

High Performance Bioinformatics in RIKEN GSC

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RIKEN Genomic Sciences Center (GSC)

- **Established as an Center of Excellence in Genome Science in 1998**
- **Located at Yokohama Campus**
- **Five Research Groups and one group for services**
 - Genome Exploration Research Group
 - Protein Research Group
 - Functional Genomics Research Group
 - Computational and Experimental Systems Biology Group
 - **Advanced Genome Information Technology Research Group**
 - Genome Core Technology Facilities

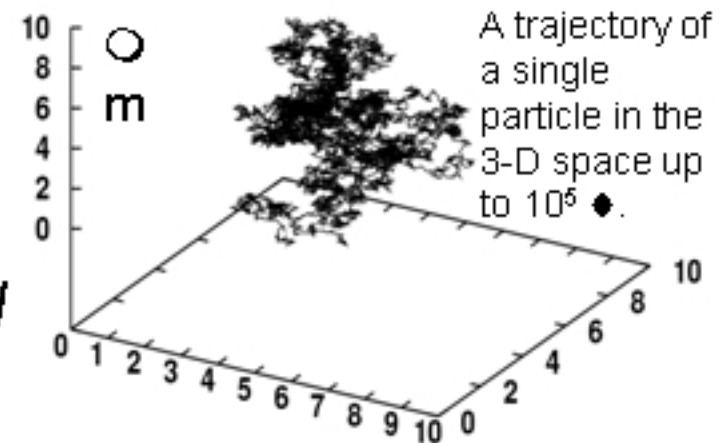
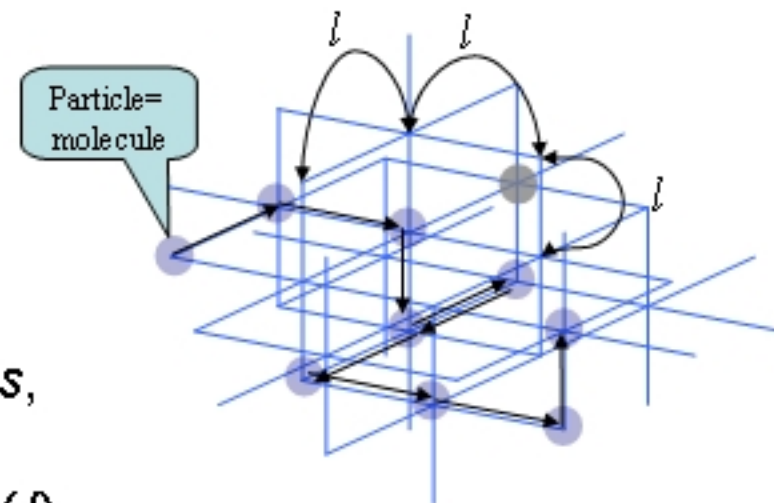


Activities related to the Gelato Consortium

- Gridification of Particle Simulation based on Monte Carlo Method (PSM)
- Parallelization of Particle Simulation based on Monte Carlo Method (PSM)

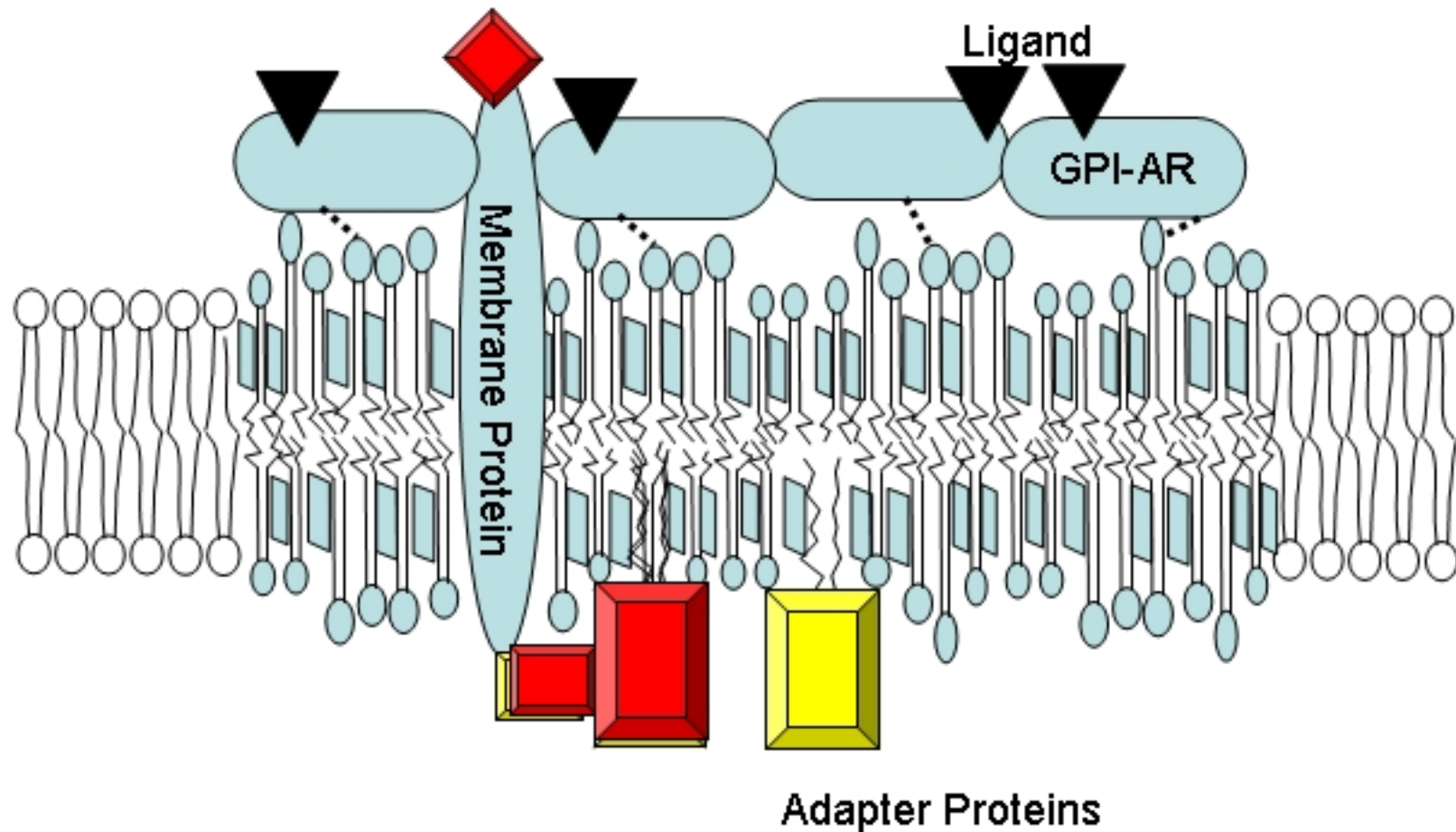
Particle Simulation on Monte Carlo Method (PSM)

- 2 or 3-D lattice space
- one particle=one molecule
- 3-D version of random walk
 - C.f. C.W. Gardiner (2004, *Handbook of Stochastic Methods*, Springer)
- Lattice distance = step length (l)
- Random selection of nearest neighbor site at random with an equal probability d ($< 1/6$).
- Diffusion coefficient D related to d
 - $D = 3fd$



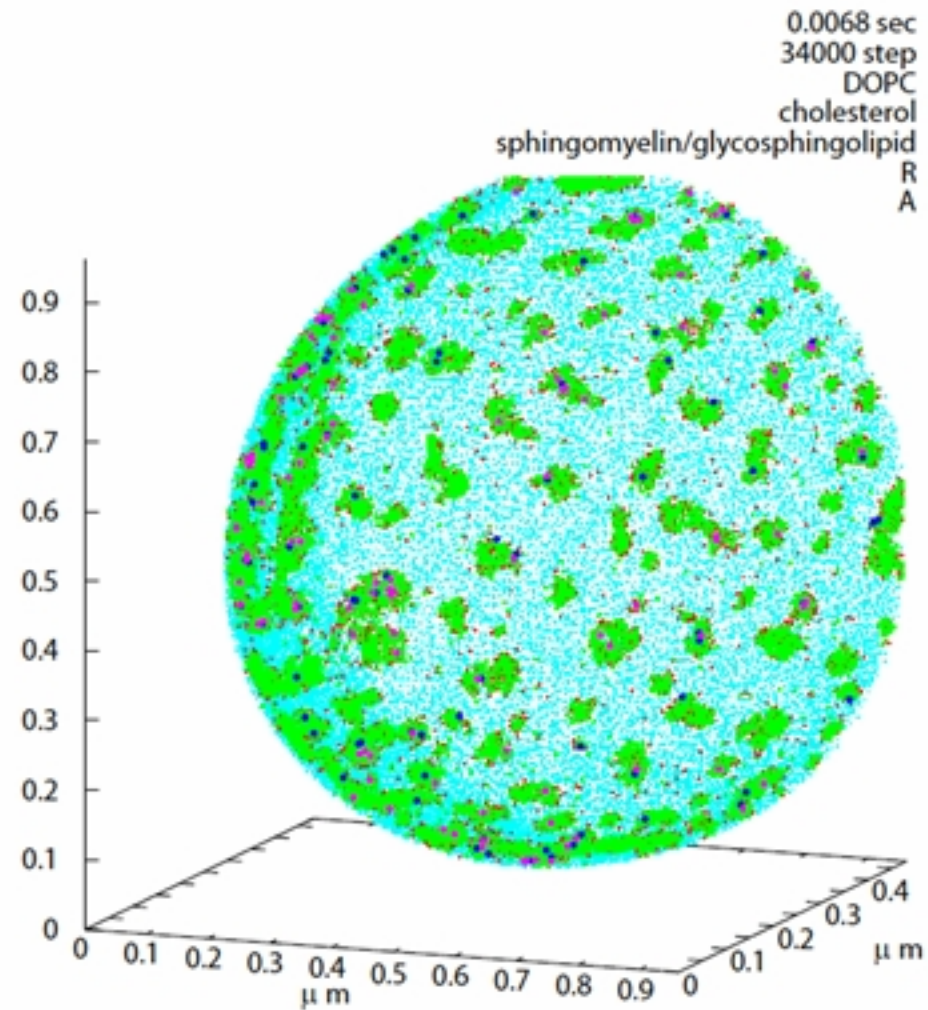
Raft Model

Enhance the possibility of the interaction between a membrane protein and its adapter proteins by constructing a raft-like structure.

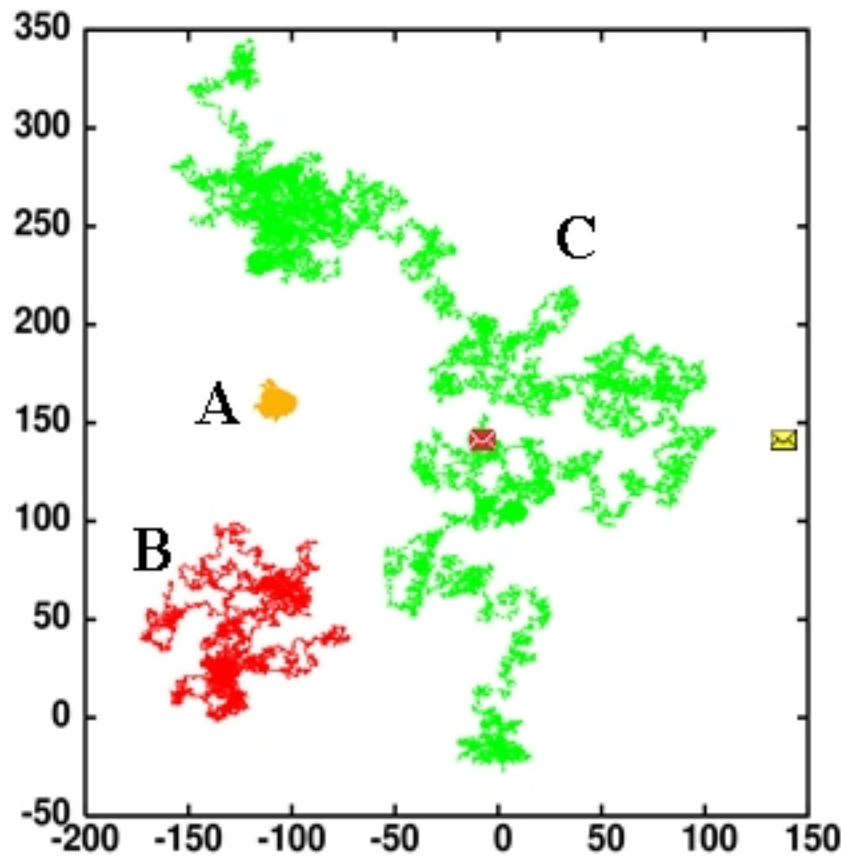


Azuma, R et al, "Particle simulation approach for sub-cellular dynamics and interactions of biological molecules", to be appeared in IMSCS06 (China, June)

Whole Membrane Simulation



Trajectory Analysis



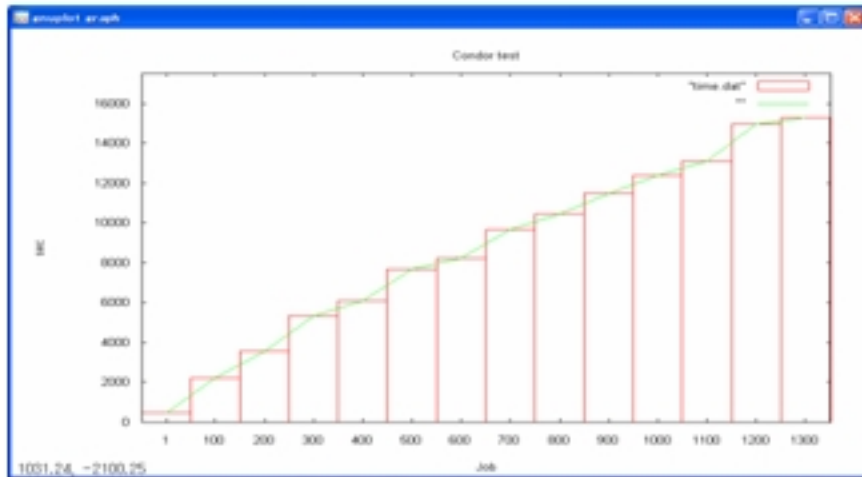
Trajectories of Cholesterol

- | | |
|----------|---|
| A | In a mini-raft (GPI-AR) |
| B | Inter-raft space
interacting with lipids |
| C | Free Cholesterol |
-

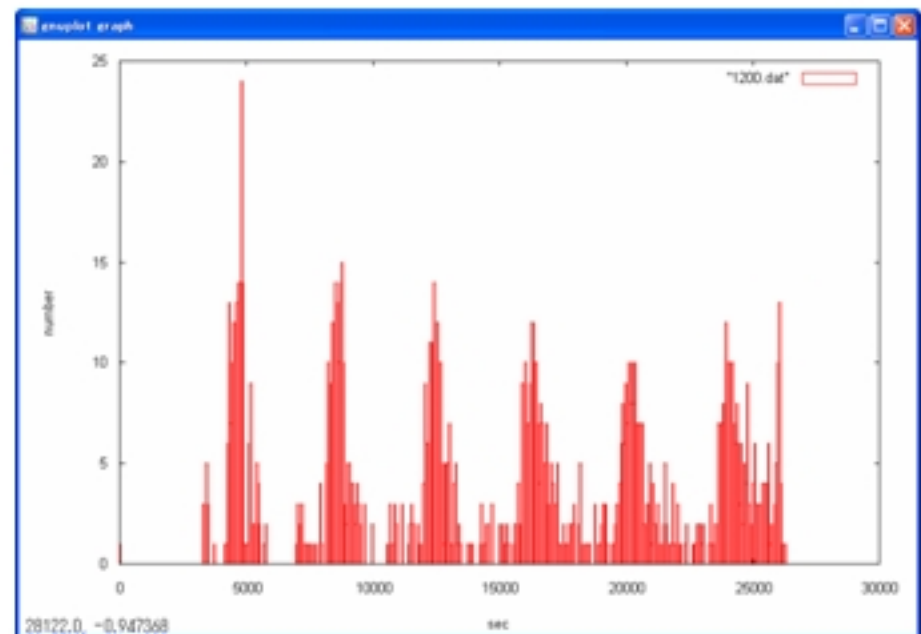
Ryuzo Azuma, Tetsuji Kitagawa, Hiroshi Kobayashi, Akihiko Konagaya:
Particle Simulation Approach for Subcellular Dynamics and interactions
of Biological Molecules, BMC Bioinformatics 2006, 7 (Suppl 4):S20

<http://www.biomedcentral.com/1471-2105/7/S4/S20>

Scalability for Knoppix Grid Computing



Throughput performance of PSM simulation running on an instant CONDOR pool (maximum 200 CPUs per user on heterogeneous computers)



Turn around time for 1200 tasks

http://big.gsc.riken.jp/index_html/Members/fumikazu/htc

Conclusion

- Whole membrane simulation requires huge computation power and storage
- Grid enables high-throughput computing for multiple trials and parameter sweep operations
- Needs parallelization to shorten the turn-around time of single run (16 days on a single Opteron 2.4GHz for whole membrane simulation)