Simulation and Analysis of Self-Assembled Silver Nanowires

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Roshell Lamug, California State University, Long Beach

Christof Teuscher, Portland State University

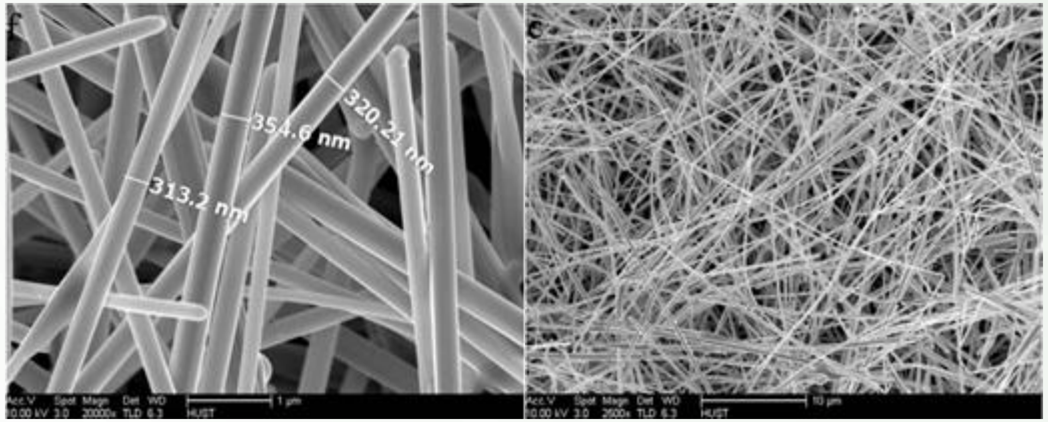
Portland State UNIVERSITY

teuscher.:Lab
teuscher-lab.com

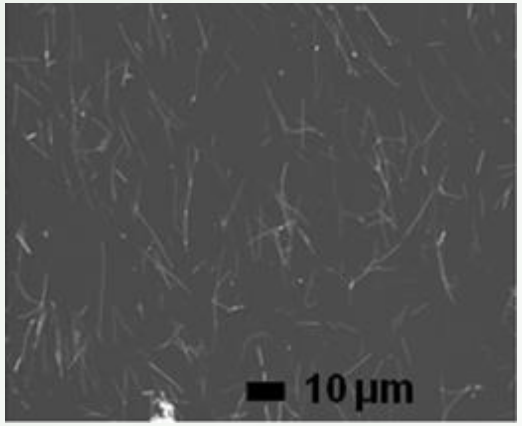
CALIFORNIA STATE UNIVERSITY LONG BEACH 1949

What are self-assembled nanowires?

- Self-assembled nanowires – nanoscale rod or tubes that are synthesized
  - Most commonly done by deposition in a solution, chemical reduction, or aggregation of polymers
- These nanowires are looked towards assembling the wires of chips



FSEM images of silver nanowires prepared with different concentrations of Na_2S at fixed temperature of T = 160 °C: (a,b) 0.3 mM[1]



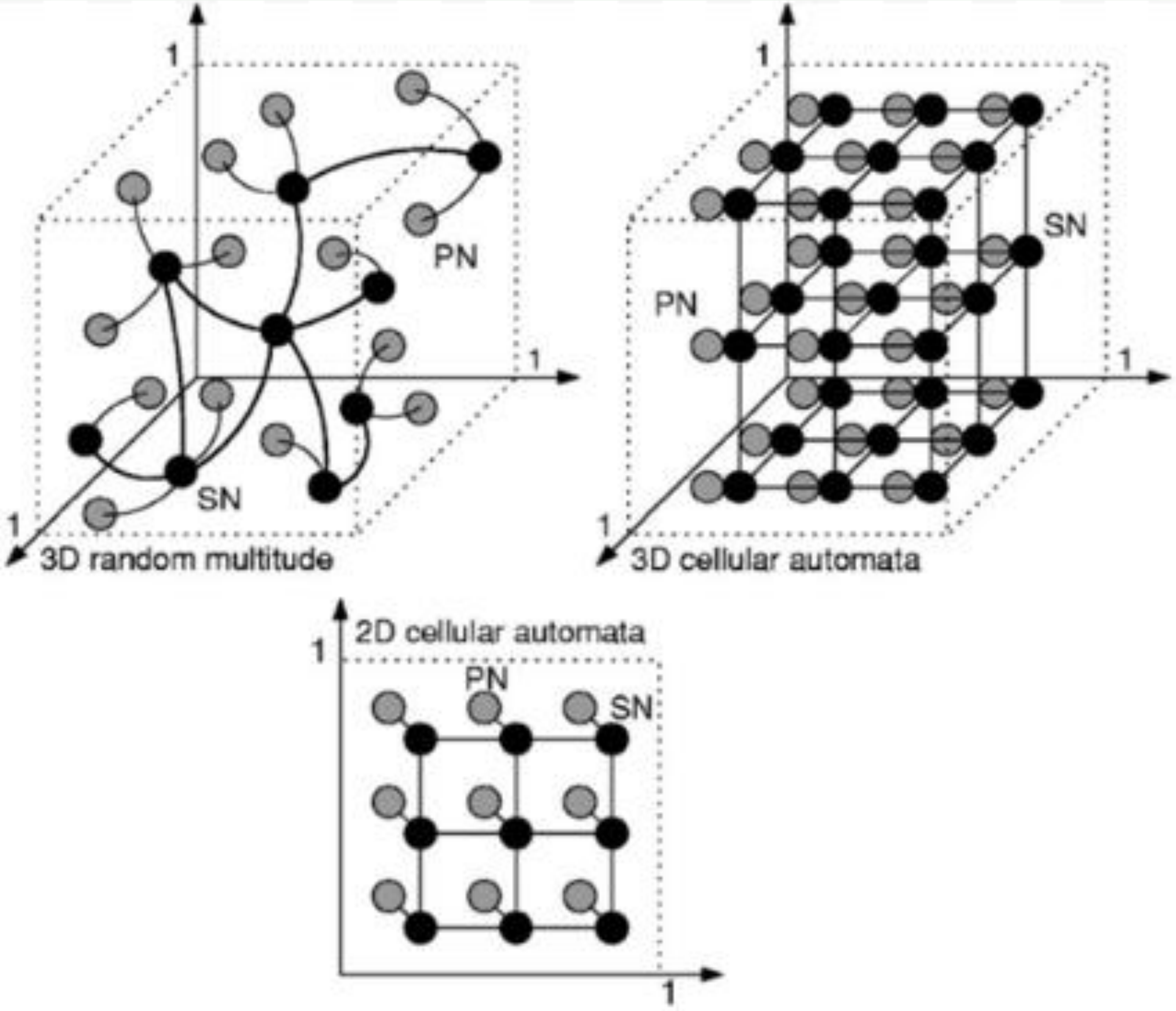
SEM images of aliquots taken at 60 min[2]

1 D. CHEN, X. QIAO, X. QIU, J. CHEN, AND R. JIANG, "CONVENIENT SYNTHESIS OF SILVER NANOWIRES WITH ADJUSTABLE DIAMETERS VIA A SOLVOTHERMAL METHOD," *J. COLLOID INTERFACE SCI.*, VOL. 344, NO. 2, PP. 286–291, APR. 2010.
2 W. M. SCHUETTE AND W. E. BUHRO, "POLYOL SYNTHESIS OF SILVER NANOWIRES BY HETEROGENEOUS NUCLEATION; MECHANISTIC ASPECTS INFLUENCING NANOWIRE DIAMETER AND LENGTH," *CHEM. MATER.*, VOL. 26, NO. 22, PP. 6410–6417, 2014.

Nanowires for Chips and Why Consider Them

- The eventual plateau of electronics: why new solutions are needed for progress
  - Shrinking size does not necessarily mean better performance
- Network-on-Chip – is an advanced scheme for organizing communication between operating modules located on the same chip.
- Why self-assembly: Nature has evolved optimized systems under limited resources and various other physical constraints[3]
  - We are looking for cost-friendly and fabrication-friendly solutions

3 C. TEUSCHER, "NATURE-INSPIRED INTERCONNECTS FOR SELF-ASSEMBLED LARGE-SCALE NETWORK-ON-CHIP DESIGNS," *CHAOS*, VOL. 17, NO. 2, 2007.



Three different interconnect topologies for Network-on-Chip[3]

Project Goal

- To simulate accurate models of silver nanowire and investigate properties of self-assembled interconnect fabrics of different length distributions for emerging nanoscale electronics.
  - The bigger goal: To be able to self-assemble well-performing Network-on-Chips that require the least amount of wires
  - All research is done on MATLAB, a numerical computing environment and programing language developed by MathWorks.

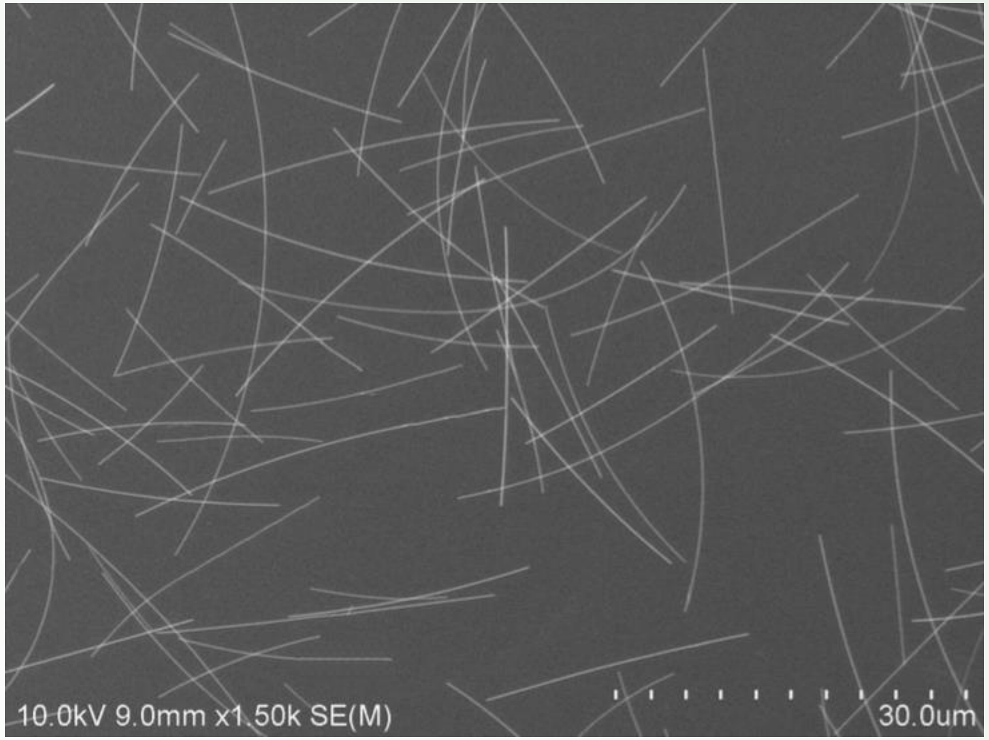
Methodology

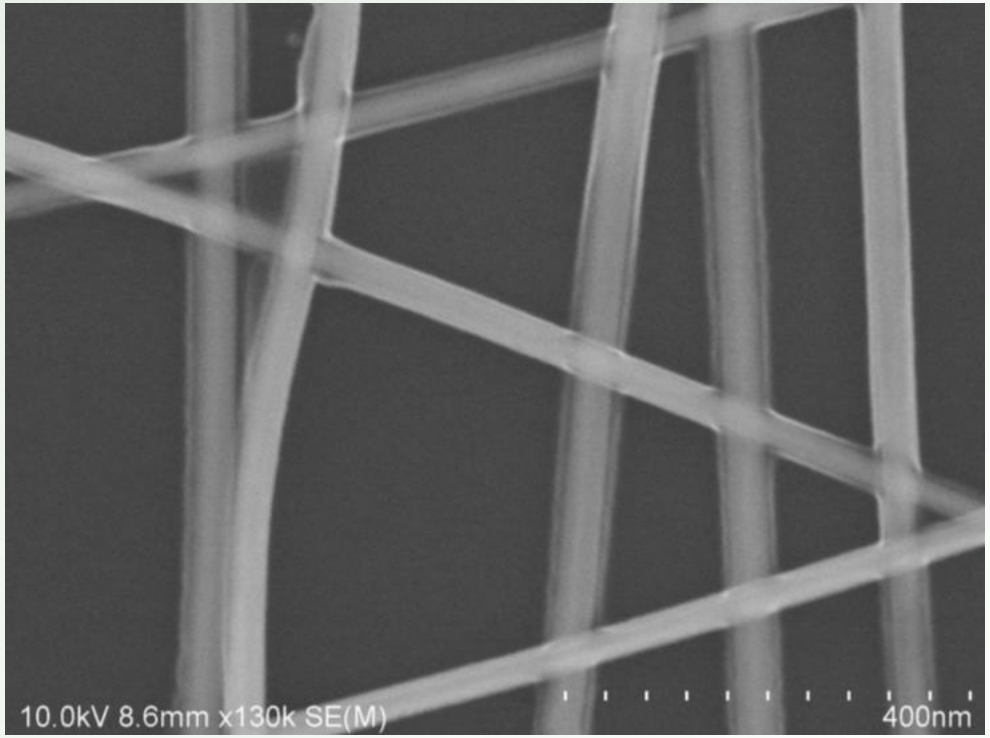
1. Visualizing the Experiment: Understanding the growth of silver nanowires
2. Generating the Model: Creating networks of wires with user-defined parameters
3. Analyzing the Model: Measuring shortest average path and wiring cost
4. Quantifying the Models: Deducing experimental parameters to create optimized application-specific Networks-on-Chips

Step 1: Visualizing the Experiment

- To generate an accurate model, the general structure and trends of silver nanowires are researched.
- Key Properties noted:
  - General direction of growth
  - Curvature
  - Wonky-ness

Visualizing the Model: Direction of Growth and Curvature

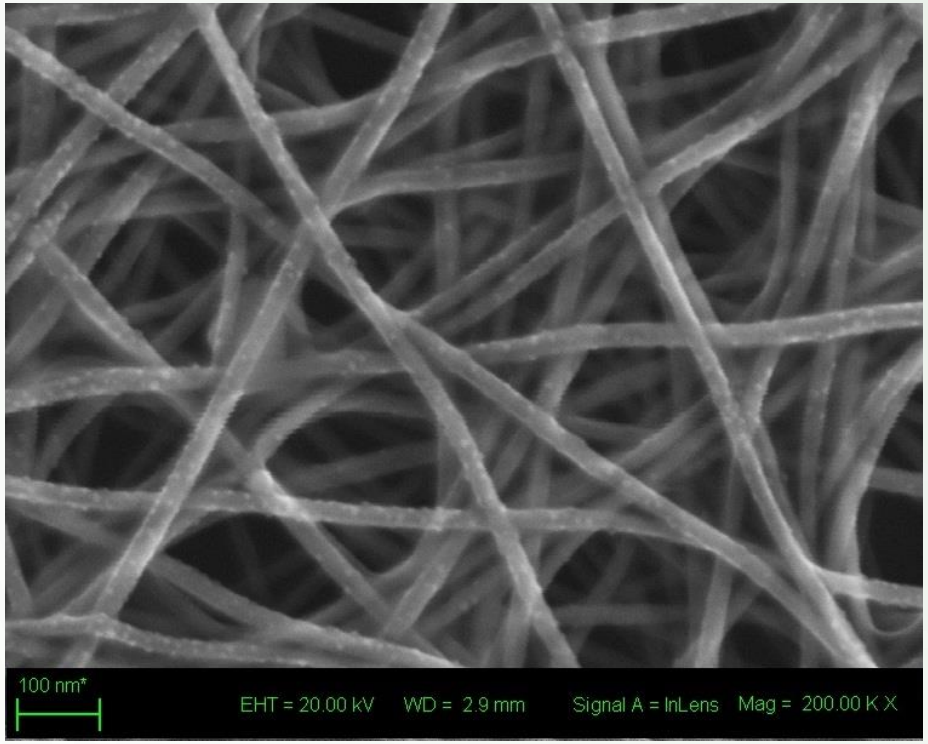




SEM images of silver nanowires (avg diameter: 40nm, length: 20-60nm, silver purity: 99.5%, concentration:20 mg/ml)

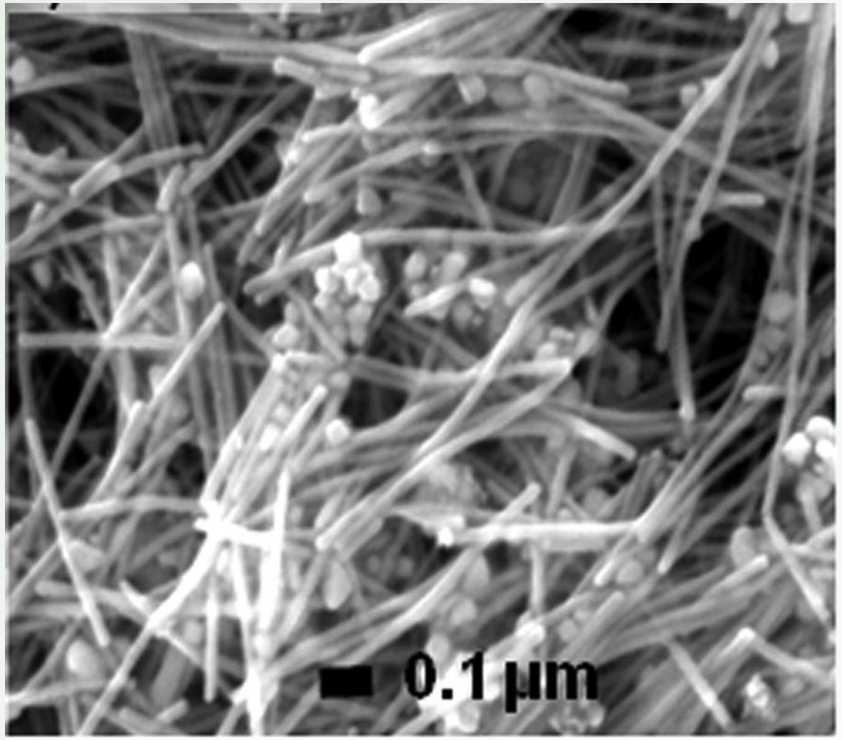
Courtesy of ACS Material
https://www.acsmaterial.com/silver-nanowire-500mg-4371.html

Visualizing the Model: Wonky-ness



SEM images of silver nanowires (diameter: 17 nm).

Courtesy of Zhejiang Kechuang Advanced Materials Co.
http://www.ke-chuang.com/productshow.asp?id=93

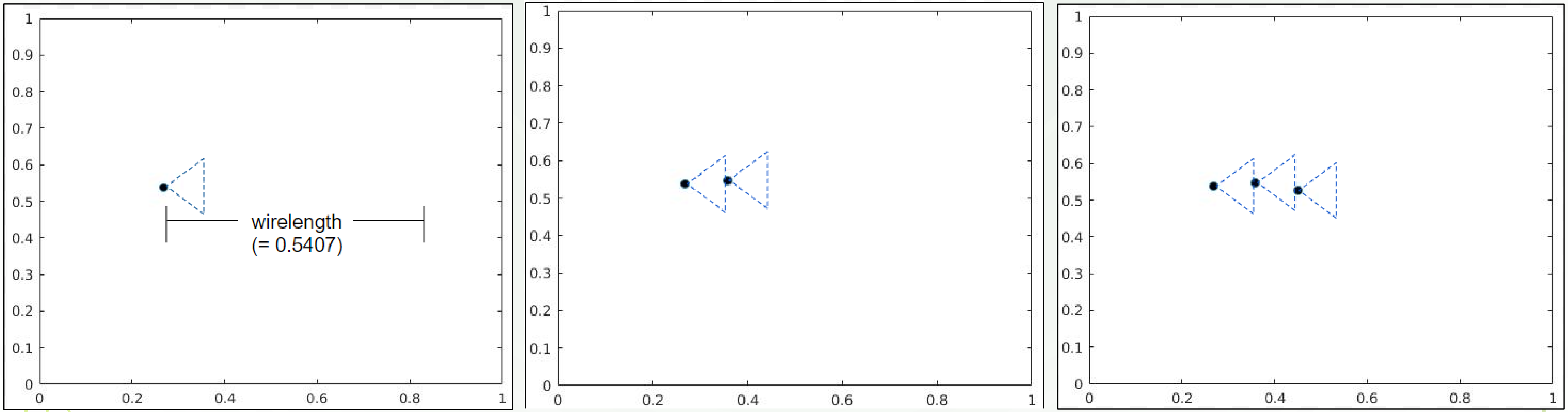


SEM images of aliquots taken at 47 min, from the Ag-NW synthesis reaction mixture at 180 °C [2]

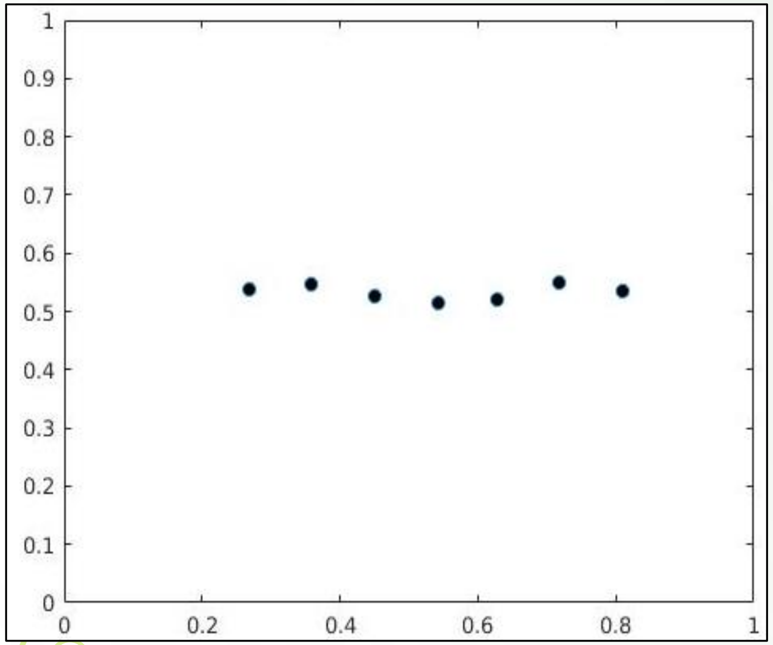
2 W. M. SCHUETTE AND W. E. BUHRO, "POLYOL SYNTHESIS OF SILVER NANOWIRES BY HETEROGENEOUS NUCLEATION; MECHANISTIC ASPECTS INFLUENCING NANOWIRE DIAMETER AND LENGTH," *CHEM. MATER.*, VOL. 26, NO. 22, PP. 6410–6417, 2014.

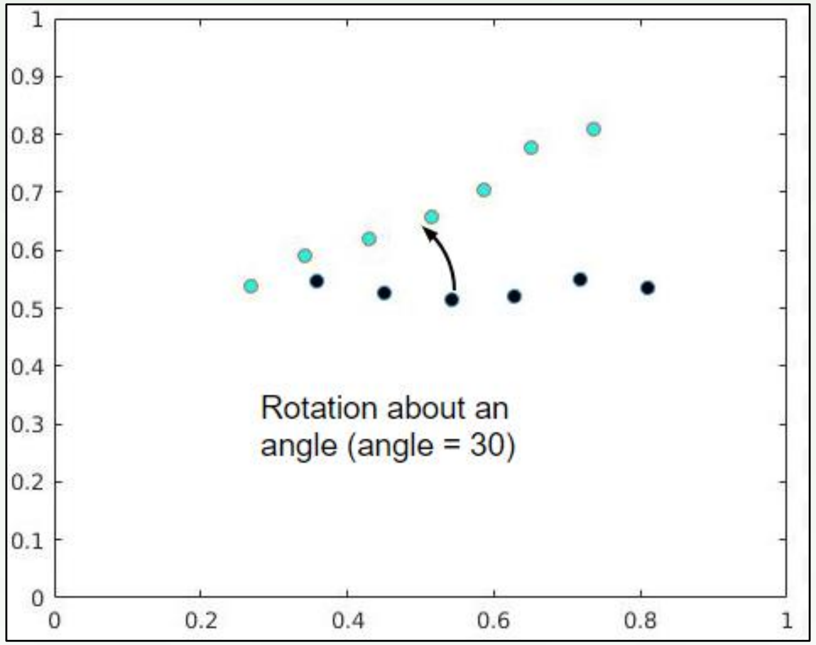
Step 2: Generating the Model

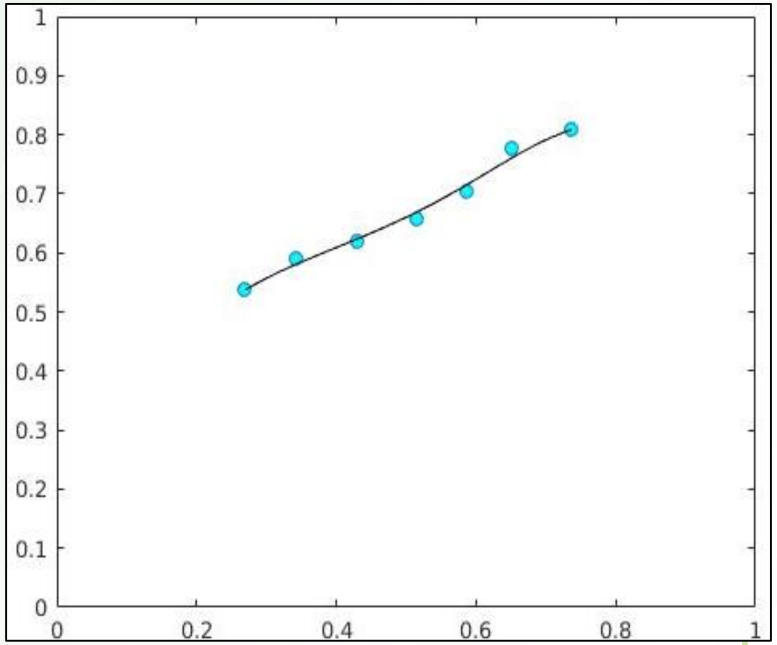
- Laying down *control points* to obtain the shape and curvature: parameters of wirelength and wonky-ness



Step 2: Generating the Model (cont.)



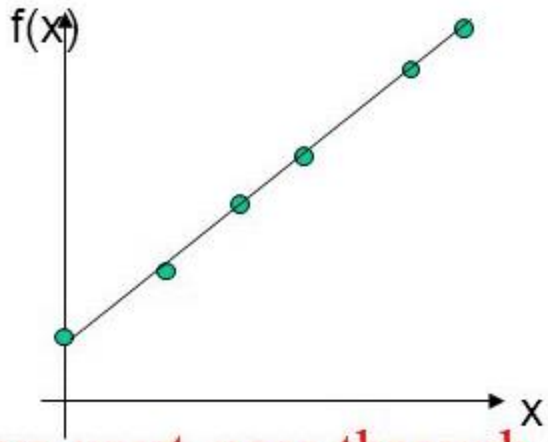




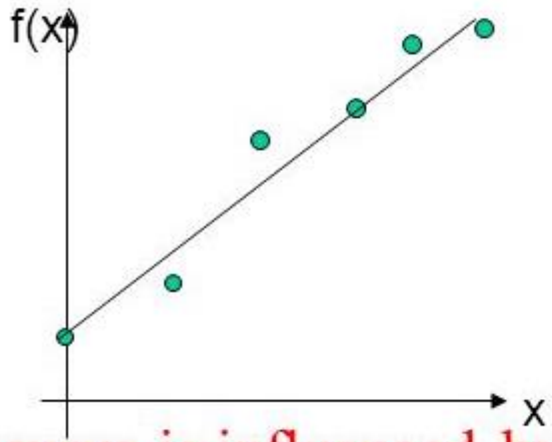
Step 2: Generating the Model (cont.)

- The set of control points are then rotated at random
- Finding the best curve fitting method: Spline vs. Bezier curves
  - Spline vs. Bezier curves is parallel to interpolation vs. approximation
  - Pros and Cons:
    - Spline has more of a defined curvature but overfitted the control points of vertical rotated nanowires
    - Bezier curves has less curvature but did not have a problem fitting vertical rotated nanowires

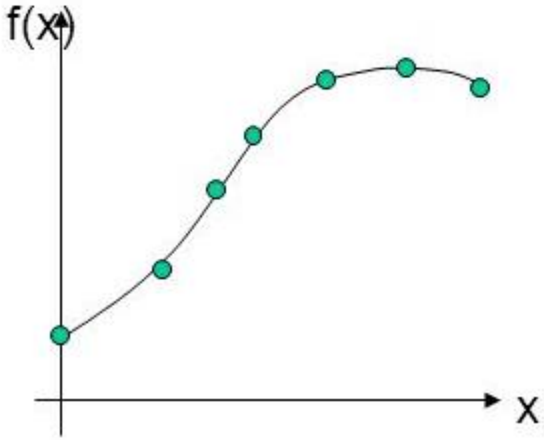
Interpolation vs approximation

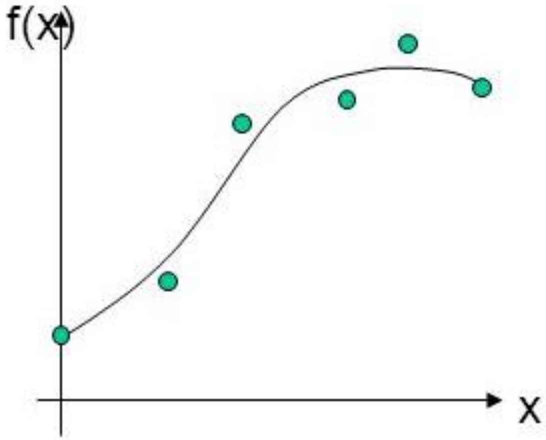


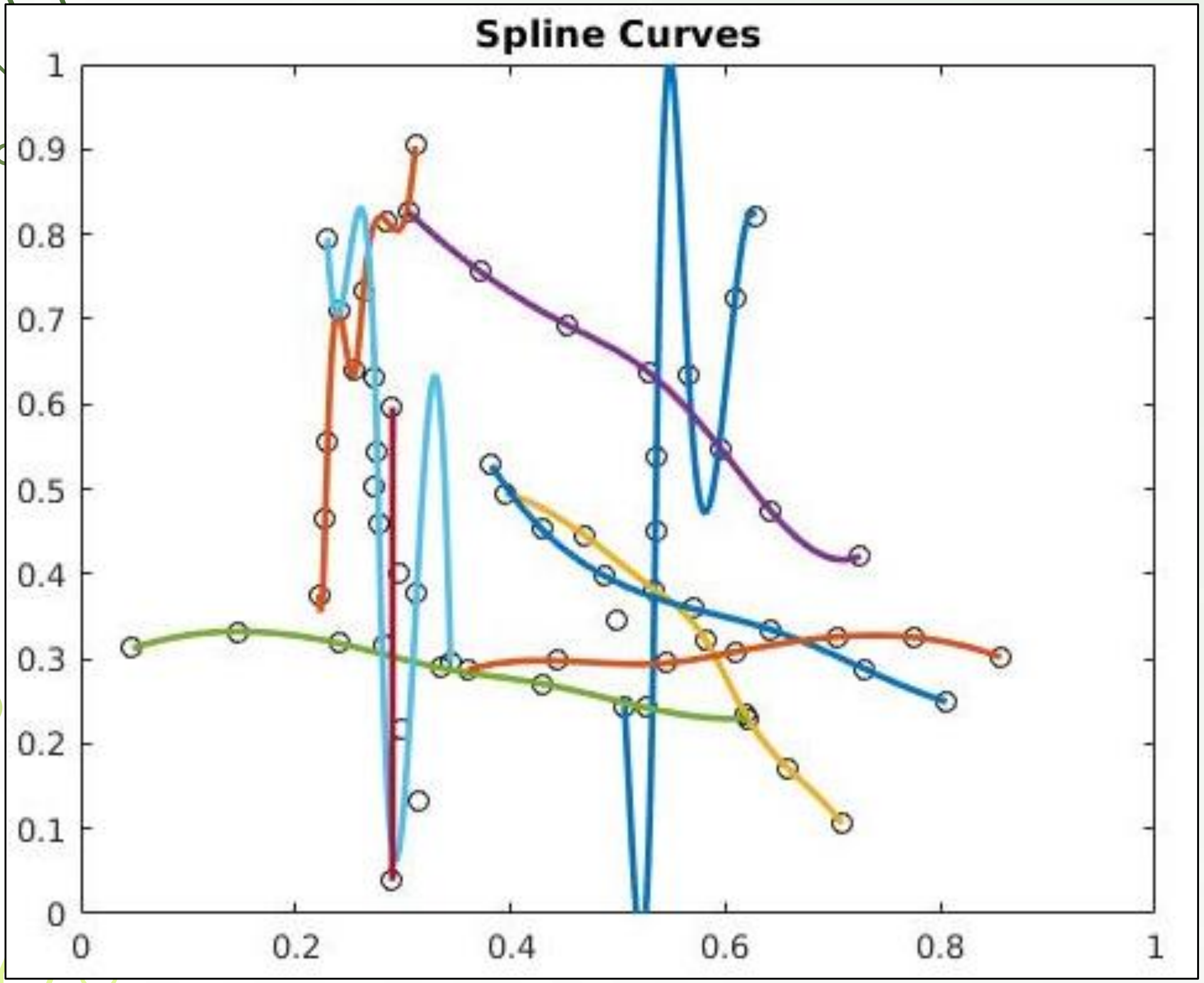
curve must pass through control points



curve is influenced by control points






Spline Curves
0
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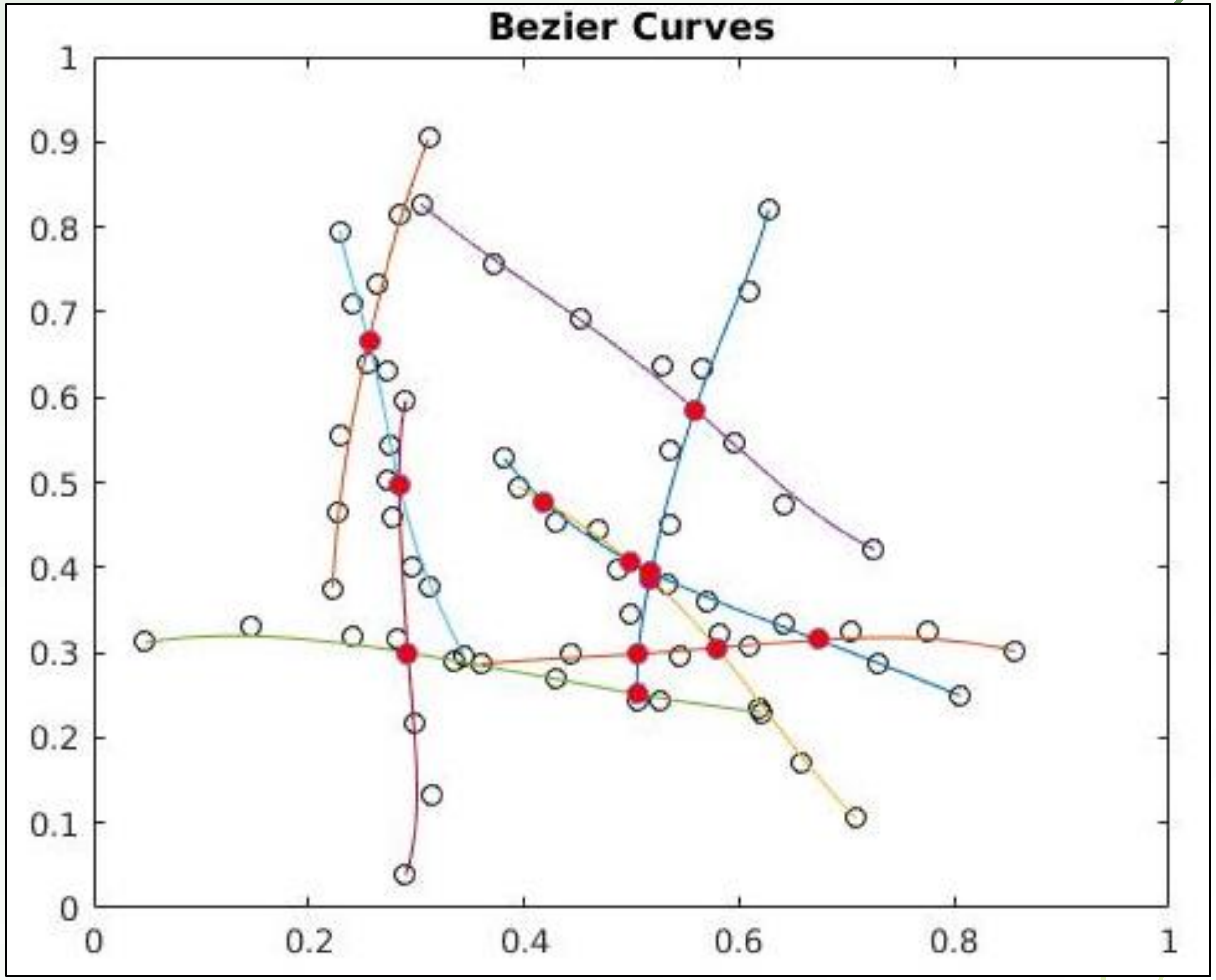
1


Bezier Curves
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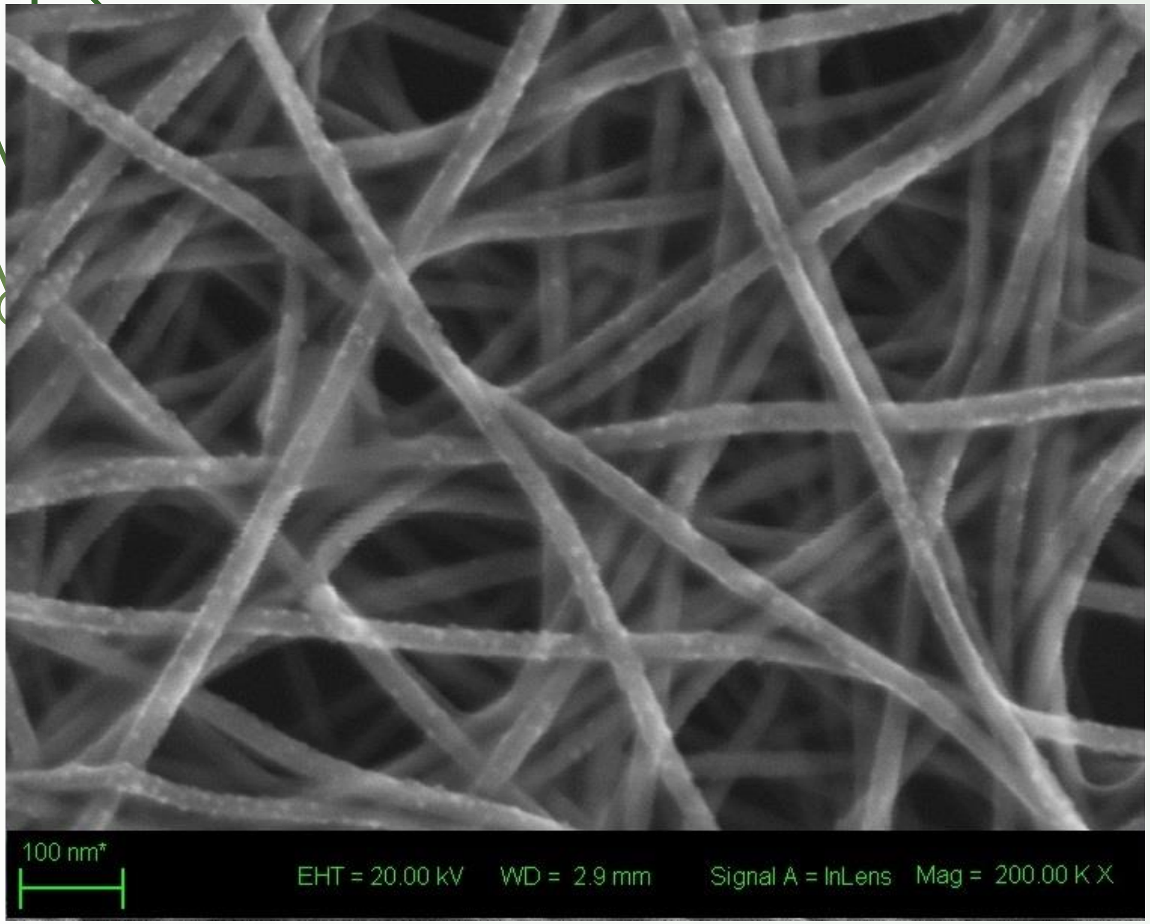

SEM images of silver nanowires (diameter: 17 nm).

Courtesy of Zhejiang Kechuang Advanced Materials Co.
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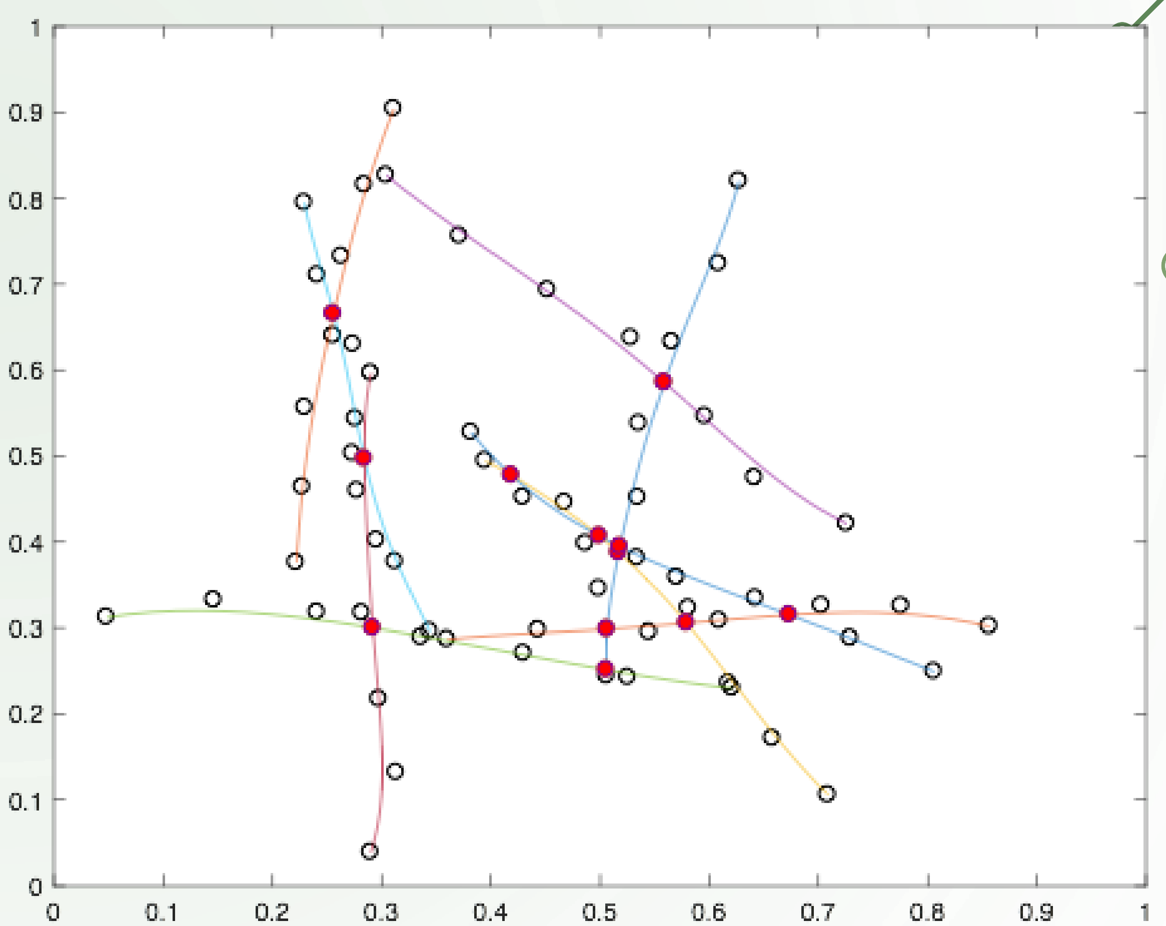


9 wires with a Gaussian distribution are generated in MATLAB. Intersection of these wires are indicated with a red filled dot.

Step 3: Analyzing the Model

- Before analysis, the intersections[4,5] of the wires needs found
  - The total wirelength[6] also needs to be calculated
  - Then the network can be represented in an adjacency matrix
- The total wiring cost and the average shortest path can then be measured
  - Total wiring cost – sum of the cost of all the wires in the network[7]
  - Average shortest path – the average number of hops in the shortest path for all possible node combinations[7]
- Parameter settings for optimized networks can then be determined: networks with short average paths and the least amount of wires

4 D. MANOCHA AND J. DEMMEL, "ALGORITHMS FOR INTERSECTING PARAMETRIC AND ALGEBRAIC CURVES II: MULTIPLE INTERSECTIONS," *GRAPH. MODEL. IMAGE PROCESS.*, VOL. 57, NO. 2, PP. 81–100, 1995.
5 D. MANOCHA AND S. KRISHNAN, "ALGEBRAIC PRUNING: A FAST TECHNIQUE FOR CURVE AND SURFACE INTERSECTION," *COMPUT. AIDED GEOM. DES.*, VOL. 14, NO. 9, PP. 823–845, 1997.
6 J. GRAVESEN, "ADAPTIVE SUBDIVISION AND THE LENGTH AND ENERGY OF BÉZIER CURVES," *COMPUT. GEOM. THEORY APPL.*, VOL. 8, NO. 1, PP. 13–31, 1997.
7 H. CHUNG, C. TEUSCHER, AND P. PANDE, "DESIGN AND EVALUATION OF TECHNOLOGY-AGNOSTIC HETEROGENEOUS NETWORKS-ON-CHIP," *ACM J. EMERG. TECHNOL. COMPUT. SYST.*, VOL. 10, NO. 3, PP. 1–27, 2014.

Step 4: Quantifying the Model

- The performance of the network can now be determined by the user's preference
  - Creates application-specific networks
  - This is done by an objective aggregate fitness function:

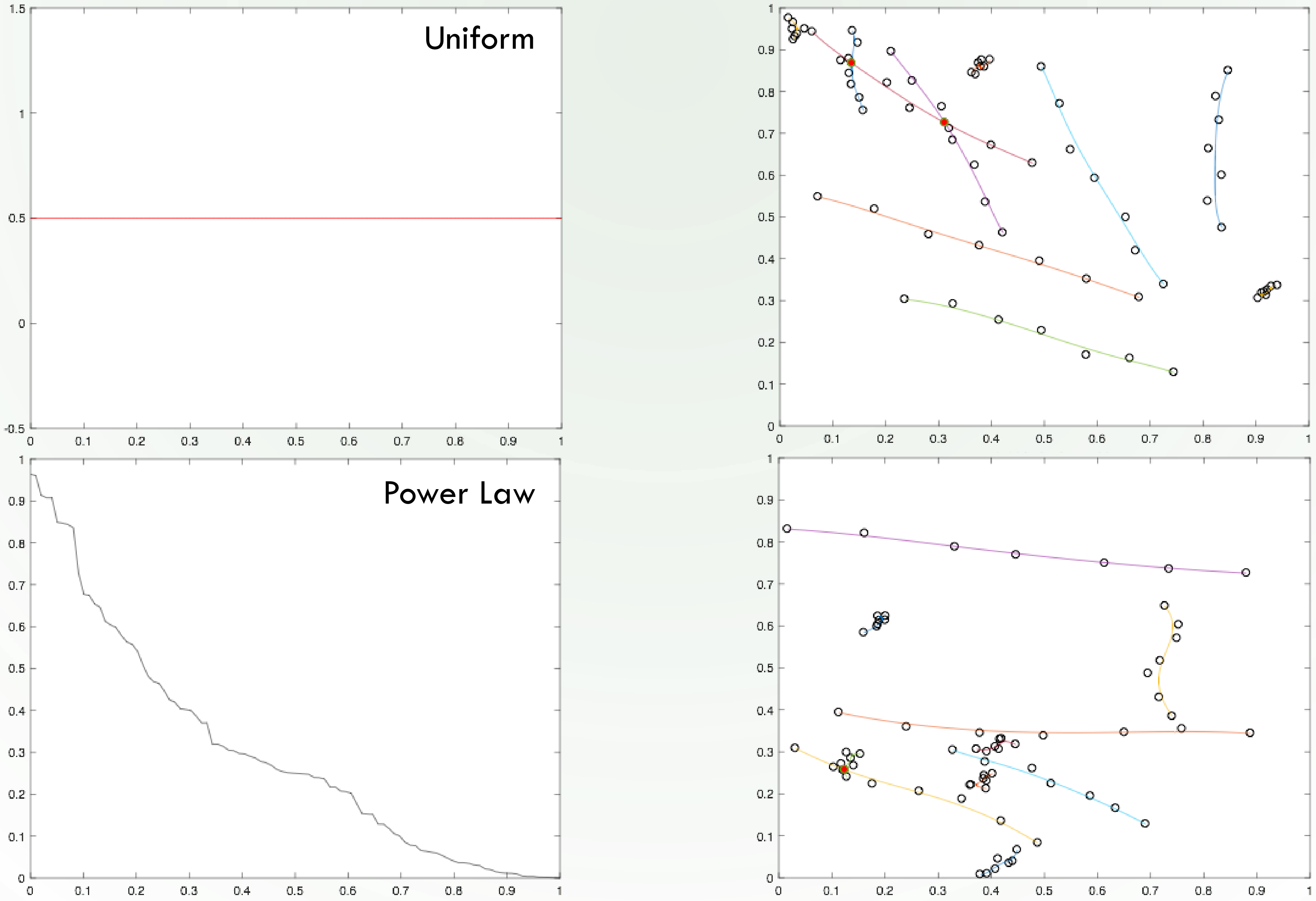
$$f(w) = w * WiringCost_{network} - (1 - w) * ASP_{network}$$

    - Where w is a weight defined by the user ($0 \leq w \leq 1$)

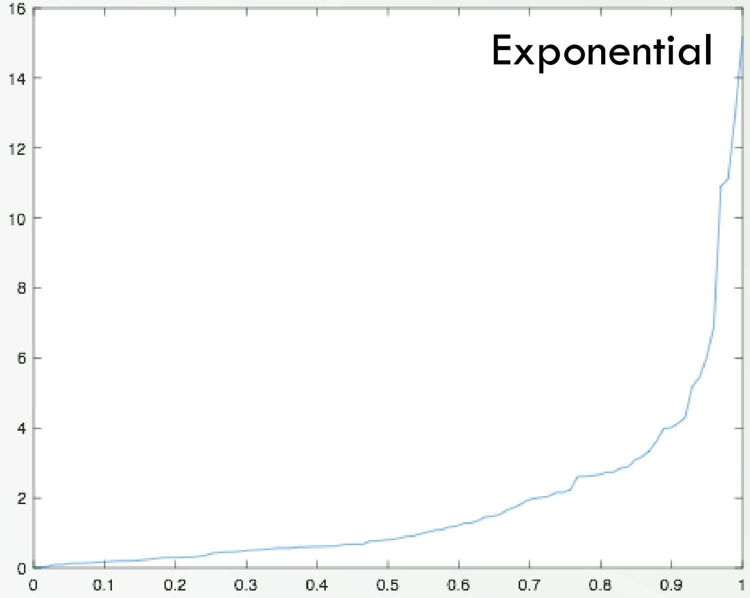
Results

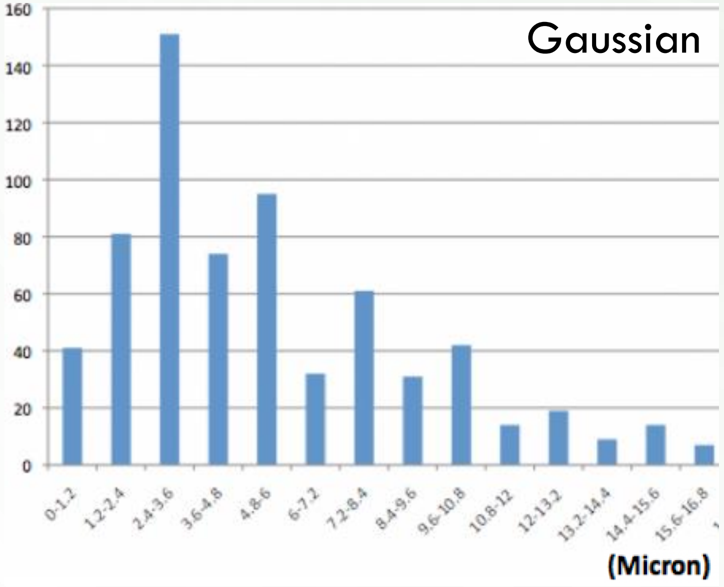
- Accurate models of silver nanowires were produced and can be varied by certain parameters
- The intersections and wirelength of the network of wires can be found
- Different length distributions of wires can be generated: uniform, power-law, exponential, and Gaussian
- Means of evaluating the performance of the network by the user’s preference is established

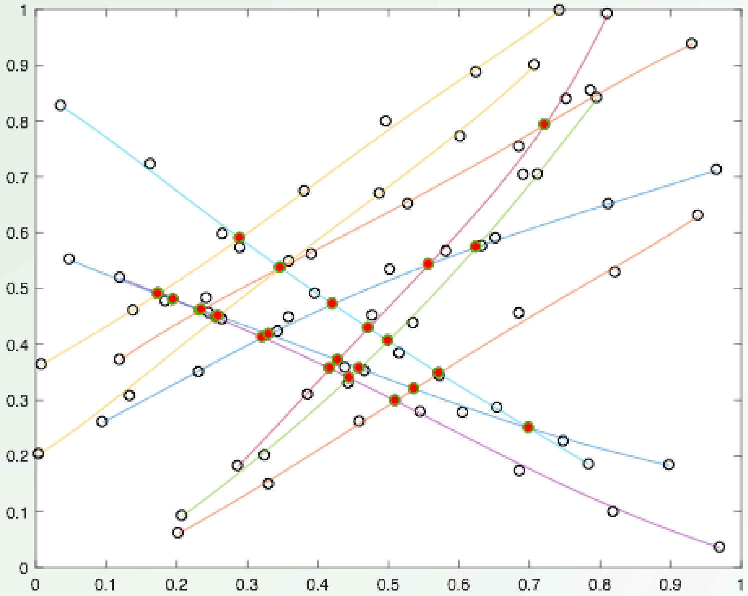
Results (cont.)

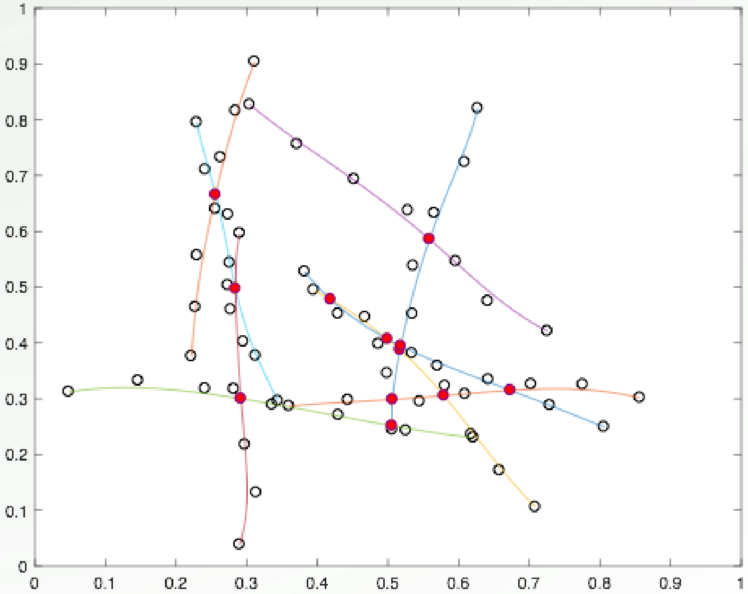


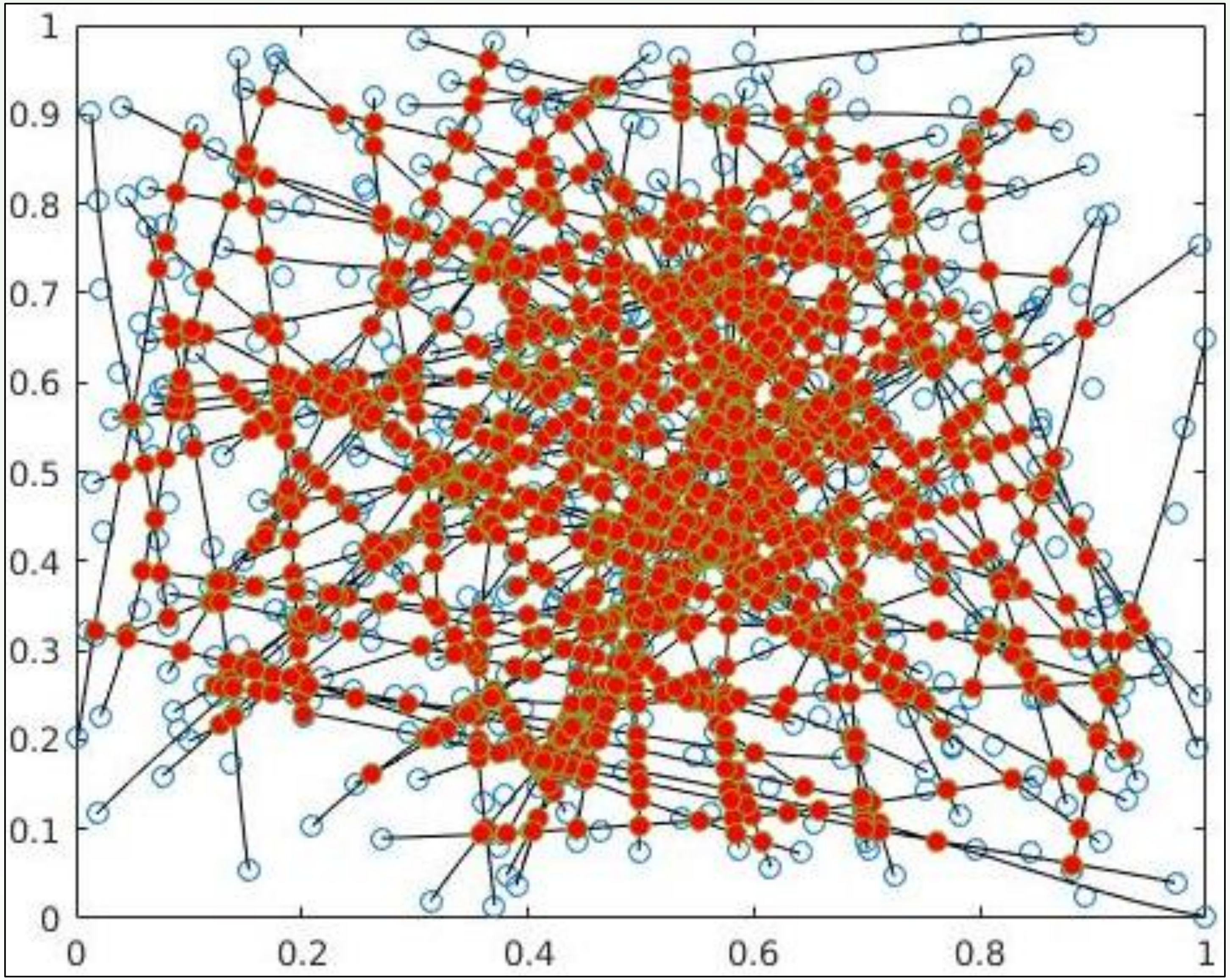
Results (cont.)







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1

Future Work/Conclusions

- Experimental trials of self assembled chips are needed before future manufacturing
- Analyzing the length distribution of different methods of synthesizing nanowires will help determine experimental parameters
- In this specific project:
  - Network representation by adjacency matrix
  - Finding parameter settings for optimized networks of different length distributions
    - The connection probability in brain networks[8,9], electronic circuits[10], the Internet, and social networks as opposed to a rat's neocortical pyramidal neurons[11].
  - Include other factors for analysis: energy consumption, latency, throughput, etc.

4 C. TEUSCHER, N. PARASHAR, M. MOTE, N. HERGERT, AND J. AHERNE, "WIRE COST AND COMMUNICATION ANALYSIS OF SELF-ASSEMBLED INTERCONNECT MODELS FOR NETWORKS-ON-CHIP," *2009 2ND INT. WORK. NETW. CHIP ARCHIT.*, PP. 83–88, 2009.
5 O. SPORNS, D. R. CHIALVO, M. KAISER, AND C. C. HILGETAG, "ORGANIZATION , DEVELOPMENT AND FUNCTION OF COMPLEX BRAIN NETWORKS," VOL. 8, NO. 9, 2004.
6 V. M. EGU, D. R. CHIALVO, G. A. CECCHI, M. BALIKI, AND A. V. APKARIAN, "SCALE-FREE BRAIN FUNCTIONAL NETWORKS," PP. 1–4, 2008.
7 B. HELLWIG, "A QUANTITATIVE ANALYSIS OF THE LOCAL CONNECTIVITY BETWEEN PYRAMIDAL NEURONS IN LAYERS 2/3 OF THE RAT VISUAL CORTEX," *BIOL. CYBERN.*, VOL. 82, NO. 2, PP. 111–121, 2000.

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