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PARALLEL TECHNOLOGIES IN SOME PROBLEMS OF NETWORK MODELING

M. H. HOVHANNISYAN *

Chair of Programming and Information Technologies YSU, Armenia

The paper is devoted to the analysis and programmatic implementation of directed evolution processes in complex networks. We describe the evolution model and present requirements for implementation. Then we display the developed system in architectural form and present the performance evaluation.

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Introduction. Complex networks are widely investigated due to various critical and collective effects [1, 2]. One of those is the first-order phase transition analogue in random networks under certain conditions [3], shed light on the analogy between random networks behavior and various physical phenomena. These results were obtained by specific modeling techniques applied to random networks. In general, modeling plays a significant role in science, since it allows to confirm or decline theoretical hypothesis. The modeling can also help to discover previously unknown and hardly predictable phenomenon. As a consequence, the programmatic modeling of random networks and various processes in them becomes actual. The results should be obtained on large networks to be correct enough, so the problem of modeling is also a resource usage optimization task.

There are many different libraries in the area of network modeling. Major mathematical packages include routines to work with graphs and networks. These can be used for various actions, but they are mostly generic, require acquaintance with specialized scripting language and do not take into account specific caveats in certain problems. This paper is devoted to analyzing usage of parallel technologies in some specific processes of modeling problems. It will be described an appropriate model and presented the architecture of developed system and main characteristics.

The structure of the paper is following. First the model description will be presented. Then we will describe, consequential requirements for software implementation. Then, we present the solution and its analysis and finally, the conclusion and some additional information on publications.

Model Description. We consider undirected graph model, which is given by the pair $G = (V,E)$, where $V(G) = \{x_1, \ldots, x_N\}$ is a non-empty finite set of vertices and $E(G)$ is a finite set of edges. Graph produces a symmetric adjacency matrix A with elements $a_{ij} = 1$ if $(x_i, x_j) \in E(G)$ and $a_{ij} = 0$ otherwise. Further, a term *network* will be used to designate undirected graph model. The vertices of the graph G, representing the network, are referred as nodes, and the edges are referred as links.

* E-mail: minas.hovhannisyan@gmail.com

Let $T(G)$ be the number of cycles of length 3 of the network G. Now consider the process of network evolution toward the growth of $T(G)$. The evolution process is a sequence of transformations of graphs $G = G_0, G_1, G_2, \dots G_k$, $k >> 1$, i.e. a random process in which each successive graph is obtained from the previous one by switching links. Switching can conserve some local or global property. We will consider the following two cases:

1. Degrees of nodes are preserved [3] (depicted on Fig. 1);
2. Degrees of nodes are not preserved [4] (depicted on Fig. 2).

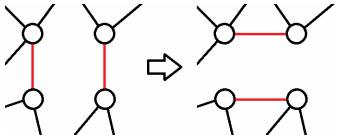

Fig. 1. Link switch with degree conservation.

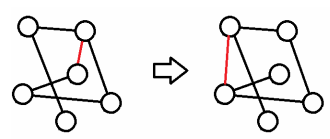

Fig. 2. Link switch without degree conservation.

The value of $T(G)$ may change during the switching. Let $\Delta_i = T(G_i) - T(G_{i-1})$, $1 \le i \le k$, which is a one-step change. To accept or reject network resulting from such a switch, we use the Metropolis-Hastings algorithm. Namely, the probability ω of acceptance or rejection of a switch is determined as follows:

$$\omega = \begin{cases} 1, & \text{if} \quad \Delta_i \ge 0, \\ e^{\mu \Delta_i}, & \text{if} \quad \Delta_i < 0, \end{cases} \tag{1}$$

where μ is the parameter of model; higher μ values correspond to lower probabilities that the network is accepted with a lower value of $T(G)$. The evolution continues until the *stabilization*, i.e. until the system reaches a state in which the number of cycles of length 3 does not tend to change over a sufficiently long series of switches, $\Psi(G, \mu)$, and the system only fluctuates around some value. It is natural to associate such a state with equilibrium. The evolution itself is represented by evolutionary *trajectory*, $\mathbb{T}(G, \mu)$, i.e. the variation of the number of cycles of length 3 along the number of elementary switches (time). $|\mathbb{T}(G, \mu)|$ will denote the length of trajectory (which coincides with overall evolution time).

The process of network directed evolution with link switching is called *randomization*.

This model discovers critical effects in random networks during the directed evolution [3–6]. In the case of node degree conservation this shows up a disintegration of the network into dense clusters with weak interconnections. If there is no node degree conservation, then one can observe a constriction of the network into single dense cluster with a vapor of nodes around it. Namely, a critical value of the model parameter, μ_c, exists and no critical effects are observed below μ_c,. Above μ_c, the evolution leads to the reconstruction of the network. Depending on the parameters of the input network the evolution requires various run-times to reach the stabilization.

As a consequence, programmatic implementation needs to satisfy several requirements in order to allow acceleration and automation of research process.

Requirements for Implementation. Initial analysis of model allows to describe requirements for programmatic implementation of the evolution modeler:

1. *Large Input Networks Support.* This requirement comes from network theory, since it requires large networks (theoretically at ∞) correct results.

2. *Long Trajectories Support.* Stabilization may require long trajectories to come on, and the requirement of generating trajectories with large $|\mathbb{T}(G, \mu)|$ is reasonable.

3. *Range-Based Parameter Investigation.* Various ranges of the model parameter should be considered to discover critical effects and their dependency from parameter. Also same range can be considered with various steps to discover critical point with necessary precision. Thus system should allow to investigate ranges of parameter with specified step.

4. *Optimal Usage of Resources.* This requirement comes out from the previous ones. Taking into account the volume of calculations for parameter value ranges in the case of large networks and long trajectories, the resource usage problem can be considered as central.

5. *Results Visualization Support.* Visualization of trajectories, local/global properties and networks/matrices allows to make initial conclusions and assumptions on the obtained output.

A deeper analysis of the network evolution model shows possible places for application of parallelization techniques:

1. The evolution process is sequential and rather difficult to parallelize. Each step is dependent on the result of previous one, the network during the step can be changed and next step of the process should consider this. But analysis of two presented modes of evolution shows that some critical parts can be parallelized to speed up process. Details are presented in next section.

2. Modeling process assumes necessity to model evolution for different values of input parameter μ on the network ensembles. There are two options of parallelization in this situation. First, parallelize over different values of model parameter μ and ensemble members. Parallel instances in this case will be memory independent and processes can be used for the purpose. Second, parallelize algorithm of evolution (or some parts of it). Parallel units in this case are memory bounded and threads usage will allow to gain high performance.

Architecture of Implementation. To model network evolution and analyze results software system was developed with accordance to presented requirements. In Tab. 1 is shown high level architecture of system.

It consists of 3 layers:

1. *User interface* provides user with command set to perform the evolution and analyze the results. Layer consists of shell scripts, which wrap core tools with user-friendly interface. Each script provides appropriate options to control the execution flow and the descriptions for them.

2. *Helper/intermediate staff* provides convenient ways to convert the formats of input and output networks, converting the output data for the follow-up analysis and for other similar functionalities. Layer includes scripts and underlying programmatic utilities.

3. *Core* implements evolution modelers, counters for different network properties, tools for network manipulation (f.e. extraction of subnetworks and clusters). Layer uses C++ programming language for high-efficient implementations of tools.

Table 1

High level architecture of system

User Interface (Shell wrapper scripts collection)
Helper Stuff (converters, scripts for third party tools, etc.)
Core (Implementation of evolution modelers, network manipulation tools, property counters, etc.)

Here we present the structure of the core part. Core consists of several specialized components:

• Central component of core is network container, which holds nodes and links in memory and provides efficient ways to manipulate them. Component implements the memory-efficient and performance-oriented representation of large networks.

• Networks and network ensembles are generated with appropriate component.

• Specific components allow to calculate various local and global properties of networks, calculate eigenvalues and eigenvalue density of network adjacency matrices and extract subnetworks to perform above-mentioned analyzes.

• Component, which is responsible for evolution modeling, is called *evolutioner*. It generates trajectories for input networks with the specified μ parameter values. To allow simultaneous generation of trajectories for a range of parameter values, parallelization with usage of MPI architecture is applied. MPI is used due to the following reasons:

– scalability from parallel computers to clusters;

– portability between various platforms;

– point-to-point and collective communication between processes;

– automatic and efficient process management.

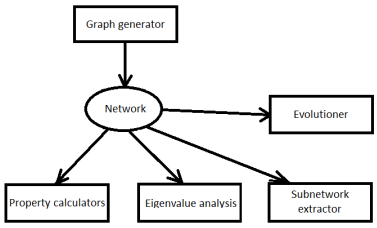

Fig. 3. Architecture of core.

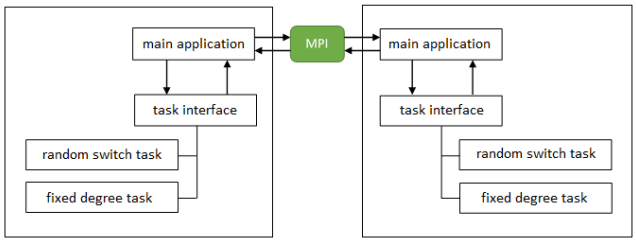

Fig. 4. Architecture and interaction diagram of core.

Structure and interaction scheme of evolutioner is presented in Fig. 4. Main application class defines routines for input data load and distribution between peers, interaction of running processes through MPI interface and results processing. Task interface defines interaction mechanism between main application and specific tasks, which define implementation details. Two tasks are implemented in the system for earlier described variants of edge switching. Each of implementations use specific caveats in according algorithm to decrease execution time and get necessary results faster.

Algorithms of Evolution. Let us describe the randomization algorithms.

Algorithm 1 . Generic Randomization Algorithm.

procedure RANDOMIZATION(G, μ)
  $trajectory \leftarrow [\,]$
  $prop \leftarrow CalculateObservedProperty(G)$
  $trajectory.append(prop)$
  while $!Stabilized(trajectory)$ **do**
    $\Delta prop \leftarrow RandomizationStep(G, \mu)$
    $prop = prop + \Delta prop$
    $trajectory.append(prop)$
  return $trajectory$

Algorithm 1 provides general view on the process of randomization. As an input this routine accepts the initial graph and the value of model parameter μ. The output contains the sequence of the observed property values on the time domain, i.e. the trajectory. The algorithm calculates the initial value of the property and during the following steps incrementally updates it. The process continues to perform randomization steps until reaching the stabilization. There are two ways to determine this. At first, the track is changed over a large count of trajectory steps and calculate the variance. This approach make additional calculations at each step and, thus, increase overall runtime of algorithm. The second, manually define the number of steps to perform and stop the process after reaching that number.

First, the case with degree-conservation of vertexes is presented. Algorithm 2 contains sequence of steps performed at each step of randomization in this case. Initially, two random edges are selected under the condition that sources and targets of those are not connected. The edges are removed and two new edges are added between the sources and the targets of the removed edges, respectively. Then, the change in the observed property is calculated. Based on it, the probability of accept/reject of the performed step is calculated according to equation 1. This probability is used as a parameter for the random generator with Bernoulli distribution. The outcome defines whether to accept or reject the current step. Finally, the procedure returns the change of the observed property.

Algorithm 2 . Algorithm of Randomization Step with Degree Conservation

```
1:  procedure RANDOMIZATIONSTEP(G, μ)
2:      e1 ← GetRandomEdge(G)
3:      e2 ← GetRandomEdge(G)
4:      RemoveEdge(e1, G)
5:      RemoveEdge(e2, G)
6:      AddEdge(e1.source, e2.source, G)
7:      AddEdge(e1.target, e2.target, G)
8:      Δ ← CalculatePropertyChange(G)
9:      p ← CalculateProbability(Δ, μ)                ▷ Calculated by 1
10:     if 0 == BernoulliDistribution(p) then
11:         RevertChanges(G)
12:         Δ ← 0
13:     return Δ
```

There are two compute-heavy parts in these algorithm. First, random edge generation (procedure *GetRandomEdge*()). To speed up random edge generation, parallel threads are used for the each generated edge. Second, property change calculation (procedure *CalculatePropertyChange*()). More advanced technique is required for parallelization of this routine. Edges to remove and add are available at the point of computation, and it is necessary to calculate count of added and removed triangles as a result of performed switches. This operation is local and requires to traverse only neighbors of nodes participating in switch and appropriately handle repeating triangles. All nodes proceed parallel, thus, this increases overall speed of calculation. Beside the addition and the removal of the edges is done by parallel threads and this also have a positive impact on process run-time.

Algorithm 3 presents the randomization without degree conservation. The randomization step at the beginning uniformly selects random edge from the set of all edges of network and removes it; after that, a disconnected pair of vertexes is selected and connected by an edge. The pair should be selected uniformly from the set of all the available pairs of the unconnected vertexes. To ensure this, the randomization algorithm should be slightly modified. Namely, after calculating the initial value of the property, it collects all pairs of the unconnected vertexes at the moment. This is done by the quadratic traversing of all vertexes

in the network and storing the necessary ones. OpenMP loop parallelization is used here for the better performance. As in previous case, property change is calculated after performed actions and the value is used for probability calculation. According to that value, decision is made to continue or revert performed changes. Finally, algorithm returns the calculated delta of property value.

Algorithm 3. Algorithm of Randomization Step without Degree Conservation

```
1:  procedure RANDOMIZATION(G, μ)
2:      trajectory←[]
3:      prop← CalculateObservedProperty(G)
4:      trajectory.append(prop)
5:      pairs ← FindAllUnconnectedVertexPairs(G)
6:      while! Stabilized(trajectory) do
7:          Δprop ← RandomizationStep(G, μ)
8:          prop = prop + Δprop
9:          trajectory.append(prop)
10:     return trajectory
11:
12: procedure RANDOMIZATIONSTEP (G, μ)
13:     e ← GetRandomEdge(G)
14:     ⟨v1, v2⟩ ← GetRandomPair(pairs)
15:     RemoveEdge(e, G)
16:     AddEdge(v1, v2, G)
17:     UpdateUnconnectedPairs(pairs)
18:     Δ ← CalculatePropertyChange(G)
19:     p ← CalculateProbability(Δ, μ)          ▷ Calculated by Eq.(1)
20:     if 0 == BernoulliDistribution(p) then
21:         RevertChanges(G)
22:         Δ ← 0
23:     return Δ
```

The main part in this algorithm, which is exposed to the parallelization, is the property change calculation routine. This, as in previous case, is a local procedure and a parallel examination of neighbors of participating vertexes is enough to get result.

Table 2

System performance results

N	64					256					1024				
p	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
R t_1, h	0.023	0.025	0.031	0.050	0.053	0.050	0.190	0.370	0.690	1.390	0.92	4.70	11.75	29.20	59.50
R t_2, h	0.012	0.014	0.016	0.018	0.020	0.040	0.120	0.240	0.340	0.390	0.84	2.50	6.60	12.70	17.40

System Performance. To perform analysis of developed system performance, Erdös-Rényi random graph model was used. In put networks were constructed with the following parameters: $N = 64;\ 256;\ 1024$ and $p = 0.1;\ 0.3;\ 0.5;\ 0.7;\ 0.9$. Tab. 2 presents appropriate run-times for two cases of randomization step for the generated networks with $|\mathbb{T}(G,\mu)| = 5 \cdot 10^6$ and t_1 shows the run-time in the cases of evolution with degree conservation and t_2 in the case of degree conservation failure. The results were obtained on Intel Core i7 processor with averaging run-times of over 20 runs with same parameters.

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