CECAM workshop

Nano-structured soft matter: a synergy of approaches to amphiphilic and block copolymer systems

June 25, 2018 - June 27, 2018
University of Lincoln, UK
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1 Description

An important class of soft materials is formed by molecules consisting of chemically distinct parts. In this workshop, we concentrate on two types of materials that possess this feature: lipid amphiphilic molecules and block copolymers. These molecules can self-assemble into nanostructures (mesophases) of similar symmetries, but on different scales [1-4].

Controlling the properties of the nano-structured soft materials is relevant for a range of industrial applications (energy materials, templates, pharmaceuticals, cosmetics, foodstuffs, detergents and advanced painting) [5]. Their phase diagrams have marked differences, for instance in their stability regions [6]; the kinetics of their formation often plays an important role [2,6]. These systems span multiple scales both in space and time. Both short amphiphiles (lipids) and block copolymers can form bilayers (membranes), which can close into vesicles (e.g. spherical), which are important systems in biology and also in technological applications, for example as drug delivery vehicles.

Both in biological and synthetic systems lipid mesophases usually contain more than one lipid species, which have a tendency to phase separate. From a biological perspective, lateral lipid organizations into domains and membrane curvatures are ubiquitous features, and are known to play an important role for the membrane functionalities [7]. From a materials perspective, this can lead to a systematic and rational functionalization of such mesophases. Most studies on lipid phase separation focus on simple membrane geometries, such as lipid vesicles and supported membranes [8-10]. Only very recently have lipids in more complex bi-continuous phases been theoretically investigated [11].

For block copolymers (BCP), due to the larger molecular sizes, mesoscale and multiscale techniques have to be involved. Much research has been done using soft, generic coarse-grained models of polymers that allow for accelerated dynamics [12]. Self-consistent field theory (SCFT) and more recently field theoretical approaches [13-16], which work with polymer densities, can address much larger system sizes [17,18] compared to molecular dynamics simulations and were able to simulate experimentally relevant systems [19-22] and molecular
weights [16]. For even larger BCP system sizes advances have been made using a variety of phase field models offering the next scale level of description [23]. For practical applications such as lithography there is an interest in defects and their removal [19,24].

Forming vesicles from amphiphilic molecules (both lipids and BCP) received much attention in recent experiments utilizing a wide range of techniques, including microfluidic templating [25], electroformation from membranes [26] and self-assembly in solution [27]. A recently developed variation on the self-assembly process is polymerisation-induced self-assembly [28], during which polymerisation continues as self-assembly is taking place. In this process, spherical micelles can grow into vesicles as the polymers from which they are formed gradually lengthen. Simplified theoretical models were proposed for BCP vesicular and micellar formation using versions of SCFT [29,30]; however, most of the progress has been driven by experiment, and there is now a need for further theory and simulation to deepen our understanding and guide future investigations.

The proposed workshop aims at bringing together experts from two different subfields of soft matter physics, namely amphiphilic and block copolymer physics which, despite the differences in their objects of enquiry, share marked similarities in the thermodynamic phases observed both numerically and experimentally and also in the modelling these highly complex systems require to complement experimental studies. The workshop will strongly encourage simulation experts of these two subfields to interact with the aim of addressing challenges in the method development and multiscale modelling necessary to understand an ever-growing body of experimental results which will be summarised by leading experts in these fields. Specific challenges to be addressed are listed in three overlapping sections. All these problems have been chosen because we believe that discussion among researchers from a range of scientific backgrounds will contribute strongly to their solution.

**Lipids**

- Formulation of models for repartition of different species (other lipids or peptides) in lipid bilayers; discussion of raft hypothesis and its controversial aspects
- Formulation of models to describe accurately the thermodynamic and kinetic pathways to transition from one lipid phase to another (e.g. from minimal gyroid to primitive or diamond)

- Modelling and understanding the role of local phase instability in facilitating or hindering aggregation (e.g. protein crystallisation in the triply periodic primitive phase)

- Modelling of the specific experimental signatures (e.g. how to experimentally test species patterning on complex surfaces such as the P-surface)

**Block copolymers**

- How to cope with defects/eliminate them/lower the annealing time in order to achieve perfect structures in applications? How to minimize the effect of box size on the defect dynamics?

- How to enhance the stability region of phases, such as the gyroid, to ease assembly of these structures? Can incorporation of additional components (e.g., nanoparticles) enhance the stability?

- Development of hybrid models with automatic numerical determination of the parameters of phase field models from self-consistent field theory

- Related to the accuracy of modelling, what is the effect of compositional fluctuations that are present in experiments, but neglected in some coarse grained models such as SCFT?

**Vesicles**

- Dynamics of vesicle formation in new experiments; e.g., polymerisation-induced self-assembly, which allows nano-objects to be formed at very high concentrations.

- Controlling the surface properties of vesicles to tune their interaction with their environment.

- The role of molecular architecture in controlling the properties and size of vesicles; for example, to allow fine control over the dosage of an encapsulated chemical.
In general

What can the communities learn from each other: simulation techniques, preparation, inspiration from biology, external fields? Development of models for lipid/polymer mixtures.

Key References


2 Program

Day 1 - Monday June 25, 2018

Welcome
- 9:00 to 9:10 - Welcome

Experimental challenges - Chair: C. Marques
- 9:10 to 9:35 - Presentation - Ian Hamley
  Self-assembly and bioactivity of polymer-peptide conjugates
- 9:35 to 10:00 - Presentation - John Seddon
  Bi-continuous and discontinuous lipid cubic phases
- 10:00 to 10:25 - Coffee Break
- 10:25 to 10:50 - Presentation - Lorenzo Di Michele
  Highly porous responsive crystalline frameworks self-assembled from amphiphilic DNA nanostructures
- 10:50 to 11:15 - Presentation - Masayuki Imai
  Morphology of a model multicellular organism
- 11:15 to 12:00 – Q&A and discussion
- 12:00 to 13:30 - Lunch
Simulation challenges - Chair: A. Sevink

- 13:30 to 13:55 - Presentation - Marcus Müller
  Kinetics of pattern formation in symmetric diblock copolymer melt

- 13:55 to 14:20 - Presentation - Friederike Schmid
  Why "bad" is "good": polydispersity in polymeric nanostructures

- 14:20 to 14:45 - Presentation - Qiang Wang
  Fluctuation/correlation effects in diblock copolymer melts: simulations and theories

- 14:45 to 15:10 - Presentation - Kris Delaney
  Progress in fully fluctuating field theoretic simulations of polymers

- 15:10 to 15:35 - Coffee Break

- 15:35 to 16:30 – Q&A and discussion

- 16:30 to 18:00 - Poster Session

- 18:00 to 20:00 – Networking reception
Day 2 - Tuesday June 26, 2018

Bringing subfields together I - Chair: A.-C. Shi

- 9:00 to 9:25 - Presentation - Toshihiro Kawakatsu
  Multiscale modeling on complex multiphase flows

- 9:25 to 9:50 - Presentation - Carlos Marques
  Transformation of lipid bilayers under photo-induced oxidation

- 9:50 to 10:15 - Presentation - Halim Kusumaatmaja
  Phase separation on curved surfaces

- 10:15 to 10:45 - Coffee Break

- 10:45 to 11:10 - Presentation - Thorsten Auth
  Nanoparticles at lipid-bilayer membranes: curvatures at play

- 11:10 to 11:35 - Presentation - Robert Vacha
  Translocation of amphiphilic peptides across phospholipid membranes

- 11:35 to 12:30 – Q&A and discussion

- 12:30 to 14:00 - Lunch
Bringing subfields together II - Chair: F. Schmid

- 14:00 to 14:25 - Presentation - Kostas Daoulas
  Top-down development of mesoscopic polymer models: aligning interactions

- 14:25 to 14:50 - Presentation - Vladimir Lobaskin
  Diblock copolymer simulations: studying inter-lamellar roughness of BCP films on a coated substrate

- 14:50 to 15:15 - Presentation - Weihua Li
  Non-classical ordered nanostructures from designed block copolymers

- 15:15 to 15:45 - Coffee Break

- 15:45 to 16:10 - Presentation - An-Chang Shi
  Frustration in block copolymer assemblies

- 16:10 to 17:00 – Q&A and discussion

- 17:00 to 18:00 - Presentation - Daan Frenkel
  Soft matter: the inner frontier

- 19:00 to 22:00 - Social Dinner
Day 3 - Wednesday June 27, 2018

Simulations vs experiments - Chair: D. Wang

- 9:00 to 9:25 - Presentation - Robert Wickham
  Simulation of chain diffusion in diblock copolymer nanostructures using dynamical self-consistent mean-field theory

- 9:25 to 9:50 - Presentation - Agur Sevink
  Efficient incorporation of momentum transfer in coarse-grained membrane simulations

- 9:50 to 10:15 - Presentation - Josep Bonet Avalos
  Kinetic exchange of copolymer surfactants in micelles

- 10:15 to 10:45 - Coffee Break

- 10:45 to 11:10 - Presentation - Takashi Honda
  SCF calculation of polymer composite materials

- 11:10 to 11:25 - Presentation - Javier Diaz
  Hybrid block copolymer/nanoparticle systems: colloidal assembly

- 11:25 to 11:40 - Presentation - Elena Patyukova
  Association model approach for description of hydrogen-bonding in block copolymers
• 11:40 to 11:55 - Presentation - **Jiajia Zhou**
  Elastic properties and line tension of bilayer membranes

• 12:00 to 13:15 – Q&A, discussion and future directions

• 13:15 to 13:30 - Closing Word

• 13:30 to 15:00 - Lunch
3 Abstracts

**Self-assembly and bioactivity of polymer-peptide conjugates**

Ian Hamley  
University of Reading, United Kingdom

Self-assembling peptides and their conjugates offer exceptional potential in nanomedicine. I will present some of our recent work on nanoscale assembled peptides and their conjugates, focussing on polymer-peptide conjugates and lipopeptides. Our work on self-assembling polymer-peptide conjugates incorporating poly(ethylene glycol), PEG [1], includes PEGylated amyloid peptides which exhibit distinct modes of self-assembly [2-5] and enzyme responsive peptide delivery systems [6]. In addition we have developed a thermoresponsive and biocompatible PEG/peptide hydrogel based on telechelic hydrophobic dipeptides [7]. Recent work on linear triblock and star PEG-tyrosine conjugates in collaboration with the group of H.Iatrou (Athens, Greece) reveals distinct modes of self-assembly, gelation behaviour and bioactivity [8,9]. Examples from our recent work on self-assembling lipopeptides (peptide amphiphiles) will also be outlined. Our focus is to investigate potential relationships between self-assembly and bioactivity, in particular in the fields of regenerative medicine, antimicrobial systems, and immune therapies.


Bicontinuous and discontinuous lipid cubic phases

John Seddon
Imperial College, UK, United Kingdom

Lytotropic liquid crystals of 1-, 2-, or 3-dimensional periodicity spontaneously assemble when lipids are mixed with solvent under various conditions of temperature, pressure and hydration. There are two quite distinct types of inverse cubic phases: bicontinuous ones based on underlying periodic minimal surfaces, and discontinuous ones based on simple or more complex packings of discreet inverse micelles. By incorporation of charged phospholipids, we have been able to swell inverse bicontinuous cubic phases to approx. 500 Å, with water channels of approx. 220 Å diameter, potentially expanding the range of usefulness of such phases for applications [1, 2]. We have studied [3] the effect of chain branching on the phase behaviour of a series of synthetic β-D-glucosides derived from Guerbet alcohols, whose total hydrocarbon chain length ranged from C8 to C24. A wide range of liquid-crystalline phases was observed, with the C16 Guerbet glucoside (i.e. β-Glc-C10C6) forming an Ia3d bicontinuous cubic phase of space group in excess aqueous solution, which is very unusual – and potentially useful - behaviour. We have formed cubosomes from bicontinuous cubic phases, and have studied the effect of incorporation of a pH-sensitive polymer, PP50, on these cubosomes using cryo-TEM, SAXS and dynamic light scattering [4].

We have previously shown that by addition of weakly-polar amphiphiles such as diacylglycerols to phospholipids, we can tune the interfacial curvature to be strongly inverse, leading to the formation of a discontinuous cubic phase of spacegroup Fd3m, with a structure based upon a complex close packing of two types of quasi-spherical inverse micelles. We have investigated the effect of hydrostatic pressure on the structure and stability of this phase, and have discovered a number of novel effects [5]. We have also studied the structure of this phase by contrast variation neutron scattering, and have been able to demonstrate that the more weakly amphiphilic diacylglycerol component is preferentially located in the smaller, more highly curved inverse micelles (A.I.I. Tyler, unpublished data).
We have dispersed this bulk Fd3m phase into ‘micellosomes’ by sonication in the presence of the amphiphilic block copolymer F127, and have used x-ray diffraction to compare their structure to that of the bulk Fd3m cubic phase (A.M. Sartor et al., unpublished data). Some time ago [6] we discovered a lyotropic phase of space group P63/mmc, whose structure is based upon a 3-D hexagonal packing of quasi-spherical inverse micelles, in a hydrated mixture of dioleoyl phosphatidylcholine, dioleoyl glycerol, and cholesterol. This phase is expected to have a greater chain packing frustration than the Fd3m cubic phase, and it appears that the cholesterol is able to relieve the chain packing frustration within the hydrophobic region of this phase, allowing the P63/mmc phase to form.


Highly porous responsive crystalline frameworks self-assembled from amphiphilic DNA nanostructures

Lorenzo Di Michele[1], Ryan A. Brady[1], Nicholas J. Brooks[2], Vito Fodera[3], Pietro Cicuta[1]

Several emerging technologies require the production of highly porous frameworks with a controlled nanoscale morphology. Due to the exquisite binding selectivity of nucleic acids, together with their facile synthesis and functionalization, DNA nanotechnology has emerged as a prime route for the production of programmable and functional nanoscale materials. Nonetheless, the preparation of 3D DNA
frameworks which are, at the same time, crystalline and highly porous remains elusive. Indeed, branched motifs prepared with DNA origami or tiles can only support long-range order in 2D, while 3D crystallization has only been demonstrated with compact building blocks forming low-porosity networks.

We introduce a novel class of amphiphilic DNA building blocks that, combining the programmability of Watson-Crick base pairing with the robustness of hydrophobic forces, self-assemble into 3D macroscopic single crystals, in which the lattice parameter can be tuned between 18.4 and 34.2 nm, and precisely prescribed by straightforward scaling of the DNA motifs [1,2]. We exploit the tunable porosity, reaching 85%, to control the partitioning of a broad range of molecular species, and create size-exclusion filters with a precise cutoff. The robustness and versatility of our approach enables the modification of the amphiphilic building blocks with responsive DNA motifs, which can be triggered to induce isothermal melting of the network [2].


**Morphology of a model multicellular organism**

Masayuki Imai[1], Ryuta Ebihara[1], Kei Murakami[1], Yuka Sakuma[1], Masayuki Imai[1], Primoz Ziherl[2,3]

A single cell system, such as red blood cell, shows a series of shape transitions, stomatocyte-discocyte-echinocyte, by applying a variety of chemical and physical stresses. This series of shapes is well described by minimization of elastic energy, i.e., area difference elasticity (ADE) model [1] [2]. By adhering vesicles, the aggregates show rich morphologies due to the competition between the elastic energy and the adhesion energy, which gives physical basis of morphology of multicellular organism or embryogenesis [3].

When two deformable spherical vesicles are adhered each other, the total energy of the doublet is expressed by a sum of the vesicles' bending energy [4] and the adhesion energy assumed to be proportional to the contact area. This theoretical model predicts that in the weak adhesion, the adhering vesicles prefer the minimum contact area morphology (flat adhesion), whereas in the strong adhesion, the doublet shows the maximum contact area morphology with curved interface [5].

In this study we show the morphology transitions of adhering giant unilamellar vesicles (GUVs) induced by the changing the reduced volume of vesicles. The GUV
is homogeneous single component vesicle composed of 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC). First we adhered two spherical GUVs by controlling the inter-vesicle interactions. Thereafter we decreased the reduced volume of the adhering vesicles by using thermal expansion of membranes. Depending on the reduced volume, the doublet deformed its shape and showed a unique morphology transitions, sphere-oblate-prolate doublet and sphere-sigmoidal doublet. We observed more complicate morphologies for the vesicle triplets. We describe the observed morphology transitions based on the competition between the bending and the adhesion energies.


**Kinetics of pattern formation in symmetric diblock copolymer melt**

**Marcus Müller**
Georg-August University, Göttingen, Germany

In equilibrium copolymers self-assemble into spatially modulated phases with long-range order. When the system is quenched far below the order-disorder transition temperature, however, such an idealized, defect-free structure is not obtained in experiments and simulations; instead a fingerprint-like structure forms.

Using large-scale simulation we have studied the kinetics of structure formation after a quench from the disordered phase. Quantitative comparing morphologies obtained in the course of structure formation in particle-based simulation with SCFT, we associate to each snapshot a free-energy basin via the identification of an associated inherent morphology. We illustrate that the ordering process can be conceived as a combination of thermally activated jumps between free-energy basins and a gradual change of morphology in response to strain-field mediated interactions. For the time scales accessible in our simulation, both processes are characterized by comparable time scales.

Why "bad" is "good": Polydispersity in polymeric nanostructures

Friederike Schmid
Johannes Gutenberg University, Mainz, Institute of Physics, Germany

Synthetic polymers almost always have some degree of polydispersity, yet the influence of polydispersity on polymeric nanostructures has received surprisingly little attention so far. In the talk, we discuss polydispersity effects in polymer brushes and in self-assembled polymeric micelles, using self-consistent field calculations, analytical theory, and Monte Carlo simulations. We first consider simple polymer brushes and show that they correspond in some sense to a multicritical state characterized by anomalously high fluctuations. These fluctuations can be reduced dramatically already by introducing small levels of polydispersity. Then we discuss two situations where polydispersity turns out to have a highly beneficial effect from a practical point of view: First, we study a certain type of smart brush-based surfaces, which change their properties in response to external stimuli. Here, polydispersity is shown to enhance the performance of the switches by reducing their response times as well as their robustness.

Second, we study the size distribution of self-assembled copolymeric micelles in solution. Polydispersity in the copolymer constituents is shown to significantly reduce the dispersity in the micelle size distribution.

Hence "bad", not very well defined polymeric materials, produce "better", more uniform nanoparticles.

[1] Polydisperse polymer brushes: Internal structure, critical behavior, and interaction with flow

[2] Tuning transition properties of stimuli-responsive brushes by polydispersity

[3] Increasing block copolymer dispersity leads to more uniform micelles
**Fluctuation/Correlation Effects in Diblock Copolymer Melts: Simulations and Theories**

Qiang Wang  
Colorado State University, USA

With the polymer self-consistent field theory well developed in terms of both theoretical formalisms and numerical methods, it is natural and timely to develop advanced theories that can properly account for the fluctuation/correlation effects neglected by this mean-field theory. In this work, we take the most commonly studied linear diblock copolymer melts as an example. Based on the same model system of discrete Gaussian chains interacting with soft, finite-range repulsions as commonly used in dissipative-particle dynamics simulations, we directly compare, without any parameter-fitting, various structural and thermodynamic properties obtained from the fast off-lattice Monte Carlo simulations[1], reference interaction site model theory, Gaussian-fluctuation theory, and self-consistent field theory[2]. Our comparisons unambiguously and quantitatively reveal the consequences of various theoretical approximations and the accuracy of these theories in describing the fluctuations/correlations in either disordered or ordered[2] diblock copolymers, and are the pre-requisite for developing advanced theories that can better capture the fluctuation/correlation effects in polymeric systems.


**Progress in fully fluctuating field theoretic simulations of polymers**

Kris Delaney, Glenn Fredrickson  
University of California, Santa Barbara, USA

A field theoretic approach for simulating assemblies of interacting polymers is discussed. By applying a Hubbard-Statonovich-Edwards transformation to a molecularly informed coarse-grained polymer model, auxiliary fluctuating fields are introduced to decouple segmental interactions, and particle degrees of freedom are integrated out. The resulting theory has several advantages for simulating dense, long-chain polymeric systems, including efficient equilibration and direct access to mesoscale phenomena without simulating the atomic/molecular scale. The theory is commonly employed in a mean-field approximation (SCFT), which is exact for asymptotically long polymer chains in the melt state. However, for intermediate-
molecular-weight melts, for solvated or charged polymers, or for systems close to critical phase transitions, the mean-field approximation is qualitatively inadequate. We discuss a stochastic computational method based on complex Langevin sampling to directly simulate the fully fluctuating field theory without approximations or critical inefficiencies from the sign problem.

Applications of the field-theoretic simulation method to the study of fluctuation corrections of block copolymer phase diagrams will be presented, including the formation of novel fluctuation-stabilized morphologies in highly asymmetric branched polymers[1]. Subsequently the application to complex coacervates and self coacervates of polyelectrolyte solutions will be presented, with a focus on phase coexistence conditions, the scaling of the critical point, and the nature of the dilute supernatant phase[2]. Finally, a recently developed extension to the FTS method for simulating soft materials involving polar or polarizable segments, potentially coexisting with charges and/or subject to applied electric fields, will be presented[3]. This new framework is suitable for simulating a vast range of soft-matter systems, including polyelectrolytes, polymerized ionic liquids, ionomers and block copolymers, with collective phenomena including van der Waals interactions, charge localization and phase-separation-driven dielectric contrast all emerging consistently from the molecular specification.


**Multiscale Modeling on Complex Multiphase Flows**

**Toshihiro Kawakatsu, Yohei Morii**
Department of Physics, Tohoku University, Sendai, Japan

As a part of a project for the next generation supercomputer named “Post-K computer”, we are developing a multiscale simulation platform for complex flows(MSSP). In this platform, one can perform multiscale simulations by coupling a mesoscopic flow simulator based on smoothed particle hydrodynamics (SPH) and microscopic simulators for constitutive equations embedded in each of the SPH particles. Here, the microscopic simulator performs either molecular dynamics simulation under deformation, or evaluation of model constitutive equation.
We performed a series of simulations on a flow around an obstacle that generate vortices behind it for a Newtonian fluid, a viscoelastic fluid and an elastic-plastic fluid. We compared the results with those of experiments and large scale molecular dynamics simulations to study Toms’ effect caused by an addition of a small amount of polymers.

For the microscopic simulators, we are developing simulators that can calculate stress-strain relations for polymer solutions, polymer melts, cavity flows and so on. One of such simulators is the self-consistent field simulators for viscoelastic flows of polymers and block copolymers. We will discuss such simulation techniques.

Acknowledgements
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Transformation of lipid bilayers under photo-induced oxidation

Carlos Marques
Institut Charles Sadron, University of Strasbourg, CNRS, Strasbourg, France

Oxidation can intimately influence and structurally compromise the levels of biological self-assembly embodied by intracellular and plasma membranes. Lipid peroxidation, a natural metabolic outcome of life with oxygen under light, is also a salient oxidation reaction in photomedicine treatments. However, the effect of peroxidation on the fate of lipid membranes remains elusive. Here we present our recent efforts to understand lipid bilayer alterations following the formation of photo-induced lipid hydroperoxides, the primary products of every oxidation mechanism.


Phase Separation on Curved Surfaces

Halim Kusumaatmaja[1], Fabien Paillusson[2], Sergiu Busuioc[3], Victor Ambrus[3]

[1] Durham University, United Kingdom

In this contribution I will discuss two recent works on phase separation on curved surfaces. In the first part of the talk, I will focus on bicontinuous cubic membranes, whereby lipids form a triply periodic bilayer that separates two percolating and non-intersecting water channels. Using Monte Carlo simulations, we find an interesting competition between a curvature favoured splitting and a line tension favoured coalescing mechanism for the membrane phase separation. With increasing the line tension contribution, we also observe a faceting of the domains that we explain with a simple argument based on the symmetry of the underlying geometry. In the second part of the talk, I will present a novel lattice Boltzmann (LB) model designed to solve the coupled Cahn-Hilliard and Navier-Stokes equations on curved surfaces. We present an application of this methodology by considering a simple Landau free energy model on the surface of a torus. I will also contrast the results to those obtained for two-dimensional flat surfaces.
Nanoparticles at Lipid-Bilayer Membranes: Curvatures at Play

Thorsten Auth, Qingfen Yu, Sabyasachi Dasgupta, Sameh Othman, Gerhard Gompper
Forschungszentrum Jülich GmbH, Germany

Lipid-bilayer membranes serve as barriers and communication interfaces for biological cells. Controlled transport of material across its membranes is therefore essential for a cell's survival. However, also viruses are abundant and have developed very different physicochemical properties and mechanisms to enter and exit cells. Similarly, engineered nanoparticles can be fabricated with various sizes, shapes, and surface characteristics for applications in therapy and diagnostics, e.g. for targeted drug delivery and as membrane markers in imaging. Biological membranes can have complex compositions and structures, and therefore can lead to a variety of different observations when particle-membrane interactions are studied. Plasma membranes, membranous organelles, nuclei, and both intracellular and extracellular vesicles—for example—typically not only have different lipid compositions, but also different morphologies. A thorough and systematic characterisation of bud formation and nanoparticle wrapping at lipid-bilayer membranes is thus essential both for understanding basic biological processes in vivo and for developing bioinspired systems in vitro.

We use a continuum membrane model to study budding and wrapping processes at lipid bilayers [1]. With the help of triangulated membranes, we numerically characterise nanoparticle-membrane systems without the need for specific symmetries. For example, we calculate wrapping diagrams that characterise the parameter regimes where particles are complete-wrapped, partial-wrapped, or non-wrapped by a membrane. Furthermore, we discuss the importance of particle curvature, membrane curvature, and membrane spontaneous curvature for wrapping of nanoparticles [2-4]. In particular, we find complex nanoparticle-wrapping behaviour at small vesicles, where particle wrapping transitions and vesicle-shape transitions are coupled. Vice versa, partial-wrapped nanoparticles stabilise oblates and stomatocytes for particle entry, and prolates and stomatocytes for particle exit. Our systematic characterisation of the interaction of nanoparticles with lipid-bilayer membranes may help to shed light on passive aspects of highly-complex biological processes.

Translocation of Amphiphilic Peptides Across Phospholipid Membranes

Robert Vacha, Ivo Kabelka
CEITEC and Faculty of Science, Masaryk University, Czech Republic

Amphiphilic peptides and polymers can translocate across lipid bilayers without significantly perturbing the membrane structure. However, the molecular properties for efficient translocation are not fully understood. We employed Metropolis Monte Carlo method together with coarse-grained models to systematically investigate free energy paths associated with the peptide translocation. We investigated alpha-helical peptides with different length, amphiphilicity, and distribution of hydrophobic content and found common translocation path consisting of adsorption, tilt, and insertion. In the adsorbed state the peptides are parallel to the membrane plane, while in the inserted state the peptides are always perpendicular to the membrane. Our simulations showed that the most easily translocating peptides balance the hydrophobic content to be able to insert but also to escape from the membrane. Minimizing the free energy of translocation we obtained a linear relationship between the peptide length and its optimal hydrophobic area. Such optimal peptides could be used as carriers of molecular cargos or as therapeutics themselves.

Top-down development of mesoscopic polymer models: aligning interactions

Kostas Daoulas[1], Jaime Martin[2], Emily Davidson[3], Cristina Greco[4], Wenmin Xu[5], James Bannock[5], Amaia Agirre[2], John C. de Mello[6], Rachel Segalman[3], Natalie Stingelin[6]

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[2] POLYMAT, University of the Basque Country, Spain
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[4] Max Planck Institute for Polymer Research, Germany
[5] Imperial College London, UK
[6] Georgia Institute of Technology, USA

Theoretical studies of polymeric materials often require drastically coarse-grained (CG) models, representing large groups of atoms with a single CG site. Interactions in drastically CG models have a pronounced free-energy character and their determination from systematic coarse-graining [1-3] is challenging. Top-down strategies offer an alternative, where CG potentials are chosen such that the model reproduces by construction [3] a set of experimentally known properties. The Edwards model of polymer blends and block-copolymers is an example, where non-bonded interactions are captured through simple binary potentials. The
incompatibility between different species is controlled by the Flory-Huggins [FH] parameter. The determination of FH parameters has attracted significant attention and many strategies are available [4]. However, the Edwards model is insufficient to address cases where phase separation combines with other ordering processes. For example, when liquid-crystalline ordering occurs models with anisotropic interactions, e.g. Maier-Saupe (MS) are needed. Top-down approaches for constructing such models are significantly less developed, although multiple ordering phenomena are observed in many interesting materials, such as conjugated [5-7] homopolymers and block-copolymers.

We discuss a method for constructing models of conjugated polymers with nematic order. Polymers are described with discrete worm-like-chains [8], while non-bonded interactions are given by a MS potential. The strength of the latter is controlled by the MS parameter, which we determine [9] by combining numerical mean-field theory [9,10] with experiments. Our calculations take explicitly into account effects of temperature on persistence length, neglected in previous studies. We address cases where temperature has different impact on molecular conformations by studying rod-like, semi-flexible, and flexible conjugated polymers. To reproduce situations considered in earlier studies, we also extract the MS parameter neglecting deliberately the temperature-dependence of the persistence length.

We demonstrate [9] that subtle assumptions made in the CG model can affect the MS parameter qualitatively. Its temperature dependence is an example. Our findings have important practical implications, because MS parameters can provide guidelines [11] for designing conjugated polymers with improved alignment behaviour.

Diblock copolymer simulations: studying interlamellar roughness of BCP films on a coated substrate

Vladimir Lobaskin, Aleksei Kabedev
University College Dublin, Ireland

Directed self-assembly of symmetric block copolymers (BCP) has a number of promising applications in nanofabrication as the polymers can microphase separate and form structures with characteristic size of less than 10 nm. One of the widely used techniques developed for directed self-assembly (DSA) of BCP is a chemical nanopatterning of the substrates with lines, preferentially attracting one of the blocks, whereas the rest of the surface is covered with a polymer brush neutral to both blocks. Apart from directing the lamellae it affects the quality of the formed structures. The period of patterning lines is usually less than that of the copolymer, which makes it possible to lower time and expenses during the manufacturing processes. In this work, we use computer simulations to study the influence of monomer-monomer and monomer-substrate interactions in BCPs, polymer brush parameters and the factor of pitch multiplication on the orientation of the lamellae and on the width of the interface between them.

We use coarse-grained molecular dynamics simulation to study the nanoscale morphologies arising due to microphase separation in symmetric BCPs. The polymers are modeled as bead-spring chains, where a single bead corresponds to several monomers of the original molecule. The beads are connected with harmonic springs and angular bonds, and interact via Lennard-Jones-type potential. We include both repulsive and attractive parts of interaction between A-B and A-A/B-B blocks. The substrate is introduced via a constraint at the bottom of the simulation box, covered by tethered polymer chains. It is represented by either neutral brush (NB) or by combination of NB and patterning lines. Guiding lines are consistent of particles, having affinity to A-block monomers, whereas neutral stripes are made of mixture A and B beads distributed randomly. We are also studying the impact of pitch multiplication on the quality of lamellae.

Depending on the difference in strength of A-B and A-A interactions, in the case of patternless brush we find vertical, horizontal or mixed alignment of lamellar structures with respect to the substrate. Where the substrate is neutral to copolymers, vertical lamellae are likely to appear. Where A-A interactions are stronger than A-B more than fourfold, the adsorption of one bead block is preferred, and film tends to self-organize in horizontal lamellae. We introduce a technique to estimate the quality of the layered structures. We use the average nematic order parameter for polymers to get the direction of the normal to the lamellae and then measure the monomer density distribution function along this normal vector. Thus, we can quantify the width of the interface. We have also found that upon the growth of the bending rigidity of copolymer chains both line edge roughness (LER) and line width roughness (LWR) are decreasing. We also report on the influence of the polymer brush chains parameters on the quality of the lamellar structures. Vertical
lamellae were observed for a variety of polymer brushes with different ratio of A-block beads in range between 50 and 70 percent.

**Nonclassical ordered nanostructures from designed block copolymers**

Weihua Li
State Key Laboratory of Molecular Engineering of Polymers, Department of Macromolecular Science, Fudan University, China

The self-assembly of block copolymers provides a powerful platform for the fabrication of rich ordered nanostructures. From the aspect of practical applications, it is more useful to design block copolymers for desired ordered structures. In recent years, my group have been focusing on designing block copolymers to target some nonclassical ordered structures based on the calculations of self-consistent field theory (SCFT). The chain architecture of block copolymers with variable number of blocks and topology has been demonstrated as an important parameter controlling their self-assembly behaviors. Furthermore, blending different block copolymers together also offers an opportunity for stabilizing new phases. With AB-type block copolymers, complex Frank-Kasper spherical phases beyond the classical body-centered-cubic (bcc) phase, square-array cylindrical phase instead of the classical hexagonal phase, and perforated lamellar phase instead of the usual double gyroid phase are predicted. With ABC-type multiblock terpolymers, a large number of binary mesocrystal phases are predicted, including the prototypes of NaCl, CsCl, ZnS, BN, CaF2, TiO2, ReO3, Al2O3, Li3Bi, Nb3Sn, and even interesting dodecagonal quasicrystalline approximants. The self-assembly mechanisms of these nonclassical phases are also instructive to other soft matter systems.
Frustration in Block Copolymer Assemblies

An-Chang Shi
Department of Physics and Astronomy McMaster University, Hamilton, Ontario, Canada

The observation of ordered phases in hard-condensed matter systems such as metallic alloys has a long history in materials physics. In recent years, intricate periodic and aperiodic order has emerged in a host of soft matter systems including supramolecular assemblies, surfactants and block copolymers. The emergence of complex ordered phases in these diverse systems underscores the universality of emergent order in condensed matter. Recent experimental and theoretical studies have revealed that non-classical ordered phases, such as the Frank-Kasper phases and quasicrystals, could be self-assembled from block copolymers as equilibrium or metastable morphologies. Therefore, block copolymers provide an ideal system to study the origins and stability of periodic and aperiodic order in condensed matter physics. We have examined the occurrence of complex spherical packing phases in block copolymer systems using the self-consistent field theory. We have showed that a key mechanism of forming complex spherical phases is the conformational asymmetry of the blocks. Furthermore, we have predicted that the segregation of different polymeric species in block copolymer blends provides another mechanism to stabilize spherical packing phases with very different sized-spherical domains. In my presentation, I will summarize recent theoretical and experimental progresses on this fascinating topic and discuss possible future research directions.

Soft Matter: the inner frontier

Daan Frenkel
University of Cambridge, United Kingdom

The term "Complexity Theory" is unfortunate. It sticks a vague label on something that has a very precise meaning, namely the fact that most (possibly all) physical laws describe phenomena that are emergent: the collective behaviour of many entities is qualitatively different from that of the entity in isolation.

The boundaries of physics are wherever new laws emerge. Soft Matter Science is a field rich in such 'internal' boundaries. It is therefore a wonderful source of new physical concepts.

Computer 'experiments' play a key role in identifying the essential ingredients of an emergent phenomenon. Simulations do not replace theory, but they help to distinguish fruitful theoretical approaches from those that are less so.

In my talk I will discuss a few examples and finish with some homework assignments.
Simulation of chain diffusion in diblock copolymer nanostructures using dynamical self-consistent mean-field theory

Robert Wickham[1], Douglas J. Grzetic[2]
[1]University of Guelph, Guelph, Canada, Canada
[2]University of California at Santa Barbara

Understanding the influence of a block copolymer nanostructure on chain diffusion and, conversely, chain diffusion on nanostructure kinetics, is important to applications involving molecular transport, and to the question of the dynamics of defected structures. This talk will present results for unentangled chain diffusion in ordered phases of a diblock copolymer melt, from simulations based on our recently-developed dynamical self-consistent mean-field theory (dSCFT) [1]. In dSCFT, a saddle-point approximation to a dynamical functional integral reduces the problem of many interacting chains to that of the motion of a single chain under the influence of a dynamical mean force field determined self-consistently from the other chains. This hybrid, particle-field, multi-scale simulation enables one to study large-length and long-time scales in dense polymeric systems, while remaining connected to the microscopic dynamics of the interacting Brownian chains. In the LAM, HEX and BCC phases, chain diffusion perpendicular to the nano-domain interface is exponentially suppressed with increasing segregation, while parallel diffusion is unaffected. In the bicontinuous gyroid phase, the diffusion constant asymptotes at high segregation to a value consistent with chain diffusion along a three-dimensional network, characterized by network tortuosity value of 1.72. We also calculate the out-of-equilibrium evolution of chain diffusion as metastable LAM transforms to stable HEX over long times.


Efficient Incorporation of Momentum Transfer in Coarse-Grained Membrane Simulations

Agur Sevink[1], Friederike Schmid[2], T. Kawakatsu[3], G. Milano[4]

Hybrid Particle-Field (HPF) methods such as single-chain in mean-field (SCMF) and MD-SCF combine a serious gain in computational efficiency with the resolution
needed for addressing relevant detail at the molecular level. They do so by smearing local chemical structure of the molecule into global concentration fields for chemical species, and subsequently replacing the calculation of two-body inter-molecular interaction forces between chemical groups by much more efficient interactions between these groups and surrounding chemical concentration fields. Due to their increased efficiency, HPF methods enable the simulation of heterogeneous lipid membrane at overall time and length scales that are directly comparable to experimental setups, thus offering a more realistic handling of key factors in complex multiple scale phenomena such as liposome fusion. Yet, the additional smoothing poses a challenge for properly incorporating momentum transfer, especially the long-range transfer between the membrane and the solvent phases that is known to be important in both membrane formation and dynamics. In this presentation, we discuss an efficient solution for reinserting effective momentum transfer by coupling MD-SCF with multi-particle collision dynamics (MPCD), a method that mimics collisions on a coarse-grained cell level.[1] We will cover both the theoretical background and some exemplary simulation results, showing that momentum transfer can be efficiently incorporated and considerably speeds up the formation of liposomes compared to the current standards.


**Kinetic exchange of copolymer surfactants in micelles**

Josep Bonet Avalos, Fabian Alonso García-Daza, Allan D. Mackie
Departament d'Enginyeria Química, ETSEQ, Universitat Rovira i Virgili, Spain

The exchange of surfactants in micelles involves several processes which are difficult to characterize experimentally [1-4]. Microscopic simulations have the potential to reveal some of the key aspects that take place when a surfactant spontaneously exits a micelle. We present a study based on a dynamic version of a single-chain mean field theory [5] using a coarse-grained model for poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) triblock copolymer systems [6]. The kinetics described in our simulations involves three different regimes which span over a large range of time [7]. After a fast initial rearrangement of the labelled chains, the system undergoes a logarithmic relaxation [8], which has been experimentally observed [1-2]. Contrary to what has been stated in previous analyses, this regime is caused by the intrinsic physical behaviour of the system, and not only due to the polydispersity of the samples. Finally, the terminal regime is characterized by an exponential decay. The exit rates predicted by our simulations are in good agreement with the ones experimentally reported. In addition, we find a subtle variation of the radius of gyration of the hydrophobic block while exiting the
micelle, which challenges the vision of either a complete collapse or a full stretching commonly accepted in current theoretical and experimental literature [9].


SCF calculation of polymer composite materials

Takashi Honda
ADMAT:Research Association of High-Throughput Design and Development for Advanced Functional Materials, Japan

The SCF method of polymeric materials was improved, and the calculations of phase separation of polymeric materials in systems with three kinds of fillers (particle, fiber, and hexahedron) were done with MPI + GPGPU[1]. For particles, diffuse Interface was introduced and simultaneous optimization of phase separation structure and particle position was enabled [2].

Acknowledgement

This presentation is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

Hybrid block copolymer/nanoparticle systems: colloidal assembly

Javier Diaz\textsuperscript{[1]}, Marco Pinna\textsuperscript{[1]}, Andrei Zvelindovsky\textsuperscript{[1]}, Ignacio Pagonabarraga\textsuperscript{[2]}

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Block Copolymers are macromolecules composed of blocks of different repeated units. In the simplest case, diblock copolymers can self-assemble into ordered structures, and its morphology and overall properties can be modified by the presence of nanoparticles. The resulting nanocomposite can be highly ordered, and its properties depend on both the pure polymeric matrix and the shape, chemistry and volume fraction of the colloids.

The effect of nanoparticles with a strong compatibility with one of the components of the block copolymer is studied, finding an induced phase transition \cite{1}. On the other hand, incompatibility with both blocks leads to close-packed hexagonal assembly of colloids within the least unlike phase \cite{1}, which is in accordance with recent experimental results by Shenhar et al. In addition to this, a quantitative analysis of the morphology and self-assembly of BCP/nanoparticle systems is presented. Ellipsoidal particles are shown to reproduce the ordering of nanorods in a block copolymer, as was found experimentally.

In addition to the block copolymer morphology in the presence of nanoparticles, we study the colloidal assembly in nanocomposite systems, to assert the conditions of nanoparticle aggregation and ordering.

\cite{1} Díaz, Javier, et al. Macromolecular Theory and Simulations (2017).
Association model approach for description of hydrogen-bonding in block copolymers

Elena Patyukova[1], Martin J. Greenall[2], Paul D. Topham[1]

[1] Aston University, United Kingdom
[2] University of Lincoln, United Kingdom

Hydrogen bonds are common in nature. Despite they are weak, their effect of physical properties can be profound. The common examples include unusual properties of water and secondary structure of proteins.

One of the most natural ways to look at hydrogen bonding is to describe it as a reversible chemical reaction. This idea is exploited in association model approach [1, 2], which considers hydrogen bond formation as a reversible chemical reaction between donor and acceptor groups that produces (at equilibrium) a population of hydrogen-bonded “polymers” of different size and structure (linear or branched).

In our work, we first develop association model approach in order to allow it to describe hydrogen bonding association in case when it produces branched hydrogen bonded aggregates [1]. Apart from development of “one constant models” in which all hydrogen bonds have the same energy, we also consider “two constant models” with the aim to take into account some degree of cooperativity of hydrogen bonding. We apply developed models to describe association in solution of acrylamide in non-hydrogen bonding solvent and determine association constants for acrylamide by means of IR spectroscopy.

Then we use association model approach in order to describe hydrogen bonding in block copolymers with one self-associating hydrogen-bonding block (such as polyacrylamide (PAM) or polyhydroxystyrene (PHS)) and one non-hydrogen bonding block and calculate the contribution of hydrogen bonding into Flory-Huggins parameter. The advantages of association model approach are that it allows correctly count the number of hydrogen-bonding contacts between hydrogen bonding groups, all expressions are analytical and the values of association constants can be measured by IR spectroscopy. We end with presenting our first SAXS data for PS-b-PHS and PS-b-PAM systems.

Elastic properties and line tension of bilayer membranes

Jiajia Zhou
Beihang University, China

The elastic properties of a self-assembled bilayer membrane are studied using the self-consistent field theory, applied to a model system composed of flexible amphiphilic chains dissolved in hydrophilic polymeric solvents. Examining the free energy of bilayer membranes with different geometries allows us to calculate their bending modulus, Gaussian modulus, two fourth-order membrane moduli, and the line tension. The dependence of these parameters on the microscopic characteristics of the amphiphilic chain, characterized by the volume fraction of the hydrophilic component, is systematically studied. The theoretical predictions are compared with the results from a simple monolayer model, which approximates a bilayer membrane by two monolayers.
4 Posters

**Coarse-Grained Potential Derivation for Modelling the Self-Assembly of Block-Copolymers in Binary Solvents**

Gerardo de Jesus Campos Villalobos, Flor Siperstein and Alessandro Patti
University of Manchester, United Kingdom

Amphiphilic block copolymers in mixtures of selective and common solvents are able to self-assemble into colloidal size aggregates such as vesicles or more complex mesophases including polymeric nanospheres with bicontinuous internal structure (BPNs)[1], which have been recognised as excellent templates for the synthesis of nano-structured porous materials[2]. Motivated by their essential role in the preparation of complex self-assembled morphologies, we herein develop new computationally efficient coarse-grained models for studying by means of molecular dynamics simulations the phase and aggregation behaviour of methacrylate-based copolymers in mixtures of THF and water (common and selective solvents, respectively). The CG potential derivation is based on a hybrid thermodynamic-structural approach which incorporates macroscopic and atomistic level information, more specifically, the target properties in the parameterisation are those that govern the self-association mechanism (i.e. interfacial tension, chain conformational entropy and excluded volume repulsive interactions [3]). The resulting transferable model allow for the reproduction of the behaviour of copolymers in aqueous and organic solutions, melts and interfaces.

In particular we focus on mapping phase diagrams of these copolymers in binary solvents with emphasis on the morphological transformations of self-assembled aggregates as a function of the selective/common solvent ratio, polymer concentration and chain architecture. Our ultimate aim is to contribute to the development of the computer-based design of nanostructured materials.

Supramolecular Self-Assembled Prebiotic Biopolymer Systems on the Early Earth

Tony Jia[1], Henderson J. Cleaves[1], Kuhan Chandru[1], Rehana Afrin[1], Ankit Jain[2], Daniela Kroiss[2], Rein Ulijn[2,3]


The emergence of life is governed by the ability for a system to develop replication and metabolism. For these purposes, extant life utilizes biopolymers such as DNA and proteins, respectively. However, early cellular life likely did not have access to large amounts of these long biopolymers due to the inability for prebiotic systems to easily replicate these molecules. One area of recent interest is the possibility of using supramolecular self-assembly to assist in or catalyze these essential reactions. These self-assembly can be assembled from simple small molecules, short oligomers such as short peptides or polyesters, or even mineral surfaces; all of these components would have likely been readily available on the early Earth (much more readily available than longer biopolymers). The resulting structures, whether they are nanofibers, uniform sheets, crystalline structures, or phase-separated compartments, potentially give rise to novel emergent properties that the smaller individual components cannot. Here, we study the self-assembly properties and resulting supramolecular structures of various prebiotically relevant supramolecular systems, including short tripeptides, coacervate droplets, hydrogels, and polyesters. Although this work mainly focuses on astrobiology and origin of life questions, we hope to also explore engineering or materials science applications as well.

Coarse-grained potential for solid-polymer interface based on first-principles simulation; application to silica-polybutadiene interface.

Hiroya Nitta, Taku Ozawa
JSOL Corporation, Japan

Composite materials, such as fiber reinforced plastics, filler dispersed rubber, and materials bound with adhesive, etc., have been attracting interests in engineering field. These materials must have interfaces where two different materials meet, and the properties near the interfaces are expected to be different from their original ones. Molecular dynamics (MD) simulation is a powerful tool to investigate properties of the materials, however, force-field (FF) parameter appropriate to the
interfacial system is not always accessible. One approach to identify FF parameter is to minimize energy differences calculated in FF and first-principles simulation [1].

In the previous study [2], we have identified FF parameters for full-atomistic (FA) and coarse-grained (CG) models for silica-polybutadiene interface, however, we found that CG potential parameters need to be revised to obtain consistent results between FA and CG MD. We will present a procedure to refine the CG parameters.

Coarse-grained model of liquid-crystal polymer with efficient electrostatic interaction

Kenji Tagashira\textsuperscript{[1]}, Kazuaki Z. Takahashi\textsuperscript{[2]}, Hideo Doi\textsuperscript{[2]}, Jun-ichi Fukuda\textsuperscript{[3]}, Takeshi Aoyagi\textsuperscript{[2]}

\textsuperscript{[1]}Panasonic Corporation, Japan  
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Liquid-Crystal Polymers (LCPs) consist of open chain compounds containing mesogenic units. They exhibit high-responsiveness to external stimuli such as an electric field and magnetic field. Even though this characteristic could be applied to functional sensor and actuators, designing LCP materials and devices is still challenging due to their complex physical nature. To tackle this problem from a molecular point of view, a simulation study is a promising approach. In this work, for future applications of molecular dynamics simulations to problems involving an electric field, we develop a coarse-grained LCP model which possesses smeared charges on the ends of the mesogenic units (Gay-Berne particles) \cite{1}. For the smearing function of the electrostatic force, the Gauss error function is introduced. This smearing is optimized to attain a reasonable accuracy for phase transition phenomena of the liquid crystal while numerical instabilities arising from the singularity of the Coulomb potential are suppressed. The MD simulation system consists of 121 LCP molecules, each molecule containing 30 mesogenic units in a cubic cell. In addition, 3630 mesogenic molecules were added as a solvent. All of the simulations were done by the coarse-grained MD program COGNAC. The results show that our model exhibits the characteristics of liquid-crystalline orientational order and Rouse-like relaxation dynamics of unentangled polymer chains.

This study is based on results obtained from a project (P16010) commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

\cite{1} K. Tagashira, K.Z. Takahashi, J. Fukuda and T. Aoyagi, Materials 11 83 (2018)
# 5 Participant list

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6 Notes:
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Cathedral and castle

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Lincoln Central Station