An Interactive Environment to Support Agent-based Graph Programming

Daniel Blashaw\textsuperscript{a} and Munehiro Fukuda\textsuperscript{b}

Division of Computing and Software Systems, University of Washington Bothell, U.S.A.

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Abstract: We apply agent-based modeling (ABM) to distributed graph analysis where a large number of reactive agents roam over a distributed graph to find its structural attributes, (e.g., significant subgraphs including triangles in a social network and network motifs in a biological network). Of importance is providing data scientists with an interactive environment to support agent-based graph programming, which enables interactive verification of agent behaviors, trial-and-error operations, and visualization of graphs and agent activities. This paper presents and evaluates our implementation techniques of these interactive features.

1 INTRODUCTION

In contrast to conventional data streaming, we apply agent-based modeling (ABM) to big-data computing (Fukuda et al., 2020). More specifically, instead of streaming data to analyzers such as Spark\textsuperscript{1}, we construct a distributed data structure, dispatch reactive agents to it as mobile analyzers, and find its structural attribute in their emergent collective group behavior. For instance, triangles in a given social network is considered as a useful factor to measure the intimacy among the network users and can be counted by walking agents three times over the network.

Distributed data structures have been facilitated for years in well-known parallel and distributed systems. GlobalArray constructs multi-dimensional arrays on top of MPI (Nieplocha et al., 2006). Pregel is a large-scale graph library based on inter-vertex message passing (Malewicz et al., 2010) and is used in Spark’s data streaming as GraphX. RepastHPC is the parallel version of Repast Simphony\textsuperscript{2} that distinguishes spatial and network projections.

Focusing on graph analysis, these systems however have substantial difficulties in implementing our agent-based approach: GlobalArray could represent a graph with an adjacency matrix but does not support element-to-element communication, thus obstructing agent communication nor movement; Pregel and GraphX nail computation in their vertices, immobilizing agents over a graph; and RepastHPC is meant for traditional ABM simulation, not considering parallel file I/Os nor interactive operations on its network projections. Given this background, we facilitated distributed graph construction, agents’ graph traversal and visualization in the MASS (multi-agent spatial simulation) library (Gilroy et al., 2020).

Of importance is providing data scientists with an interactive environment to support agent-based graph programming, which includes interactive verification of agent behaviors, capability of trial-and-error operations, and visualization of graphs and agent activities. This paper presents and evaluates our implementation techniques of these interactive features.

The rest of this paper is organized as follows: Section 2 differentiates our interactive environment from the related work in graph programming; Section 3 gives technical details on the MASS interactive features and their implementation; Section 4 evaluates MASS execution overheads, programmability improvements, and visualization; and Section 5 concludes our discussions as mentioning our future plans.

2 RELATED WORK

This section compares related systems from the following four viewpoints: (1) potential of distributed graph analysis with agents, (2) agent tracking over a distributed graph, (3) forward and backward graph analysis, and (4) visualization of graphs and agents.
2.1 Distributed Graph Analysis with Agents

NetLogo\(^3\) and Repast Simphony are capable of simulating networked agents or agent movements over a network, respectively using network extensions or network projections. However, the biggest challenge results from their single-computing execution that limits graph scalability. In fact, our scalability test shows that Repast Simphony suffers from counting the number of triangles in a graph only with 3,000 vertices (Wenger et al., 2021).

RepastHPC and FLAME\(^4\) are MPI-supported parallel ABM simulators. Since their paramount goal is parallel performance in native execution, their MPI-based C/C++ implementation does not consider interactive operations that are essential to the speed or the serving layer in big-data computing. Furthermore, they cannot initialize a graph in parallel as rank 0 must read an input file sequentially.

WAVE (Sapaty and Borst, 1996) and UCI Messengers (Bic et al., 1996) are mobile-agent execution platforms, both allowing their agents to construct and to roam over a distributed graph at run-time. Their drawback is the necessity of describing graph construction logics in their agent code, which in turn means that they are incapable of automating graph construction from an input file and are thus unsuited to big-data computing.

2.2 Agent Tracking

ProvMASS (Davis et al., 2018) provides MASS users with a novel approach for tracking data provenance in a distributed setting. This data provenance includes agent data, simulation space, and cluster node information, and is captured to file at run-time. Although these data provenance features contribute to analyzing agent behavior, they have a significant impact on simulation performance.

Repast Simphony, on the other hand, has a lightweight implementation for tracking agent data, but settings must be pre-configured before running the simulation and recorded agent data can only be written to console or file. This is useful for reviewing agent information but does not facilitate interactive uses nor operations on the agent data in a running simulation.

IBM Aglets (Lange and Oshima, 1998) allows users to communicate with the agent servers named Tahiti. Through Tahiti’s GUI, users can create, clone, inspect, dialogue with, retract, and destroy agents. However, since Aglets are intended to work on Internet tasks, they do not distinguish distributed data structures nor duplicate too many instances through the GUI menus.

2.3 Forward and Backward Graph Analysis

We anticipate that data scientists may want to conduct various analyses on the same graph, (e.g., centrality and clustering analyses on the same biological network). These operations need to retract agents or even roll back computation, which are then followed by a new analysis. Some systems indirectly or directly implement such forward and backward computation as follows:

Optimistic synchronization in parallel simulators (Wang and Zhang, 2017) allows each computing node to take repetitive snapshots of ongoing computation for the purpose of rolling back to the computation and accepting tardy messages from slower computing nodes. As their checkpointing and rollback operations are system-initiated features, users cannot use them intentionally for their trial-and-error analysis.

The UCI Messengers system implements the optimistic synchronization in the execution platforms so that agents can automatically go back to a network node they previously visited. Needless to say, agent checkpointing and rollback are carried out automatically and thus not user-controllable.

Looking at single-CPU execution, Repast Simphony requires that all graph and agent information be set prior to execution of the simulation and does not support incremental backtracking or manipulation of a running simulation.

2.4 Graph Visualization

Single-CPU ABM simulators furnish non-computing users with a plenty of graph analyzing and visualization features. NetLogo arranges an IDE-based graph visualization with its network extension, while forcing users to pre-configure visualizations and lacks the mid-simulation control features. Repast Simphony is equipped with JUNG (O’Madadhain et al., 2003) as its internal graph tool, which in turn means that data scientists need to embed visualization logics in their graph programming.

Cytoscape\(^5\) is an open-source network visualization tool with the following three graph-programming supports: (1) extensive file support for importing

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\(^3\)https://ccl.northwestern.edu/netlogo/
\(^4\)http://www.flame.ac.uk/
\(^5\)http://cytoscape.org/
graphs into Cytoscape, (2) native functionality for dynamic manipulation of existing graph structures, and (3) the use of the OSGi framework to make its components modular and easily extensible. Needless to say, Cytoscape is not concerned with agent activities on a Cytoscape graph.

We should emphasize that all these graph visualization endeavors are limited to single-CPU execution, thus unable to address the demand for large-scale graph analysis.

In summary of this section, agent-based graph programming needs to address interactive and scalability problems in the following three areas:

1. **Agent Tracking**: quickly observing a large number of agents traversing a graph;
2. **Forward and Backward Computation**: interactively retracting active agents, restoring former graph states, and dispatching new agents; and
3. **Graph Visualization**: dynamically modifying graphs through GUI and visualizing agent activities on a graph.

## 3 Interactive Features and Their Implementation

In the following, we briefly introduce the MASS library and thereafter explain our technical solutions to three interactive graph-programming features: (1) agent tracking, (2) forward and backward computation, and (3) graph visualization.

### 3.1 MASS Library

The MASS library represents ABM using the two modeling objects: *Places* and *Agents*. *Places* is a computational space implemented with a multi-dimensional array, distributed over a cluster system. *Agents* is a collection of reactive agents within the computation. An agent has navigational autonomy of traversing places. The MASS library functions using a master-worker pattern to control the computation. User applications interact with the MASS master node that runs their main() function; starts MASS workers with MASS.init(); invokes a parallel function call at each place or each agent with Places.callAll(func) or Agents.callAll(func); exchanges data among places in an inter-place RPC form with Places.exchangeAll(func); clones, kills, and moves agents within Agents.manageAll(); and terminates the MASS workers with MASS.finish().

To ease graph programming, MASS derives GraphPlaces from the Places base (Gilroy et al., 2020). Using this class, users can initialize a distributed graph with an input file in XML, HIPPIE, CSV, and text formats. As GraphPlaces can grow by adding a new Places instance to itself, users can incrementally construct the graph with addVertext() and addEdge(). The MASS library interfaces with Cytoscape for GUI-enabled graph construction and visualization as well as with JShell (Oracle, 2017) for interactive agent deployment over the graph.

### 3.2 Agent Tracking

We implemented an agent-tracking feature in MASS, based on the following three design strategies: (1) enabling quick observation of many agent activities, (2) generating consistent agent propagation history, and (3) facilitating a straightforward, easy-to-use agent-tracking API.

To pursue the performance consideration, instead of allowing each agent to carry its travel history with it, we added to each place the AgentHistoryManager class that is responsible for managing which agents or classes of agents are being tracked and then recording history each time a tracked agent visits that place. Importantly, this means agent history is stored on the Places but not on the Agents; this maintains execution performance by ensuring agents remain lightweight for serialization and transfer between computing nodes. The trade-off is that agent history is distributed amongst the cluster nodes during execution which introduces some complications when extracting the data, especially when child agents are involved.

In many applications, agents will come to decision points at which their instructions indicate they need to travel to multiple places at once. In these instances, the parent agent will move to one place, and then a child agent will be spawned for each of the other available places. At this point, if agents are being tracked by their class name, then places will begin gathering data on the newly spawned child agents. This pattern may continue throughout the computation, causing multiple waves of child agents to spawn at various times in the computation. The issue that arises from this process is that the child agents will have an incomplete history, because they did not exist at the beginning of execution.

To help illustrate this problem, consider the Triangle Counting benchmark application running on a sample graph shown in Figure 1. Triangle Counting is solved in four ABM simulation cycles: *(time 0)* one agent is spawned on each available place; *(time 1-2)* each agent propagates itself to all neighboring places with a lessor index value than the current place
Listing 1 shows a code snippet to initiate agent tracking and to collect agent travel history. The `main()` program creates a graph (line 5) and initializes `AgentHistoryManager` at each graph place (line 6). Once an agent class is registered for tracking, the user program may continue execution without worrying about tracking data. Each time the `manageAll()` function is invoked, the MASS library will keep track of all associated agent movements. Although the code invokes `manageAll()` twice for each loop iteration, one in line 10 for spawning children and the other in line 12 for moving all the agents to neighboring places, `manageAll()` internally counts these two invocations as one logical time event. This gives users a simple view of agent dissemination. Finally, `main()` can retrieve all the agent travel histories through `graph.callAll(AGENT_TRACE_GET)` (line 14). This retrieval process internally consolidates all collected results into a single, cleaned, and sorted `AgentHistoryCollection` object. It is at this step that parent-data propagation occurs.

### 3.3 Forward and Backward Computation

We have leveraged the MASS library’s interface to JShell named InMASS (Alghamdi, 2020) for forward and backward computation.

In conventional data streaming, Spark addresses forward/backward computation with immutable RDDs that create new versions upon any transformation applied to them, and thus keeps old RDDs retrievable with their references. This strategy takes the same effect as checkpointing and rollback of computation. To avoid generating too many snapshots of RDD, Spark carries out lazy evaluation.
of RDD transformations until they really need to be evaluated for passing their changes to RDD actions (which produce non-RDD values). In agent-based graph programming, agents travel or propagate over a graph as changing each data item. This in turn means that, if we use the same strategy as Spark’s dataset immutability, we need to take a snapshot every time an agent changes each vertex. Furthermore, unlike Spark’s RDD, (i.e., a collection of data items), a graph needs more disk space for storing its serialized data upon a checkpointing and more time for de-serializing it upon a rollback. Taking these overheads in consideration, we implemented interactive parallelization in the MASS library as follows:

1. **Maintaining only One Snapshot of Computation**: MASS users are supposed to commit their operations to an in-memory graph once they have no intention to roll back beyond this checkpoint. This saves the secondary storage space.

2. **Maintaining a History of Previous MASS Function Calls**: The MASS library will keep recording any MASS functions invoked since the last snapshot was taken, so that MASS can rebuild any past graph structure between the snapshot and the latest graph state.

3. **Rolling Back Computation by Re-executing Functions in History**: Upon a user-specified rollback, the MASS library will re-apply previous function calls to the snapshot in a chronological order all the way to the rollback point. While this rollback scheme needs a substantial time to rebuild a past graph, the normal computation can run faster without continuously taking a snapshot of ongoing executions onto disk.

At the highest level, InMASS is simply a wrapper class that initializes a JShell window and receives MASS statements from users. The challenges of InMASS implementation, however, revolve around (1) making JShell function properly for all cluster nodes in a distributed environment and (2) deciding how to save and reload computation state for checkpoint and rollback functionality.

To address issue 1, we customized a Java class loader named `InMASSLoader` that facilitates distribution of new classes’ bytecode from the MASS master to worker nodes. Once all computing nodes are aware of the new classes, they use new `MASSObjectInputStream` and `MASSObjectOutputStream` functions to assist in serialization and deserialization of these dynamic classes.

To address issue 2, we had `Agents` and `Places` inherit `AgentsInternal` and `PlacesInternal` serializable classes to facilitate serialization and deserialization of all agents and places data. Then, each MASS worker process gathers all hash tables containing all `Agents` and `Places` instances, and holds them in one single object named `MState`. This is the object to be saved and updated on checkpoint and rollback. (Note that users can choose a checkpoint storage from active memory, temporary disk location, or a specified file in disk.) To facilitate user ability to rollback to states other than the original checkpoint, the MASS master process prepares the `MHistory` object to keep a log of all API calls to `Agents` and `Places` and to store their bytecode to enable re-execution on demand. Consequently, when a user requests rollback to “step 5”, for example, the original snapshot will be loaded from `MState`, and then `MHistory` will execute the next five API calls that follow the snapshot.

### 3.4 Graph and Agent Visualization

To facilitate visualization and validation of agent activities over a distributed graph, we have extended the existing MASS-Cytoscape integration, based on the following three implementation strategies: (1) allowing users to focus on programming their graph application, (2) following the OSGi framework to modularize MASS-related plugins, and (3) allowing large-scale graphs to be visualized by retrieving partial graphs from MASS.

#### 3.4.1 Usability Enhancement

Figure 4 presents an overview of the MASS-Cytoscape architecture. We have illustrated the user’s two points of interaction on the left side of the figure, with the JShell window for running their code in MASS and with the MASS Control Panel for managing their data flow and visualization in Cytoscape.

The MASS Control Panel serves three main functions. First, it provides a single point of interaction for the user by internally managing the data transfer plugins: `import-network`, `export-network`, and `import-agents`. Second, it provides the ability to manipulate the MASS Configuration tables that inform the data transfer plugins of how to find the MASS computation and what data to pull back into Cytoscape. Lastly, it provides the interface and logic for visualizing agent movement through manipulation of the Cytoscape data tables and network view.

In MASS, the CytoscapeListener class must be started by the user application to open a TCP-based communication port for MASS-Cytoscape communication. This listener will then field any requests from Cytoscape by first parsing the request, then obtaining reference to the corresponding `GraphPlaces` method, and finally invoking that method and returning the results to the requesting Cytoscape plugin. Internally,
the GraphPlaces methods utilize standard MASS internal APIs, such as callAll(), to communicate with the rest of the cluster and set or retrieve the appropriate information.

Visualizations in Cytoscape are all controlled by two factors: the layout and the network view. While we utilized the “Circular” layout, (i.e., one of Cytoscape’s defaults), we customized the network view to change edge thickness and vertex color for visualizing agent travel histories.

### 3.4.2 Modularity and Expandability

Cytoscape plugin components must follow OSGi to modularize them in a bundle. Since each bundle is self-contained, plugin developers are responsible to coordinate bundle invocations and to provide bundle-to-bundle data communication. We handle this communication using a shared table named “MASSConfiguration table” within the Cytoscape environment. The table includes fields for the MASS host name and port as well as other fields used for partial graph streaming. The MASS Control Panel writes new values to the table after taking inputs from the UI and the data transfer plugins read in relevant information each time a new data transfer task is created. To tolerate any ordered start-up of bundle, the panel also maintains a reference to each of the data transfer plugins and the ability to test and reacquire the reference.

### 3.4.3 Graph Scalability

Visualization of a partial graph is important in situations where the MASS cluster is operating on a graph too large to be stored in a single machine. To allow the visualization environment to support the scale of these graphs, we have implemented an optional “N-Neighbors” approach to graph retrieval from MASS. This requires the user to provide a centroid node ID as well as determine the degrees of separation (DoS) that should be imported. DoS is interpreted as the number of neighbor rings that we would like to visualize. Shown in Figure 5, if the user selects “1” DoS then the graph retrieval will bring back the centroid node as well as one ring of immediate neighbors.

To manage this request on the MASS side of the program, the MASS master node first receives the request, saves centroid and DoS information, and then invokes GraphPlaces’s getGraphNNeighbors() method. This method iteratively queries the remote workers for each DoS requested, passing a list each time to ensure only the required graph vertices are sent back. This approach is critical when a given graph is too large for a single machine.

### 4 EVALUATION

We evaluated the MASS interactive environment in the following three criteria: (1) execution performance, (2) ease of programming, and (3) usefulness of visualization. Our evaluation used a cluster of eight computing nodes, each with an Intel Xeon Gold 6130 CPU at 2.10GHz and 20GB memory.

#### 4.1 Execution Performance

We first compared the execution performance between the agent-tracking API and the conventional history-passing technique (i.e., maintaining and pass-
Since the agent population increases exponentially when the graph expands, we use the total number of agents to provide context to our results. Figure 6 shows Triangle Counting’s execution time as increasing the number of agents. Note that we calculated the average of five measurements. Beyond 140K agents, we observe approximately 1,700ms (11-18%) slower performance when using the agent-tracking API. This increase in processing time is due to the added overhead from data capture methods invoked when agents are spawning and moving. This gap widens slightly when running in multi-node configurations due to network latency, but the correlation between the two techniques remains consistent.

Figure 7 compares agent-tracking API and the history-passing technique in their overheads when extracting agent data. We conversely observe a significant gap in performance between the two techniques regarding agent-data extraction time. This is because the agent-tracking API returns all agent data from places and takes additional step to clean, sort, and propagate the data upon retrieval.

4.2 Programmability Evaluation

The following qualitatively compares the history-passing technique and the agent-tracking API:

1. **History-passing Technique**: only works for agents that are alive upon data extraction and requires the user to have additional understanding of the MASS library, which resulted in more lines of code, (i.e., 15 lines)

2. **Agent-tracking API**: presents history for all registered agents at any point of execution, can be initiated and then ignored until needed, which is more intuitive with 13 lines of code for inexperienced MASS users.

4.3 Graph and Agent Visualization

We have implemented two agent visualizations in Cytoscape: Agent Path and Heat Map. Both visualizations are generated using the MASS Control Panel and each can be manipulated in the network view. Agent Path is shown in Figure 8 and provides the user with the ability to review the complete path of any individual agent. The more recent movements are represented with a darker node and thicker edge. If an agent ever traverses a non-existing edge, then a dashed line is created to signal the issue to the user. This view is particularly useful in computation, such as Triangle Counting, where the pattern of agent movement determines the success of the application.

The Heat Map visualization, shown in Figure 9, provides the user a representation of all agents active in the simulation at a point in time with darker nodes representing higher concentrations of agents. The user is then able to cycle through the time variable of the computation to observe movement patterns of the entire group. This visualization is best applied to use cases such as in network centrality analyses, in which we seek to observe aggregate movement patterns centralized around particular vertices of interest.
in graph analysis.

In comparison with MASS, Repast Simphony provides a GUI for both execution and visualization of graph analysis through their integration with the Eclipse IDE. This integration also provides plugin support for 2D/3D visualization of the simulation “Context”, (which corresponds to MASS Places and Agents). The visualizations, known as “Projections”, (which includes “Network Projections”) are configured through the IDE before starting the simulation and are strictly synchronized with simulation execution. Repast Simphony does provide statistics and logging features for reviewing historical data, but the simulation itself is limited to only stepping forward through execution or running the simulation at full speed.

Contrary to that, MASS separates the execution and visualization aspects of the system into two windows. Computation is handled through the command-line interface, which also enables forward and backward stepping through the inclusion of JShell with checkpointing and rollback features. Visualization is then managed separately through the Cytoscape GUI and MASS-specific extensions. Adding support for agent visualization in this work brings MASS on par with Repast Simphony as far as what objects can be visualized, but our visualizations are still limited to 2D views. Most importantly, the separation of view and execution concerns allows for the visualization to be completed asynchronously and the visualizations to be adjusted as desired through the Cytoscape GUI without the need to pre-configure or restart a computation.

5 CONCLUSIONS

To enable more rapid development and exploration when building agent-based graph programs, we introduced new APIs for tracking agent data, incorporated an interface for forward and backward computation with JShell, and expanded integration of Cytoscape for visualization of MASS GraphPlaces and associated Agents. Verification using Triangle Counting showed minimal impact on execution performance, though increased overheads on agent-data extraction times.

Our future work is two-fold in Cytoscape expansion: (1) visualization capabilities of multi-dimensional arrays and binary/quad trees and (2) filtering capabilities of agents to capture for their graph traverse, (e.g., those alive at a particular time or marked as a successful traveler).

REFERENCES


