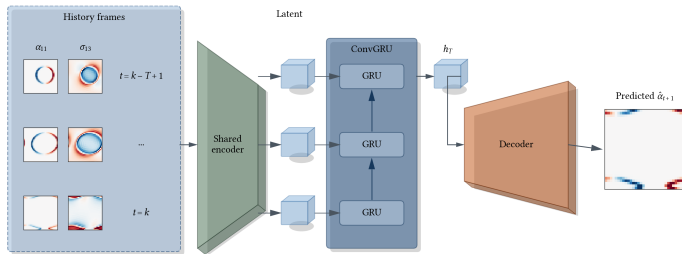
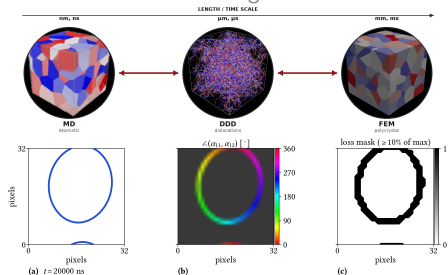


Learning a Nye-field update for mesoscale dislocation dynamics

Multiscale modeling of materials.

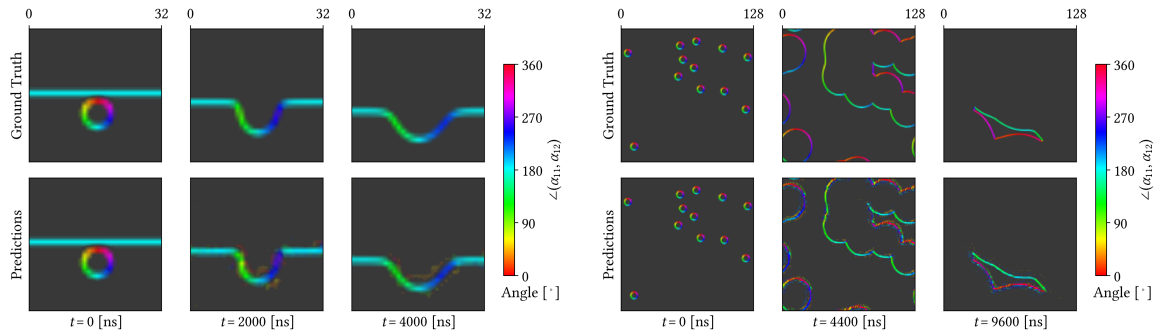


CNN-ConvGRU maps history of α & $\sigma \mapsto \hat{\alpha}_{t+1}$.

DDD graph $\rightarrow$ midplane $\alpha \rightarrow$ loss mask.

- Dislocations are **line defects** in materials that controls crystal plasticity.
- Discrete dislocation dynamics (DDD) is accurate, but long runs are expensive.
- The Nye tensor α stores dislocation Burgers vector and line direction as a voxelized field.
- We learn Nye dynamical update: $\hat{\alpha}_{t+1} = f_{\theta}(\alpha_{t-T+1:t}, \sigma_{t-T+1:t})$ with $T = 10$.
- Train on $\mathbb{R}^{32 \times 32}$ only. The network is fully convolutional, the trained model is evaluated at larger box.

The trained model transfers to larger boxes without retraining



Line and loop on 32×32 . Top: DDD benchmark. Bottom: CNN2D–ConvGRU predictions. Times 0/2000/4000 ns. Twelve loops on 128×128 (larger box), no retraining of the model. Times 0/4400/9600 ns.

- The trained model generalizes across different physical scenarios, e.g., annihilation, junction formations.
- The predictions preserve the dislocation core structure. Expansion and merging follow basic dislocation topological rules. Results show dislocation interactions on the glide plane.