NIST Workshop on
Complex Systems Chemistry at the Nexus of Chaos, Emergence, and Information Theory
October 22-24, 2018

NIST Gaithersburg, MD Campus

Organizers: Carlos Gonzalez and André Striegel, NIST

DAY 1 – Monday, October 22

7:30 – 8:15 Arrive/Check-in//Etc.

8:15 – 8:30 NIST welcome: *Eric Lin, Director, Material Measurement Laboratory, NIST*

8:30 – 9:00 *Carlos Gonzalez/André Striegel*

9:00 – 9:45 Keynote 1: "Machine learning for analysis and prediction of chaotic dynamics." *Edward Ott, University of Maryland*

9:45 – 10:30 Keynote 2: "Quantum information and quantum computing for complex chemical systems." *Sabre Kais, Purdue University*

10:30 – 11:00 Break

11:00 – 12:00 Plenary 1: "Chemistry and the computational universe." *Stephen Wolfram, Wolfram Research*.

12:00 – 1:00 Lunch (on own)

1:00 – 1:45 Keynote 3: "Towards predicting the combustion chemistry of real, multicomponent fuels: Simplicity amid complexity." *Hai Wang, Stanford University*

1:45 – 2:30 Keynote 4: "Emergent space, emergent time, emergent descriptions: Data and the computer-assisted modeling of complex systems." *Yannis Kevrekidis, Johns Hopkins University*

2:30 – 3:00 Break

3:00 – 3:45 Keynote 5: "Quantifying pancreatic islet network pattern emergence during development." *Deborah Striegel, Henry Jackson Foundation*

3:45 – 4:30 Keynote 6: "Synchronization measurements for decrypting the complex response of chemical reaction networks." *Istvan Kiss, St. Louis University*

4:30 – 5:00 NIST talk 1: "Uncertainty quantification in complex chemical systems." *David Sheen, NIST*

5:15 Adjourn

DAY 2

8:15 – 8:30 Welcome Day 2: *Carlos Gonzalez/André Striegel*

8:30 – 9:30 Plenary 2: “Complexity as a self-generated property of multidimensional systems.” *Antonio Politi, University of Aberdeen*

9:30 – 10:15 Keynote 7: “System inference with small sample size in stochastic systems.” *Vipul Periwal, National Institute of Health (NIH)*

10:15 – 10:45 Break

10:45 – 11:30 Keynote 8: “Chemical selforganization: Macroscopic order from microscopic processes.” *Oliver Steinbock, Florida State University*

11:30 – 12:15 Keynote 9: "Complex behavior in complex reaction-diffusion systems.” *Irving Epstein, Brandeis University*

12:15 – 1:30 Lunch (on own)

1:30 – 2:15 Keynote 10: “Emergent collective behavior of self-powered single molecules and nanoparticles.” *Ayusman Sen, Pennsylvania State University*

2:15 – 3:00 Keynote 11: “Chimera states in populations of coupled chemical oscillators.” *Kenneth Showalter, West Virginia University*

3:00 – 3:30 Break

3:30 – 4:15 Keynote 12: “Time-lapse and cure-on-demand polymerizations for adhesives, wood repair and art.” *John Pojman, Louisiana State University*

4:15 – 4:45 NIST talk 2: “Bayes Markov Monte Carlo applied to NIST chemical measurements.” *Blaza Tolman, NIST*

5:00 PM Adjourn

DAY 3

8:30 – 9:00 Statement of purpose: *Carlos Gonzalez/André Striegel*

9:00 – 10:00 Breakout group discussions

10:00 – 10:30 Break

10:30 – 11:30 Breakout group discussions/Assembling notes for presentations

11:30 – 12:30 Lunch (on own)

12:30 – 1:30 Presentations by groups

1:30 – 3:00 Discussion

3:00 – 3:15 Farewell/Adjourn