The main focus of the group concerns hierarchical self-assembly, and how such processes can be modelled. The first project with this theme was "Creating a framework for modelling the hierarchical self-assembly of anisotropic building blocks".
The current project of the group is "Coordination chemistry on the nanoscale: Computational design of supramolecular building blocks capable of highly specific, orientation-dependent interactions", financed by UEFISCDI (project number PN-III-P1-1.1-TE-2016-1279). The project runs between May 2018 and April 2020.

Abstract:

With the advent of modern synthetic methods of nano- and mesoscale building blocks, it is now possible to encode complex self-assembling behaviour in relatively simple particles. However, the parameter space available for experimentalists is huge: one has to tune the building block anisotropy, interaction anisotropies, range, type etc. Computational methods can add valuable insight into the rational design of such building blocks. Coarse-grained modelling of anisotropic interactions can guide experiments into regions of the parameter space relevant to the desired target self-assembled structure.

The present project aims to establish a new field for the self-assembly of nanoscale building blocks, through applying concepts from coordination chemistry into designs of nanoparticles, which will become capable of highly specific coordination to other nanoparticles. Although the concept of 'colloidal molecules' exists, experimental realizations are still in their infancy. In order to understand the behaviour of such building blocks, and to create the simplest possible models for them, we will be using and further developing state-of-the-art methods in energy landscape theory (global optimization within the rigid body framework, discrete path sampling and rigid body MD).

In the first stage, we aim to explore the minimal physics required for assembly of hollow cages formed by nanoscale analogues of M_nL_{2n}-type Goldberg polyhedra, which are experimentally realized by square planar coordinated transition metal complexes with nonlinear bidentate ligands. We propose that cages with the same symmetry can be obtained using a combination of excluded volume and Coulombic interactions, and we will investigate the dynamics of hollow shell formation and transition between competing structures.

The second stage involves the design of novel anisotropic nanoparticles capable of tetrahedral, planar and linear coordination, giving rise to mesoscale structures analogous to hydrocarbons.

Group members working on the project:

- Dr Zoltan Antal
- Dr Lorand Czipa
- Janos Szoverfi

Computing resources:

Our computations are done on a small compute cluster by Supermicro, with three performant Nvidia Tesla K40M GPUs, and 44 CPU cores. Details of the architecture can be found here .

Contact:

The project is implemented in the R&D department of Provitam Foundation. Address: 16 Muncitorilor street, Sfantu Gheorghe, Romania.

Info about the previous research project (PN-II-RU-TE-2014-4-1176, October 2015 to September 2017)

The two years of the project enabled the establishment of the research group, which is now growing hierarchically. The project was financed by UEFISCDI (project number PN-II-RU-TE-2014-4-1176)

Objectives:

- creating a framework for modelling anisotropic building blocks across length scales, using advanced coarse-graining techniques

- studying the energy landscapes of selected hierarchically self-assembling systems

Abstract:

Hierarchical self-assembly is one of the most promising tools in nanotechnology. In biological systems, such processes have been already perfected during evolution, and involve successive formation of building blocks from smaller units, which in turn self-assemble into larger structures in a hierarchical fashion (e.g. virus capsid proteins, keratin filaments, amyloid fibrils etc.). Prese ntly, computational modelling of assembly processes on the nanoscale is possible only with coarse-grained methods, chosen appropriately for the size of the system and the particular problem. However, hierarchical self-assembly often happens across multiple scales, and each layer of the process has to be modelled differently: molecular mechanics force fields for protein folding, united atom force fields for oligomerization, shape-based coarse-grained models (e.g. bead models) for successive assembly of protein oligomers. To this date, no framework exists supporting modelling such processes across length scales.

The aim of the project is to use the experience of the PI with modelling anisotropic building blocks using the rigid body framework, and extend the method to bridge the gap between the different length scales. The method will involve a hierarchical calculation of building block parameters, obtained from extensively studying the energy landscape of their components. This

approach will be scale-independent, and will allow bottom-up design of novel complex structures on the nanoscale.

Project results:

During the project, we will created new methods and algorithms for determining coarse-grained parameters representing the shape of a building block modelled with atomistic potentials. Another priority was to determine the necessary conditions for selected building block shapes that determine their hierarchical self-assembling properties. We have created minimal physical models enabling hierarchical self-assembly into exotic structures such as Goldberg polyhedra, stacked rings, dodecahedral cages etc.

Summary of scientific activities between 01.10.2015 - 01.12.2016:

- development of hierarchical coarse-graining methods

- studying the aggregation of CCMV capsid proteins

- devising new design principles for hierarchical self-assembly by using macroions

A detailed version of the progress report can be downloaded from here .

Summary of scientific activities between 01.12.2016-30.09.2017:

- adaptation of the developed hierarchical coarse-graining methods for capsid proteins

- studying the dynamics of CCMV protein dimers, microsecond MD simulations

- designing addressable building blocks capable of hierarchical self-assembly

- creating a minimalistic model for hierarchical self-assembly of polyhedral shells of exotic symmetries

- coarse-grained modelling of spherical 'Blackberry' structures

Media

This video illustrates how kinetically trapped structures form in a system capable of forming a Kagome lattice (triblock Janus particles). This is a constant energy MD run adapted for ellipsoidal rigid bodies. Videos about large-scale rearrangements of self-assembling coarse-grained systems can be found on my Youtube channel .