

Supplementary Material for

**3D Electro-elastic Modeling of the Nucleation and
Propagation of the Spin Domains in Spin Transition
Materials**

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1 Movies

In this supplementary material we provide six different movies to shed light on the results already presented in the main manuscript by giving complementary information.

Movie S1: corresponds to spatiotemporal configurations of the lattice during the thermal cycle for $A_{1n} = 50$, related to Figure 6 of the main paper. Yellow (blue) spheres represent HS (LS) sites.

Movie S2: corresponds to spatiotemporal configurations of the lattice during the thermal cycle for $A_{1n} = 3\,000$, related to Figure 7 of the main paper. Yellow (blue) spheres represent HS (LS) sites.

Movie S3: corresponds to spatiotemporal configurations of the lattice during the relaxation process at $T = 1K$ from an initial HS phase for $A_{1n} = 7\,000$, related to Figure 13 of the main paper. Yellow (blue) spheres represent HS (LS) sites.

Movie S4: corresponds to spatiotemporal configurations of the lattice during the relaxation process at $T = 10K$ from an initial HS phase for $A_{1n} = 8\,000$, related to Figure 14 of the main paper. Yellow (blue) spheres represent HS (LS) sites.

Movie S5: corresponds to the spatial distribution of the local pressure field of the lattice during the relaxation process at $T = 10K$ from an initial HS phase for $A_{1n} = 8\,000$, related to Figure 15 of the main paper. We only display the tensile strain (negative pressure): remark the convexity of the propagating pressure wave along the x direction.

Movie S6: corresponds to the spatial distribution of the local elastic energy field during the relaxation process at $T = 10K$ from an initial HS phase for $A_{1n} = 8\,000$, related to Figure 18 of the main paper.

2 Figures

2.1 Thermal cycle

2.1.1 Interplay between dynamics of the spin and lattice degrees of freedom

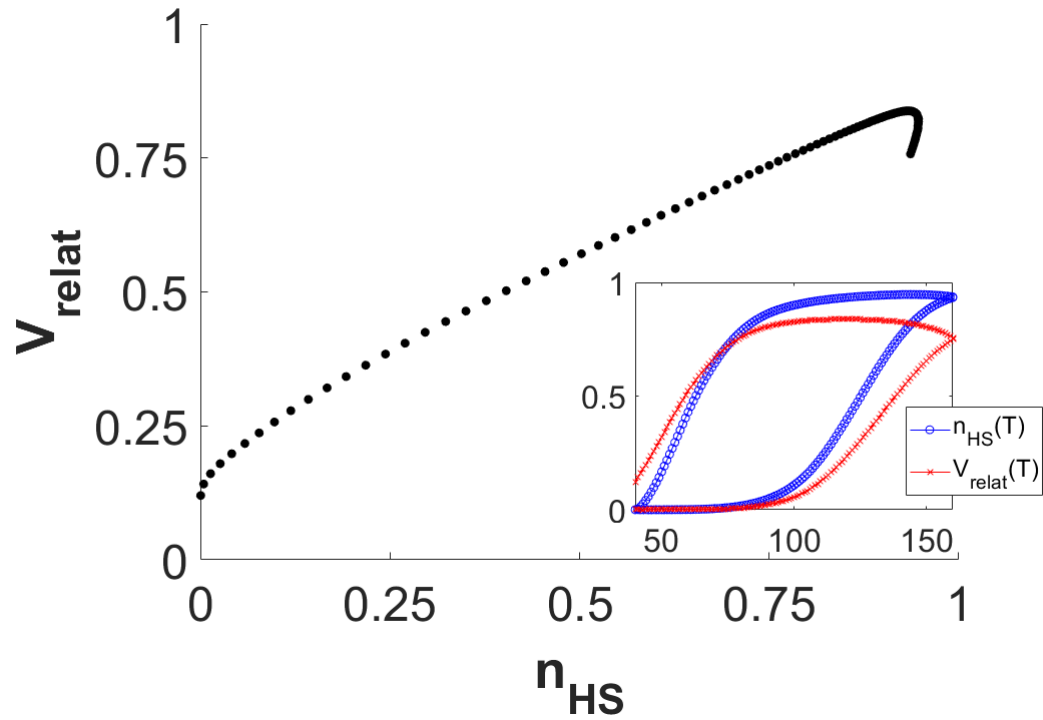


Figure S1 – Elastic variations of the lattice V_{relat} as a function of electronic variations n_{HS} during hysteresis loop presented for the case of the cooling branch for $A_{1n} = 3\ 000$ for 10 molecular dynamics runs after each spin flip. All other model parameters are the same as for 300 runs presented in the main paper.

2.1.2 Averaged distances of neighbouring pairs

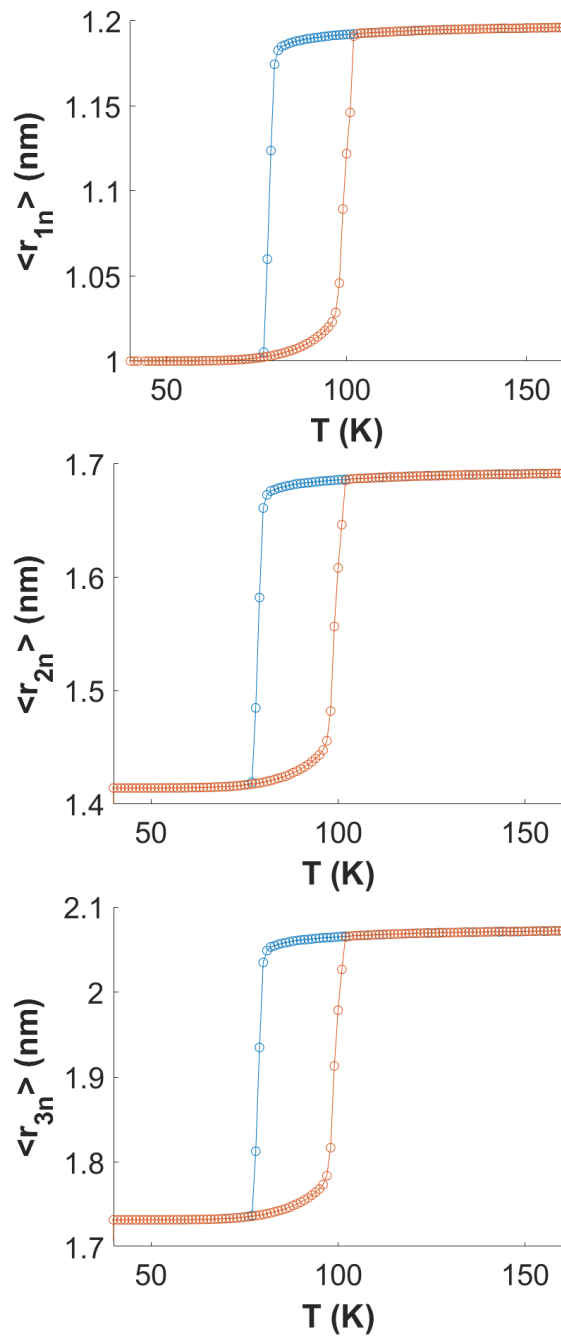


Figure S2 – Thermal evolution of the averaged distances of the neighbouring pairs throughout the lattice for $A_{1n} = 3000$. Top to down: $1n$, $2n$ and $3n$ nearest-neighbours.

2.1.3 Divergence of the displacement field

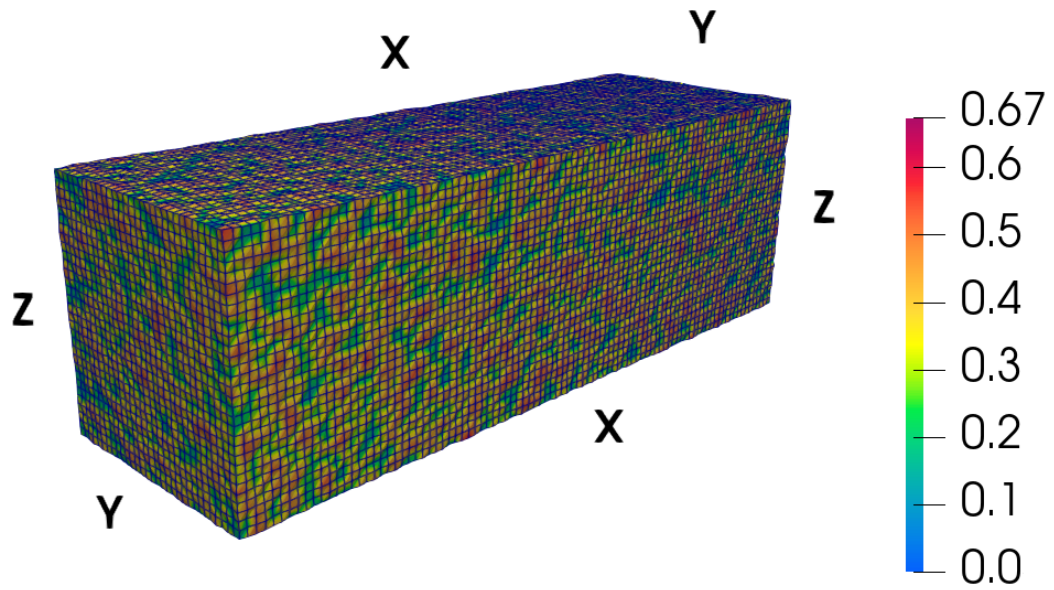


Figure S3 – Snapshot showing the spatial distribution of the divergence of the displacement field corresponding to the gradual transition during the cooling branch at $n_{HS} = 0.55$ and $T = 92K$ for $A_{1n} = 50$.

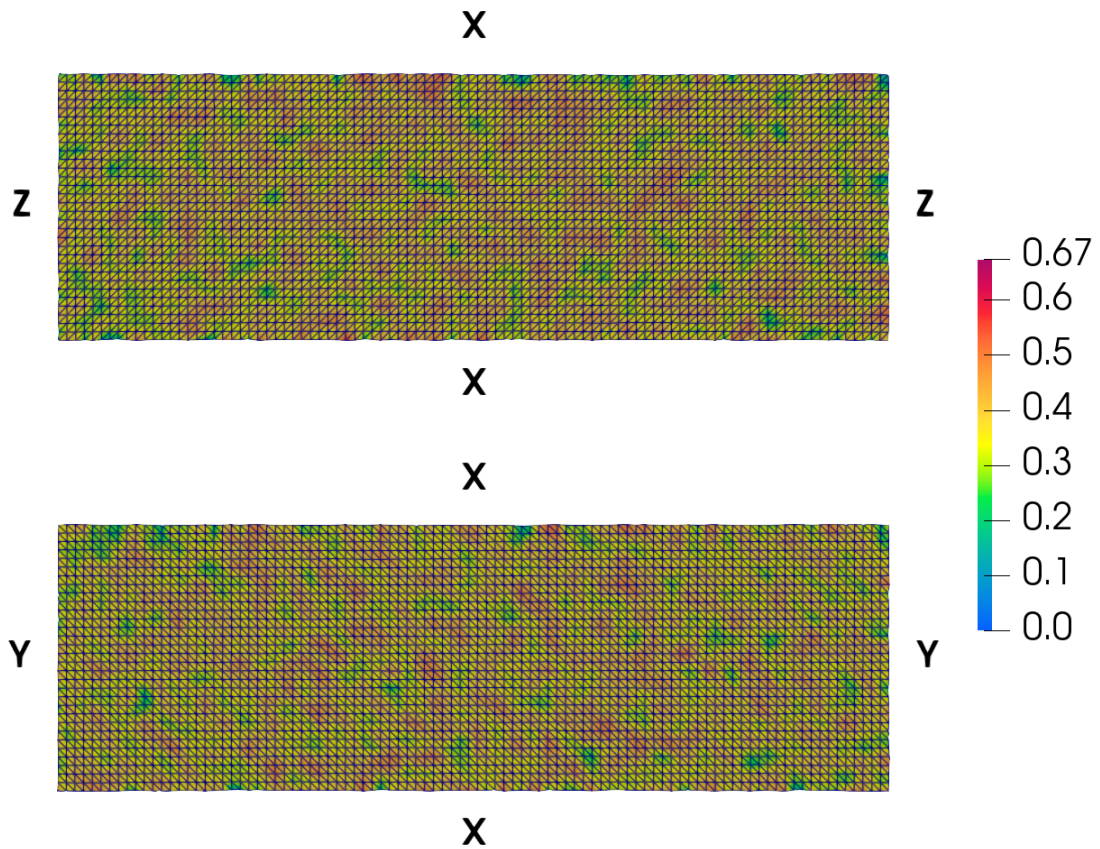


Figure S4 – Sectional view in the planes (xOz) at $\frac{N_y}{2}$ (top) and (xOy) at $\frac{N_z}{2}$ (bottom) of the spatial distribution of the divergence of the displacement field corresponding to snapshot of S3.

2.1.4 Curl and divergence of the displacement field

Remark for FigureS5, S6, S7, S8, S9: along the thermal transition, there is a difference in the curl of the displacement field (vector field) between the heating and the cooling branches.

As depicted in these figures, we show the magnitude of the curl of the displacement field at various n_{HS} values around T_{up} (for $T = 97, 98, 99, 100, 101K$), and the spatial distribution of the divergence of the displacement field as an indicator of the propagation front. As the transition spin occurs, the magnitude of the curl field is higher in the regions of the interface splitting up the LS and the HS states, and these regions follow thermally the front. Hence, the distortion of the lattice (shear stresses) seems to occur mainly alongside the front and at the intersection of the front and the surface of the simulation cell.

However, during the cooling branch, the changes in the curl don't occur during the thermal propagation of the transition front, but some degrees before.

In particular, in the same interval of temperatures as the distortion of the lattice occurs during the heating branch, i.e. around the equilibrium temperature of the heating branch which is $T_{up} \approx 99K$ at $n_{HS} = \frac{1}{2}$

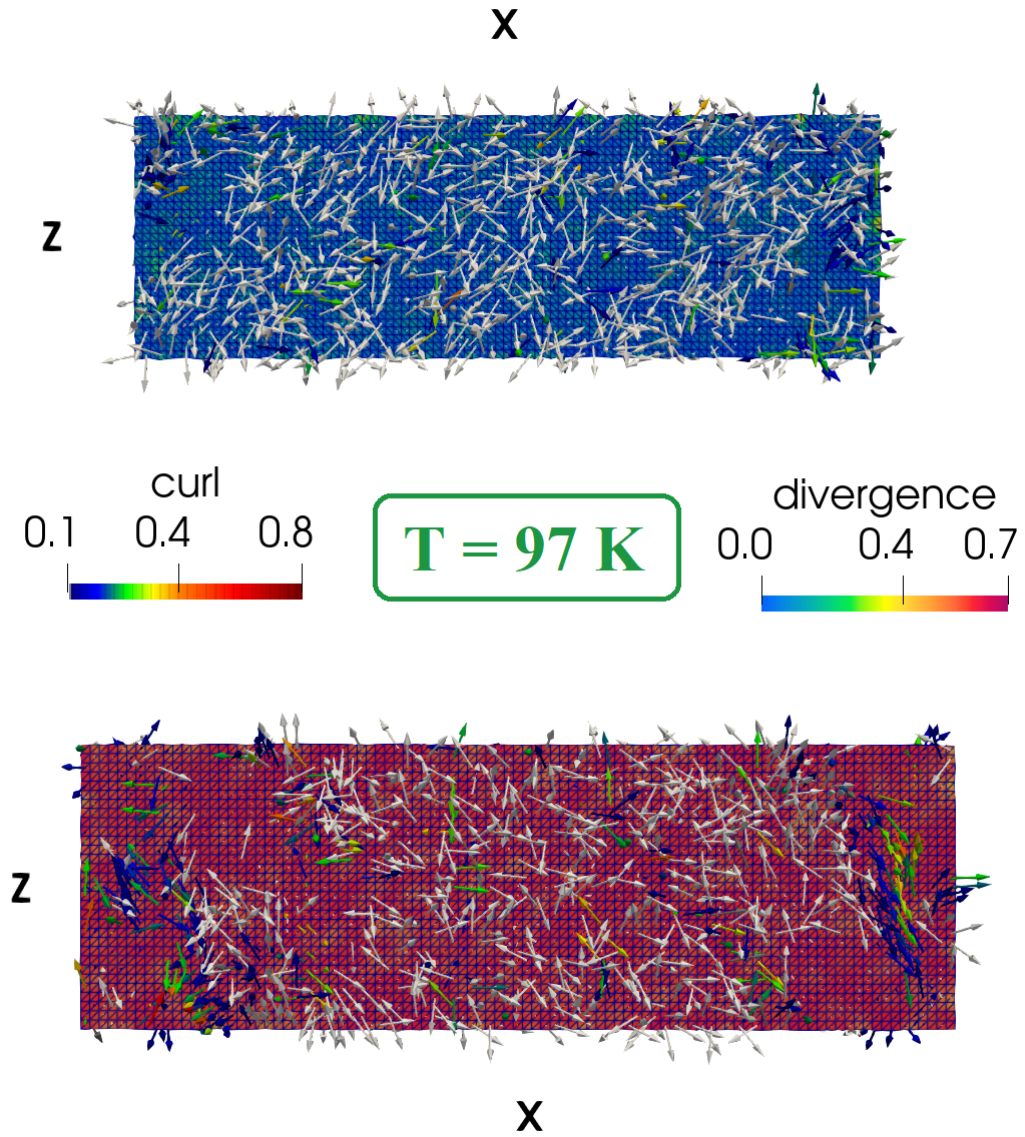


Figure S5 – Snapshots taken for $A_{1n} = 3\,000$ at $T = 97\text{ K}$ during the heating branch (top) and during the cooling branch (bottom), showing sectional view in the plane (xOz) at $\frac{N_y}{2}$ of the magnitude of the vectorial field of the curl of the displacement field (represented by colored arrows). Spatial distribution of the divergence of the displacement field have been added as an indicator of the propagation front. Remark that whitish arrows indicate a value almost equal to zero.

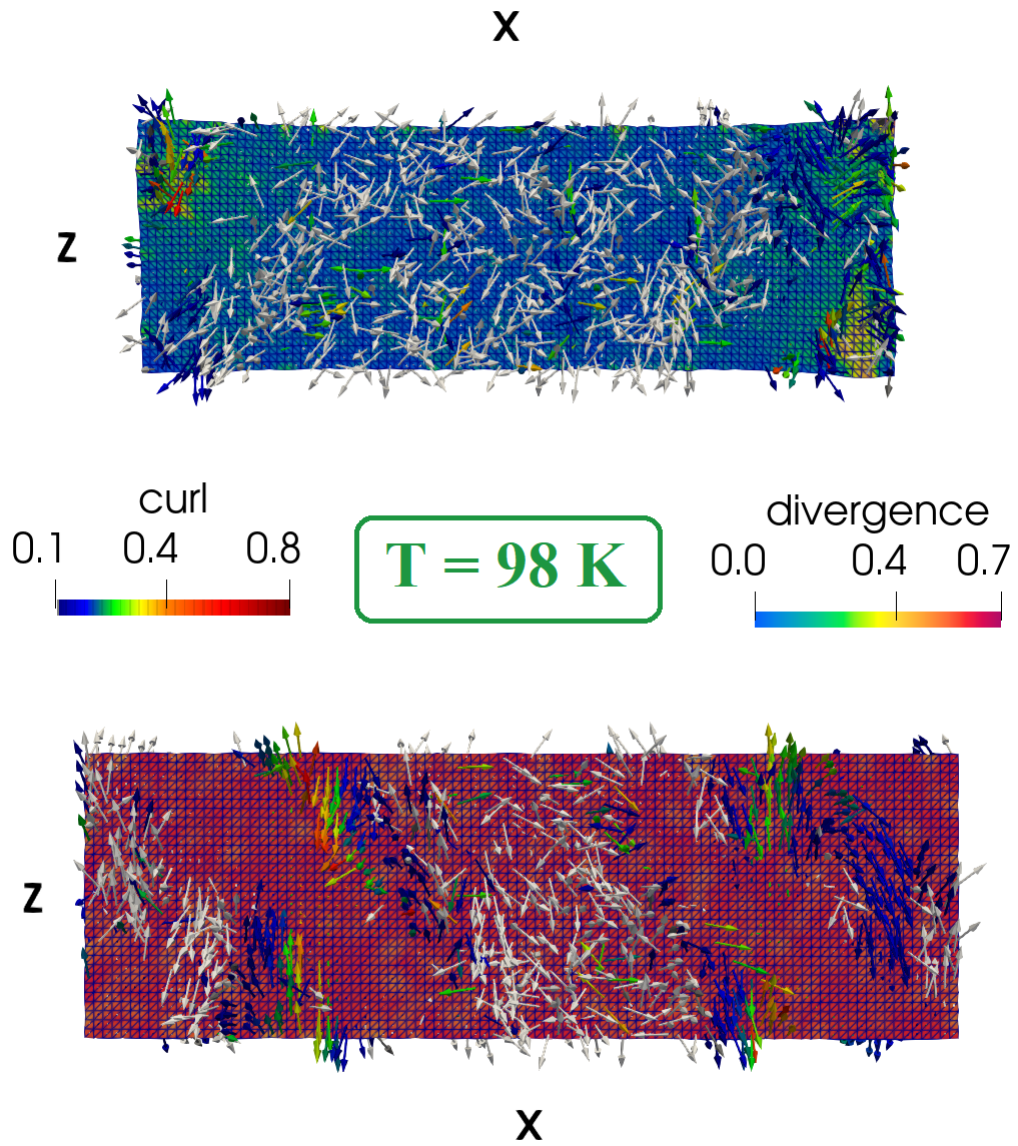


Figure S6 – Snapshots taken for $A_{1n} = 3\,000$ at $T = 98K$ during the heating branch (top) and during the cooling branch (bottom), showing sectional view in the plane (xOz) at $\frac{N_y}{2}$ of the magnitude of the vectorial field of the curl of the displacement field (represented by colored arrows). Spatial distribution of the divergence of the displacement field have been added as an indicator of the propagation front. Remark that whitish arrows indicate a value almost equal to zero.

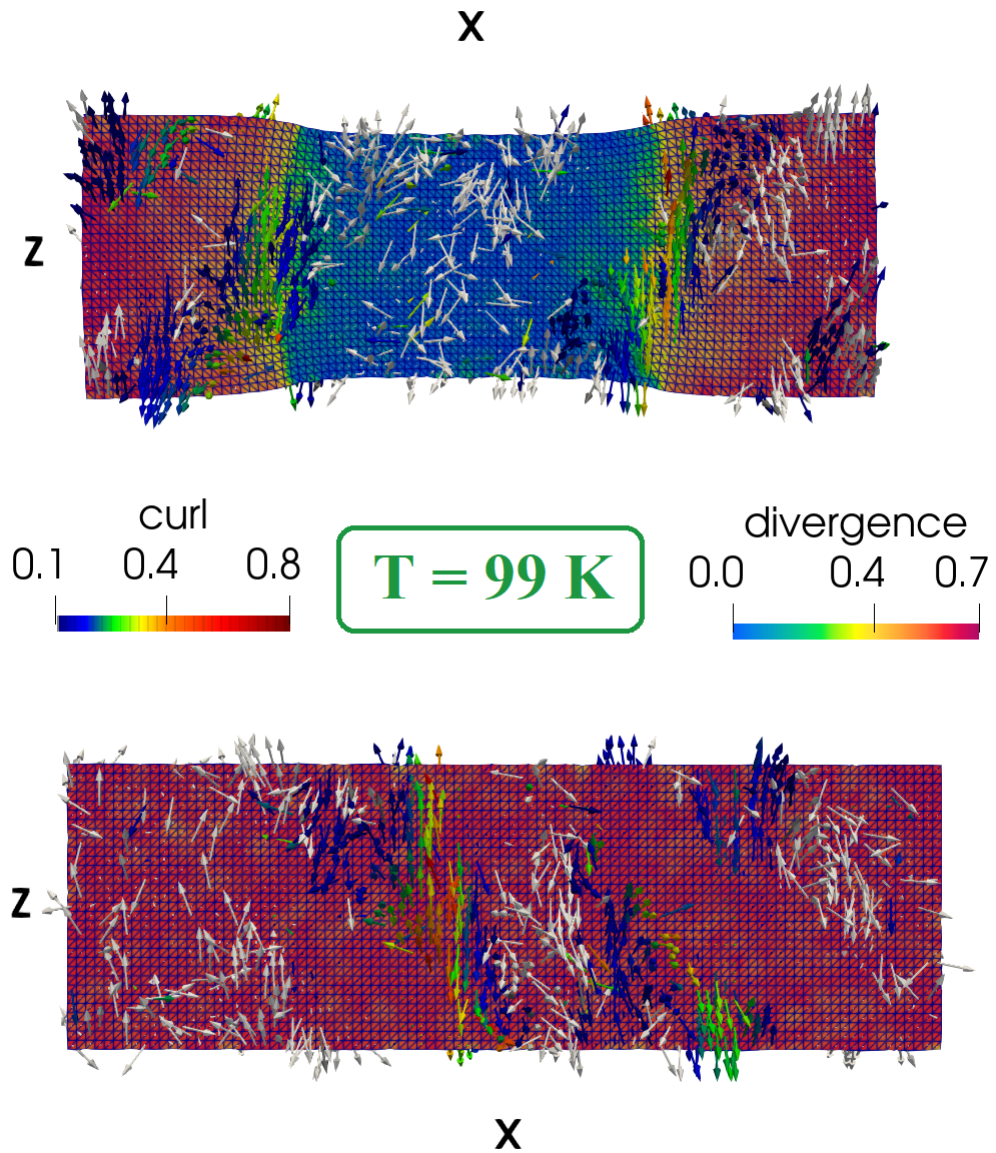


Figure S7 – Snapshots taken for $A_{1n} = 3\,000$ at $T = 99K$ during the heating branch (top) and during the cooling branch (bottom), showing sectional view in the plane (xOz) at $\frac{N_y}{2}$ of the magnitude of the vectorial field of the curl of the displacement field (represented by colored arrows). Spatial distribution of the divergence of the displacement field have been added as an indicator of the propagation front. Remark that whitish arrows indicate a value almost equal to zero.

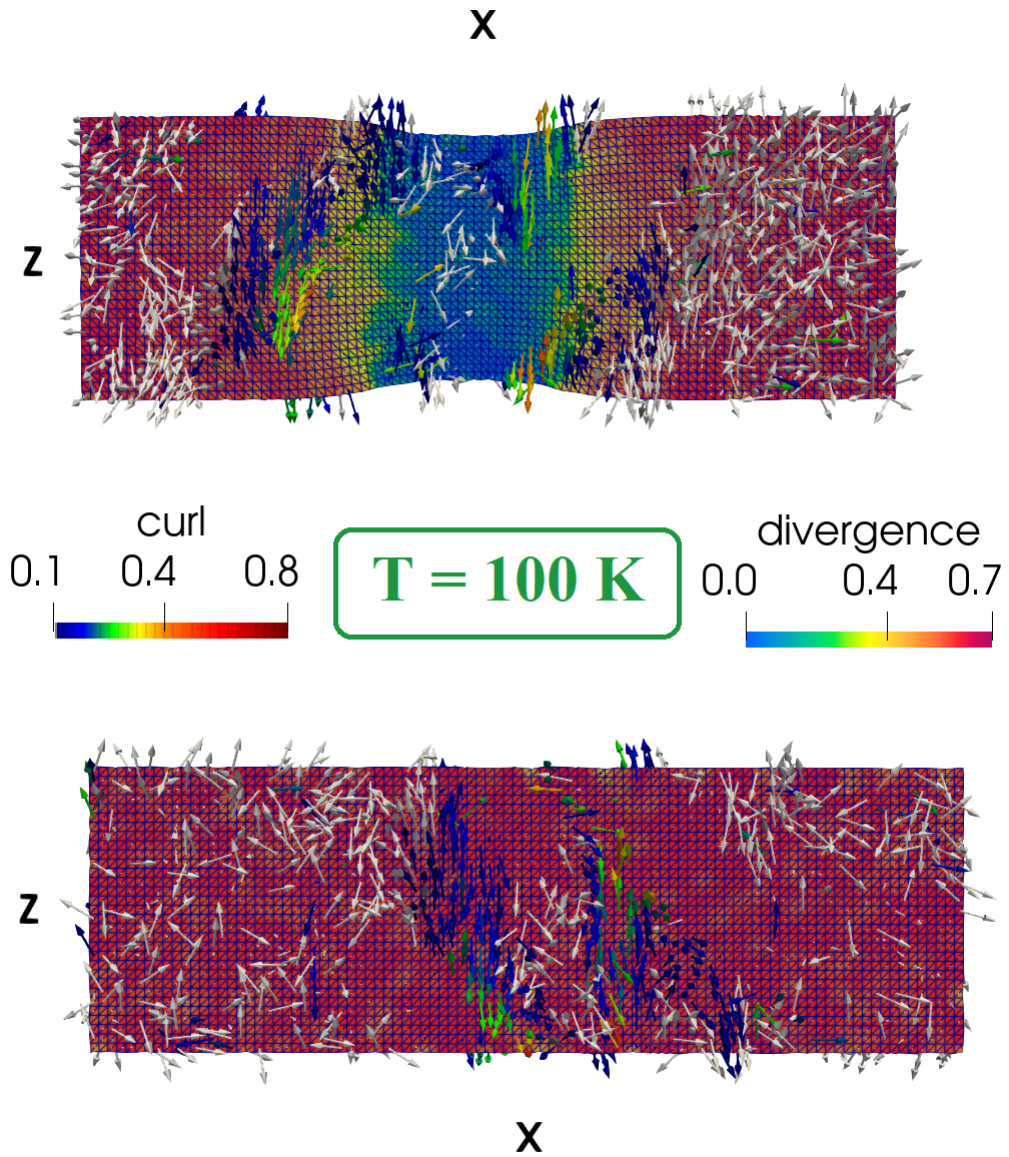


Figure S8 – Snapshots taken for $A_{1n} = 3\,000$ at $T = 100\text{ K}$ during the heating branch (top) and during the cooling branch (bottom), showing sectional view in the plane (xOz) at $\frac{N_y}{2}$ of the magnitude of the vectorial field of the curl of the displacement field (represented by colored arrows). Spatial distribution of the divergence of the displacement field have been added as an indicator of the propagation front. Remark that whitish arrows indicate a value almost equal to zero.

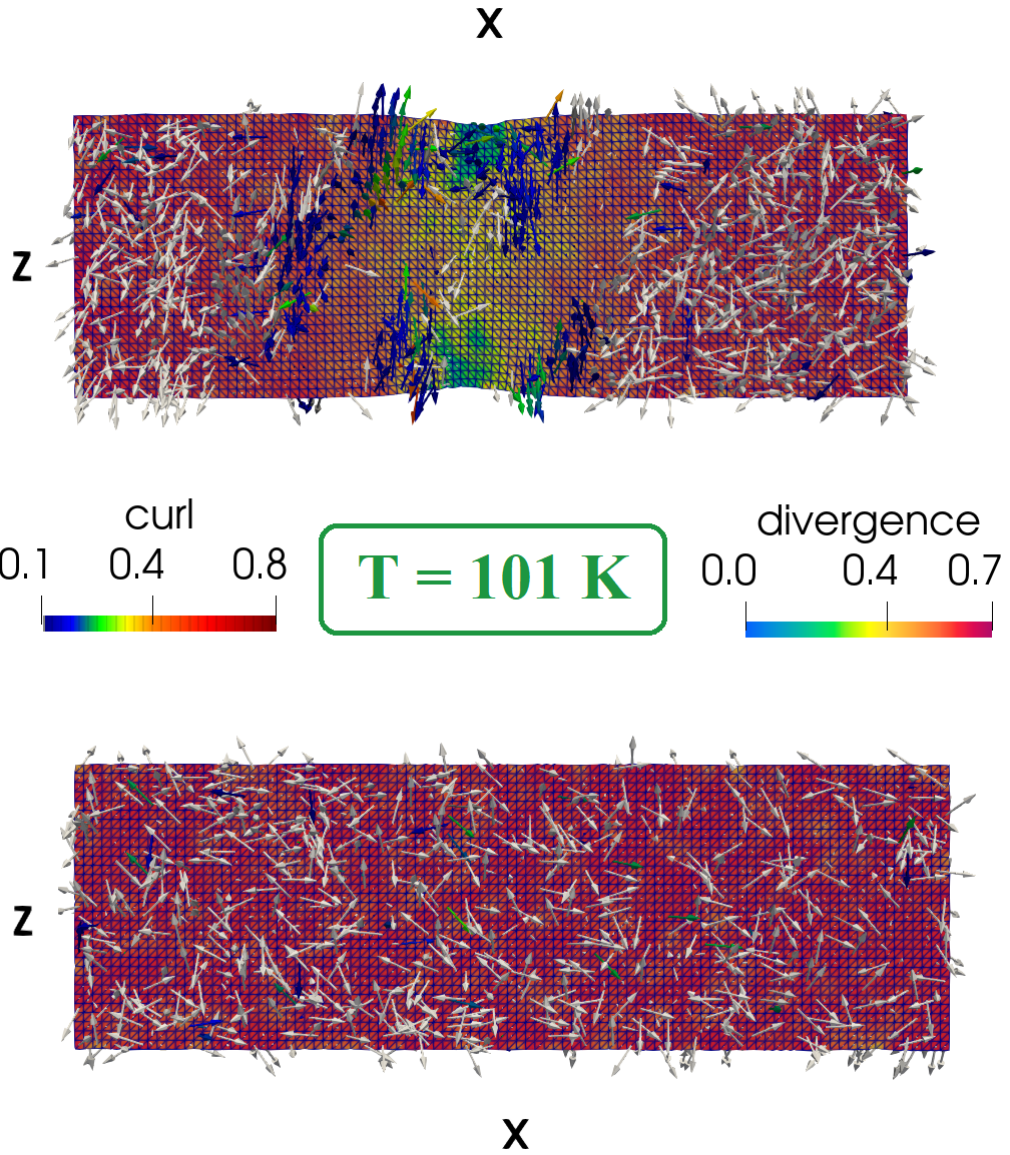


Figure S9 – Snapshots taken for $A_{1n} = 3\,000$ at $T = 101\text{ K}$ during the heating branch (top) and during the cooling branch (bottom), showing sectional view in the plane (xOz) at $\frac{N_y}{2}$ of the magnitude of the vectorial field of the curl of the displacement field (represented by colored arrows). Spatial distribution of the divergence of the displacement field have been added as an indicator of the propagation front. Remark that whitish arrows indicate a value almost equal to zero.

2.2 Relaxation process

2.2.1 Spatiotemporal configuration

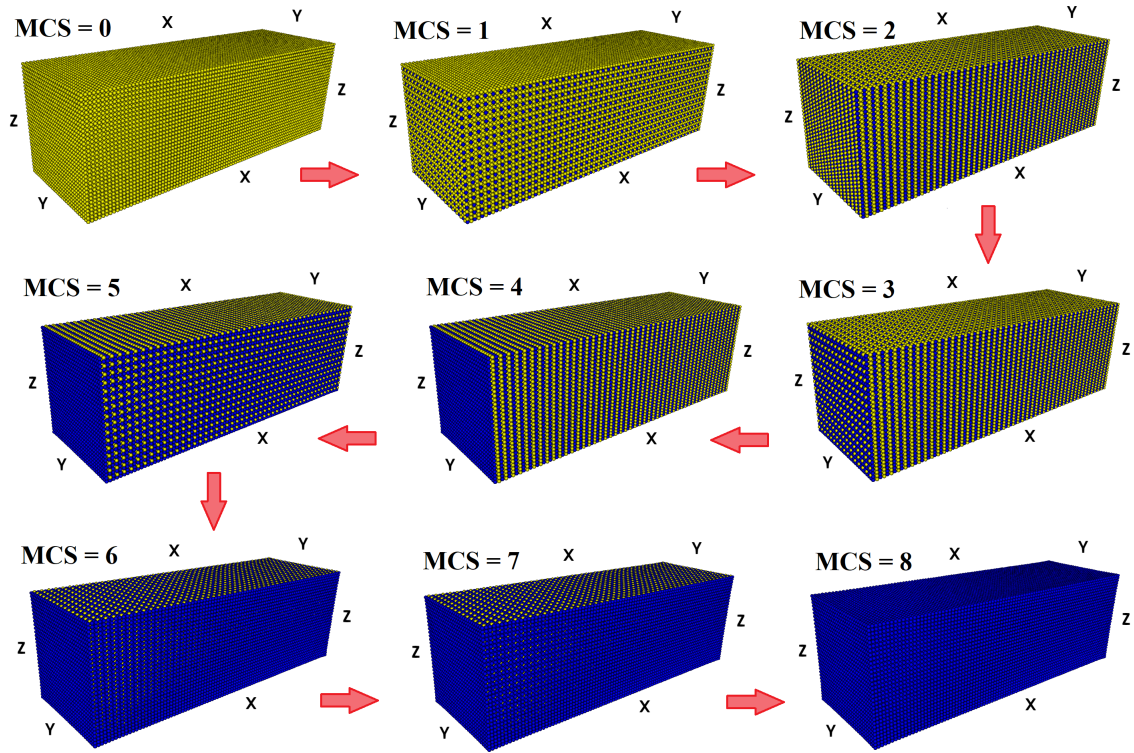


Figure S10 – Snapshots showing the spatiotemporal configurations of the lattice during the relaxation process at $T = 1K$ from an initial HS phase for a weak value $A_{1n} = 100$. Yellow (blue) spheres represent HS (LS) sites.

2.2.2 Local pressure field

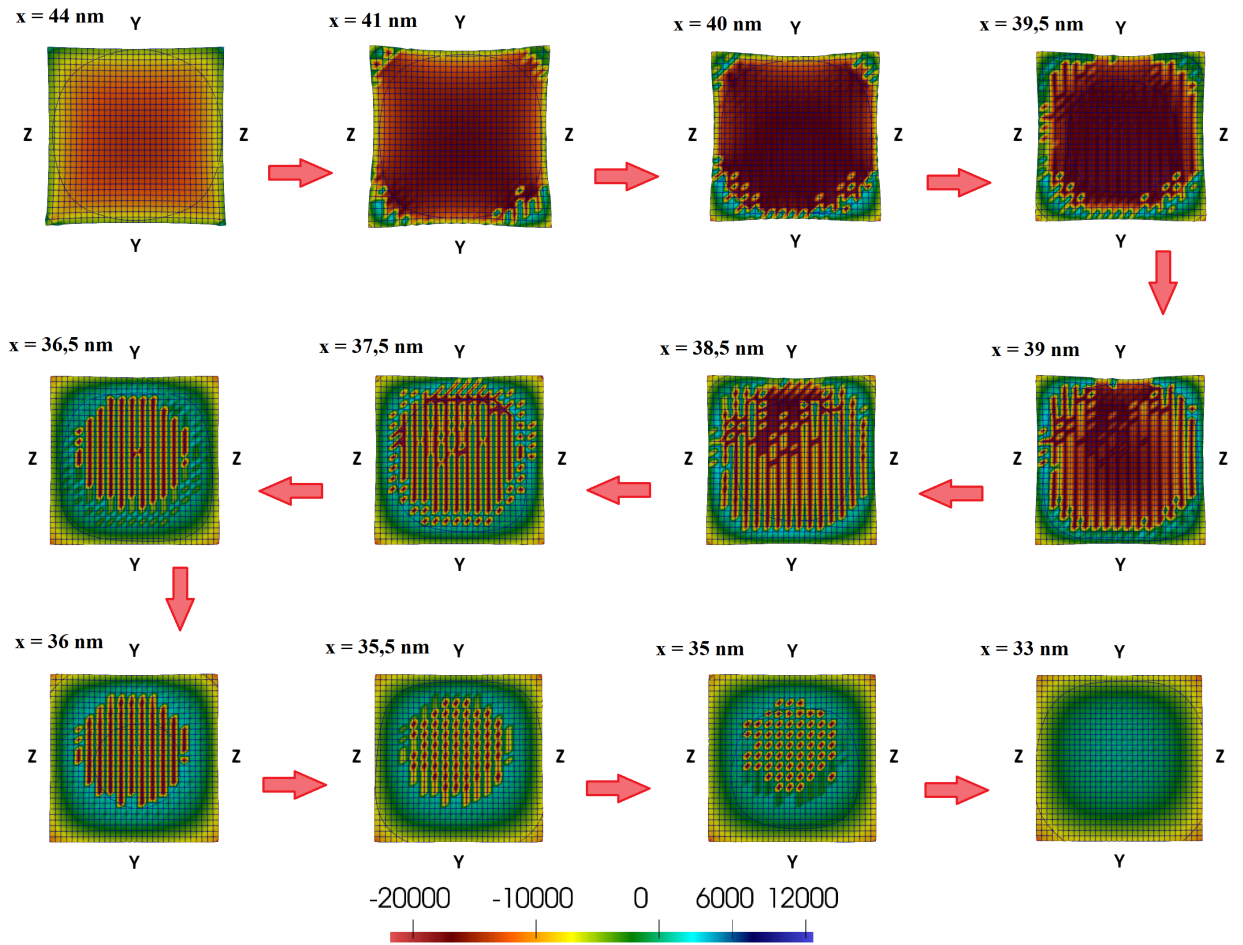


Figure S11 – Sectional view, related to Figure 15 of the main paper, showing the spatial distribution of the local pressure field of the lattice during the relaxation process at $T = 10K$ from an initial HS phase for a large value $A_{1n} = 8\,000$, in the planes (yOz) at various x direction values in front of and behind the interface, for 4 151 MCS.

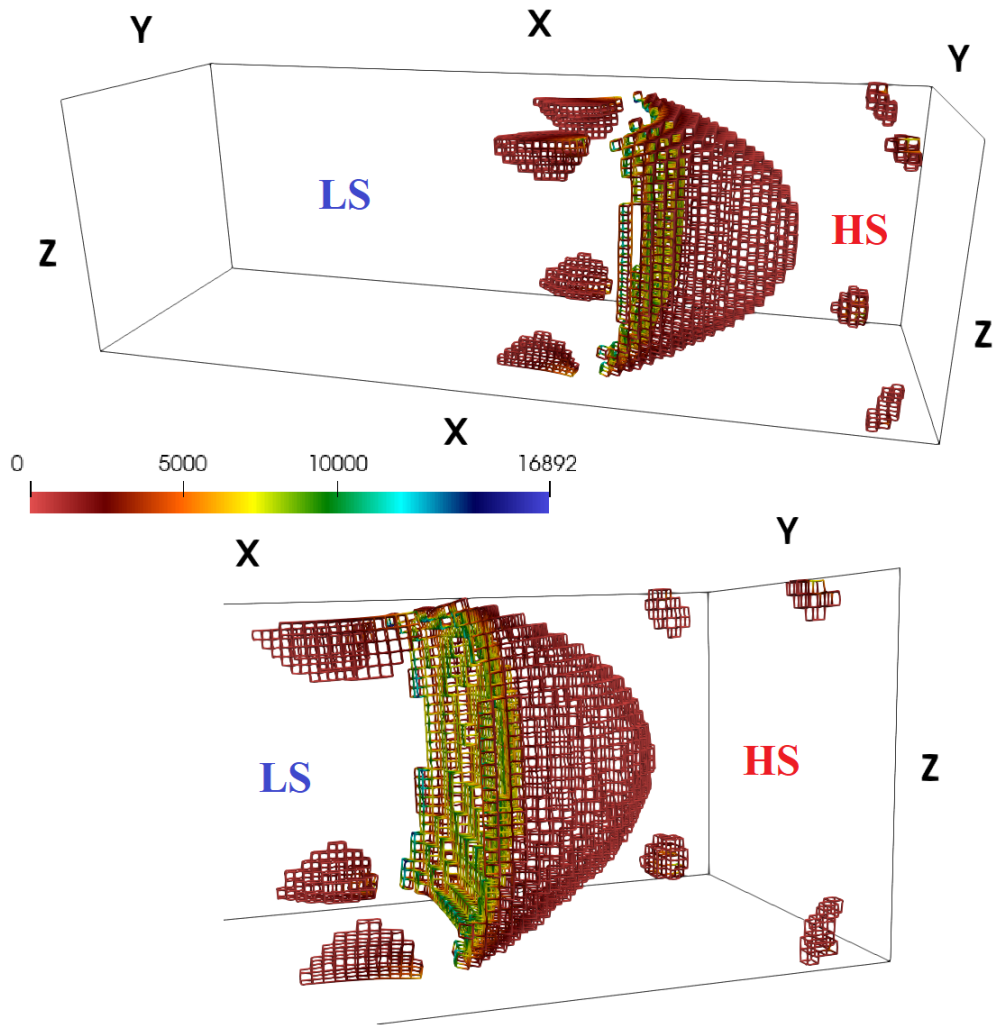


Figure S12 – Specific spatial distribution, related to Figure 15 of the main paper, of the local pressure field of the lattice during the relaxation process at $T = 10K$ from an initial HS phase for a large value $A_{1n} = 8\,000$ for 4 151 MCS: we only display the compressive strain (positive pressure). Remark the convexity of the propagating pressure wave along the x direction.

2.2.3 Local elastic energy field

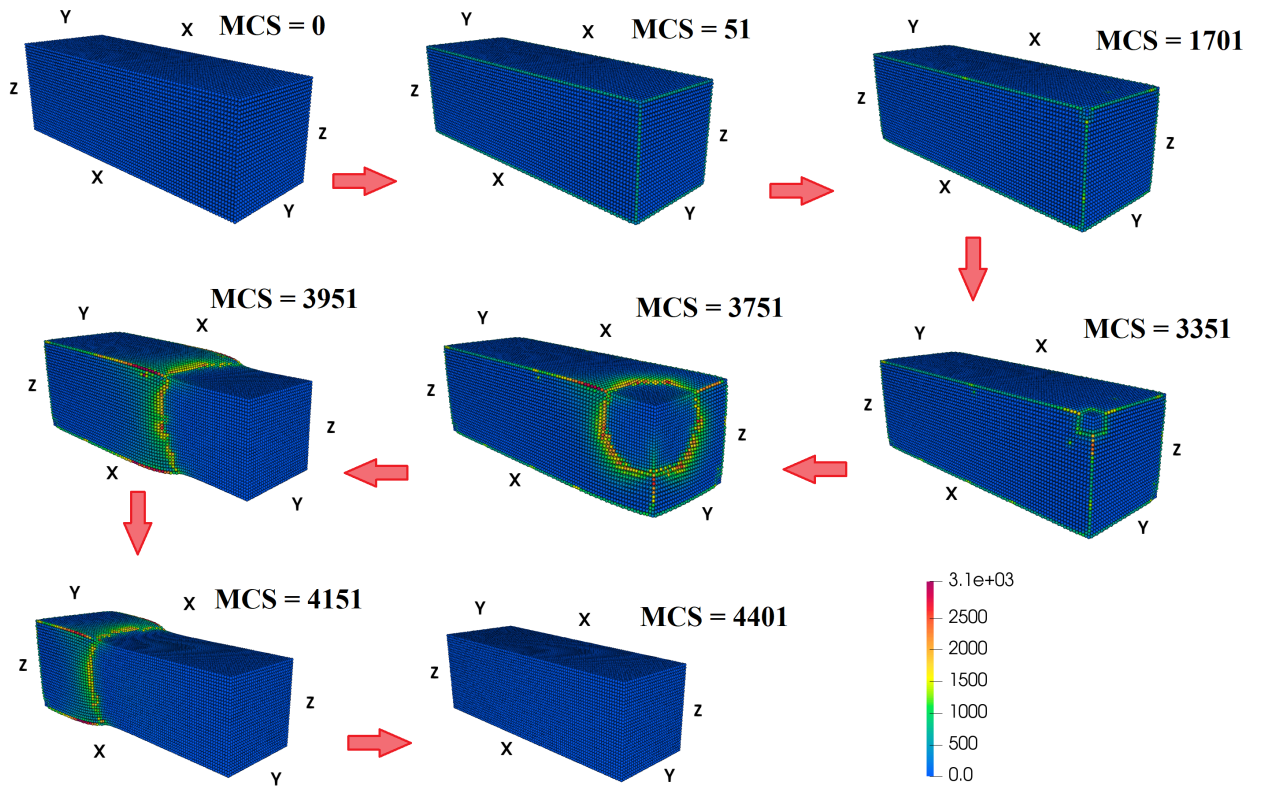


Figure S13 – Snapshots, related to Figure 18 of the main paper, showing the spatial distribution of the local elastic energy field during the relaxation process at $T = 10K$ from an initial HS phase for a large value $A_{1n} = 8\,000$.