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Application form mySNF

Instrument	**Spark**

Part 1: General Information

Basic data

Project Title	Deep generative modelling for gravitational lensing fields from 3D models of galaxies
Project title in English	Deep generative modelling for gravitational lensing fields from 3D models of galaxies

Research Field	Mathematics, natural sciences
Main Discipline	20200 Astronomy, Astrophysics and Space Sciences
University	Zürcher Hochschule f. Angew. Wissenschaften - ZHAW

Applicant(s)

Main Applicant	**Philipp Denzel**

Grant Application

Amount requested (CHF)	Total	**96'968**

Requested starting date	**01.11.2023**
Duration (6-12 months)	**12**

Attachments

Project description	gl3dgen_spark_23.pdf
CV	CV_Denzel_i01gz647k49tvcwzfy4xsvhpk3q8.pdf
Employment confirmation	confirmation_of_employment_letter_Denzel_signed.pdf

1. Responsible applicant

Last name	**Denzel**
First name	**Philipp**
Function (title)	
Academic degree	Dr./PhD
Date of birth	19.08.1991
Gender	männlich
Swiss social security number	756.7165.9375.87
Language	Deutsch
Nationality	Deutschland
Correspondence address of application	Address of workplace

Home address

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Street, No.	Breitwiesstrasse 61
P.O. Box	
Postcode / Zipcode	8135
Place	Langnau am Albis
Country	Schweiz

Current work address (if available)

Designation 1 (lab/research group)*	Center for Artificial Intelligence
Designation 2 (inst /dept.)*	School of Engineering
Designation 3 (University)*	ZHAW
Street, No.	Technikumstrasse 71
Address supplement 1 (e.g. building)	TN
Host (Head of the institute/ department, Grants Office) *	Prof. Dr. Thilo Stadelmann
P.O. Box	
Postcode / Zipcode	8400
Place	Winterthur
State, canton, etc.	ZH
Country	Schweiz

Communication

Secretariat line	
Switchboard	
Direct line	
Fax office	
Home telephone number	
Cellphone	+41 76 211 19 08
Website	
E-mail address	phdenzel@gmail.com

2. Host research group

General information

Designation 1 (lab/research group)*	**Centre for Artificial Intelligence**
Designation 2 (inst /dept.)*	**School of Engineering**
Designation 3 (University)*	**ZHAW**
Address supplement 1 (e.g. building)	TN
Host (Head of the institute/ department, Grants Office) *	Prof. Dr. Thilo Stadelmann
Street, No.	Technikumstrasse, 71
P.O. Box	
Postcode / Zipcode	8400
Place	Winterthur
State, canton, etc.	ZH
Country	Switzerland
Planned start of the project	01.11.2023
Planned end of the project	02.08.2024

Communication

Secretariat line	+41 58 934 72 08
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Website	www.zhaw.ch/cai
E-mail address	thilo.stadelmann@zhaw.ch

3. Applicant's employment

Information on employment and function at the anticipated starting date of the grant

Name	**Denzel, Philipp**
Employment at the anticipated starting date of the grant	befristet bis...
fixed-term contract until	30.06.2025
Level of employment %	100
Function in the context of this grant application	Postdoktorand/in, Research associate, Assistenzärztin/Assistenzarzt
Professorship	Keine
Doctorate (PhD)?	Yes
Date of doctorate (PhD)	29.10.2020
PhD supervisor	Prof. Dr. Prasenjit Saha
Country of doctorate	Schweiz
Remarks	
Further employments	

4. Basic data I

Title in English	Deep generative modelling for gravitational lensing fields from 3D models of galaxies
Original title (if different)	
Requested starting date	01.11.2023
Duration (6-12 months)	12
Research field	Mathematics, natural sciences
Further research fields	Engineering sciences
Main discipline	20200 Astronomy, Astrophysics and Space Sciences
Sub-discipline(s)	20506 Information Technology

5. Basic data II

Summary (copy of the summary in the project description)

This is a research proposal for the development of a novel technique using generative deep learning for modelling galaxies of gravitational lens systems in 3D, opposed to conventional methods limited to 2D.
Gravitational lensing is a phenomenon that occurs when rays of light from a distant background source are deflected by the gravitational field of a massive foreground object, e.g. a galaxy, which almost perfectly aligns with the observer. While such occurrences are rare, they are scientifically significant, because they provide the only opportunity to directly infer the lensing galaxy's mass distribution, including its dark matter content. This unique perspective on a galaxy's dark matter distribution offers exceptional insights into the mysteries surrounding galaxy evolution, the nature of dark matter,
galaxy substructures, and even the expansion of the Universe.
Accurately predicting the deflection field of a strong gravitational lens is a complex task that requires a detailed understanding of the distribution of matter in the lensing galaxy. Conventional methods for calculating these deflection fields, such as ray-tracing, are computationally expensive, can take a long time to generate results, and typically have to be fine-tuned by an experienced expert.

In recent years, deep learning methods have emerged as a promising approach for generating and processing image-based data in various scientific fields, often with super-human proficiency. These methods employ neural networks to learn the mapping between the input properties (for instance, the lensing galaxy) and the resulting image (in this instance, the deflection field).

In this research proposal, I outline the usage of generative deep learning methods to produce strongly lensing deflection fields of 3D galaxy models from existing hydrodynamical simulation suites for the purpose of creating mock observations, observational fits, and corresponding source reconstructions. Specifically, we will explore various state-of-the-art deep learning architectures, including diffusion models, vision transformers, generative adversarial networks (GANs), and variational autoencoders (VAEs) to develop a model that can accurately generate the deflection field from a given 3D galaxy
model. The resulting deep learning model will be used to create synthetic observations that can be compared to existing observational data to test the accuracy of the lens model, and in particular investigate the theoretical properties of the observed lensing galaxies and their corresponding background source reconstructions, within a Bayesian framework.

Lens modelling is inherently considered as a (degenerate) 2D inverse problem. The novelty of this project consists of introducing 3D models as direct input, which requires methods able to cover a broad range in solution space due to the degeneracy introduced thereby. Conventional modelling methods are insufficient due to the typically low complexity of their models whereas deep learning methods increase the model complexity with a high number of parameters, thus able to span a wider range in solution space.

As of today, roughly 10^3 lenses have been discovered, only a fraction of those properly analysed. Moreover, it is anticipated that the next-generation satellites and telescopes such as JWST, Euclid, SKA, or ELT may increase this number to 10^5. Thus, it is crucial to devise novel techniques that can scale with big data efficiently.

Keywords	Gravitational lensing
	Artificial Intelligence
	Deep Learning
	Galaxy formation
	Hydrodynamical simulations
	Astronomical data
Language of correspondence	German
Financial administration	ZHAW Zürcher Hochschule für Angewandte Wissenschaften

6. Host institution

University	Zürcher Hochschule f. Angew. Wissenschaften - ZHAW
Remarks	

7. Requested funding

Requested funding	**Total (CHF)**	**Year 1**
Total (CHF)	**96'968**	**96'968**

Salaries	**Total (CHF)**	**Year 1**
The applicants' own salaries	12'165	12'165
Salary for further employees	71'429	71'429
Total (CHF)	**83'594**	**83'594**
Total (%)	**86%**	**86%**

Social security contributions	**Total (CHF)**	**Year 1**
Social security contributions	13'374	13'374
Total (CHF)	**13'374**	**13'374**
Total (%)	**14%**	**14%**

Details

The applicants' own salaries	**Total (CHF)**	**Year 1**
Denzel, Philipp: n.n.	12'165	12'165
Work-time percentage: Year 1: 10.00% Social security contributions: Year 1: 16.00%		
Total (CHF)	**12'165**	**12'165**
Total (%)	**13%**	**13%**

Salary for further employees	**Total (CHF)**	**Year 1**
Advisor/AI Development: Frank-Peter Schilling	9'732	9'732
Work-time percentage: Year 1: 4.00% Social security contributions: Year 1: 16.00% Comments / Additions: Frank-Peter Schilling has expertise in AI, specifically 3D deep learning approaches, and will help with the implementation of the AI components of this project. Person: Frank-Peter Schilling male / 06.08.1970 German / Germany Academic degree: Prof.		

AI/software development: n.n.		52'138	52'138
Work-time percentage	Year 1: 65.00%		
Social security contributions	Year 1: 16.00%		
Comments / Additions	This person will have expertise in AI and (scientific) software development. She or he will mainly be in charge of code implementations, and run tests of the different deep learning methods.		
Co-PI: Elena Gavagnin		9'559	9'559
Work-time percentage	Year 1: 5.00%		
Social security contributions	Year 1: 16.00%		
Comments / Additions	Elena Gavagnin agreed to act as Co-PI for this project. She has expertise in both astrophysics and artificial intelligence. She will help with any administrative work, contribute to the AI development, normally act in an advisory role, and as my replacement in the out of ordinary case.		
Person	Elena Gavagnin female / 19.07.1988 Number of children 1 / English / Italy		
Academic degree	Dr./PhD		
Total (CHF)		**71'429**	**71'429**
Total (%)		**74%**	**74%**

Social security contributions	**Total (CHF)**	**Year 1**
Advisor/AI Development: Frank-Peter Schilling	1'557	1'557
AI/software development: n.n.	8'342	8'342
Co-PI: Elena Gavagnin	1'529	1'529
Denzel, Philipp	1'946	1'946
Total (CHF)	**13'374**	**13'374**
Total (%)	**14%**	**14%**

8. Collaboration (national and international)

Person/Institution	Prof. Dr. Prasenjit Saha/University of Zurich
Country	Switzerland
Context	Prof. Saha agreed to provide his expertise in the field of gravitational lensing. He will take an adivsory role and help in writing the scientific publications.
Types of collaboration	in-depth/constructive exchanges on approaches, methods or results
	Publication

Person/Institution	Dr. Elena Gavagnin/ZHAW
Country	Switzerland
Context	Dr. Gavagnin agreed to assist in almost any aspects of the project (and will act as Co-PI). She can share her expertise in astrophysical hydrodynamical simulations and artifical intelligence, refer research assistants, host meetings if necessary, and will help in writing the scientific publications.
Types of collaboration	in-depth/constructive exchanges on approaches, methods or results
	Publication
	Research Infrastructures
	Exchange of personnel

Person/Institution	Prof. Dr. Frank-Peter Schilling/ZHAW
Country	Switzerland
Context	Prof. Dr. Schilling agreed to assist in almost any aspects of the project. He can share his expertise in artifical intelligence and deep learning, refer research assistants, and will help in writing the scientific publications.
Types of collaboration	in-depth/constructive exchanges on approaches, methods or results
	Publication
	Research Infrastructures

Exchange of personnel

9. Research requiring authorisation or notification

HRA-relevant and HRA-irrelevant research involving humans	No
Research on human embryonic stem cells	No
Research on animals	No
Research on GMO or pathogens	No

10. 3R – Replace, Reduce, Refine

Project does not involve any animal experiments	Yes
Project involves experiments with animals that fall under the Animal Welfare Act (vertebrates, cephalopods, crayfish) and takes account of the 3R	No
Project is a 3R research project focusing on "Replace"	No
Project is a 3R research project focusing on "Reduce"	No
Project is a 3R research project focusing on "Refine"	No
Project involves experiments with animals that do not fall under the Animal Welfare Act (insects, worms)	No

11. Access and Benefit Sharing (ABS)

The research project plans to use genetic resources that are governed by the ABS provisions of the Nagoya Protocol	No

12. Fellowships for a research stay abroad

Project involves experiments that require authorisation and notification. I hereby confirm compliance with Swiss laws and ethical guidelines.	No

13. Awareness of the relevant regulations

Relevant regulations noted and accepted	Yes

Deep generative modelling for gravitational lensing fields from 3D models of galaxies

1 Project summary

This is a research proposal for the development of a novel technique using generative deep learning for modelling galaxies of gravitational lens systems in 3D, opposed to conventional methods limited to 2D. Gravitational lensing is a phenomenon that occurs when rays of light from a distant background source are deflected by the gravitational field of a massive foreground object, e.g. a galaxy, which almost perfectly aligns with the observer. While such occurrences are rare, they are scientifically significant, because they provide the only opportunity to directly infer the lensing galaxy's mass distribution, including its dark matter content. This unique perspective on a galaxy's dark matter distribution offers exceptional insights into the mysteries surrounding galaxy evolution, the nature of dark matter, galaxy substructures, and even the expansion of the Universe.
Accurately predicting the deflection field of a strong gravitational lens is a complex task that requires a detailed understanding of the distribution of matter in the lensing galaxy. Conventional methods for calculating these deflection fields, such as ray-tracing, are computationally expensive, can take a long time to generate results, and typically have to be fine-tuned by an experienced expert.

In recent years, deep learning methods have emerged as a promising approach for generating and processing image-based data in various scientific fields, often with super-human proficiency. These methods employ neural networks to learn the mapping between the input properties (for instance, the lensing galaxy) and the resulting image (in this instance, the deflection field).

In this research proposal, I outline the usage of generative deep learning methods to produce strongly lensing deflection fields of 3D galaxy models from existing hydrodynamical simulation suites for the purpose of creating mock observations, observational fits, and corresponding source reconstructions. Specifically, we will explore various state-of-the-art deep learning architectures, including diffusion models, vision transformers, generative adversarial networks (GANs), and variational autoencoders (VAEs) to develop a model that can accurately generate the deflection field from a given 3D galaxy model. The resulting deep learning model will be used to create synthetic observations that can be compared to existing observational data to test the accuracy of the lens model, and in particular investigate the theoretical properties of the observed lensing galaxies and their corresponding background source reconstructions, within a Bayesian framework.

Lens modelling is inherently considered as a (degenerate) 2D inverse problem. The novelty of this project consists of introducing 3D models as direct input, which requires methods able to cover a broad range in solution space due to the degeneracy introduced thereby. Conventional modelling methods are insufficient due to the typically low complexity of their models whereas deep learning methods increase the model complexity with a high number of parameters, thus able to span a wider range in solution space.

As of today, roughly 10^3 lenses have been discovered, only a fraction of those properly analysed. Moreover, it is anticipated that the next-generation satellites and telescopes such as JWST[1], Euclid, SKA[2], or ELT[3] may increase this number to 10^5. Thus, it is crucial to devise novel techniques that can scale with big data efficiently.

[1]James Webb Space Telescope
[2]Square Kilometer Array
[3]Extremely Large Telescope

2 Project plan

2.1 State of research

Although gravitational lensing is often regarded as an optical illusion that shows the same source in multiple images, lensing systems possess distinct visual features which make them relatively easy to spot by the trained eye. Nevertheless, wide-field surveys capture billions of light sources, and over 100'000 strongly lensing systems may still await discovery (Taak and Im, 2020; Taak and Treu, 2023; Collett, 2015). Not all these instances can be examined by humans with the same level of scrutiny.
Deep learning methods have emerged as a promising approach for the automated detection of strong gravitational lenses. In fact, recent studies have demonstrated that deep learning techniques have led to a significant increase in the number of identified strong lensing candidates by more than threefold (Storfer et al., 2022; Huang et al., 2021; Rezaei et al., 2022; Wilde et al., 2022).

Contrary to the automated discovery of strong gravitational lenses using deep learning, advancements for lens modelling have been more restrained in that aspect. Still, the scientific community is actively investigating how deep learning can be integrated into lens modelling.
In a recent study by Gu et al. (2022), the same optimization methods utilized in the backward propagation algorithm for training neural networks were employed in a Bayesian framework. Through a Hamiltonian Monte-Carlo sampling scheme, they obtained posterior estimates for their lens model parameters, albeit with mediocre efficiency. Based on the previous study, Mishra-Sharma and Yang (2022) use continuous neural fields to reconstruct strongly lensing sources from parametric lens models.
Similarly, Morningstar et al. (2019) designed a custom recurrent neural network (RNN) architecture, the recurrent inference machine (RIM), to construct reconstructed source priors for fitting lens model parameters. A subsequent study by Adam et al. (2022) incorporates the lens modelling procedure in the RIM architecture.
In an automated pipeline setting, Schuldt et al. (2022); Chianese et al. (2019) demonstrate that incorporating a simple CNN-based residual network (ResNet) for estimating lens model parameters is comparable in performance to traditional parametric lens modelling techniques.
Furthermore, Park et al. (2020) use a Bayesian neural network (BNN) to characterize the posterior probabilities of lens model parameters for the purpose of inferring the Hubble constant.

The very first gravitational lens discovered by Walsh et al. (1979) was simultaneously confirmed and modelled by Young et al. (1980). They used a simple spherically symmetric lens model using 4 parameters to fit the observation. Ever since then, even modern lens modelling tools (as mentioned above) employ some type of parametric model (with typically no more than 8 parameters) to fit the density distribution of the lens (cf. Birrer and Amara, 2018; Hezaveh et al., 2017; Tessore et al., 2016; Oguri, 2010). Note that Hezaveh et al. (2017) use convolutional neural networks (CNNs) to fit mass distribution parameters to lens observations. However, this still prescribes the same parametric constraints on the complexity of the lensing galaxy's shape.

Young et al. (1981) already recognized that a major obstacle in lens modelling is that numerous mass distributions could plausibly explain observed data. This fact manifests as parameter degeneracies when interpreting observations as discussed by Saha (2000); Saha and Williams (2006); Schneider and Sluse (2014); Birrer (2021). An often ignored issue with parametric models is that they assume to cover enough of the solution space to encompass the "truth". Cognizant of this fact, free-form lens modelling, as presented by (Saha and Williams, 2004), uses an over-parameterization trick to sample a wide range of solution space. Despite, this technique is not efficient at higher resolutions and the majority of fits are still not considered realistic or physically viable.

All conventional lens modelling techniques rely on recipes which aim to efficiently reproduce shapes and slopes of galaxies, as they are usually observed. These methods therefore suppress or even completely ignore the evolutionary processes of galaxies and the physical properties which form and drive them (cf. Naab and Ostriker, 2017). In contrast, cosmological hydrodynamical simulations have made significant strides in recent years, incorporating semi-analytical models which simulate star formation and feedback effects at small scales, enabling exploration of various galaxy-formation scenarios (e.g. Pillepich et al., 2017; Weinberger et al., 2016; Vogelsberger et al., 2014).

Despite the apparent benefits of directly integrating these galaxy models to lens modelling, the already difficult computational and algorithmic challenges persist. However, it has been shown that deep learning neural networks are universal approximators (Hornik et al., 1989; Kratsios and Bilokopytov, 2020) and often outperform conventional, computationally complex operations in efficiency and accuracy. Hence, I propose a novel data-driven deep learning approach to lens modelling that generates deflection fields directly from 3D galaxy models sampled from hydrodynamical simulations.
While there were previous attempts at harnessing realistic galaxy models from hydrodynamical simulations (see Adam et al., 2022; Denzel et al., 2021), these studies used predetermined 2D projections at fixed orientations of the galaxy. The novelty in this proposal lies in the direct processing of the 3D data from such galaxy models as input to a deep neural network architecture, which essentially serves as a data augmentation method. This approach allows for an increase in possible lens model fits due to the multiplicity of orientations from which a galaxy model can be projected onto a 2D plane (as shown by these previous studies).

In astrophysical, hydrodynamical simulations, the commonly-used data format is called *smooth-particle hydrodynamics* (Gingold and Monaghan, 1977; Lucy, 1977; Monaghan, 1992). Basically, the same data type is referred to as *point clouds* in the computer vision field. They are most commonly produced by LiDARs, 3D scanners, or multi-channel depth camera systems. Parsing and knowledge extraction from point cloud data is considered an exceptionally difficult task as they are fundamentally unstructured data (cf. Vinyals et al., 2015; Armeni et al., 2016; Rufus et al., 2020; Zhang and Singh, 2015; Nüchter et al., 2007; Rusinkiewicz and Levoy, 2000). Qi et al. (2016) pioneered deep learning with 3D point cloud data, and subsequent studies built upon this idea (see Qi et al., 2017; Ben-Shabat et al., 2017; Klokov and Lempitsky, 2017; Kaul et al., 2021; Abad-Rocamora and Ruiz-Hidalgo, 2022).
At the same time, recent studies by Quessard et al. (2020); Keurti et al. (2022) demonstrate the feasibility of efficiently learning spatial group operators, such as rotation, through regularization and mapping of the latent space with neural networks.

Integrating computer vision deep learning techniques with astrophysical data within the context of gravitational lensing poses a significant challenge, but holds the potential for substantial scientific advancement across all disciplines.

2.2 Project description

2.2.1 Goals & expected results

The main objectives of this research are:

1. To develop a generative deep learning model that can efficiently and accurately predict gravitational lensing deflection fields from a 3D galaxy model, optimizing for its orientation and alignment.
    - To this end, we construct a custom training dataset of ray-traced, synthetic lenses from observed source images, such as quasars, and manually projected galaxy models from publicly available hydrodynamical simulation suites (Springel et al., 2017; Nelson et al., 2018; Davé et al., 2019).

2. To embed the generative deep learning model in a (for the most part autonomous) Bayesian lens modelling framework analogous to Adam et al. (2022); Denzel et al. (2021); Morningstar et al. (2019); Hezaveh et al. (2017) to fit observations for galaxy models.
   - We will compare its accuracy and efficiency against existing lens modelling and source reconstruction techniques. Note that the proposed scheme will be able to directly draw conclusions on the 3D structure of lenses, which is a novel capability no other existing lens modelling tool possesses.
   - This test can be performed with corresponding gravitational lens datasets from surveys such as the Strong Lensing Legacy Survey (SL2S: Gavazzi et al., 2012; Sonnenfeld et al., 2015), the Sloan Lens ACS Survey (SLACS: Bolton et al., 2006; Shu et al., 2017), or the Baryon Oscillation Spectroscopic Survey (BOSS) Emission-Line Lens Survey (BELLS: Brownstein et al., 2011; Shu et al., 2016).
   - The modelling tools, as well as the trained deep learning models, and custom training dataset will be made available for the community as an open-source software package for reproducibility of scientific results, and detailed in scientific publications.
3. To test the generative lens modelling scheme on new unseen gravitational lens observations in a "real-world" setting, and to investigate the relative impact of 3D dark matter distributions, galaxy shape, orientation, galaxy formation scenarios, and other properties on these observations.[4]

2.2.2 Methods

Formally, the deflection field $\boldsymbol{\alpha}(\boldsymbol{\theta}, \xi)$ can be expressed through a given angle on the observer's sky $\boldsymbol{\theta}$, and an orientation ξ of the 3D density $\rho(\boldsymbol{\theta}, z)$. The convergence map (that is, the lensing mass distribution in dimensionless form) is given by the usual projection of the 3D mass density as

$$\kappa(\boldsymbol{\theta}, \xi) = \frac{4\pi G}{cH_0} \frac{D_{\mathrm{LS}} D_{\mathrm{L}}}{D_{\mathrm{S}}} \int \rho(\boldsymbol{\theta}, \xi, z)\, \mathrm{d}z\,. \tag{1}$$

Here, D_{LS} is the dimensionless angular-diameter distance from the lens to the source, D_L and D_S are analogous. Through the Poisson equation, we can connect the deflection field in Equation (1) to the convergence as

$$\boldsymbol{\alpha}(\boldsymbol{\theta}, \xi) = \nabla_{\boldsymbol{\theta}} \psi(\boldsymbol{\theta}, \xi) = 2\nabla_{\boldsymbol{\theta}}^{-1} \kappa(\boldsymbol{\theta}, \xi)\,. \tag{2}$$

Angular positions on the source plane $\boldsymbol{\beta}$ are connected to the image plane positions $\boldsymbol{\theta}$ through the ray-tracing lens equation

$$\boldsymbol{\beta} = \boldsymbol{\theta} - \boldsymbol{\alpha}\,. \tag{3}$$

This translates to a mapping between image and source plane $L(\boldsymbol{\theta}, \boldsymbol{\beta})$ that can be discretized in matrix form according to

$$I(\boldsymbol{\theta}) = \int L(\boldsymbol{\theta}, \boldsymbol{\beta}) s(\boldsymbol{\beta}) \mathrm{d}^2\boldsymbol{\beta}\,, \tag{4}$$

where $s(\boldsymbol{\beta})$ source-brightness and $I(\boldsymbol{\theta})$ image-brightness distributions; see Appendix A and B in Treu and Koopmans (2004) for details on how to construct this matrix.

Forward modelling these equations is trivial and can be accomplished with well-established algorithms such as Fast Fourier Transform, multi-grid, or iterative relaxation methods.
Solving the inverse problem is considerably more challenging however, and requires convex optimization involving repeated, computationally expensive operations such as matrix inversions. This task is further complicated if the orientation of the 3D galaxy density distribution in Equations (2) & (3) has to be marginalized.

[4] This could also be considered part of a follow-up project.

My proposed technique controls these optimizations using conditional, generative neural networks. There are various deep learning approaches which can deal with such problems, each with advantages and trade-offs:

- VAEs (Kingma and Welling, 2013) are considered fast, and explicitly construct a latent representation of the input, but trade accuracy for the sake of prior matching. VAE models could be good candidates for initial tests as they are comparatively easy to train, and give insights in the compression, i.e. abstraction process.
- GANs (Goodfellow et al., 2014) play a minimax game between a generator network and a discriminator network that critiques the generator during training. They tend to be fast during inference and generate high-quality outputs, but are prone to the issue of mode collapse. Since these models are relatively complicated to train, they will be explored during later stages of the project.
- Autoregressive models (Parmar et al., 2018) have been shown to consistently outperform other types of models when it comes to accuracy, but tend to be extremely slow, especially during inference. Since these models hold the potential to deliver high-quality results, they will be investigated relatively early, despite their extended training phases.
- Diffusion models (Sohl-Dickstein et al., 2015; Ho et al., 2020) are latent variable models whose variables keep the dimensionality of the input data. Inspired by the physical effect of the same denomination, the approximate posterior is fixed to a Markov chain with Gaussian noise transitions. These models have recently shown great success in generating high-quality samples, but similar to autoregressive models are slow in comparison to GANs or VAEs. Depending on the project timeline, this method may be skipped altogether.

In addition, hybrid approaches that combine the strengths of the aforementioned methods while mitigating their weaknesses are also often employed. The choice of deep learning architecture and method will ultimately depend on the accuracy and scalability to the lensing galaxy data, and has to be investigated.

2.2.3 Approach

The project is organized in a work package of sequential tasks (WP[1-5]) as follows:

- WP1: *gathering publicly available base datasets* (duration: $<$ 1 month)
  1. source plane images of quasars (QSOs) from the Sloan Digital Sky Survey Quasar Catalog (Schneider et al., 2010; Pâris et al., 2018) and other sources (Flesch, 2021). In total, these catalogs have over a million classified type-I/II QSO entries, but for this project only a small sub-sample around 1'000–10'000 at preferentially higher redshifts should suffice.
  2. lensing galaxy models (3D) from the *IllustrisTNG* (Nelson et al., 2018) and *simba* (Davé et al., 2019) simulation suites. These are available as raw HDF5 data at up to 2.7 TB per snapshot containing roughly 3000 appropriate galaxy models. Again, roughly 3-4 snapshots should suffice and fit on the available storage devices.
  3. the test datasets SL2S, SLACS, and BELLS (see Section 2.2.1) have a direct comparison with corresponding existing lens modelling tools. Here, only a small subset is needed corresponding to the samples tested in the studies by Adam et al. (2022); Denzel et al. (2021); Morningstar et al. (2019); Hezaveh et al. (2017).
- WP2: *building the training dataset* (duration: 1-2 months)
  - simulated lens images and deflection fields from the base datasets in WP1. These can be simulated with existing, open-source software (see Section 2.1), but as explained in Section 2.2.2 could easily be implemented to run on the available GPU cluster available to us.
- WP3: *testing and training deep learning architecture* (duration: 4-5 months)

- this is the most compute-intensive task and will be run in parallel on our GPU science cluster of 8 NVIDIA A100 GPUs and 24 V100 GPUs. The network architectures mentioned in Section 2.2.2 are typically designed for processing 2D or voxel data, so significant adjustments and novelty will be necessary to adapt them to our specific data requirements.

- WP4: *integration into a lens modelling framework* (duration: 2-3 months)
  - strategies from studies mentioned in WP2 may be adapted for this purpose, or a new strategy could be explored.
- WP5: *benchmarking and real-world testing* (duration: 1 month)
  1. benchmarking the generative lens modelling performance on the test dataset and comparison of the results with existing lens modelling techniques mentioned above.
  2. once proof-of-concept has been established, the generative lens modelling scheme can be tested on new gravitational lens observations in a "real-world" setting, such as lens candidates from Huang et al. (2021); Storfer et al. (2022).

2.2.4 Possible risks

The potential risks of this project mainly comprise of undesirable outcomes which either impact the model's autonomy and efficiency, or extend the project timeline due to additional work, but can be ameliorated:

- The principal idea of the proposed method relies on the degeneracy problem in lens systems. While in theory there should be an infinite amount of lens solutions to a particular observations, the selected training dataset may not be large enough for the true data distribution. In that case, the training dataset may need to be reworked.
- Previous attempts to integrate 3D point-cloud data into the aforemention deep learning models have been met with challenges and considerable trade-offs in efficiency at times. Poor choices in architecture and model design could prevent the proposed technique from being scalable for large datasets.
- In addition, deep learning is often categorized as black-box model, and it is necessary to take significant caution when presenting any results from a deep generative model. To increase its trustworthiness, well-established methods such as saliency maps, surrogate modelling, or uncertainty estimation should be employed. Moreover, the deep learning model should be designed for robustness against noise (and adversarial examples). If these considerations are not sufficiently addressed, the lens modelling community may not accept any results from the method.

2.2.5 Potential impact

Demonstrating the feasibility of the proposed method would mark a significant achievement as it would be the first instance of a strong-lensing modelling technique capable of directly inferring 3D matter distributions and its individual components (dark matter, stars, gas, and dust). In particular, it will model the first-ever 3D map of a dark matter halo for strong-lens observations, a crucial, still missing component for studying the astrophysical and cosmological properties of our Universe.
Moreover, the method could provide prior constraints for time-delay tomography studies, possibly enabling a much-needed determination of the Hubble constant at the 1%-precision level.
Designed with efficiency in mind, the method is also capable of autonomously processing vast amounts of new lensing data. This is especially critical in light of the gravitational lens discoveries anticipated from next-generation telescopes, such as SKA or Euclid. The SKA, in particular, prepares for data rates of several PB/day, and a deep learning technology capable of performing dimensionality reduction (i.e. compression) of unstructured data could significantly contribute to achieving this objective.

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CV

Philipp Denzel
Current position(s): Junior researcher / Postdoc
Academic age: 2 year(s) 8 month(s)

Education

Degree	Organisation	Duration
PhD / Dr.: Physics Prof. Dr. Prasenjit Saha	Universität Zürich - ZH, CH Institute for Computational Science	08.2016 - 10.2020 4 year(s) 3 month(s)
Master: Computational Science Prof. Dr. Romain Teyssier	Universität Zürich - ZH, CH Institute for Computational Science	09.2015 - 07.2016 11 month(s)
Bachelor: Physics Prof. Dr. Jürg Diemand	Universität Zürich - ZH, CH Institute for Physics	09.2010 - 06.2015 4 year(s) 10 month(s)

Employment

Role	Organisation	Duration
Junior researcher / Postdoc Prof. Dr. Frank-Peter Schilling	Zürcher Hochschule f. Angew. Wissenschaften - ZHAW, CH Centre for Artificial Intelligence	07.2022 - Present 10 month(s)
-	Self-employed	12.2020 - 06.2022 1 year(s) 7 month(s)
Doctoral student / PhD student Prof. Dr. Prasenjit Saha	Universität Zürich - ZH, CH Institute for Computational Science	08.2016 - 10.2020 4 year(s) 3 month(s)

SNSF

Major achievements

Achievement 1

My research presents a new estimate of the Hubble parameter, which quantifies the expansion rate and age of the Universe, completely independent from previous methods. This is particularly relevant in light of the ongoing crisis in cosmology, where precise measurements of the Hubble parameter exhibit discrepancies beyond the 5-sigma uncertainty level. Through a comprehensive, free-form analysis of eight strongly, quadruply lensing systems, I obtained an estimate of H0=71.8+3.9-3.3 kms-1Mpc-1 with a precision of 4.97 per cent in the concordance cosmology. This study is designed to be agnostic of any inferential uncertainties which may arise from the interaction between aleatoric and epistemic uncertainties in the data and inference methods. Moreover, it demonstrates that current measurements close the 1%-precision mark might be less robust as previously thought.

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Achievement 2

I pioneered a novel lens modelling approach, known as the lens "matching" technique, which directly connects galaxy simulations to lensing galaxies in observations.
Traditional lens modelling techniques rely on recipes which aim to efficiently reproduce shapes and slopes of galaxies, as they are usually observed. These methods therefore suppress or even completely ignore the evolutionary processes of galaxies and the physical properties which form and drive them. In contrast, cosmological hydrodynamical simulations have made significant strides in recent years, incorporating semi-analytical models which simulate star formation and feedback effects at small scales, enabling exploration of various galaxy-formation scenarios.
Through proof-of-concept, I demonstrate that enhancing the complexity and realism of the galaxy models underlying the lens models can lead to plausible matches with observations. Additionally, by embedding the lens matching technique within a Bayesian framework, it becomes feasible to infer the relative posterior probabilities of two different galaxy-formation scenarios, a task that was previously deemed nearly impossible.

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Achievement 3

Bubble chambers and droplet detectors used in dosimetry and dark matter particle search experiments use a superheated metastable liquid in which nuclear recoils trigger bubble nucleation. This process is described by the classical heat spike model of F. Seitz [Phys. Fluids (1958-1988) 1, 2 (1958)], which uses classical nucleation theory to estimate the amount and the localization of the deposited energy required for bubble formation. Here we report on direct molecular dynamics simulations of heat-spike-induced bubble formation. They allow us to test the nanoscale process described in the classical heat spike model. 40 simulations were performed, each containing about 20 million atoms, which interact by a truncated force-shifted Lennard-Jones potential. We find that the energy per length unit needed for bubble nucleation agrees quite well with theoretical predictions, but the allowed spike length and the required total energy are about twice as large as predicted. This could be explained by the rapid energy diffusion measured in the simulation: contrary to the assumption in the classical model, we observe significantly faster heat diffusion than the bubble formation time scale. Finally we examine α-particle tracks, which are much longer than those of neutrons and potential dark matter particles. Empirically, α events were recently found to result in louder acoustic signals than neutron events. This distinction is crucial for the background rejection in dark matter searches. We show that a large number of individual bubbles can form along an α track, which explains the observed larger acoustic amplitudes.

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April 29, 2023

Prof. Dr. Thilo Stadelmann
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The **Centre for Artificial Intelligence** confirms the following employment situation of the applicant **Dr. Philipp Denzel** of the proposal entitled "*Deep generative modelling for gravitational lensing fields from 3D models of galaxies*":

- Level of employment at the anticipated start of the planned Spark project: 100%
- Percentage of the salary covered by the institution: 90%
- Percentage of the salary covered by the Spark grant: 10%

Prof. Dr. Thilo Stadelmann (Director of the Centre for Artificial Intelligence)