# Active Learning-Assisted Optimization of Magnetic Nanostructures

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## ABSTRACT

**Micro- and nanostructural design of magnetic materials is the most promising strategy for future high-performance but rare earth-lean permanent magnets. Exchange coupled composites combine materials with high magnetocrystalline anisotropy and others with high spontaneous magnetization. It is still unclear, which nanostructural spatial distribution of these materials is advantageous for a high energy density.**

**We use a Convolutional Neural Network, trained by micromagnetic simulations, to predict the energy density from a given distribution. The neural network serves as a surrogate model for optimizing the spatial distribution and is retrained in an active learning cycle.**

## COOPERATION

MATHEMATICS - MAGNETISM - MATERIALS

wpi

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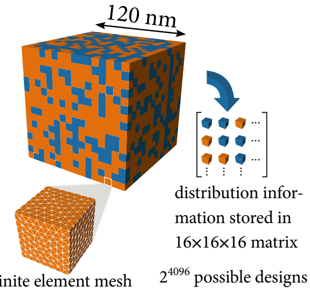
## 1 Micromagnetic simulations

A cube with an edge length of 120 nm is divided into 16 × 16 × 16 cuboid cells of 7.5 nm, each of which can take the properties of either hard or soft magnetic material. After further discretization into a finite-element mesh, a massively parallelized micromagnetic code[1] is used to compute the demagnetization curves of arbitrary phase distributions. The energy density product $BH_{max}$ is extracted from the curve.

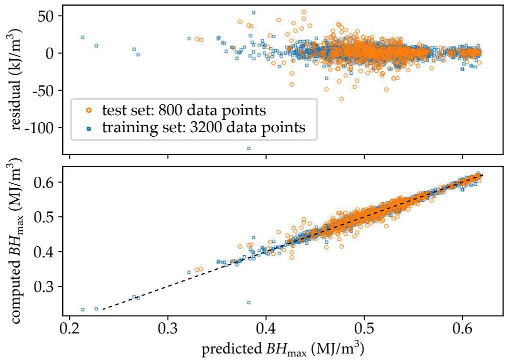
**$Fe_{65}Co_{35}$** (Soft magnetic):
$\mu_0 M_s = 2.54$ T
$A_x = 35$ pJ/m
$K_u = 0$ MJ/m$^3$

**$Nd_2Fe_{14}B$** (Hard magnetic):
$\mu_0 M_s = 1.61$ T
$A_x = 7.7$ pJ/m
$K_u = 4.3$ MJ/m$^3$



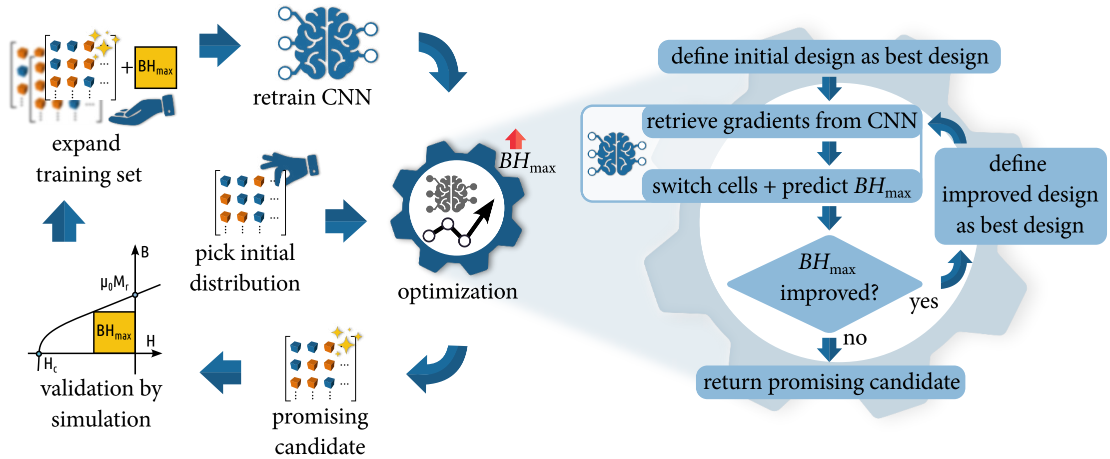

## 2 Convolutional Neural Network

A neural network was designed[3] to predict the energy density product $BH_{max}$ of the magnet by a given phase distribution. The model was trained using both random phase distributions and specific distributions assumed to perform well. After tuning of hyper-parameters, an $R^2$-score of 95% was achieved for the unseen test set.



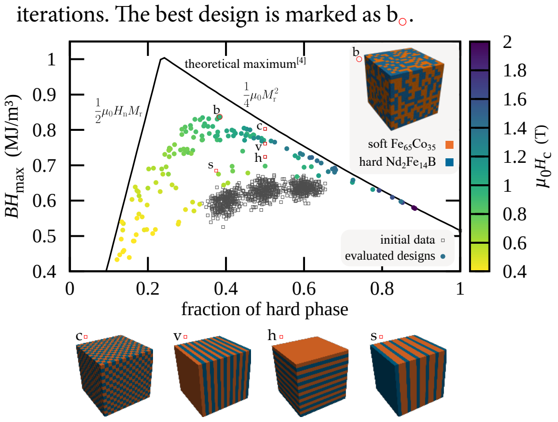

## 3 Optimization

The Convolutional Neural Network is used as a surrogate model in an optimization loop to accelerate the search for the best spatial distribution of hard and soft magnetic phases. An adapted binary search algorithm[2] is applied, with the maximization of $BH_{max}$ as the objective function. The algorithm takes advantage of the gradients provided by the CNN to determine which cells should change material in order to enhance $BH_{max}$. Additionally, the CNN is used for a rapid evaluation of $BH_{max}$ during optimization.




## 4 Results

The colored dots represent the validated designs proposed by the active learning scheme at different iterations. The best design is marked as b.




## 5 Conclusion

- Key magnetic properties can be predicted from the magnetic phase distribution by a CNN.
- Fast predictions and an active learning scheme can be used in an optimization framework to find beneficial phase distributions.
- The active learning optimization scheme found superior phase distributions beyond kown ones, including the checkerboard pattern (see c in Results).

## References

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