few numbers



components/chains (0)

loops/cycles (1)

NG: number of generators

Lifespan: average distance to the diagonal

TP: total persistence, sum of all lifespans

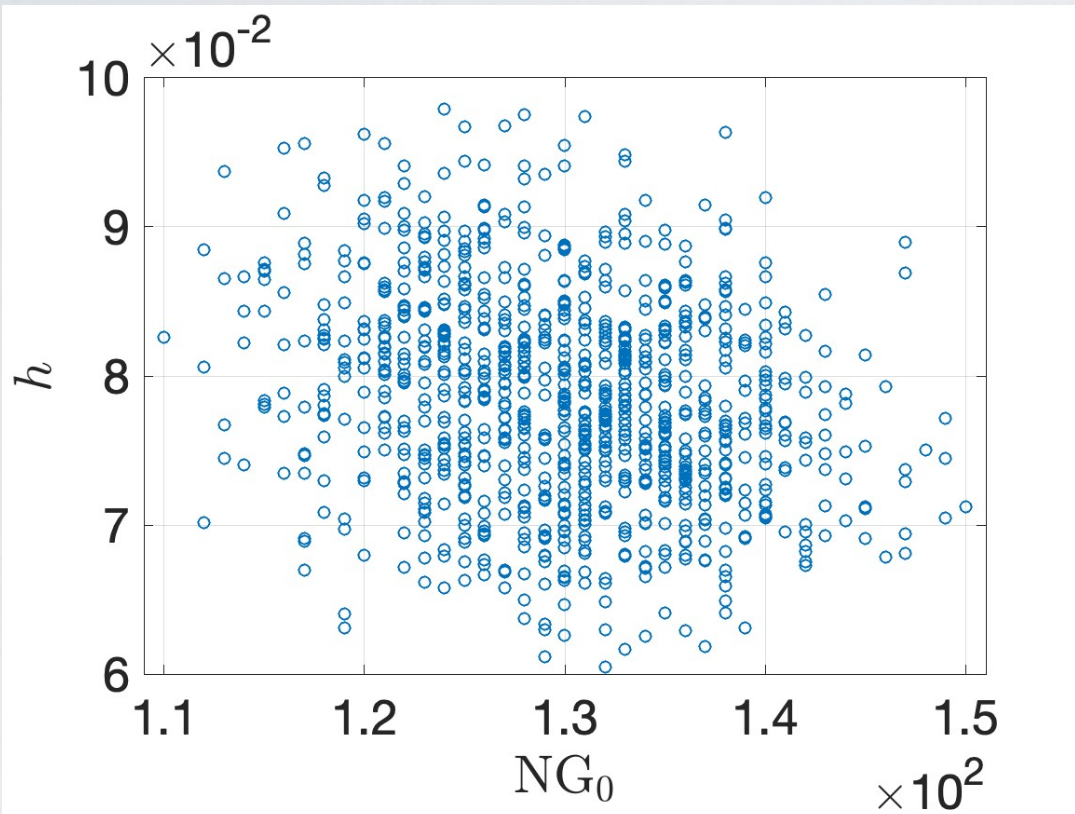
Kaczynski, Mischaikow, Mrozek, Computational Homology

Kramar, LK, Mischaikow, Physica D (2014)

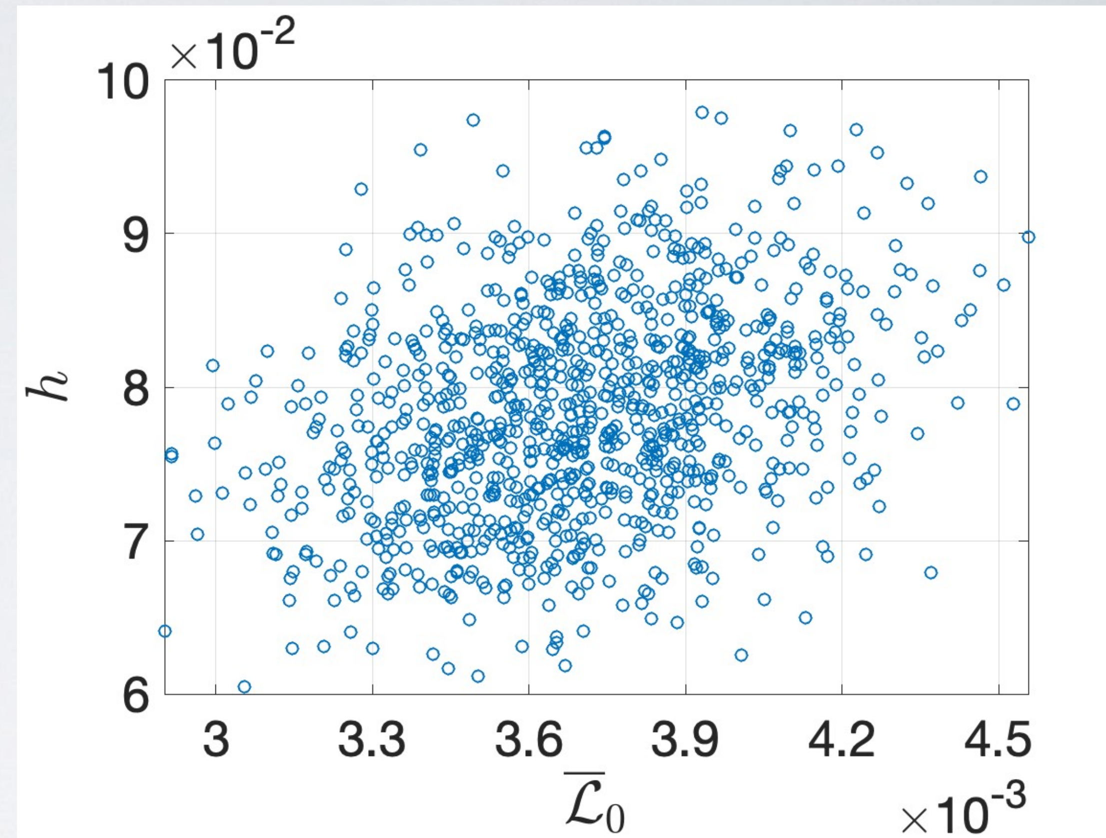
Computations: Gudhi Library, INRIA

RESULTS: THROUGHPUT VERSUS (OPEN) COMPONENTS

throughput



number of generators

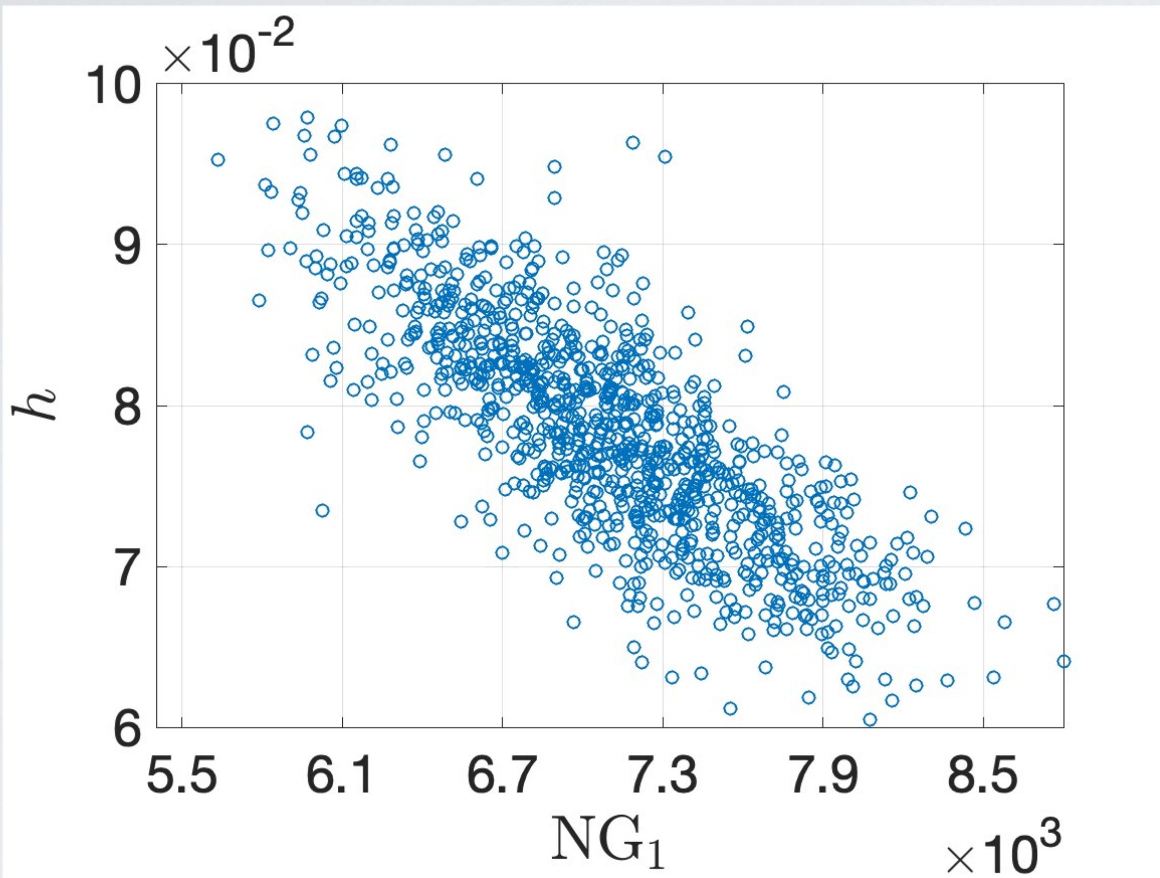


lifespan

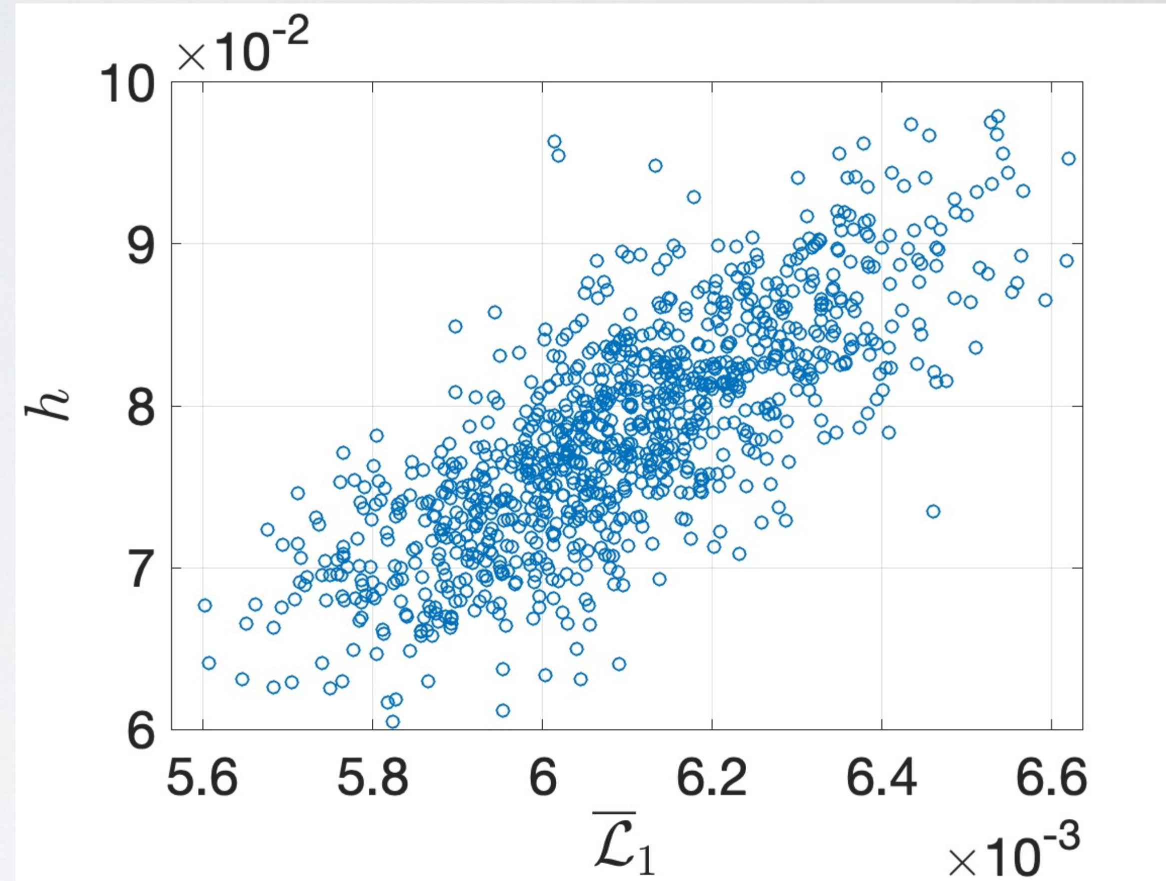
- No correlation!
- Are topological measures actually useful?

RESULTS: THROUGHPUT VERSUS LOOPS

throughput



number of loops



loop lifespan

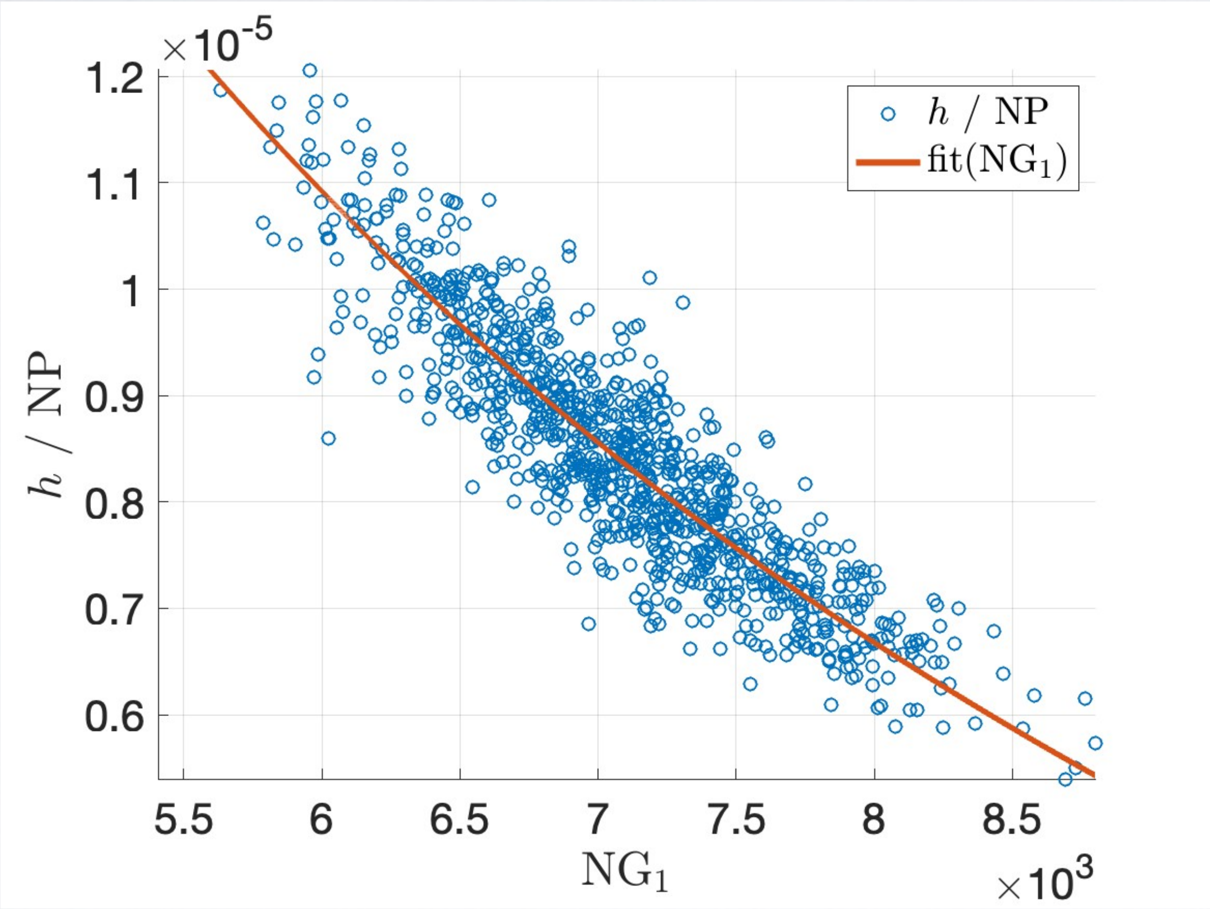
- Correlation!
- Topological measures describing loops can be correlated with throughput!

But: is it topology or geometry that matters?

GEOMETRY VERSUS TOPOLOGY

- Scale throughput by number of pores (NP) and ask how it depends on number of loop generators

throuphput/no. of pores



number of loops

- Topology matters!

Illingworth, Gu, Cummings, LK
PRE 2026

- fit: obtained by assuming linear relation between the number of pores and number of loop generators

CONCLUSIONS

- Modeling a filter as a network of connected pores allows for efficient computation of both flow and the adsorption of particles
- Ability to carry out large number of realizations permits the use of statistical analysis to identify the important parameters in the problem
- *Topological measures allow for correlating initial filter morphology and its performance: `loopiness' of the filtration networks appears to be particularly useful measure*
  - Future work:
    - consider time-dependent topological measures and their correlation with filtration performance
    - consider clogging and its influence on the time-dependent network topology
    - *think of other systems such that important insight can be reached by considering topology of the interactions, in particular in the context of weighted networks*

Thank you for listening

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