

Parameter studies on heterogeneous computing infrastructures with the Scalarm platform

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Agenda

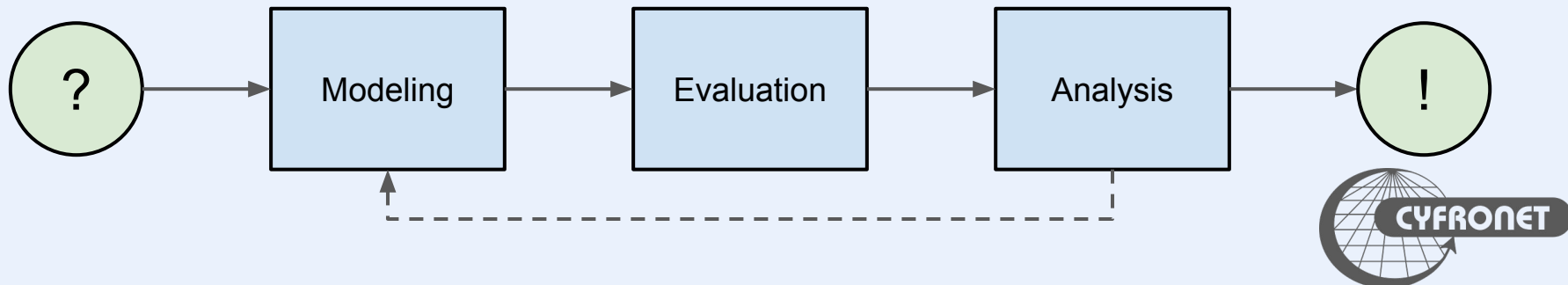
- Parameter studies methodology
 - Computer simulation as a tool for researchers
 - Sample applications
- Interactive parameter studies with Scalarm
 - Scalarm overview
 - The process in practice
- Summary



Parameter studies

Computer simulation as a tool for researchers

- Scientific research methods often rely on executing numerous simulations each with different input parameter values
 - Behavior study in various configurations
 - Optimal simulation configuration discovery
- Model executions can be treated as bag-of-tasks computations
- Large-scale parameter studies can use heterogeneous geographically and organizationally distributed computing
- Challenges:
 - Distribution of tasks among different resources
 - Computation progress monitoring
 - Results collection



Parameter studies

Sample applications

- Behavior analysis of security forces

- M. Kvassay, L. Hluchý, S. Dlugolinský, B. Schneider, H. Bracker, A. Tavčar, M. Gams, M. Contat, L. Dutka, D. Król, M. Wrzeszcz, J. Kitowski, A Novel Way of Using Simulations to Support Urban Security Operations. COMPUTING AND INFORMATICS, 34(6), 2015.

- Molecular dynamics - nano droplet simulation

- D. Król, M. Orzechowski, J. Kitowski, Ch. Niethammer, A. Sulisto, A. Wafai, A Cloud-Based Data Farming Platform for Molecular Dynamics Simulations, in: proc. 7th IEEE/ACM International Conference on Utility and Cloud Computing (UCC), 8-11, London UK, IEEE 2014, pp. 579 – 584.

- Immunological Evolutionary Multi-Agent System (IEMAS)

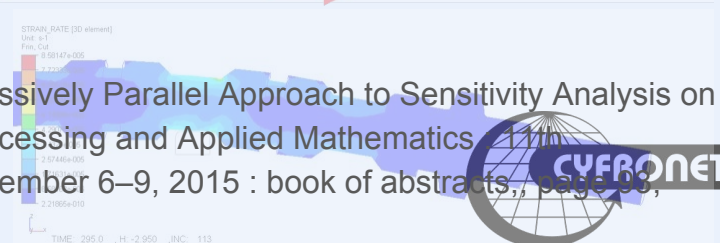
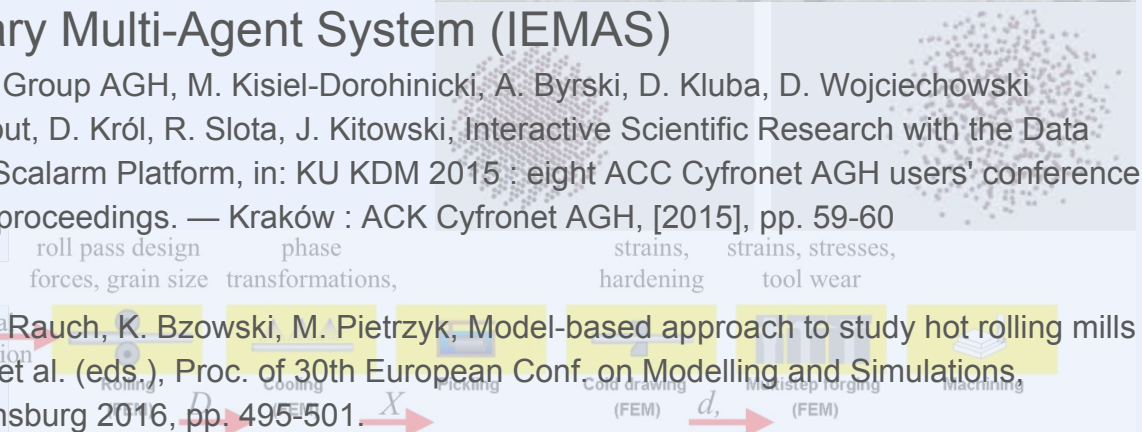
- Intelligent Information Systems Group AGH, M. Kisiel-Dorohinicki, A. Byrski, D. Kluba, D. Wojciechowski
- G. Skiba, M. Wojakowski, J. Liput, D. Król, R. Słota, J. Kitowski, Interactive Scientific Research with the Data Farming Methodology and the Scalarm Platform, in: KU KDM 2015 : eight ACC Cyfronet AGH users' conference : Zakopane, 11-13 Mar, 2015 : proceedings. — Kraków : ACK Cyfronet AGH, [2015], pp. 59-60

- Hot rolling mill design

- D. Król, R. Słota, J. Kitowski, L. Rauch, K. Bzowski, M. Pietrzyk, Model-based approach to study hot rolling mills with data farming, in: T. Claus, et al. (eds.), Proc. of 30th European Conf. on Modelling and Simulations, Regensburg, 2016, OTH Regensburg 2016, pp. 495-501.

- Sensitivity analysis

- D. Bachniak, J. Liput, L. Rauch, R. Słota, and J. Kitowski. Massively Parallel Approach to Sensitivity Analysis on HPC Architectures by using Scalarm Platform. In Parallel Processing and Applied Mathematics 11th international conference, PPAM 2015 : Kraków, Poland, September 6–9, 2015 : book of abstracts, page 93, 2015.



Interactive parameter studies with Scalarm

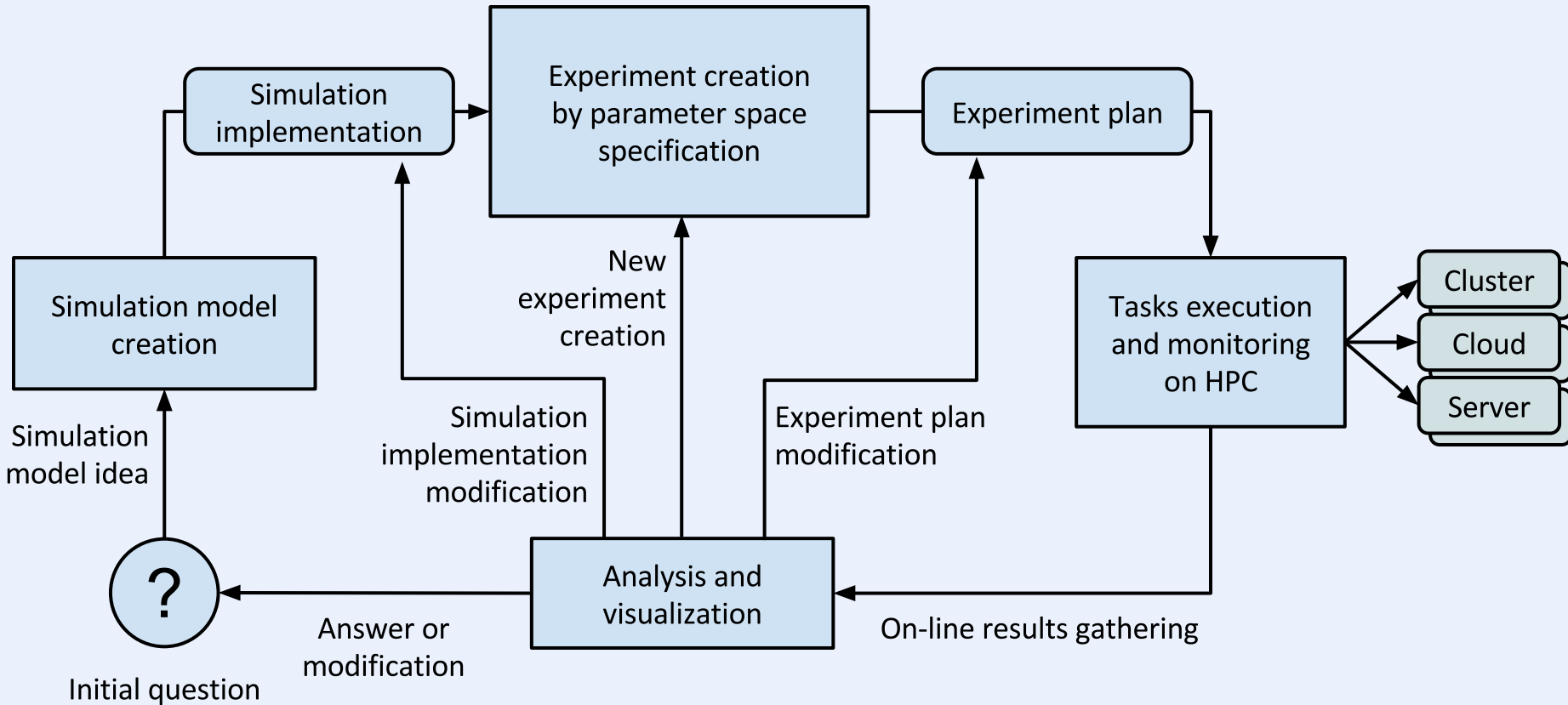
Scalarm overview

- Main goal: execution of the same application with different input parameter values
- More precisely: support different steps of a parameter studies process:
 - input parameter space specification
 - application execution with different input parameter values
 - collecting results and analysis
 - optimization and sensitivity analysis
- Web-browser front-end, HTTP API
- Support for clusters, IaaS clouds and private Linux or OSX machines



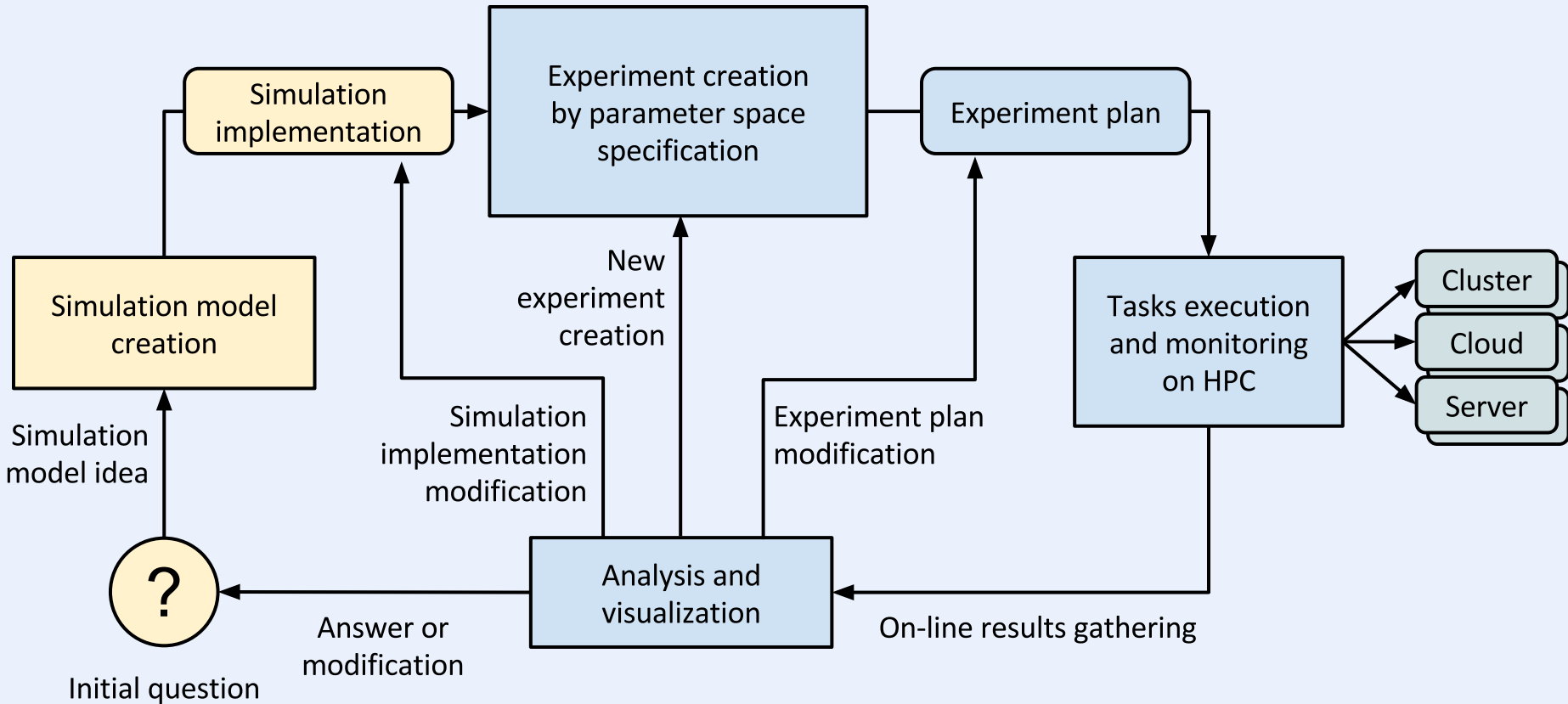
Interactive parameter studies with Scalarm

The process



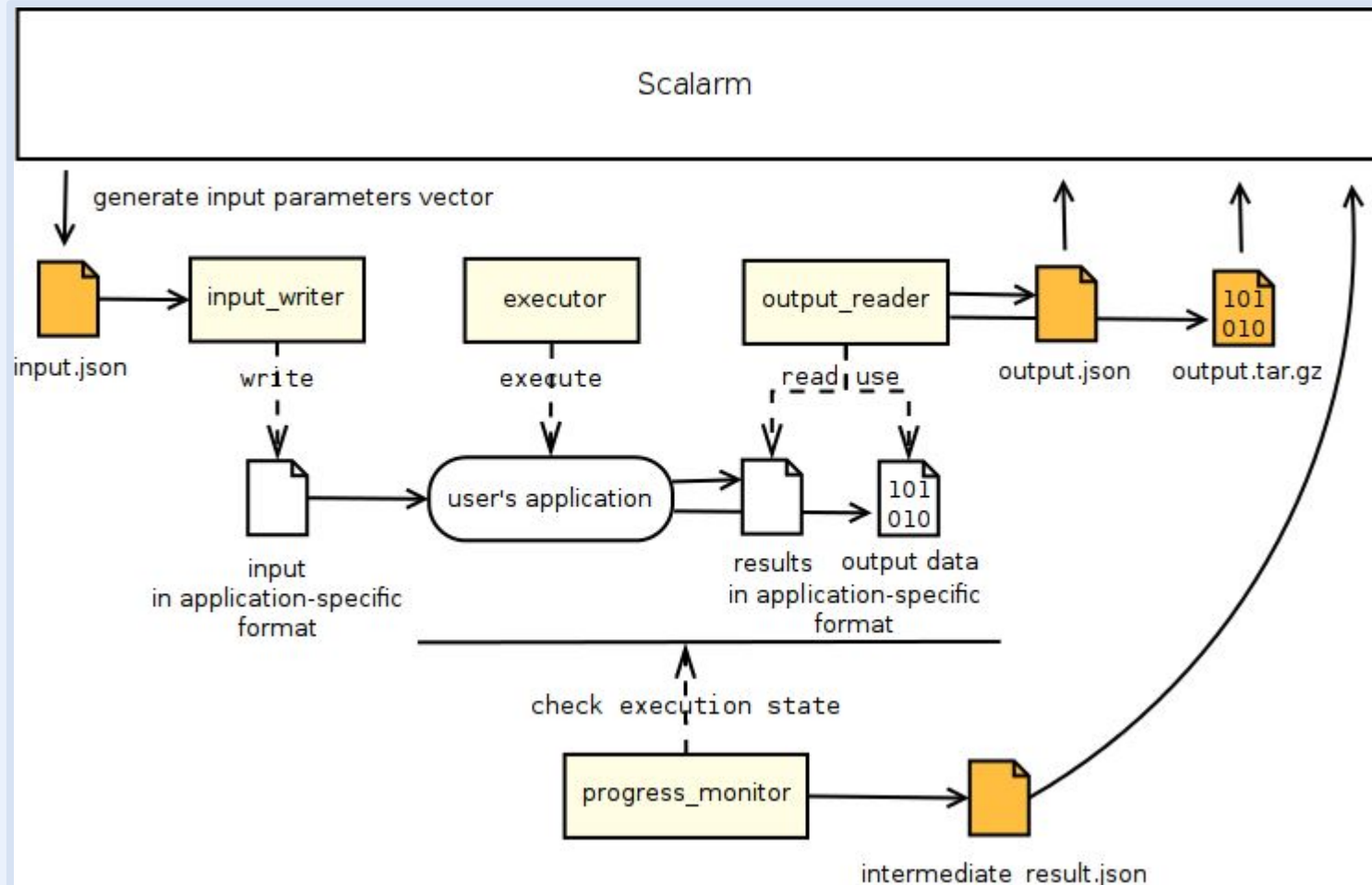
Interactive parameter studies with Scalarm

The process: modeling



Interactive parameter studies with Scalarm

The process: modeling



Interactive parameter studies with Scalarm

The process: modeling

Input definition Design Upload JSON

Parameters

[+ Add](#) [- Remove](#)

- Reproduction ... (reproducti...)**
- Newborn energ... (newborn_en...)
- Transferred e... (transfere...)
- Amount of ite... (amount_of_...)
- Immunological... (immunologi...)
- Bite transfer (bite_trans...)
- Mahalanobis s... (mahalanobi...)
- Immunological... (immunologi...)
- Good agent en... (good_agent...)
- Evaluation me... (evaluation...)

Parameter specification

Parameter ID:

Label:

Type:

Min: Max:

[Save changes](#) [Discard changes](#)

Files

Simulation binaries

Current file: simulation_binaries.zip

Upload new file: [Wybierz plik](#) Nie wybrano pliku

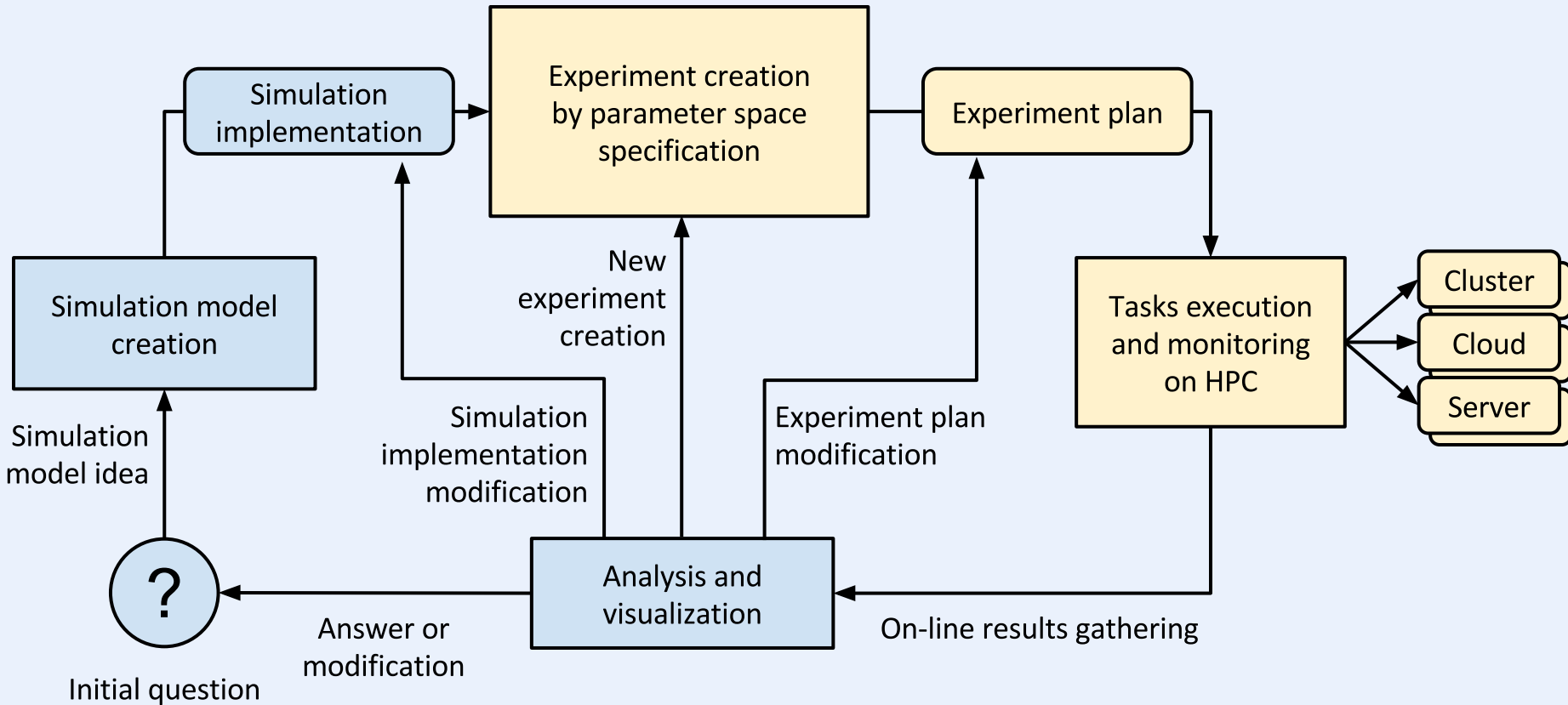
Executor

Select a registered name:

or insert file: [Wybierz plik](#) Nie wybrano pliku

Interactive parameter studies with Scalarm

The process: evaluation



Interactive parameter studies with Scalarm

The process: evaluation

Input space - manual specification On Off

1. Parametrization 2. Design of Experiment 3. Parameter constraints

Specify parametrization for each input parameter below

Group: Default group

Entity: Default entity

Parameter 'Reproduction minimum' - Value constraints: [0, 1000]

Set parametrization type:

Specify values based on the selected parametrization type

Set value:

Parameter 'Newborn energy' - Value constraints: [0, 1000]

Set parametrization type:

Specify values based on the selected parametrization type

Set minimum:

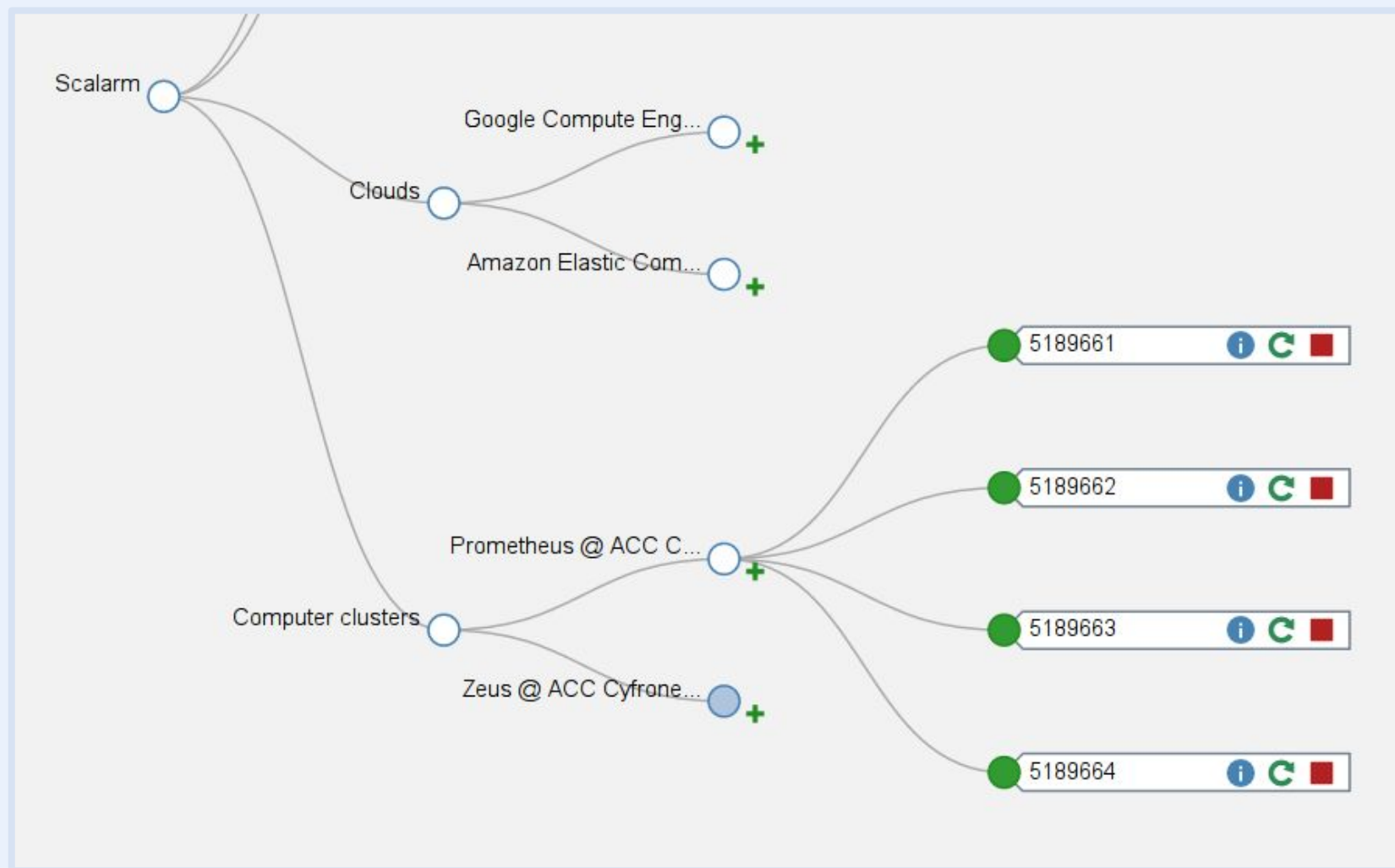
Set maximum:

Set step:



Interactive parameter studies with Scalarm

The process: evaluation



Interactive parameter studies with Scalarm

The process: evaluation

Progress information

Show/Hide completed

Show/Hide running

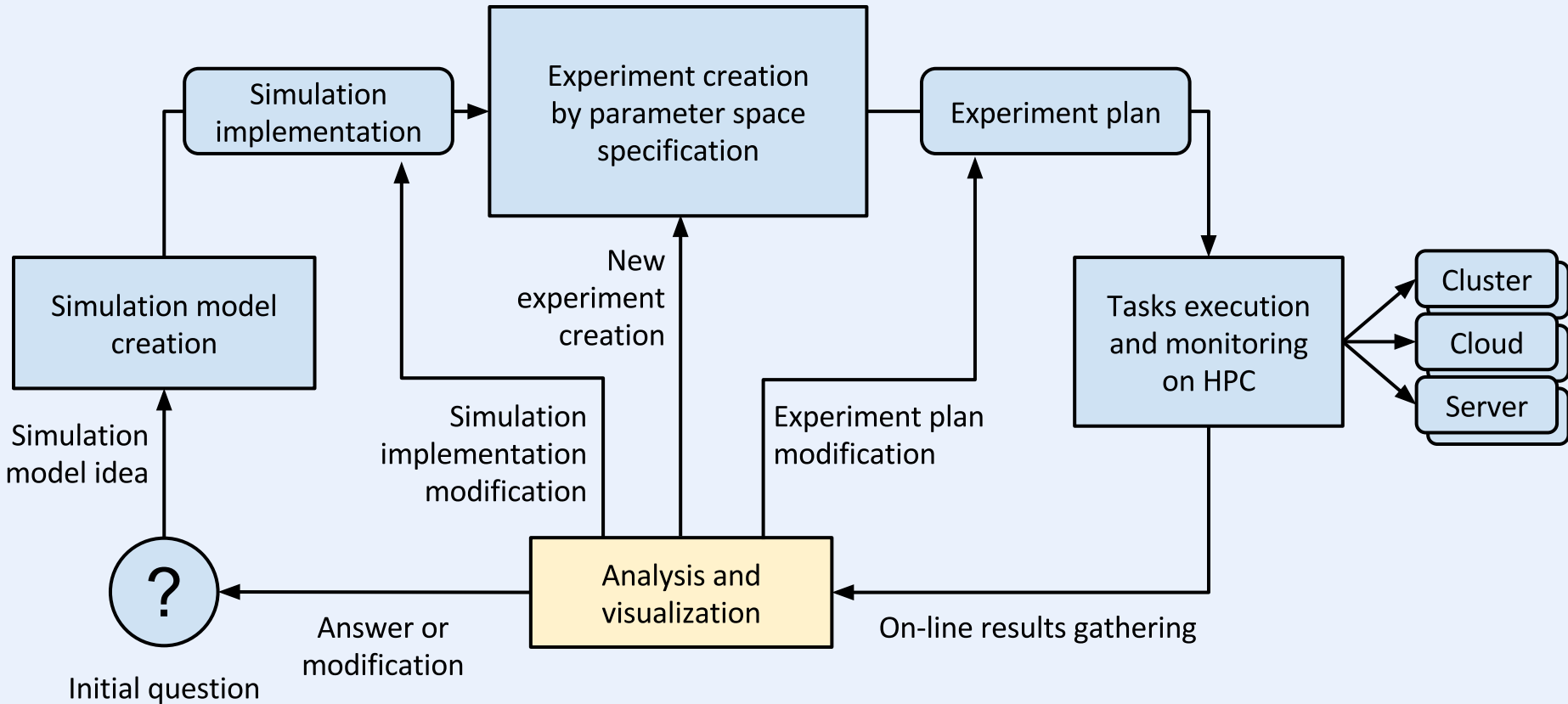
Complete simulation runs

#	Execution time	Final results	Transferred energy	Amount of iterations (replication)
1	98.112 [s]	{"fitness_calls"=>72, "iemas_fitness"=>692.112086227, "time_elapsed"=>50}	0	1
2	136.69 [s]	{"fitness_calls"=>57, "iemas_fitness"=>740.62615994, "time_elapsed"=>100}	0	2
3	191.722 [s]	{"fitness_calls"=>66, "iemas_fitness"=>724.829450338, "time_elapsed"=>140}	0	3



Interactive parameter studies with Scalarm

The process: analysis



Interactive parameter studies with Scalarm

The process: analysis

Progress information

Show/Hide completed

Show/Hide running

Complete simulation runs

#	Execution time	Final results	Transferred energy
1	98.112 [s]	{"fitness_calls"=>72, "iemas_fitness"=>692.112086227, "time_elapsed"=>50}	0
2	136.69 [s]	{"fitness_calls"=>57, "iemas_fitness"=>740.62615994, "time_elapsed"=>100}	0
3	191.722 [s]	{"fitness_calls"=>66, "iemas_fitness"=>724.829450338, "time_elapsed"=>140}	0

Simulation 2

Status: completed

Started at: 2015-02-25 17:25:22 UTC

Completed at: 2015-02-25 17:27:38 UTC

Input:

- **Reproduction minimum:** 0
- **Newborn energy:** 0
- **Transferred energy:** 0
- **Amount of iterations (replication):** 2
- **Immunological time span:** 1
- **Bite transfer:** 1
- **Mahalanobis similarity:** 0.8
- **Immunological maturity time:** 1
- **Good agent energy:** 1
- **Evaluation method:** rastrigin

Output:

- **fitness_calls:** 57
- **iemas_fitness:** 740.62615994
- **time_elapsed:** 100

Binary output:

[click to download](#)

File size: 685 [kB]

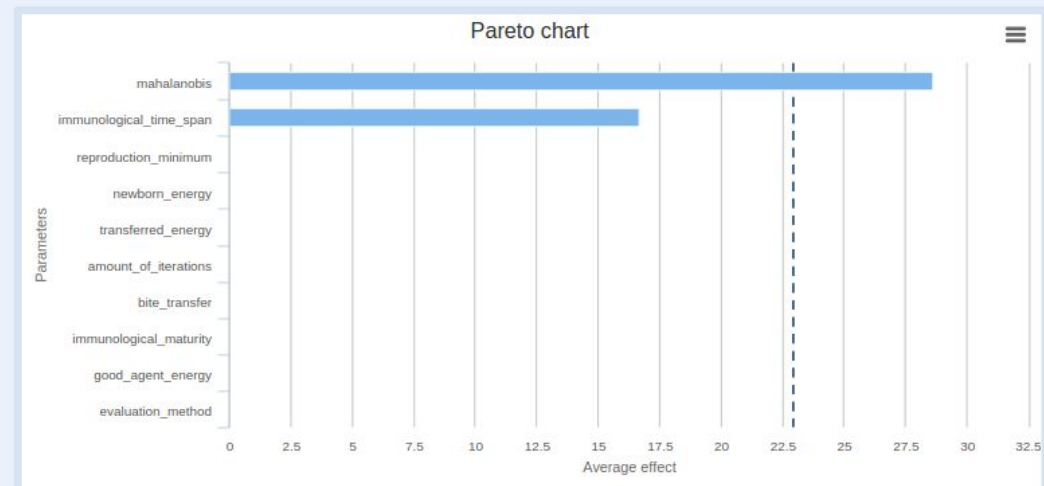
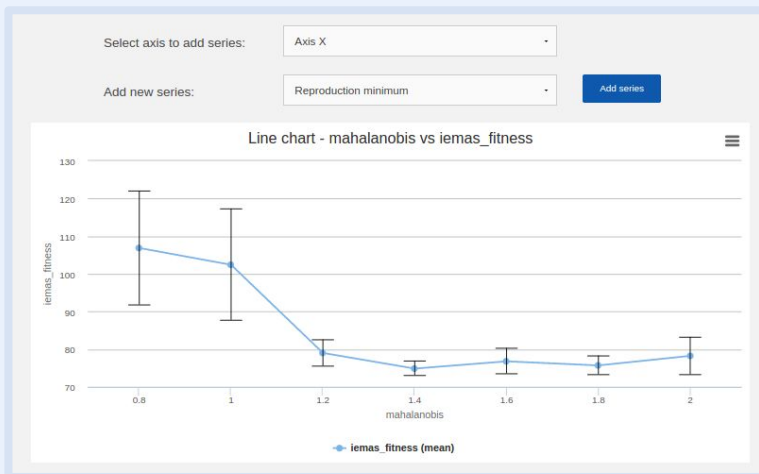
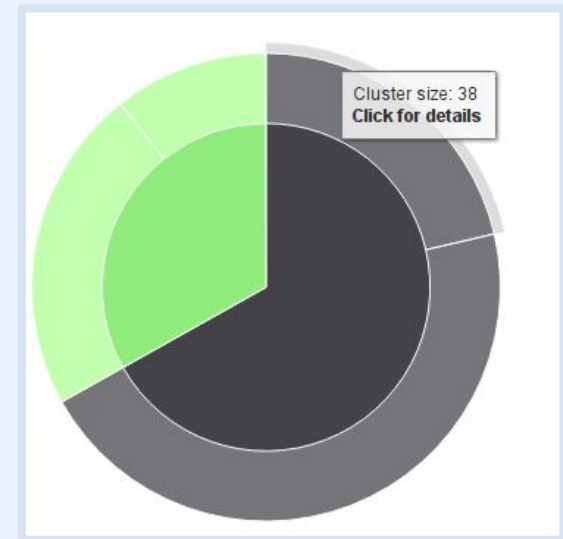
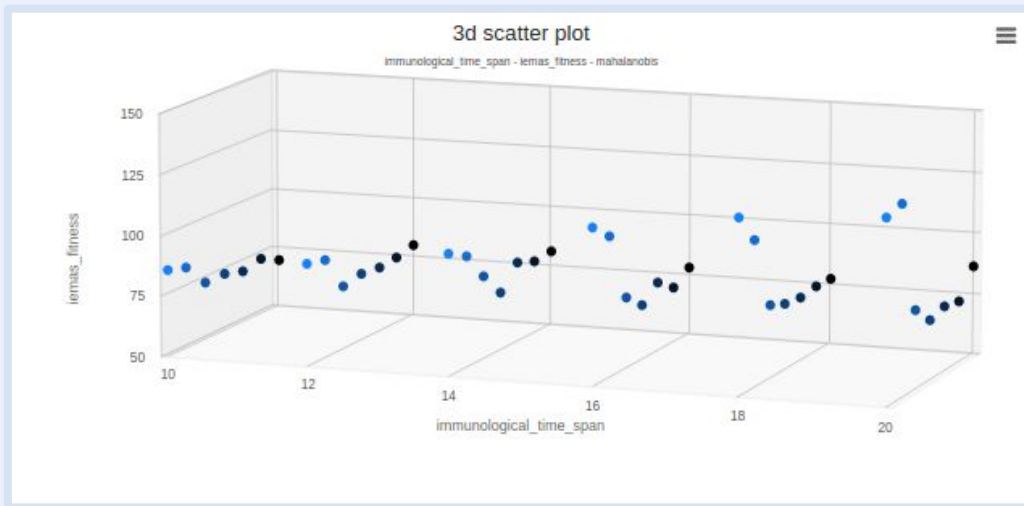
Simulation STDOUT:

[click to download](#)

File size: 365 [B]

Interactive parameter studies with Scalarm

The process: analysis



Summary

- Scalarm is a platform for conducting parameter studies based on any simulation model provided
- Scalarm is developed and used in ACK Cyfronet AGH
- Scalarm has been successfully used in PLGrid NG, PLGrid CORE and VirtROLL (funded by EU RFCS) projects implemented by ACK Cyfronet AGH
- Element of PaaS environment (EU FP7)
 - M. Orzechowski, J. Liput, R. Slota, and J. Kitowski, Manageability of Deployment of Multi-Cloud Scientific Applications: Data Farming Use-case, in: M. Bubak, M. Turała, K. Wiatr (Eds.), Proceedings of Cracow Grid Workshop - CGW'15, October 26-28 2015, ACC-Cyfronet AGH, 2015, Krakow, pp. 107-108
- PhD Thesis D. Król
 - D. Król, J.Kitowski, Self-scalable Services in Service Oriented Software for Cost-effective Data Farming, Future Generation Computer Systems, 54 (2016), pp. 1-15.



Summary

We invite you to use Scalarm in your work
to make research more efficient!

**Currently it is available to all PL-Grid users
as a service:**

<https://scalarm.plgrid.pl>



Thank you!

<https://scalarm.plgrid.pl>

<http://scalarm.com>

