Workflow-based Simulation of Solids

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Monte Carlo-Simulation for Solid Bodies

The Monte Carlo simulation of solid bodies investigates the thermal ageing of copper-alloyed steel on an atomistic scale. The steel changes its material behavior during the ageing process when being operated at temperatures > 300°C. The simulated system is a body-centered cubic (bcc) crystal lattice with different atom types and a single vacancy. Atoms jump into the vacancy with a certain probability. Over time, precipitations develop in the alloy which decreases the material strength [1].

initial state　　　*precipitations*
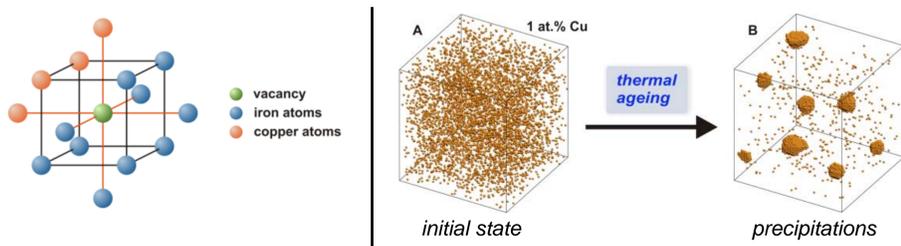
The system is solved numerically with a Kinetic Monte-Carlo approach [2]. As a start configuration, a number of iron atoms is substituted by copper atoms in a fixed bcc lattice. In every Monte-Carlo step, the vacancy changes its position with an adjacent atom dependent on the jump frequencies of all neighbors. A long series of vacancy jumps results in the formation of precipitates with mean radii above 1 nm.

Simulation Applications

The simulation is conducted with a legacy tool called opal (Ostwald-Ripening of Precipitates on an Atomic Lattice) [3]. The opal application consists of five monolithic Fortran 77 programs. The simulation results can be visualized, e.g. with Gnuplot.
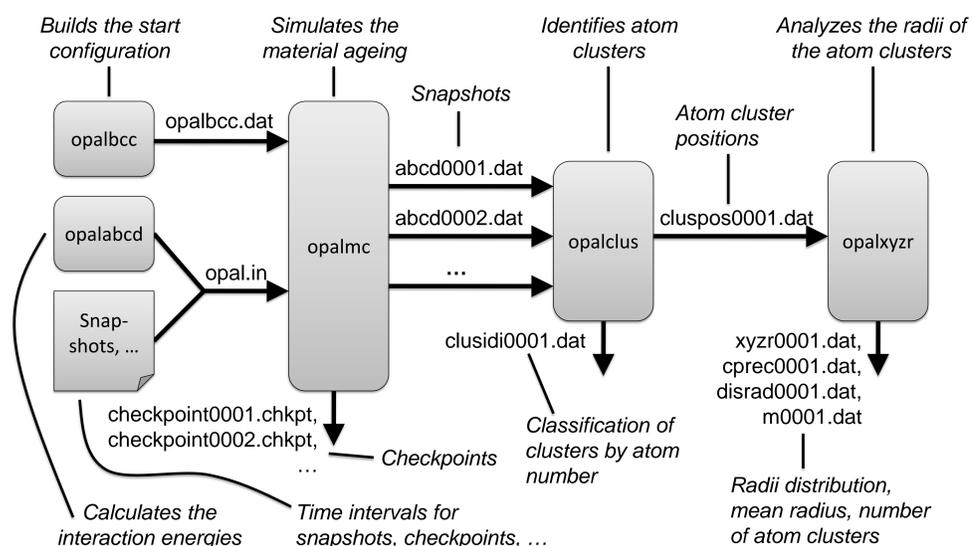

Disadvantages

■ The programs are started manually by the scientists – a tedious and time-consuming task as there can be hundreds of snapshots.

■ The tools have no GUI and some parameters are hard-coded.

■ The simulation runs only sequentially on single workstations because opalmc allocates a complete processor for the simulation.

■ Due to a limitation of Fortran 77 opal is not able to benefit from multi-core processor architectures.

References

[1] Molnar, D., Binkele, P., Hocker, S., Schmauder, S.: Multiscale Modelling of Nano Tensile Tests for Different Cu-precipitation States in α-Fe. Proc. of the 5th Int. Conf. on Multiscale Materials Modelling, pp. 235-239, Fraunhofer Verlag (2010)
[2] Soisson, F., Barbu, A., Martin, G.: Monte-Carlo Simulations of Copper Precipitates in Dilute Iron-Copper Alloys During Thermal Ageing and Under Electron Irradiation. Acta Materialia, 44, pp. 3789-3800 (1996)
[3] Binkele, P., Schmauder, S.: An atomistic Monte Carlo simulation for precipitation in a binary system. International Journal for Materials Research, 94, pp. 1-6 (2003)

Workflow-based Re-Engineering

We improved this situation by applying the workflow technology, Web services (WS) and software engineering concepts. The opal programs were extended so that parameters are not hard-coded any more but can be passed during invocation. We created thin WS wrappers for the programs that makes them accessible in a network. A new resource manager (RM) supervises the registered servers in the network, their properties and installed services. It controls utilization of the services and also works as logically centralized data storage for simulation context data. Two BPEL workflows implement and automate the simulation logic. They invoke the opal WSs. An opal manager on top of the BPEL engine is used to start and control simulations.

Former situation　　　*Workflow-based solution*
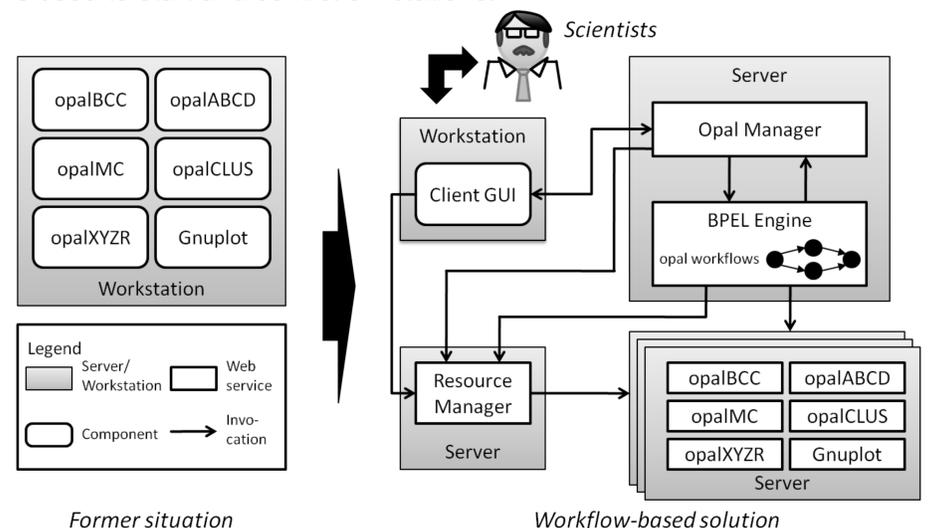
The scientists interact solely with the client GUI. Servers and WSs can be registered, the work load of the environment can be monitored, and simulations can be started or aborted. With a file explorer the user can access and open all files related to a simulation run. It is also possible to display previews of the lattice snapshots (i.e. the intermediary results of the simulation) based on Java 3D. File explorer and snapshot preview give the scientists a sense how the simulation and atom structure of the steel is developing.
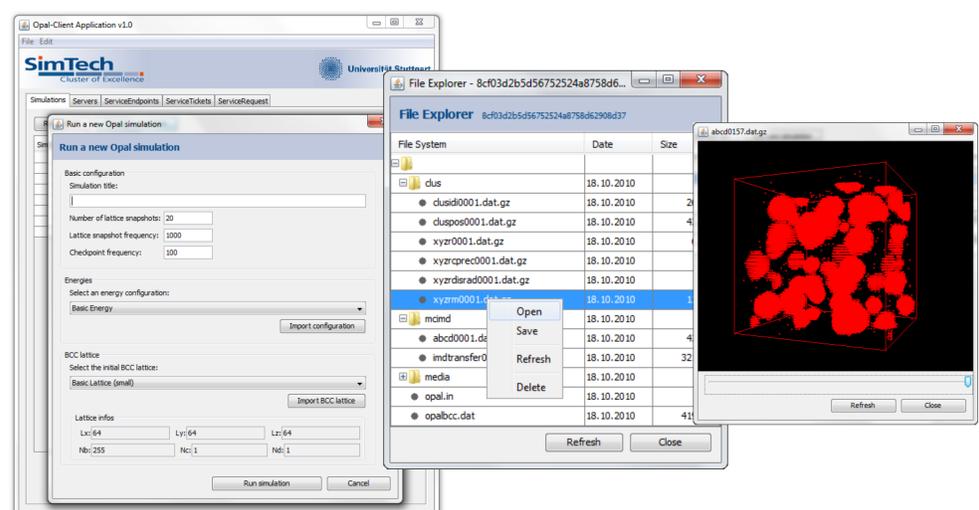
Benefits

■ The GUI improves the software ergonomics. Scientists can configure, start and monitor a simulation.

■ Distributed, parallel execution of the simulation on different servers, exploiting multi-core processors. Post-processing of intermediate results can be done in parallel to the main simulation.

■ Automation of the simulation.

■ Decrease of the overall execution time of a simulation.

■ The scientists control the servers in the simulation infrastructure.

■ Efficient utilization of the resources.

■ Usual commodity hardware can be used to conduct the simulations.