Assessing the feasibility of OpenCL CPU implementations for agent-based simulations

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ABSTRACT

Agent-based modeling (ABM) is a bottom-up modeling approach, where each entity of the system being modeled is uniquely represented as a self-determining agent. Large scale emergent behavior in ABMs is population sensitive. As such, it is advisable that the number of agents in a simulation is able to reflect the reality of the system being modeled. This means that in domains such as social modeling, ecology, and biology, systems can contain millions or billions of individuals. Such large scale simulations are only feasible in non-distributed scenarios when the computational power of commodity processors, such as GPUs and multi-core CPUs, is fully exploited. In this paper we evaluate the feasibility of using CPU-oriented OpenCL for high-performance simulations of agent-based models. We compare a CPU-oriented OpenCL implementation of a reference ABM against a parallel Java version of the same model. We show that there are considerable gains in using CPU-based OpenCL for developing and implementing ABMs, with speedups up to 10× over the parallel Java version on a 10-core hyper-threaded CPU.

CCS CONCEPTS

•**Computing methodologies** → **Shared memory algorithms; Agent / discrete models; Massively parallel and high-performance simulations; Parallel programming languages; Model verification and validation; Artificial life;**

KEYWORDS

Parallel simulation, Agent-based model, PPHPC, OpenCL, cf4ocl

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1 INTRODUCTION

Agent-based modeling (ABM) is a bottom-up modeling approach, where each entity of the system being modeled is uniquely represented as a self-determining agent. When prompted to act, each agent examines its current situation (e.g. what resources are available, what other agents are in the vicinity), and acts accordingly, based on a set of rules (e.g., if-then-else rules, differential equations, neural networks). These rules incorporate knowledge or theories about the respective low-level components. The global behavior of the system then emerges from the simple, self-organized local relationships between the agents [13]. As such, ABM is a useful tool in simulating and exploring systems that can be modeled in terms of interactions between individual agents, for example, biological cell cultures, ants foraging for food or humans in a crowd.

Spatial agent-based models (SABMs) are a subset of ABMs in which a spatial topology determines how agents interact [56]. For example, an agent may be limited to interact with agents located within a specific radius, or may only move to a near physical or geographical location [45]. SABMs have been extensively used to study a range of phenomena in the biological and social sciences [36, 56].

Large scale emergent behavior in ABMs is population sensitive. As such, it is advisable that the number of agents in a simulation is able to reflect the reality of the system being modeled [35, 38, 44]. Otherwise, accurate simulation behavior may not be attainable, and model validation becomes difficult [31, 35]. This means that in domains such as social modeling, ecology, and biology, systems can contain millions or billions of individuals [9, 10, 38, 53]. Consequently, simulating realistic models will involve as much agents being processed per time step [9]. Such large scale simulations generate a very high demand for computing power [30] and are impractical on typical ABM frameworks such as NetLogo [69] or Repast Symphony [49], which run on a single CPU core or compute unit [9, 10]. Considering that commodity processors, such as GPUs and multi-core CPUs, are nowadays composed of several compute units, a natural solution to reach acceptable scalability in ABMs consists of decomposing models such that each component can be autonomously processed by a logical processor (LP¹) in a concurrent manner [5, 31, 56, 60–62, 66]. However, in order to minimize communication between LPs and obtain optimal performance, model partitioning should guarantee that individual model components are as independent as possible.

¹In shared memory architectures, LPs are usually represented by threads, which communicate via synchronized access to shared variables. In distributed memory scenarios, LPs are commonly represented by processes, which communicate via message passing.

In this paper we evaluate the feasibility of using CPU-oriented OpenCL for high-performance simulations of agent-based models. OpenCL is an open standard for general-purpose parallel programming across CPUs, GPUs, FPGAs and other processors, giving software developers portable and efficient access to the power of these heterogeneous processing platforms [34, 57]. OpenCL implementations are provided by a large and increasing number of CPU, GPU and FPGA vendors². We test a CPU-oriented OpenCL implementation of the reference PPHPC ABM [16] over two proprietary OpenCL CPU runtimes, provided by Intel and AMD, respectively. We compare this implementation against a parallel Java version of the same model [20], both in terms of performance and statistical accuracy. Leveraging on the fact that the PPHPC model captures important characteristics of SABMs, such as agent movement and local agent interactions, several conclusions on SABM parallelization techniques using OpenCL are drawn.

The rest of the paper is organized as follows. First, in Section 2, previous work on SABM parallelization is presented and the associated issues are discussed. Next, Section 3, Methods, is composed of five parts: 1) an overview of the PPHPC model; 2) a discussion on how to generically parallelize it; 3) a description of the model's parallel Java implementation; 4) a thorough presentation of the CPU-oriented OpenCL implementation of PPHPC; and, 5) a summary on how to compare the outputs collected from two model implementations in order to assert their statistical equivalence. Results, Section 4, show that there are considerable gains in using CPU-based OpenCL for developing and implementing ABMs, and at the same time guaranteeing simulation reproducibility and statistical accuracy with the original model. Section 5 provides some conclusion of what was accomplished in this paper, outlining directions for future work.

2 BACKGROUND

The distributed memory programming model is widely used for parallelizing ABMs [4, 5, 30, 55, 56, 62]. This approach allows models to scale to thousands of cores, usually found in supercomputer-type setups or computing clusters. However, communication issues for larger models [56] and a more complex programming paradigm (when compared with multithreading on shared memory architectures) [41] often restrict this approach.

Recently, the trend has been on hybrid [1, 59], GPU [3, 44, 54, 68] and heterogeneous [65, 67] methods. While these approaches allow concrete gains in simulation performance on commodity hardware, they come with an increased cost in implementation time due to the considerably more complex programming models. Hybrid methods, combining distributed and shared memory programming models, require modelers to master both paradigms, as well as specific multi-level model decomposition. GPU architectures require the reformulation of ABMs in terms of stream SIMD computation and offer limited control flow constructs [44]. Heterogeneous methods, in which both CPU and GPU are utilized, require careful model decomposition so that components can be efficiently processed. Furthermore, costly data transfers between the two processors can only be avoided by using integrated GPUs, which are typically much less powerful than their discrete counterparts.

The computing potential of GPUs and the apparent massively parallel nature of SABMs make general-purpose GPU (GPGPU) implementations of such models an interesting proposal [52]. However, in order to express ABMs in terms of stream SIMD computation, each type of agent should be processed by the same code (single instruction) and multiple instances of each type of agent should exist in the simulation (multiple data) [32, 42]. Optimal performance requires that the processing of one agent is causally independent of the processing of any other agent in the same time step [9]. This can be difficult to achieve with ABMs, since the behavior of an agent is frequently associated with the dynamic environment and with the actions of other agents [42]. A common case in SABMs is that of mobile agents in a discrete grid, which poses several difficulties. If there is a unique location constraint (maximum of one agent per grid cell), the implementation must explicitly handle collisions which result from agents concurrently moving to the same location [44, 54]. However, the absence of this constraint creates a different problem. More specifically, agents need to determine the location of other agents in their neighborhood. The typical solution consists of having a sorted array of agents, with each grid cell holding a pointer to the first agent it contains. This solution requires a sorting step in each iteration, which can deteriorate performance [2, 12, 14, 28, 51]. The agent life-cycle is another difficult aspect of ABM on GPUs, requiring adequate memory management patterns, such as allocation and garbage collection, which are unavailable within GPGPU kernels [44]. For more complex models, with different agent types and dynamic environments which influence agent behavior, it will be difficult to find an efficient SIMD solution at all [42]. Having this into account, the use of SIMD architectures may lead to good results for simpler ABMs [42], such as cellular automata and homogeneous agent models [4, 24, 54]. A number of proposed GPGPU ABM frameworks rely on these assumptions or simplifications [4, 35, 44, 54].

Among the possible parallelization techniques, multithreading is arguably the simplest to implement [41, 66], with the added bonus of portability. For example, modern threading APIs, such as OpenMP [8] for C, C++ and Fortran or the Java concurrency API [25] greatly simplify multithreaded ABM implementations, and are available for a number of different shared memory CPU architectures and operating systems. For example, the ABM of opinion exchange presented by Gong et al. [27], implemented in C++ and parallelized with OpenMP, was tested in a 32-core CPU (AMD Opteron), with impressive speedups. Java is also a common choice for parallelizing ABMs, as exemplified by Fachada et al. [13, 20] and Goldsby and Pancerella [26].

A few ABMs have also been developed in OpenCL in recent years. However, most have either been focused on GPGPU [6, 48] or implemented without apparent CPU-specific optimizations when also tested on CPUs [24, 37, 39, 40]. The work of Wang et al. [67] is an exception, leveraging OpenCL's versatility by targeting heterogeneous processors, i.e., CPUs with integrated GPUs.

²<https://www.khronos.org/conformance/adopters/conformant-products#opencl>

Algorithm 1 Simulation algorithm for the PPHPC model.

```

1: INIT()
2: GETSTATS()
3:  $i \leftarrow 1$ 
4: for  $i \leq m$  do
5:   for all agent do
6:     MOVE()
7:   end for
8:   for all grid cell do
9:     GROWFOOD()
10:  end for
11:  for all agent do
12:    ACT()
13:  end for
14:  GETSTATS()
15:   $i \leftarrow i + 1$ 
16: end for

```

3 METHODS

3.1 The PPHPC agent-based model

The Predator–Prey for High-Performance Computing (PPHPC) model is a reference model for studying and evaluating SABM implementation strategies, capturing important characteristics such as agent movement and local agent interactions. It is used in this work as a test case for ABM parallelization using CPU-oriented OpenCL. The model is thoroughly described in reference [16] using the ODD protocol [29]. Here we present a summarized description of the model.

PPHPC is a predator–prey model composed of three entity classes: *agents*, *grid cells* and *environment*. *Agents* can be of type prey or predator. While prey consume passive cell-bound food, predators consume prey. Agents have an energy state variable, E , which increases when feeding and decreases when moving and reproducing. When energy reaches zero, the agent is removed from the simulation. Instances of the *grid cell* entity class are where agents act, namely where they try to feed and reproduce. Grid cells have a fixed grid position and contain only one resource, cell-bound food (*grass*), which can be consumed by prey, and is represented by the countdown state variable C . The C state variable specifies the number of iterations left for the cell-bound food to become available. Food becomes available when $C = 0$, and when a prey consumes it, C is set to c_r (an initial simulation parameter). The set of all grid cells forms the *environment* entity, a toroidal square grid where the simulation takes place. The environment is defined by its size and by the restart parameter, c_r . The temporal scale is represented by a positive integer m , which represents the number of iterations.

Simulations start with an initialization process, where a predetermined number of agents are randomly placed in the simulation environment. Cell-bound food is also initialized at this stage. After initialization, and to get the simulation state at iteration zero, outputs are collected. The scheduler then enters the main simulation loop, where each iteration is sub-divided into four steps: 1) agent movement; 2) food growth in grid cells; 3) agent actions; and, 4) gathering of simulation outputs. This process is summarized in Algorithm 1.

Six outputs are collected at each iteration i : prey population (P_i^s), predator population (P_i^w), quantity of cell-bound food (P_i^c), mean prey energy ($\bar{E}_i^s$), mean predator energy ($\bar{E}_i^w$) and mean value of the C state variable in all grid cells ($\bar{C}_i$).

Reference parameters for the PPHPC model are qualitatively separated into size-related and dynamics-related groups [16]. Although size-related parameters also influence model dynamics, this separation is useful for parameterizing simulations. Concerning size-related parameters, a base grid size of 100×100 is associated with 400 prey and 200 predators. Different grid sizes should have proportionally assigned agent population sizes, such that the initial agent density and the initial ratio between prey and predators remains constant. Thus, *model size* is the relation between grid size and initial agent population. For example, model size 400 corresponds to a grid size of 400×400 with 6400 prey and 3200 predators at iteration 0.

For the dynamics-related parameters, two parameter sets, 1 and 2, are proposed. The two parameterizations generate distinct dynamics, with the second set typically yielding more than twice the number of agents than the first during the course of a simulation. The combination of model size and parameter set will be referred as “size/set”, e.g., 400/1 for model size 400, parameter set 1. The reference number of iterations, m , is 4000, not counting with the initial simulation state at iteration 0.

3.2 A generic parallelization approach

The components that constitute a SABM can be split among LPs according to two broad patterns: agent-parallel (AP) and environment-parallel (EP) [50]. Even though these patterns are not mutually exclusive, they constitute a convenient basis for evaluating SABM parallelization techniques. In the AP criterion each LP processes a set of agents, i.e., the model is divided at the agent-level, as shown in Figure 1a. Load balancing is simplified since agents, and the associated computational tasks, can be equally distributed among LPs [7, 50]. However, in a moving agents scenario, additional communication between LPs is required in order to guarantee that spatially localized agent interactions are processed in a consistent fashion, as co-location on a LP does not guarantee co-location in space [50]. Model partitioning occurs at the spatial environment level in the EP criterion, i.e., each LP is assigned a slice of the simulation space, together with the agents it contains [7], as shown in Figure 1b. As such, local agent interactions will mostly occur in the same LPs. Unfortunately, load balancing issues may occur if spatial agent density is mostly non-uniform. This typically occurs in models involving agent grouping phenomena such as flocking or chemotaxis [7, 21, 26, 50].

As shown in Algorithm 2, the parallelization approach followed by the PPHPC implementations discussed here is essentially based on the EP pattern (cell initialization and main simulation loop), with the AP paradigm used only for agent initialization.

The `Init()` process of Algorithm 1 is represented in lines 1–3 of Algorithm 2 by the `InitCells()`, `InitPrey()` and `InitPredators()` subprocesses. The first is executed in EP fashion, since there are no dependencies on initializing the cells and setting the initial cell-bound food. The two agent initialization processes are executed in AP fashion, i.e., each LP manages the initialization and

Figure 1: The SABM parallelization patterns.

Algorithm 2 Generic parallelization of Algorithm 1 using an EP approach for the main simulation loop.

```

1: INITCELLS()           ▶ Environment-parallel
2: INITPREY()            ▶ Agent-parallel
3: INITPREDATORS()       ▶ Agent-parallel
4: GETSTATS()            ▶ Environment-parallel
5:  $i \leftarrow 1$ 
6: for  $i \leq m$  do
7:   MOVE() + GROWFOOD()  ▶ Environment-parallel
8:   ACT() + GETSTATS()   ▶ Environment-parallel
9:    $i \leftarrow i + 1$ 
10: end for

```

deployment of a number of agents, although, as we shall discuss, this is done differently in the Java and OpenCL implementations.

The `GetStats()` process (line 2 of Algorithm 1 and line 4 of Algorithm 2) collects the initial simulation output using an EP strategy, since at this stage cells are independent of each other.

Lines 5–10 of Algorithm 1, which include agent movement and growth of cell-bound food, are combined into a single EP loop (line 7 of Algorithm 2). This is possible because the `Move()` and `GrowFood()` processes are independent; i.e., the outcomes of either will only influence the `Act()` process, which occurs later. Basically, both `Move()` and `GrowFood()` are cell-wise independent and can be processed autonomously for each cell in an EP loop. When a cell is evaluated, agents located within are prompted to move, and then the cell is asked to execute its `GrowFood()` process. Care must be taken so that agents that already moved are not prompted to move again.

Finally, lines 11–14 of Algorithm 1, containing the `Act()` and `GetStats()` processes, are also condensed into one EP loop, as shown in line 8 of Algorithm 2. While agent actions and statistics gathering are not independent events (i.e., the former must occur before end-of-iteration data is collected), they are cell-wise independent. As described in Section 3.1, the actions of an agent are limited to the cell it occupies. Thus, after agent actions take place in a cell, end-of-iteration cell data can be collected.

PS	Rep.	Description
ST	Yes	Serial execution (no parallelization).
EQ	No	Partition grid between LPs, cell-level sync.
EX	Yes	Same as previous, with ordered agent insertion.
ER	Yes	LPs simultaneously process grid rows, sync. at end of row.
OD	No	LPs continuously process blocks of grid cells while they are available, cell-level sync.

Table 1: Parallelization strategies (PS) in the Java implementation. The second column (Rep.) indicates if simulations performed with the respective PS are numerically reproducible.

3.3 A Java implementation

Java is a well-known language within the ABM community, powering popular toolkits such as NetLogo [69], Repast Symphony [49] and MASON [43]. The Java implementation of PPHPC [20] is based on the concept of units of work, which are processed by one or more worker threads. The basic units of work are grid cells in the EP sections of Algorithm 2, and agents in the AP sections. This implementation was designed using a modular and scalable approach, following relatively high-level object-oriented programming concepts and design patterns [23]. However, care has been taken so that performance was not compromised. Consequently, the implementation has shown speedups up to 40× on a six-core hyper-threaded processor against a serial version implemented in NetLogo [20].

This implementation of PPHPC follows the Model-View-Controller design pattern. The Model component represents the actual ABM logic, and can be manipulated and observed using one or more views. Work factories, implementing the factory pattern, are responsible for creating and configuring the controller and work providers, which handle how units of work are processed. The controller spawns a specified number of worker threads, which in turn rely on the controller for synchronization. The work providers determine the amount of work each worker processes. Five work factories are provided, each implementing a specific parallelization strategy, as shown in Table 1.

The EX strategy is selected for this comparison, as it allows for numerically reproducible simulations while offering a level of performance close to that of the top-performing OD strategy [20]. The general idea of the EX parallelization strategy is that each worker always processes the same work. Work distribution is performed once at the beginning of the simulation by the associated work providers, and then the workers are always given the same exact units of work, i.e., they always process the same cells in the EP sections. Cell-level synchronization is required because more than one worker may potentially access the same cell at the same time for agent movement or initial agent placement purposes. Agents are orderly placed in cells, allowing them to posteriorly move or act in the same sequence, making numerically reproducible simulations possible. The maximum number of units of work to be processed by each worker, n , is given by

$$n = \lceil T/N \rceil \quad (1)$$

where T is the total number of units of work to be processed in a parallel work cycle, and N is the number of worker threads. If T is not equally divisible between the available workers, the last worker will process less work than the remaining workers, as shown in Eq. 2,

$$n \cdot i \leq t_i < \min(n \cdot (i + 1), T) \quad (2)$$

where i identifies the i^{th} worker, and t_i corresponds to the range of units of work which will be processed by the i^{th} worker.

Parallel pseudo-random generation is carried out in the following manner. The i^{th} worker thread obtains its own subsequence of a global random sequence by using a unique seed, S_i , through a random spacing approach [33]. Each seed S_i is derived from the worker's unique identifier, i , and from a user specified global seed, S , according to Eq. 3,

$$S_i = \begin{cases} S, & \text{if } i = 0 \\ S \oplus \text{SHA256}(i), & \text{if } i > 0 \end{cases} \quad (3)$$

where $\oplus$ is the bitwise XOR operator and $\text{SHA256}()$ is the SHA-256 cryptographic hash function. Since each worker thread has its own PRNG subsequence, simulation reproducibility is guaranteed.

3.4 A CPU-oriented OpenCL implementation

The OpenCL CPU-oriented PPHPC realization uses OpenCL 1.2 kernels for maximum compatibility across vendor OpenCL CPU implementations. Additionally, host-side code was developed in C99, using the following libraries:

- GLib [63] - Used for command-line option parsing, error handling, pseudo-random number generation (host-side) and string manipulation.
- cf4ocl [18] - Simplifies OpenCL host-side programming and offers an integrated profiler.
- cl_ops [15] - Provides device-side pseudo-random number generators.

Due to the close-to-hardware nature of OpenCL, this PPHPC realization is implemented using a low-level approach, especially when compared with the Java version. First, the C99-based OpenCL kernel language does not allow for memory allocation inside kernels, meaning that: a) all the memory required for newly born agents must be host-side allocated upfront; and, b) the insertion of new agents in the simulation must be manually handled within the OpenCL kernels.

This PPHPC realization uses two data structures, more specifically two large arrays, in order to perform this management: 1) an array of grid cells; and, 2) an array of agents. While number of grid cells is fixed and known before the simulation begins, the same is not true for the number agents. As such, this array of agents should be made large enough to accommodate the maximum number of agents ever existing in the simulation.

Each element of the cells array is a structure containing two fields: 1) the grass countdown value, C ; and, 2) the location (in the agents array) of the first agent in the cell. The array index implicitly identifies the cell position in the grid. In turn, each

element of the agents array is a structure with the following fields: 1) the agent energy; 2) the agent type (predator or prey); and, 3) the index of the next agent in the same cell. The last agent in the cell points to a sentinel constant identifying the end of the list. As a consequence of this arrangement, agents in the same cell are scattered along the agents array, each agent holding a pointer to the next. These data structures are optimized for a CPU device. They would not be appropriate for GPU targets, due to the way the agents are scattered along the memory, and due to the use of the array of structures pattern (a structure of arrays is preferred for GPUs). Both approaches are not friendly towards coalesced memory accesses, one of the first optimizations to be considered for GPU targets.

Contrary to the Java version, the use of the EX strategy is not straightforward here. Following that approach, the insertion of an agent in a cell would require an atomic exchange between the first agent in the cell and the newly arrived agent. The latter would then become the first agent, pointing to the previously first agent – now the second agent in the cell. This would work, providing the equivalent of Java's EQ strategy, also sharing one of its caveats: it does not allow reproducible simulations. In order to obtain the equivalent of the EX strategy, new agents should be inserted in an orderly fashion. Since OpenCL does not provide Java-like explicitly synchronized blocks, this would have to be accomplished in one of two ways: a) via a spinlock implemented with atomics or a similar approach [58]; or, b) using an additional kernel, executed before agent movement and agent actions (i.e., before line 7 and before line 8 of Algorithm 2), to sort the agents within each cell according to a pseudo-random, but deterministic order. The former approach is somewhat against the spirit of OpenCL, is prone to deadlocks and may not be portable. The latter method may incur in severe computational overhead.

Given these considerations, we find that the ER (Equal with Row synchronization) parallelization strategy is a better fit to the OpenCL workflow. In the ER strategy, each worker serially processes rows of the simulation grid, leaving a distance of at least three rows (including the row to be processed) to the next worker (see Figure 2). More generally, this distance is given by

$$d_{\min} = 2r + 1 \quad (4)$$

where r is the agent movement radius, which is 1 for the PPHPC model. This approach allows workers to run in parallel without cell-level synchronization, since they synchronize at the end of each row at the host level (i.e., between kernel invocations), as shown in Figure 2. Thus, agents always move to neighboring cells in the same order, making simulations reproducible.

An initial estimate of the number of rows to be processed by each worker, Δy , is given by

$$\Delta y = \left\lceil \frac{y_{\text{env}}}{N} \right\rceil \quad (5)$$

where y_{env} is the total number of rows in the simulation grid. This estimate can be incremented if: 1) the number of rows is not equally divisible by the number of workers; and, 2) after incrementing it, there are enough rows for the last worker to process. This is shown in Eq. 6, where Δy_f is the final number of rows per worker:

Figure 2: Equal with Row synchronization (ER): example of three workers processing nine rows of the simulation grid in parallel.

$$\Delta y_f = \begin{cases} \Delta y + 1, & \text{if } y_{env} \bmod N > 0 \wedge \\ & (N - 1) \cdot (\Delta y + 1) \leq y_{env} - d_{min} \\ \Delta y, & \text{otherwise.} \end{cases} \quad (6)$$

All workers, except possibly the last one, will process n cells, according to Eq. 7. The exact number of cells that the i^{th} worker will process are given in Eq. 8. Note that any adjustment due to the number of rows not being exactly divisible by the number of workers is performed on the last worker.

$$n = x_{env} \cdot \Delta y_f \quad (7)$$

$$n \cdot i \leq t_i < t_f, \text{ where } t_f = \begin{cases} n \cdot (i + 1), & \text{if } i < N - 1 \\ x_{env} \times y_{env}, & \text{if } i = N - 1 \end{cases} \quad (8)$$

The OpenCL CPU implementation uses three kernels, `init()`, `step1()` and `step2()`, as shown in Algorithm 3. The ER strategy is implemented by kernels `step1()` and `step2()` in the main simulation loop, lines 4–13 of Algorithm 3. Each time these kernels are invoked, they process a row of the simulation environment, in accordance with the ER strategy. However, during the initialization stage, performed by the `init()` kernel (line 1 of Algorithm 3), a different parallelization approach, similar to Java’s EX strategy, is used. The `init()` kernel implements the functionality of lines 1–4 of Algorithm 2, initializing grid cells, prey agents and predator agents, and collecting statistics for iteration 0. Each worker executing the `init()` kernel is assigned part of the environment grid. From here, workers initialize grid cells in EP fashion, and then proceed to initialize the agents. As in the case of cells, each worker initializes a similar amount of agents. However, in order to avoid conflicts, workers only insert agents in the cells assigned to them. This dispenses the use of atomics and ensures agents are deterministically placed in cells. In practice this goes beyond the PPHPC model specification, since it forces an even distribution of agents along the vertical axis of the environment grid at the beginning of the simulation.

Continuing to the main simulation loop kernels, `step1()` performs agent movement and grows cell food (line 7 of Algorithm 2), and `step2()` performs agent actions and gathering of end-of-iteration statistics (line 8 of Algorithm 2). In both cases, care is taken so that: a) agents that already moved/acted are not prompted to

Algorithm 3 CPU-oriented OpenCL implementation of Algorithm 2. Function names correspond to the actual OpenCL kernels invoked.

```

1: INIT()                                ▶ Env./Agent-parallel
2:  $i \leftarrow 1$ 
3: for  $i \leq m$  do
4:    $j \leftarrow 0$ 
5:   for  $j < \Delta y_f$  do
6:     STEP1()                            ▶ Environment-parallel
7:      $j \leftarrow j + 1$ 
8:   end for
9:    $j \leftarrow 0$ 
10:  for  $j < \Delta y_f$  do
11:    STEP2()                            ▶ Environment-parallel
12:     $j \leftarrow j + 1$ 
13:  end for
14:   $i \leftarrow i + 1$ 
15: end for

```

do so again; and, b) agents with zero energy or killed by predators are immediately removed from the simulation. Within work-items, i.e., OpenCL threads, agents are processed serially, maintaining simulation consistency.

Allocation of newly born agents in `step2()` is performed with an atomic compare-exchange instruction. A position in the agents array is randomly obtained, with two possible outcomes: 1) the position is empty, in which case it is atomically set as occupied; or, 2) the position is not empty, in which case random allocation is attempted again, up to a predefined, user-controllable maximum number of times. Only when allocation is successful are the state variables of the new agent written to the selected position. Although not deterministic, the positions of new agents are nonetheless irrelevant for simulation reproducibility.

The `GetStats()` process, executed in the `step2()` kernel, is performed by atomically updating a global array of structures. While this approach is not scalable for GPU targets – which favor reduction for this type of operation – it does not cause visible performance degradation in the CPU case, mostly likely due to the limited number of work-items executing in parallel.

Similar to the Java implementation, individual OpenCL work-items have their own subsequence of a global random sequence obtained via a random spacing approach. However, in this case the initial PRNG state for each work-item is determined serially at host-side with the Mersenne Twister PRNG [46] – in turn seeded with a user-specified value. Work-items then use and update their exclusive PRNG states with one of the PRNG algorithms provided by the `cl_ops` library, specifiable at run time.

3.5 Statistical equivalence of model implementations

The parallelization of ABMs is of no use if the parallel implementations do not produce statistically equivalent results with respect to the original serial version. It is very easy to inadvertently introduce changes which modify the model dynamic. This is a more complex type of model replication, which in itself is not a straightforward

process [11, 70]. ABMs are very sensitive to implementation details: the impact that seemingly unimportant aspects such as data structures, algorithms, discrete time representation, floating point arithmetic or order of events can have on results is tremendous [47, 70]. The situation becomes more difficult with model parallelization, which by definition requires considerable changes in many of these aspects. Parry and Bithell [50] provide an informative account in which they were unable to successfully replicate a serial model when converting it to a parallel one.

In order to guarantee that the Java and OpenCL implementations display statistically indistinguishable behavior, we compare their output using a technique described in reference [19]. This model comparison method uses principal component analysis to convert simulation output into a set of linearly uncorrelated statistical measures, analyzable in a consistent, model-independent fashion. It is appropriate for ascertaining distributional equivalence of two or more model implementations, automatically selecting output features that best explain implementation differences.

4 RESULTS AND DISCUSSION

4.1 Experimental setup

A total of 10 replications were performed with the following combination of parameters:

- *Implementations:*
 - Java: 20 threads, Mersenne Twister PRNG
 - OpenCL: 20 work-items/work-groups (1 work-item per work-group), MWC64X PRNG [64]
- *Parameter sets:* 1, 2
- *Model sizes:* 400, 800, 1600, 3200, 6400

For each combination of parameters, the 10 replications were performed with distinct PRNG seeds. These replications are the basis for both the performance and statistical analysis performed in the next sections. All performance results are based on the mean run time of the 10 replications. Replications were performed in “headless” mode for both implementations, i.e., without any graphical component. All replications were performed on a machine with the following hardware and software configuration:

- Intel Xeon CPU E5-2650 v3 @ 2.30GHz (ten cores, two logical processors per core), 64GB RAM
- Ubuntu 16.04.1 LTS, OpenJDK Java 1.8.0, Intel OpenCL CPU Runtime 16.1.1, AMD APP SDK 3.0

The source code of both PPHPC implementations is available at <https://github.com/fakenmc/pphpc>. The data produced by this computational experiment, as well as the scripts used to set up and analyze the experiment, are available at <https://zenodo.org/record/293014>.

4.2 Performance comparison

Figure 3 shows how the Java and OpenCL implementations scale for increasingly larger model sizes. Speedups of the OpenCL implementation (on Intel and AMD runtimes) against the Java implementation for the tested model sizes are displayed in Figure 4. Table 2 provides more detailed data, including simulation times and relative standard deviations. These figures and table were generated with PerfAndPubTools [17].

(a) Parameter set 1.

(b) Parameter set 2.

Figure 3: Scalability of the Java and OpenCL implementations for increasing model sizes.

With respect to the scalability of the several versions, it is clear the OpenCL implementation, on both Intel and AMD runtimes, is consistently more performant than the parallel Java realization. In other words, there is no noticeable relative approximation between OpenCL and Java for increasing model sizes. Interestingly, and while the Intel runtime is more efficient than AMD’s for all tested size/parameter combinations, their relative performance differences seem to decrease for larger sizes.

Concerning speedups, the OpenCL implementation running on the Intel runtime is between 5× and 10× faster than the Java realization for parameter set 1, stabilizing at 8× for the larger sizes. A similar speedup pattern is observed when running the OpenCL

(a) Parameter set 1.

(b) Parameter set 2.

Figure 4: Speedups of the OpenCL implementation (on Intel and AMD runtimes) against the Java implementation for the tested model sizes. Error bars show the maximum and minimum speedups.

version on the AMD runtime, although the effective speedups are only 60%–75% of those verified on the Intel driver.

The speedups for second parameter set have less variation. For the OpenCL simulations performed with the Intel runtime, speedups over the Java implementation vary between 5× and 7×. The AMD replications follow the trend observed for parameter set 1, displaying a similar pattern to the Intel runs, with smaller speedups between 65% and 80% of Intel’s runs. Thus, not only are the observed speedups more stable for the second parameter set, but the performance gap between the Intel and AMD runtimes is smaller.

Impl.	Size	Param. set 1			Param. set 2		
		$\bar{t}(s)$	$s(\%)$	S_p^{Java}	$\bar{t}(s)$	$s(\%)$	S_p^{Java}
Java	400	17.85	8.49	1.00	29.21	2.19	1.00
	800	74.79	1.54	1.00	113.70	5.23	1.00
	1600	238.73	2.87	1.00	467.57	3.88	1.00
	3200	873.28	0.91	1.00	1982.88	1.44	1.00
	6400	3815.88	2.40	1.00	7545.00	3.55	1.00
CL-I	400	3.34	1.33	5.34	5.63	1.88	5.19
	800	7.07	0.65	10.57	16.02	0.55	7.10
	1600	22.44	0.38	10.64	79.90	0.14	5.85
	3200	108.07	0.11	8.08	320.20	0.05	6.19
	6400	448.16	0.07	8.51	1288.89	0.02	5.85
CL-A	400	4.34	0.65	4.11	8.38	0.70	3.49
	800	11.69	0.99	6.40	24.78	0.72	4.59
	1600	35.89	0.58	6.65	108.45	0.34	4.31
	3200	149.23	0.12	5.85	411.79	0.13	4.82
	6400	581.49	0.08	6.56	1573.80	0.06	4.79

Table 2: Times and speedups for the different versions using both parameter sets and tested model sizes. The $\bar{t}(s)$ column specifies the mean simulation time for each version and model size combination. The $s(\%)$ column shows the associated relative standard deviation, given by $100 \cdot s/\bar{t}(s)$, where s is the sample standard deviation. The S_p^{Java} column displays the speedups observed against the Java version.

Since parameter set 2 involves considerably more agents than the first, and thus entails more computationally expensive runs, API overheads seem to diminish and relative performance becomes more consistent.

From this comparison it becomes clear that using CPU-based OpenCL for implementing ABMs is a worthwhile endeavor. The speedups obtained against the parallel Java implementation offset the extra work required for developing a lower-level, CPU-optimized OpenCL implementation.

4.3 Statistical comparison

The OpenCL PPHPC implementation produces numerical equal results whether it is running on the Intel or AMD OpenCL runtimes. Thus, it is sufficient to compare the outputs of one or the other with the Java implementation, since they are the same.

The p -values obtained from the model-independent comparison of the Java and OpenCL PPHPC implementations for all combinations of parameter sets and model sizes are provided in Table 3. The p -values result from applying the MANOVA test on the first principal components which explain at least 90% of the respective output variance. The null hypothesis in this test is that the specified outputs from the two PPHPC versions are drawn from the same distribution. This comparison was performed with the `micompR` package [22].

In a total of 60 p -values (6 outputs, 2 parameter sets, 5 model sizes), 4 are below the 0.05 significance level, and none below 0.01. The p -values do not appear to follow any trend or pattern, e.g.,

Size/set	Outputs					
	p^s	p^w	p^c	$\bar{E}^s$	$\bar{E}^w$	$\bar{C}$
400/1	0.062	0.285	<u>0.029</u>	0.241	0.446	<u>0.030</u>
800/1	0.863	0.482	<u>0.865</u>	<u>0.047</u>	0.494	<u>0.864</u>
1600/1	0.532	0.816	0.759	0.332	0.382	0.768
3200/1	0.125	0.212	0.174	0.119	0.189	0.171
6400/1	0.189	0.117	0.218	<u>0.015</u>	0.452	0.218
400/2	0.557	0.639	0.717	0.735	0.535	0.721
800/2	0.522	0.560	0.558	0.289	0.724	0.559
1600/2	0.623	0.822	0.787	0.297	0.655	0.786
3200/2	0.153	0.567	0.715	0.830	0.654	0.715
6400/2	0.996	0.989	0.990	0.997	0.882	0.990

Table 3: P-values for the model-independent comparison of the Java and OpenCL PPHPC implementations (MANOVA test on the principal components which explain at least 90% of the respective output variance). Values lower than 0.05 are underlined.

smaller p -values do not seem to be associated with any particular output, parameter set or model size.

From these results, it is possible to conclude that the two model realizations seem to produce similar dynamic behavior. Thus, reimplementing PPHPC with OpenCL does not appear to have introduced any observable bias for the tested parameter sets.

5 CONCLUSIONS AND FUTURE WORK

In this paper we have compared a CPU-oriented OpenCL realization of the reference PPHPC ABM against a parallel Java implementation, which was already shown to be substantially faster than a serial NetLogo version. The OpenCL realization offered speedups up to 10 $\times$ against the Java implementation on a 10-core hyper-threaded Xeon processor, while also providing fully reproducible simulations. Thus, it is possible to conclude that CPU variants of the OpenCL standard are appropriate for developing high-performance ABMs.

The presented OpenCL realization of the PPHPC model has the potential to be improved by using the nested parallelism capabilities introduced OpenCL 2.0. More specifically, these capabilities allow device-side kernel invocations, thus avoiding host-side row synchronization, shown in the inner *for* loops of Algorithm 3.

We are currently working on an agent-parallel GPU realization of PPHPC, which, at the time of writing requires a number of performance and simulation accuracy improvements [14].

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