

Exploring strategies to streamline the development of cellular automata algorithms by reducing neighborhood-dependent calibration

Armin Golesch¹[0009–0000–7535–9198], Peter Raninger¹[0000–0002–2631–3422], and Thomas Antretter²[0000–0002–6538–5090]

¹ Materials Center Leoben Forschung GmbH, Vordernbergerstraße 12, 8700 Leoben, Austria

`mclburo@mcl.at`

² Chair of Mechanics, Montanuniversität Leoben, Franz Josef-Straße 18/III, 8700 Leoben, Austria

`mechanik@unileoben.ac.at`

In microstructure simulation using Cellular Automata (CA), the choice of neighborhood prominently influences the behavior of a generic implementation [1-3]. Moore and von Neumann neighborhoods can yield diverging results, and directional bias may be reduced using pseudo-pentagonal or pseudo-hexagonal neighborhood patterns. The work of Łach and Svyetlichnyy [3] demonstrates that not only basic implementations, but even advanced hybrid approaches show sensitivity to neighborhood choice. The need for calibration to mitigate numerical artifacts is common in CA literature and the desire to minimize this problem was emphasized by Zhi et al. [1].

This work aims to establish a Frontal Cellular Automata (FCA) framework with coupling to concentration fields via the Finite Volume Method (FVM), while maintaining high adaptability by avoiding reliance on a specific neighborhood type. The core concept is the development of a consistent neighborhood-interpretation scheme based on the Cahn-Hilliard equation. On-demand solutions of the Cahn-Hilliard equation are used for neighborhood interpretation, while relevant integrals are evaluated locally and results are stored for reuse to keep computational cost low. The dependence on neighborhood selection is minimized and a user-friendly system is established. The explicit representation of grain boundaries within a neighborhood enables a tailored evaluation of the free-energy change associated with defined cell transitions, which supports further advances in simulating anisotropic processes.

A decoupled treatment of phase/grain pairings is utilized to reduce overall computational time through parallel execution on a HPC cluster. All information regarding specific pairings is computed locally on-demand and stored for reuse.

References

1. Zhi, Y., Jiang, Y., Ke, D., Hu, X., Liu, X.: Review on Cellular Automata for Microstructure Simulation of Metallic Materials. *Materials* **17**, 1370 (2024)

2. Sieradzki, L., Madej, L.: A perspective comparison of the cellular automata and Monte Carlo techniques in application to static recrystallization modelling in polycrystalline materials. *Computational Materials Science* **67**, 156-173 (2013)
3. Łach, Ł., Svyetlichnyy, D.: 3D Model of Carbon Diffusion during Diffusional Phase Transformations. *Materials* **17**, 674 (2024)