Discrete Multiscale Modelling and Future Research Plans concerning Metals

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My CV

Eindhoven University of Technology (Ron Peerlings & Marc Geers)

10 years PhD, MSc (cum laude), BSc (cum laude)

Mechanics of Materials, Mechanical Engineering

Cardiff University (Pierre Kerfriden & Stephane Bordas)

1.5 years Assistant Prof, Institute of Mechanics & Advanced Materials

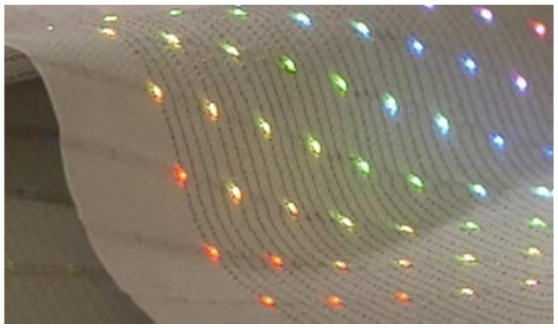
University of Luxembourg (Hussein Rappel, Jack Hale, Stephane Bordas)

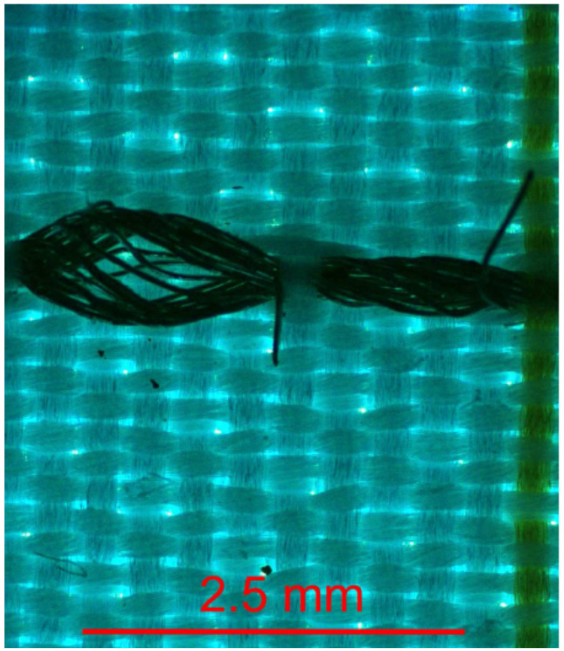
4 months Research Fellow, Computational Mechanics

Outline

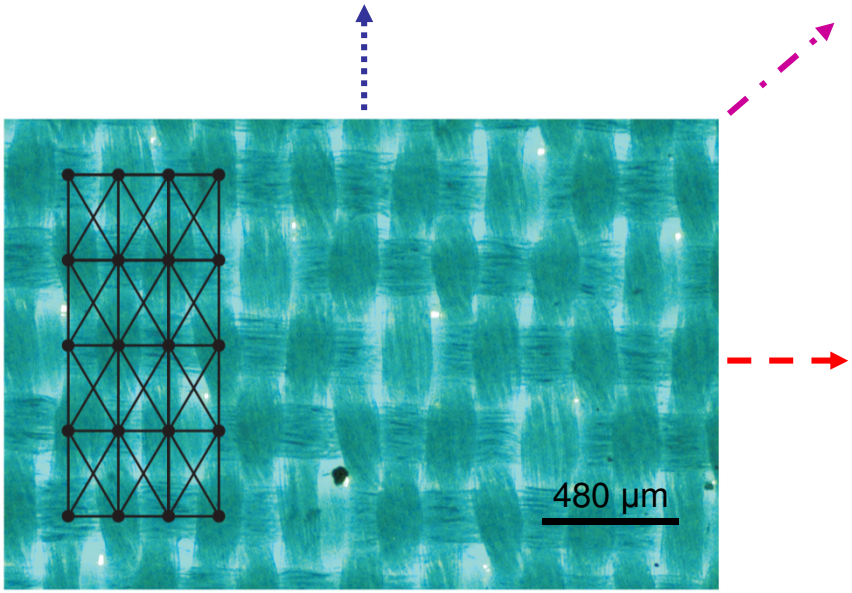
1. Discrete multiscale models for fibrous materials
2. Discrete multiscale models for metals
3. Future research plans for metals

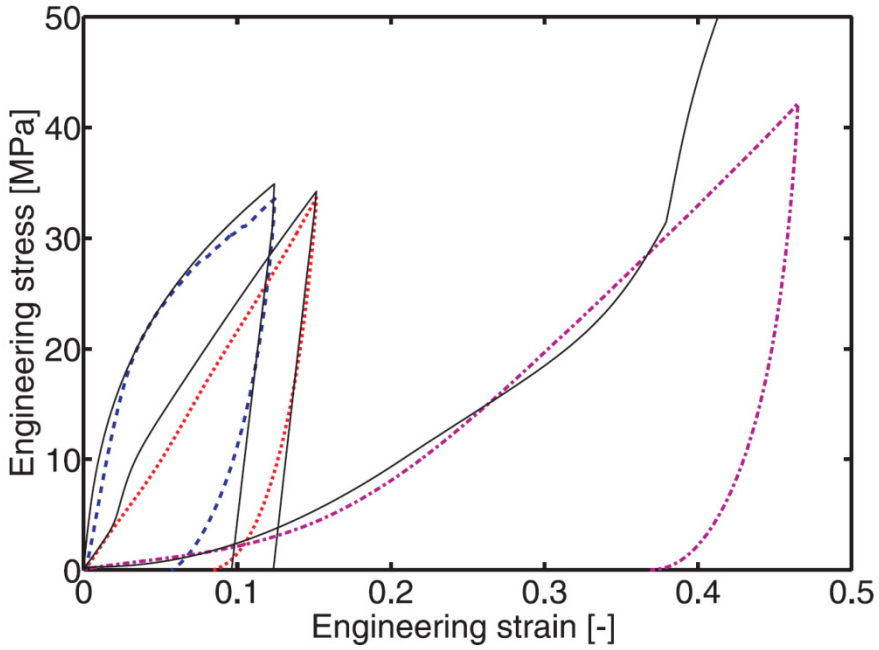
Fibrous material 1: electronic textile





Fibrous material 1: electronic textile





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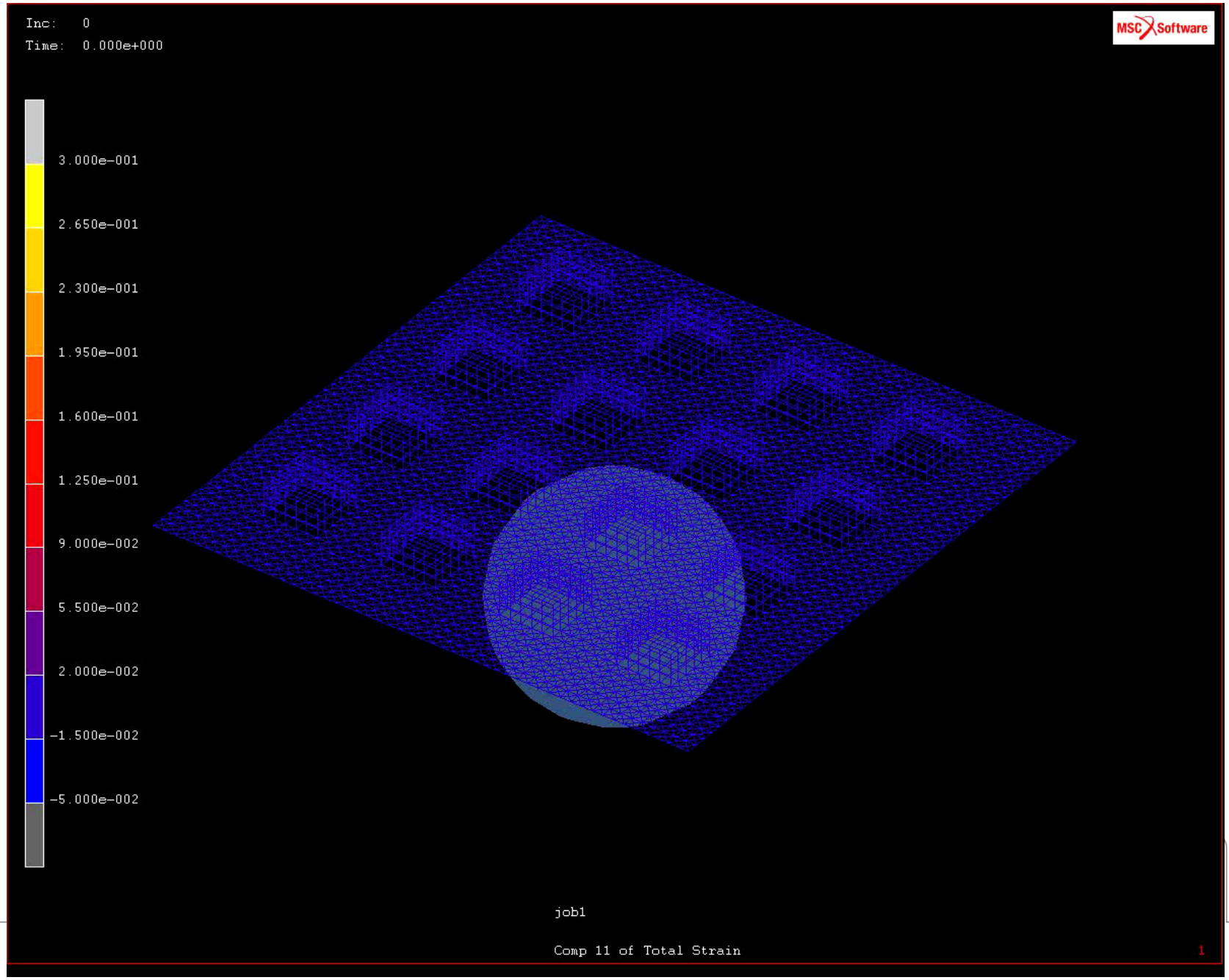
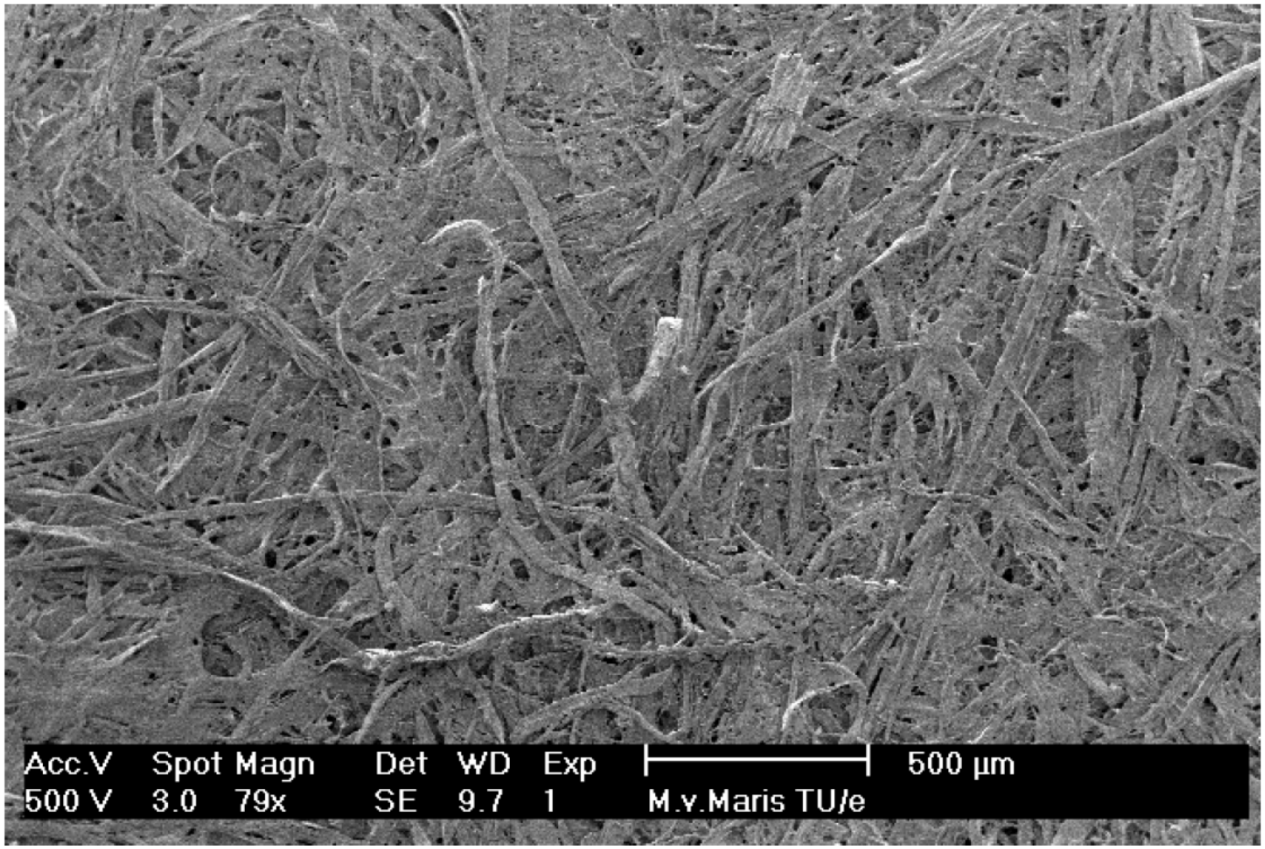


Fibrous material 2: paper materials



TU/e Technische Universiteit Eindhoven University of Technology

océ Canon CANON GROUP

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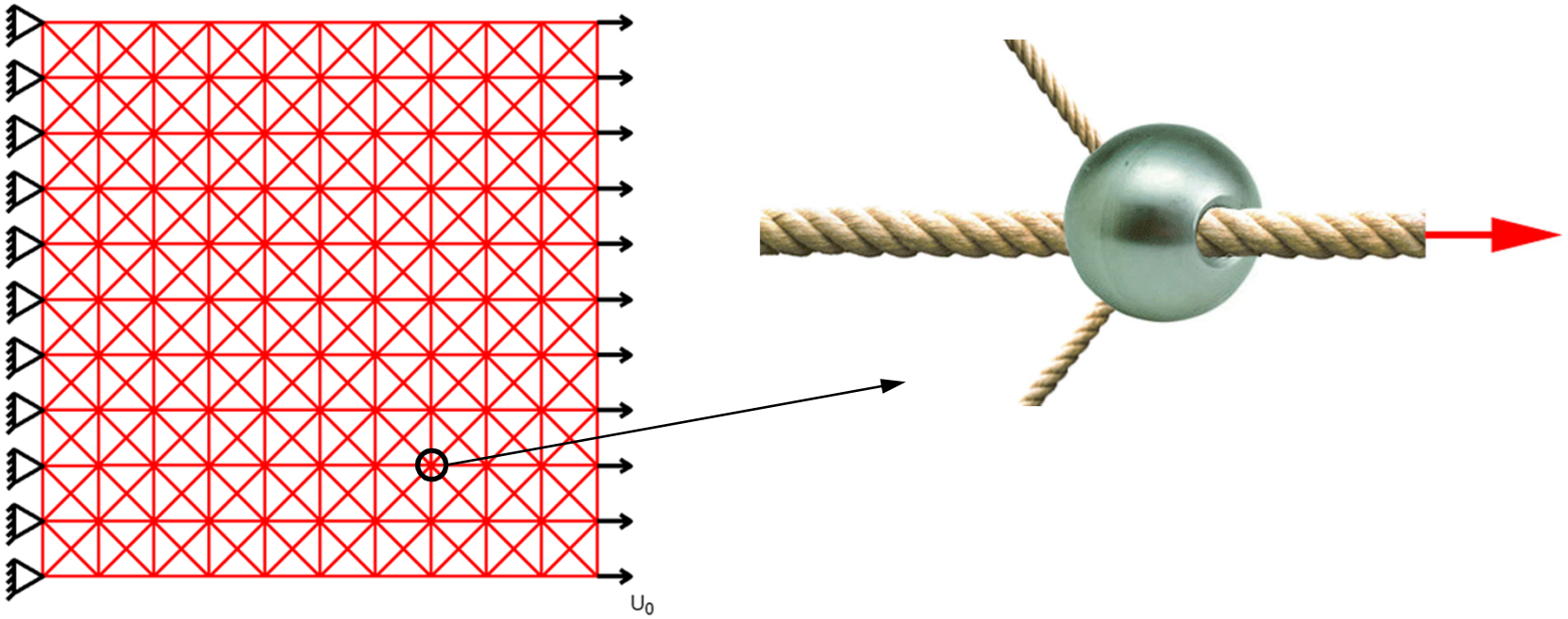
Fibrous material 2: paper materials



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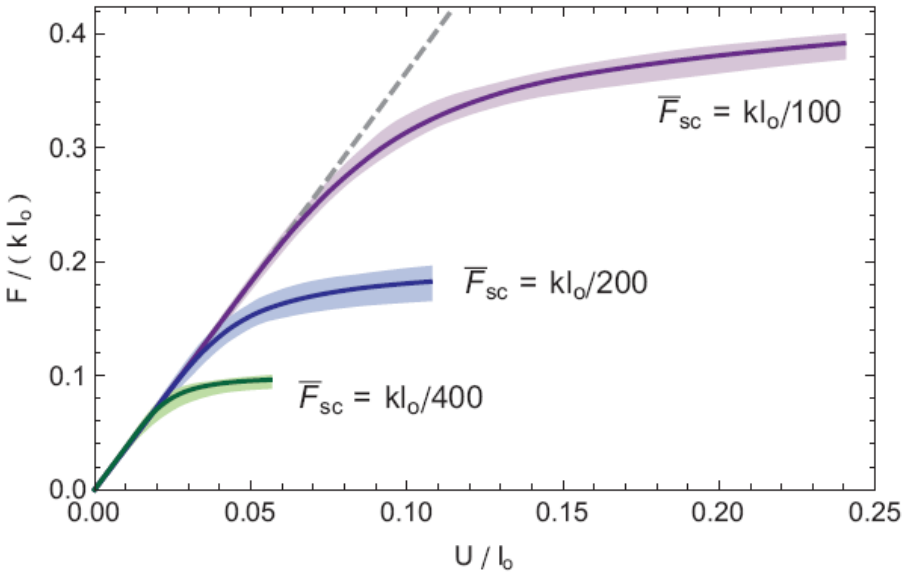
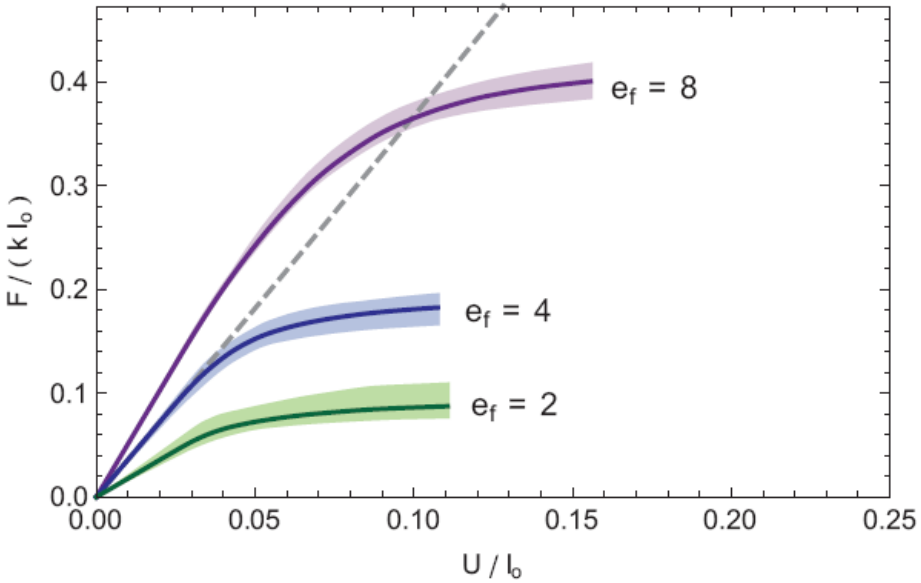
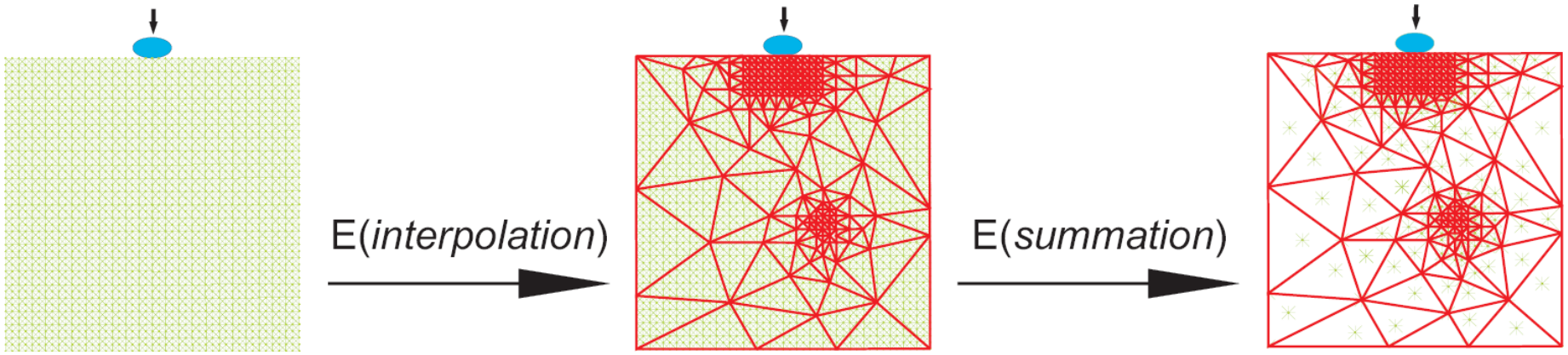


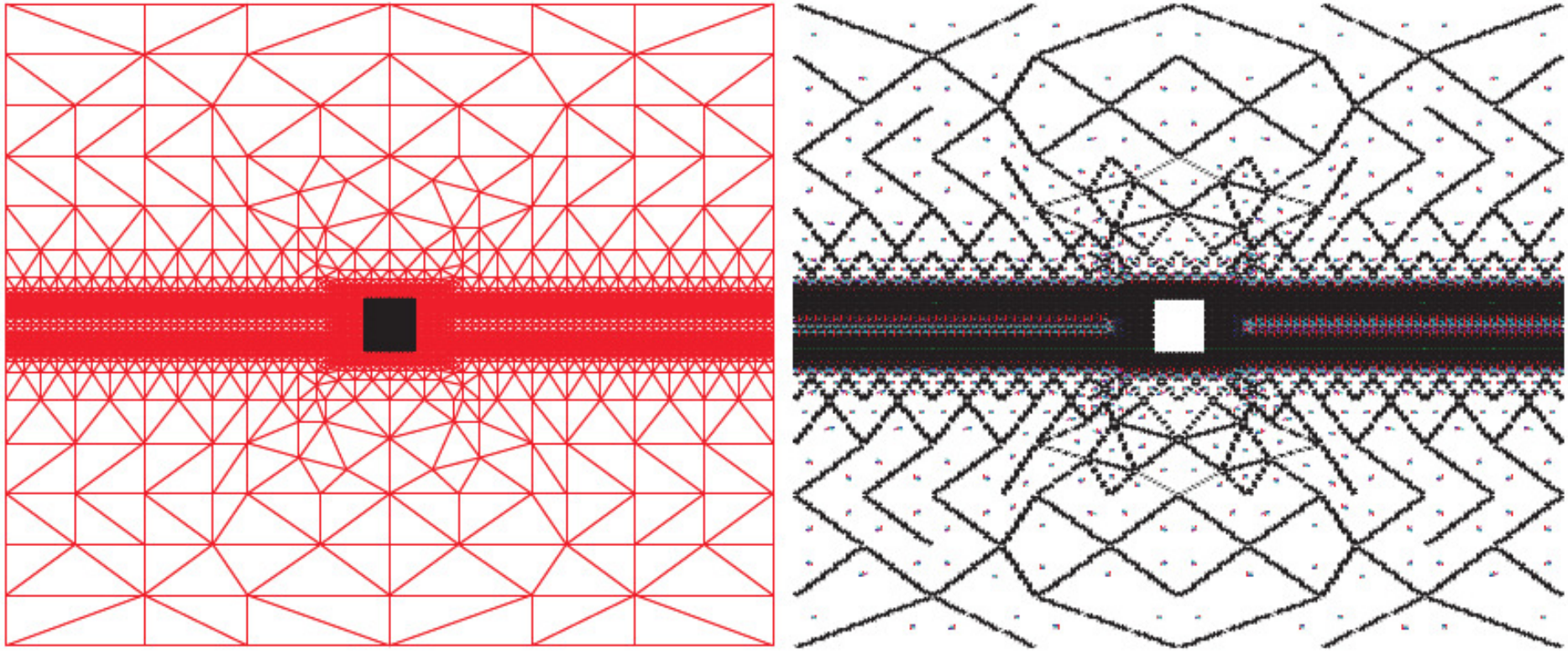


Quasicontinuum method (Tadmor et al, 1996)

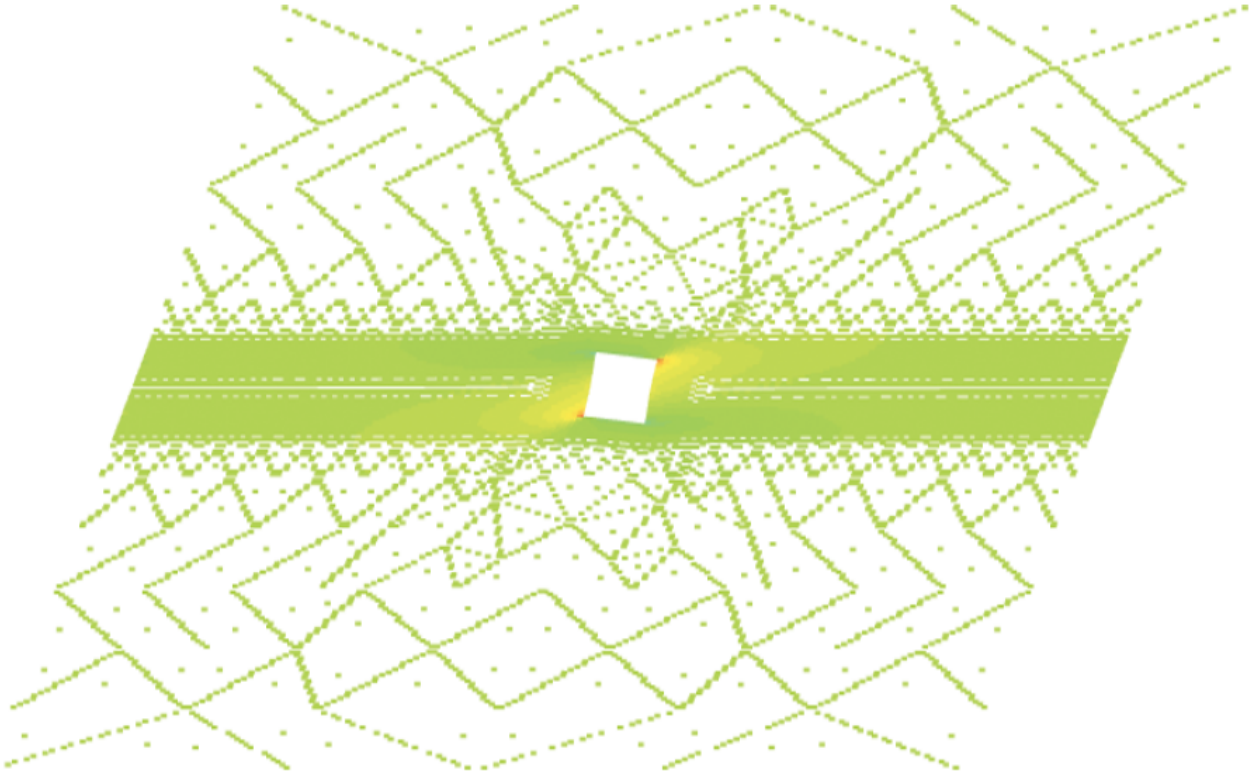


- Ideal for local events in large-scale lattice computations
- Underlying lattice fully resolved where needed
- No continuum/constitutive assumptions

Electronic textile

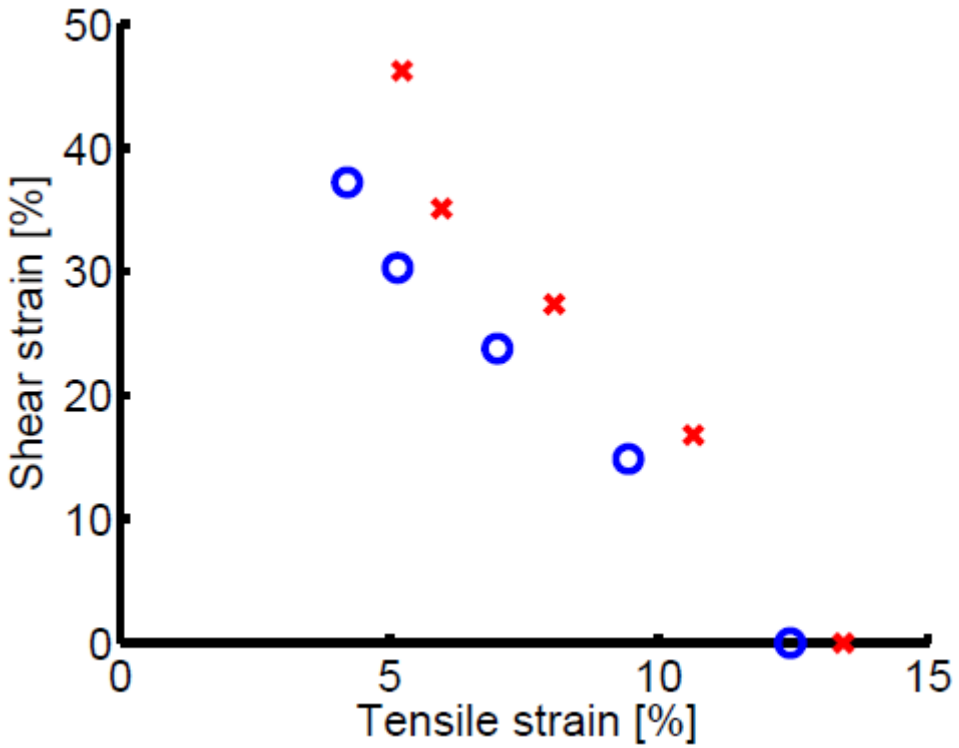


Results: electronic textile

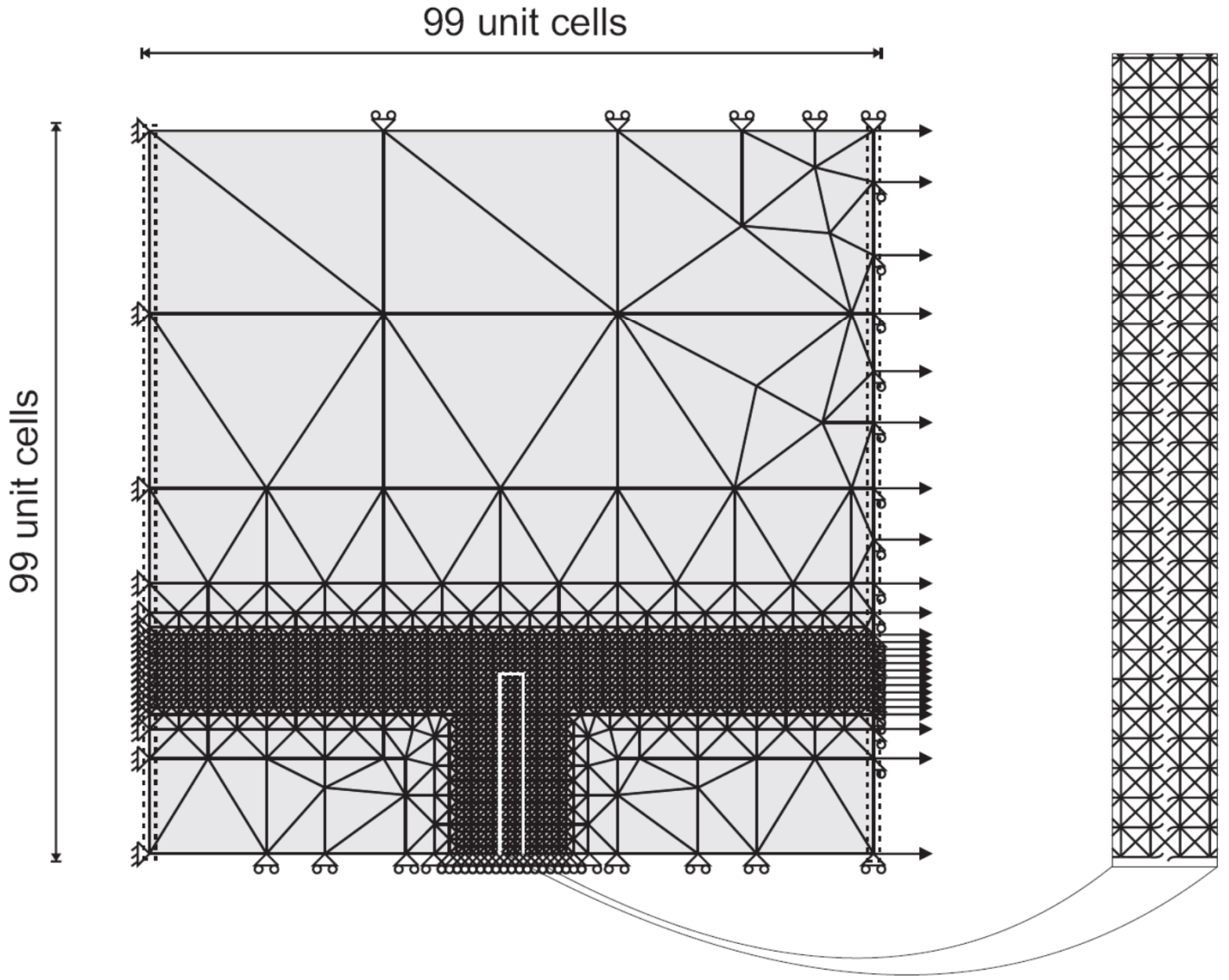


Results: electronic textile

Failure surfaces

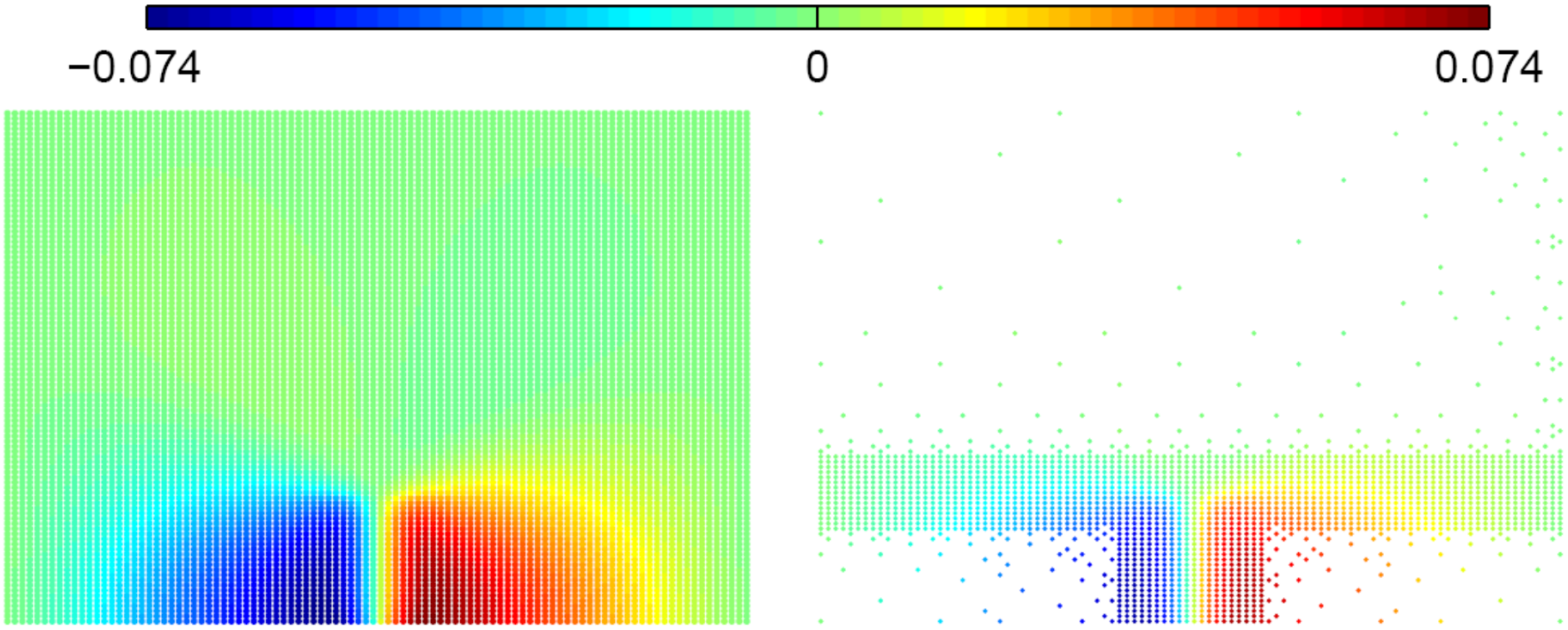


Results: fiber sliding in paper materials

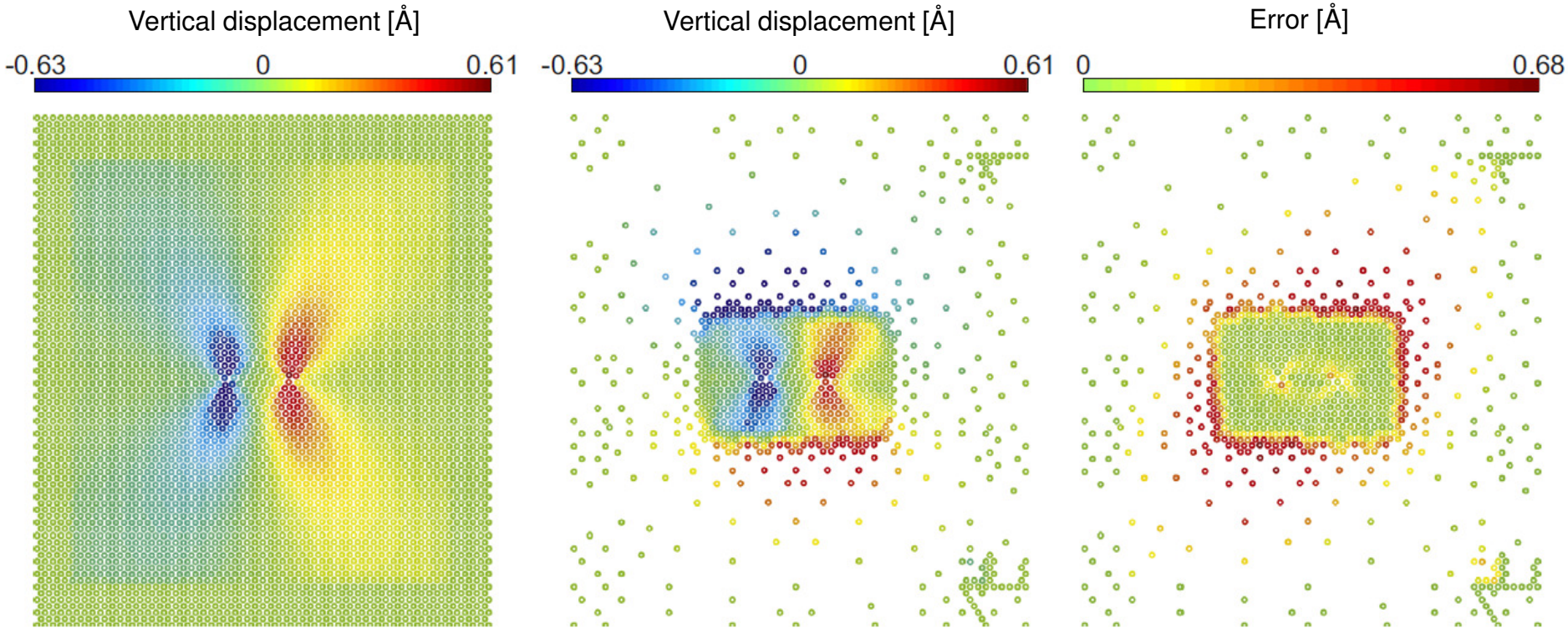


Results: fiber sliding in paper materials

Horizontal displacement, relative to the uniform displacement



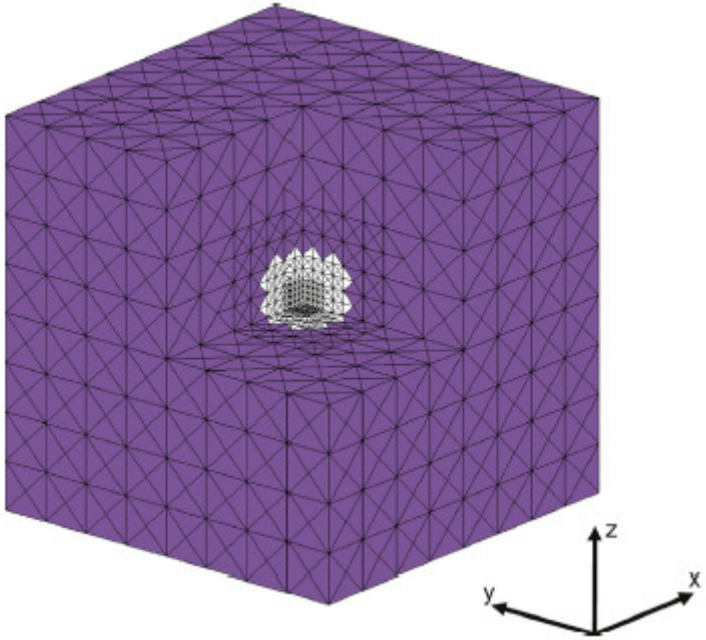
Lomer di-pole in 2.5D FCC system (EAM)



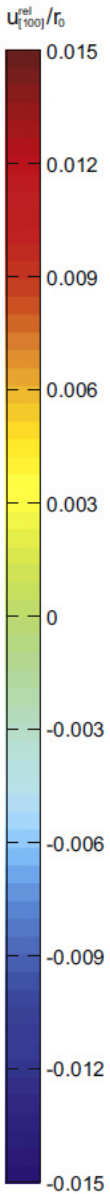
QC for atomistics

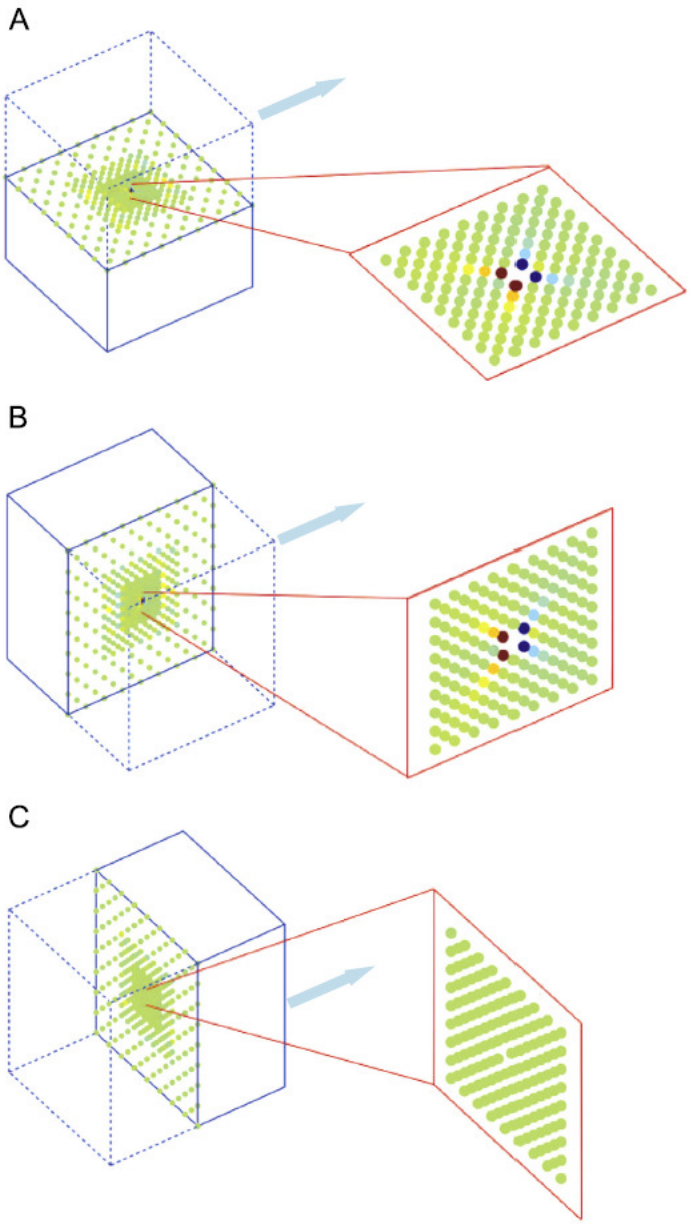
Vacancy in 3D FCC system

(LJ-potential)



Total number of atoms:	1,074,344
Atoms for DOFs:	8732 (0.8%)
Sampling atoms:	55,744 (5.1%)





Research plans for QC method applied to metals

√ Elastoplastic trusses (local dissipative mechanism)

√ Nodal sliding (non-local dissipative mechanism)

√ Atomistics (conservative but highly nonlocal)

√ Beams

√ Irregularity

- Adaptivity

- Applications: 1. Technically relevant atomistic problems,

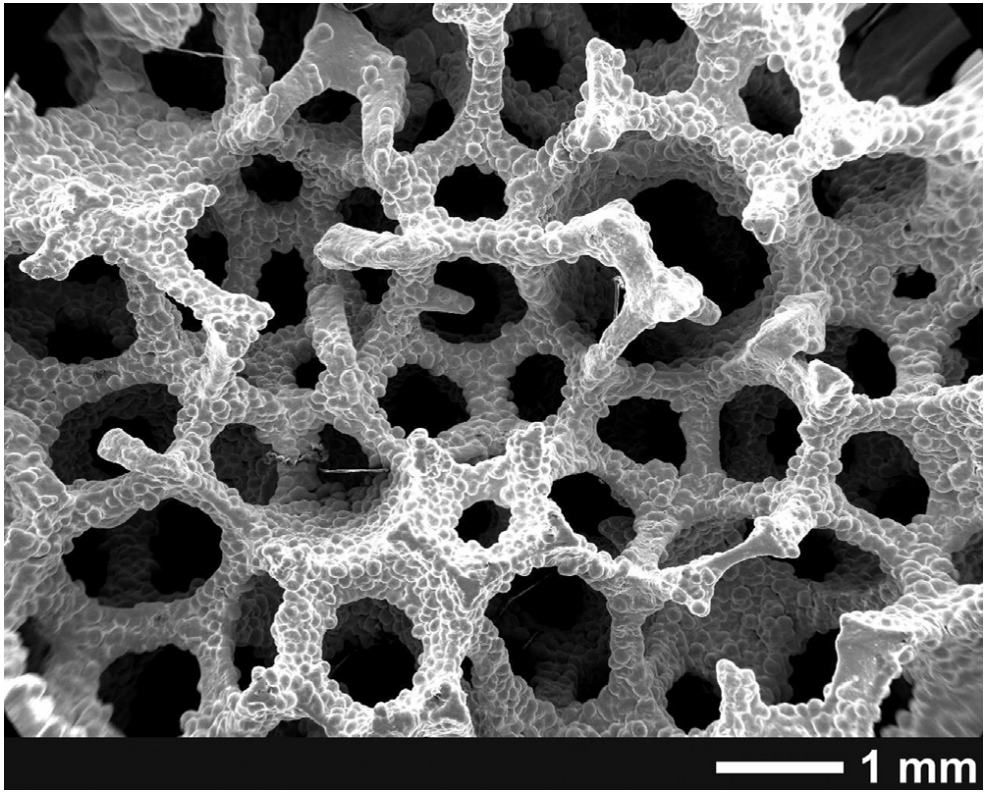
2. Open-cell Al foams with functionally graded Ni coatings.

Open-cell Al foams with functionally graded Ni coatings

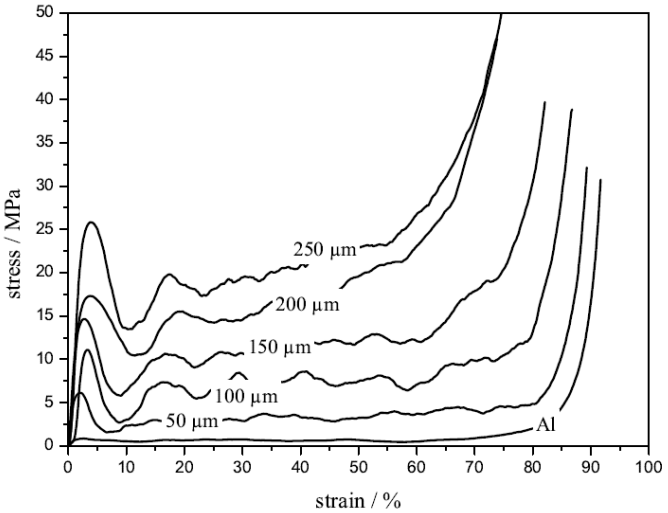
Anne Jung

Stefan Diebels

SAARLAND UNIVERSITY



(Jung, 2012)



(Jung, 2014)

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Open-cell Al foams with functionally graded Ni coatings

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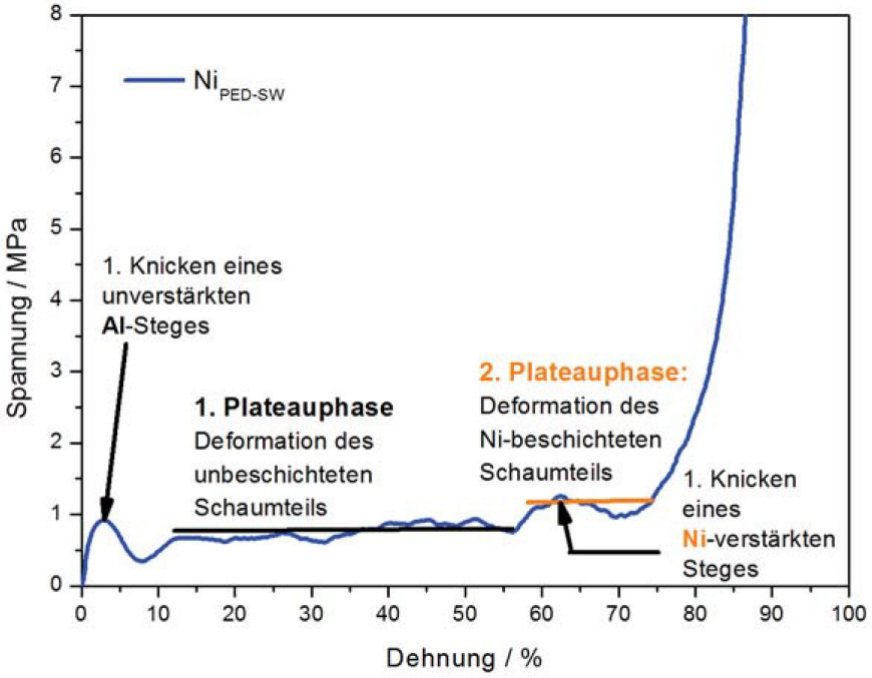

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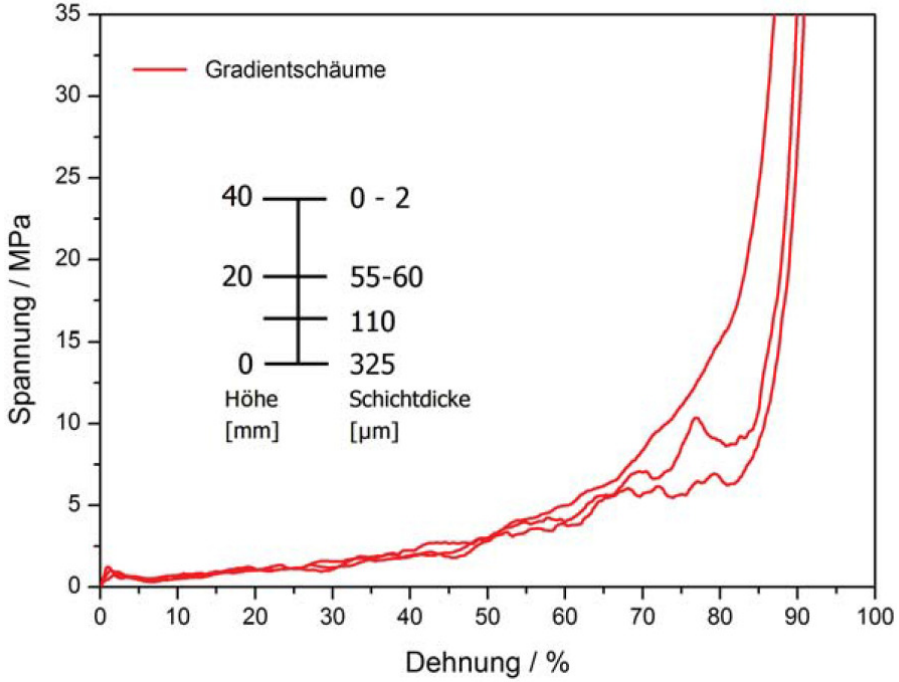


(Jung, 2012)

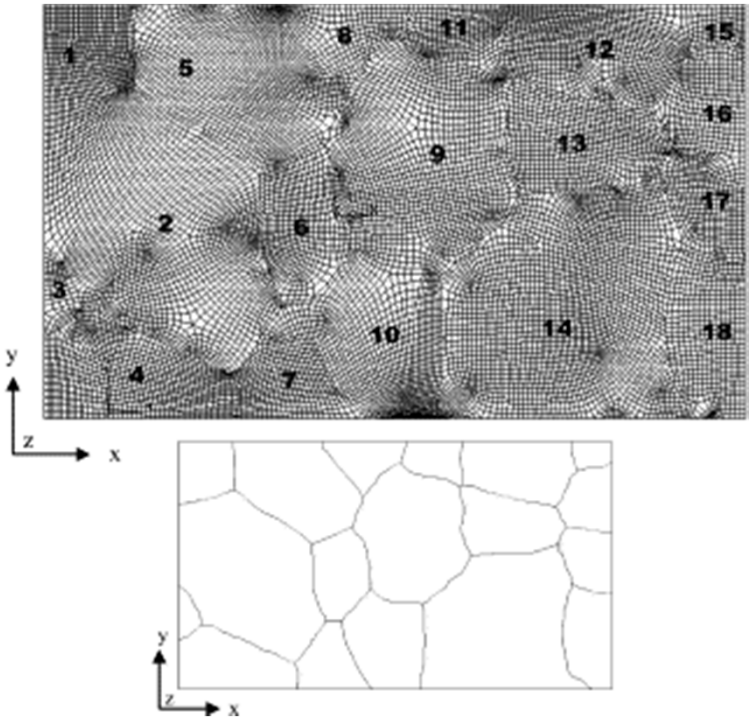
Enhanced discretisation technique for crystal plasticity

Hussein Rappel

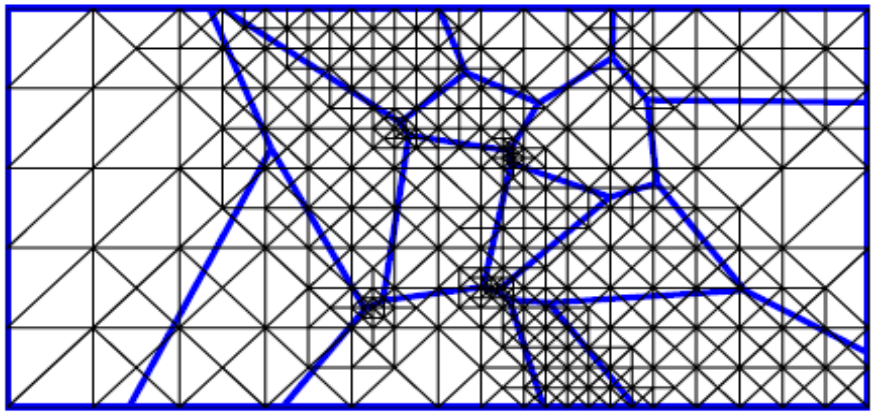
Daniel Balint

ArcelorMittal

Imperial College London



(Raabe, 2012)



Advantages:

1. Easy remeshing
2. Grain boundary fracture
3. Growth/shrinkage of crystals

Multitime modelling for low cycle fatigue of crystal plasticity

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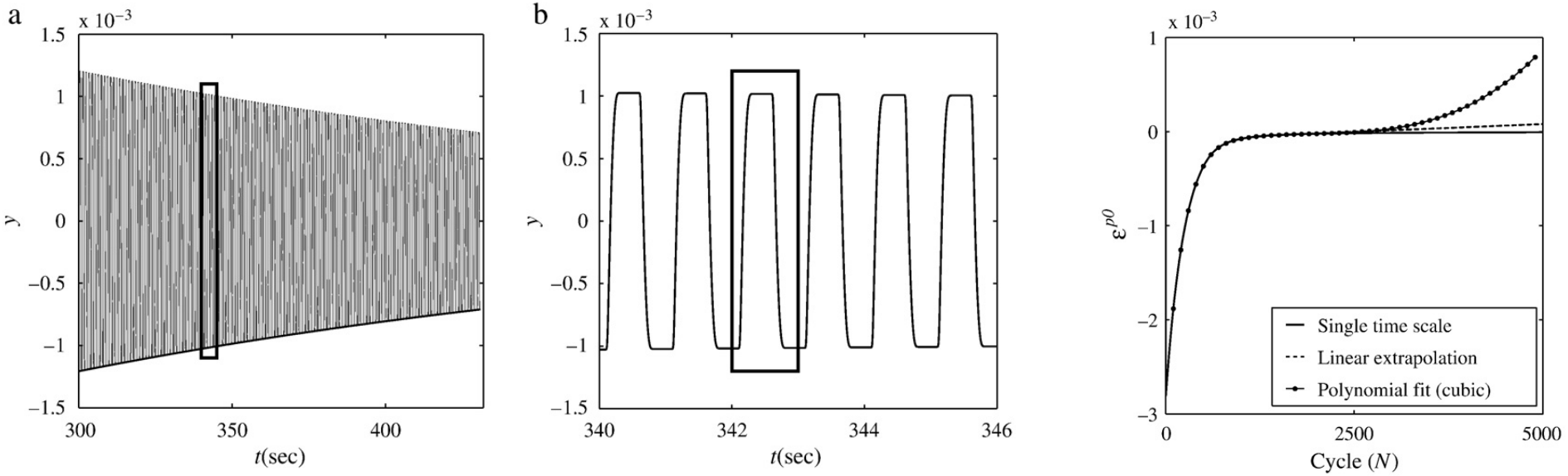
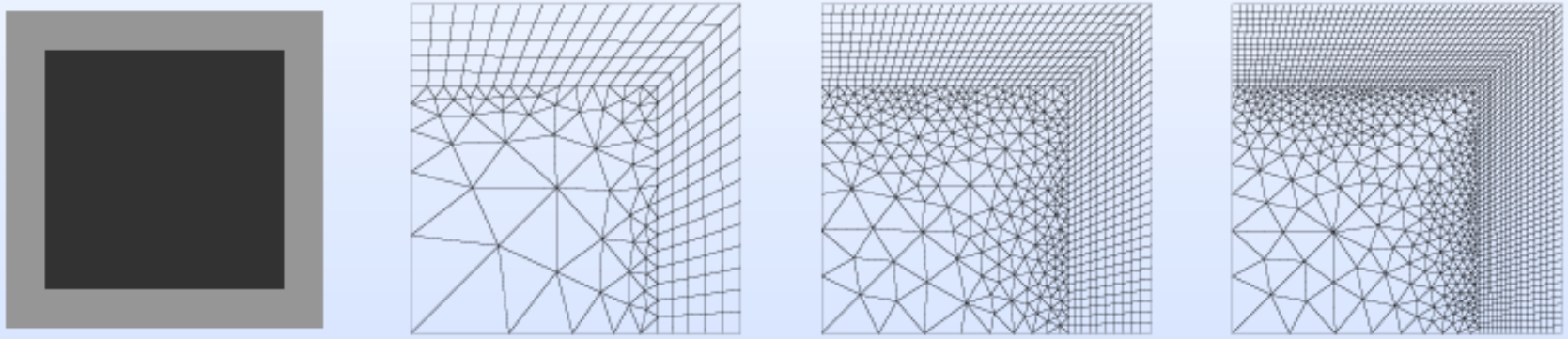


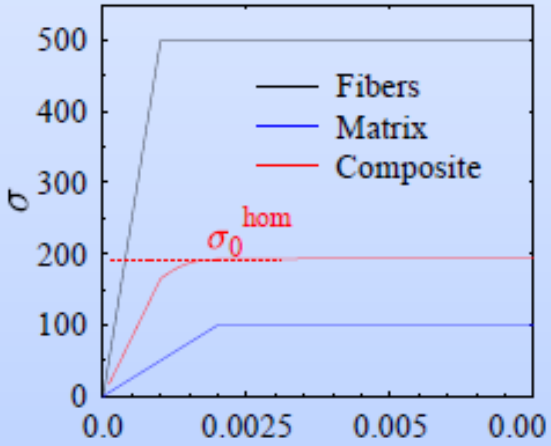
(Joseph, 2010)

Fast Fourier Transformation for RVEs

Comparison FFT/FEM 2 elastic plastic phases $\sigma_0^m = 100$ Mpa, $\sigma_0^f = 500$ Mpa.



Resol. N	FFT σ_0^{hom} MPa	FFT CPU time s	Dof's	FEM σ_0^{hom} MPa	FEM CPU time s
16	160.34	1.64	*	*	*
32	160.66	3.02	1402	162.36	267.69
64	160.07	12.21	5710	160.62	2170.28
128	159.55	53.53	11370	160.37	6464.47
256	159.29	253.31	*	*	*
512	159.13	1075.60	*	*	*



(Moulinec & Suquet)

Summary

√ QC method for dissipative systems (springs/beams, regular/irregular)

√ QC method for conservative systems (atomistics)

- QC method for dissipative graded systems (open-cell Al foams)

- Enhanced disretisation technique for crystal plasticity

- Multitime modelling for low cycle fatigue

- FFT modelling for RVEs

Virtual-power-based QC framework

Dissipative lattice model based on a Coleman-Noll procedure

Kinematic variables $\boldsymbol{u}$ & history variables $\boldsymbol{z}$

Internal energy $E = \sum_{i=1}^{n} E_i$

Virtual-power $\dot{\boldsymbol{u}}^T \boldsymbol{f}_{int} = \dot{\boldsymbol{u}}^T \boldsymbol{f}_{ext} \quad \forall \dot{\boldsymbol{u}}$

Internal power $P_{int} = \dot{E} + \dot{D}$

Energy rate $\dot{E} = \dot{\boldsymbol{u}}^T \frac{\partial E}{\partial \boldsymbol{u}} + \dot{\boldsymbol{z}}^T \frac{\partial E}{\partial \boldsymbol{z}}$

Dissipation rate $\dot{D} = \dot{\boldsymbol{u}}^T \left(\boldsymbol{f}_{int} - \frac{\partial E}{\partial \boldsymbol{u}} \right) - \dot{\boldsymbol{z}}^T \frac{\partial E}{\partial \boldsymbol{z}} \geq 0$

Virtual-power-based QC framework

Apply 2 QC reduction steps to

Dissipative lattice model based on a Coleman-Noll procedure

Kinematic variables $\boldsymbol{u} = \Psi \overline{\boldsymbol{u}}$ & history variables $\boldsymbol{z}$

Internal energy $E = \sum_{i \in S} E_i$

Virtual-power $\dot{\overline{\boldsymbol{u}}}^T \Psi^T \boldsymbol{f}_{int} = \dot{\overline{\boldsymbol{u}}}^T \Psi^T \boldsymbol{f}_{ext} \quad \forall \dot{\overline{\boldsymbol{u}}}$

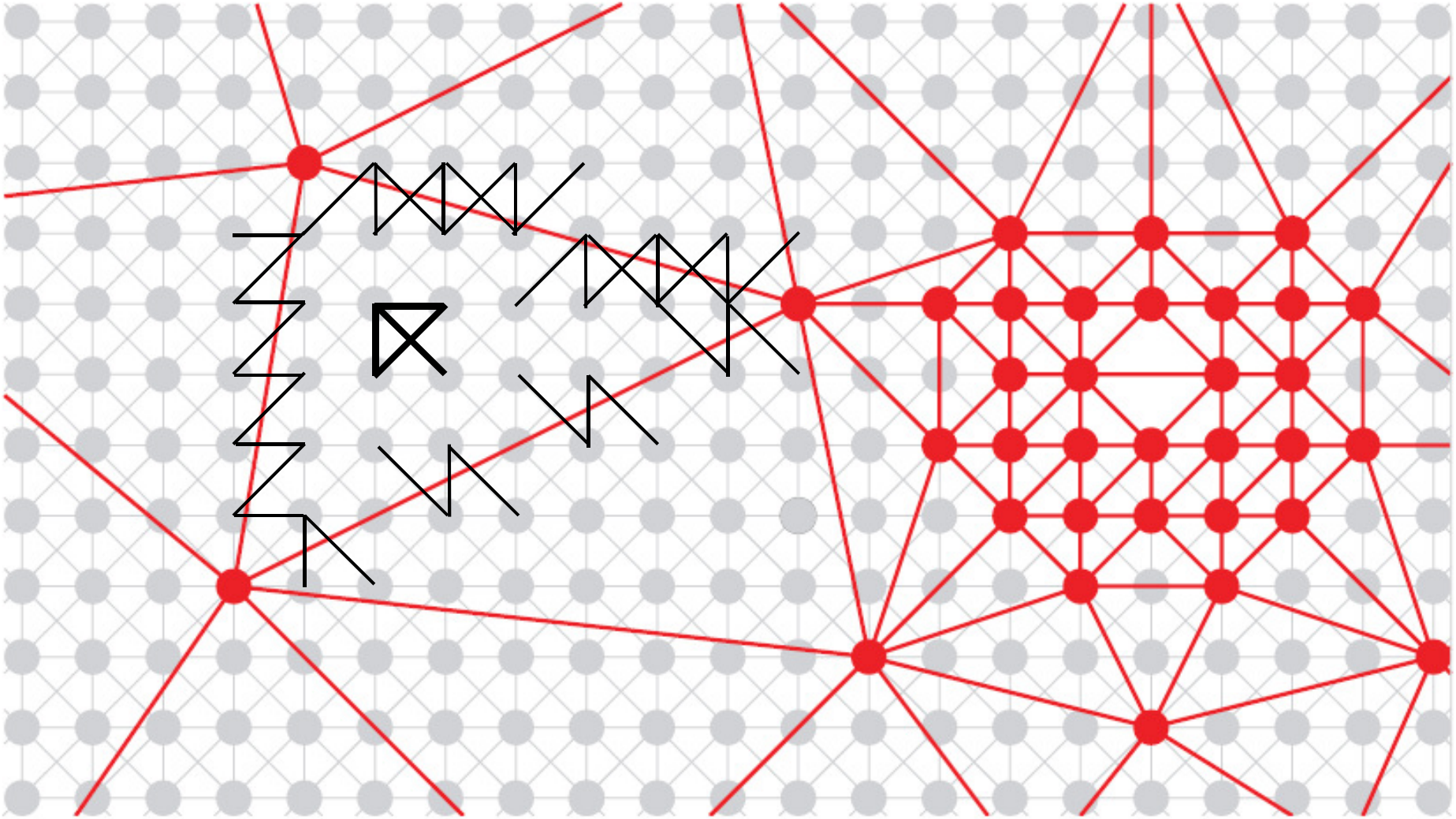
Internal power $P_{int} = \dot{E} + \dot{D}$

Energy rate $\dot{E} = \dot{\overline{\boldsymbol{u}}}^T \Psi^T \frac{\partial E}{\partial \boldsymbol{u}} + \dot{\boldsymbol{z}}^T \frac{\partial E}{\partial \boldsymbol{z}}$

Dissipation rate $\dot{D} = \dot{\overline{\boldsymbol{u}}}^T \left(\boldsymbol{f}_{int} - \Psi^T \frac{\partial E}{\partial \boldsymbol{u}} \right) - \dot{\boldsymbol{z}}^T \frac{\partial E}{\partial \boldsymbol{z}} \geq 0$

Virtual-power-based QC framework

Summation



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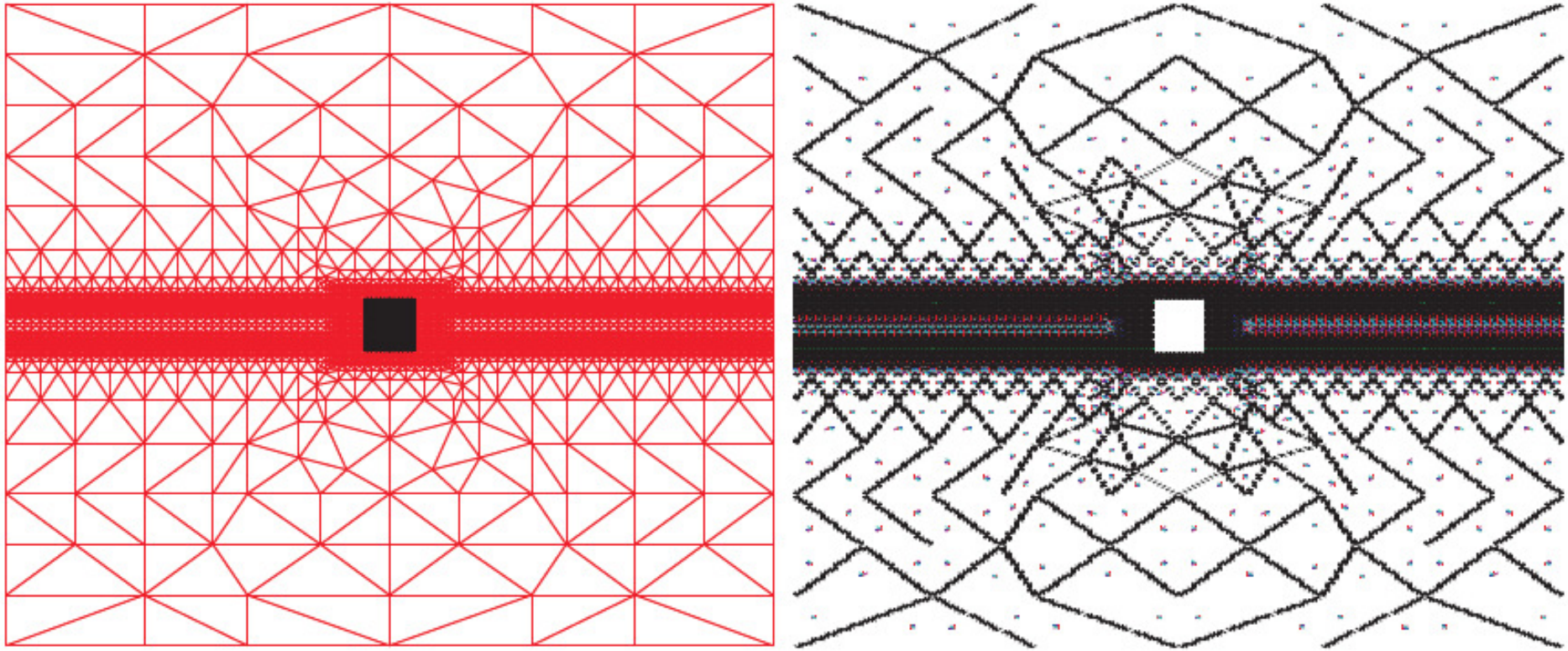

Virtual-power-based QC framework

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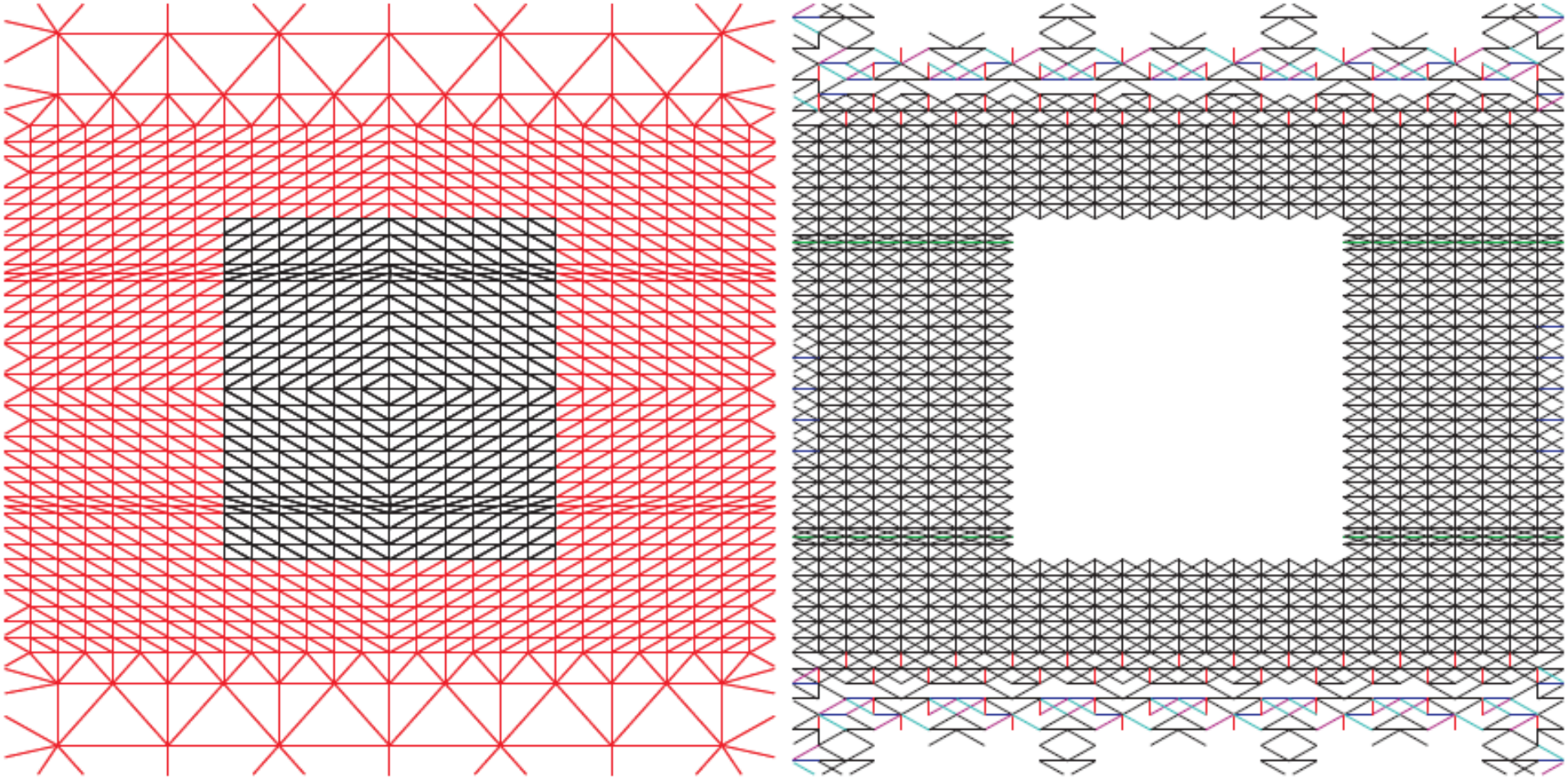

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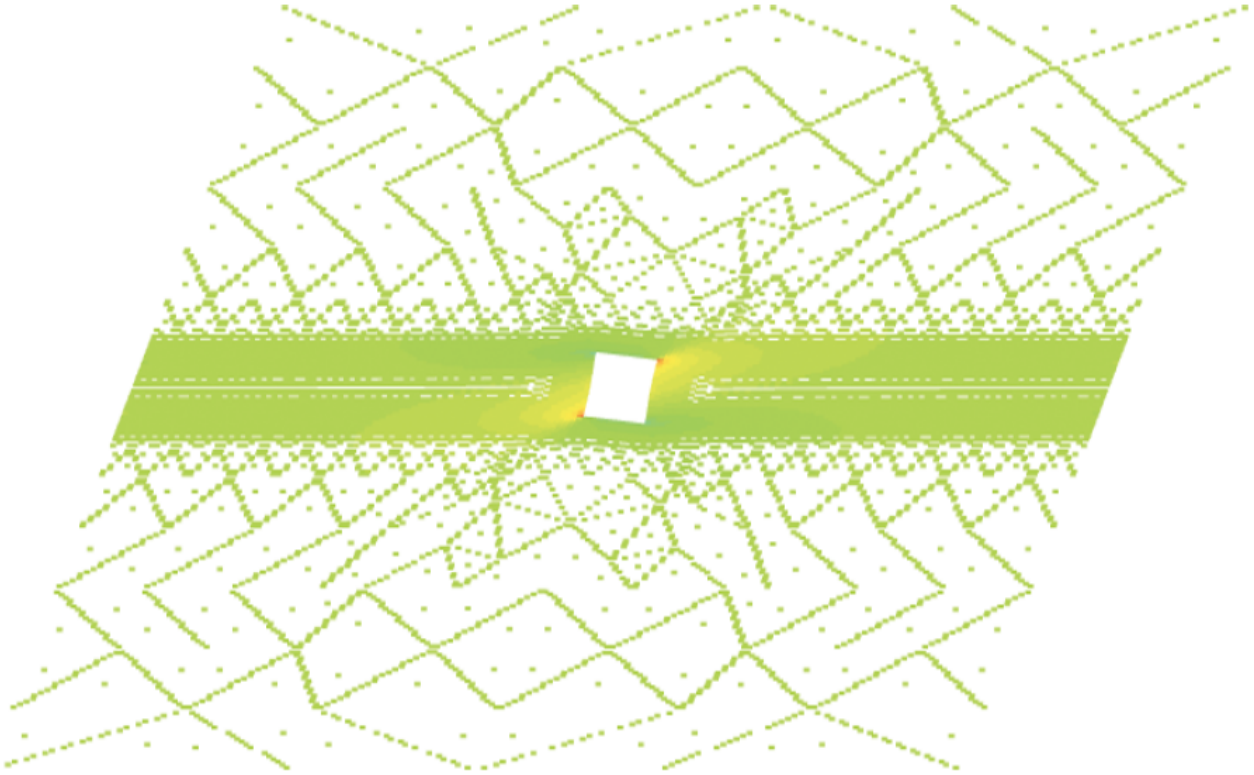

Results: electronic textile

Failure surfaces