Introduction: The processes of monomer aggregation in clusters 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 a cluster aggregation scenario takes several days on a single modern processor, depending on the number of Monte Carlo steps (MCS). The parallel execution environment can reduce the waiting time and scale up the simulated system to the desirable realistic values. The main aim of the work was to test the applicability and everyday efficiency of the Desktop Grid computing technology in an ordinary materials science lab with heterogeneous distribution of desktop computing resources. For this purpose, the ported parallel version of the sequential application was developed and tested on the worker nodes of Desktop Grid (DG) installed on BOINC software platform [4] and Distributed Computing Application Programming Interface (DC-API) [5].

1. Problem Description

Typical heterogeneous distributed computing infrastructure

<table>
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<tr>
<th>Category</th>
<th>Floating point MIPS (Whetstone)</th>
<th>Integer point MIPS (Dhrystone)</th>
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<td>Newest (4-core CPU)</td>
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<td>New (2-core CPU)</td>
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<tr>
<td>Labs</td>
<td>876</td>
<td>1285</td>
</tr>
</tbody>
</table>

Distribution of PCs in our lab under usual work schedule:

Red lines: only local manual management routes in sequential run

Main hardships in such an infrastructure are caused by human factor -> some users...
- do not like to provide remote access to their PCs and housekeeping operations
- can be done manually and on site only;
- forgot about background sequential application and switch-off their PCs after working hours;
- do not allow use PCs in the absence of their owners.

It is very hard to do input/output housekeeping operations, and even plan them reliably.

How to resolve these hardships? (Don’t worry, see to the right side... →)

2. Efficient Way to Solution - Desktop Grid

- Performance Analysis of Desktop Grid Solution

3. Example of Typical Simulation in Our Material Science Lab with Heterogeneous Distribution of Computing Resources

Create Kinetic Monte Carlo model

Run in local Desktop Grid

Master on BOINC DG-server

Client-sides on BOINC workers

Obtain Scientific Results:
- scaling regimes in defect aggregation - proved
- plant uptake decrease of the whole number of plants with iterations
- wide decrease of the whole number of plants with iterations

4. Performance Analysis of Desktop Grid Solution

Much lower housekeeping time

Linear speedup

5. Drawbacks

- order of magnitude increase in performance speedup
- problems with “ad hoc” dynamical memory allocation;
- bottlenecks in heterogeneous distributed computing infrastructure created by slow and greedy PCs.

6. Acknowledgements

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