Structure formation in soft, polymer materials: Role of Data & Analytics

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outline:
• Introduction – some criteria for the potential of Data & Analytics from a perspective of a scientists
• Models, data and algorithms for structure formation in soft, polymer materials
• Concluding remarks
Some criteria for potential of Data & Analytics

• **local aspects on the scale of working groups:**
  – re-use of data, collaborations and transfer of knowledge
  – program and data documentation / good scientific practice
  – compliance with mandates of funding agencies / government

  important, needs low-barrier software solution to facilitate documentation of work processes, can use problem-specific formats

• **large-scale collaborations:**
  – an established example – high-energy physics (CERN)
  – synergistic collaborations of groups in different disciplines and locations
  – parallel development of experiment, theory, and computational infrastructure
  – building of community by common data and algorithms
Some criteria for the potential of Data & Analytics

- Scientific problem / large-scale collaboration
- Scientific framework – models, data, algorithms
- Need and availability of complex data
- Scientific community
Soft, polymer materials – scientific problem

- **dense copolymer materials** (personal bias … there are many more)
  - microphase separation on the length scale from 5-100 nm
  - can be tailored in geometry and length scale by molecular
  - applications:
    - photonic materials
    - solar and fuel cells
    - DSA – microelectronic device fabrication

Soft, polymer materials – scientific problem

- **dense copolymer materials**
  (personal bias … there are many more)

- **self-assembly of amphilpic molecules in solution**
  (lipid membranes, lipid-protein assembly)

- **colloidal self-assembly**
  (role of shape and depletion interactions, DNA-mediated interactions)

**common ingredients that control the structure formation in soft materials** (characteristic free-energy scale $k_B T$)
- kinetics of structure formation/transformation is crucial
- multitude of metastable states and intermediates
- process-directed self-assembly
Process-directed self-assembly

direct the kinetics of structure formation as to reproducibly trap the morphology in the desired metastable state

free energy, $F[m]$

unstable BCC

metastable I-WP

stable BCC

free-energy barrier

configuration space, $m$

stable LAM

alchemical trans. for $T$ quench

$10^3$ s

$10^3$ s

stable BCC

$f_{\text{start}} = 0.15$

$f_{\text{end}} = 1/2$
Process-directed self-assembly

- **process-directed self-assembly by pressure jump**
- Fabrication of I-WP network morphology from BCC structure
- **Local conservation of density** is crucial to predict pathway Jacobian of transformation from particle-based coordinates to densities
- **Importance of chain conformations being not in equilibrium** with instantaneous density distribution

Process-directed self-assembly

- **process-directed self-assembly by alchemical (photochemical) transformation**

![Diagram showing process-directed self-assembly](image)

- **variety of periodic structures:**
  - (a) FCC, (b) F-RD, (c) BCC, (d) I-WP, (e) I-WP-S, (f) HEX, (g) HEX2, (h) GYR-S, (i) GYR, (j) DIA, (k) DIA-S, (l) LAM
Multitude of stable and metastable structures

- Broadly accessible self-consistent field theory for block polymer materials discovery, Arora, Qin, Morse, Delaney, Fredrickson, Bates, Dorfman, Macromolecules 49, 4675 (2016)
Scientific framework – models, data & algorithms

- **Time scale**
  - 1ps
  - 1ms
  - 1s

- **Length scale**
  - 1nm
  - 100 nm
  - 1 µm

- **Models**
  - Atomistic models
  - Coarse-grained models (particle-based)
  - Reduced models (phenomenological)

- **Scientific framework**
  - Models, data & algorithms
minimal coarse-grained model that captures only
relevant interactions: connectivity, excluded volume, repulsion of unlike segments

- incorporate essential interactions through a
  minimal, soft, coarse-grained model
  chain extension, $R_e$, compressibility $\kappa N$ and
  Flory-Huggins parameter $\chi N \rightarrow universality$
- elimination of degrees of freedom
  top-down model

Scientific framework – models, data & algorithms

a small number of atoms is lumped into an effective segment (interaction center) MC, MD, DPD, LB, SCFT

diffusion $\sim 10^{-9} - 10^{-4}$ s

conformational rearrangements $\sim 10^{-12} - 10^{-10}$ s

bond vibrations $\sim 10^{-15}$ s

$t = 3$ hours

Scientific framework – models, data & algorithms

$t = 12$ hours

Daoulas, Müller, JCP 125, 184904 (2006)
effective interactions become weaker for large degree of coarse-graining

no (strict) excluded volume, soft, effective segments can overlap, rather enforce low compressibility on length scale of interest, $R_{eo}$

-terms generate pairwise interactions

particle-based description for MC, BD, DPD, or SCMF simulations

The standard Gaussian model for block copolymer melts

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• “universal standard model” that defines a framework to categorize models for particle simulation, polymer DFT, molecular theory and SCFT
• starting point for generalizations (molecular architecture, EOS-effects and solvents, charges or supramolecular interactions, dynamical properties)
Scientific framework – models, data & algorithms

• **equilibrium data:**
  - phase diagrams as a function of molecular architecture (SCFT)
  - effects of compressibility and local packing structure (p-DFT)
  - exploration of potential structure (particle simulation)
  - scattering experiments
  - real-space imaging techniques (TEM/AFM/tomography+SIS)

• **dynamic equilibrium data:**
  - rheology data
  - diffusion constant, single-chain motion in spatially modulated structure

• **non-equilibrium collective dynamics:**
  - structure formation, reorientation dynamics in external fields
  - defect motion and annihilation
  - process-directed structure formation

**multitude techniques:** SCFT, p-DFT, molecular theory, particle simulation, GISAX/GISAS, TEM, AFM, tomography+SIS
Scientific framework – models, data & algorithms

example: particle simulations on GPUs

- **MPI**
  - no domain decomposition
  - polymer block parallel
- **OpenACC 2.5**
  - fine grain parallel (polymer)
  - #pragma GPU parallel
  - Imemory offloading
  - PGI compiler
- **OpenMP**
  - like OpenACC
  - any compiler

- **features**
  - Smart Monte-Carlo moves
  - Distributed computation via MPI / OpenMP
  - single source code multiple architectures: CPU and GPU (via OpenACC)
  - *hdf5 i/o format*, parallel i/o
  - up to 64 polymer types

→ synergies in co-development of programs and unified data formats: GROMACS, LAMMPS, ESPRESSO, HOOMD
Need and availability of complex data

\[ 0.88R_e \times 240.64R_e \times 135.36R_e \]
\[ nN \approx 500 \times 10^6 \text{ time: } 4 \tau_P \]
\[ 10 \text{ nvidia K80 devices} \]
\[ 20 \text{h computation time} \]
Need and availability of complex data
wealth of information (even in this deceptively simple example):
• single-chain motion in spatially modulated environment
• kinetics of collective structure formation (initial, spinodal)
• defect motion and annihilation
• grain growth and grain boundary motion
• large-scale connectivity of domains

requires analysis on different scales, using different models and comparison to various experimental techniques;
interaction between simulation (theory) and experiment

“computing gets more and more intertwined with data analysis”

involvement of different scientific communities using common standards
Opportunities for Data & Analytics in Soft Matter research

- need and availability of complex data
- scientific framework – models, data, algorithms
- scientific problem / large-scale collaboration
- scientific community

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Opportunities for Data & Analytics in Soft Matter research

- **scientific problem:**
  - relevant for technological applications
  - complex, rich behavior due to multitude of competing structure

- **framework:**
  - universal standard model (top-down approach)
    connecting computational models to experiments

- **availability of data:**
  - advances in numerical methods (SCFT, GPU-based simulation) and experiments
  - wealth of information (from single-molecule motion to large-scale morphology)

- **scientific community:**
  - numerous groups in America, Europe, and Asia
  - common standards and community-building required
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Disclaimer – specific case of structure formation in dense copolymer materials
but similar for other Soft Matter areas