Cellular Automata Simulation for Microstructural Estimation during Wire-Arc Additive Manufacturing

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Motivation

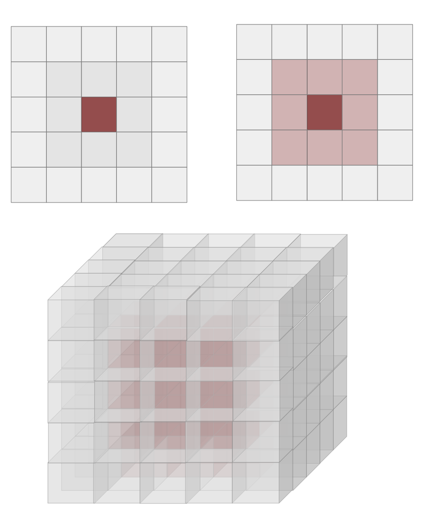
Controlling the microstructure of material requires developing a multi-scale framework that allows multiple deformation and damage processes to occur over discrete-time and length scales.

Introduction

Scientific modeling using the cellular automata method is well-established and holds great amplitude in research, but most applications are in two dimensions. Since there are processes that two-dimensional models can not represent, a three-dimensional CA estimation of the microstructure is instrumental to making better microstructural analyses. This work aims to simulate the microstructural behavior and mechanical response of metallic components with a three-dimensional multi-scale framework using the cellular automata method.

Cellular Automata

Fig. 2. 2D and 3D Moore's Neighborhood



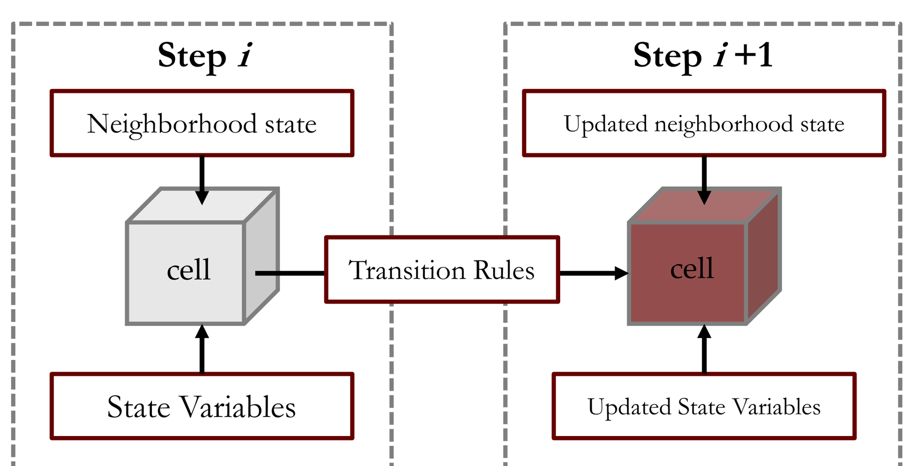


Fig 1. The state of a cell is determined upon the state of the surrounding cells through each iteration

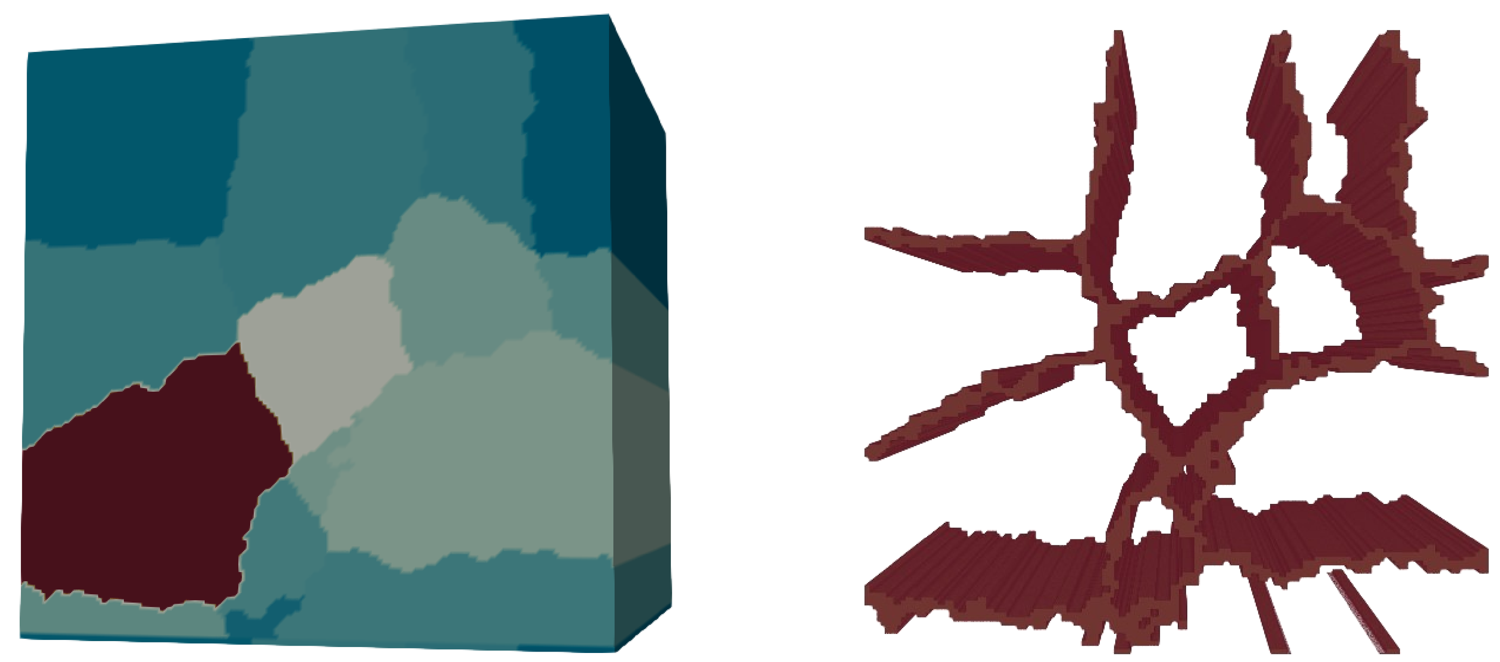
Method	Characteristics	CA Comparison
Monte Carlo	• Discrete method • Arbitrary units • Single phase grain growth • Unable to track RX front	• Physical parameter negation results in irregular RX front • CA tracks RX front and has real time interaction with analytical equations
Vertex	• Complex calculation of driving force • Computationally intensive • Tracks RX front	• RX depends on grain growth • Grain growth's complexity results in simulation time consumption
Phase Field	• Computationally intensive • No need for RX front tracking	• Inefficient parallelization compared to MC and CA • Less applicable in studies of texture evolution

*Recrystallization (RX)

Cellular Automata for Super Computers (CASUP)

- Cellular automata library for high-performance computing systems [1]
- Microstructure evolution, solidification, recrystallization, ductile damage and brittle fracture, and magnetization.
- Fortran 2018, Fortran coarrays, Intel Fortran Compiler and MPI Library

Fig. 3. Simulation of formation and cleavage fracture of polycrystalline microstructure [1]



3.a. Grain size/shape

3.b. Grain boundary

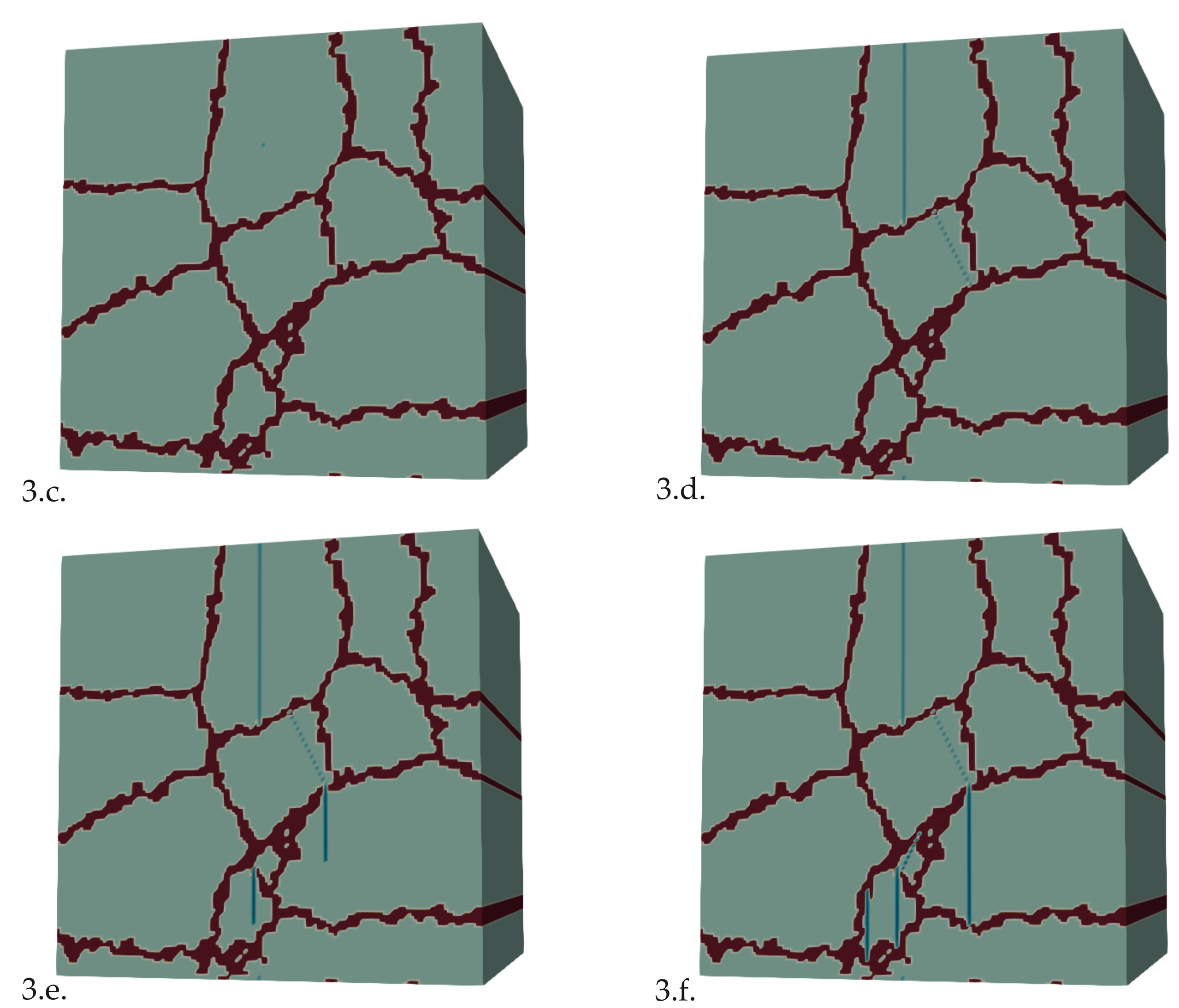


Fig. 3.c.-3.f. Stages of fatigue crack

References

1. Shterenlikht, A., & Cebamanos, L. (2011). Cellular automata library for supercomputers.
2. Li, H., Sun, X., & Yang, H. (2016). A three-dimensional cellular automata-crystal plasticity finite element model for predicting the multiscale interaction among heterogeneous deformation, DRX microstructural evolution and mechanical responses in titanium alloys.

Future Work

The computationally efficient cellular automata structured grid works well for parallelization making the method scalable for a multi-scale framework. Using the cellular automata library, CASUP, developed with Fortran coarrays, a framework will be assembled and integrated with the macro-scale finite element and crystal plasticity finite element solvers ParaFEM and Abaqus.

- Assemble the existing library, which includes a coupled CAFE method integrated with ParaFEM to create a Multi-scale Framework for fracture and deformation
- Development of CACPFEM to simulate deformation, mechanical response, and microstructural evolution

Cellular Automata Finite Element (CAFE)

- 3D CA and FE to predict deformation & fracture
- Miniapps
  - Represent multiscale fracture models of polycrystalline solids
  - Allow user customization
- FE (ParaFEM)
  - Solves macro-scale continuum mechanics problem
  - Communicate stress, strain variables to CA
- CA (CASUP)
  - Simulates micro-scale damage and fracture
  - Communicates damage variables to FE

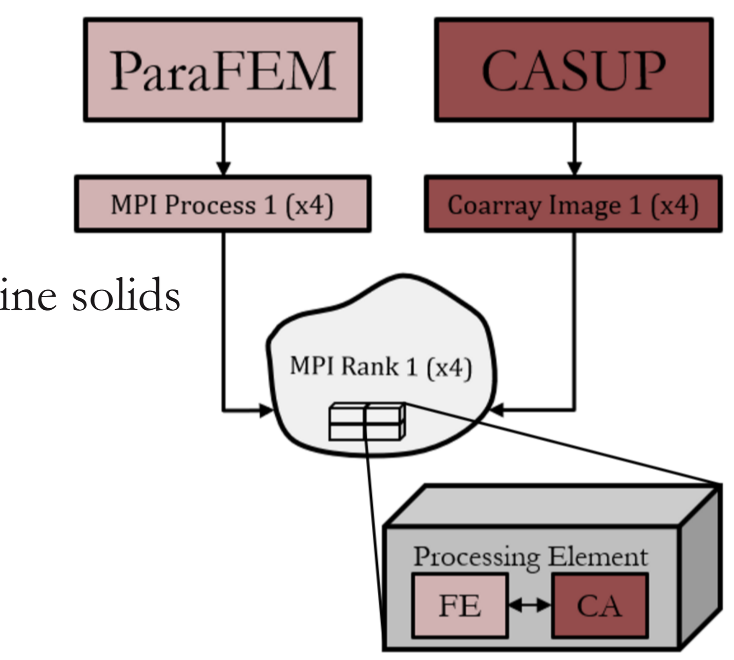


Fig. 4. Processing elements transfer data between CA and FE

CA Crystal Plasticity Finite Element Method (CACPFEM)

- 3D CA and CPFEM coupled to predict deformation, mechanical response, and microstructural evolution
- DRX interacts with deformation
- CASUP linked with ABAQUS
- CA algorithm assigned to DRX evolution
- CPFEM assigned to multiscale heterogeneous deformation

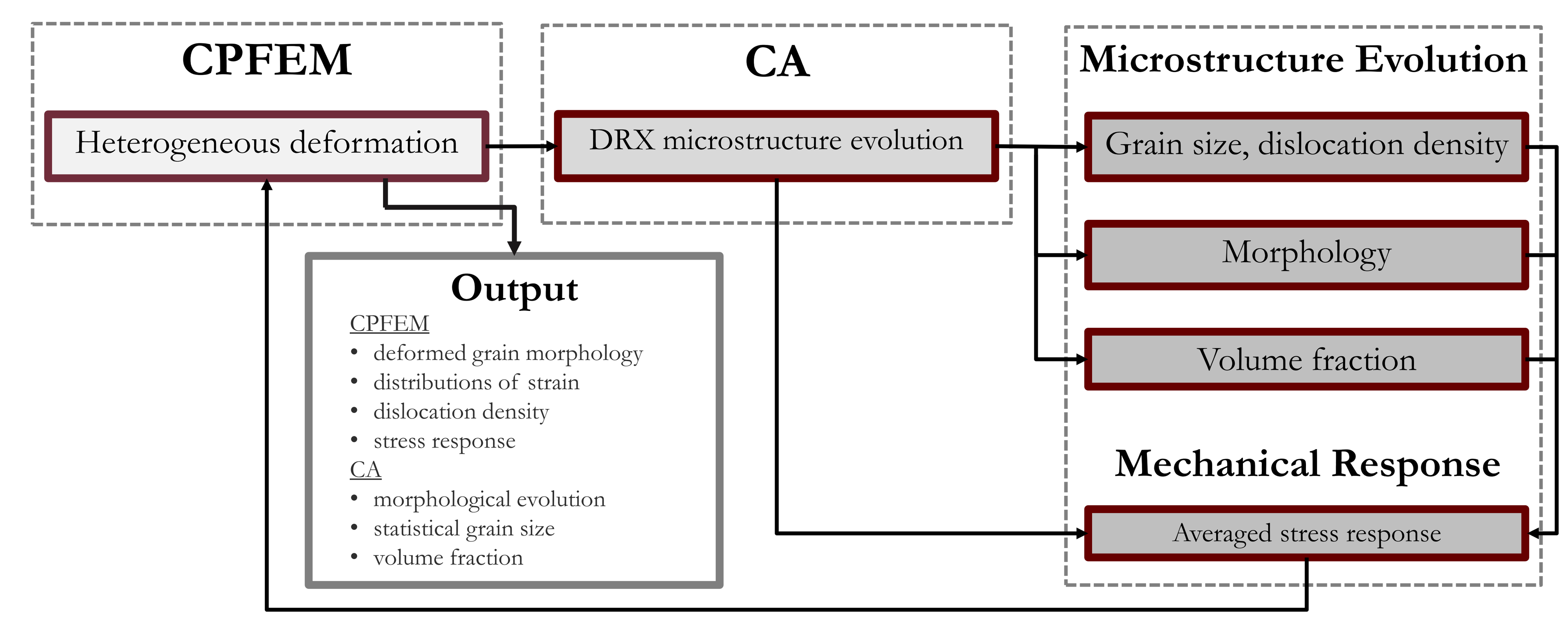


Fig. 5. CACPFEM simulation outline [2]