

Care HPS: A High Performance Simulation Methodology for Complex Agent-Based Models

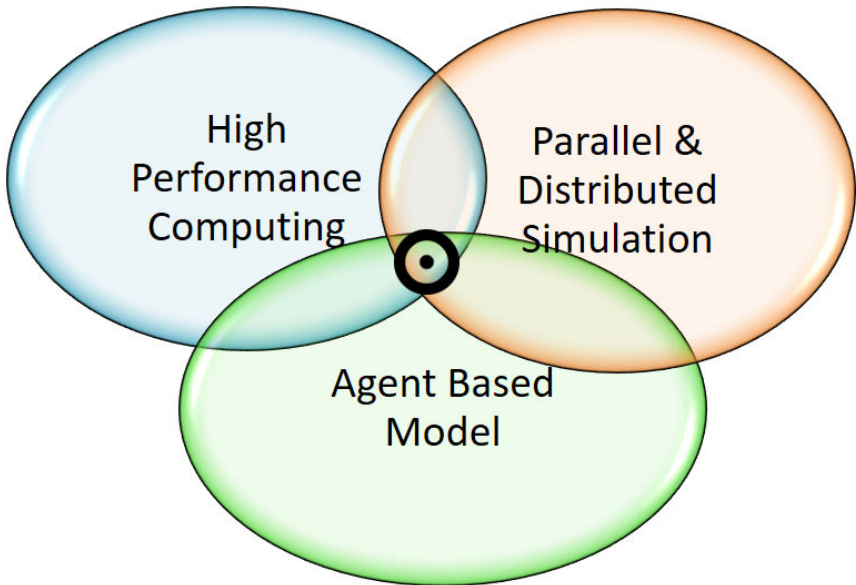
Francisco Borges

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Federal Institute of Bahia
and

Universitat Autònoma de Barcelona
Computer Architecture & Operating Systems Department
February 21, 2017, Salvador





High
Performance
Computing

Parallel &
Distributed
Simulation

Agent Based
Model

What is agent-based model?

- ▶ A fixed number of discrete and autonomous agents.
- ▶ Local rules are applied to each agent.
- ▶ An environment.
- ▶ Collective behaviors emerge as a result of local interaction between agents.

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As an example: fish schooling

Requirements for simulating complex system using ABMS

- ▶ Simulations must offer realistic results.
- ▶ It means simulations whose results are valid in reality, and which can also be used for prediction or to explain some phenomenon.
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- ▶ Moreover, they have a high computational complexity because thousands of agents model them, their higher level of parameters and their behavior complexity. Thus, this kind of simulation **requires a long execution time**.

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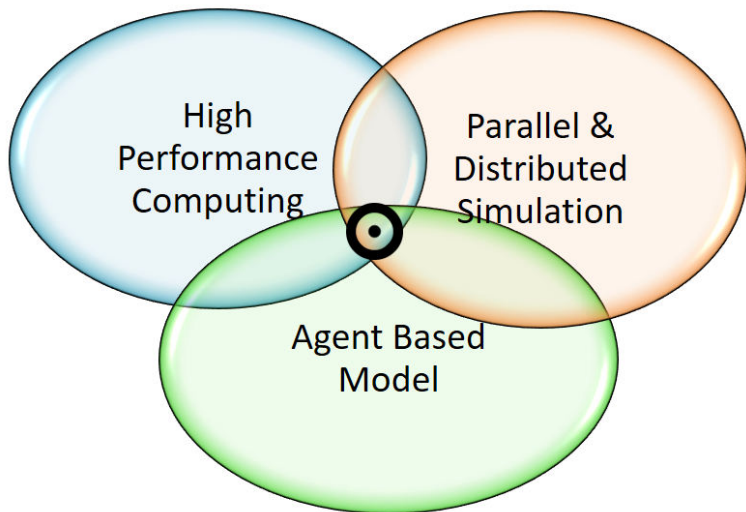
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Outline

- ① Introduction
- ② ABMs case study
- ③ HPC approaches
- ④ Care HPS
- ⑤ Results
- ⑥ Publications
- ⑦ Conclusion
- ⑧ Future work

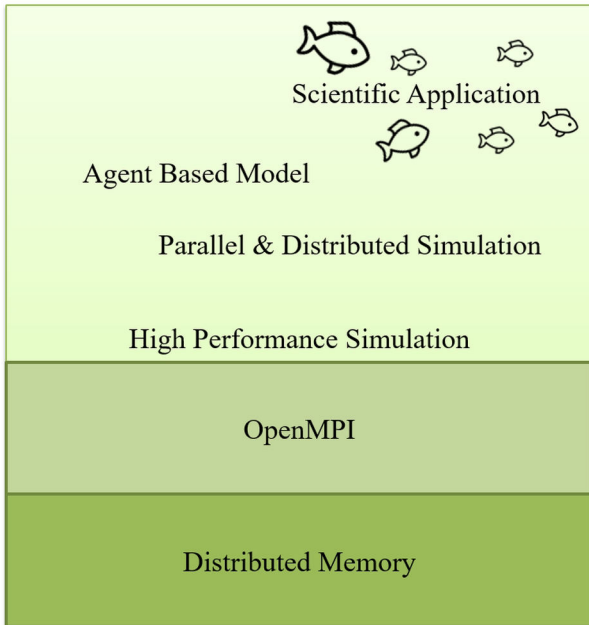
① Introduction

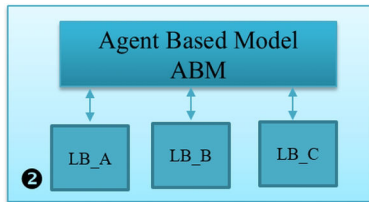
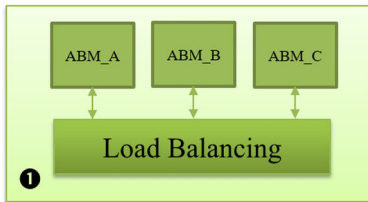
- Motivation and justification

- Research question

- Literature review

- Objective





- ▶ How to generalize our HPC techniques and approaches for agent-based models that demand high performance solutions?

- ▶ We can find several ABMS tools.
- ▶ A few of them **use HPC** to **execute** agent-based models.
- ▶ Although exist many consolidated ABMS tools **none of them** enable the **experimentation** in HPC.

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We introduce a methodology called Care High Performance Simulation (HPS). The main objective of Care HPS is:

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 - ▶ to enable application area researchers to study, design and implement complex ABM models that require an HPC solution; and,
 - ▶ to enable HPC experts to develop techniques and solutions of high performance distributed simulation for agent-based models.

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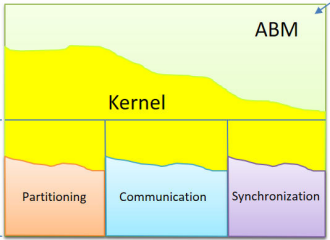
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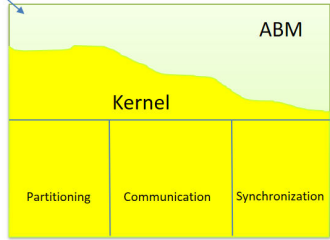
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Uses/Create



Care HPS



Other ABM Tools

Uses/Creates/
Extend HPC
Approaches

Uses HPC
Approaches

- ② ABMs case study
- ③ HPC approaches
- ④ Care HPS

② ABMs case study

- Overview

- Fish schooling

- Ant colony

- Shopping agent

- Assessment of *Aedes Aegypti* pupal productivity

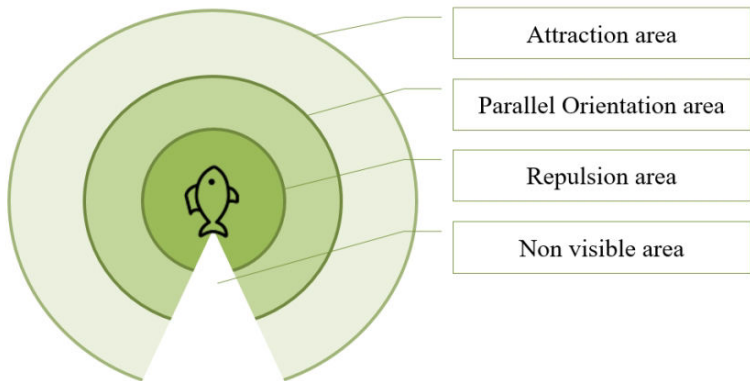
③ HPC approaches

④ Care HPS

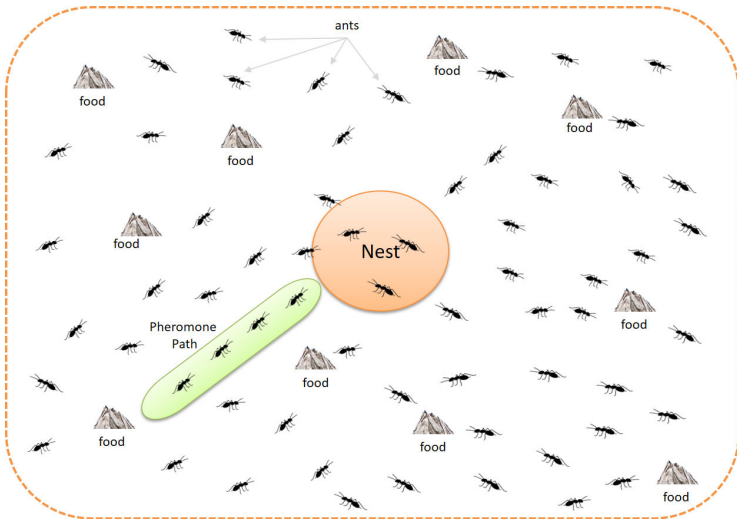
Agent-based models overview

| Model | Agents | Type | Real Application? |
|--------------------------|---------------------------------|--------------|-------------------|
| Fish Schooling | Fish | Biological | No |
| Ant colony | Ant | Biological | No |
| Shopping agent | Buyer | Sociological | No |
| Aedes Aegypti (mosquito) | Mosquito, Persons, Health Agent | Biological | Yes |

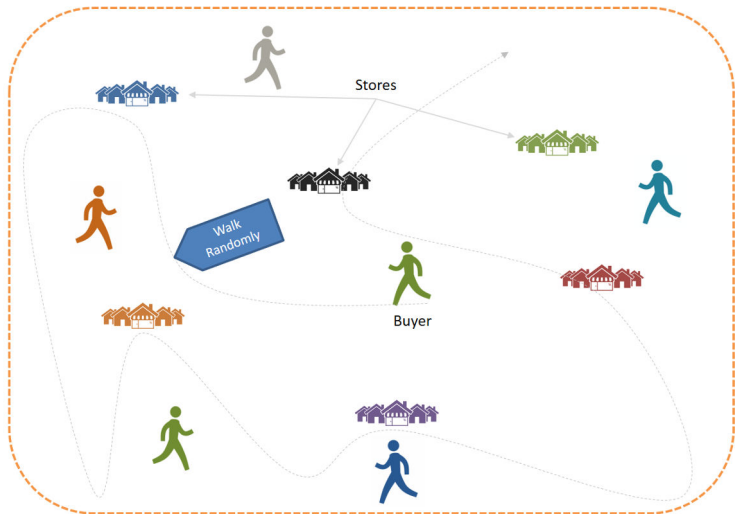
Huth and Wissel model



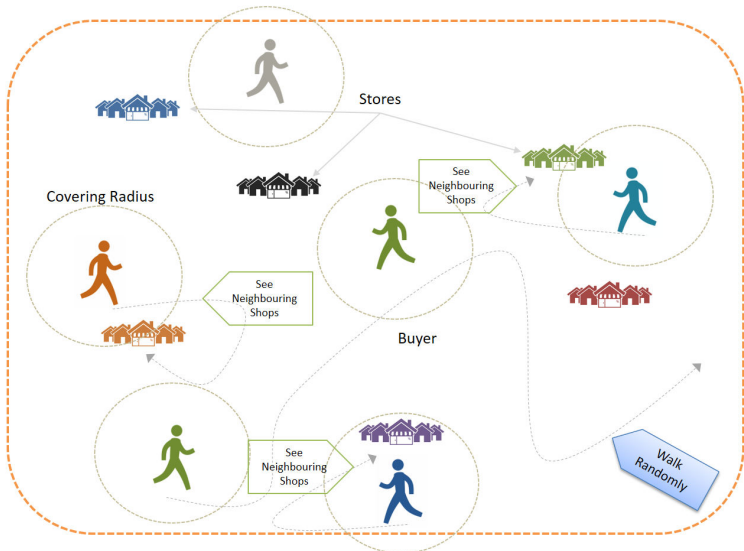
Wilensky model



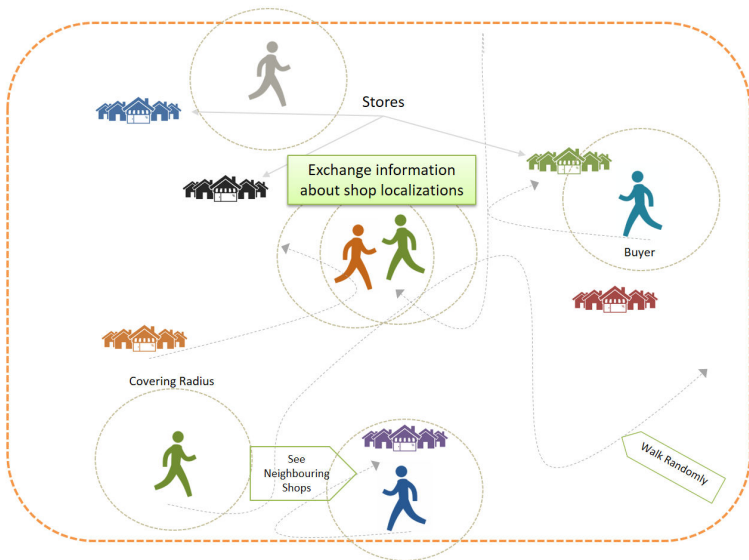
Gilbert and Troitzsch Model - simplest version



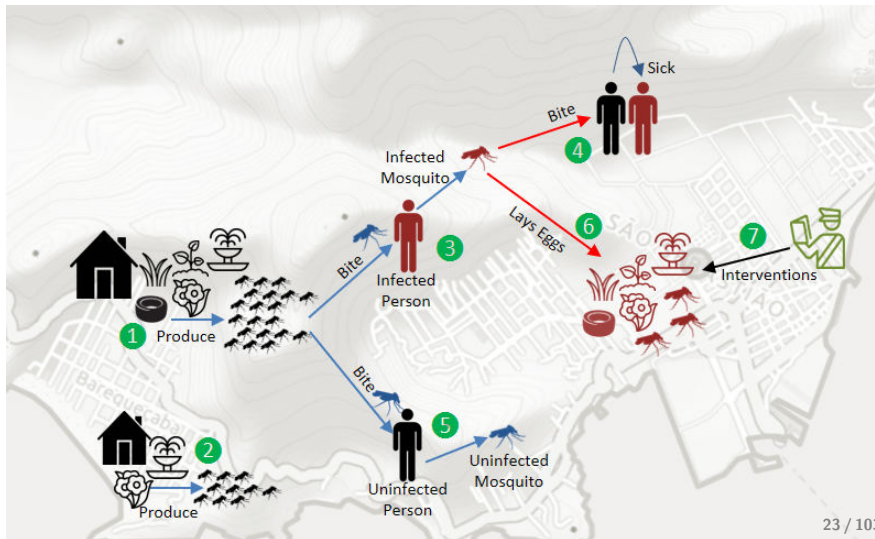
Gilbert and Troitzsch model - add another behavior



Gilbert and Troitzsch model - smartest agents

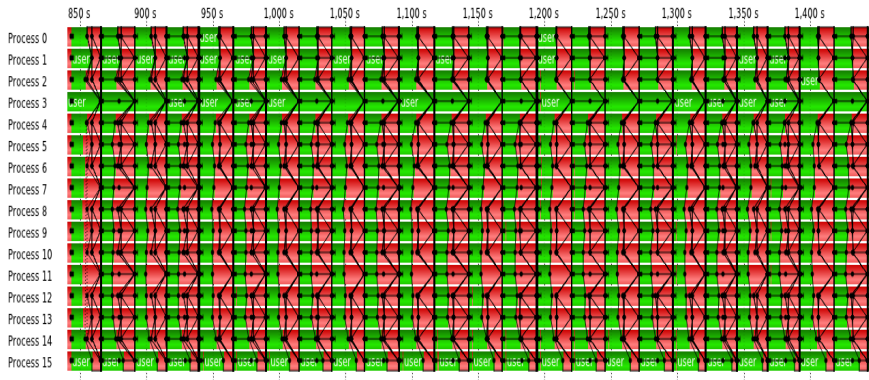


Assessment of Aedes Aegypti pupal productivity model



- ② ABMs case study
- ③ HPC approaches
 - Communication patterns
 - Strip partitioning
 - Hybrid strip partitioning
 - Optimal run length for simulations
 - Hybrid cluster-based partitioning
- ④ Care HPS

HPC approaches: Communication patterns



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Primary goals

We have compared three communication strategies:

- ▶ Asynchronous and synchronous message passing.
- ▶ Bulk-synchronous parallel (BSP) for communication.

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- ▶ Therefore, we implemented different methods of communication to evaluate the scalability.

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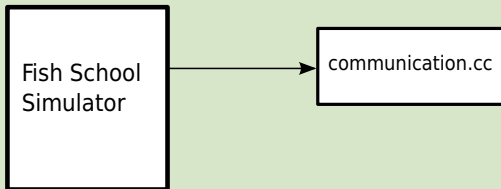
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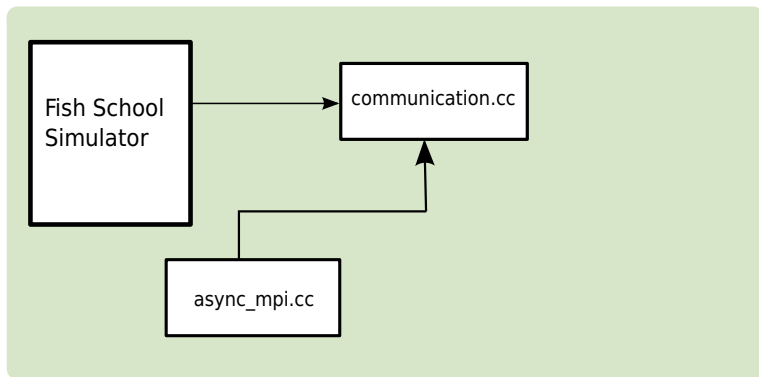
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Implementation



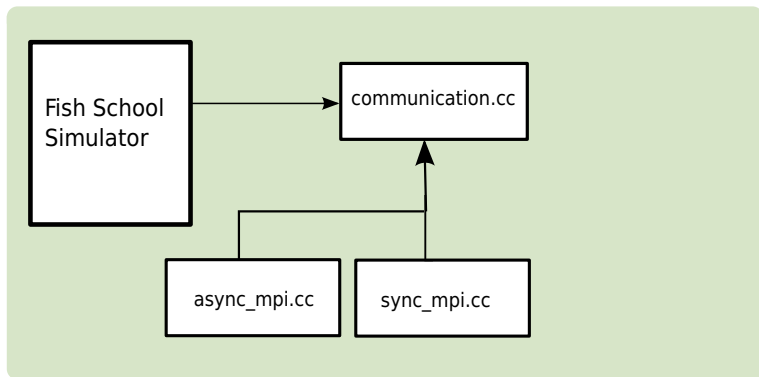
Implementation



Message passing via MPI

- ▶ MPI_Isend
- ▶ MPI_Irecv

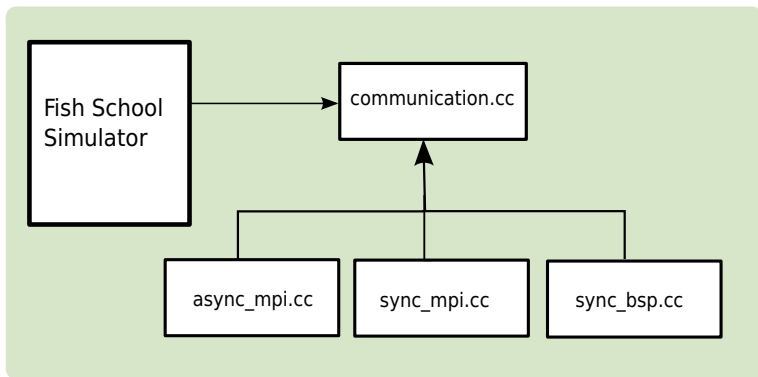
Implementation



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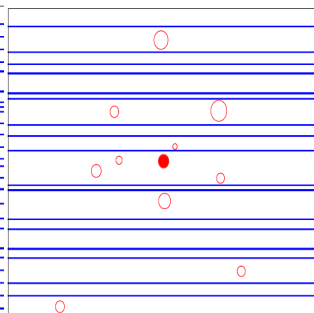
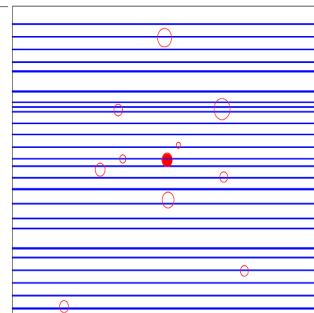
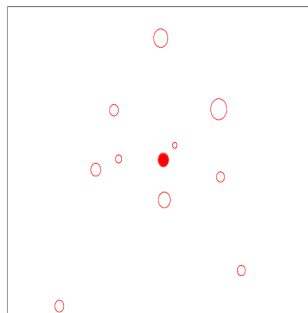
Implementation



Bulk-synchronous parallel via BSPonMPI

- ▶ BSPonMPI is a small communications library for BSP which consists of only 20 basic operations on top of MPI.

HPC approaches: Strip partitioning

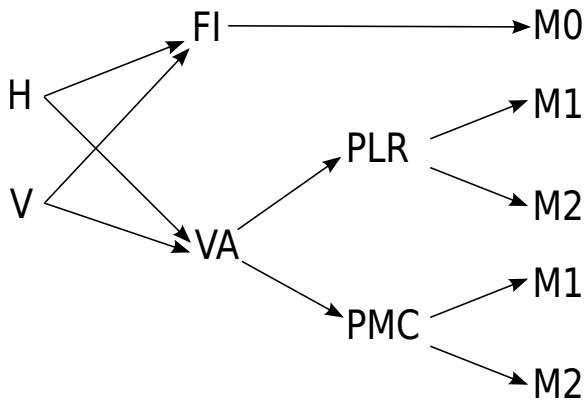


Ant colony environment

Environment partitioned
with sharing objects

Environment partitioned
with no sharing objects

Partitioning Scheme



HPC approaches: Hybrid strip partitioning approach

- ▶ We extended the strip partitioning algorithm.
- ▶ We decrease the idleness of these cores through the creation of OpenMP threads which are used to compute the extra agents that are in other cores.
- ▶ This partitioning checks the proportion of the quantity of agents inside a strip and dynamically creates a number of threads.

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HPC approaches: Optimal run length for simulations

- ▶ In simulations the results usually come from a stochastic process.
- ▶ How to compare these solutions since the results are not deterministic?
- ▶ Consequently how to guarantee that the output results are statistically trusted?
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Method steps

1 Identify the steady state

2 Identify the run length

- Identify the non significant correlation lag size

- Make a batch ten times the size of the lag

- Make the steady state replication run length ten batches long

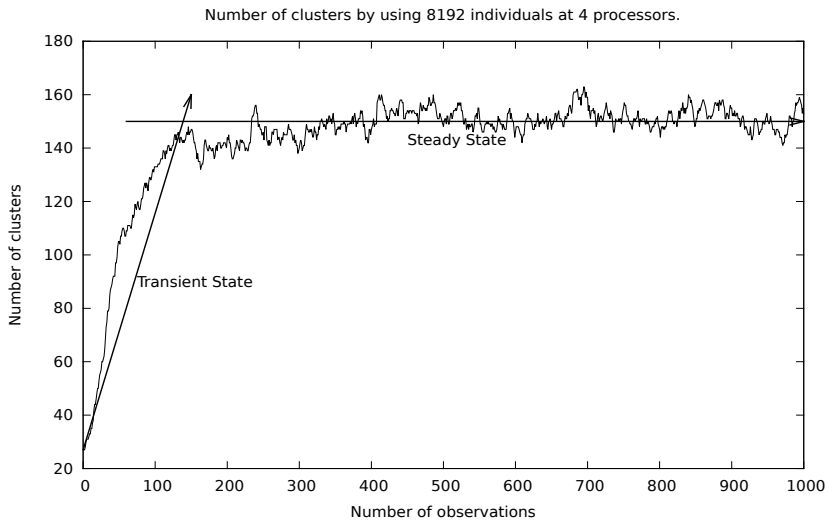
3 Replication analysis

- Ensure that the number of replication is enough

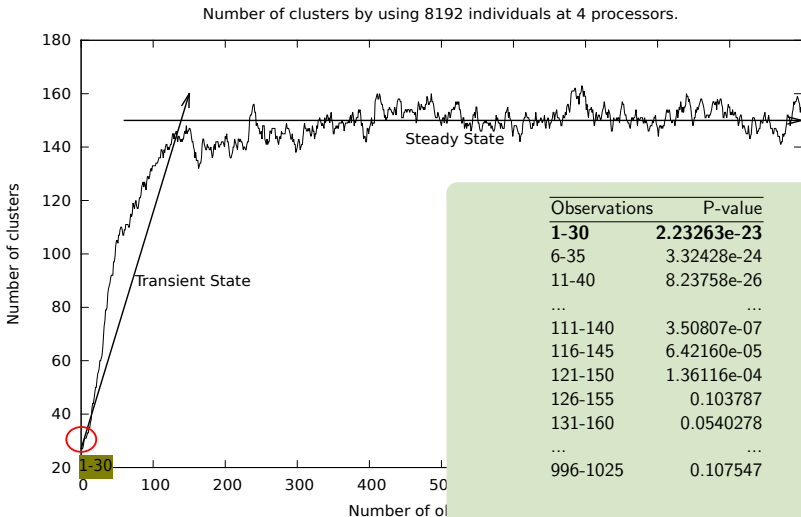
- Determine if the means are statistically significantly different from the others

- Identify which means are different

Optimal run length for simulations

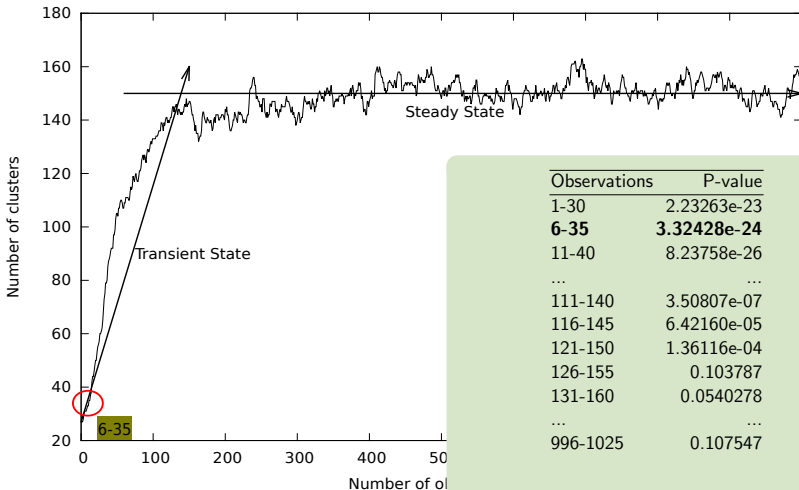


Optimal run length for simulations

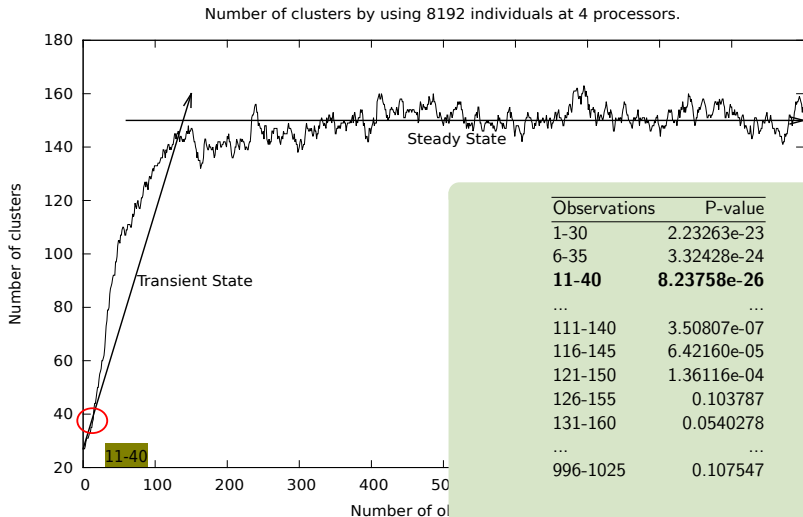


Optimal run length for simulations

Number of clusters by using 8192 individuals at 4 processors.

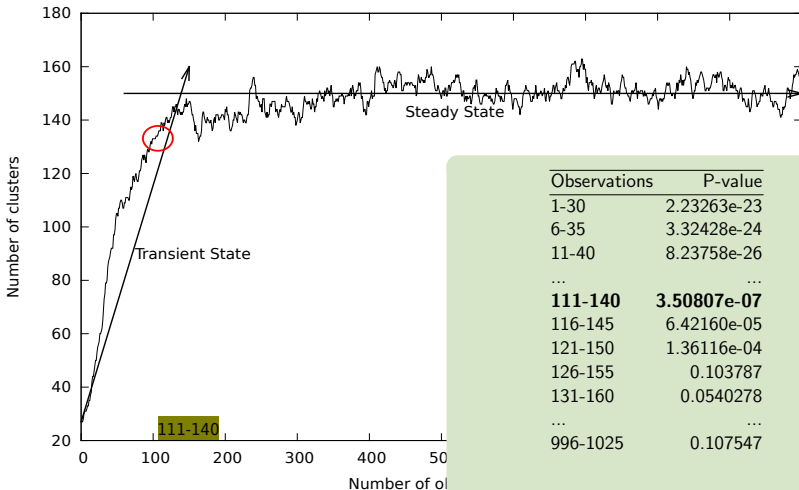


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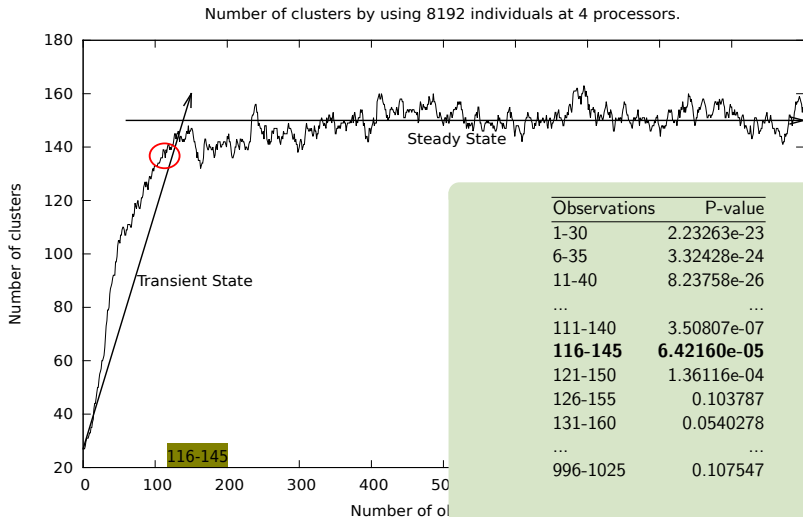


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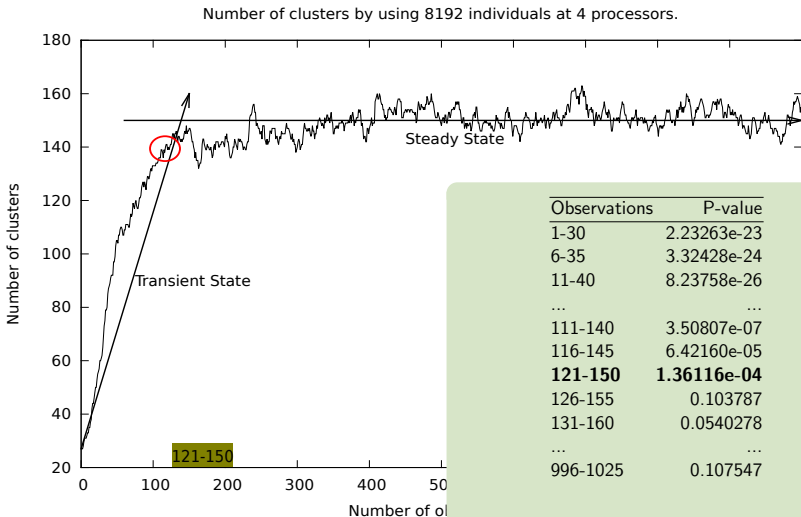
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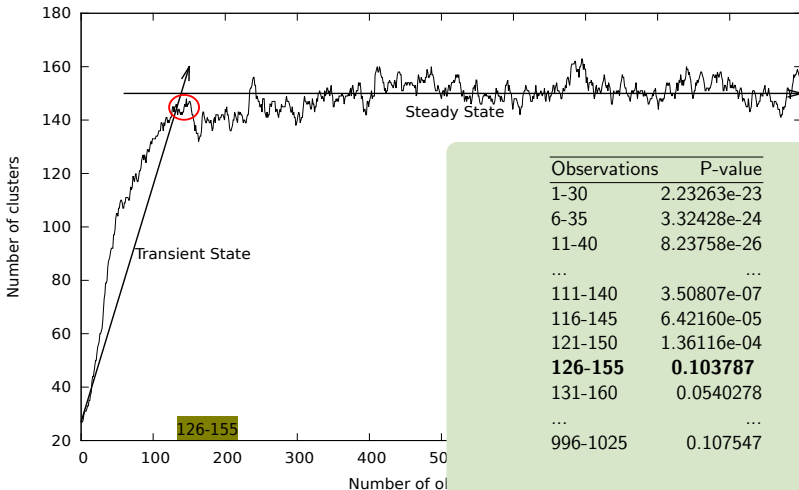
Optimal run length for simulations



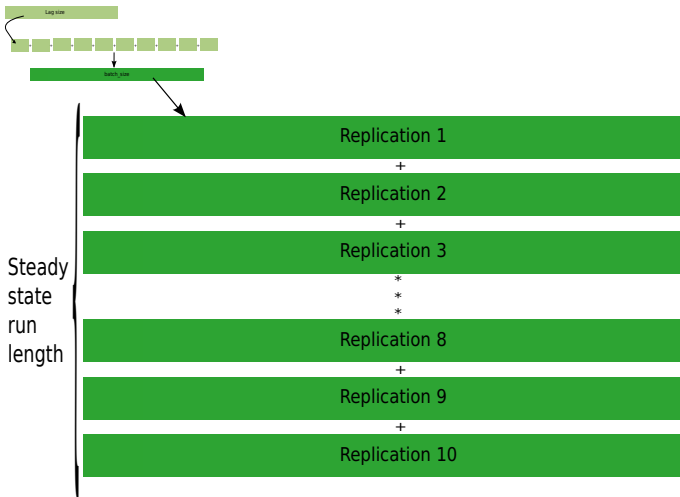
Optimal run length for simulations



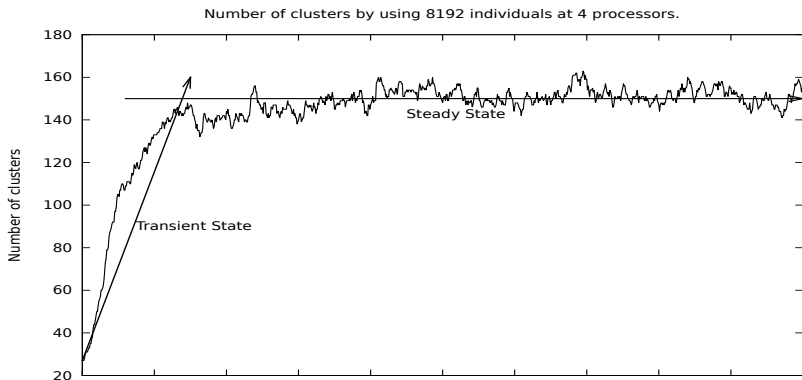
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Optimal run length for simulations



Optimal run length for simulations



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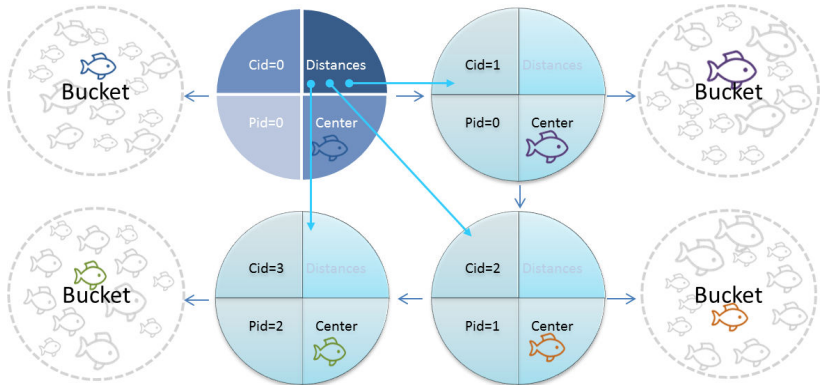
22,300

Lag size = 223

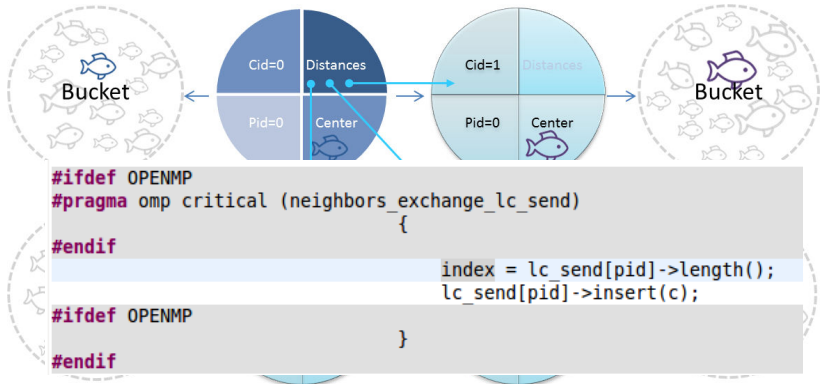
Batch size = 2,230

Total number of observations = 22,426

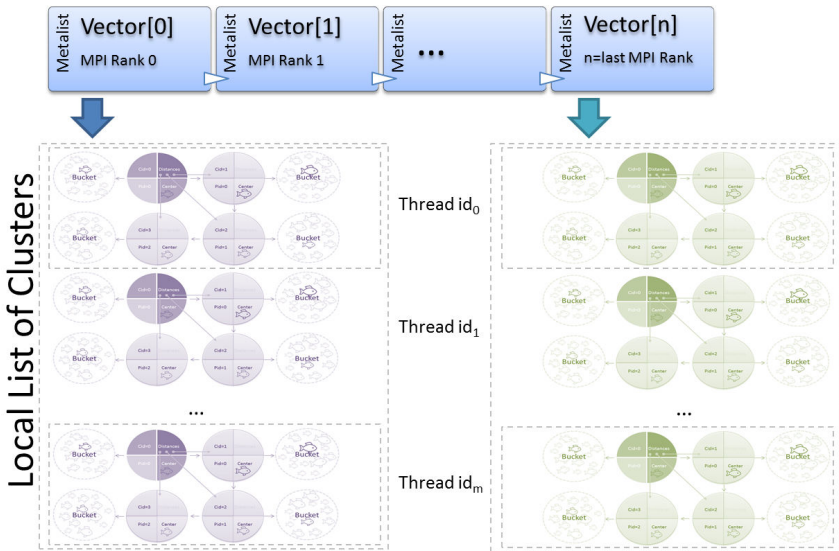
Distributed memory data structure



Distributed memory data structure



Shared memory data structure



② ABMs case study

③ HPC approaches

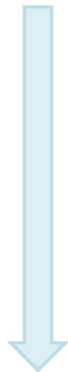
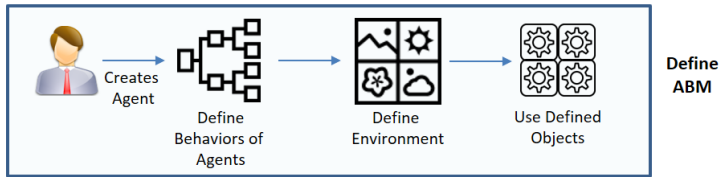
④ Care HPS

Methodology

Architecture

Care HPS as a scientific instrument

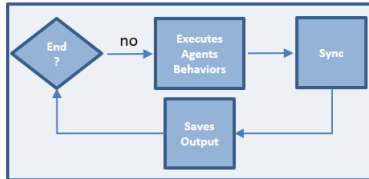
Methodology for application area user



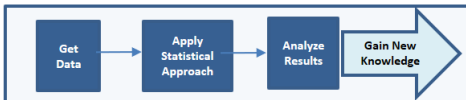
Configure Simulation



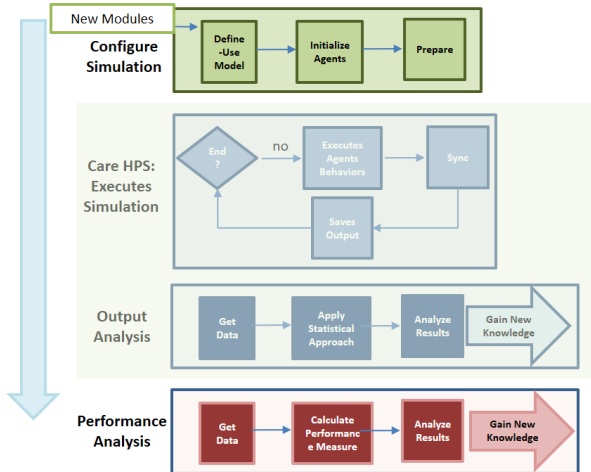
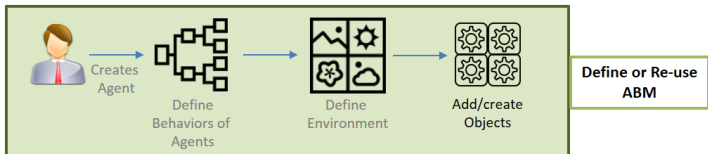
Care HPS: Executes Simulation



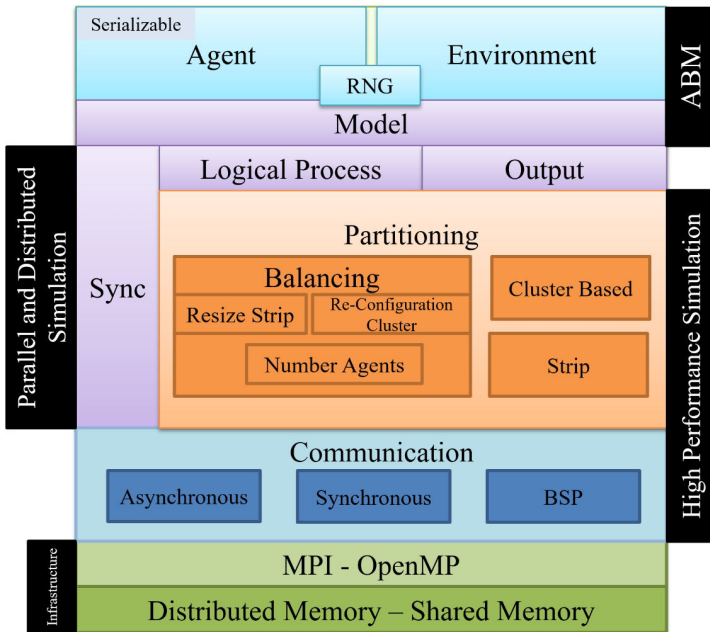
Output Analysis



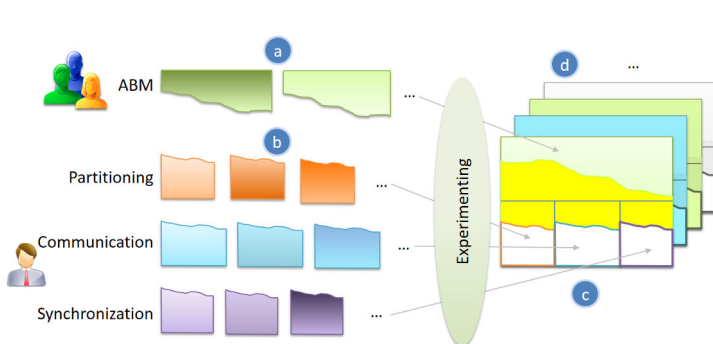
Methodology for HPC expert



Care HPS architecture



Several scenarios can be represented



Design and programming issues

Object-oriented design

- ▶ Design pattern

Design and programming issues

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Design and programming issues

Object-oriented design

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Object-oriented programming

- ▶ Inheritance
- ▶ Polymorphism
- ▶ Interface

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Creating an environment for the fish

```
pds_fish* PDS_FISH=NULL;
ABM_fish* ABM=NULL;
environment* ENV=NULL;
PDS_FISH = new pds_fish ();
ABM = PDS_FISH->createABM ();

/** Creates an environment with a
plan( $ax + by + cz + d = 0$ ) defined by
equation:  $2*x - 13*y + 5$  */

ENV = PDS_FISH → createEnvironment(new linear_plan( 2,-13,0,5));

/** The user can create how many objects inside of
the environment that are required. */
/** Code that creates other objects inside of
the environment defined by the equation:  $2*y-3$  */

// ENV → createObject(new linear_plan(0,2,0,-3)); //
```

Implements the interaction with environment

```
vector<object*> obj_env;  
obj_env = ENV->getObjects();  
for (vector<object*>::iterator ob=obj_env.begin();  
      ob!=obj_env.end();  
      ob++)  
  
    if ( (*ob)->check_collision(this->get_position(),  
                                this->get_velocity(),  
                                MAXIMUM_VISION_RANGE)  
        this->repulsion(*this);  
}
```

Creating the partitioning class

```
class partitioning_strip_hybrid : public
    partitioning_strip{

public :
    // Constructor methods

    // Override the execute method
    void execute(int);

};
```

Defining the partitioning strategy

```
//here goes other the factory methods of the model class.  
partitioning* model_ant::factory_partitioning(){  
    return new partitioning_strip_hybrid();  
}
```

- 5 Results
- 6 Publications

5 Results

- Verification of Pupal productivity model

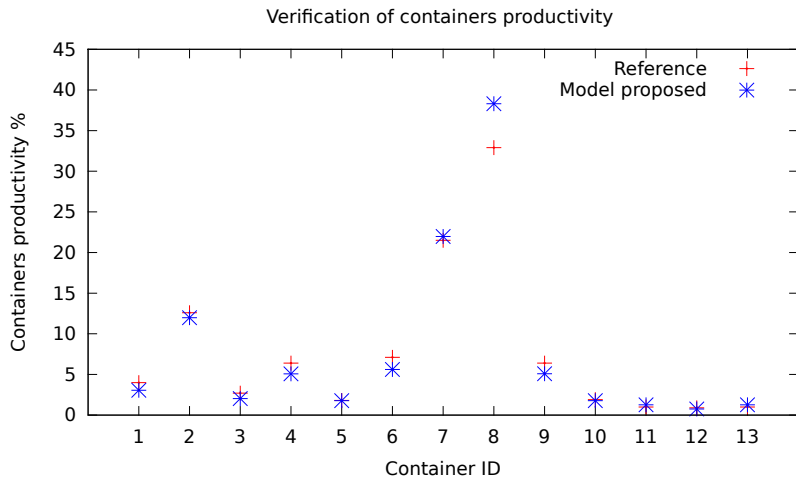
- HPC techniques

- Care HPS features

- Care HPS scalability

6 Publications

Verification of containers productivity





Results: Container pupal productivity

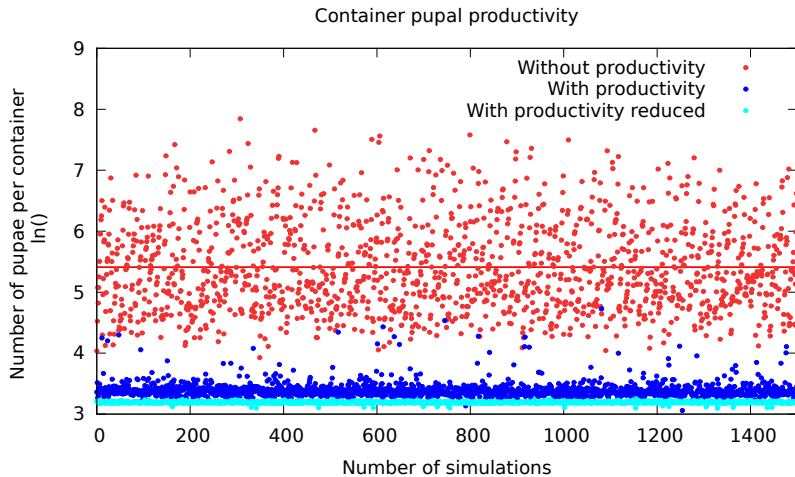
Objective

Present the effects of consider the pupal productivity issue in the number of pupae per container.

Data and parameters

| | |
|-----------------------|---|
| Number of simulations | 1500 |
| Days simulated | 100 |
| Measure analyzed | Number of pupal per containers ln() scale. |

Container pupal productivity





Verification of Pupal productivity model

Results: What-if

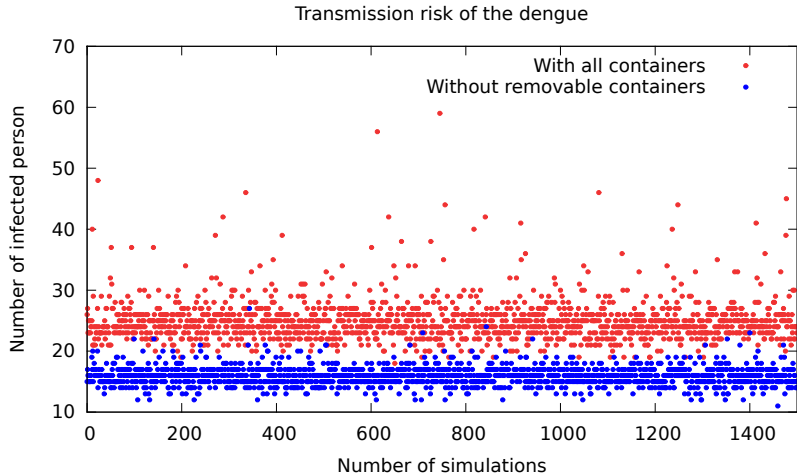
Objective

Hypothetical situation where a health agent changes the model parameters in order to simulate actions for decisions made.

Data and parameters

| | |
|-----------------------|---------------------------|
| Number of simulations | 1500 |
| Days simulated | 100 |
| Measure analyzed | Number of infected person |

What-if





Results: Area of the mosquito actuation.

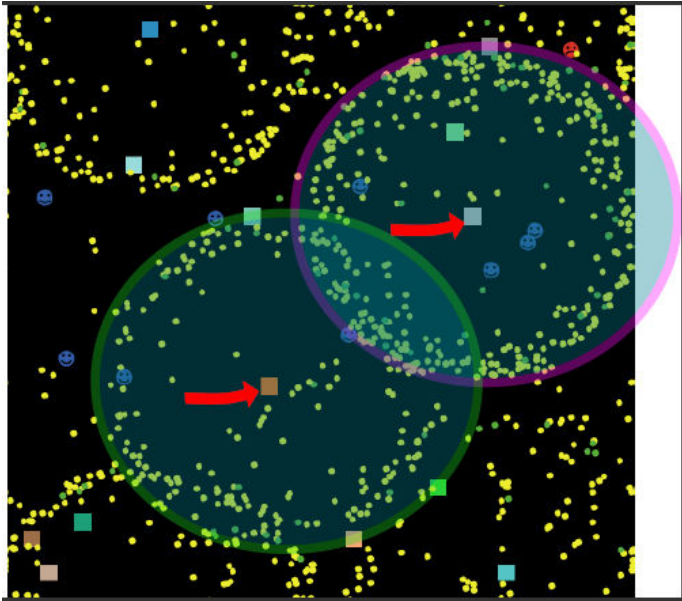
Objective

Emergent behavior of the mosquitoes.

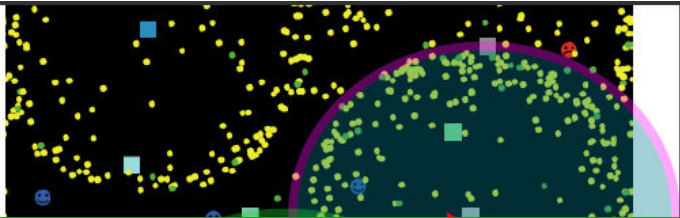
Data and parameters

| | |
|-----------------------|------------------|
| Number of simulations | 1500 |
| Days simulated | 100 |
| Measure analyzed | radius of flight |

Area of the mosquito actuation.



Area of the mosquito actuation.



Francisco Borges, Albert Gutierrez-Milla, Remo Suppi, Emilio Luque, Marylene de Brito Arduino. An Agent-Based Model for Assessment of *Aedes Aegypti* Pupal Productivity. WSC 2015. (CORE B)



5 Results

- Verification of Pupal productivity model

- HPC techniques

 - Communication patterns

 - Hybrid cluster-based partitioning

 - Strip partitioning

 - Hybrid Strip partitioning

- Care HPS features

- Care HPS scalability

6 Publications



Results: Communication patterns

Objective

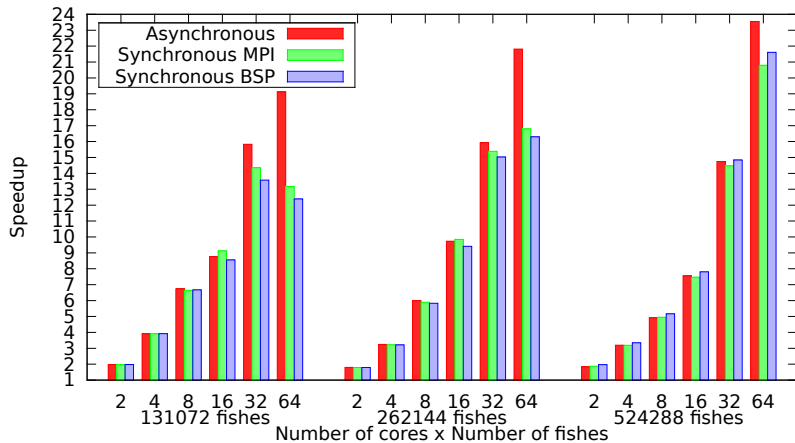
Speedups comparison of the communication strategies: asynchronous, synchronous BSP, and synchronous MPI.

Data and parameters

| | |
|------------------|------------------------|
| ABM | Fish schooling |
| Number of agents | 131K, 262K and 524K |
| Number of cores | 2, 4, 8, 16, 32 and 64 |
| Measure analyzed | Speedup |

Speedup of each communication strategy

Speedup by number of fishes and cores





Results: Communication patterns

Objective

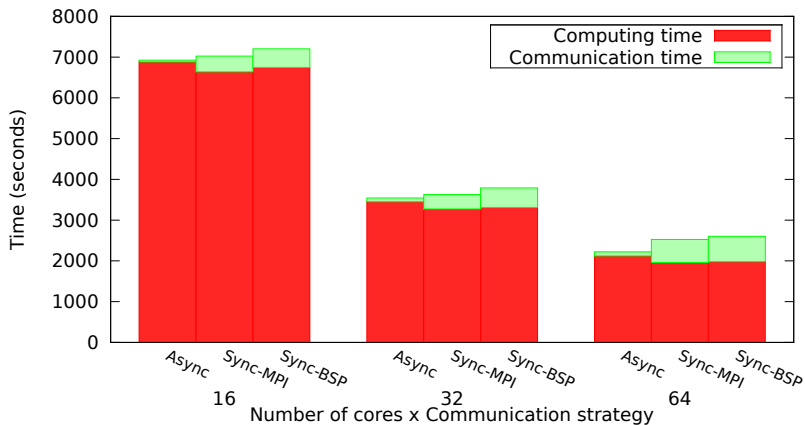
Computing time and communication time of communication strategies.

Data and parameters

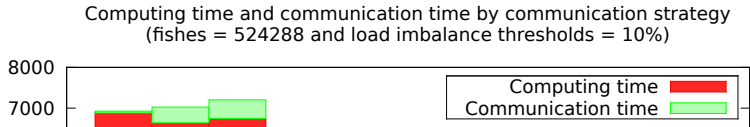
| | |
|------------------|--------------------------------------|
| ABM | Fish schooling |
| Number of agents | 524K |
| Number of cores | 16, 32 and 64 |
| Measure analyzed | Computing and communication time (s) |

Computing time and communication time x communication strategies

Computing time and communication time by communication strategy
(fishes = 524288 and load imbalance thresholds = 10%)



Computing time and communication time x communication strategies



Roberto Solar, Francisco Borges, Remo Suppi, Emilio Luque. Improving Communication Patterns for Distributed Cluster-Based Individual-Oriented Fish School Simulations. Procedia Computer Science. ICCS 2013: 702-711. (CORE A)

sync sync-MPI sync-BSP sync sync-MPI sync-BSP sync sync-MPI sync-BSP
16 32 64
Number of cores x Communication strategy



Results: Hybrid cluster-based partitioning

Objective

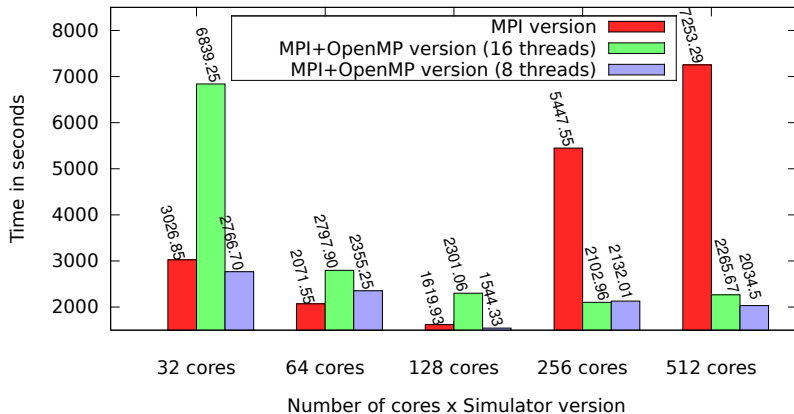
Total execution time comparison between the partitioning approaches: Pure MPI and Hybrid.

Data and parameters

| | |
|-------------------|--------------------------|
| ABM | Fish schooling |
| Number of agents | 131K |
| Number of cores | 32, 64, 128, 256 and 512 |
| Number of threads | No threads, 8 and 16. |
| Measure analyzed | Execution time (s) |

Total execution time comparison between the MPI and the MPI+OpenMP

Total execution time
Simulation of 131,072 individuals





Results: Hybrid cluster-based partitioning

Objective

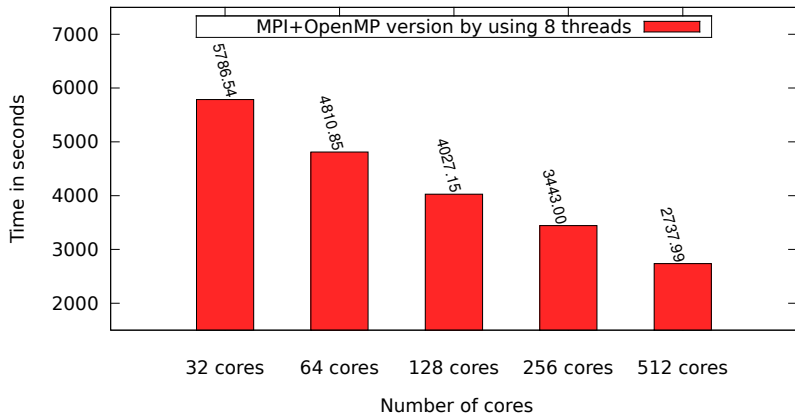
Scalability of the hybrid version.

Data and parameters

| ABM | Fish schooling |
|-------------------|--------------------------|
| Number of agents | 262K |
| Number of cores | 32, 64, 128, 256 and 512 |
| Number of threads | 8 |
| Measure analyzed | Execution time (s) |

Scalability of the hybrid version by using 8 threads per MPI process

Total execution time
Simulation of 262,144 individuals





Results: Hybrid cluster-based partitioning

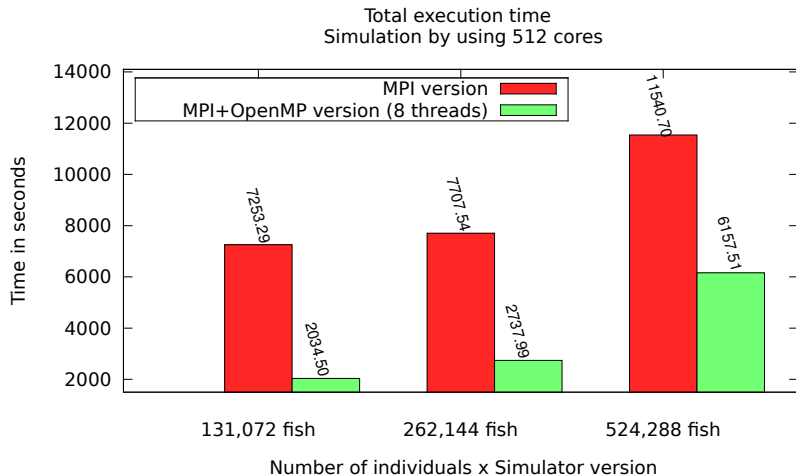
Objective

Total execution time comparison between the MPI and the MPI+OpenMP versions by using 512 cores.

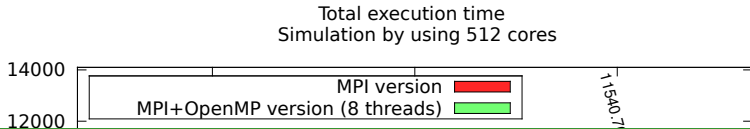
Data and parameters

| | |
|-------------------|--------------------|
| ABM | Fish schooling |
| Number of agents | 131k, 262K, 524k |
| Number of cores | 512 |
| Number of threads | 8 |
| Measure analyzed | Execution time (s) |

Total execution time comparison between the MPI and the MPI+OpenMP versions by using 512 cores



Total execution time comparison between the MPI and the MPI+OpenMP versions by using 512 cores



Francisco Borges, Albert Gutierrez-Milla, Remo Suppi, Emilio Luque. A Hybrid MPI+OpenMP Solution of the Distributed Cluster-Based Fish Schooling Simulator. Procedia Computer Science. ICCS 2014. (CORE A)

131,072 fish

262,144 fish

524,288 fish

Number of individuals x Simulator version



Results: Strip partitioning

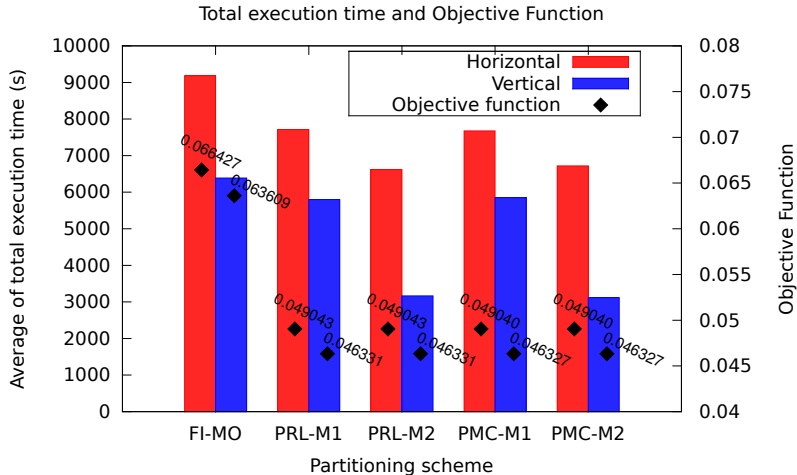
Objective

Total execution time average and objective function of each partitioning strategies.

Data and parameters

| | |
|------------------|--------------------|
| ABM | Ant colony |
| Number of agents | 10k |
| Number of cores | 64 |
| Measure analyzed | Execution time (s) |

Total execution time average and objective function of the partitioning strategies





Results: Strip partitioning

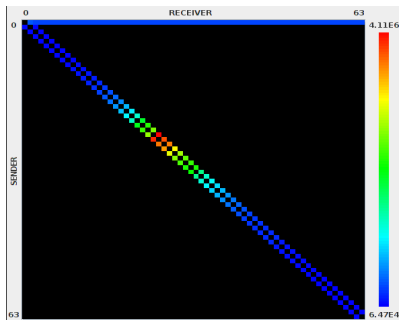
Objective

Comparison of total volume bytes of the worst and best strategies with heat maps.

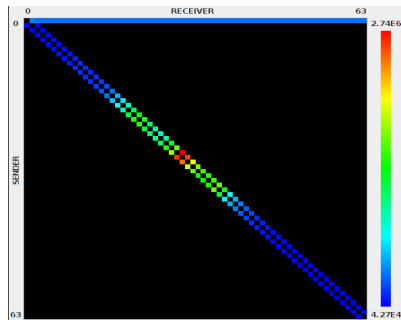
Data and parameters

| | |
|------------------|-------------------|
| ABM | Ant colony |
| Number of agents | 10k |
| Number of cores | 64 |
| Strategies | best and worst |
| Measure analyzed | Total volume data |

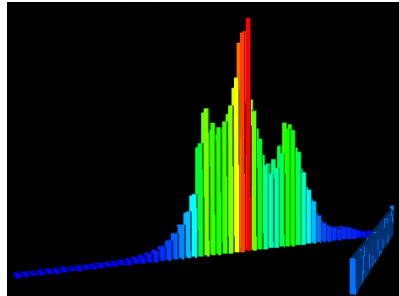
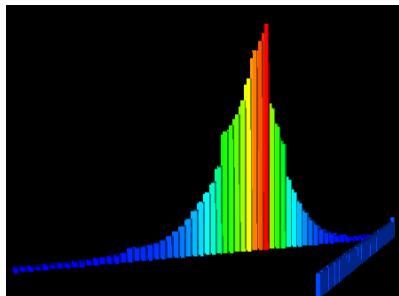
Comparison of total volume bytes with heat maps



(a1) H-FI-M0



(b1) V-PMC-M2





Results: Strip partitioning

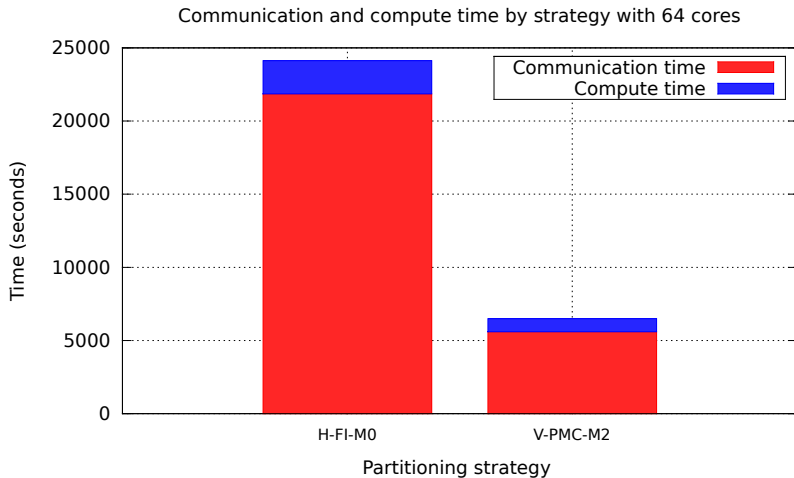
Objective

Communication and computing time of the worst and best strategies.

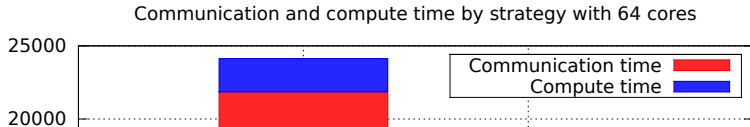
Data and parameters

| | |
|------------------|--------------------|
| ABM | Ant colony |
| Number of agents | 10k |
| Number of cores | 64 |
| Strategies | best and worst |
| Measure analyzed | Execution time (s) |

Communication and computing time of the worst and best strategies



Communication and computing time of the worst and best strategies



Francisco Borges, Albert Gutierrez-Milla, Remo Suppi, Emilio Luque.
Strip Partitioning for Ant Colony Parallel and Distributed
Discrete-Event Simulation. Procedia Computer Science. ICCS 2015.
(CORE A)

H-FI-M0

V-PMC-M2

Partitioning strategy



Results: Hybrid Strip partitioning

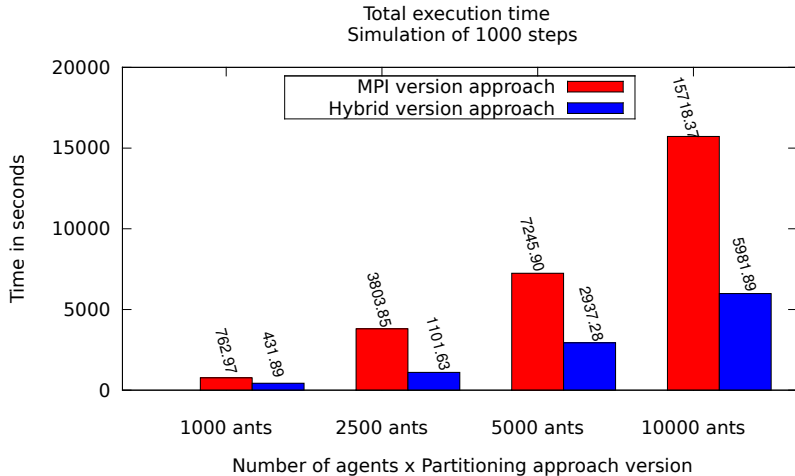
Objective

Total execution time of pure MPI and Hybrid strip partitioning algorithm.

Data and parameters

| | |
|-------------------|--------------------|
| ABM | Ant colony |
| Number of agents | 1k, 2.5k, 5k, 10k |
| Number of cores | 64 |
| Number of threads | No threads, [2..8] |
| Measure analyzed | Execution time (s) |

Total execution time of pure MPI and Hybrid strip partitioning algorithm



Results: Hybrid Strip partitioning

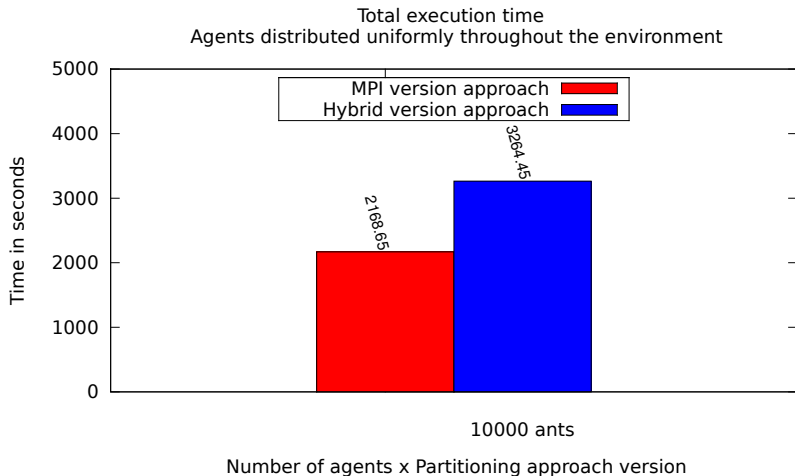
Objective

Total execution of pure MPI and hybrid strip partitioning algorithm. Agents distributed uniformly throughout the environment

Data and parameters

| | |
|-------------------|---|
| ABM | Ant colony |
| Number of agents | 10k |
| Number of cores | 64 |
| Number of threads | No threads; [2..8] threads dynamically created. |
| Measure analyzed | Execution time (s) |

Total execution of pure MPI and hybrid strip partitioning algorithm. Agents distributed uniformly throughout the environment.



5 Results

- Verification of Pupal productivity model

- HPC techniques

- Care HPS features

 - Agent layer

 - Environment layer

- Care HPS scalability

6 Publications

Results: Agent layer

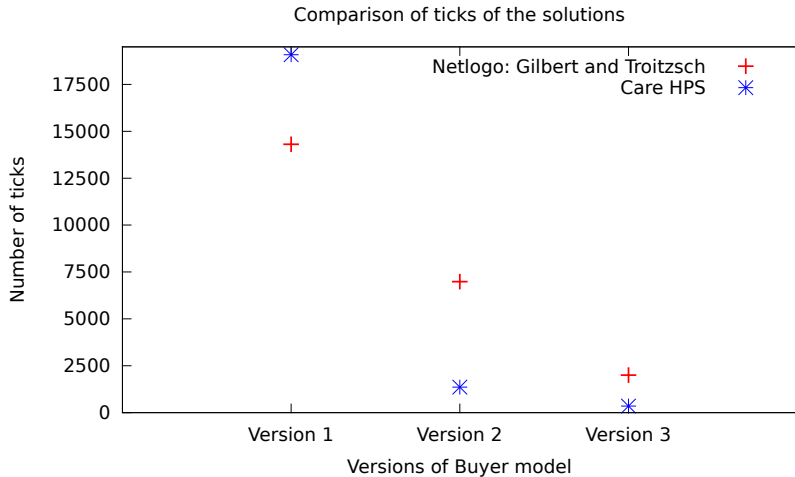
Objective

ABMS tools must be able to model agent rules and behaviors. So, this model can create collective and emergent behavior. It is important that these tools can reflect the interaction among agents

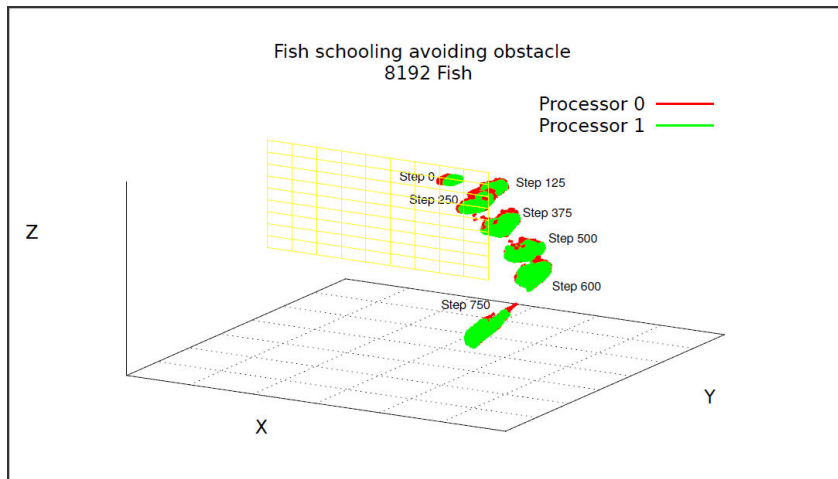
Data and parameters

| ABM | Shopping agent |
|----------------------|-----------------|
| Number of agents | 10 |
| Number of cores | 1 |
| Size of list product | 10 |
| Number of stores | 12 |
| Measure analyzed | Number of ticks |

Ticks of Gilbert and Troitzsch Netlogo version and Care HPS



Fish repulsion behavior to avoid the collision. This experimentation was executed in two cores using 8192 agents





Results: Care HPS scalability

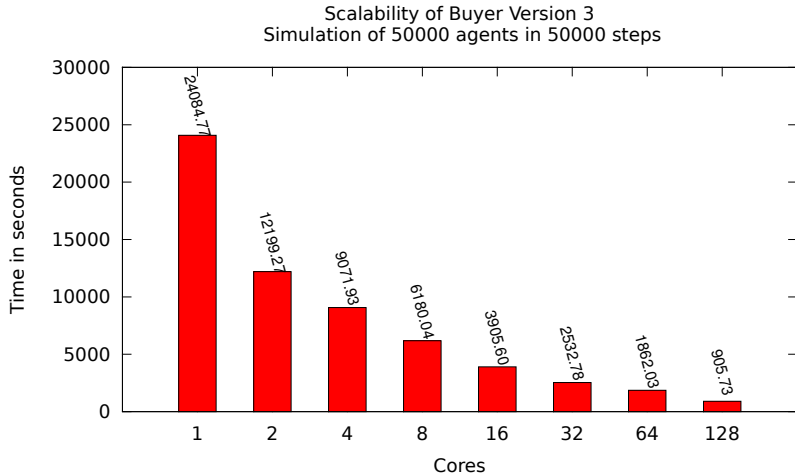
Objective

Present the scalability of Care HPS.

Data and parameters

| | |
|------------------|--------------------------------|
| ABM | Shopping agent |
| Number of agents | 50K |
| Number of cores | 1, 2, 4, 8, 16, 32, 64 and 128 |
| Measure analyzed | Execution time (s) |

Scalability of Buyer Version 3 with 50000 agents in 50000 steps





Results: Care HPS scalability

Objective

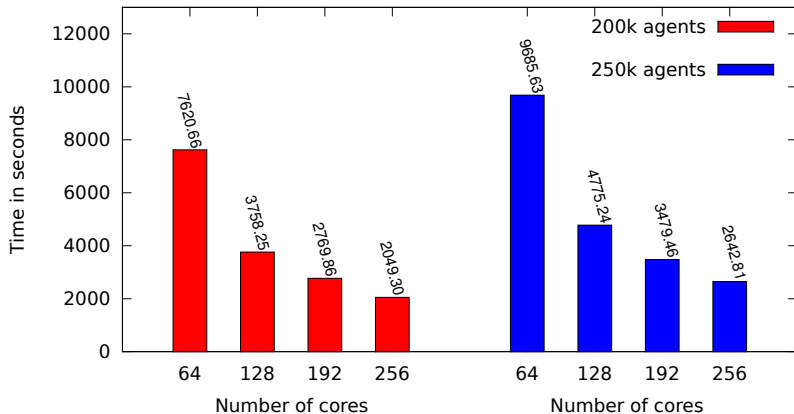
Present the scalability of Care HPS.

Data and parameters

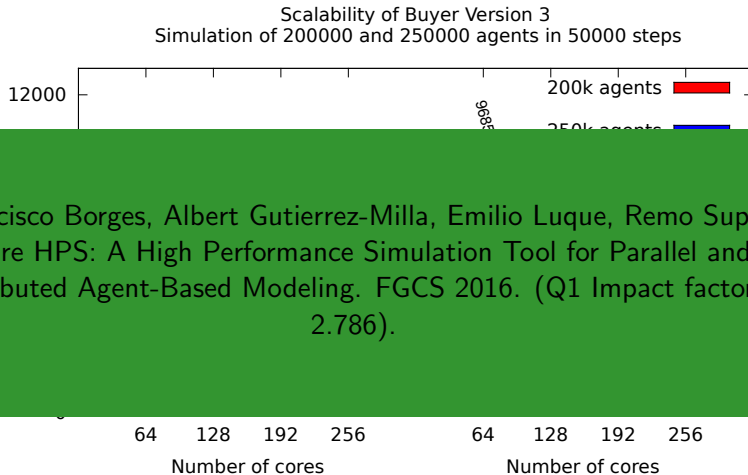
| | |
|------------------|----------------------|
| ABM | Shopping agent |
| Number of agents | 200K and 250K |
| Number of cores | 64, 128, 192 and 256 |
| Measure analyzed | Execution time (s) |

Scalability of Buyer Version 3 in 50000 steps to 200k and 250k agents executed in 64, 128, 192 and 256 cores

Scalability of Buyer Version 3
Simulation of 200000 and 250000 agents in 50000 steps



Scalability of Buyer Version 3 in 50000 steps to 200k and 250k agents executed in 64, 128, 192 and 256 cores



Francisco Borges, Albert Gutierrez-Milla, Emilio Luque, Remo Suppi.
Care HPS: A High Performance Simulation Tool for Parallel and
Distributed Agent-Based Modeling. FGCS 2016. (Q1 Impact factor of
2.786).

5 Results

6 Publications

The following papers are strictly related with this research.

- ▶ Roberto Solar, **Francisco Borges**, Remo Suppi, Emilio Luque. **Improving Communication Patterns for Distributed Cluster-Based Individual-Oriented Fish School Simulations**. ICCS 2013: 702-711. (CORE A)
- ▶ **Francisco Borges**, Roberto Solar, Remo Suppi y Emilio Luque. **Performance and scalability in distributed cluster-based individual-oriented fish school simulations**. Actas de las XXIV Jornadas de Paralelismo, Madrid (Madrid), 17-20 Septiembre 2013:401-406.
- ▶ Gallo, S., **Borges, F.**, Suppi, R., Luque Fadón, E., De Giusti, L. C., and Naiouf, M. (2013). **Mejoras en la eficiencia mediante Hardware Locality en la simulación distribuida de modelos orientados al individuo**. In XVIII Congreso Argentino de Ciencias de la Computación.
- ▶ **Francisco Borges**, Albert Gutierrez-Milla, Remo Suppi, Emilio Luque. **A Hybrid MPI+OpenMP Solution of the Distributed Cluster-Based Fish Schooling Simulator**. ICCS 2014. (CORE A)

- ▶ **Francisco Borges**, Albert Gutierrez-Milla, Remo Suppi, Emilio Luque. **Optimal Run Length for Discrete-Event Distributed Cluster-Based Simulations**. ICCS 2014. (CORE A)
- ▶ **Francisco Borges**, Albert Gutierrez-Milla, Remo Suppi, Emilio Luque. **Strip Partitioning for Ant Colony Parallel and Distributed Discrete-Event Simulation**. ICCS 2015. (CORE A)
- ▶ **Francisco Borges**, Albert Gutierrez-Milla, Remo Suppi, Emilio Luque, Marylene de Brito Arduino. **An Agent-Based Model for Assessment of Aedes Aegypti Pupal Productivity**. WSC 2015. (CORE B)
- ▶ **Francisco Borges**, Albert Gutierrez-Milla, Emilio Luque, Remo Suppi. **Care HPS: A High Performance Simulation Tool for Parallel and Distributed Agent-Based Modeling**. FGCS 2016. (Q1 Impact factor of 2.786).

The following papers are other publications with our research group related with ABM and HPC.

- ▶ Albert Gutierrez-Milla, **Francisco Borges**, Remo Suppi, Emilio Luque. **Individual-Oriented Model Crowd Evacuations Distributed Simulation**. ICCS 2014. (CORE A)
- ▶ Albert Gutierrez-Milla, **Francisco Borges**, Remo Suppi, Emilio Luque. **Crowd evacuations SaaS: an ABM approach**. ICCS 2014. (CORE A)
- ▶ Albert Gutierrez-Milla, **Francisco Borges**, Remo Suppi, Emilio Luque. **Simulació de evacuaciones multitudinarias basadas en modelos orientados al individuo**. Actas de las XXV Jornadas de Paralelismo, Valladolid, 17-19 Septiembre 2014.
- ▶ Albert Gutierrez-Milla, **Francisco Borges**, Remo Suppi, Emilio Luque. **Crowd Dynamics Modeling and Collision Avoidance with OpenMP**. WSC 2015. (CORE B)
- ▶ Albert Gutierrez-Milla, **Francisco Borges**, Remo Suppi, Emilio Luque. **Crowd turbulence with ABM and Verlet Integration on GPU cards**. ICCS 2016. (CORE A)

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7 Conclusion

8 Future work

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- ▶ We introduce Care High Performance Simulation (HPS).
- ▶ The initial idea of Care HPS comes up as a methodology to support our research group, with the aim of answering the following question: how can we generalize our HPC techniques and approaches for agent-based models that demand high performance?
- ▶ Care HPS is a methodology to execute agent-based modeling and simulation in a parallel and distributed architecture.

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- ▶ Care HPS is a scientific instrument to do research on HPC for agent-based models that demand high performance solutions. Care HPS enables both:
 - ▶ application area researchers to gain knowledge about the system under study using ABMs that require high performance computing solutions. This is possible because Care HPS offers well-defined and simple interfaces for this type of user in which all HPC complexity is hidden;
 - ▶ and, HPC expert users to develop approaches of high performance parallel and distributed simulation for ABM problems without high programming effort. Care HPS was projected using good object-oriented design practices which allow for the extension and reuse of the main HPS features.

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- ▶ As part of our main findings and contributions, we present Care HPS, and we show through experimentation that Care HPS meets its objective and can be used as a scientific instrument for agent-based modeling that requires high performance parallel and distributed simulations.

7 Conclusion

8 Future work

- ▶ Currently, we are doing a comprehensive study of the ABM for the assessment of *Aedes Aegypti* pupal productivity.
- ▶ There are still room for improvement: components, models, HPC strategies, features.

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Care HPS: A High Performance Simulation Methodology for Complex Agent-Based Models

Francisco Borges

Advisor: Dr. Remo Suppi

Federal Institute of Bahia
and

Universitat Autònoma de Barcelona
Computer Architecture & Operating Systems Department
February 21, 2017, Salvador

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Thank you for your attention!