Kinetics of Defect Aggregation in Materials Science Simulated in Desktop Grid Computing Environment Installed in Ordinary Material Science Lab

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Introduction: Aggregation processes are investigated in many branches of science: defect aggregation in materials science, population dynamics in biology, city growth and evolution in sociology, etc [1-3]. The typical simulation of crystal defect aggregation by our application *SLinCA* (Scaling Laws in Cluster Aggregation) takes several days and weeks on a single modern CPU, depending on the number of Monte Carlo steps (MCS). However, thousands of scenarios have to be simulated with different initial configurations to get statistically reliable results. Porting to distributed computing infrastructure (DCI) and parallel execution can reduce waiting time and scale up simulated systems to the desirable realistic values.

The main aims of the work:

- to verify feasibility of porting the sequential version of *SLinCA* to DCI by ordinary (non-expert) end-users;
- to test different target desktop grid platforms and utilize larger number of global EGEE resources at robust production level.

1.Porting the Sequential Version of *SLinCA* Application to Distributed Computing Infrastructure (DCI)

What do you need to do **in practice for setting DCI environment in an ordinary lab and porting the sequential version of** SLinCA **application to the DCI environment [4]:**

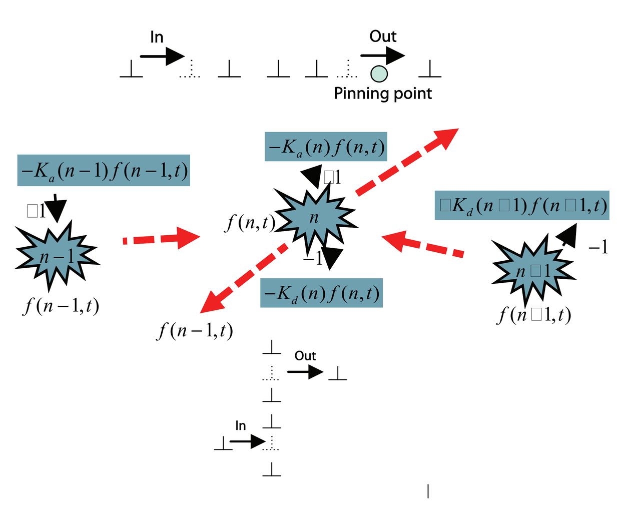
1. Install Desktop Grid (DG) with a BOINC-DG server and BOINC-worker.
2. Port your sequential application to parallel version using the simple and intuitive DC-API [5].
3. Deploy an application (master and client parts) on the DG server.
4. Connect BOINC-workers to the DG-server.
5. Start your application and enjoy automatic job distribution, resource allocation, result management, etc.

Minimal pre-requisites **for setting local DCI environment:**

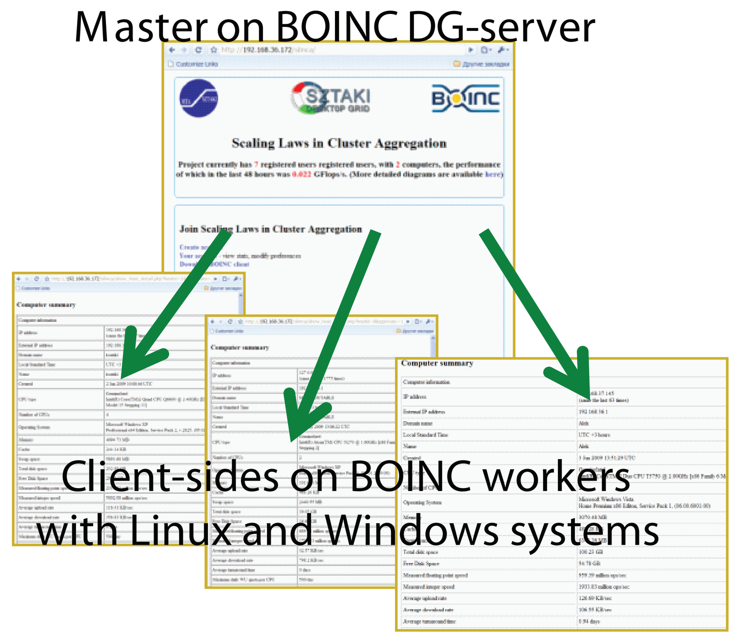
Download and install free software:
- Apache Web-server (freeware);
- MySQL database (freeware, GPL);
- BOINC software (freeware, LGPL);
- DC-API libraries for DG by SZTAKI (freeware) [5].

2.Typical Workflow for *SLinCA* application in DCI on the basis of local DG in Our Material Science Lab

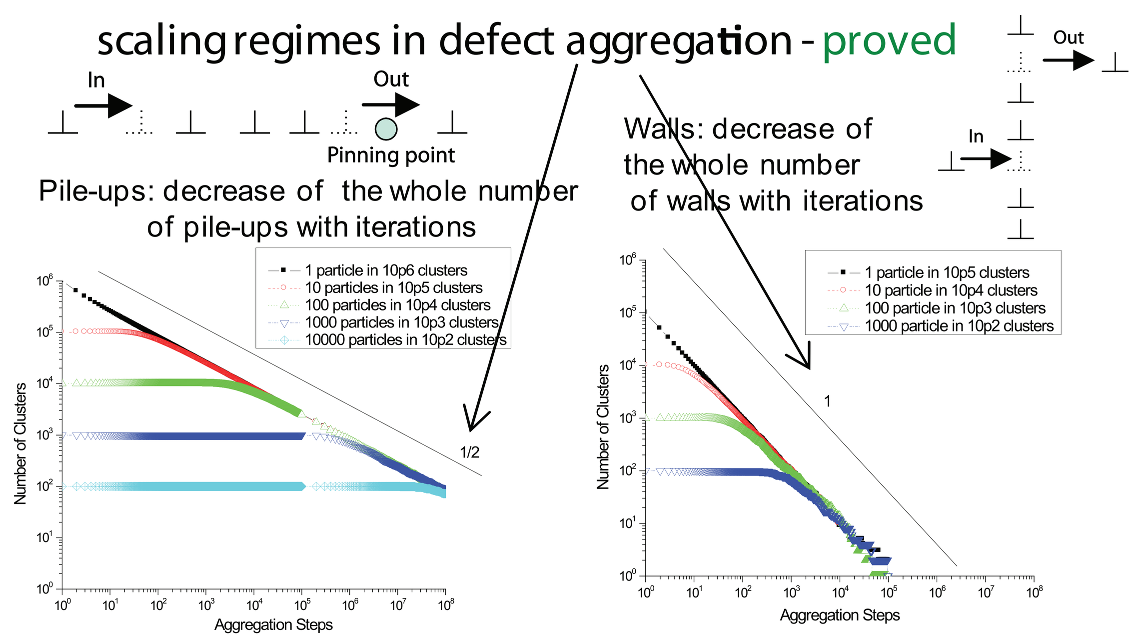
Adopt SlinCA **application (with kinetic Monte Carlo model) to "parameter sweeping" mode of parallel execution**



Install and run in local Desktop Grid

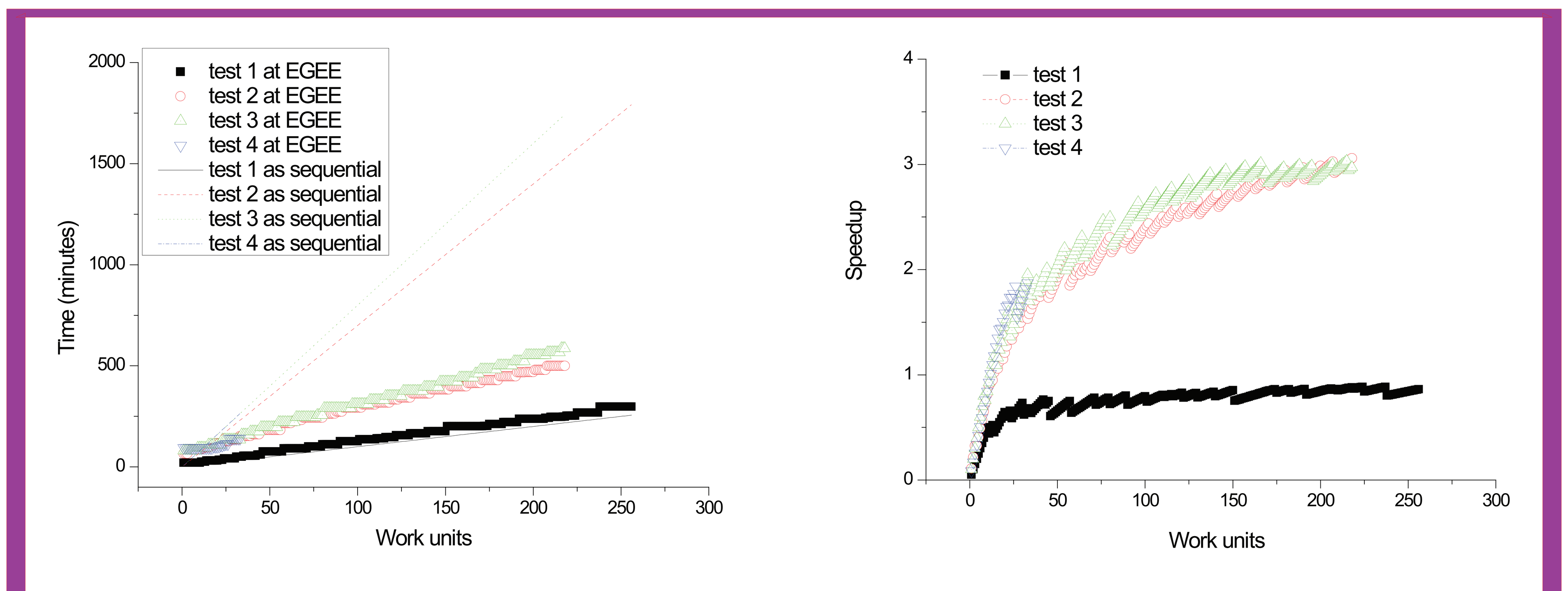


Obtain Scientific Results:



3.Running the Ported *SLinCA* application on Global EGEE Resources

The further increase of performance is possible by usage of EGEE computing resources through EDGeS DG->EGEE Bridge [6] on BOINC and XtremWeb [7] platforms:

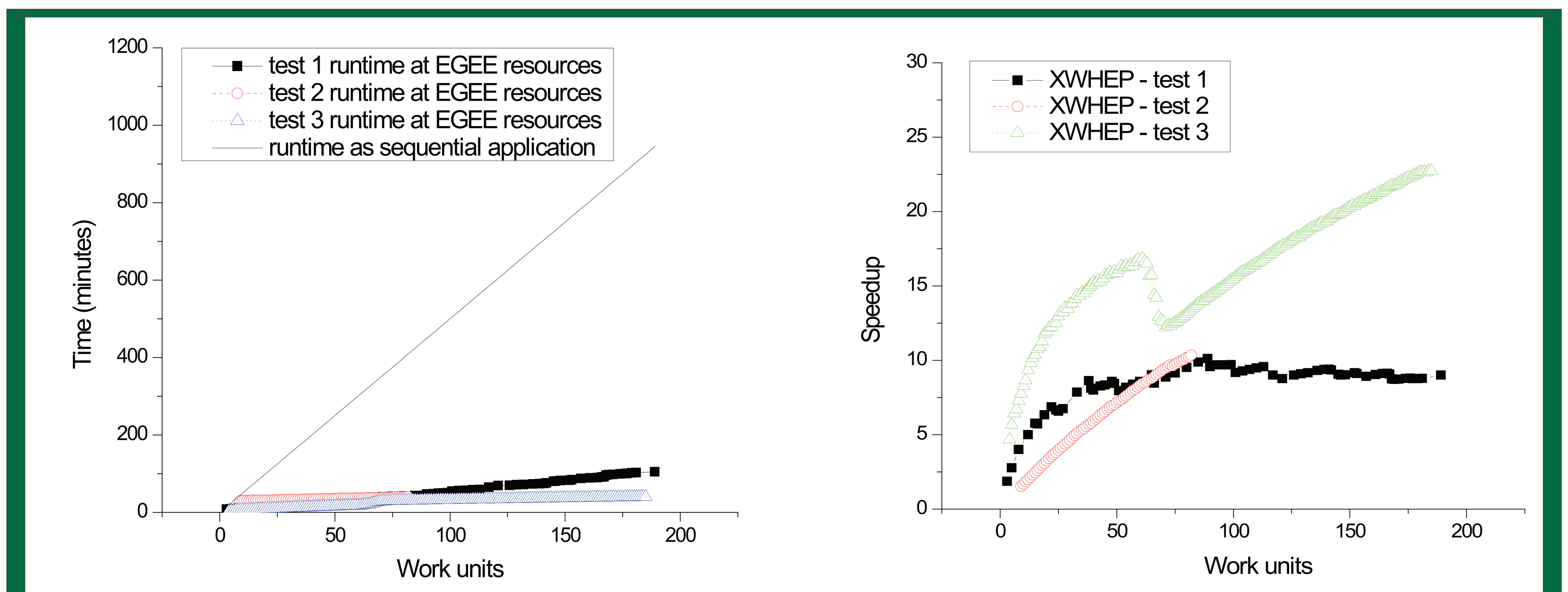


a) comparison of sequential and parallel versions

b) actual speedup with the number of work units

Tests through BOINC DG->EGEE bridge at CETA-CIEMAT test infrastructure (>800 work units successfully passed and calculated on 10 available EGEE workers).

Note: actual speedup (~3) was lower than theoretical (~10), because the work units with short runtimes (1,3,5,7 min) were used in the tests and were shadowed by overheads (~20 min) related with necessary EGEE-related operations.



a) comparison of sequential and parallel versions

b) actual speedup with the number of work units

Tests through XtremWeb DG->EGEE bridge at IN2P3 infrastructure at LAL (>1100 work units successfully fulfilled during the test phase at local XtremWeb DG and >256 work units - over XtremWeb->EGEE bridge).

Conclusions

The main achievement: BOINC-DG and XtremWeb-DG ideologies of high-performance distributed computing were proved to be effectively used by non-expert developers in an ordinary science lab with significant increase of productivity.

The easy increase of performance: absence of significant performance difference between Windows and Linux versions of *SLinCA* application allows us to increase its performance significantly by delivering *SLinCA* application to EGEE resources through EDGeS BOINC->EGEE and to EDGeS XtremWeb->EGEE Bridges.

The further reserves of improvement are related with development of 64-bit client parts, versions enabled for Graphic Processing Units (GPUs), and usage of parameter sweep workflow for P-GRADE portal.

Acknowledgements

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