

Speaker Notes – Master’s Thesis Status Talk

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February 20, 2026

Slide 1: Title

Today I present the current status of my master’s thesis. The focus of this talk is not on final performance numbers, but on understanding how well machine-learning-based surrogate models can generalize to increasingly complex geometries in a physically constrained flow problem.

I will mainly discuss what already works reliably, where current limitations appear, and how these observations motivate the next steps of the project.

Slide 2: Outlook

We will start with a brief motivation and introduce the central research question. I will then outline the relevant physical background and the chosen learning strategy. After that, I will present selected results focusing on generalization behavior. Finally, I will discuss current limitations and possible next steps.

Slide 3: Motivation

In magmatic systems, changes in temperature, pressure, and chemical composition can lead to crystallization along well-known differentiation and unmixing sequences. Once formed, these crystals are typically denser than the surrounding melt and start to sink.

During this process, crystals interact with the surrounding viscous magma and with each other through the induced flow field. Over geological timescales, this leads to crystal accumulation at the chamber floor and can contribute to the formation of economically relevant ore deposits.

Crystal sedimentation in viscous magmas therefore plays a key role in magmatic differentiation, the formation of cumulates, and the internal dynamics of magma chambers.

Even at very low Reynolds numbers — meaning that inertial effects are negligible and viscous forces dominate — individual crystals induce long-range flow perturbations in the surrounding melt.

When multiple crystals are present, these perturbations interact in a highly non-trivial way. Even in the Stokes regime, particles do not simply sediment independently.

Instead, hydrodynamic interactions can lead to complex collective dynamics such as drafting–kissing–tumbling behavior, wake capture, and repeated particle reordering. Small changes in relative position, orientation, or particle shape can qualitatively change the interaction outcome.

As a result, the flow field is extremely sensitive to geometry, even though the governing Stokes equations themselves are linear.

Understanding and efficiently predicting these interactions is therefore a relevant challenge in geophysical modeling.

In this thesis, I address this challenge by investigating whether physically informed convolutional neural networks can act as surrogate models for viscous flow, and—crucially—how well such models generalize as geometric complexity increases.

Slide 4: Why This is a Hard Problem

Although Stokes flow is linear, it is not local. Instead, it is:

- globally coupled,
- highly sensitive to geometric details,
- dominated by long-range interactions.

Already a small number of crystals can lead to complex interaction patterns. Well-known examples include drafting–kissing–tumbling dynamics, clustering, and screening effects.

These interaction patterns depend strongly on relative positions and distances, which makes the problem particularly challenging for data-driven models.

Slide 5: Computational Challenge

Accurately resolving these flow fields requires fully resolved Stokes simulations. While such simulations are feasible for individual configurations, they become computationally expensive when used for systematic parameter studies or large ensembles of geometries.

In particular, the computational cost increases rapidly with the number of crystals.

This practical limitation strongly shaped the direction of this thesis. Rather than aiming to replace high-fidelity simulations, the goal is to explore whether fast surrogate models can reproduce their essential flow characteristics and, crucially, generalize beyond the configurations they were trained on.

This motivates the use of surrogate models that can approximate full flow fields much faster, while still respecting the underlying physical structure of the problem.

The central research question of this thesis is therefore:

How well can convolutional neural networks generalize flow-field predictions as geometric complexity increases?

Importantly, the goal is not interpolation between nearly identical configurations, but generalization to qualitatively new crystal arrangements.

Slide 6: Physical Background

The considered flows are governed by the incompressible Stokes equations. In this regime, inertial terms are negligible and the balance is dominated by viscous stresses and body forces.

A key constraint is incompressibility:

$$\nabla \cdot \mathbf{v} = 0$$

Physically, this means that the fluid cannot locally accumulate or vanish: any inflow into a region must be balanced by an equal outflow.

This constraint plays a central role when choosing a physically meaningful learning target for neural networks.

Slide 7: Stream Function

In two dimensions, incompressible flow can be represented using a stream function $\psi(x, z)$.

The velocity components are obtained as:

$$v_x = \frac{\partial \psi}{\partial z}, \quad v_z = -\frac{\partial \psi}{\partial x}.$$

By construction, this formulation satisfies the incompressibility condition exactly.

A second advantage is that the learning target is reduced from a vector-valued field to a single scalar field with smoother spatial structure.

For these reasons, the stream function is a natural and physically motivated learning target for convolutional neural networks.

Slide 8: Stream Function Solution

The stream function is obtained by solving a Poisson equation of the form

$$\Delta \psi = -\omega,$$

where ω denotes the vorticity.

In this project, LaMEM directly provides the necessary quantities. The stream function is therefore treated as a derived but physically consistent output of the reference simulations.

Due to the extremely small magnitude of ψ (typically 10^{-12} – 10^{-15}), each sample is RMS-normalized individually to ensure numerical stability during training.

Slide 9: Learning Strategy

In principle, three learning strategies are possible:

- direct prediction of velocities,
- prediction of the stream function,
- residual learning relative to an analytical reference solution.

All approaches use the same network architecture and training setup. Only the learning target is changed.

At the current stage of the project, I focus exclusively on the stream function approach, as it provides the most physically consistent and interpretable results so far.

Slide 10: Data

All training and evaluation data are generated using LaMEM as a reference solver. The simulations are performed in two dimensions on a fixed 256×256 grid, representing a 2×2 km magma chamber cross-section.

At the current stage, the training data consists of configurations with one, two, or three crystals. Crystal positions are randomized, while material parameters are kept fixed.

This setup allows for a controlled investigation of geometric generalization while keeping computational costs manageable. Extensions to larger crystal numbers are ongoing.

Slide 11: Input Representation

The input to the neural network consists of five channels.

A binary crystal mask encodes the phase distribution. Geometric proximity is represented using a signed distance field expressed in units of the nearest crystal radius, which provides a scale-invariant description of the geometry.

In addition, the radius of the nearest crystal is supplied as an explicit input channel, allowing the network to model size-dependent effects.

Finally, normalized spatial coordinates are included to encode absolute position within the domain and to reduce grid-aligned artefacts.

All input channels are normalized to comparable magnitudes to improve numerical stability and training convergence.

Slide 12: Architecture

A U-Net architecture is used throughout the thesis. Its encoder-decoder structure with skip connections provides multi-scale receptive fields, which align well with the long-range nature of Stokes flow.

The network consists of four encoder blocks, a bottleneck layer, and four decoder blocks.

Strided convolutions are used instead of max pooling, allowing the network to learn how spatial information is downsampled. This improves accuracy for geometrically sensitive problems.

The same architecture is used for all experiments to ensure comparability.

Slide 13: Training Setup

For each crystal configuration, approximately 4000 training samples are used. The models are trained for 300 epochs with a fixed learning rate and batch size.

All evaluations shown in this talk are performed on geometries that were not seen during training, ensuring that the reported errors reflect true generalization performance.

The Adam optimizer is used as a robust default choice.

In addition to a mean-squared error loss on the stream function, a gradient-based loss term is introduced. This term penalizes errors in the spatial derivatives of ψ .

The gradient loss is computed in physical units using the grid spacing, ensuring scale-consistent regularization of the reconstructed velocity field. This is motivated by the fact that small errors in ψ can be strongly amplified by numerical differentiation.

Slide 14: Results – Single Crystal

For the single-crystal case, the stream function is predicted with relative L^2 errors on the order of 10^{-2} . The large-scale structure and symmetry of the flow field are well reproduced.

Velocities reconstructed from the predicted stream function show larger relative errors, as expected due to the amplifying effect of numerical differentiation.

Quantitatively, the results are:

$$\text{rel } L^2(\psi) : \quad \mu = 2.09 \times 10^{-2}, \quad \sigma = 1.13 \times 10^{-2},$$

$$\text{rel } L^2(|\mathbf{v}|) : \quad \mu = 1.67 \times 10^{-1}.$$

Slide 16: Visualization – One Crystal

[Arbeit/Bilder/sample_0002_psi.png]
 Arbeit/Bilder/sample_0002_speed_frompsi_psi.png

Slide 17: First Generalization – Two Crystals

Based on the strong single-crystal results, the same model is evaluated on configurations with two crystals.

[Arbeit/Bilder/sample_00015_psi.png]
 Arbeit/Bilder/sample_00015_speed_frompsi_psi.png

Slide 18: First Generalization – Three Crystals

The same evaluation is performed for three-crystal configurations.

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 Arbeit/Bilder/sample_00021_speed_frompsi_psi.png

Slide 19: Results – Multiple Crystals

When increasing the number of crystals from one to three, the stream function error remains remarkably stable.

This indicates that the model captures dominant interaction patterns rather than memorizing individual configurations. However, certain interaction regions remain challenging.

Slide 23: Velocity Artefacts

Why do line-like artefacts appear in the velocity magnitude?

The neural network predicts the stream function ψ , not the velocity directly. Velocities are reconstructed via spatial derivatives:

$$v_x = \partial_z \psi, \quad v_z = -\partial_x \psi.$$

Although the predicted stream function is visually smooth, small grid-aligned errors remain. These errors are barely visible in ψ itself, but are strongly amplified by numerical differentiation, which acts as a high-pass filter.

As a result, stripe-like artefacts appear in the velocity magnitude. This is not a physical effect, but a numerical consequence of differentiating a learned field without explicitly constraining its gradients.

The gradient-based loss significantly reduces these artefacts by enforcing derivative consistency during training.

Slide 24: Outlook

The next major step of the thesis is residual learning relative to an analytical stream function.

In this approach, the neural network learns only the deviation between a known analytical solution and the numerical reference. This reduces the dynamic range of the learning target and focuses the model on interaction-driven corrections.

Initial experiments with this approach are currently starting.

Backup: Fourier Neural Operators

Fourier Neural Operators are a powerful class of models for learning global operators. However, they implicitly assume translation invariance and global smoothness.

The present problem is dominated by localized geometric inclusions and non-periodic boundary conditions. At this stage, a U-Net provides better control over locality and interpretability.

Fourier-based operator learning remains an interesting future direction, but establishing a physically interpretable baseline is the current priority.