AKADEMIA GÓRNICZO-HUTNICZA
IM. STANISŁAWA STASZICA W KRAKOWIE

AGH UNIVERSITY OF SCIENCE
AND TECHNOLOGY

Wydajny obliczeniowo model automatów komórkowych do symulacji rekrystalizacji statycznej

dr inż. Mateusz Sitko

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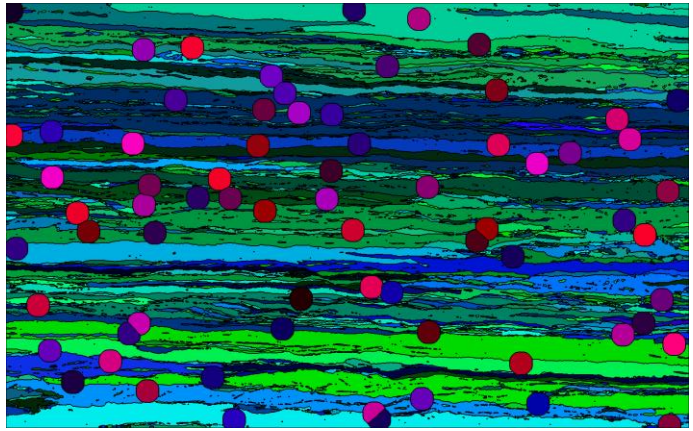
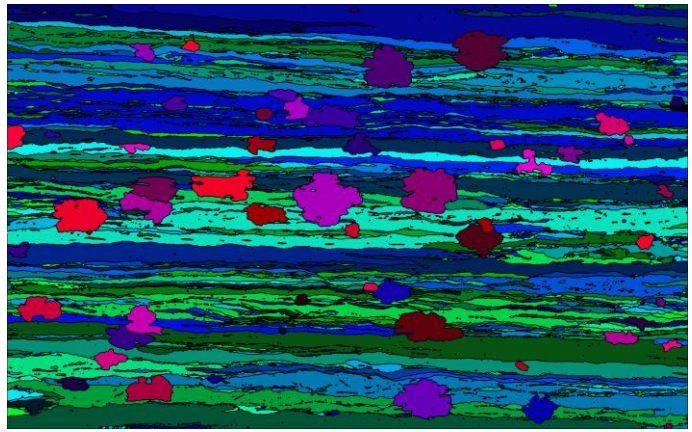
Agenda

1. Motywacja
2. Opracowanie modelu SRX
3. Identyfikacja modelu SRX
4. Zrównoleglenie modelu SRX
5. Analiza wydajności
6. Podsumowanie





SRX – rekrystalizacja statyczna (ang. Static Recrystallization)

Motywacja

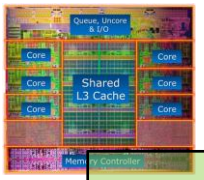
Modele analityczne i pól uśrednionych (mean field)

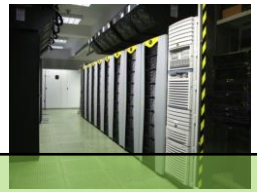
Modele pól pełnych (full field)

a materiału

Obliczenia wysokiej wydajności

CPU - openMP **GPU - CUDA** **grid - MPI**





M.J. Gibson, et al., J. Parallel Distrib. Comput. 77 (2015) 11–25.
A. Kolnoochenko, et al., Comput. Aided Chem. Eng. 37 (2015) 551–556.
L. Rauch, et al., Procedia Comput. Sci. 108 (2017) 1813–1822.

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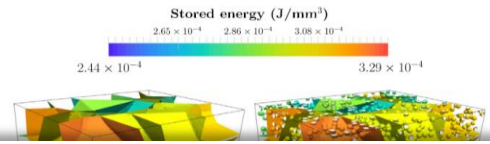
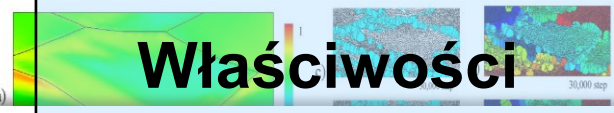
Operacje cieplno - mechaniczne

Metoda poziomic

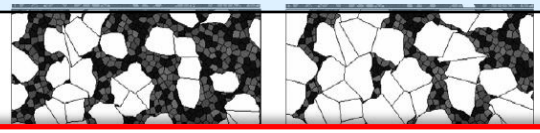


Metoda pola fazowego



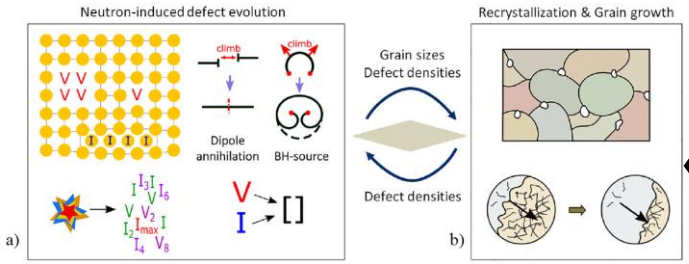
Właściwości użytkowe

Metoda wierzchołków



R. Pokharel, et a
Z. Liu, et al., Ma

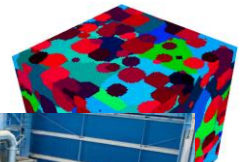
JMAK + cluster dynamics

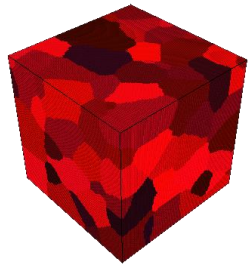


A. Mannheim, J.A.W. van Dommelen, M.G.D. Geers, Mech. Mater. 123 (2018) 43–58.

Czas obliczeń analizow fragme materia

Automaty komórkowe Monte Carlo





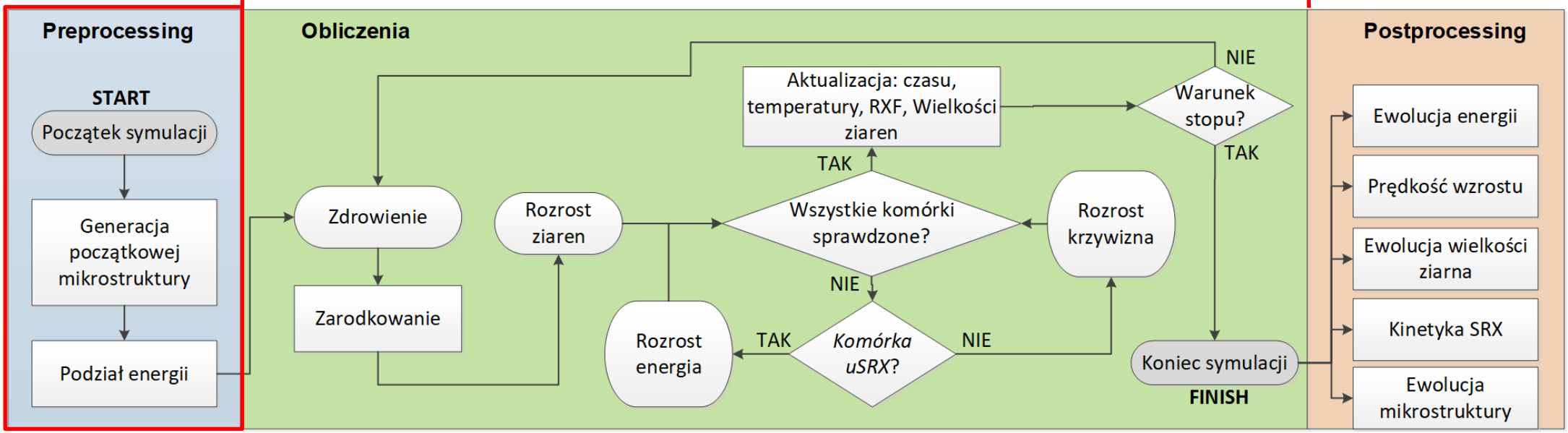
ej, *Comput. Mater. Sci.*, 2013, 67,

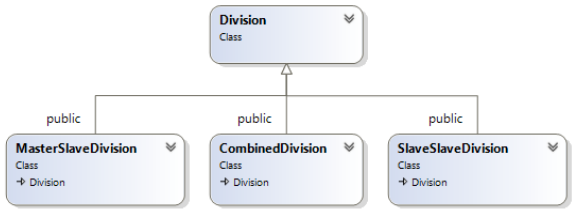
Mater. Sci. Eng. A, 2006, 433, 216–

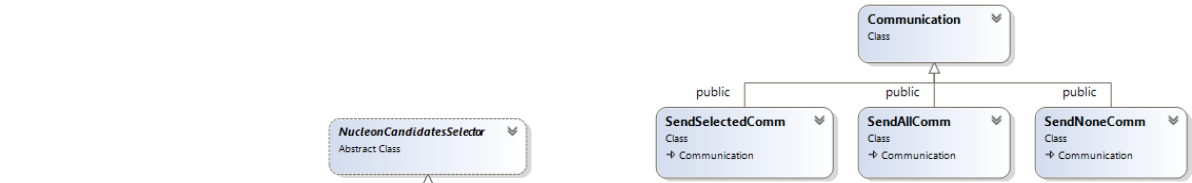
SRX – założenia modelu

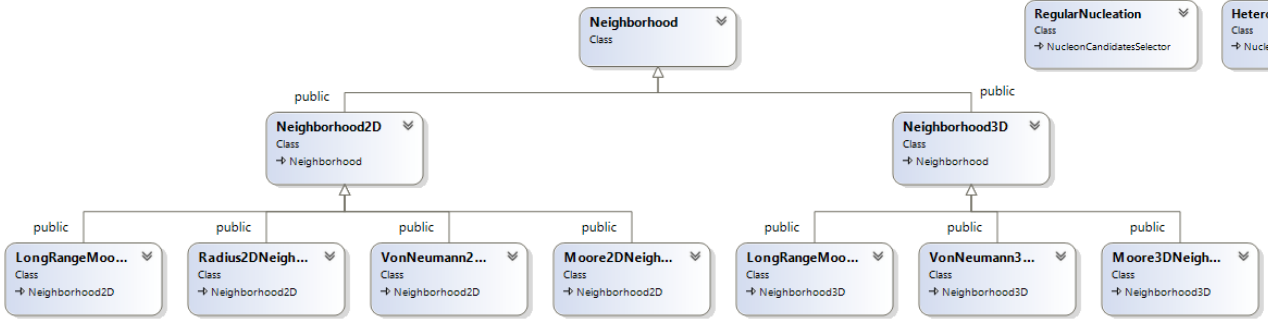
Mapowanie na architektury wysokowydajne

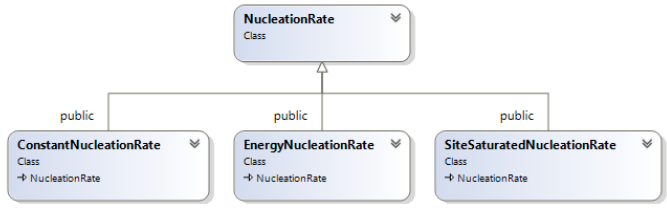
Preprocessing | Obliczenia | Postprocessing





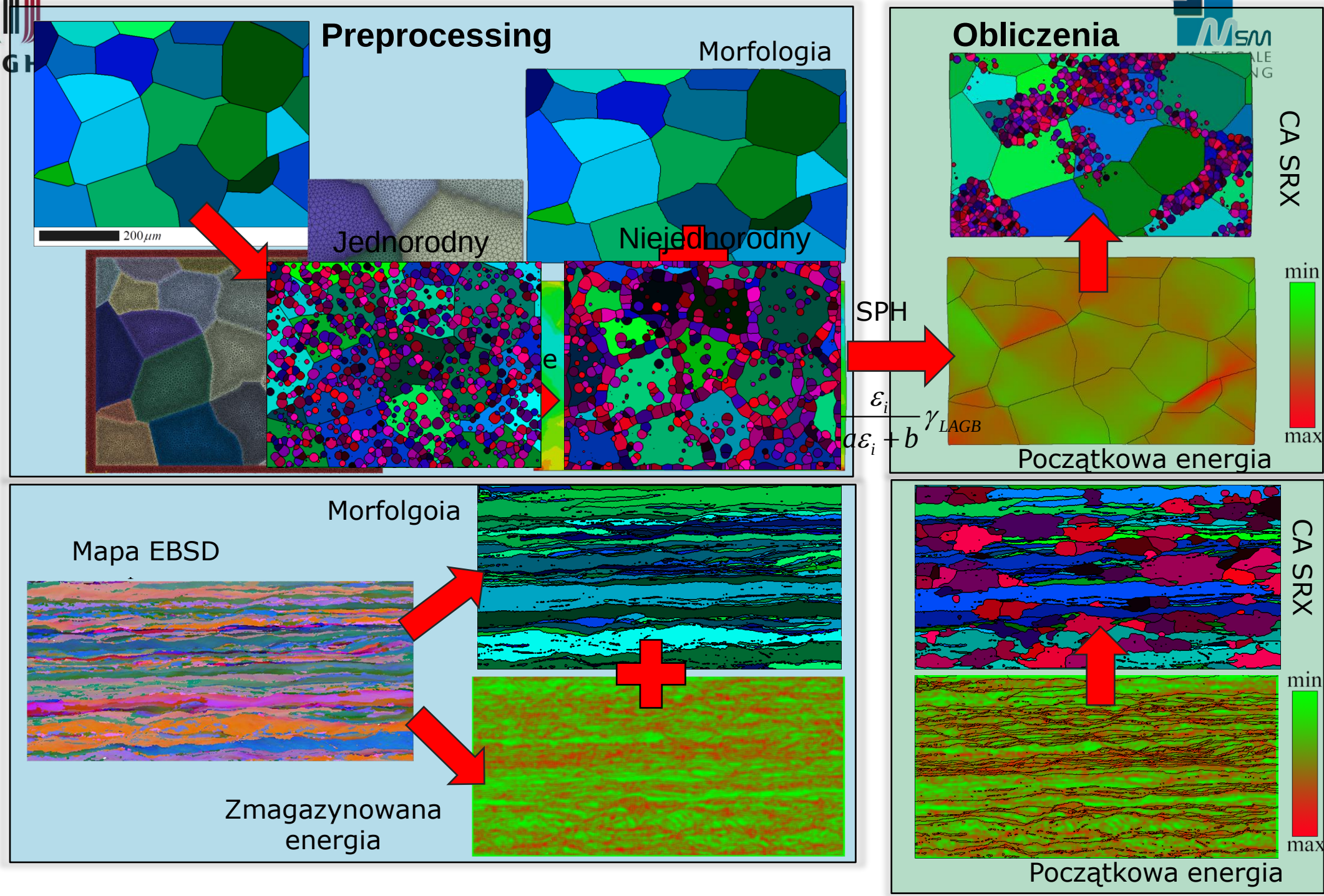






SRX – podział energii

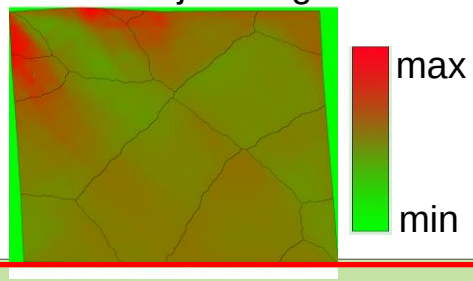
Preprocessing



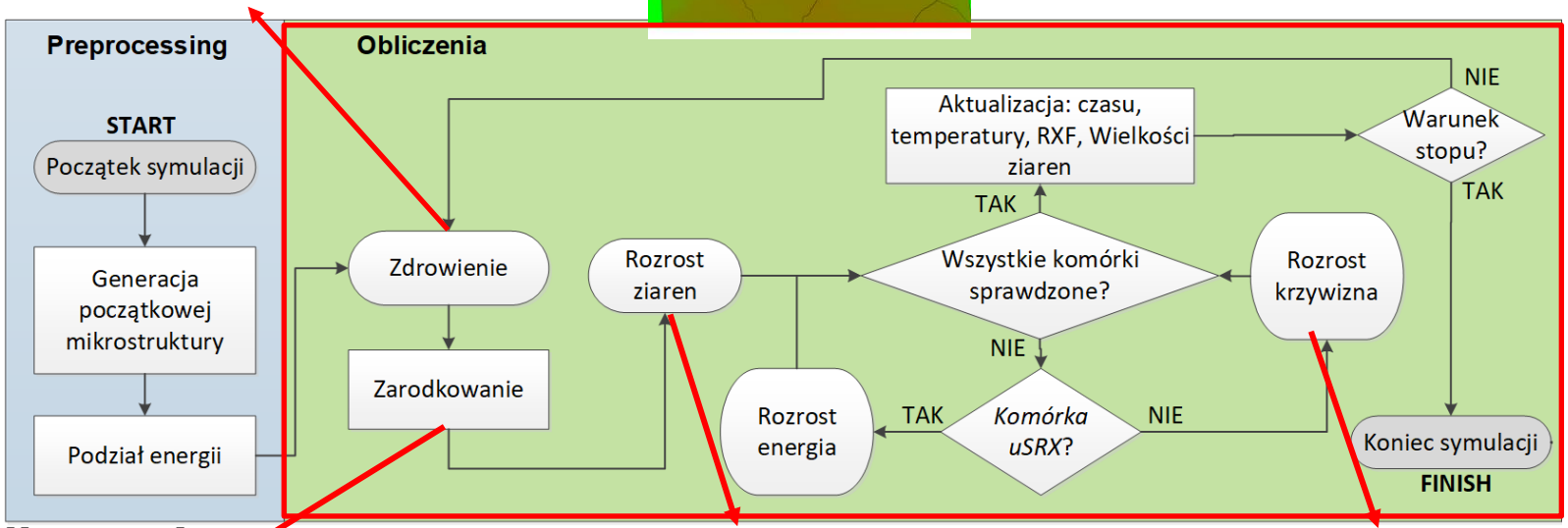
SRX – założenia modelu

$$H(t)=\left[H(t_0)^{1/2}-C_0\mu^{-1/2}kT\ln\left(1+\frac{t}{\tau_0}\right)\right]^2$$

Redukcja energii



Obliczenia

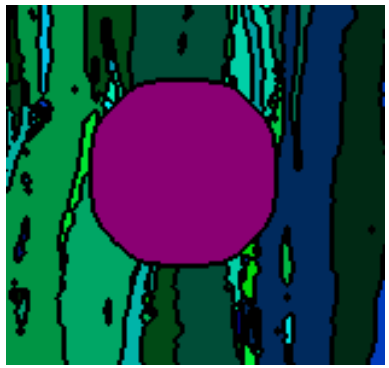


Zarodkowanie:

Rozrost ziaren RX→uRX:

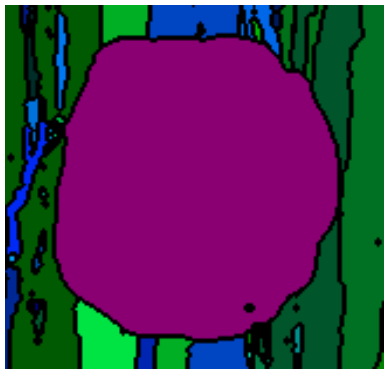
Rozrost ziaren RX→RX:

Energia jednorodna bez uwzględnienia orientacji

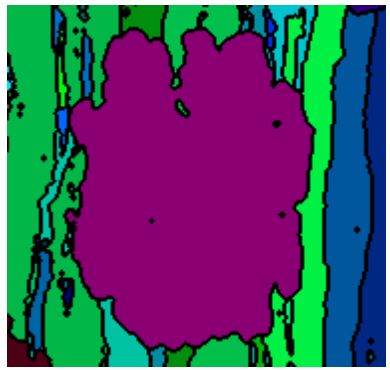


Energia heterogeniczna bez uwzględnienia orientacji

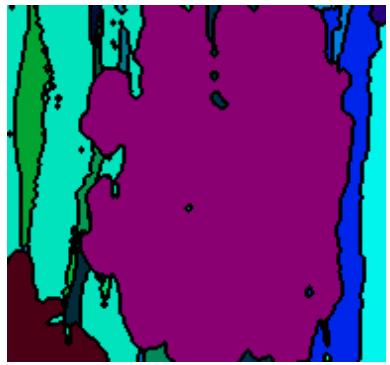
Energia jednorodna z wpływem orientacji



Energia heterogeniczna z wpływem orientacji

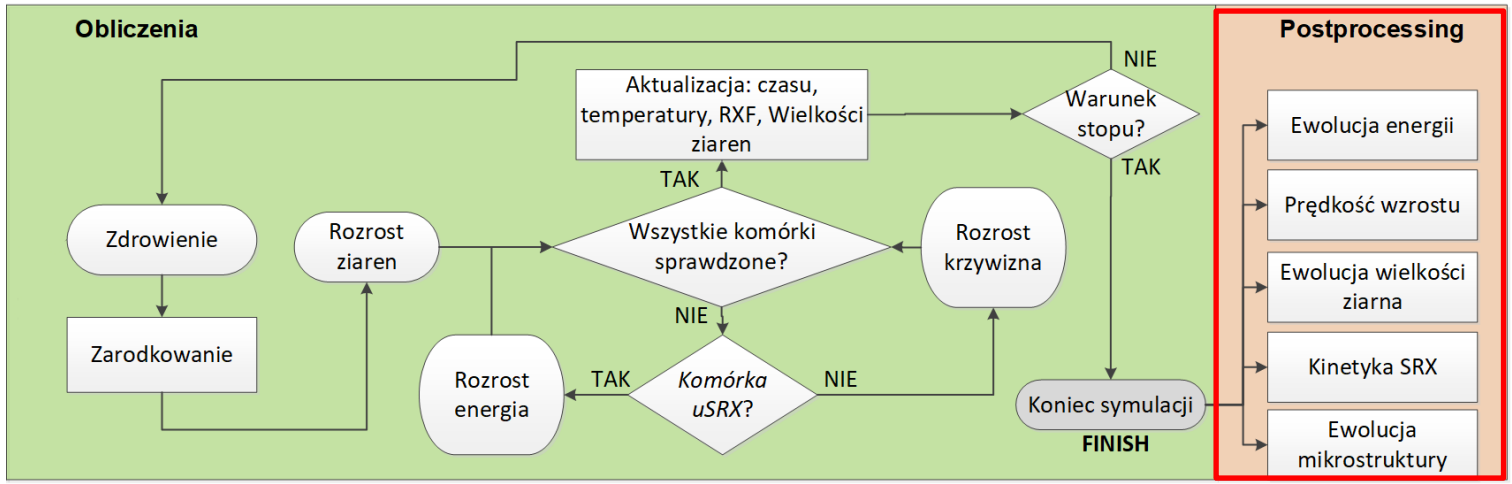


Energia heterogeniczna z wpływem orientacji i krzywizny

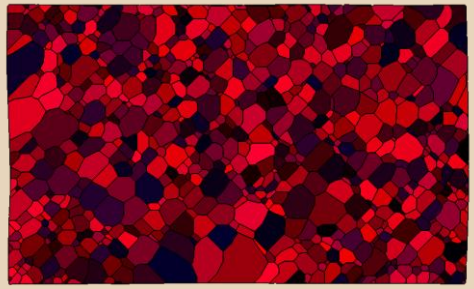


SRX – dane po symulacji

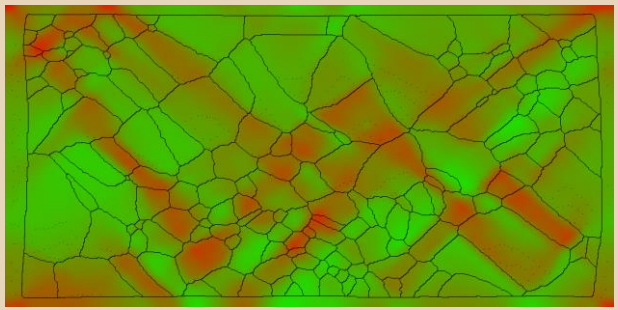
Postprocessing



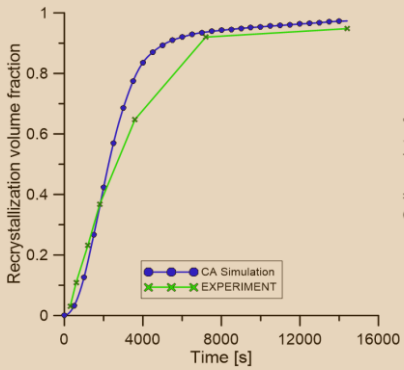
Końcowa morfologia



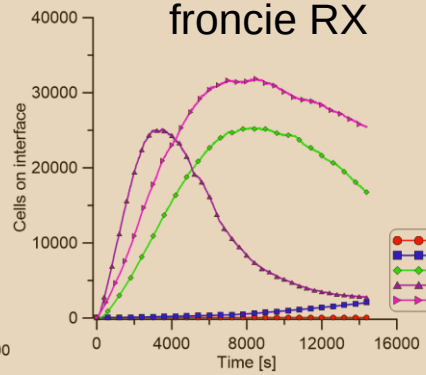
Ewolucja mikrostruktury



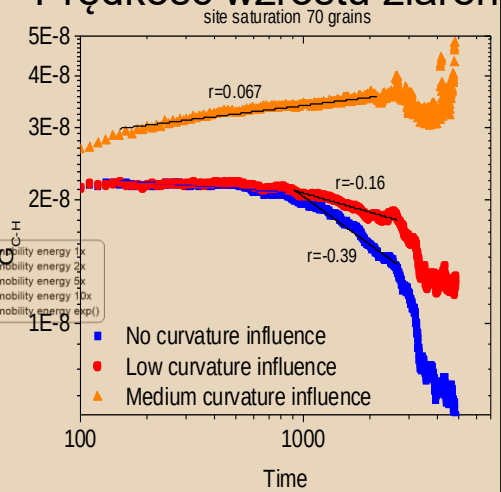
Kinetyka



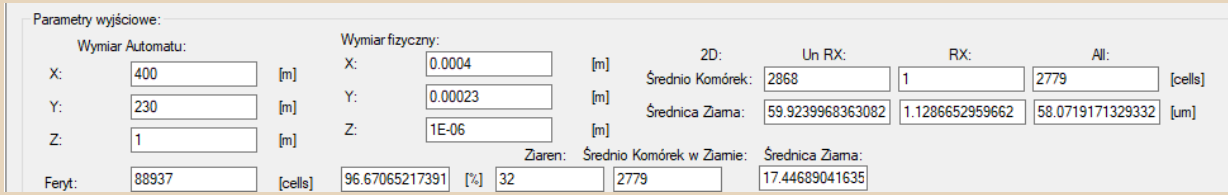
Komórki na froncie RX



Prędkość wzrostu ziaren



Dane statystyczne



Parametry wyjściowe:

Wymiar Automatu:			Wymiar fizyczny:			2D:	Un RX:	RX:	All:	
X:	400	[m]	X:	0.0004	[m]	Średnio Komórek:	2868	1	2779	[cells]
Y:	230	[m]	Y:	0.00023	[m]	Średnica Ziarna:	59.9239968363082	1.1286652959662	58.0719171329332	[um]
Z:	1	[m]	Z:	1E-06	[m]					
Feryt:	88937	[cells]	96.67065217391	[%]	Ziaren: 32	Średnio Komórek w Ziarnie: 2779	Średnica Ziarna: 17.44689041635			

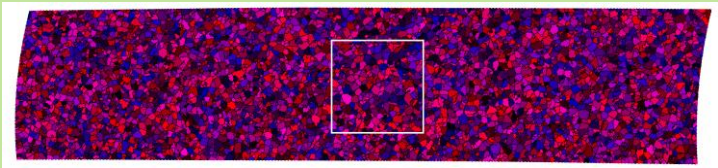
SRX – identyfikacja parametrów modelu

Badania eksperymentalne

	625 °C	675 °C	725 °C	775 °C	825 °C
RXF	0%	~3%	~41%	~84%	~99%
GS, µm	0	6.185	7.478	9.3431	8.9744

Materiał	C	Ni	Si	Mn	Ti	P	S	N
Fe30%Ni	0.089	29.8	0.27	1.73	0.003	0.01	0.016	0.004

Symulacja



Eksperyment

Problem bezpośredni

$\varphi(x) < err$

TAK

Parametry zidentyfikowane

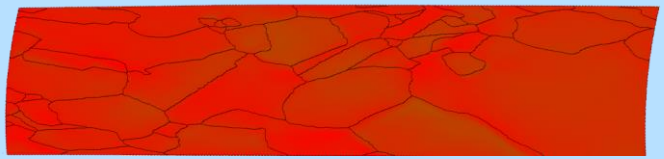
NIE

Nowe parametry

Preprocessing

Morfologia

Początkowy rozkład energii

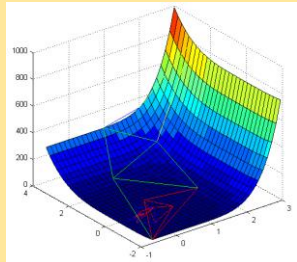


Optymalizacja

$$N = M_N \exp\left(-\frac{Q_a}{RT}\right) \qquad \kappa = \frac{A}{c_s}\frac{Kink - c_i}{N'}$$

$$M = M_0 \frac{D_0 b_B^2}{kT} \exp\left(-\frac{Q_b}{RT}\right)\left(1 - \exp\left(-\left(\frac{\theta}{n}\right)^m\right)\right)$$

$$H(t) = \left[H(t_0)^{1/2} - C_0 \mu^{1/2} kT \ln\left(1 + \frac{t}{\tau_0}\right)\right]^2$$

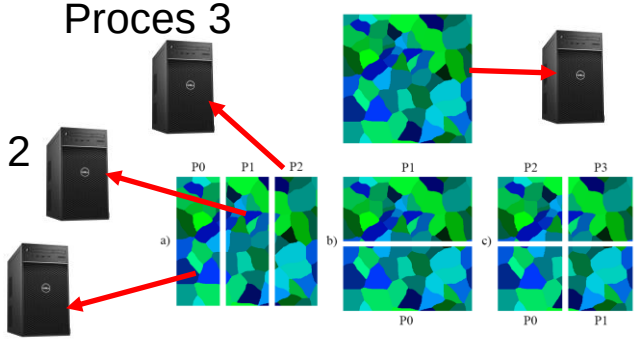


Modyfikacje wprowadzone do algorytmu

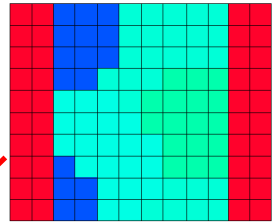
Proces 3

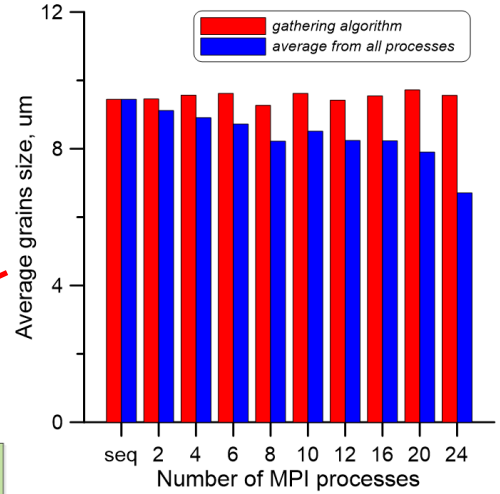
Proces 2

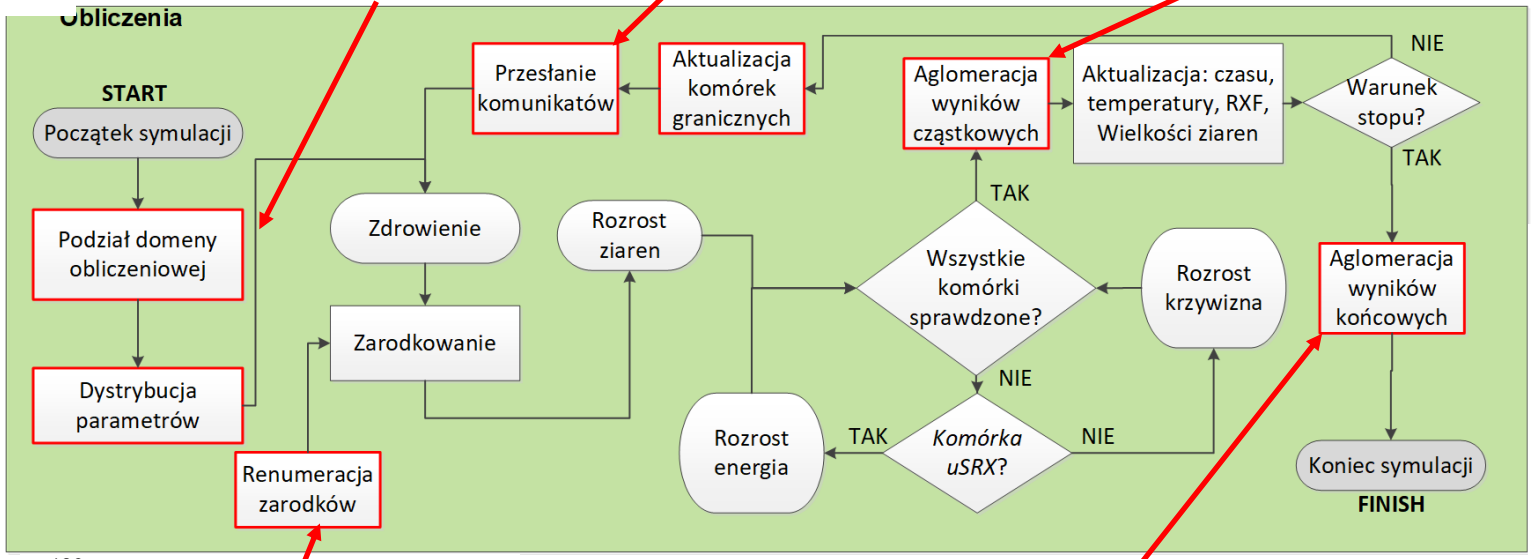
Proces 1



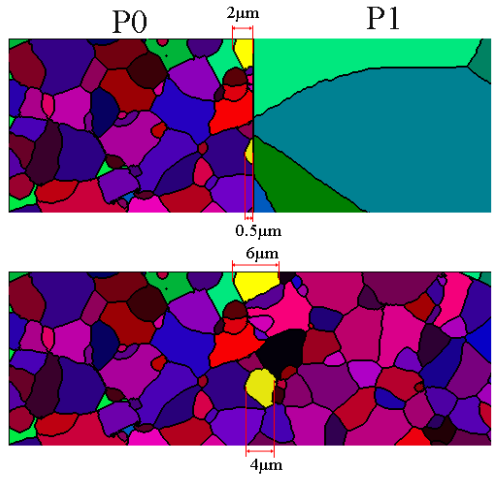
komunikacja





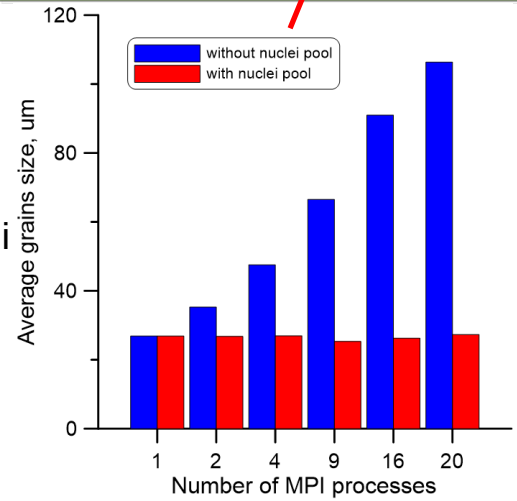


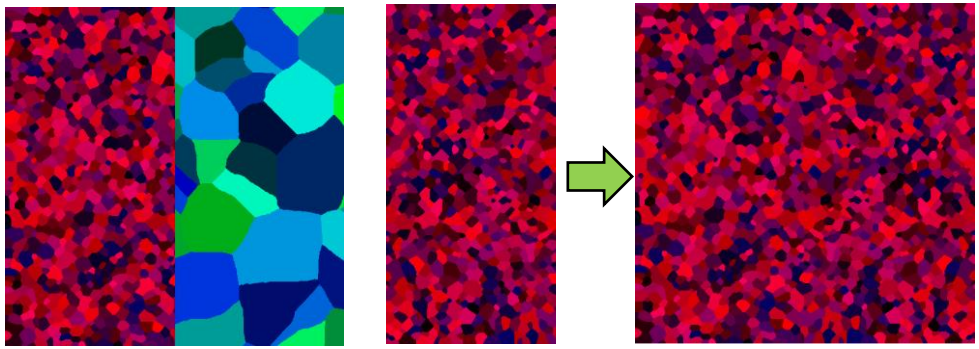
Zbieranie wyników artefakty



Cała mikrostruktura

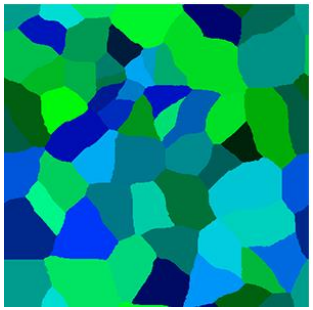
Brak renumeracji ziaren

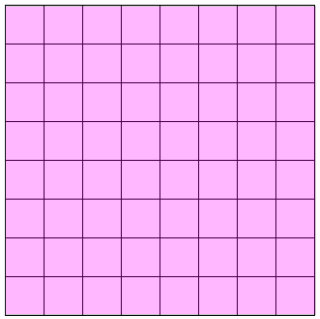


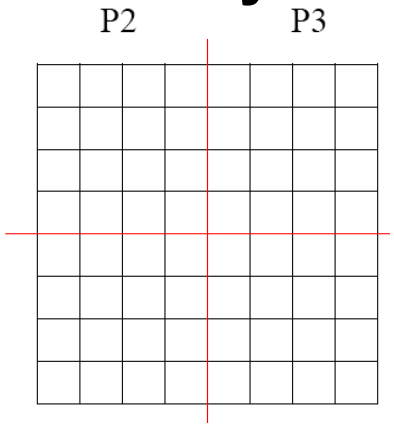


Zaimplementowane schematy zrównoleglenia

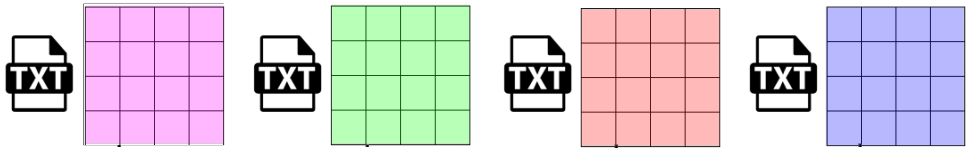
Master - slave

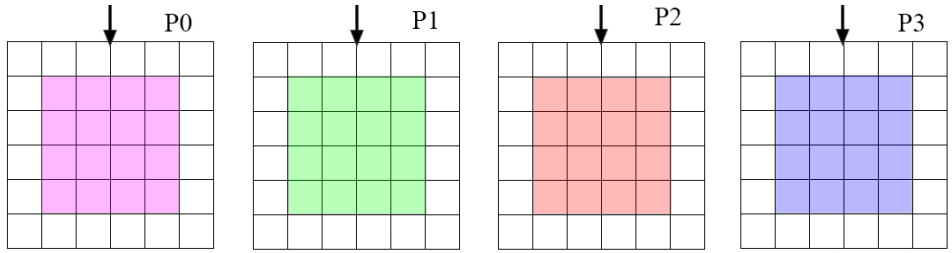


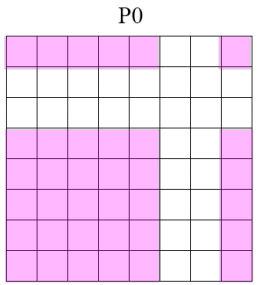


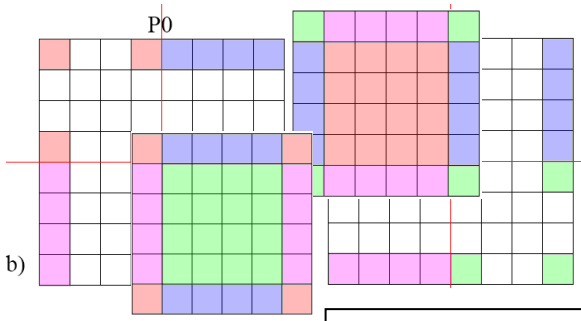


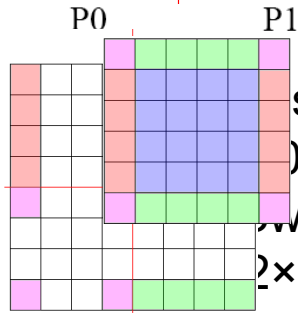
Slave - slave





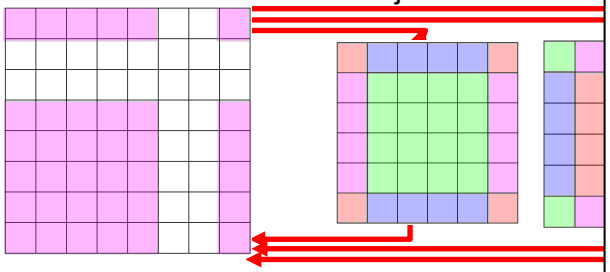






strze
)
w MPI.
2×2)

P0 komunikacja P1



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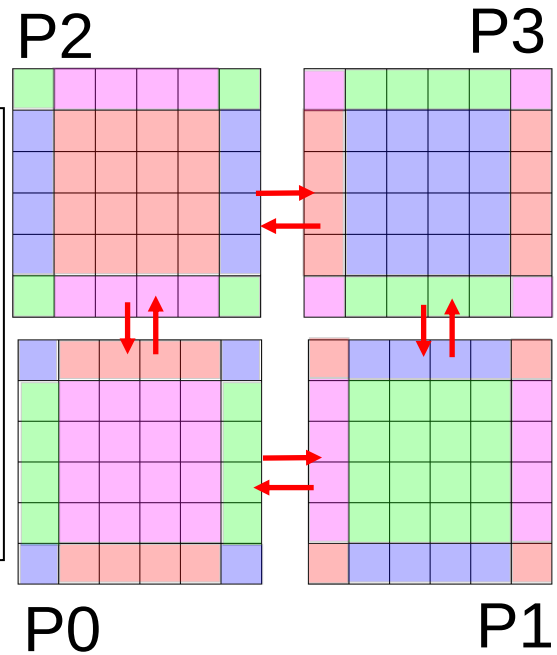
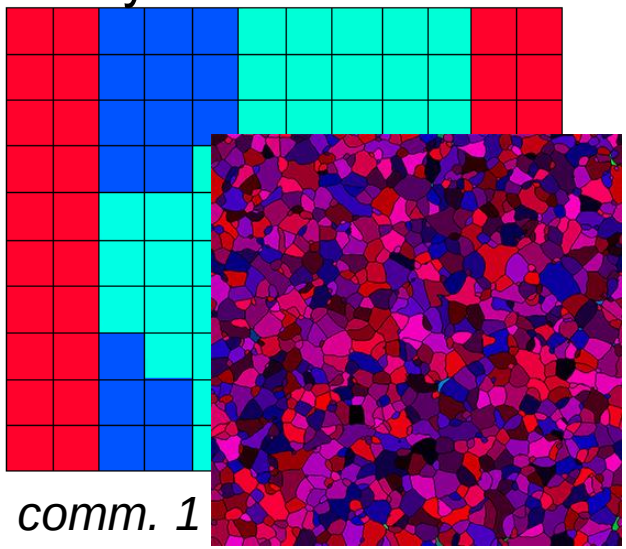


P0 P1

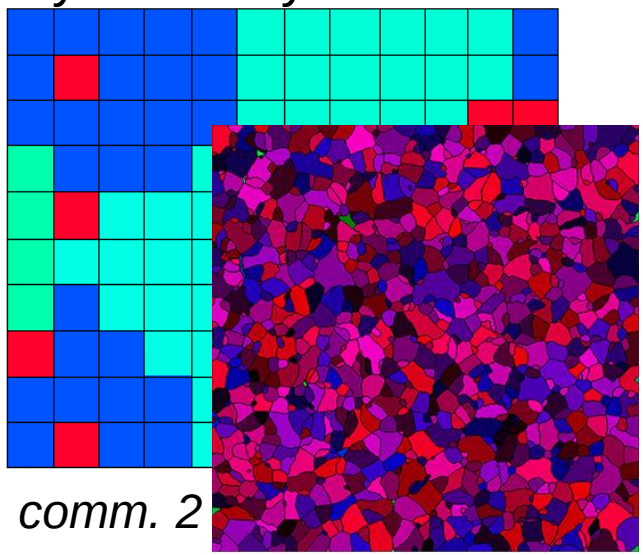
Rodzaje komunikacji pomiędzy procesami MPI

Wszystkie komórki



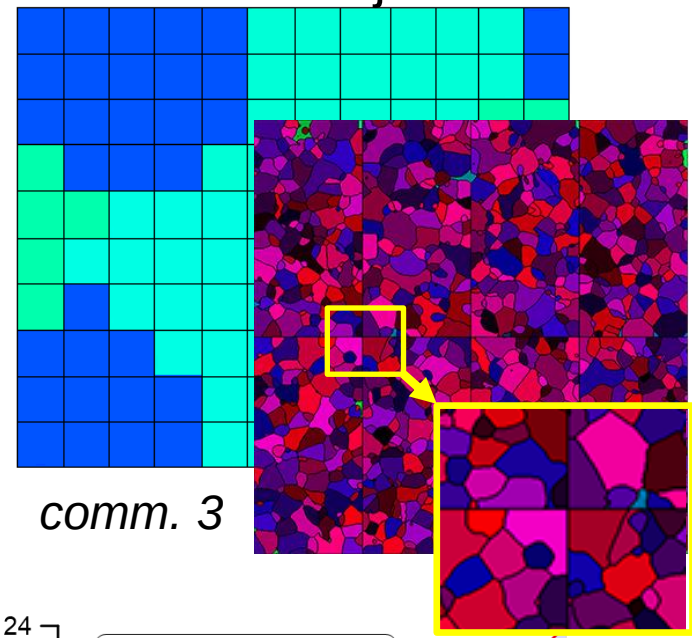
comm. 1

Tylko zrekrystalizowane

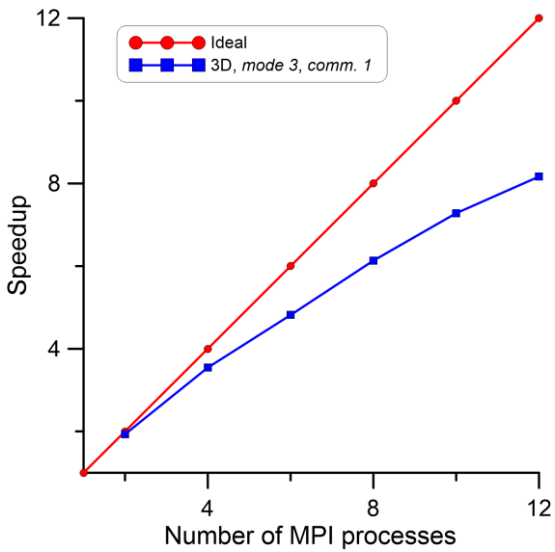


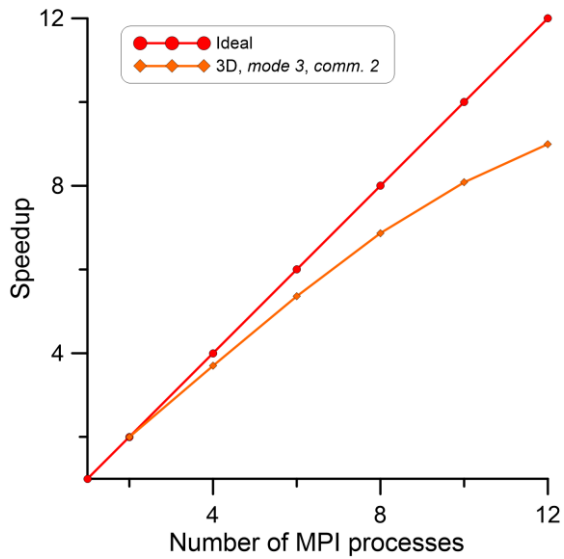
comm. 2

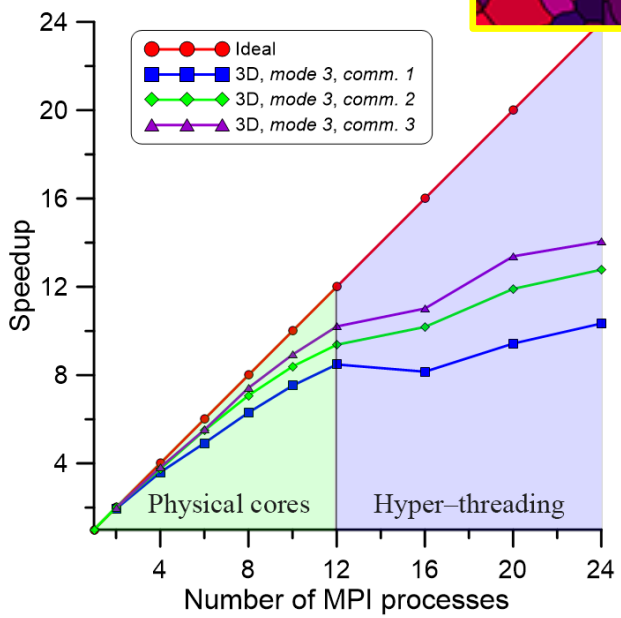
Bez aktualizacji



comm. 3

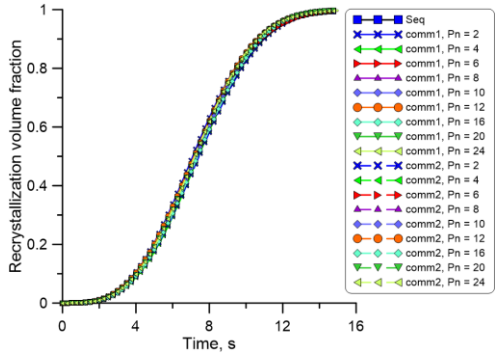


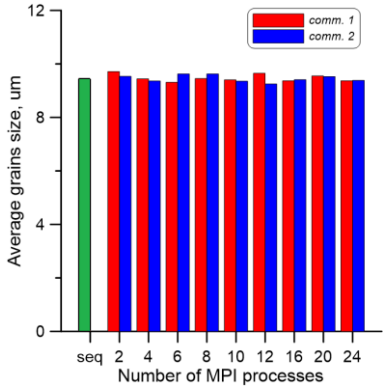


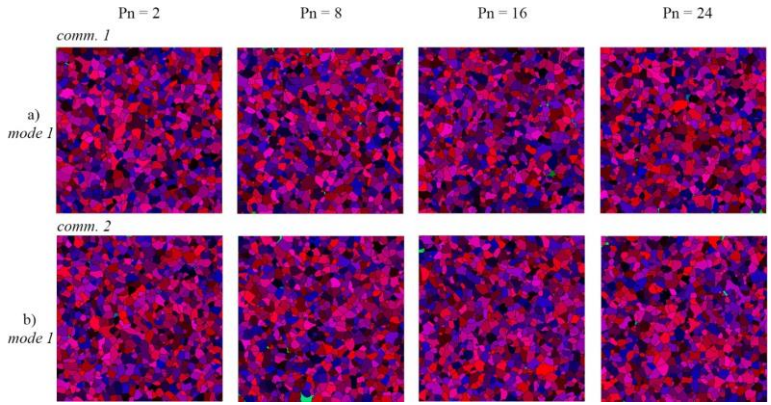


Weryfikacja zrównoleglenia

mode 1







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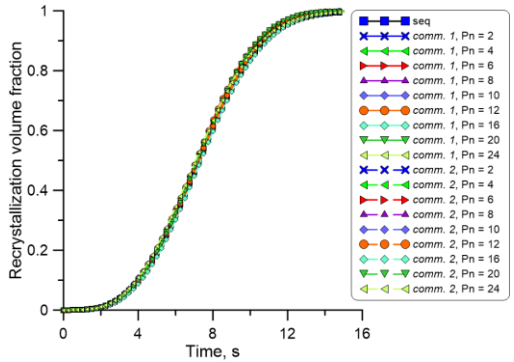
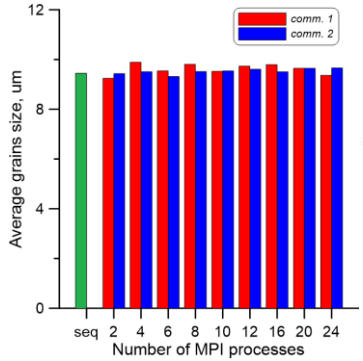
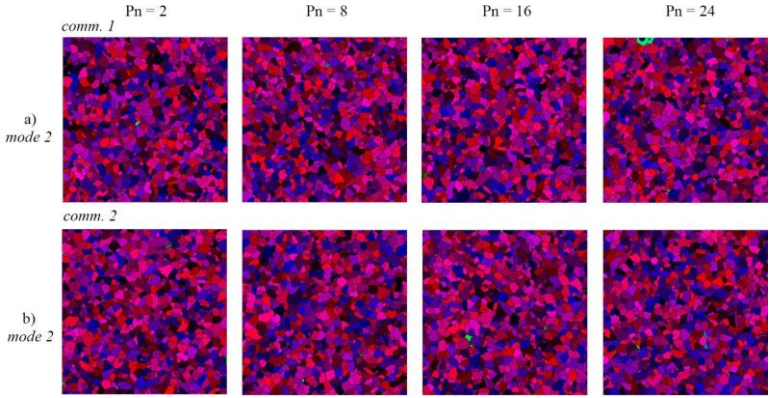
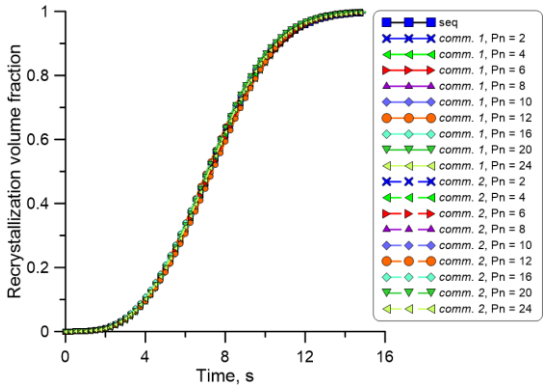
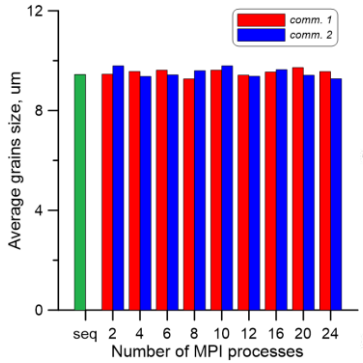


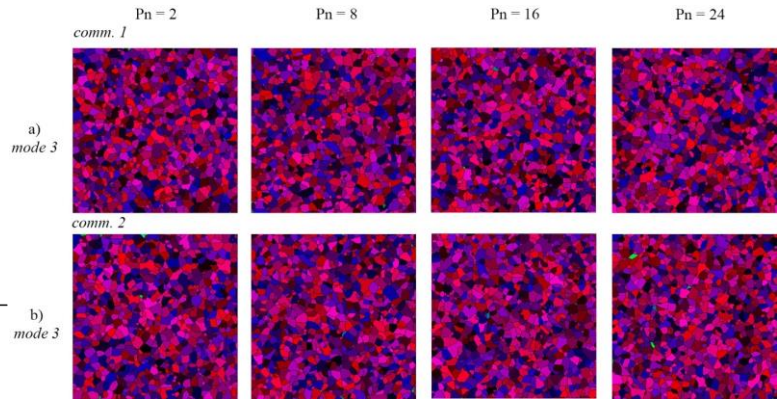


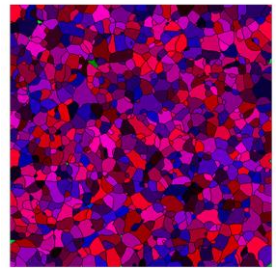


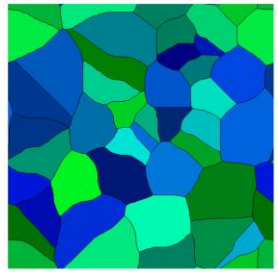
mode 3

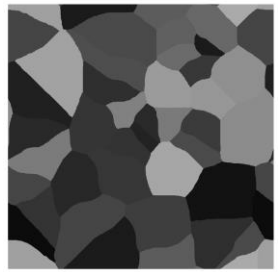


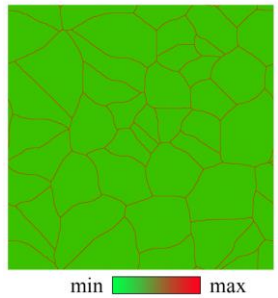








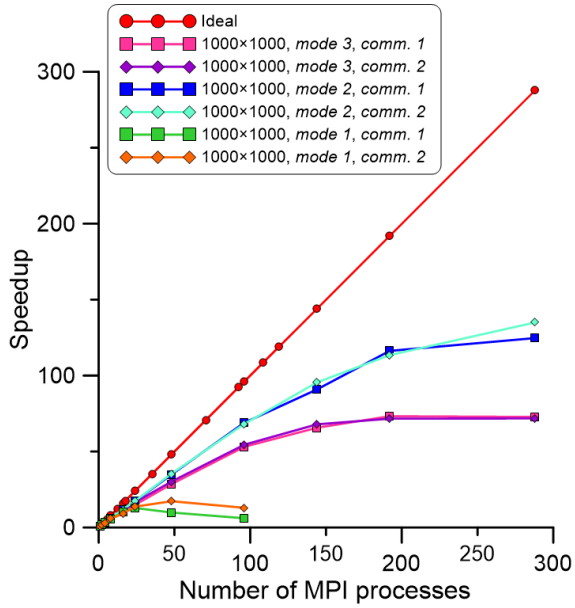


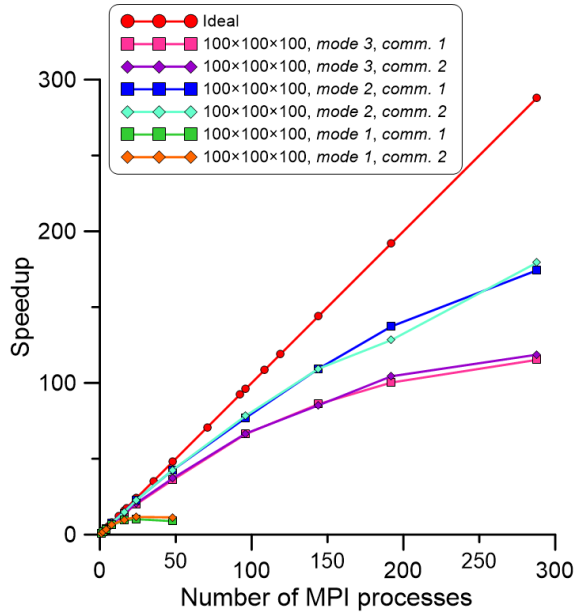


sekwencyjnie

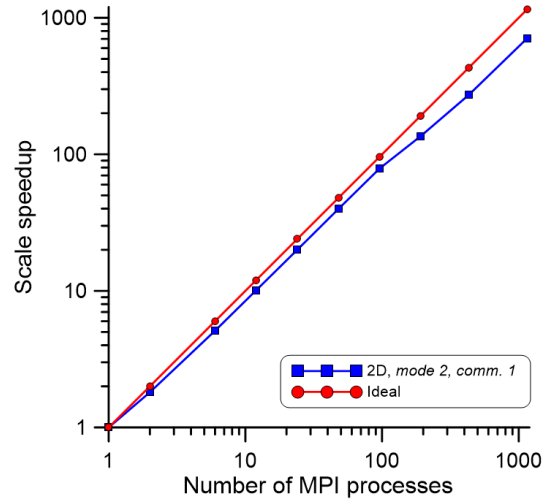
Analiza wydajności

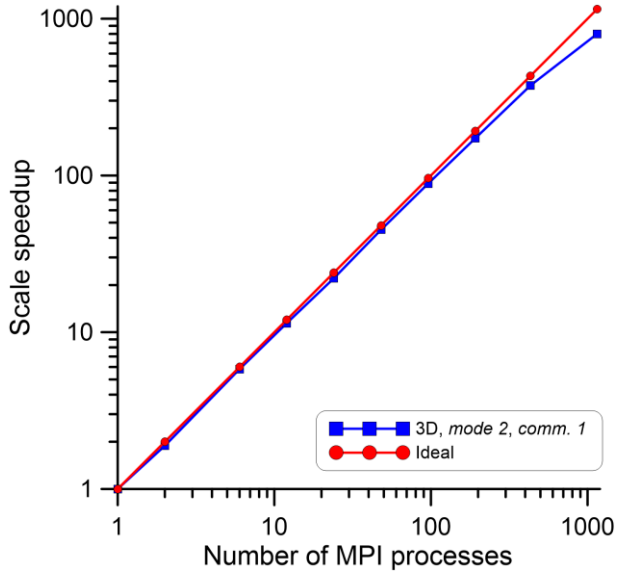
Testy jednostkowe dla
przestrzeni 1mln komórek CA





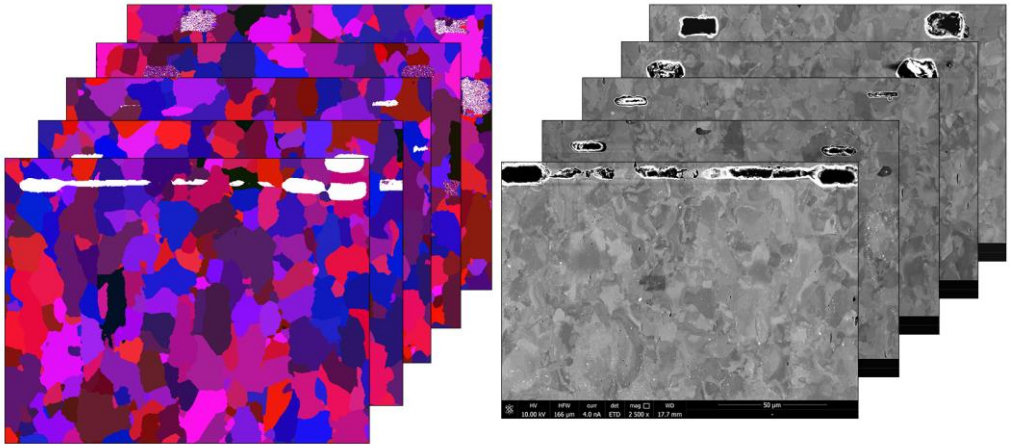
Wzrastający rozmiar
przestrzeni 1mln -1mld

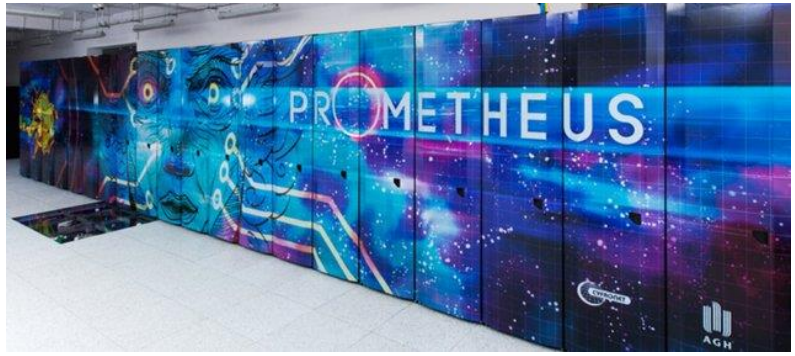




Praktyczne wykorzystanie

Dane wejściowe 10.4 GB

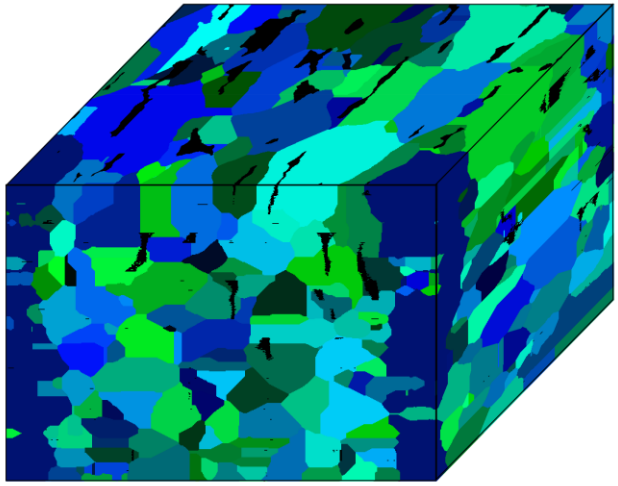




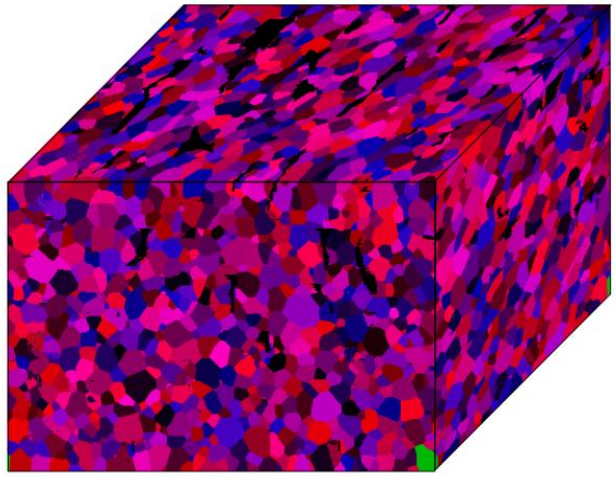
1200×700×808 komórek CA

150×87×101 μm

~5h (60 węzłów po 24 procesy)



SRX



M. Sitko, M. Mojzeszko, L. Rychlowski, G. Cios, P. Bala, K. Muszka, L. Madej, Procedia Manufacturing. 47 (2020) 1217–1222. https://doi.org/10.1016/j.promfg.2020.04.183.

Wnioski – model SRX

- Dane początkowe do symulacji CA powinny uwzględniać niejednorodności zarówno w energii zmagazynowanej podczas przeróbki plastycznej jak i morfologii mikrostruktury.

- Wykorzystanie cyfrowej reprezentacji materiału wraz z metodą elementów skończonych, pozwala odwzorować niejednorodność akumulacji energii w materiale podczas odkształcenia plastycznego, a tym samym pozwala uzyskać wiarygodne dane wejściowe do symulacji SRX zarówno w 2D jak i 3D.

- Uwzględnienie w symulacji takich parametrów jak lokalne wartości kątów Eulera, krzywizny granicy ziarna, zdrowienia czy też niejednorodności energii zmagazynowanej do wyznaczenia prędkości rosnących zrekrystalizowanych ziaren wyraźnie zmienia charakter rozrostu.

- W przypadku zaproponowanego podejścia z głównym procesem zarządzającym narzut na komunikacje jest tak duży, że powyżej 24 procesów czas symulacji diametralnie wzrasta, natomiast podejście z procesami równoważnymi jest najlepszym rozwiązaniem do symulacji z wykorzystaniem dużej liczby komórek CA.

- Opracowany model pozwala uzyskać przyspieszenie skalowalne na poziomie 700 razy dla przypadku 2D oraz ponad 800 razy dla wariantu 3D, jest to kluczowe dla przyszłego wykorzystania takich modeli w praktyce przemysłowej.

- Przy użyciu opracowanego modelu możliwa jest wydajna symulacja najważniejszych mechanizmów procesu rekrystalizacji z wykorzystaniem ponad miliarda komórek CA, zapewnia to perspektywę symulacji przestrzeni 3D z dużą liczbą ziaren w szerokim zakresie ich początkowego rozmiaru.

Dziękuję za uwagę

dr inż. Mateusz Sitko

msitko@agh.edu.pl