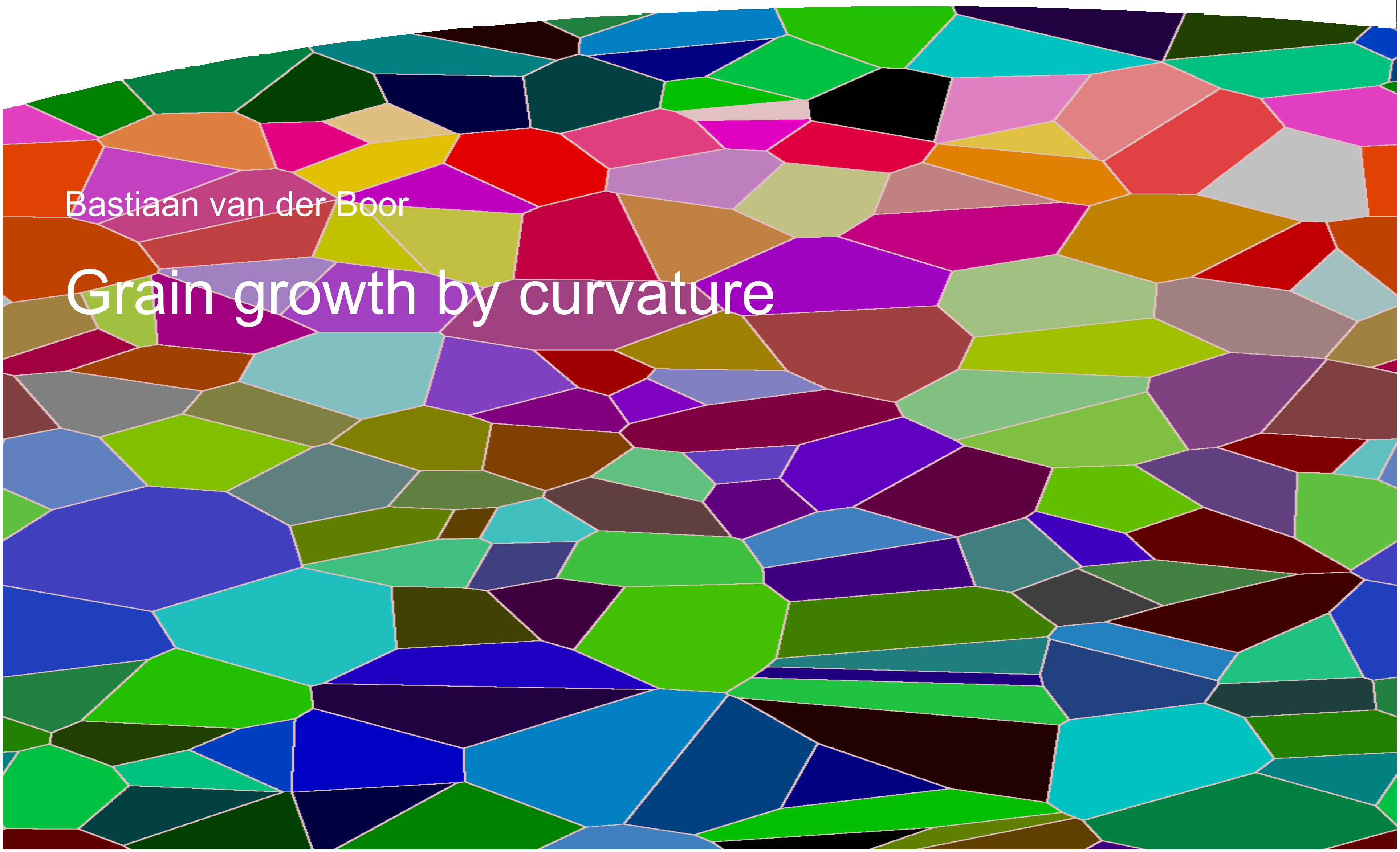
Bastiaan van der Boor

Grain growth by curvature

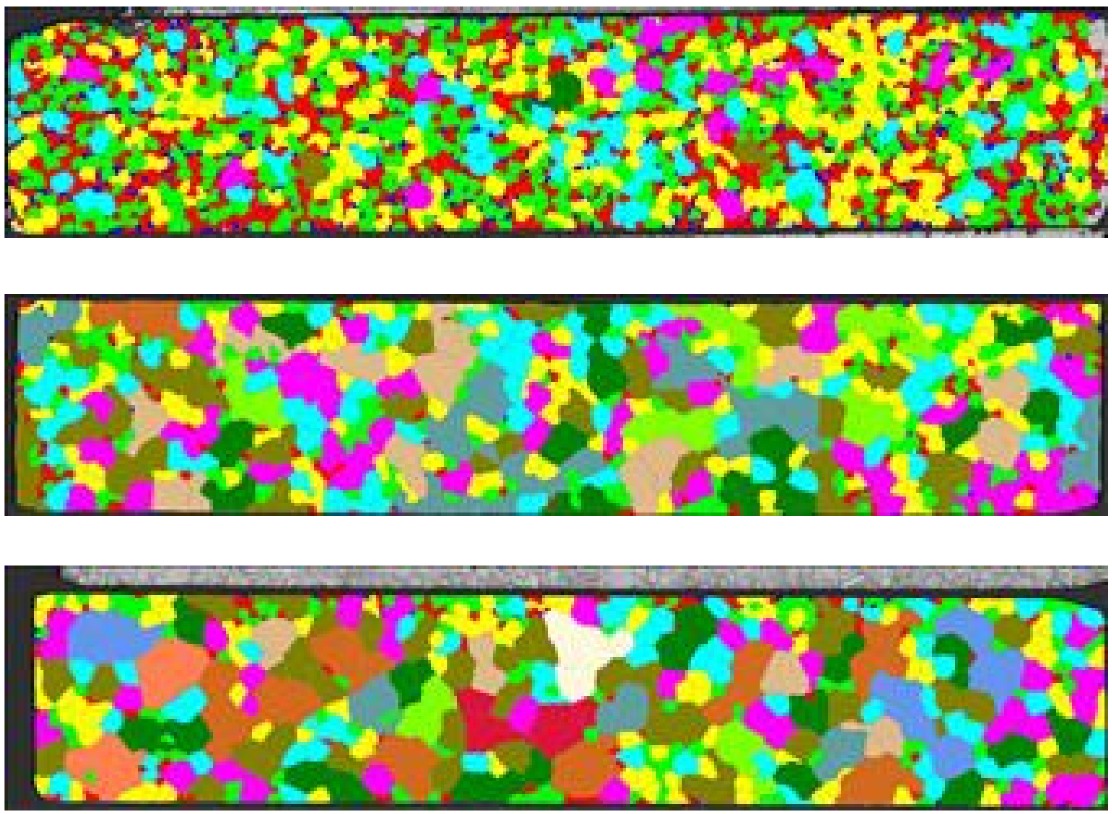


Content

Micro-structure

Micro-structure determines the mechanical properties of steel

Example of grain growth in a micro-structure of austenite at 1200°C



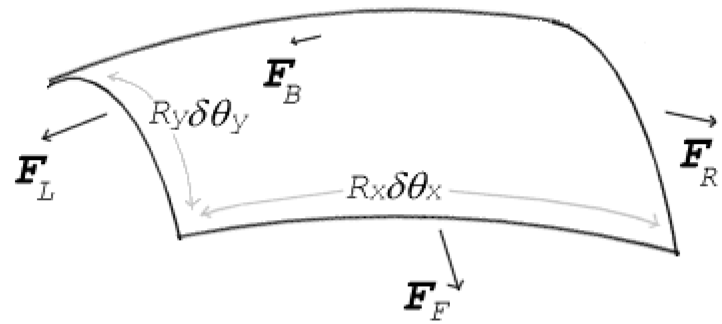
Three processes that determines the micro-structure

Goal of this master thesis is to extend the existing model of Tata Steel with grain growth by curvature

1. Phase transformations ✓
   - Austenite to ferrite transformation
2. Recrystallization & Recovery ✓
   - Austenite to austenite
3. Grain growth by curvature **T.B.D.**
   - Austenite to austenite

Soap froth

The growth of metal grains is similar to soap bubbles



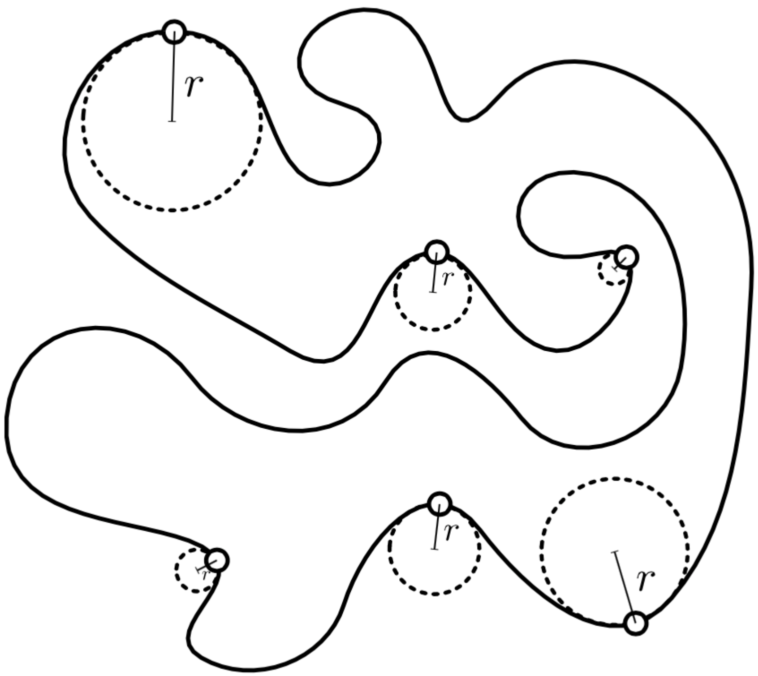
Young-Laplace equation

$$\Delta G = \gamma\left(\frac{1}{R_x} + \frac{1}{R_y}\right)$$

$$\Rightarrow \quad v = \alpha M \frac{2\gamma}{R_x}$$

Curvature

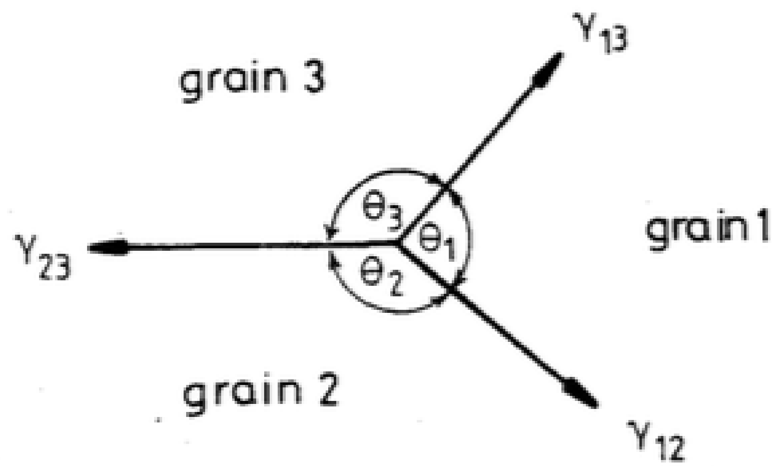
An arbitrarily simple, closed curve with a point P on it, there is a unique circle which most closely approximates the curve near P



$$\kappa = \frac{1}{R}$$

Triple points, where three grains meet

Every triple point seeks it equilibrium state, which depends on the grain boundary energy γ



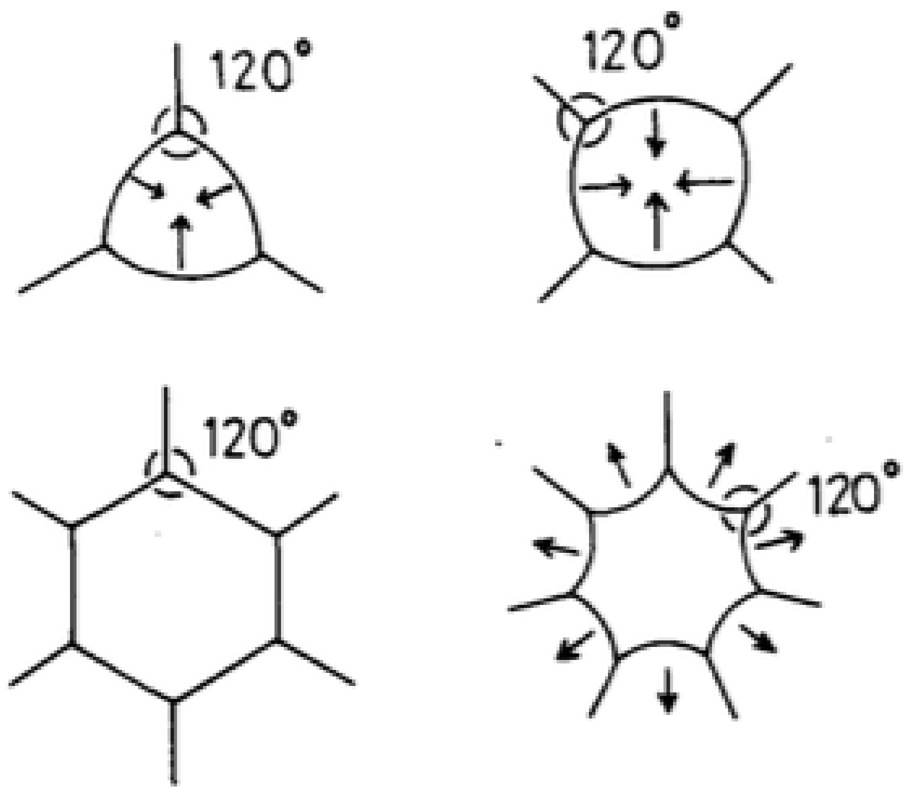
$$\gamma_{12} = \gamma_{13} = \gamma_{23}$$

Equilibrium if $\theta_i = 120^\circ \quad i = 1,2,3$

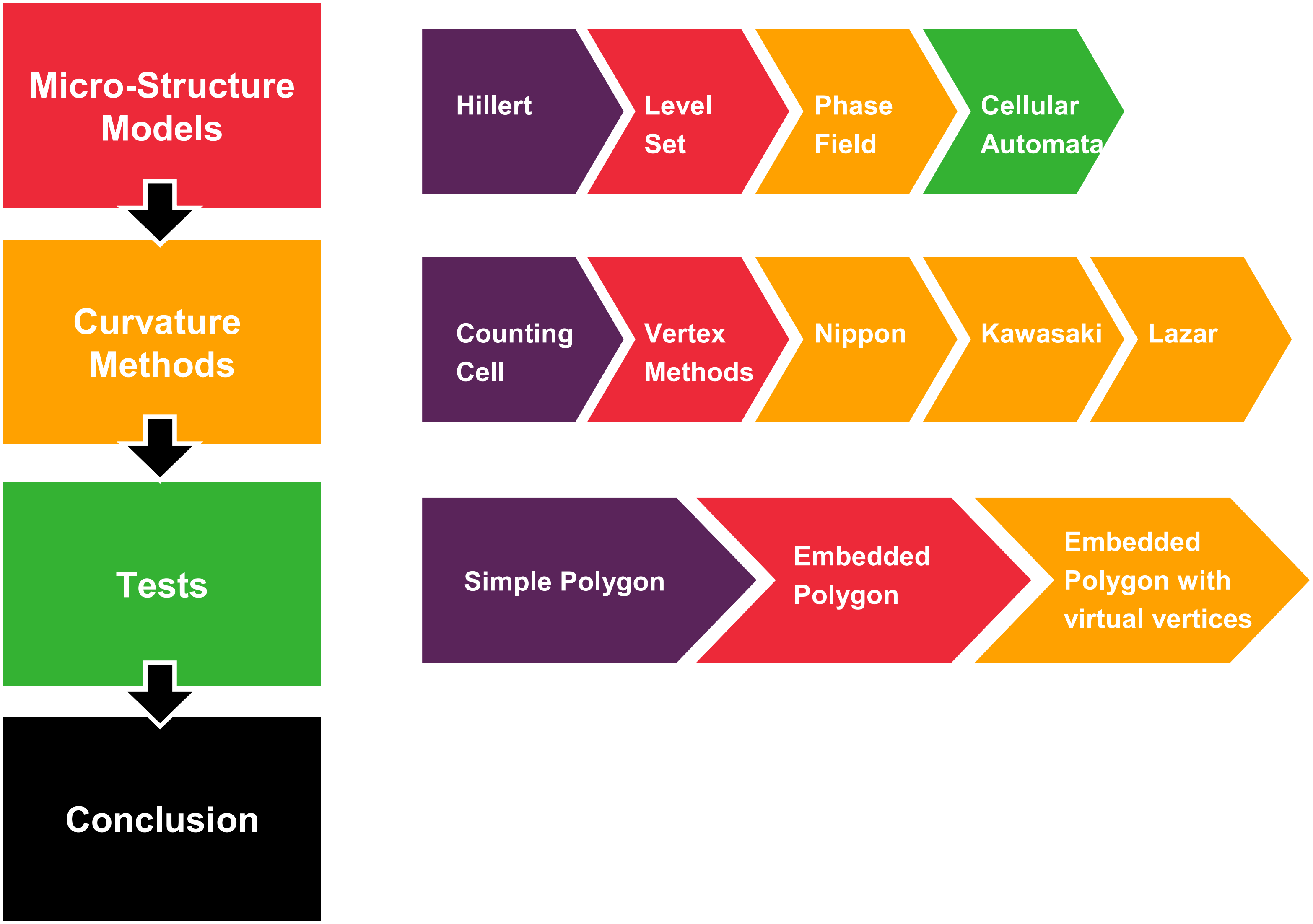
Examples

A grain with 6 corners is in equilibrium state if the angle is 120 degrees

Two vertices determine the curvature of a grainboundary



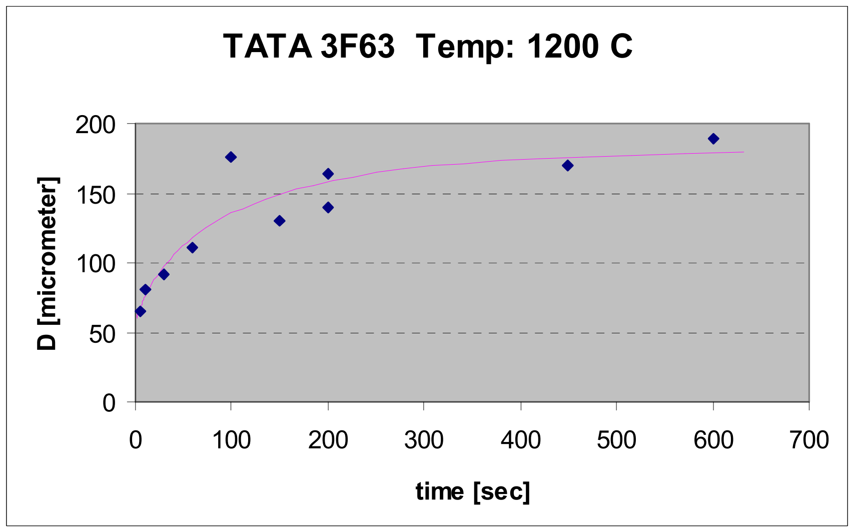
Structure of Literature Study



Hillert

A very good approximation of the average grain size distribution

Assumption

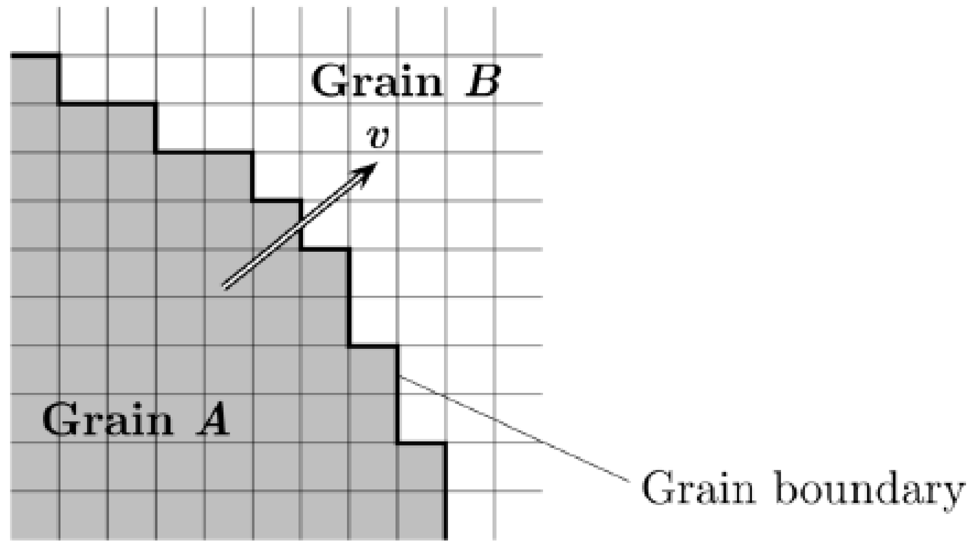


Grain Size Distribution (GSD)

$$P(u) = (2e)^{\beta} \frac{\beta u}{(2-u)^{2+\beta}} \exp\left(\frac{-2\beta}{2-u}\right)$$

Cellular Automata

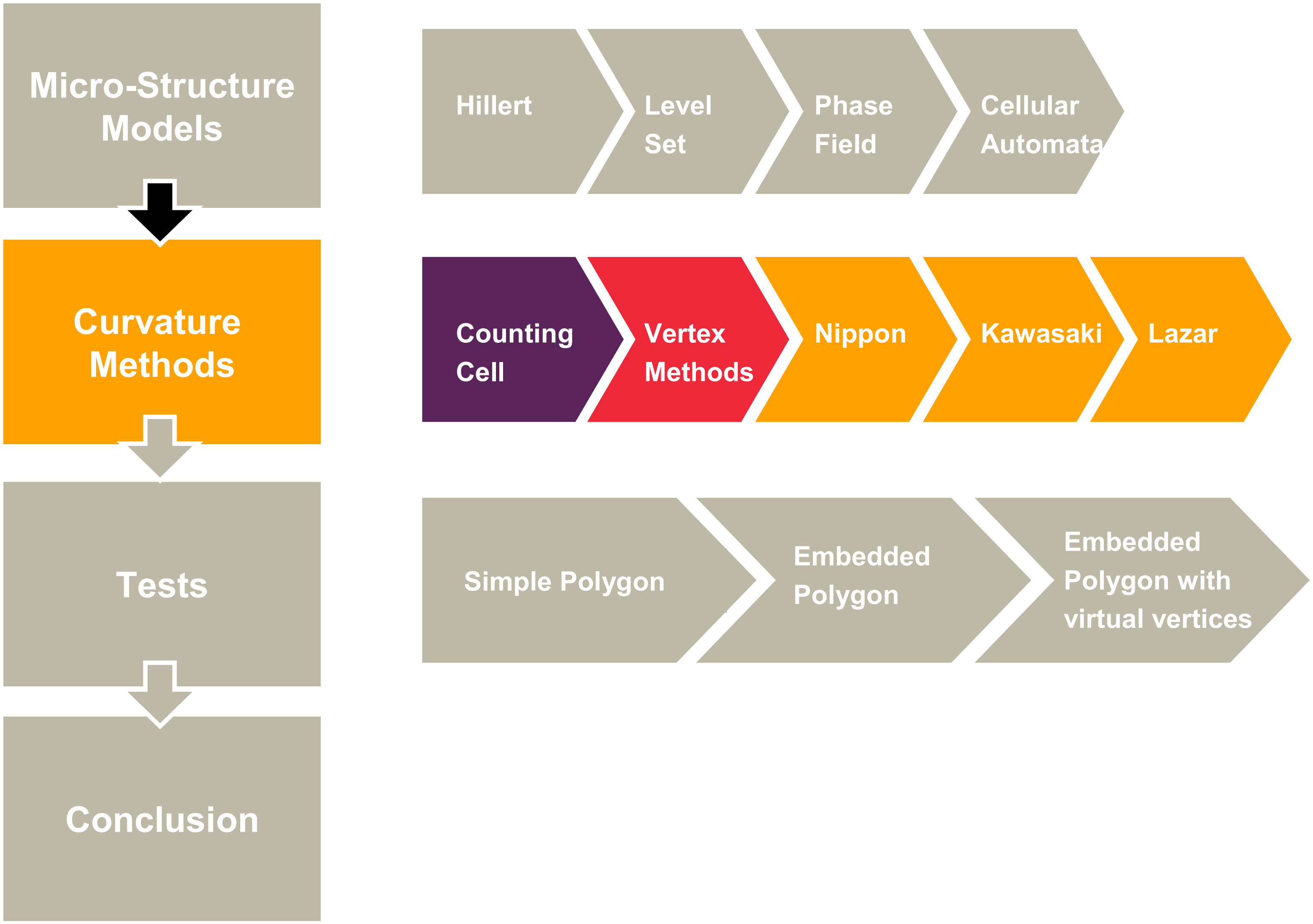
CA model first developed by John von Neumann



Each cell has assigned a

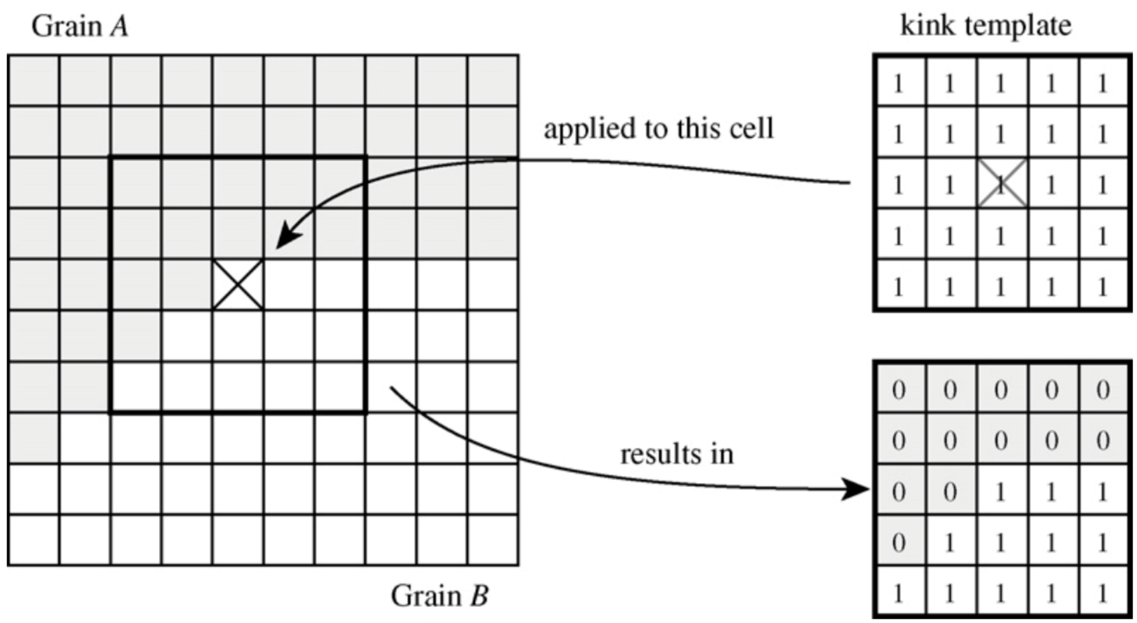
- State
- Neighborhood definition
- Transformation rule

Structure of Literature Study



Counting cell method

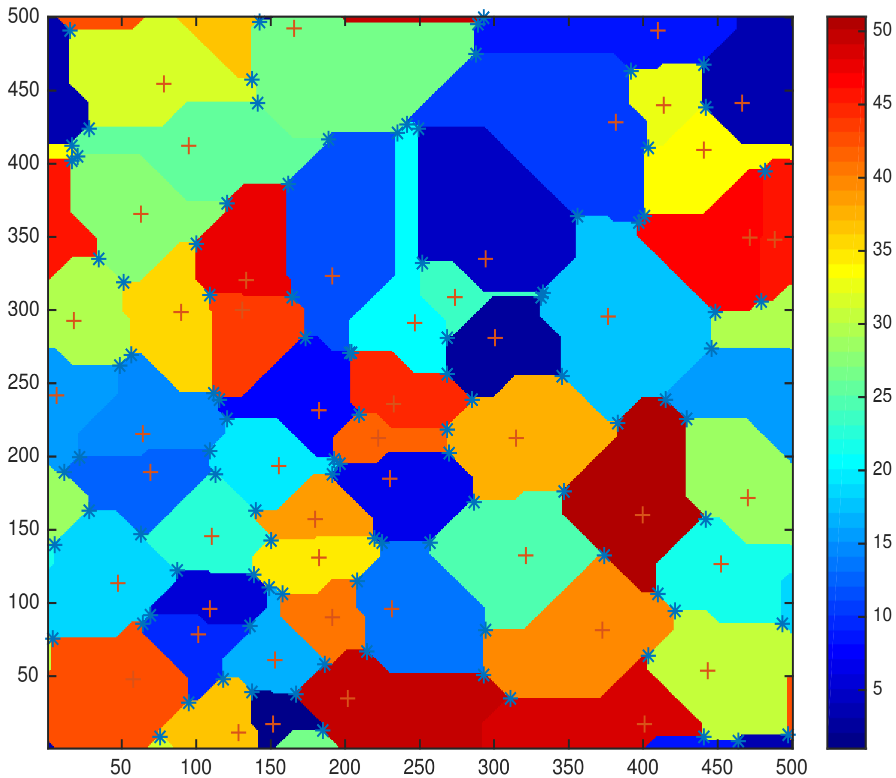
Due to the sharp interface, interpolation is needed. Hence, a lot of calculations have to be made



Computational costly

Vertex method

Using vertices is the most efficient method to calculate the effect of curvature



Advantages

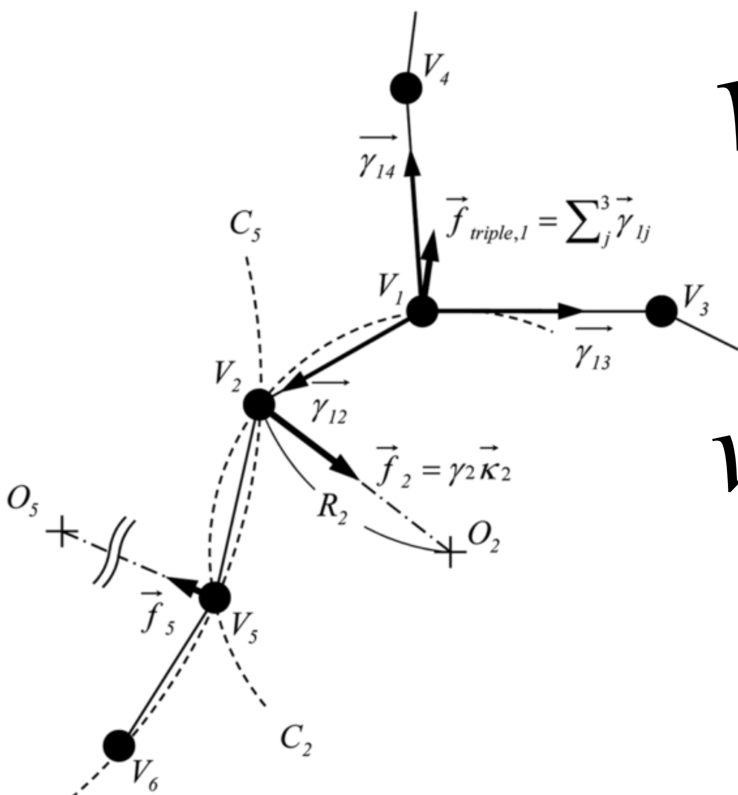
- Less points are needed to calculate
- Vertex points are most influential in grain growth
- When more points are needed, virtual vertices can be added

A hybrid model

- Run CA model
- Extract vertices
- Run vertex method
- Update states using the position of the vertices

Vertex by Nippon Steel

Method that is heavily dependent on the specific grain boundary energy



$$v_{virtual,i} = M\gamma_i \kappa_i$$

$$v_{triple,i} = M\sum_{j=1}^{3}\gamma_{ij}\frac{r_{ij}}{\left\| r_{ij} \right\|}$$

Vertex method based on Minimization of Grain Boundary Energy (1/2)

Method first introduced by Kawasaki (1952), based on idea from Phase Field Method

Dissipation Energy + Potential Energy = 0

$$\frac{1}{2}\int_{GB} \frac{v(s)^2}{M_{GB}} ds + \int_{GB} \gamma(s) ds = 0$$

Minimize energy over position

Vertex method based on Minimization of Grain Boundary Energy (2/2)

Governing equations

$$D_i v_i = f_i - \frac{1}{2}\sum_j^{(i)} D_{ij} v_j$$

$$D_{ij} = \frac{1}{3M_{ij}\left\|r_{ij}\right\|}\begin{bmatrix} {y_{ij}}^2 & -x_{ij}y_{ij} \\ -x_{ij}y_{ij} & {x_{ij}}^2 \end{bmatrix}$$

$$D_i = \sum_j^{(i)} D_{ij}$$

$$f_i = \sum_j^{(i)} \gamma_{ij} \frac{r_{ij}}{\left\|r_{ij}\right\|}$$

Neumann-Mullins (1/3)

2D Neumann-Mullins (1956) revived by expansion to 3D in 2007 by MacPherson and Srolovitz

2D: Neumann-Mullins

- Closed curve, enclosing area grows with the same rate
- Growth of a grain enclosed by others:

$$\frac{dA}{dt} = -M\gamma \frac{\pi}{3}(6-n)$$

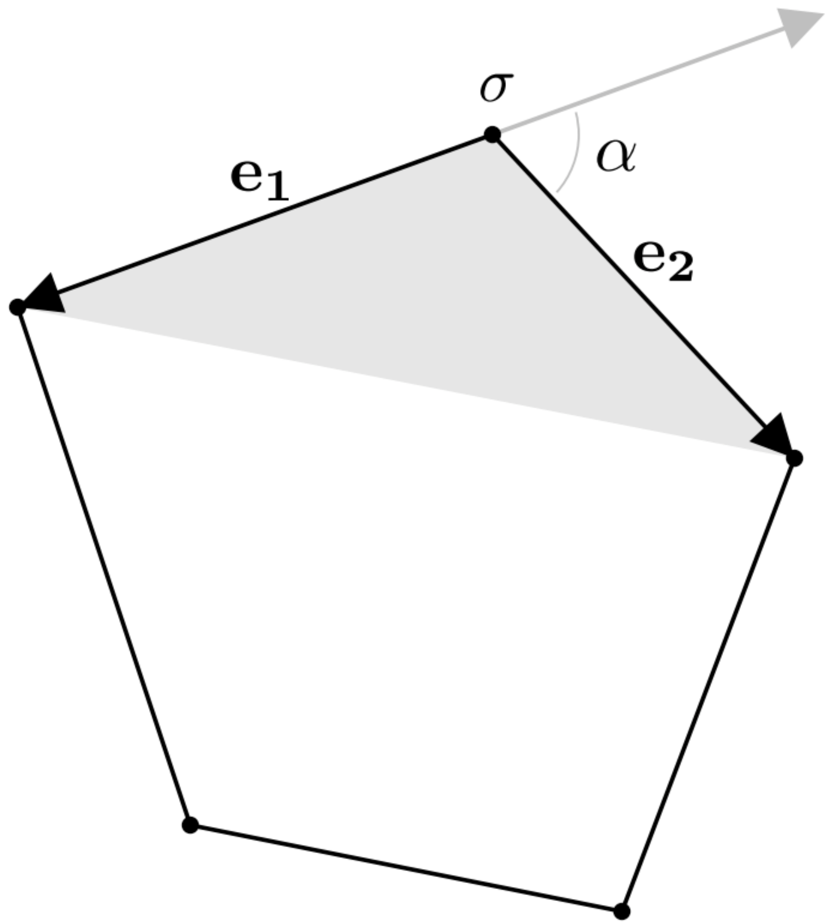
3D MacPherson & Srolovitz

- Grain growth of a grain in 3D:

$$\frac{dV(\mathbf{D})}{dt} = -2\pi M\gamma \left(\mathcal{L}(\mathbf{D}) - \frac{1}{6}\sum_i e_i(\mathbf{D})\right)$$

Neumann-Mullins (2/3)

Governing equation of a virtual vertex (arbitrary point between only two grains), satisfies Neumann-Mullins relation

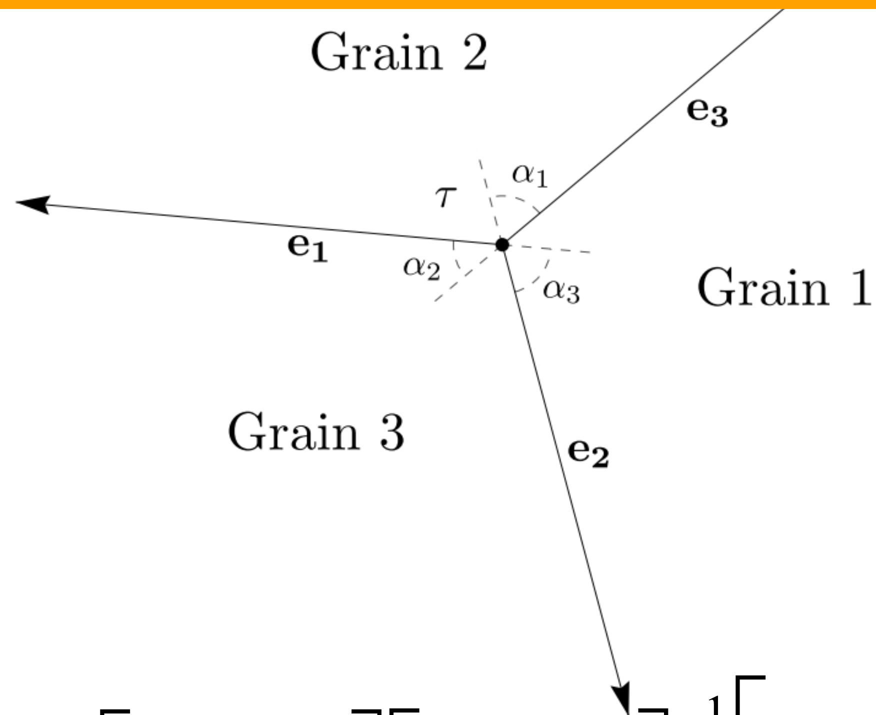


$$v_i = \alpha M \gamma \Delta t \frac{e_1 + e_2}{|e_1 \times e_2|}$$

$$\sum_{i=1}^{n} \alpha_i = 2\pi$$

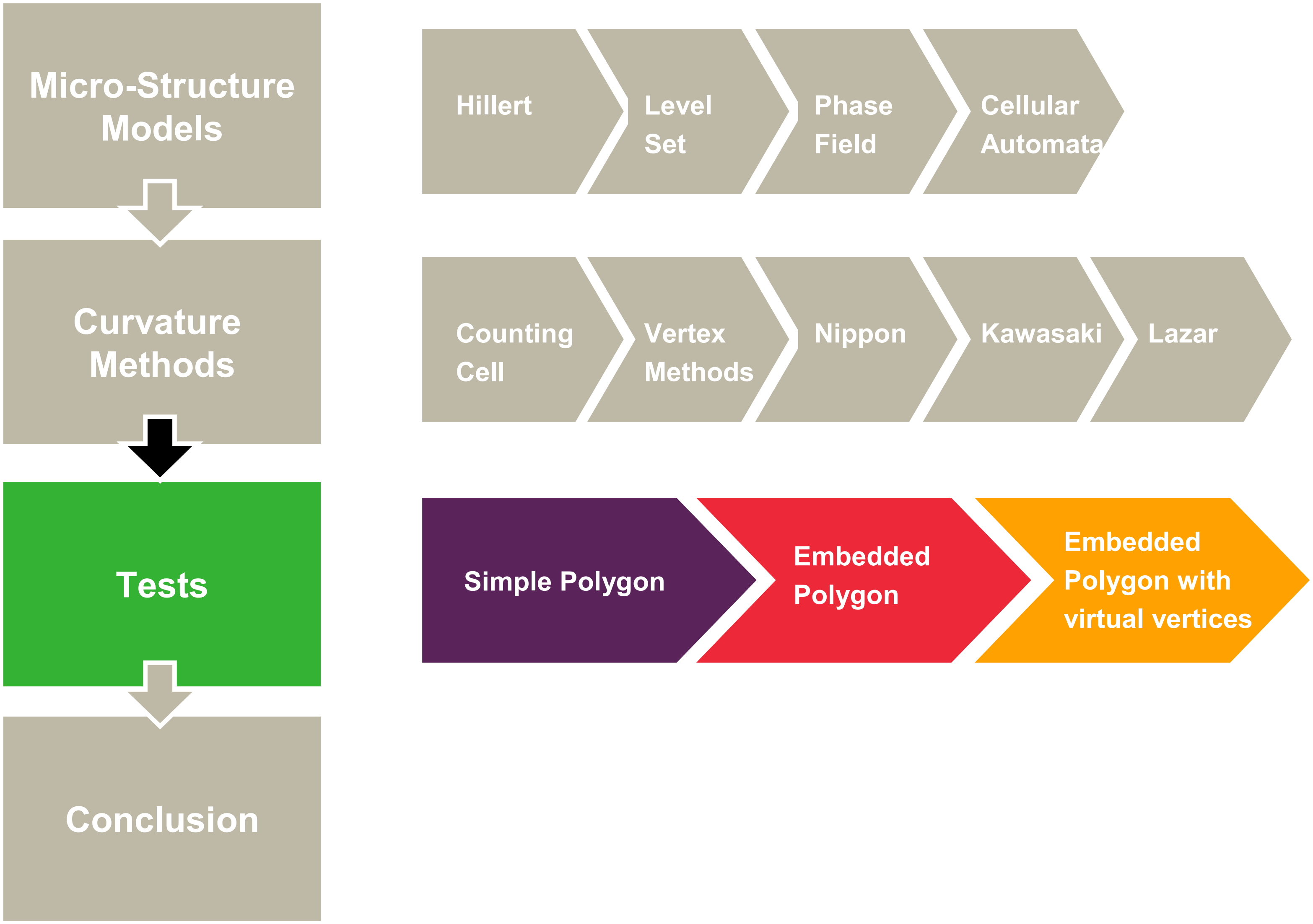
Neumann-Mullins (3/3)

Governing equations of a triple point, who satisfy the Neumann-Mullins relation



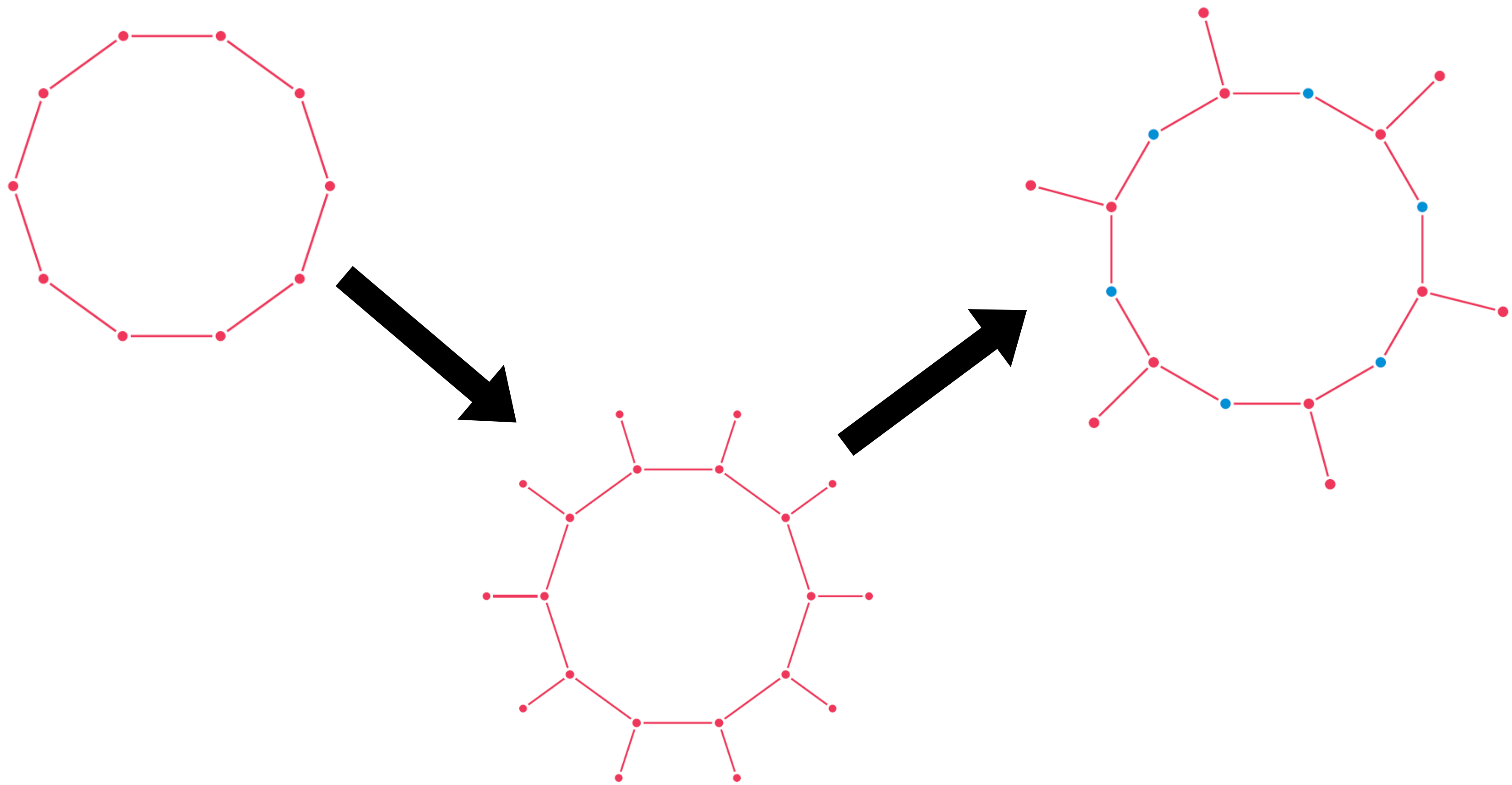
$$v_i = 2M\gamma\Delta t \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} e_1 - e_2 \\ e_2 - e_3 \end{bmatrix}^{-1} \begin{bmatrix} \alpha_1 - -\pi/3 \\ \alpha_2 - -\pi/3 \end{bmatrix}$$

Structure of Literature Study



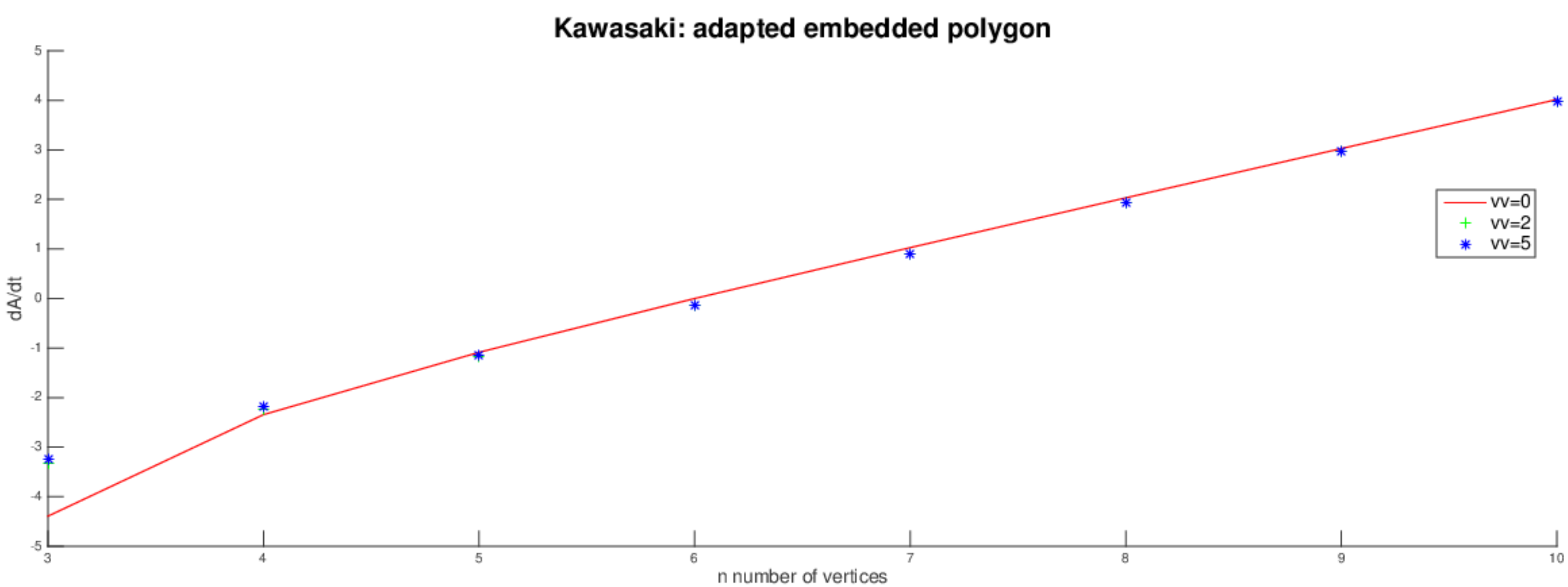
Tests

Three polygon have been constructed to test the different methods on their performance



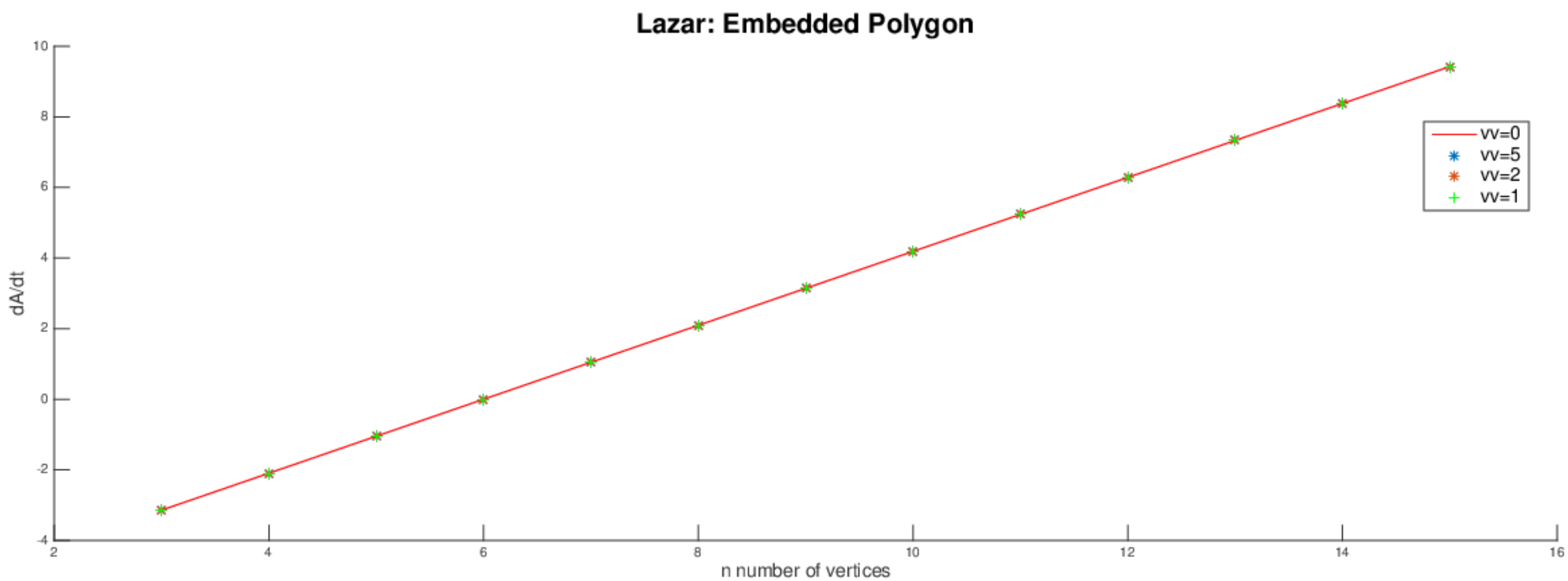
Results (1/3)

Embedded Polygon: Kawasaki vs exact Neumann-Mullins relation



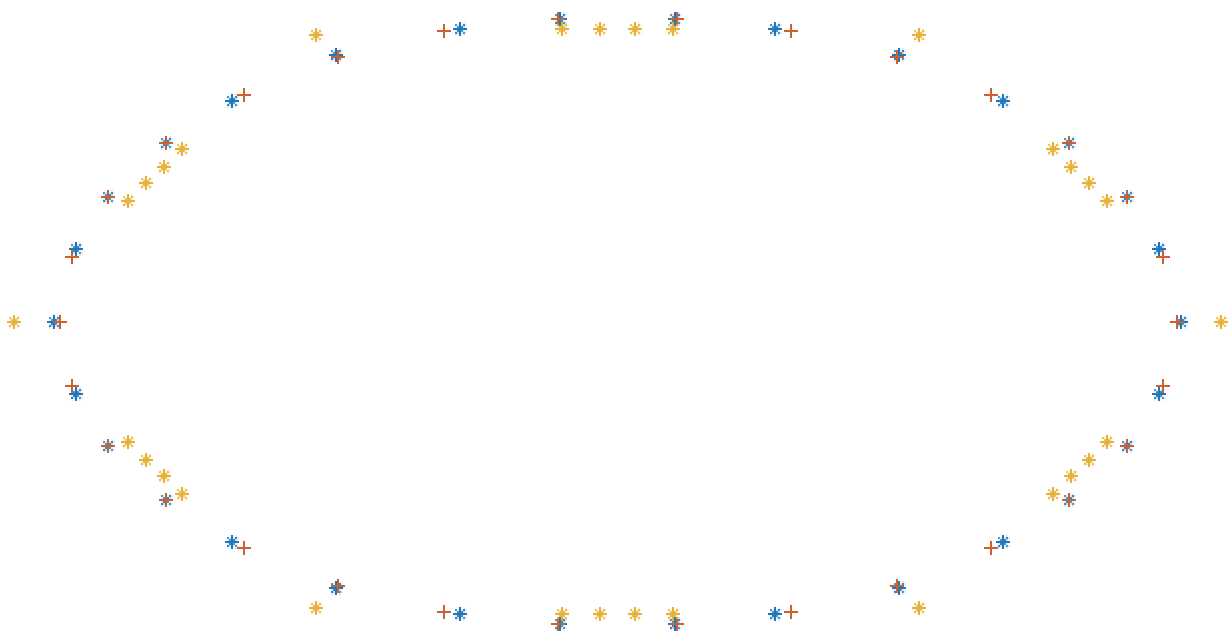
Results (2/3)

Embedded Polygon: Lazar vs exact Neumann-Mullins relation



Results (3/3)

Problem in Kawasaki: the connection of a triple point with a virtual vertex



Overview & Conclusion

The method by Lazar shows the best results

Method	Computation time	Circle	Neumann-Mullins n=6	NM, variable n, virtuals on a straight line	NM variable n virtuals virtues on the circle
Counting Cell	**--**	?	?	?	?
Vertex methods:					
Nippon	**++**	**+**	**--**	**--**	**--**
Kawasaki	**++**	**+/-**	**++**	**+**	**--**
Lazar	**++**	**++**	**++**	**++**	**++**

Further Research

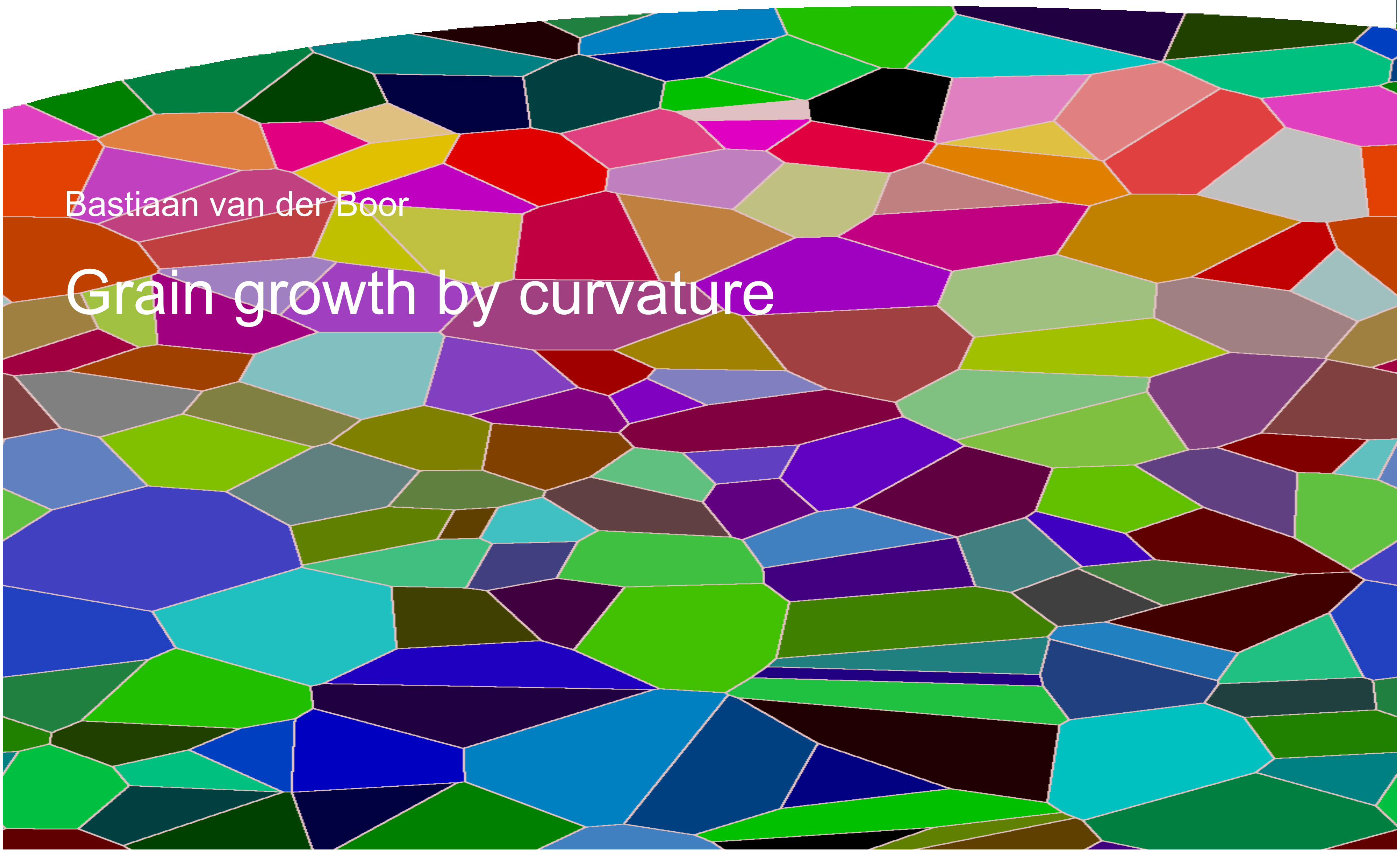
Ready to implement in cellular automata model of Tata Steel

- Implementation of 2D and 3D in cellular automata model of Tata Steel
  - Extract vertices from CA grid
  - Solve motion equations for vertices
  - Update CA grid from vertices motion
- Anisotropic variant of Lazars method

TATA STEEL

TU Delft

TATA



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