U.S. Department of Homeland Security
U.S. Citizenship and Immigration Services
03.05.2023

RE: Dr. Ryan-Rhys Griffiths

Dear Officer,

I am delighted to recommend Ryan-Rhys Griffiths to be designated as an outstanding scholar in machine learning research. Ryan-Rhys Griffiths is an internationally-recognized expert in Gaussian process models and their applications to problems in materials science and engineering.

Regarding my own qualifications to make this recommendation, since 2019 I have served as a Staff Scientist at xxxxx, a US government agency. I am a Principal Investigator (PI) in the Center for Applied Scientific Computing (CASC) at xxxxx where I am co-PI of a Strategic Initiative (SI) Lab Directed Research and Development (LDRD) grant of $2 million a year for 3 years on Digital Twins for Advanced Manufacturing. From 2017-2019 I was a Postdoctoral Researcher at xxxxx and from 2012-2017 I completed my Ph.D under the supervision of Prof. xxxxx at UC Davis. I'm a scientific AI researcher and manager with a track record of building product vision, executing technical strategy, and presenting to customers and government stakeholders. My team engineers next-generation additive manufacturing platforms and digital twins to inspect and assess the quality of 3D printed components using state-of-the-art computer vision techniques. My Postdoctoral and Ph.D research focused on computational physics and applied mathematics where I developed computational fluid dynamic simulations for high-performance computing (HPC) applications and accelerated physics simulations of laser-based metal 3D printing processes. I have previously served as a researcher in the Space Science Division (SST) of the NASA Ames Research Center where I worked on statistical models for the processing of computational fluid dynamics simulations and statistical analysis of high-dimensional turbulence data from 3D incompressible and isotropic direct numerical simulations (DNS).

I became familiar with the work of Ryan-Rhys Griffiths when working on an applied problem in material design optimization which benefited from Bayesian optimization to accelerate

the search for high-performant materials. The broad goal of Bayesian optimization is to use a probabilistic surrogate model of a figure of merit (such as the printing quality of a 3D printer) to guide the search for promising design components e.g. printer parts. The probability distribution maintained by the surrogate model allows an experimentalist to trade off what they already know about promising design components with what they don't know about regions of the design component space that have yet to be explored. In Bayesian optimization terminology this is termed the exploration/exploitation tradeoff. The effect of such a methodology is to identify promising material designs much more rapidly compared to trial-and-error testing. While I have given a specific example in materials design, the Bayesian optimization methodology is completely general and holds the potential to impact a broad range of industrial problems in science and engineering.

Following his PhD work at the University of Cambridge, Ryan-Rhys Griffiths has taken up a position as a Postdoctoral Research Scientist at Meta Research where he continues to further the state-of-the-art in Bayesian optimization as part of the Adaptive Experimentation team in the Core Data Science organization. The Adaptive Experimentation team is responsible for the development and maintenance of the open-source software library BoTorch which is the world's leading software solution for Bayesian optimization.

Concretely, in terms of Ryan-Rhys Griffiths's research contributions, the works most relevant for my own work at LLNL are his papers on 'Achieving Robustness to Aleatoric Uncertainty with Heteroscedastic Bayesian Optimization', 'HEBO: Pushing the Limits of Sample-Efficient Hyperparameter Optimisation", and "GAUCHE: A Library for Gaussian Processes in Chemistry. In the first of these works, Ryan-Rhys Griffiths introduces a novel scheme for Bayesian optimization where the goal is to minimize measurement noise in the suggestions from the Bayesian optimization algorithm. Such a scheme is highly beneficial for materials design such as the search for performant 3D printing components where robustness to large-scale manufacture is a core design consideration. The scheme operates by maintaining a heteroscedastic Gaussian process which models input-dependent noise. This model is then paired with an acquisition function that penalizes areas of the input space with large noise with the net effect that the scheme proposes solutions that are robust to perturbations introduced by a manufacturing process. The paper was published in Machine Learning: Science and Technology, a prestigious international journal in the field of machine learning.

Ryan-Rhys Griffiths's second work is related to the Heteroscedastic Evolutionary Bayesian Optimization (HEBO) algorithm. This algorithm won the 2020 NeurIPS Black-Box Optimization Competition. The NeurIPS conference is the top international venue for machine learning research. The HEBO algorithm currently has 108 citations and has been published in the prestigious Journal of Artificial Intelligence Research. The algorithm showed the strongest performance on machine learning hyperparameter tuning tasks in the competition by introducing novel methods for considering heteroscedasticity and non-stationarity of the underlying data via input warping using a Beta Kumaraswamy distribution function and Yeo-Johnson and Box-Cox transforms to correct for heteroscedasticity.

Lastly, Ryan-Rhys Griffiths's work on FLowMO (published as a NeurIPS workshop spotlight - top 5% of submitted papers) and GAUCHE: A Library for Gaussian Processes in Chemistry have extended the Bayesian optimization framework to operate on molecules and chemical reactions. By considering kernels over discrete molecular spaces, the software library allows users to model molecules in a probabilistic fashion with exact Bayesian inference and judging

from the citing papers, has already seen use by pharmaceuticals researchers including the Artificial Intelligence group at AstraZeneca. GAUCHE was recently accepted to the main track at NeurIPS 2023, the world's leading machine learning conference.

Dr. Griffiths has served as a reviewer for over 50 scientific articles and has received a trusted reviewer award from the Institute of Physics. Some of the most important journals and conferences Dr. Griffiths has reviewed for have included the Nature Machine Intelligence journal, the Chemical Science journal, and the Neural Information Processing Systems conference, all of which maintain very high standards for reviewer selection.

In conclusion, Ryan-Rhys Griffiths's research has helped to inform the progression of projects at Lawrence Livermore National Laboratory and his continued work at Meta Research will no doubt continue to benefit our work. Dr. Griffiths has made outstanding contributions of great impact to the field of machine learning and the natural sciences marking him out as having risen to the very top of his field. Furthermore, Dr. Griffiths has sustained his contributions to the international research community over time, as evidenced by achieving over 450 citations in the past year alone. It is typically considered an achievement to have a single paper accepted to NeurIPS, but this year Dr. Griffiths had two papers accepted to this top tier conference. I have no hesitation in recommending that Ryan-Rhys Griffiths be awarded an EB-1A green card based on his outstanding research scholarship in machine learning.

Sincerely,

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Dr. xxxxx
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