IEEE TCSIM Newsletter

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Editorial Board

Chair's Message

By Dr. Dave Cavalcanti, Chair of TCSIM

Dear TCSIM colleagues,

First, I'd like to thank you for the support and opportunity to lead the TCSIM for another 3 year term. We have achieved a lot, but still have a long way to go, and I count on your contributions to make TCSIM even stronger in the coming years.

I'd like to introduce the new TCSIM Officers and newsletter editorial team appointed for the 2011-2013 term:

Prof. Kaushik Chowdhury, Vice-chair for North America,

Dr. Tommaso Mazza, Vice-chair for Europe

Dr. Chittabrata Ghosh, Vice-chair for Asia

Prof. Mostafa El-Said, Vice-chair for Africa/Middle East

I'm very excited to work with fellow colleagues who have been contributing to TCSIM for sometime and also to welcome new members to the team. I hope to see even more participation of the TCSIM membership in setting up the directions and plans.

Last but not least, I'd like to thank the authors and editorial team who have selected two new articles for this issue. The first article presents an overview of the N3Sim, a simulation framework for diffusion-based molecular communications. The second article discusses the framework for stochastic simulation of biological systems. Enjoy the reading!

Inside this issue:

TCSIM mailing list

In order to facilitate communication and information sharing with TC members, a new TCSIM mailing list has been created using the IEEE Listserv system.

To send a message to the new TCSIM list, just send mail to TCSIM@LISTSERV.IEEE.ORG

If you are not currently subscribed to the list please send a message to *Prof. Kaushik Chowdhury* at krc@ece.neu.edu who is currently managing all the subscriptions to the new TCSIM list. You can also search for the TCSIM list at http://listserv.ieee.org/

We hope you can make use of this new list to share simulation related information with the TCSIM community.

Upcoming TCSIM Sponsored Events

16 th International Conference on Computer Games: AI, Animation, Mobile, Interactive Multimedia, Educational & Serious Games (CGAMES 2011)
http://www.cgamesusa.com/index.php?choice=Home

9th International Conference on Computational Methods in Systems Biology (CMSB 2011)
http://contraintes.inria.fr/CMSB11

TCSIM Student Awards

"TCSIM supports students presenting ideas on exciting research frontiers through performance appreciation and travel awards."

In 2011, TCSIM will be sponsoring Student Awards in the Following Events:

- CGAMES 2011: http://www.cgamesusa.com/index.php?choice=Home
- CMSB 2011: http://contraintes.inria.fr/CMSB11
- MASS 2011: http://www.massconf.org/2011/

For more information on the TCSIM Student Awards, please visit the TCSIM web page (http://tab.computer.org/tcsim) or contact the TCSIM Chair.

Call for TCSIM Officer (Secretary)

TCSIM is seeking volunteers to join the TCSIM Officer's team as Secretary. Please contact the TCSIM Chair if you'd like to volunteer or learn more about the open position.

TCSIM 2010 Report and 2011 Operating Plan

TCSIM report and new operating plans can be found at:
http://tab.computer.org/tcsim/REPORT2010.pdf

N3Sim: A Simulation Framework for Diffusion-based Molecular Communication

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1. Introduction

Nanotechnology, the study of nanometer-scale systems, is a multidisciplinary field with potential applications in the biomedical, environmental and industrial fields [1, 2]. A nanomachine is the most basic functional unit able to perform very simple tasks at the nanoscale. These tasks include computing, data storage, sensing and actuation.

Nanonetworks, the interconnection of nanomachines, provide means for cooperation and information sharing among them, allowing nanomachines to fulfill more complex tasks [3]. Several techniques have been proposed to interconnect nanomachines. For the short range (nm to μm), one of the most promising techniques is diffusion-based molecular communication, a bio-inspired paradigm based on the use of molecules to encode and transmit information.

Several authors have developed analytical models of diffusion-based molecular communication [4, 5]. N3Sim (available at www.n3cat.upc.edu/n3sim) is a simulation framework for the general case of diffusion-based molecular communication, which allows validation the existing theoretical models and development of novel, more accurate models.

2. Simulator Architecture

We designed N3Sim in order to simulate a set of nanomachines which communicate through molecular diffusion in a fluid medium [4]. The information to be sent by the transmitter nanomachines modulates the rate at which they release particles to the medium. The variation in the local concentration generated by the transmitters propagates throughout the medium. The receivers are able to estimate the concentration of particles in their neighborhood by counting the number of particles in the environment. From this measurement, they can decode the transmitted information.

Figure 1 shows a block diagram of the steps needed to run a simulation. First, the user specifies the simulation parameters in a configuration file. These parameters include the number and location of transmitters and receivers, the size of the emitted particles and the diffusion coefficient of the medium, amongst others.

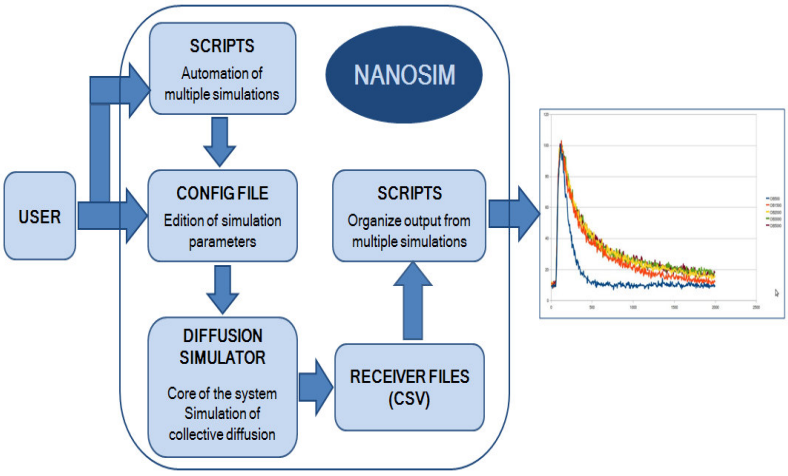

Figure 1. Block diagram for the N3Sim simulator

A set of scripts allows the user to run multiple simulations automatically, which is useful to easily evaluate the influence of a specific parameter (e.g. the number of transmitted particles) in the system output. Next, the diffusion simulator takes the configuration file and the automation scripts as input, and performs the actual simulation of the diffusion-based molecular communication scenario. When the simulation is finished, its outputs are stored in receiver files (one per receiver), which contain the concentration measured by each receiver as a function of time. Last, another set of scripts may be used to organize the results from several receivers and graphically represent them into a single plot.

3. Simulation results

In order to illustrate the capabilities of the simulator, we show the results of a simple simulation performed in a 2-dimensional space with a circular transmitter and receiver of 100 nm in radius. Figure 2 shows the transmission of a Gaussian pulse consisting of 106 molecules, and the received signal, defined as the number of particles detected by a receiver as a function of time, at 500 and 1000 nm from the transmitter location, respectively.

We observed that the molecular channel alters the shape of the pulse. As the transmission distance increases, the received pulse is lower, wider and has a longer tail, due to the effect of diffusion.

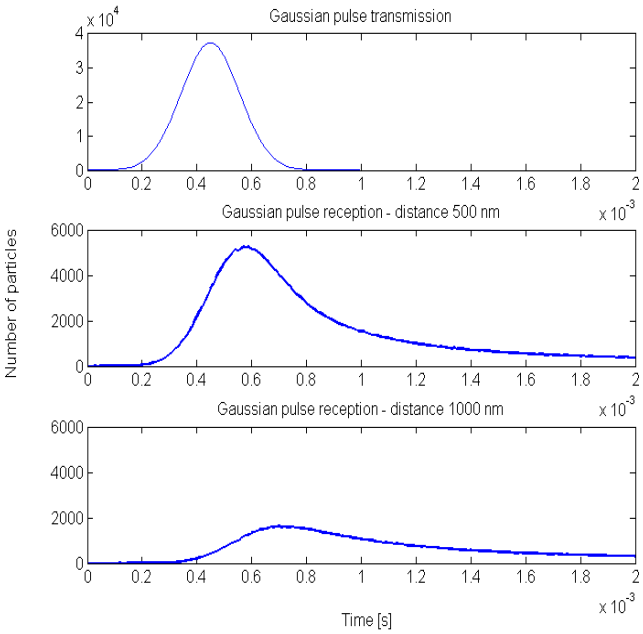

Figure 2. Transmission of a Gaussian pulse

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Anatomy of parallel stochastic simulation of biological reactive systems

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1. Introduction

In computational biology, the interest in multi-processors computing has been growing over the years. The additional computing power provided by high performance computers allowed scientists to face the Monte Carlo simulation task from two different points of view: (i) by parallelizing across the simulation, namely computing different stochastic trajectories to execute simultaneous and independent simulations of the same system (Multiple Replications in Parallel, MRiP); (ii) by parallelizing across the method, namely by distributing the realization of a stochastic trajectory to the available processors and coordinating the overall process (Single Replication in Parallel, SRiP) [1]. SRiP methods can be further divided into two sub-categories: (a) the one that aims at dividing the physical space in a finite grid, whose cells are handled by individual processors [2, 3]; (b) the one that aims at orchestrating multi-processors to simulate the trajectories of the same system in a controlled manner. Whereas MRiP found straightforward application to real case studies [4, 5], the latter lacks of a guideline and is a rather vague task. Despite all the successes achieved in other research fields, the parallel processing community did not still provide an efficient tool for distributing the stochastic simulation of a biological system. Thus, we sketch here the skeleton of a plausible framework.

2. Methods

Parallel simulation requires that a biological system to be divided into sub-systems and that each of them to be assigned to one processor to be simulated independently. Partitioning is hence a critical task.

Our partitioning solution deals with a *metabolic dependency graph* (mdg), which is a kind of workload graph obtained by a deterministic transformation of a *metabolic graph* (mg). An mdg is a lightweight data structure where vertices represent biochemical reactions and edges correspond to dynamical dependencies (Let R be the set of chemical reactions, reaction R_A depends on another reaction R_B if and only if:
$\exists\, r_i \in reactants\{R_A\} \mid r_i \in reactants\{R_B\} \cup products\{R_B\}$, where i = 1,...,|R| [6]). Weights over the edges stand for the kinetic propensities of the reactions where they issue from.

In Table 1, the six biggest mgs, gathered from six different biological repositories, have been considered. We got them as SBML [7] records and transformed into mdgs. Connectivity properties have been preliminarily assessed (see Table 1) for diagnostic purposes. If favorable, a graph has been divided into sub-graphs and simulated in a time-controlled environment and in a hybrid way by as many computational units.

The paper introduces a non-conventional and ad hoc greedy clustering algorithm which reconfigures a mdg in sub-networks, by fulfilling the following critical steps: (i) the generator node of each cluster must have the higher centrality measure; (ii) the number and weight of cut-edges among clusters must be minimized; (iii) cut-edges weights must be balanced as much as possible and (iv) paths among clusters must be the shortest.

The first is the condition that a generator node of a new cluster is chosen for. We considered (e.g.) the degree as a measure of centrality, and chosen the first vertex ũ of the i_{th} cluster by computing the following measure:

$$\tilde{u} = \underset{u \in \mathcal{P}_i}{argmax}(d_{out}(u)).$$

Here, d_{out} corresponds to the outgoing degree of the vertex ũ, and P_i is the set of chemical reactions with the same maximum propensity value.

Since edges represent synchronizations among clusters, the second condition guarantees a minimum overhead of communication. The more communication among clusters, the more relevant a synchronization load would be. In minimizing the inter-fluxes, we also tried to balance the communications load. As long ago as 1984, Jefferson [8] conjectured that a (balanced) realistic system rollback is not as costly on the average as one might fear because most programs obey a temporal locality principle. The third condition kept the rollback cascade problem under control, by minimizing the number of inter-clusters paths.

Once clustered, each sub-graph is assigned to a computational unit, called *local process* (LP), to be simulated. LPs enclose an operational logics designed to switch between a deterministic and a stochastic simulation modality. Holding the same units of measurement (in terms of number of molecules and time), the switch between both modalities is guided by demons, which ceaselessly monitor a permutation condition accurately justified by Vasudeva and Bhalla in [9]. Each LP initializes the computation by setting the starting species quantities and the simulation time to the values updated by the previously preempted execution. They run separately as if they were alone.

Database	Model	Reactions	Dependencies	Sparseness	E(Degree)	E(H&A)	C
JWS Online	*Kinetics of human erythrocytes*	38	176	0.12	3.38	2.82	0.75
	$G_{38,38}$	38	361	0.25	3.64	3.64	0.00
Kegg	*Purine metabolism*	48	111	0.05	3.75	2.72	0.78
	$G_{48,48}$	48	576	0.25	3.87	3.87	0.00
PANTHER	*Wnt Pathway*	62	132	0.03	3.95	2.26	0.74
	$G_{62,62}$	62	961	0.25	4.13	4.13	0.00
BioModels	*3-stage MAPK*	300	7101	0.08	5.36	5.27	0.50
	$G_{300,300}$	300	22500	0.25	5.70	5.70	0.00
Reactome	*Reactome of Homo Sapiens*	1917	77951	0.02	6.49	5.57	0,80
	$G_{1917,1917}$	1917	918722	0.25	7.56	7.56	0.00
Gepasi	*100 Yeast Cells*	2000	11200	0.003	7.45	6.98	0.79
	$G_{2000,2000}$	2000	1000000	0.250	7.60	7.60	0.00

Table 1: Topology properties of mdg_s and $G_{k,k}$ (complete regular bipartite graphs) in comparison. Sparseness accounts of the ratio between the number of dependencies/edges and the square of reactions/vertices; Degree and H&A are rankers based respectively on the node degree and the *hubs-and-authorities* importance measures. The latter index corresponds to the mean value of the clustering coefficient computed for each node. The entropy function is applied to the Degree and H&A distributions to estimate their homogeneity.

According to the workloads, some LPs can run faster than others. This is often the cause of an unpredictable race-condition, according to some inter-node interactions, which can be disregarded. A way of overcoming this issue is to globally monitor and synchronize the local executions, by computing and handling a Global Virtual Time [10].

Due to the greedy nature of the algorithm and to the dynamicity of the dependencies, the obtained partitioning could not always be optimal, along the simulation. We envisage post-refinement phases, which would migrate the critical nodes through the clusters in run time.

3. Results

Since the sparseness index [11] computed for the first model in Table 1 was favorable (0.12 vs 0.25 of a complete bipartite graph with the same number of vertices), we applied our algorithm and successfully divided it.

Firstly, the algorithm looked for the most important node of the network and grouped its closest neighbors over it (a).

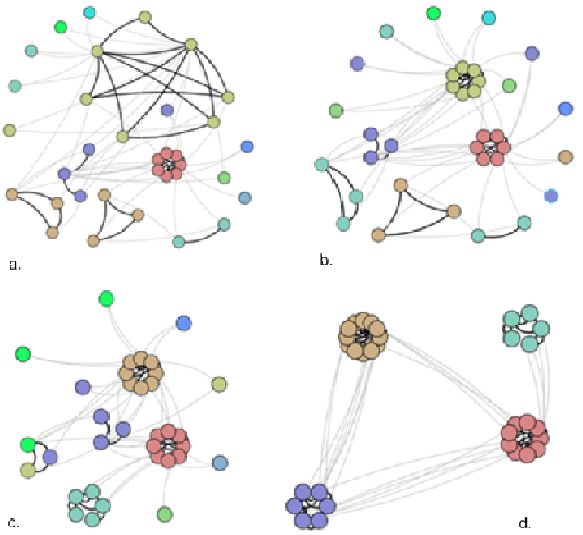

Figure 1: Energy metabolism of human erythrocytes – clustering

Then, it looked for the second most important node among the remaining nodes, making this the center of a new cluster (b). This routine looped until all nodes were grouped (c, d). Since we had chosen to finally have 4 clusters, then the algorithm looked for and picked 4 hubs during the partitioning step. This partitioning did not require any further refinement. It was optimal.

Future studies will focus on optimal rollback strategies, load balancing, and graph rearrangement benchmarks with the aim to provide quantitative insights, as well. *Any form of collaboration is welcome!*

4. References

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Call for Papers – IEEE TCSIM Newsletter

The IEEE TCSIM Newsletters will publish short technical papers. The submissions should emphasize modeling, design, and analysis of computational methods for simulations and its applications in various areas, including, but not limited to, computer science, engineering, communications, and simulation applications. The submissions are invited covering, but not limited to, the following topics:

- Simulation architecture modeling and prototyping
- Simulation algorithm design, implementation, and analysis
- Simulation complexity in computing
- Parallel and distributed simulation
- Design and usage of simulation tools
- Real-time simulation monitoring
- Simulation tools for communications and networks
- Simulation of computer systems and applications
- Agent-based simulation tools focus on the use of agents in engineering, human and social dynamics, military applications
- Systems and process simulation
- Simulation of ubiquitous networking and computing
- Simulation of transportation systems
- Automotive simulation applications
- Building and energy management simulations
- Machine learning
- Virtual reality systems
- Knowledge and data systems
- Systems optimization
- Web-based simulation and applications
- Department of Defense Architecture Framework (DoDAF)-based network simulations
- DoDAF-based vulnerability assessment

Submission

All papers must be submitted to elsaidm@gvsu.edu in four pages or fewer, including all figures, tables, and references. A manuscript submitted for publication should be original work that should not have been previously published and should not be under consideration for publication elsewhere. If an author uses charts, photographs, or other graphics from previously printed material, he/she is responsible for obtaining written permission from the publisher to use the material in his/her manuscript. The maximal number of figures and tables are five, and the number of reference is limited to ten.

Please submit electronically in DOC/PDF file, and ensure that the submitted file can be viewed in Acrobat Reader 9.0. A standard IEEE copyright release will also be required before full acceptance.

Article submissions are encouraged throughout the year, though the deadline for the next quarterly newsletter is four weeks from its publication date. Submitted articles go through a quick peer review, and authors are notified of the result within three weeks.

In the event that a particular cycle has large number of submissions, the editors reserve the right to schedule their publication in the subsequent editions of the newsletter.

All papers must include the authors' affiliation and e-mail addresses of all authors. All papers will be fully refereed for accuracy, technical content, and relevance. Contact Dr. El-Said at elsaidm@gvsu.edu with any questions concerning the paper submission and review process, or questions regarding the relevance of a paper to the IEEE TCSIM Newsletters.

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