Computational Thermodynamics - OpenCalphad: Simulations using OCASI using OpenMP

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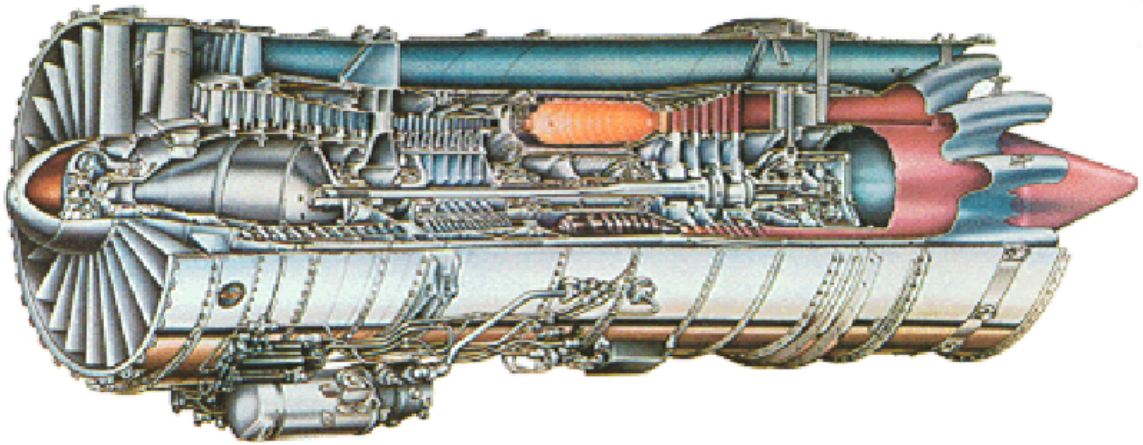
Surface coating

An example is a simulation using parallel calculation (OpenMP) of equilibria using a very simple diffusion model for a ternary Al-Ni-Pt system in a single fcc phase region.
Pt is sometimes used as coating of Al-Ni turbine blades in jet engines to improve corrosion resistance.



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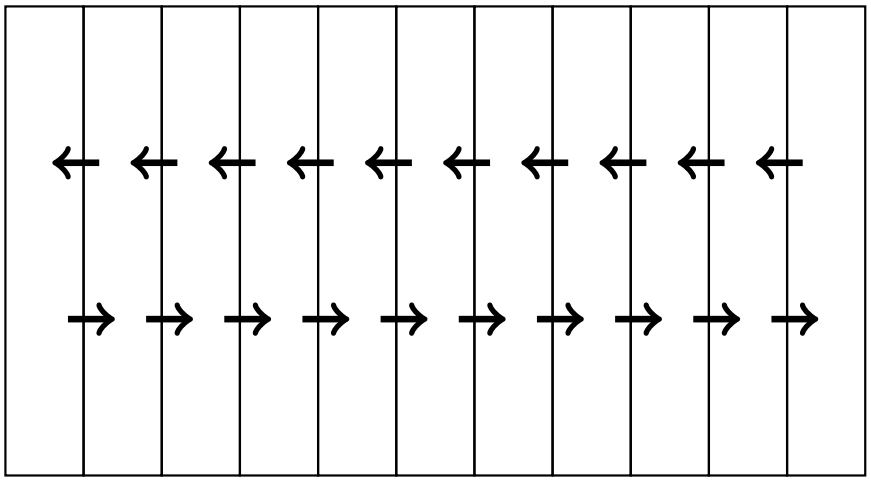
The chemical potential of Al in Pt is lower than in Ni and thus Al will diffuse to the Pt coated surface and form a protective layer of Al_2O_3 which will be renewed by diffusion of Al from the interior.
As will be shown in the simulation Al prefers the region with hight fraction of Pt.
The ordering transformations in Al-Ni-Pt has been ignored in this simulation, the calculations are made for disordered fcc.
This example is not provided with OC but it uses the OCASI interface which is part of OpenCalphad.

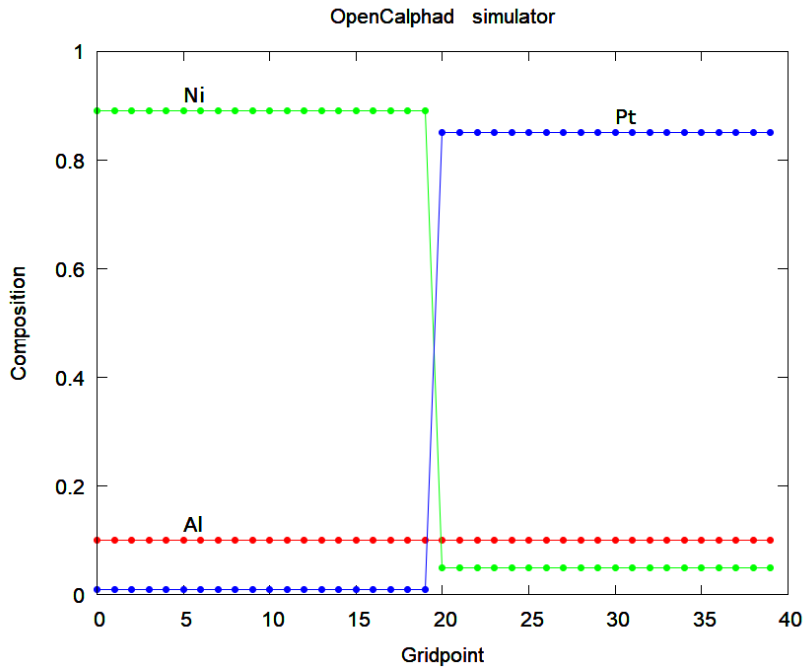
Simulation of 1D ternary diffusion Al-Ni-Pt

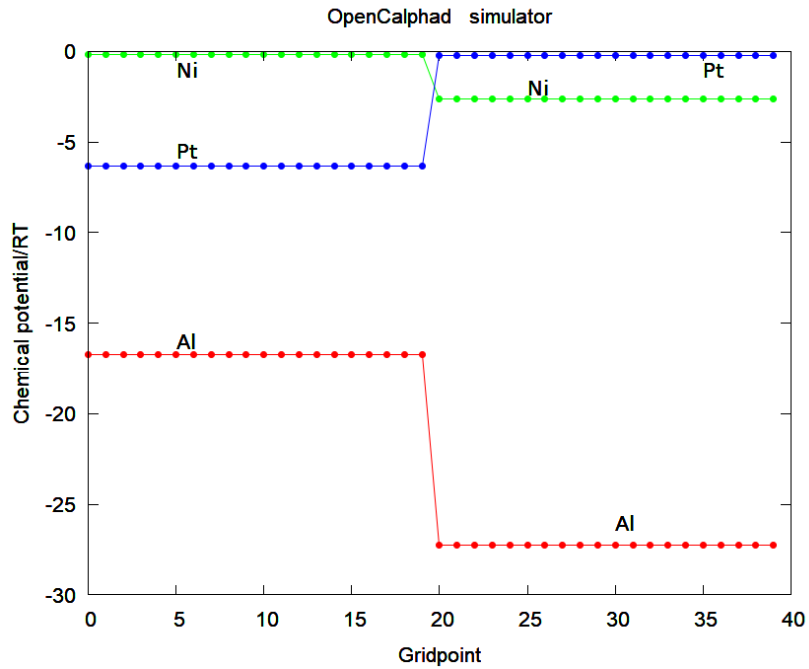
The diffusion couple has 10% Al and 1% Pt (per mole) on the left hand side and 10% Al and 85% Pt on the right hand side, rest Ni.
At the left hand side of the diffusion couple the chemical potential of Al, $\mu_{\mathrm{Al}}/RT = -16.7$
and at the right hand side $\mu_{\mathrm{Al}}/RT = -27.2$.
The left and right boundaries the system is closed. $T = 1073$ K.



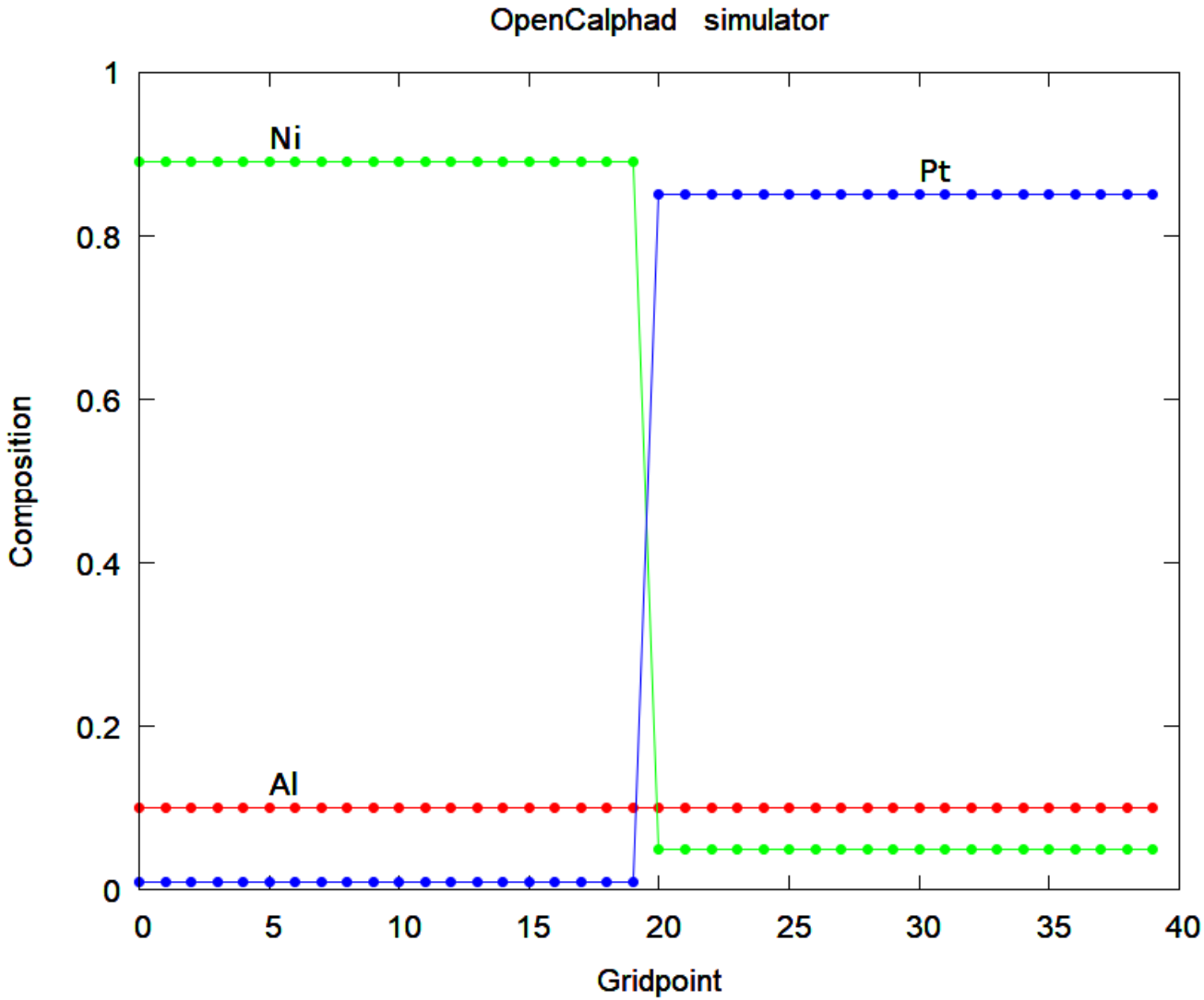
Initial composition profile and chemical potentials

The initial composition profile is the figure to the left, the Pt-rich surface is on the right hand side.
The initial chemical potentials in the figure to the right, the chemical potential of Al is lower in the Pt rich region even if its composition is the same as in the Ni-rich region.





Simulation of ternary diffusion Al-Ni-Pt



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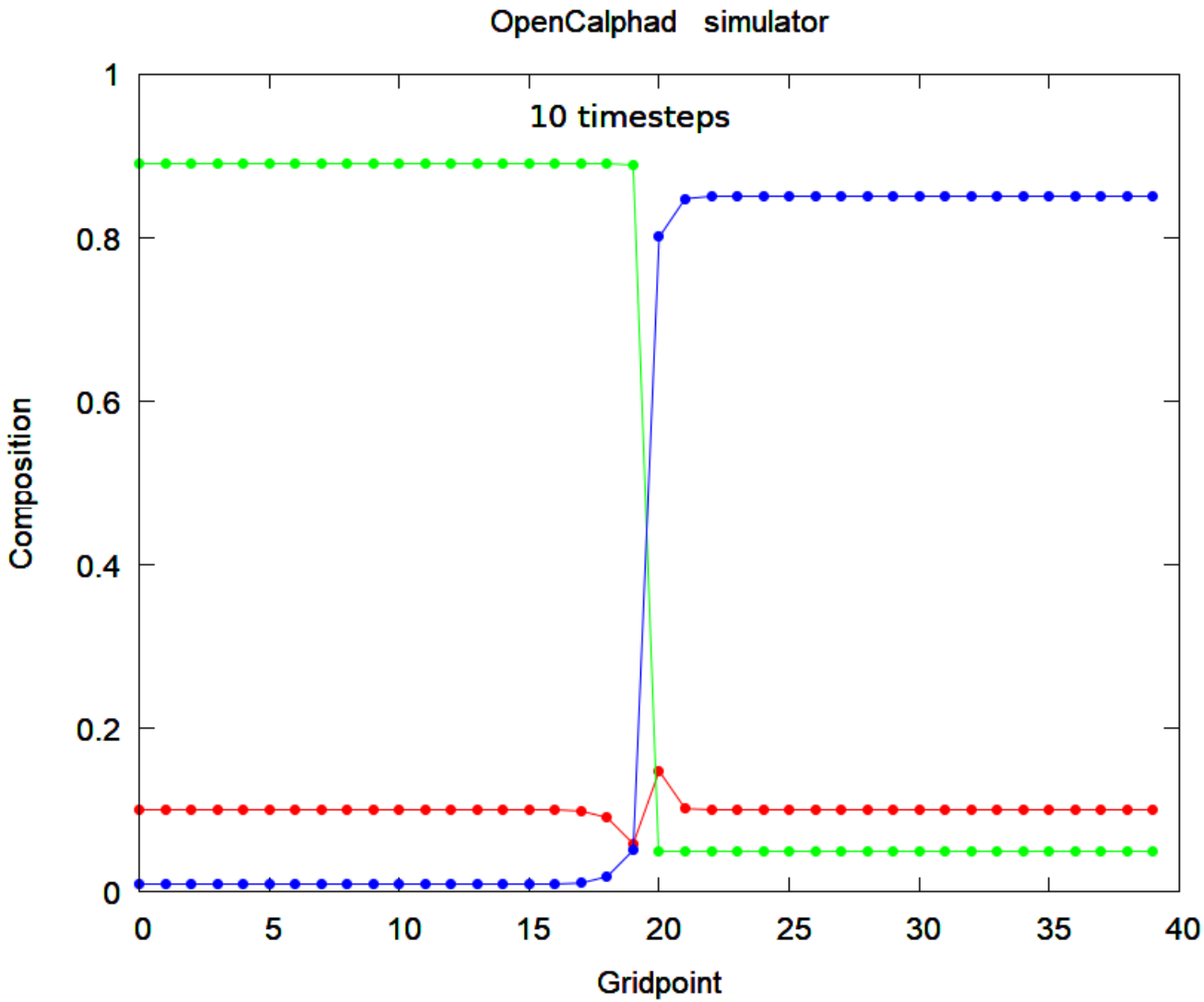

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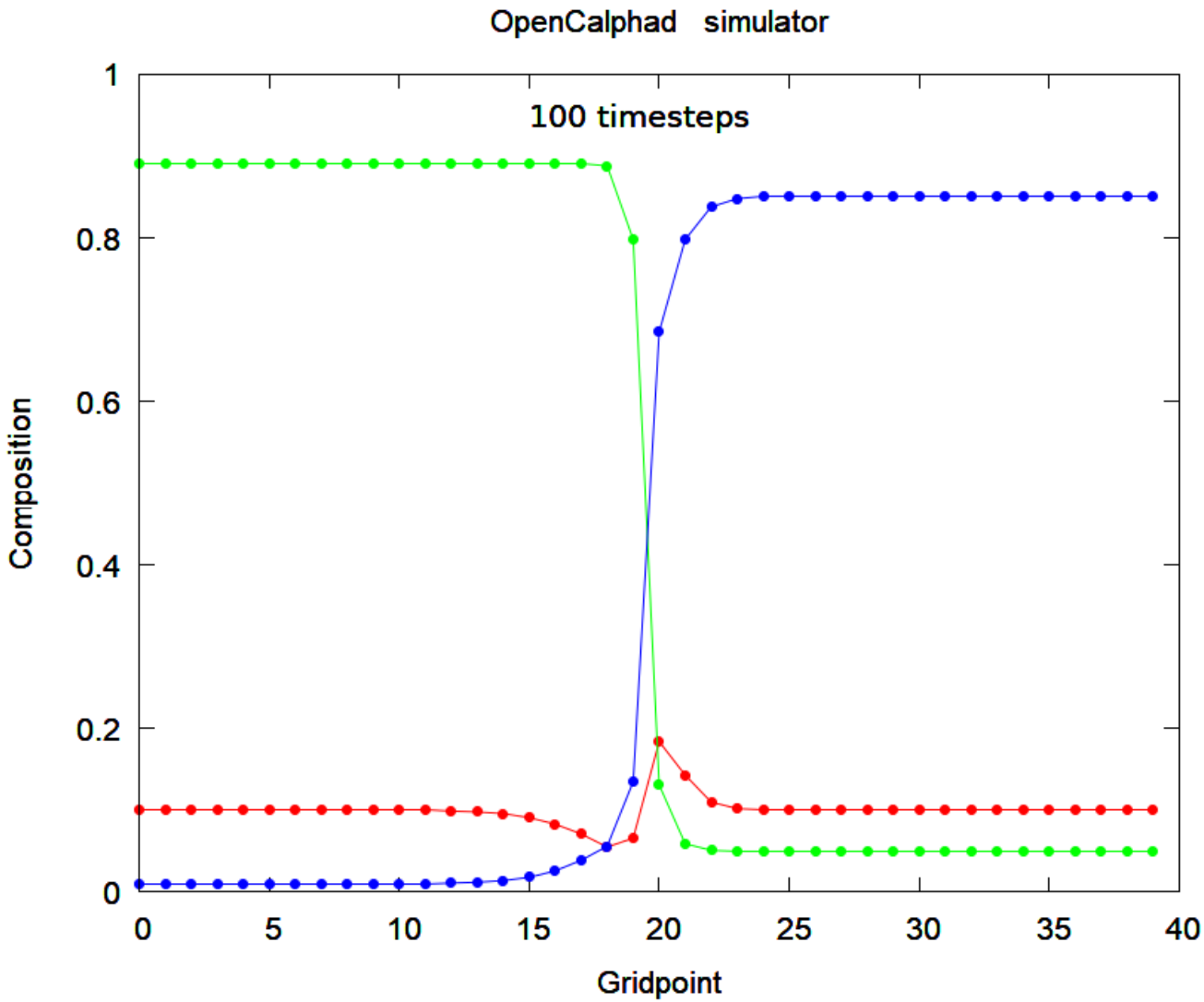

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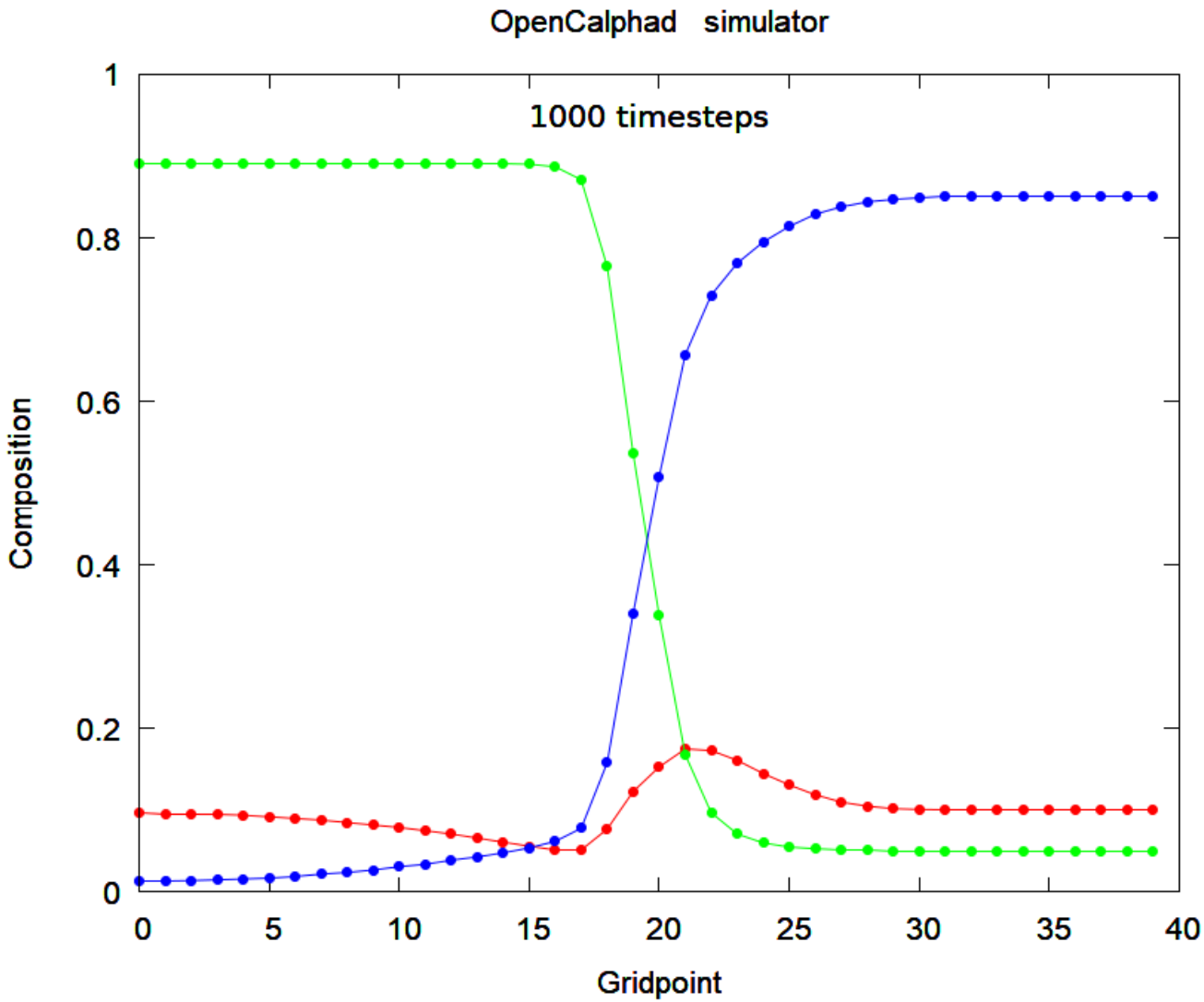

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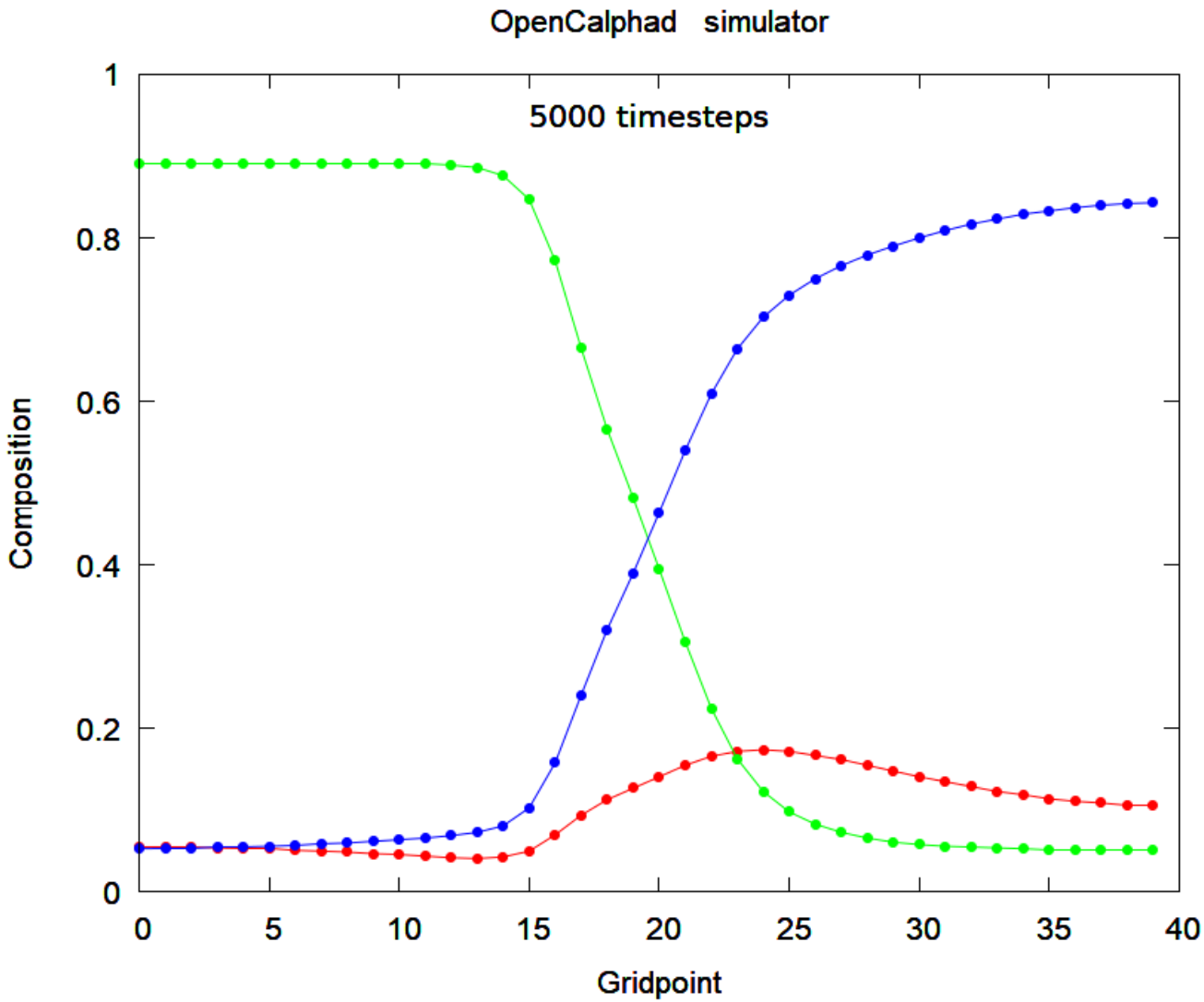

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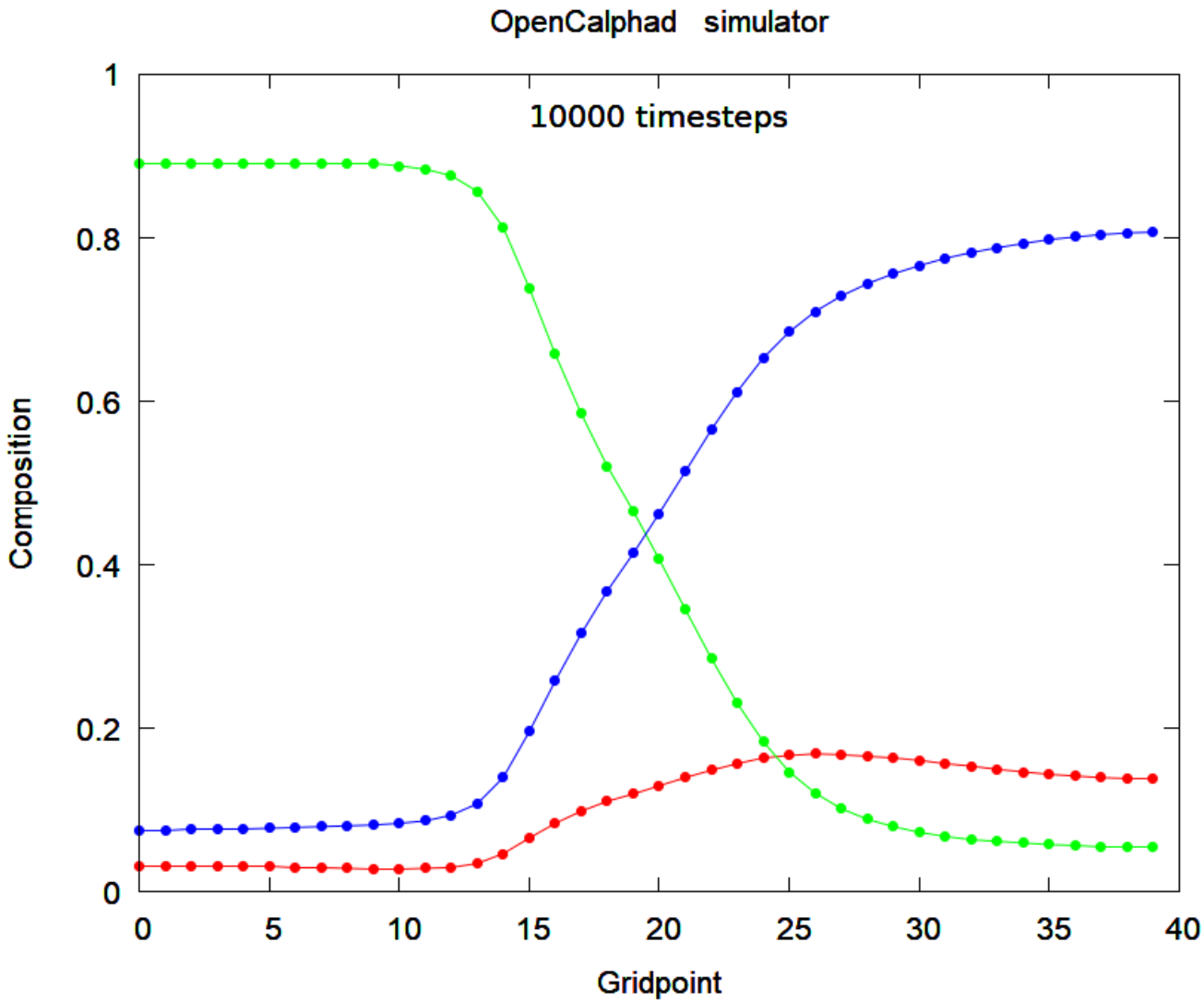

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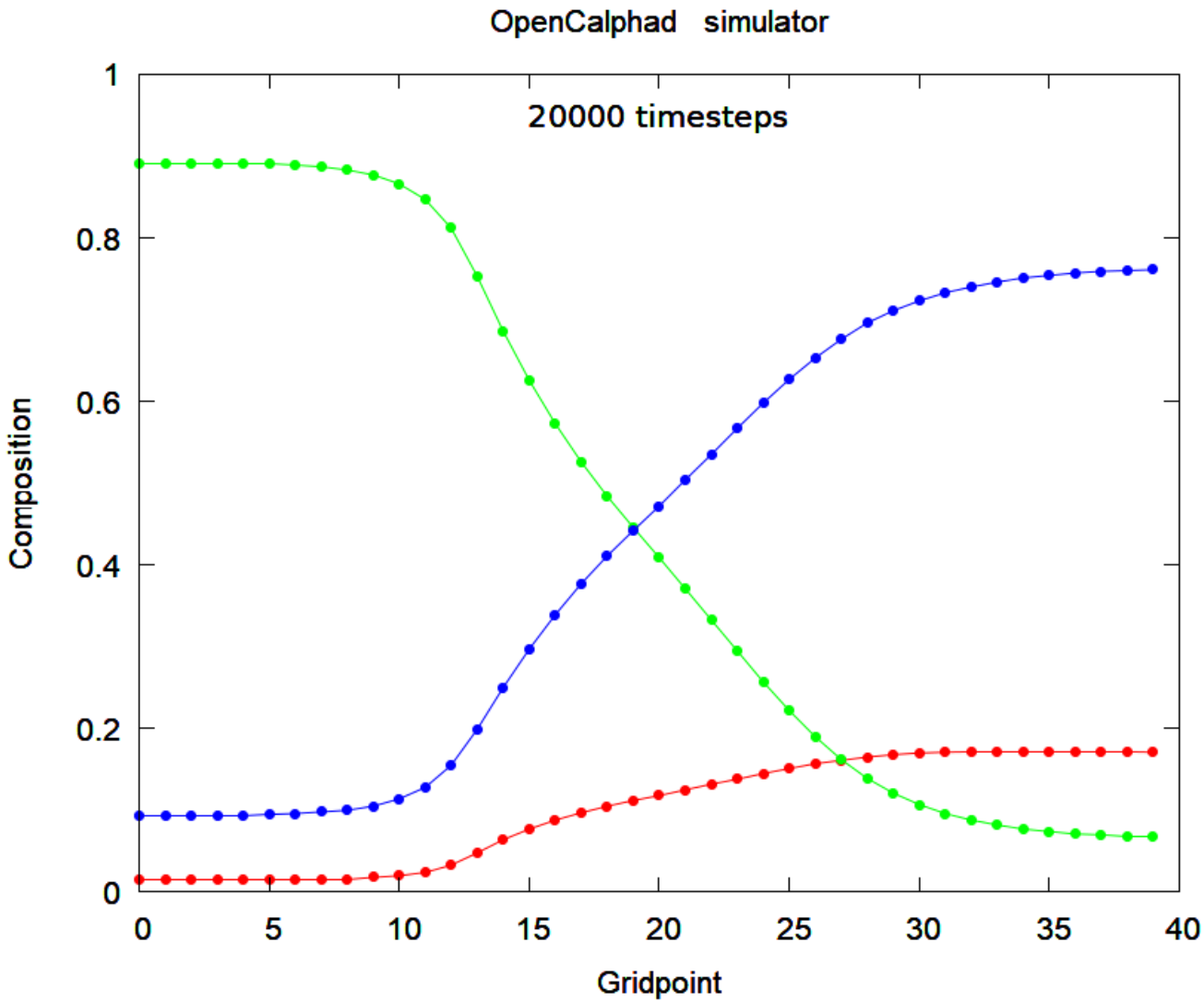

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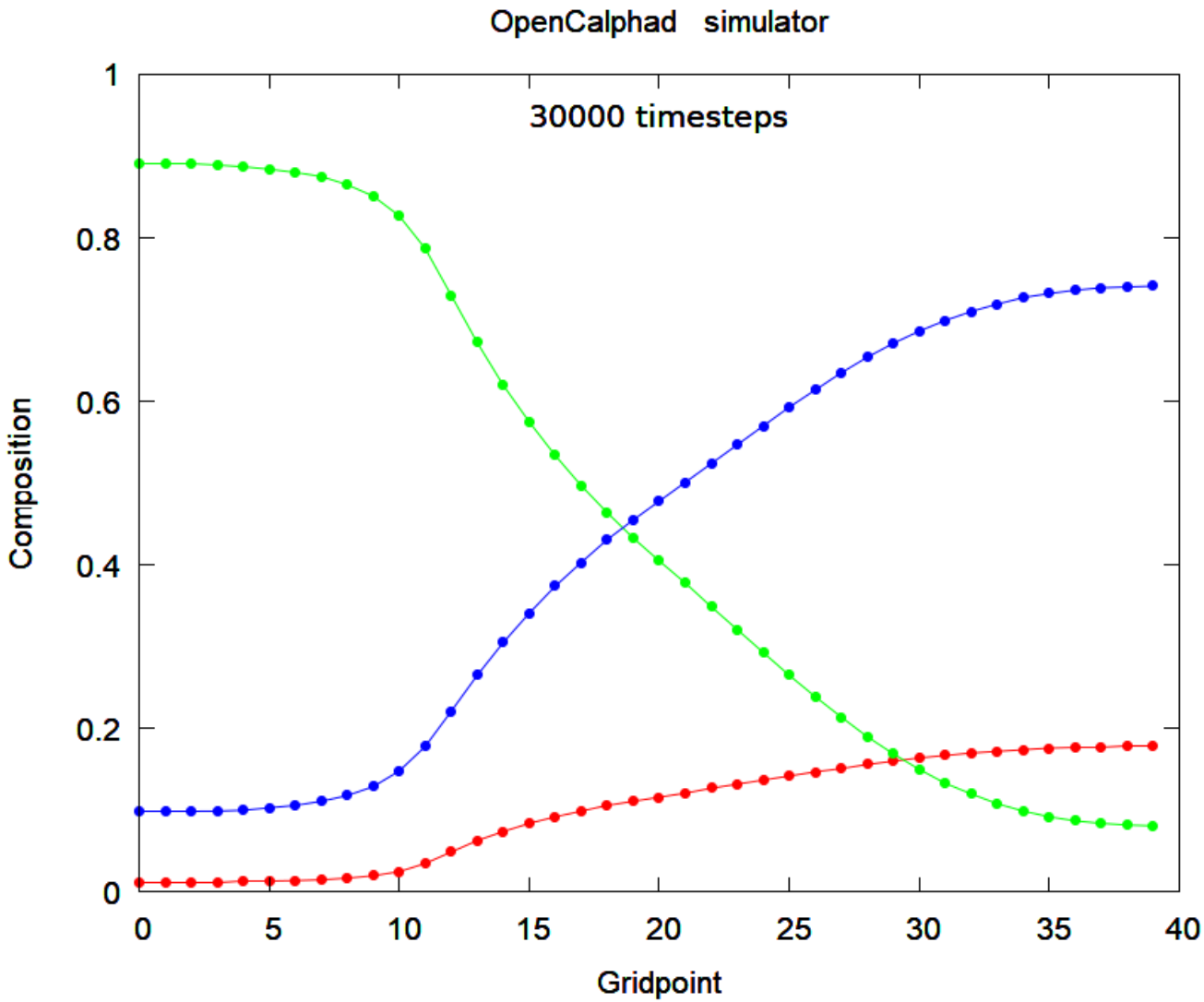

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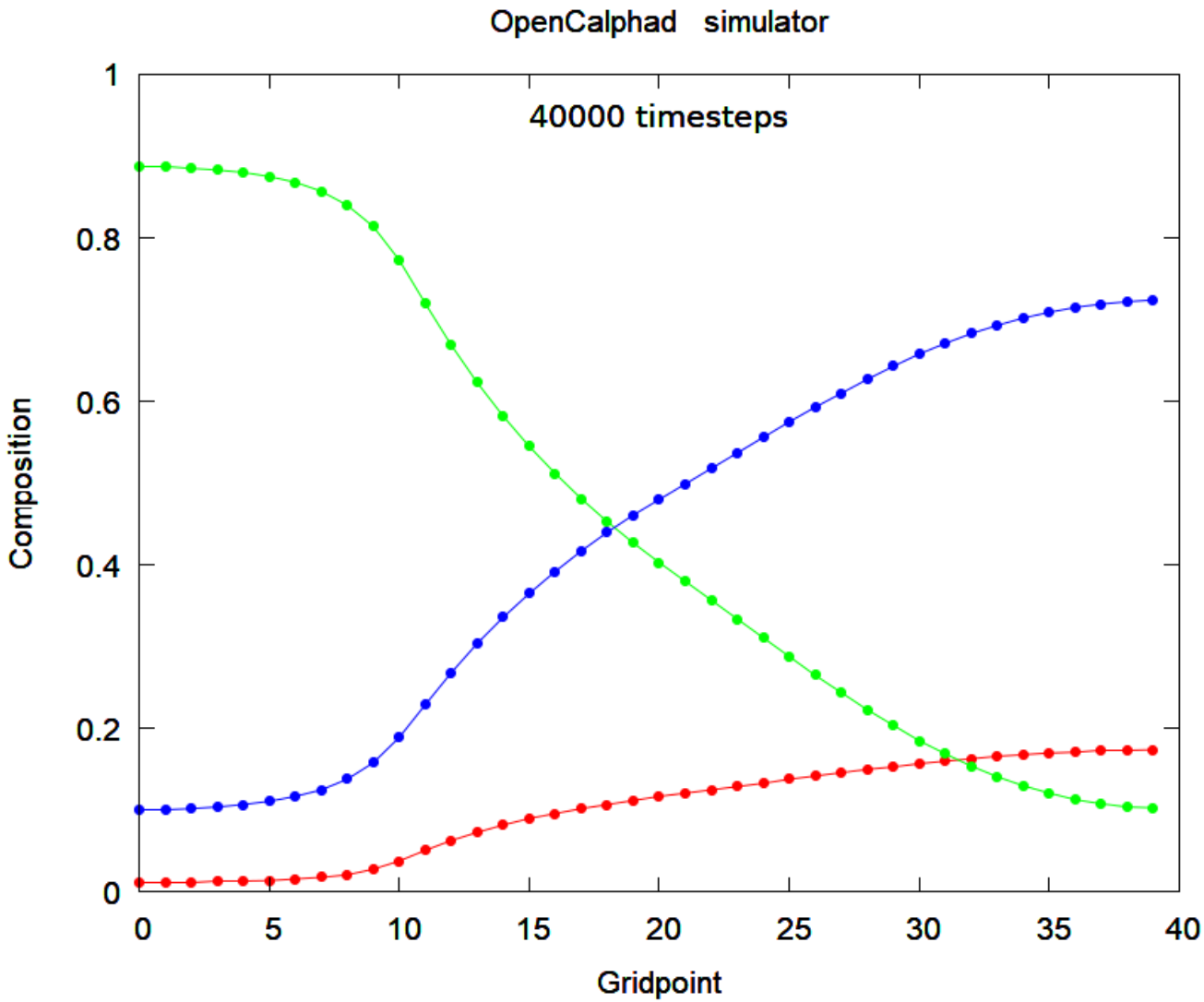

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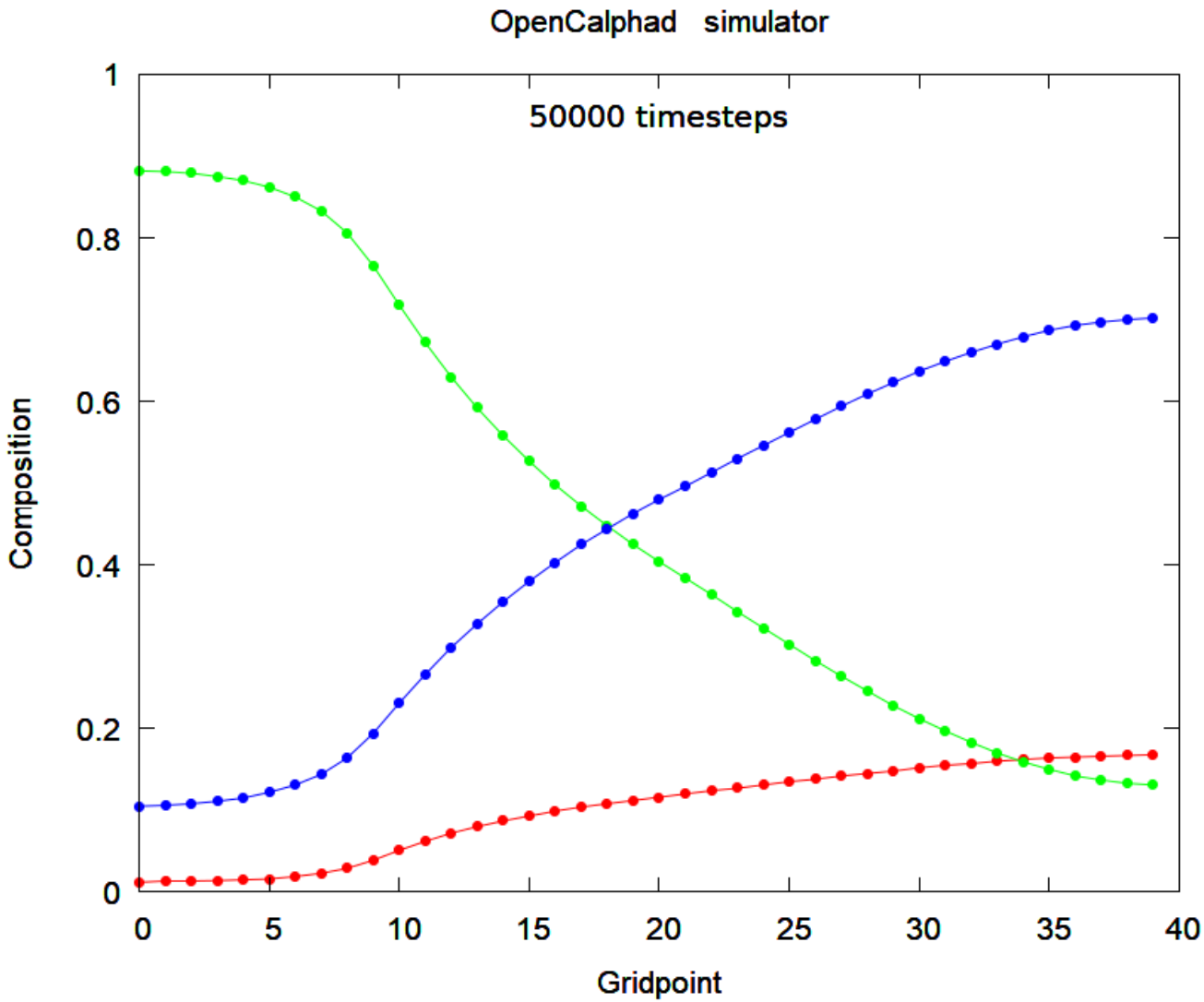
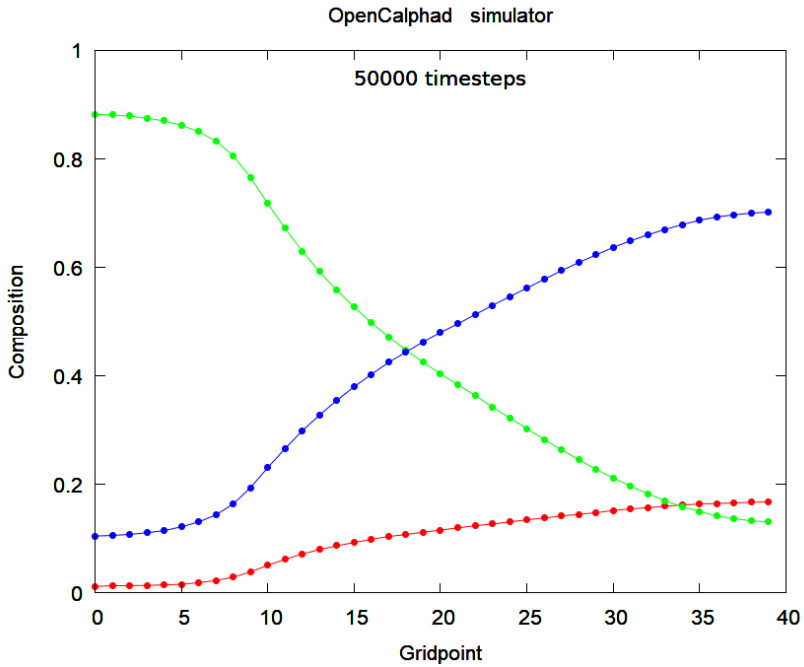
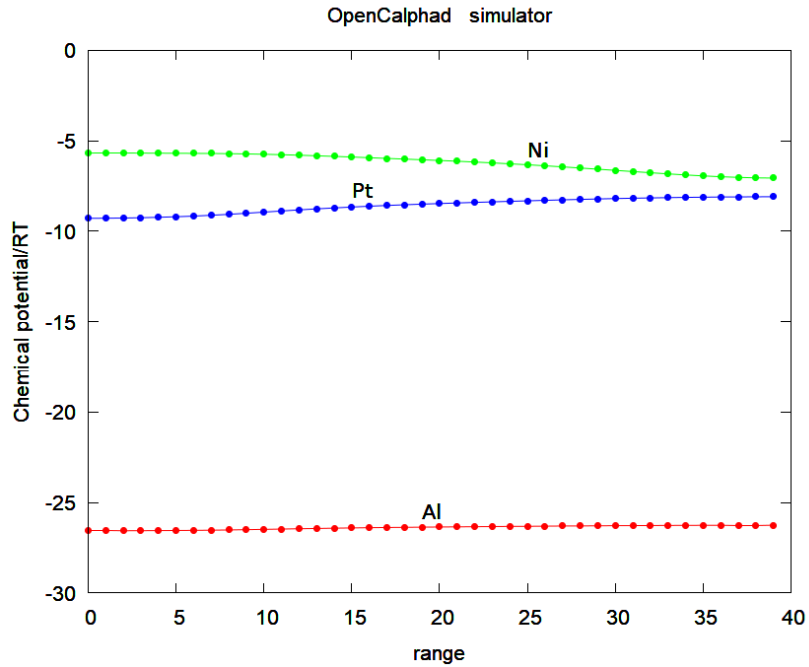


Final composition profile and chemical potentials

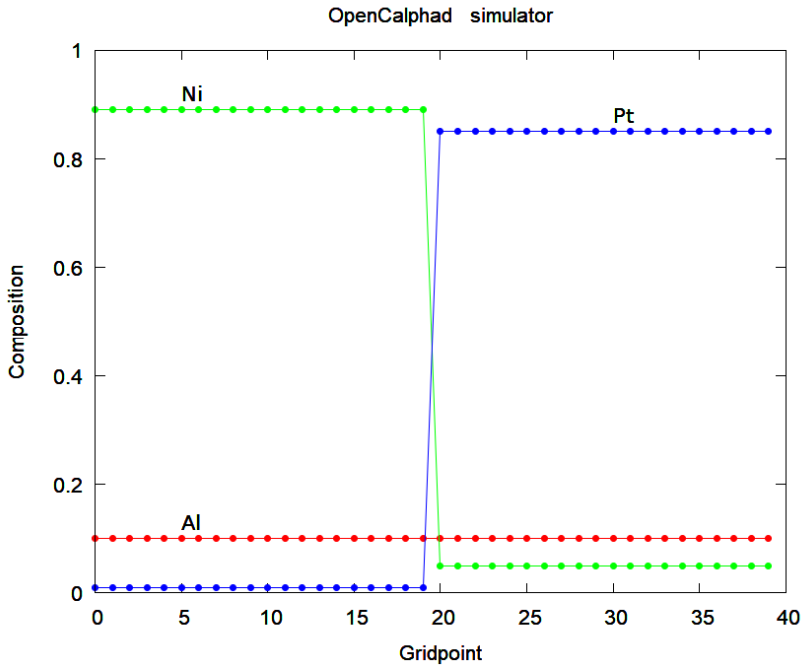
At the final timestep the composition profile vary significantly but the chemical potentials are fairly flat.

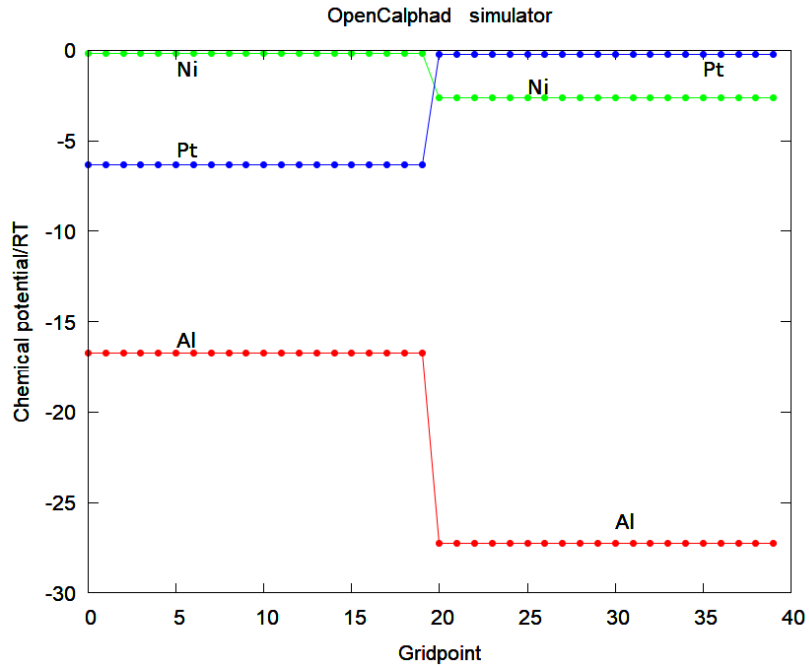




Final composition profile and chemical potentials

These were the inital profiles for composition and chemical potentials.





Simulation of ternary diffusion Al-Ni-Pt

The same simulation was run in parallel using OpenMP and sequentially. The gain in time was impressive.

Threads	timesteps	CPU (s)	Clockcycles	Clock time ratio
1	50000	1535	1606981	1
12	50000	2860	247227	0.16

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I used a very simple kinetic model and about 95% of the CPU time was spent calculating equilibria in the gridpoints. Calculating in parallel reduced the clock time by 1/6. Simulations that take a week to run sequentially can be made in a day!

Flowchart of simulation program

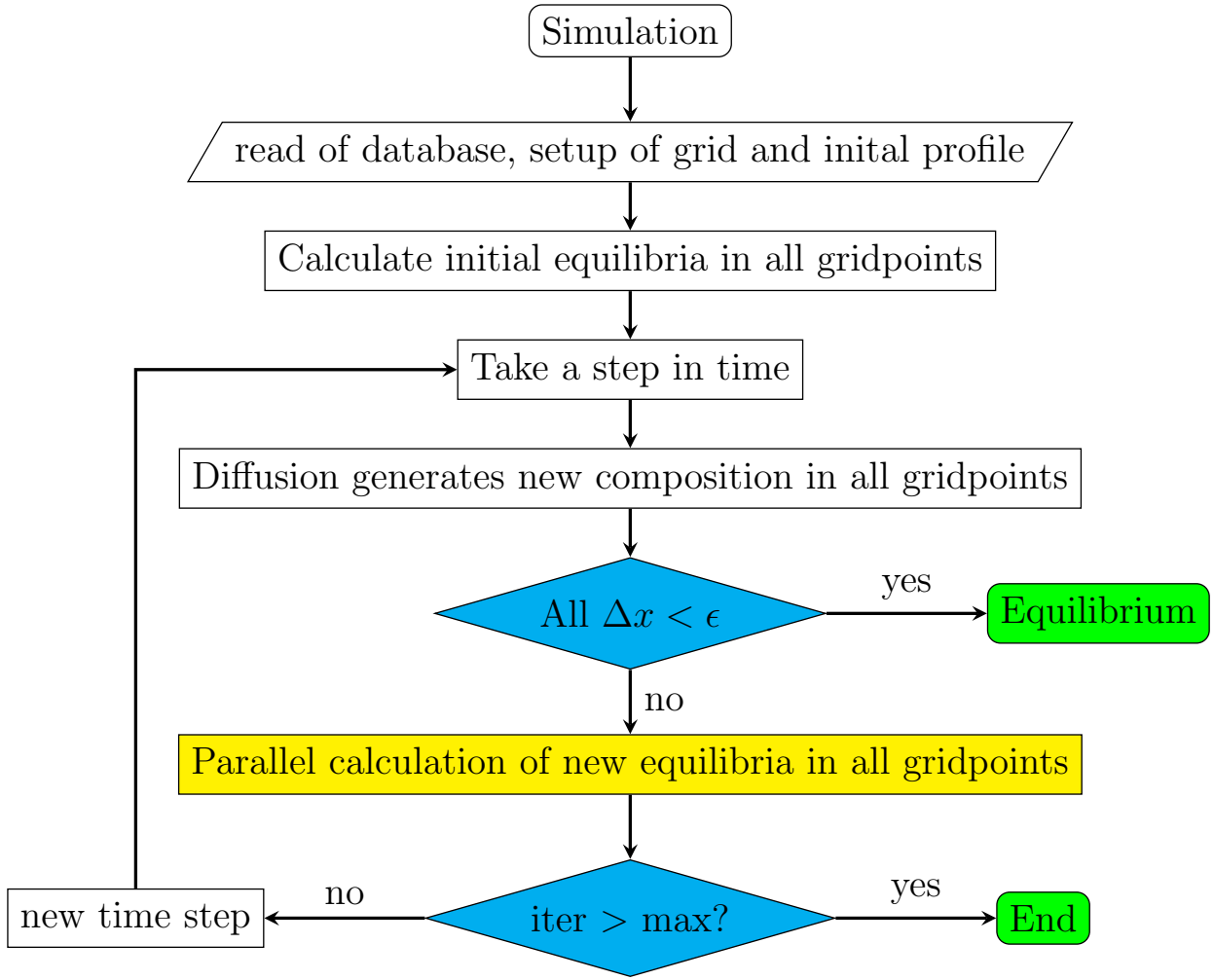

Figure 1: Flowchart of simulation