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Variational Autoencoder Performance Study

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1. Abstract

This project leverages a Variational Autoencoder (VAE) architecture to generate novel microstructure images for material science applications. The primary goal is to enhance the understanding of microstructures by synthesizing realistic and diverse images that can be used for simulation, analysis, and material design. The VAE model, a generative deep learning approach, is trained on a dataset of existing microstructure images to learn the underlying distribution of the material features, including grain patterns, porosity, and other microstructural characteristics. By encoding the images into a latent space and sampling from this space, the model generates new images that retain the statistical properties of the training data while offering variations that could represent different material configurations. The generated images are evaluated through visual inspection and quantitative metrics to assess their quality and relevance. This work aims to push the boundaries of computational material science, providing a tool for researchers to explore new microstructural configurations and gain deeper insights into material behaviors.

2. Model Problem

The dataset Brands et al. [2016] used for training the VAE consists of reconstructed dual-phase steel microstructures obtained from EBSD measurements.

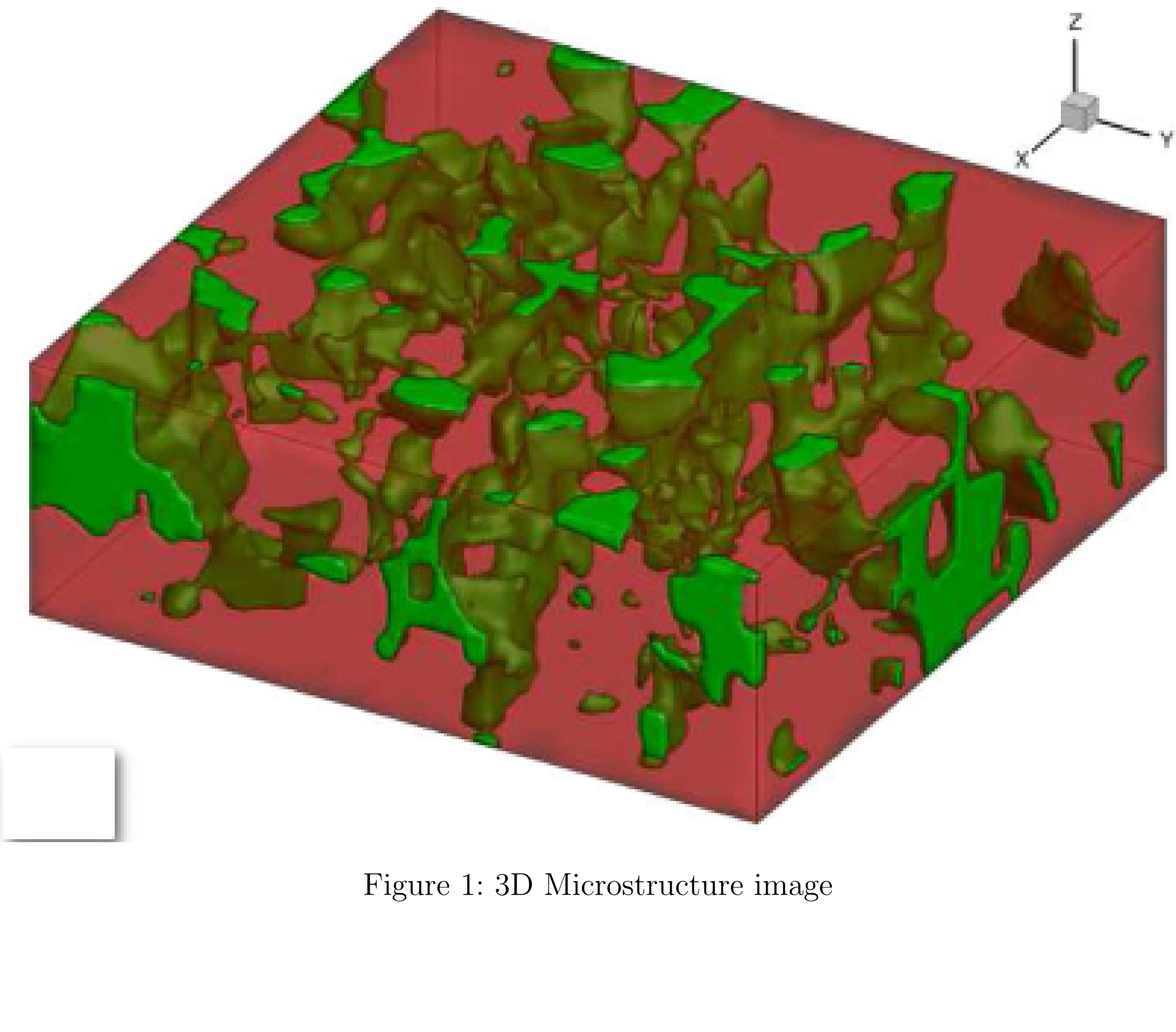

Figure 1: 3D Microstructure image

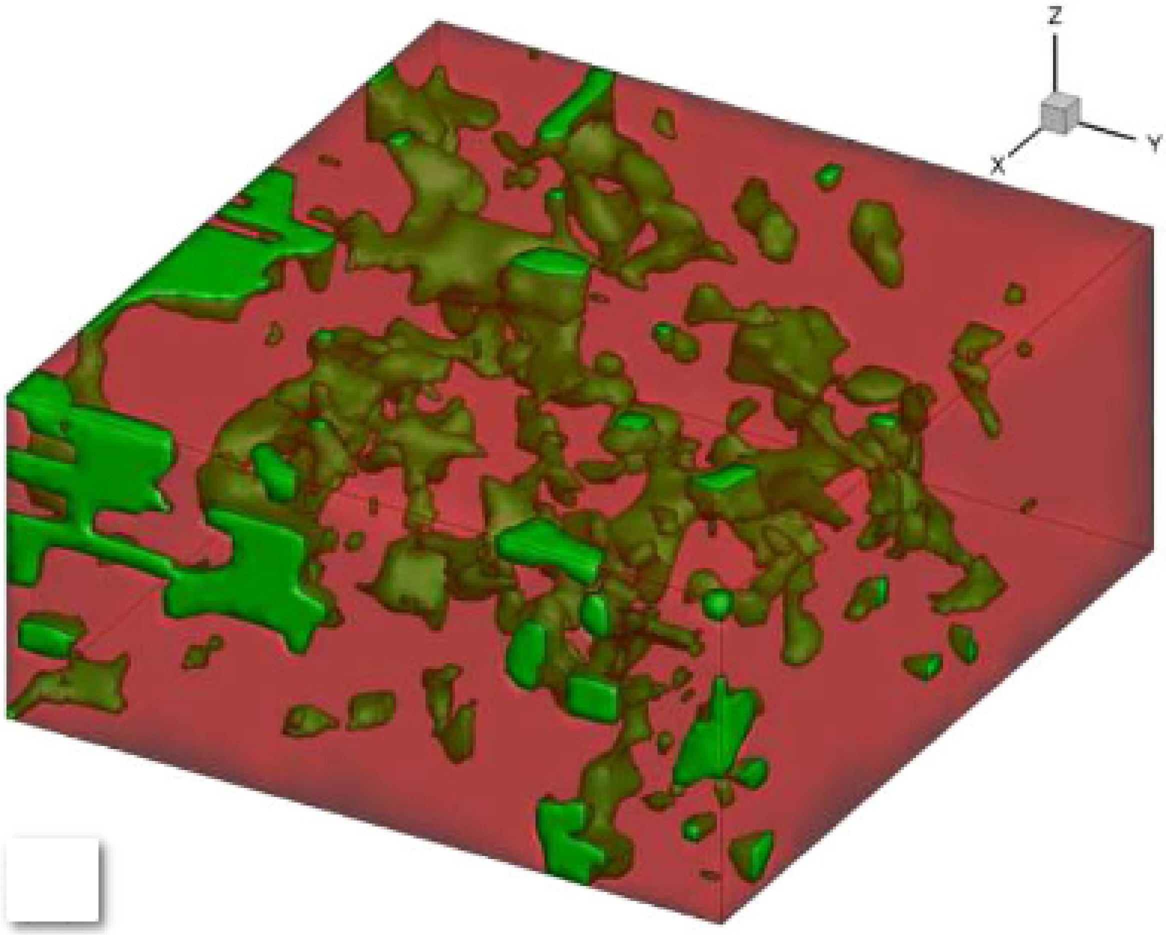

Figure 2: 3D Microstructure image

The reconstruction process involves large-area scans with a two-step electron beam movement and segmentation of phases based on the image-quality factor, which differentiates ferrite and martensite. Thresholding, region filling, and erosion-dilation operations are applied to create binary representations of the microstructures

Figure 3: Microstructure images

Figure 4: Microstructure images

The archietecture of the variational autoencoder network used in the study is shown in Figure 2 and Table 1. We have also experiemnted with latent space dimension 12 and 64 but as the latent space dimension decreases the information loss increases which results in higher loss.

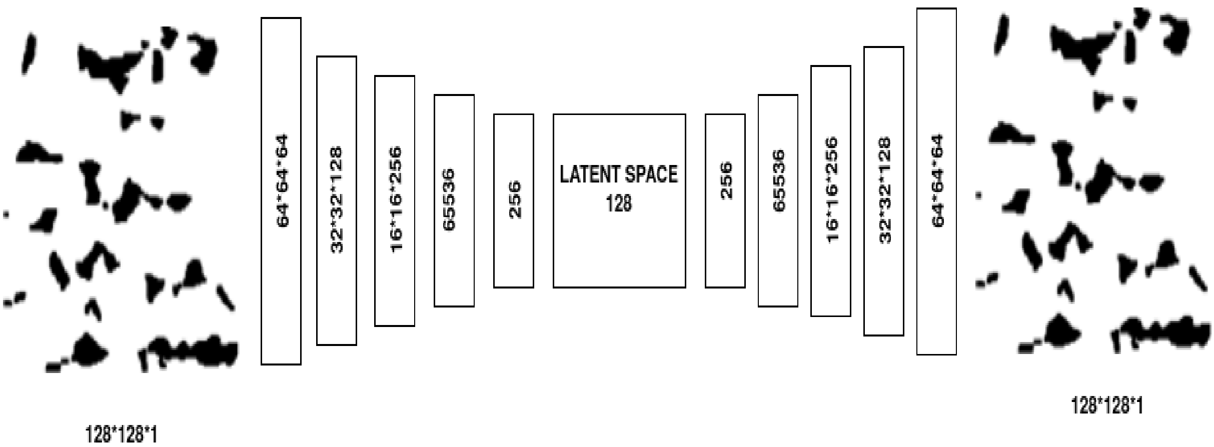

Figure 5: Variational Autoencoder Archietecture

Component	Layer Type	Details
Encoder	Input Layer	Input shape: (image_shape)
	Conv2D	64 filters, 3x3 kernel, ReLU, stride 2, padding=same
	Conv2D	128 filters, 3x3 kernel, ReLU, stride 2, padding=same
	Conv2D	256 filters, 3x3 kernel, ReLU, stride 2, padding=same
	Dense	256 units, ReLU
	Latent Variables	Dense (z_mean, z_log_var) → Sampling Layer
Decoder	Input Layer	Input shape: (latent_dim)
	Dense	16x16x256 units, ReLU
	Reshape	Reshape to (16,16,256)
	Conv2DTranspose	256 filters, 3x3 kernel, ReLU, stride 2, padding=same
	Conv2DTranspose	128 filters, 3x3 kernel, ReLU, stride 2, padding=same
	Conv2DTranspose	64 filters, 3x3 kernel, ReLU, stride 2, padding=same
	Output Layer	Conv2DTranspose, activation=sigmoid, shape=(original_shape)
VAE	Encoder	Outputs (z_mean, z_log_var, z)
	Decoder	Takes sampled z, reconstructs image
	Loss Function	Binary Cross-Entropy + KL Divergence (weighted by 0.1)

Table 1: Variational Autoencoder (VAE) Architecture

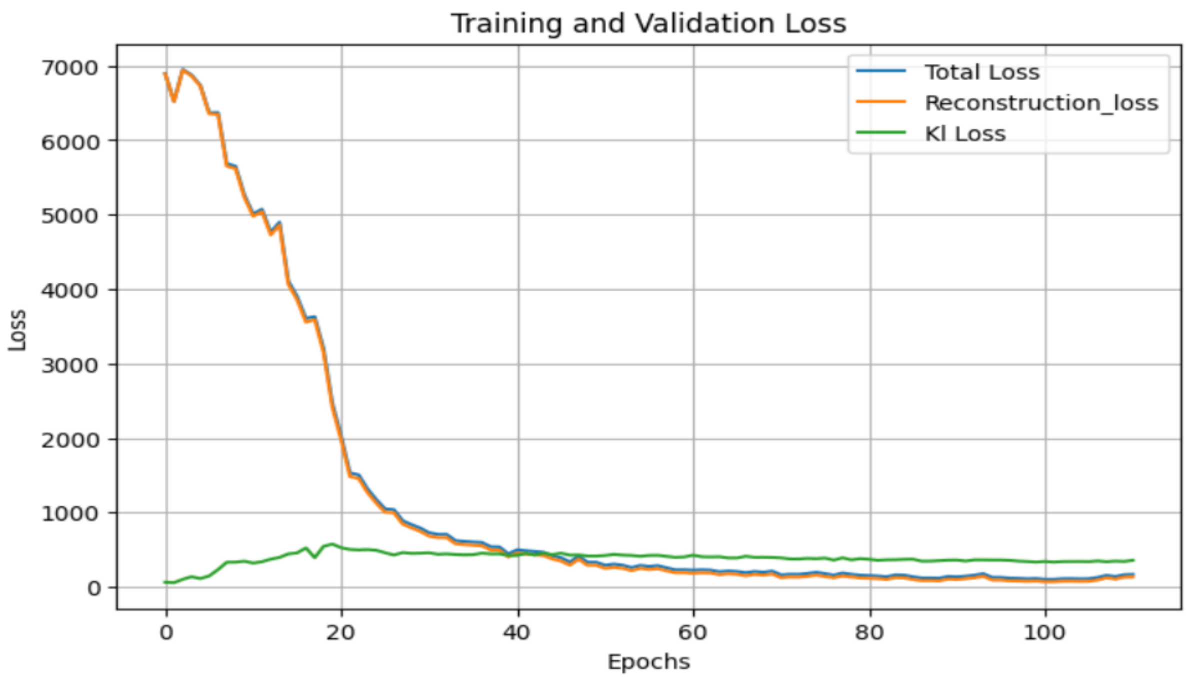

Figure 6: Loss curves for the VAE

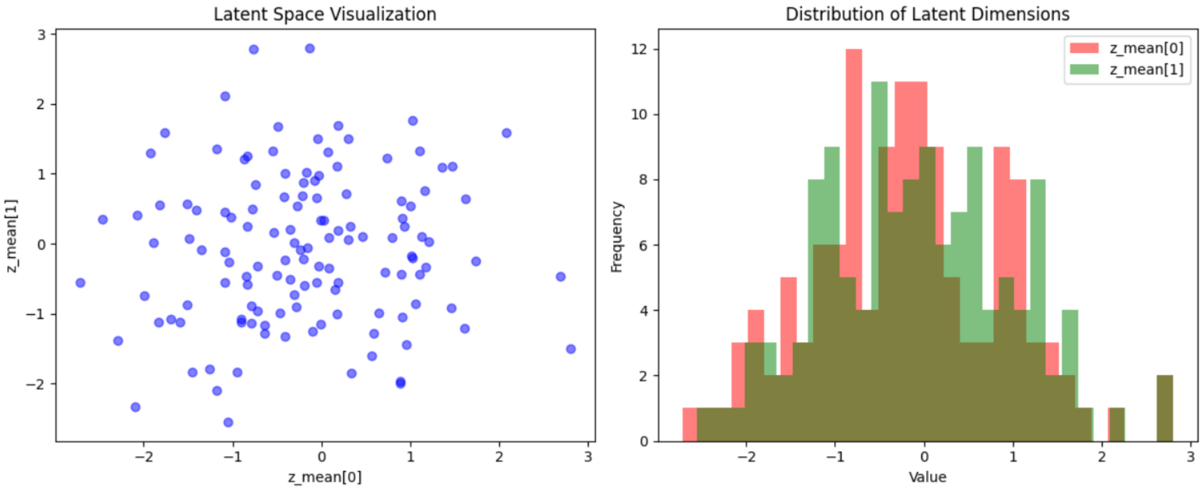

Figure 7: Latent space visualization

3. Generation of new microstructures

The process to generate new images using the Variational Autoencoder (VAE) involves encoding input images into a latent space, sampling from the latent distribution, and reconstructing new images. Initially, a random set of input images is selected and passed through the encoder, which outputs two key components: the latent mean vector z_{mean} and log variance vector $z_{\text{log\_var}}$. These represent the learned probabilistic distribution of the image features in the latent space.

Using the reparameterization trick, random noise (ϵ) sampled from a standard normal distribution N(0,1) is combined with the latent mean and variance to create sampled latent vectors. The formula used is

$$z = z_{\text{mean}} + (\text{var})^{\frac{1}{2}} \cdot \epsilon \tag{1}$$

These latent vectors introduce controlled randomness while preserving the underlying distribution learned by the encoder. The sampled latent vectors are then passed through the decoder, which reconstructs images from this latent representation.

The result is a set of generated images that retain key features of the original dataset but also exhibit variations due to the random noise. This method enables the creation of new, diverse, and realistic microstructures, useful for material design and exploration.

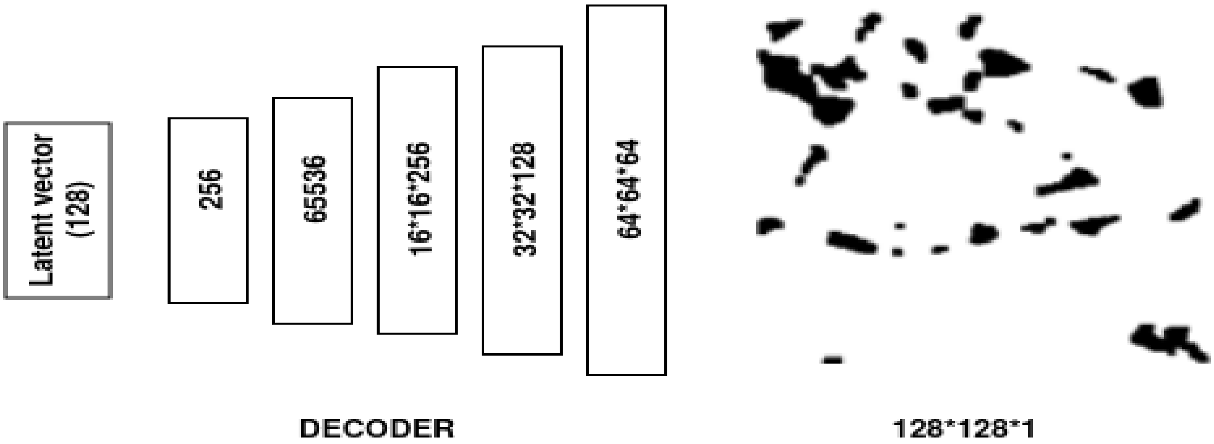

Figure 8: Generation of new image using learned latent space

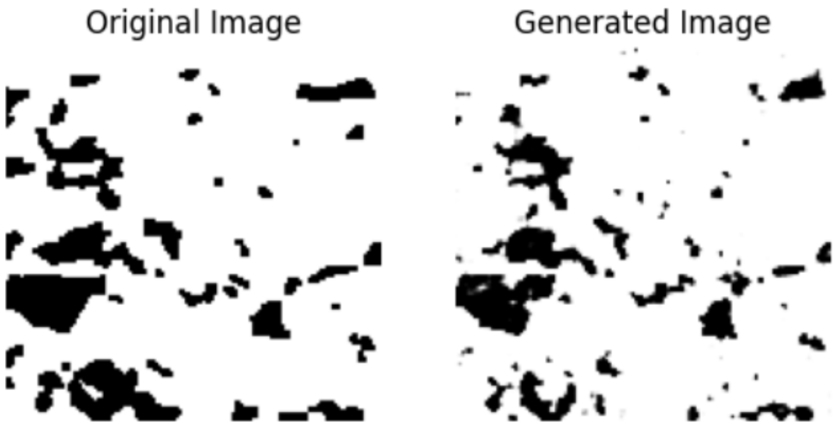

Figure 9: New generated microstructure by adding some noise

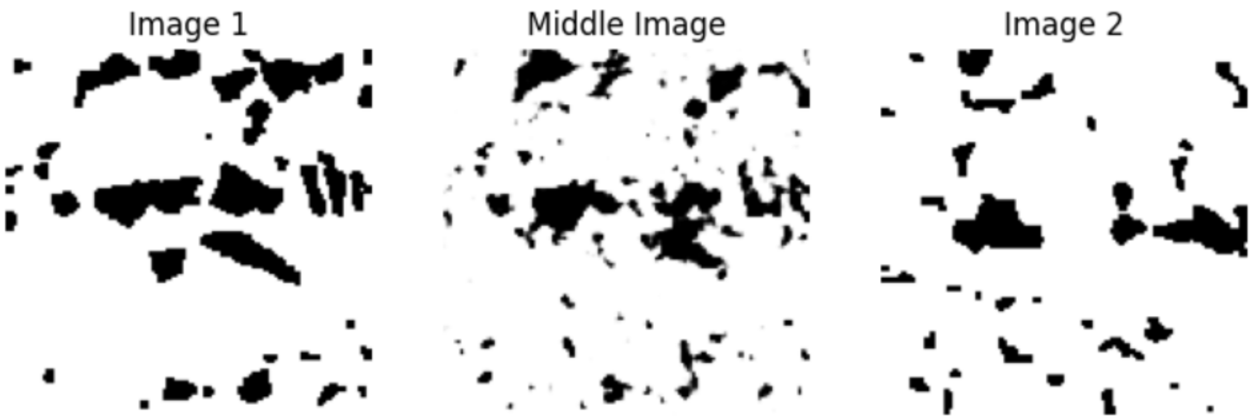

Figure 10: Middle image generation by averaging two latent space vectors

References

D. Brands, D. Balzani, L. Scheunemann, J. Schröder, H. Richter, and D. Raabe. *Computational modeling of dual-phase steels based on representative three-dimensional microstructures obtained from EBSD data*. Archive of Applied Mechanics, volume 86, pages 575–598, Springer, 2016.

A Appendix

A.1 Inkscape handling and export

In sub-directory `make_figures` the inkscape-template file `template_tm.svg` can be found. It includes predefined arrows indicating forces, coordinate systems, velocities, etc. corresponding to the "Technische Mechanik" books.

Thus, open the above mentioned file an start drawing your sketch, see Figure 11. All text should be written, as you do it in LaTeX. To add the template permanently to the list of templates directly in inkscape unter "Datei → Vorlagen..." copy the file `template_tm.svg` to following directoy depending on your operating system:

- For Linux and Mac it is `~/.config/inkscape` , where ~ is representing the path to user's home-directory
- For Windows it is `%APPDATA%\\Inkscape` (just use it in Explorer as is)

Figure 11: Example of drawing in inkscape

To keep an editable picture, please save it to an inkscape-SVG file via "Datei → Speichern unter..." or "File → Save as...“ and choose "Inkscape-SVG (*.svg)" as file format.

For the export to a file format, which can be include to a LaTeX document while the text in the picture is interpreted by the LaTeX processor, please use "Datei → Kopie speichern ..." or "File → Save a copy“. There you should choose "Encapsulated Postscript (*.eps)“ as file format and enter a filename. After a click on "Speichern“ or "Save“ an additional window with save options is shown. Please active/deactivate the option as shown in Figure 12 and click "OK“. Choosing "Seitengröße von Dokument nutzen“ will cause a (wrong) scaling of all graphic objects during LaTeXprocessing.

After this two files will be saved. One file with the extension "eps“ including all graphic objects and another file with the extension "eps_tex“ including all text objects. Please see Figure **??** regarding the LaTeX-include.

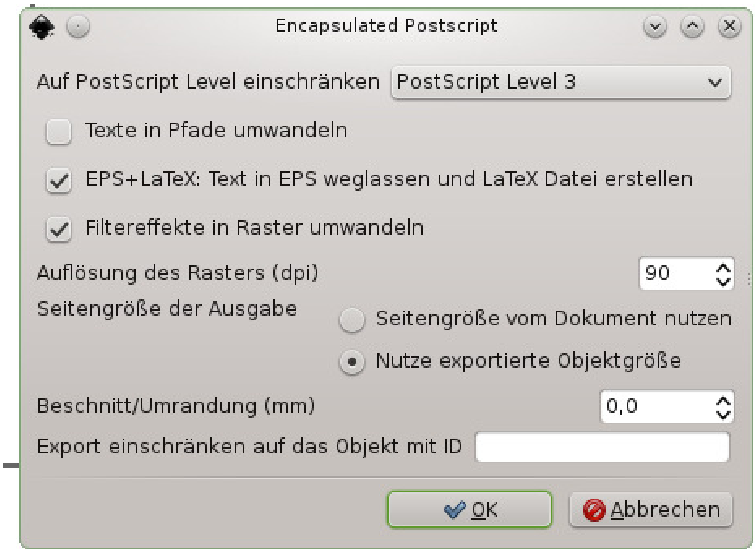

Figure 12: Example of drawing in inkscape