

Extending a Physics-based Recrystallization Model using Genetic Programming

J. Kronsteiner¹, S. Raaber², S. Hovden¹, **G. Kronberger²**

Symposium on Symbolic Regression for Materials Science and Engineering,
29th September 2026, MSE Congress, Darmstadt

¹ LKR Light Metals Technologies, AIT Austrian Institute of Technology, Ranshofen, Austria

² University of Applied Sciences Upper Austria, Hagenberg, Austria

Extending a Physics-based Recrystallization Model using ~~Genetic Programming~~ LLM-based Symbolic Regression

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Introduction: Why microstructure prediction?

- Final grain structure affected by **extrusion parameters**.
- **Grain structure** controls **mechanical properties**.
- Experimental optimization is expensive.
- Predictive models needed for digital twins and **process optimization**:
 - **Physics-based** models provide **extrapolation** capability.
 - But: **calibration** parameters often have unknown process dependencies.

Process → FEM → **Microstructure** → Flow+ReX → **Mechanical Properties**

Prior work: Metal Extrusion Simulation Workflow

1. FEM process model

- Aluminum billet is pushed through a ruler-shaped die.
- Temperatures, strains, strain rates are exported.

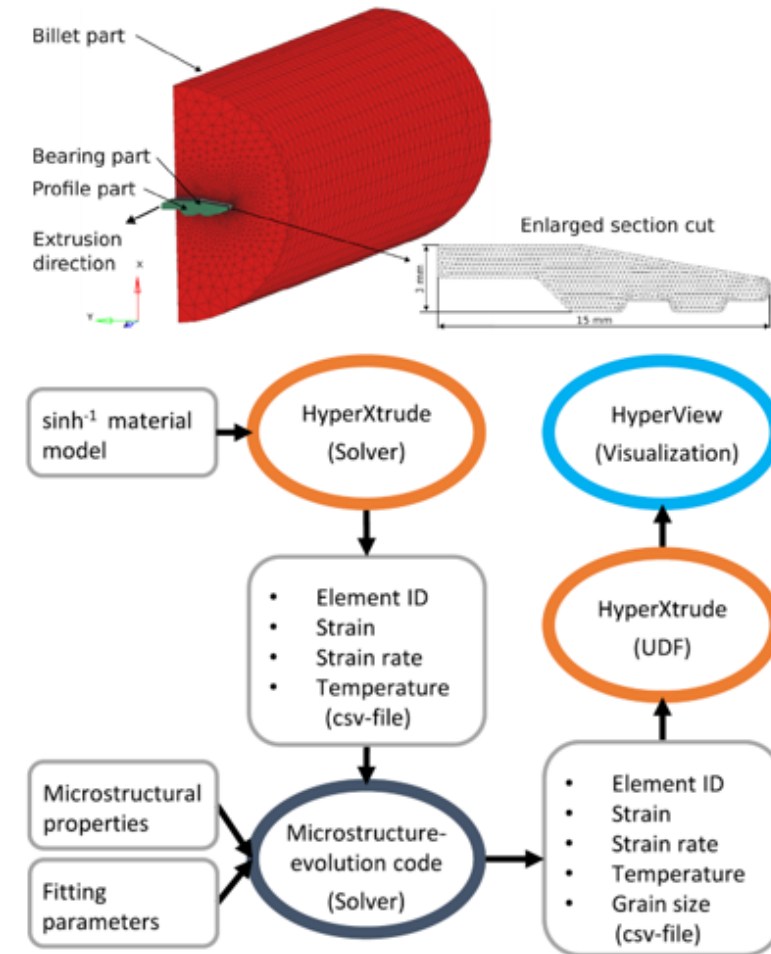
2. Streamline extraction

- Process parameters extracted from FEM model streamlines.
- Grain size evolution by parallel microstructure calculations.

3. Physics-based microstructure model tailored for 6xxx aluminum alloys

- deformation history (dislocation density-based flow stress)
- grain morphology (static and dynamic recrystallization)

Hovden, S. et. al. Parameter study of extrusion simulation and grain structure prediction for 6xxx alloys with varied Fe content, 2024-03, Materials Today Communications, Vol. 38, Elsevier BV, p. 108128



Prior work: Using Symbolic Regression to Extend a Physics-based Flow Stress Model

Workflow:

1. **Physics-based mean dislocation density-based flow stress model (MD²M)** with calibration parameters A,B,C
 - Current local flow stress $\sigma^t = f(\rho^t)$
 - $\Delta\rho^t = \rho^{t-1} + (\mathbf{A}\sqrt{\rho^{t-1}} - \mathbf{B}\rho^{t-1})\varphi - \mathbf{C}T^{-1}[(\rho^{t-1})^2 - \rho_{eq}^2] \cdot \Delta t$
 - t: time, ρ : dislocation density, φ : strain rate, T: temperature
2. Collect **experimental data** from compression tests (temperature and strain-rate dependent)
3. Use **genetic programming and symbolic regression**
 - find **short expressions** for $A(\dot{\varphi}, T, \theta_A)$, $B(\dot{\varphi}, T, \theta_B)$, $C(\dot{\varphi}, T, \theta_C)$
 - simulate and
 - fit predicted flow stress to experimental data.

Kronberger, Kablman, Kronsteiner, Kommenda, Extending a physics-based constitutive model using genetic programming, 2022-03, Applications in Engineering Science , Vol. 9, Elsevier BV, p. 100080

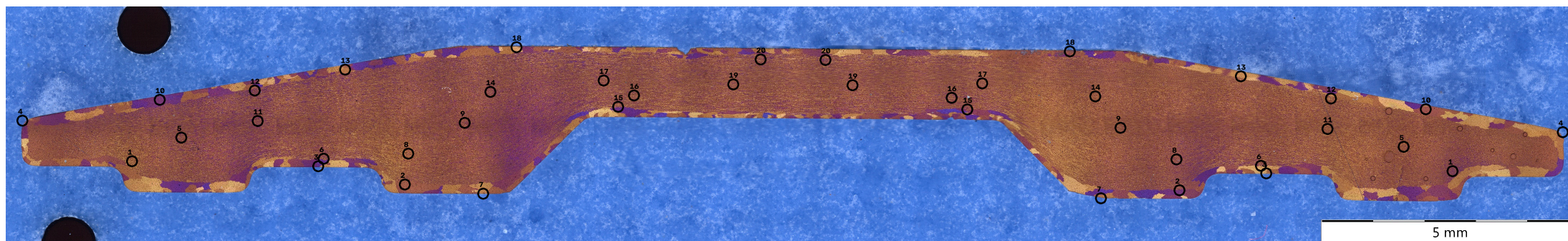
Can this approach be applied to the recrystallization model?

Original Goal: predict grain size

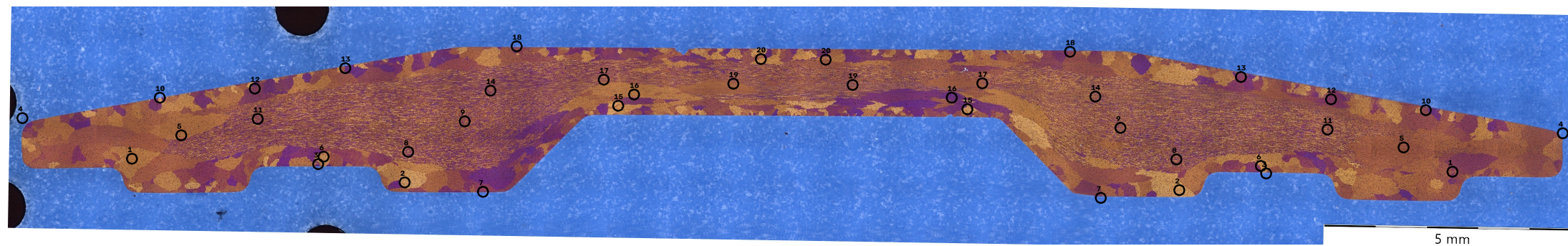
Method

- Data
 - **FEM extrusion simulations** with varied process parameters (Ram speed)
 - **Cross-section images** of the extruded profile
 - Currently limited to a single alloy (AA6005A)
- **Physics-based recrystallization model** with multiple components (in Fortran / translated to Julia)
 - Static and dynamic recrystallization: Johnson-Mehl-Avrami-Kolmogorov (JMAK) and Kocks-Mecking
 - Geometric dynamic recrystallization (**gDRX**): breakage during forming
 - Continuous dynamic recrystallization (**CDRX**): lattice rotations
 - Improved static recrystallization (**SRX**): grain-boundary and particle-stimulated nucleation (**PSN**),
- Replace selected **calibration parameters** by short **physics-based expressions** to improve the model's predictive capabilities.

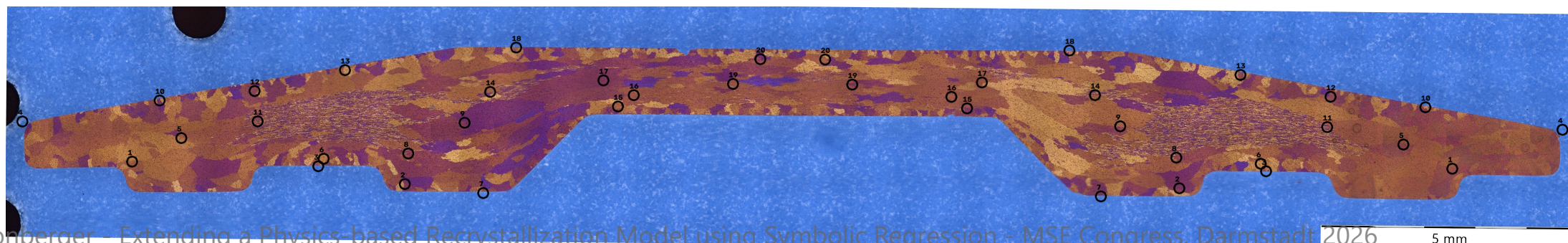
RS 1mm/s:

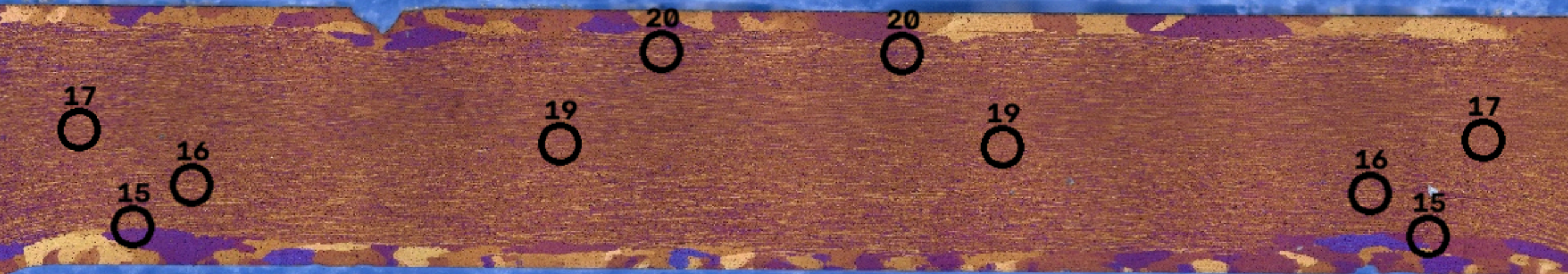


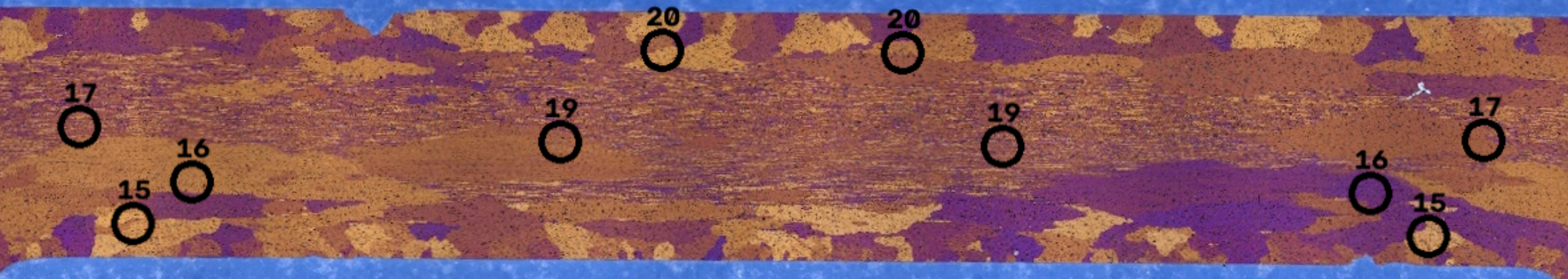
RS 2mm/s:



RS 4mm/s:







Updated Method

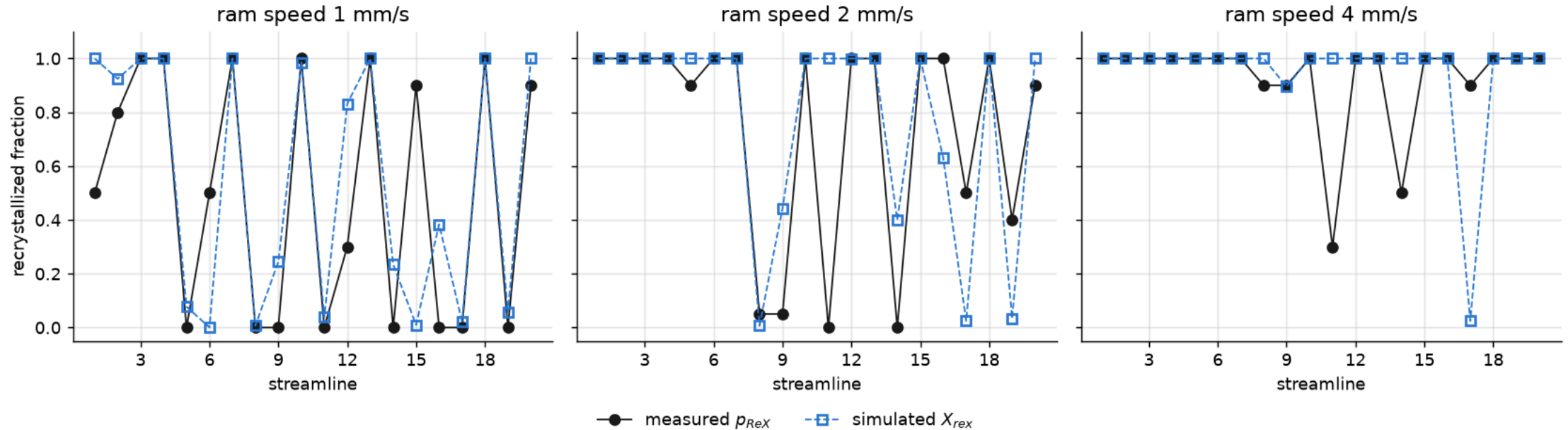
New (simplified) goal: **predict recrystallized fraction**

- Optimization objective: binary crossentropy of **predicted recrystallized fraction** p_{ReX} and **eyeball-based ground truth** from cross-section images.
- Use **agentic AI** in an **evolutionary loop** to propose adaptations to the model:
 - Improve predictive accuracy.
 - Adaptations must be **physics-driven and interpretable**.
 - Reduce number of calibration parameters
 - Optimize calibration parameters using CMA-ES (Covariance Matrix Adaptation Evolution Strategy) to fit the model to the experimental data.

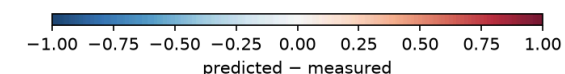
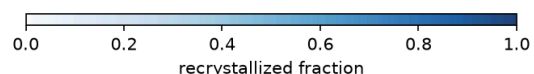
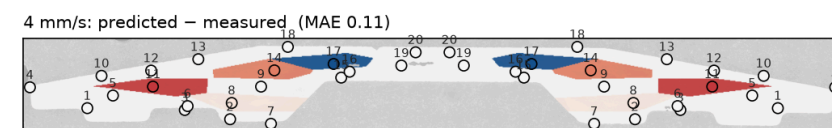
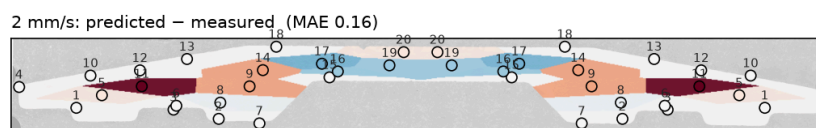
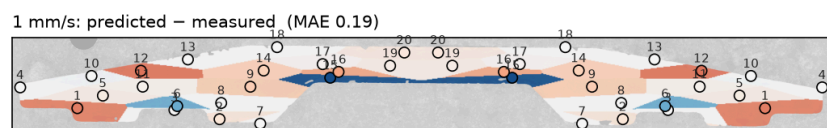
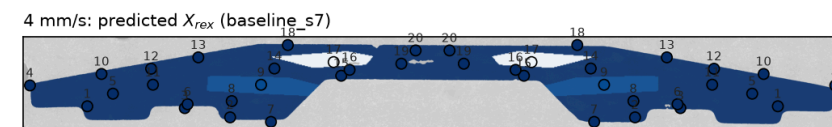
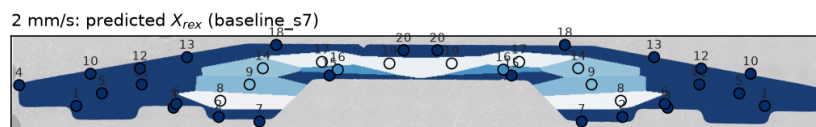
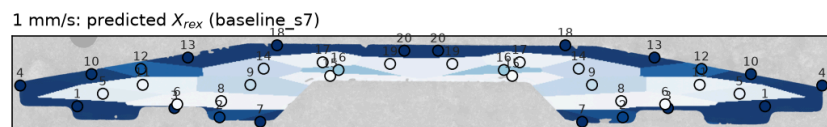
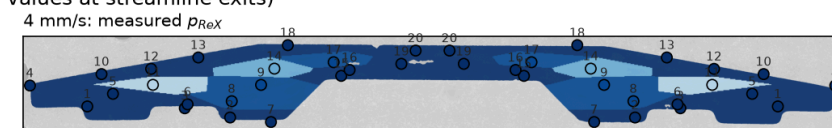
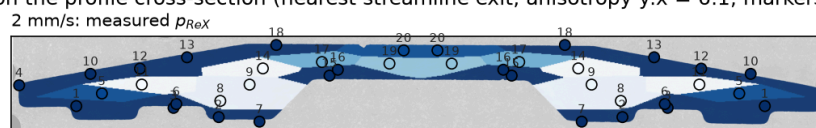
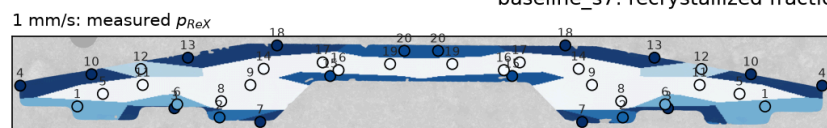
Results: Starting point

Carefully extended model by human expert + AI bugfixing

baseline_s7: best fit (BCE = 1.044)
xC_cdrx=4.44, CGB_fit=4.96e+04, Qn=1.75, N_v=4.57e+16
gamma_star=1.63

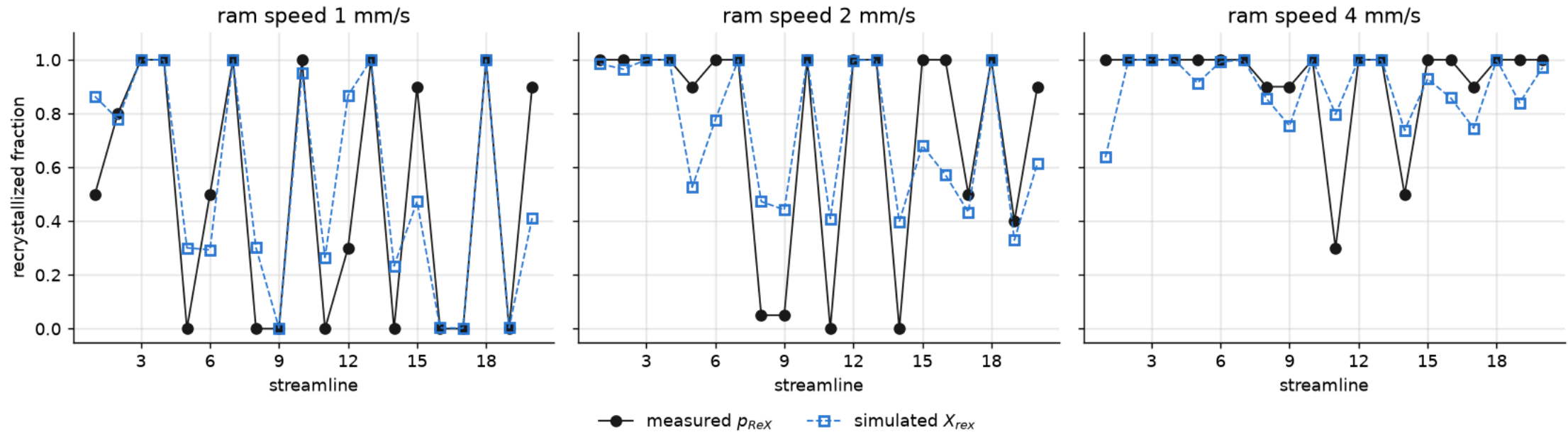


baseline_s7: recrystallized fraction on the profile cross-section (nearest streamline exit, anisotropy y:x = 6:1; markers = values at streamline exits)



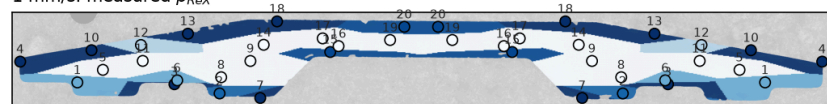
Results: Improved model

es_rec_gs: best fit (BCE = 0.283)
xC_cdrx=0.163, Qn=2.5, N_v=3.06e+16, CGB_ref=1.13e-03
gb_mob_fac=2.36, rec_fac=9.46e-03

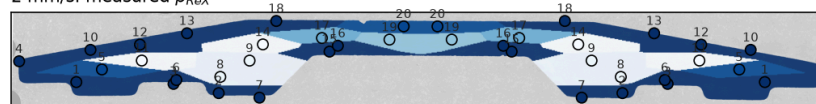


es_rec_gs: recrystallized fraction on the profile cross-section (nearest streamline exit, anisotropy y:x = 6:1; markers = values at streamline exits)

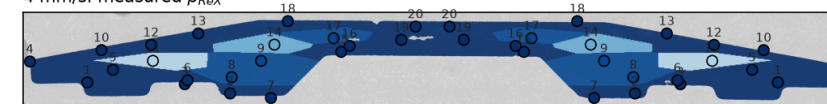
1 mm/s: measured p_{ReX}



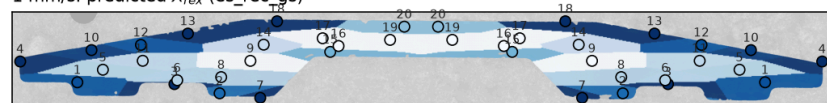
2 mm/s: measured p_{ReX}



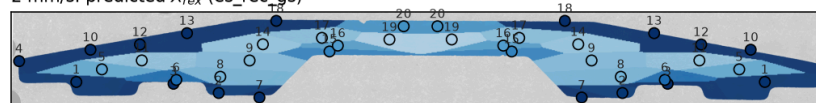
4 mm/s: measured p_{ReX}



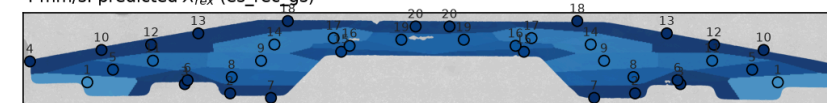
1 mm/s: predicted X_{rex} (es_rec_gs)



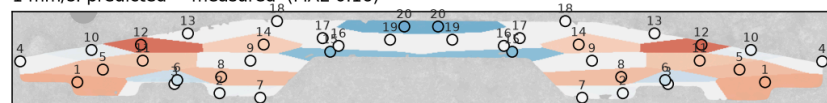
2 mm/s: predicted X_{rex} (es_rec_gs)



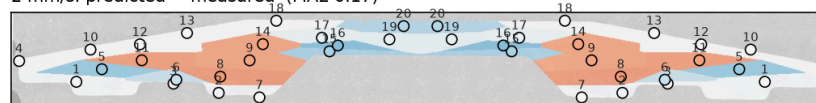
4 mm/s: predicted X_{rex} (es_rec_gs)



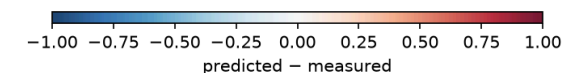
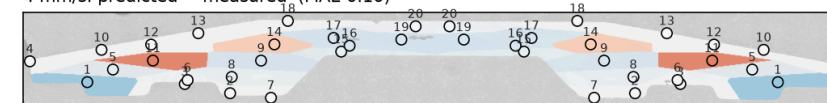
1 mm/s: predicted – measured (MAE 0.16)



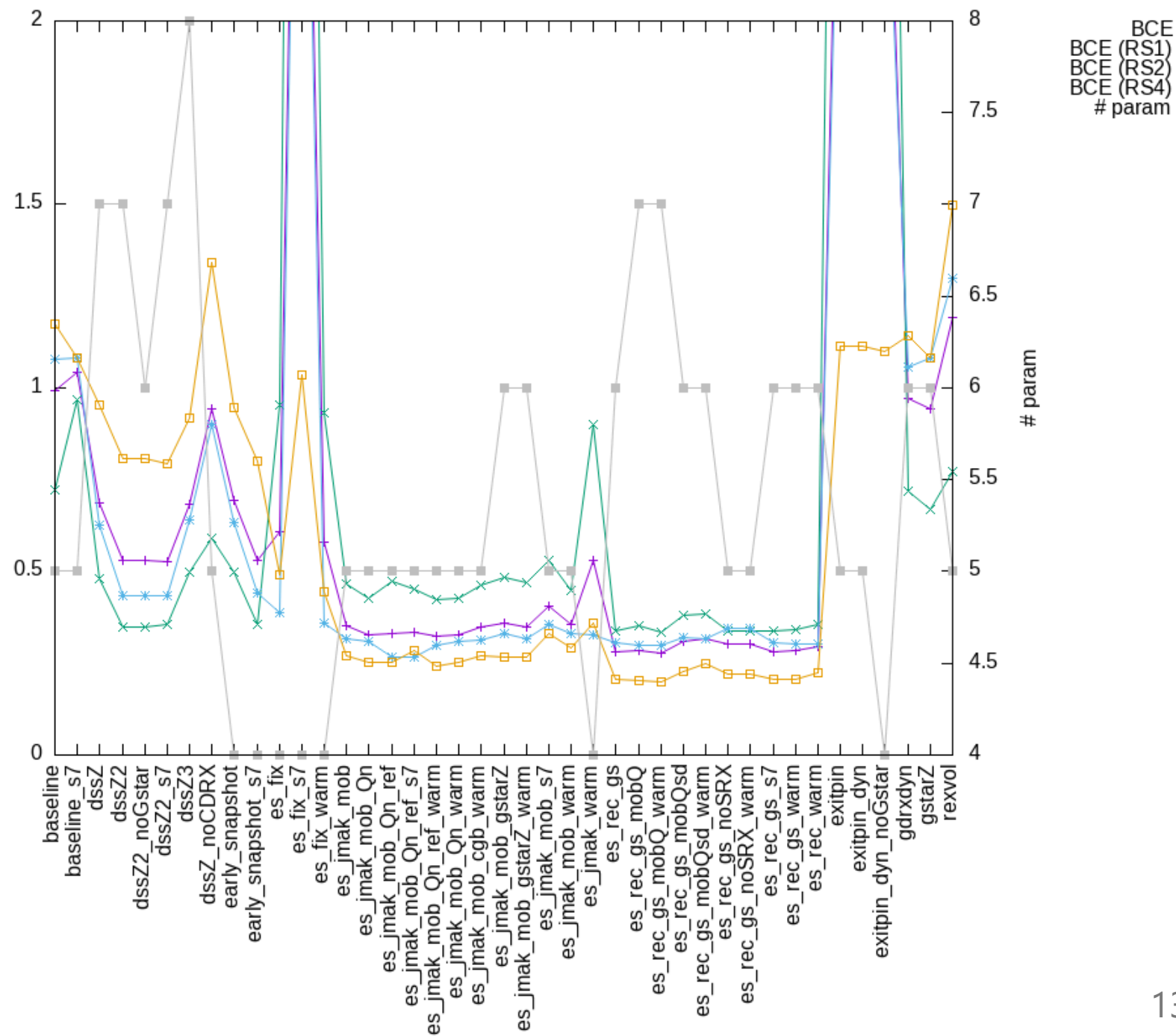
2 mm/s: predicted – measured (MAE 0.17)



4 mm/s: predicted – measured (MAE 0.10)



Evolutionary progress



Conclusions

- AI-driven SR was able to find several **bug-fixes and physics-driven improvements** to the model
- Data **uncertainty and sharp transitions** make it hard to fit the model to the data
- Competing physical mechanisms make it hard to calibrate model parameters
- AI-driven SR is also **prone to overfitting**, trying to optimize the loss even though the data is limited.

Conclusions

- AI-driven SR was able to find several **bug-fixes and physics-driven improvements** to the model
- Data **uncertainty and sharp transitions** make it hard to fit the model to the data
- Competing mechanisms make it hard to calibrate model parameters
- AI-driven SR is also **prone to overfitting**, trying to optimize the loss even though the data is limited.

Outlook

- **Increase data quality and quantity**: higher spatial resolution, better ground truth labels, more alloy variants
- **Sensitivity analysis** for each part of the model:
 - Use the **automatically differentiable model to backpropagate the loss** through the model
- **Vision**:
 - Minimum description length provides **principled model selection**
 - LLM-based agentic evolutionary loops provides automated physics-based model adaptations

Questions

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gabriel.kronberger@fh-ooe.at

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