Application of Heterogeneous Computing to CAFE Simulations of Production Processes

Rauch Łukasz, Bzowski Krzysztof, Rodzaj Artur

Department of Applied Computer Science and Modelling

Faculty of Metals Engineering and Industrial Computer Science
Agenda

1. Motivation
2. Aim of the work
3. Tools
   - DMR Multiscale Computations
   - Heterogeneous architectures
4. Implementation details
   - Cellular Automata for Grain Growth
   - Finite Element Method for Heat Transfer
5. Results and discussion
Finite Element Method

- Shape
- Loads
- Stresses
- Strains
- Temperatures

- Microstructure
- Grain size
- SRX
- DRX

- $R_e$
- $R_m$
- fatigue resistance,
- crash resistance,
- etc.

4D MODELING

optimization
Constitutive models at higher scales are constructed from observation and models at lower, more elementary scales.

Problem is solved simultaneously at several scales (in practice two-scales) by an a priori decomposition.

Concurrent

Constitutive models at higher scales are constructed from observation and models at lower, more elementary scales.

Upscaling

FE - finite element
XFE - extended finite element
MS - multi scale
CA - cellular automata
MD - molecular dynamics
Fig. Initial 3D DMR with uniform mesh and deformed mesh

Fig. Example of grain growth

Fig. Illustration of the finite element mesh generated on the basis of the DMR.
DMR Multiscale Computations

Software development
- Algorithms
- Parallelization

Microstructure simplification
- (SS)RVE

Hardware usage
- heterogeneous computing
Heterogeneous architectures - idea

- Physical constraints in the construction of standard processors
- Reducing energy consumption
- Maximizing performance

Using different processing cores
Heterogeneous architectures

CBEA

CPU in combination with GPU

CPU in combination with FPGA

Fig. Brodtkorb A., Dyken C., State-of-the-art in heterogeneous computing, Scientific Programming, vol. 18

OpenCL
Main objectives

To propose efficient parallel multiscale CAFE approach, composed of CA (micro scale) and FEM (macro scale) methods, working on heterogeneous architectures.

Implementation for heterogeneous platform using OpenCL.

To apply implemented CAFE approach to simulate selected real production process.
Finite Element Method (FEM) – basic idea

1. Discretize the domain
2. Determine interpolation functions
3. Compute the element matrices and vectors
4. Assemble the element equations
5. Solve the global equation system
The main idea of the cellular automata technique is to divide a specific part of the material into one-, two-, or three-dimensional lattices of finite cells.

Each cell is characterized by its state and transition rules are defined to determine the new state of the cell on the basis of previous states of neighbours and the cell itself.
Grains growth

Temperatures

Heat transfer

The coefficients of thermal conductivity

Grains growth

CAFE construction – practice
Numerical model

FEM

Heat equation

\[
\frac{\partial}{\partial x} \left( k_x \frac{\partial t}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial t}{\partial x} \right) - c_p \rho \frac{\partial t}{\partial \tau} = 0
\]

\[ q \]

CA

Probability of state change

\[
p = \exp \left( -\frac{Q_b}{RT} \right) \cdot \frac{K}{K_{\text{max}}}
\]
CAFE implementation details
The quantitative results – different devices

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**Speedups - f16**

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TOTAL TIME:

- **CA** = 820,553
- **FEM** = 475,754
- **FEM -> CA** = 269,093
- **CA** = 34,709
- **Solver** = 74.146
- **Ideal** = 475.754
- **Total** = 269.093
- **Solver + CA** = 29,649
- **Ideal + CA** = 21.621

**Solver**

- **Ideal** = 1.00
- **Solver** = 1.00
- **FEM->CA** = 1.00
- **CA** = 1.00

**CA**

- **Ideal** = 1.00
- **Solver** = 1.00
- **FEM->CA** = 1.00
- **CA** = 1.00

**TOTAL TIME**

- **CA** = 820,553
- **FEM** = 475,754
- **FEM -> CA** = 269,093
- **CA** = 34,709
The quantitative results – different number of iterations and LD

GPU

CPU
The quantitative results – scalability of CA calculations

\[ S_n = 1 - \frac{T_n - D_n}{T_1 - D_1} \]
Scheduling between CPU and GPGPU

Objective function vs. CPU/GPGPU ratio

- Intel i5 GTX 460
CA model verification

\[ T_{G1} = T_{G2} = T_{G3} = \text{const} \]

\[ T_{G1} > T_{G2} > T_{G3} \]
FEM model verification

\[ k_{G1} \gg k_{G2} \gg k_{G3} \]
The qualitative results of CAFE

\[ k_{G1} > k_{G2} > k_{G3} \]

Fig. Temperature-controlled grain growth

Fig. Heat transfer
$T_{G1} = T_{G2} = T_{G3} = \text{const}$

$T_{G1} > T_{G2} > T_{G3}$

CAFE
Conclusions and further research

- Good qualitative results were obtained in comparison to physical simulations.
- The character of material models implemented in micro scale strongly influences the efficiency of CA performance on GPGPU.
- Deeper analysis of scheduling CA, FEM and CAFE.
- Performance of computational tests on heterogeneous cluster environments.