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Qualitative and quantitative protein complex prediction through parallel simulations

In the last few decades due to the new high-throughput techniques and the Mass spectrometry we gained a big amount of data about Protein-Protein Interactions (PPI) and Domain-Domain Interactions (DDI). This opened the opportunity for computational methods to predicts protein complexes. Clustering algorithms can predict qualitative information about protein complexes, but it is important in the cases of proteins with many possible binding partners and with low abundance, the number of complexes formed are limited.

An approach to solve this problem is the SiComPre[1]. It uses stochastic simulation named Gillespie Multiparticle algorithm (GMP) [2], which has two parts, the classic Gillespie algorithm and the diffusion. The simulation runs in sub-volumes, that can be defined by the user and every SV belongs to a compartment. Proteins can react only in the same SVs and can change position by diffusion. The possible interactions are determined from DDI and PPI databases.

The SiComPre program has some weakness. The cell model is only two dimensional, the membranes are represented as a barrier, and through that only limited interactions can happen. In the new version, we want to implement a three dimensional cell model, the membranes are going to have a sub-volumes in which the membrane proteins and the trans-locating proteins can diffuse and interact.

We have implemented the core Gillespie algorithm that works on multiple sub-volumes and I started to parallelize on CPU first. We plan to finish and the fully parallelize our code during summer. We also want to predict the diffusion coefficients of the proteins and the complexes from the mass of the species. The reaction coefficients will depend on the protein complex.

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Summary

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