# 2022 IEEE/ACM International Workshop on Artificial Intelligence and Machine Learning for Scientific Applications (AI4S 2022)

Dallas, Texas, USA 13-18 November 2022



**IEEE Catalog Number: ISBN:** 

CFP22Z85-POD 978-1-6654-6208-2

## Copyright © 2022 by the Institute of Electrical and Electronics Engineers, Inc. All Rights Reserved

Copyright and Reprint Permissions: Abstracting is permitted with credit to the source. Libraries are permitted to photocopy beyond the limit of U.S. copyright law for private use of patrons those articles in this volume that carry a code at the bottom of the first page, provided the per-copy fee indicated in the code is paid through Copyright Clearance Center, 222 Rosewood Drive, Danvers, MA 01923.

For other copying, reprint or republication permission, write to IEEE Copyrights Manager, IEEE Service Center, 445 Hoes Lane, Piscataway, NJ 08854. All rights reserved.

\*\*\* This is a print representation of what appears in the IEEE Digital Library. Some format issues inherent in the e-media version may also appear in this print version.

 IEEE Catalog Number:
 CFP22Z85-POD

 ISBN (Print-On-Demand):
 978-1-6654-6208-2

 ISBN (Online):
 978-1-6654-6207-5

### Additional Copies of This Publication Are Available From:

Curran Associates, Inc 57 Morehouse Lane Red Hook, NY 12571 USA Phone: (845) 758-0400

Fax: (845) 758-2633

E-mail: curran@proceedings.com Web: www.proceedings.com



# 2022 IEEE/ACM International Workshop on Artificial Intelligence and Machine Learning for Scientific Applications (AI4S) AI4S 2022

## **Table of Contents**

| Message from the Workshop Chairs Vorkshop Organization  |    |
|---|----|
| Session 1   |    |
| Automated Continual Learning of Defect Identification in Coherent Diffraction Imaging Orcun Yildiz (Argonne National Laboratory, USA), Henry Chan (Argonne National Laboratory, USA), Krishnan Raghavan (Argonne National Laboratory, USA), William Judge (Formerly of University of Illinois Chicago, USA), Mathew J. Cherukara (Argonne National Laboratory, USA), Prasanna Balaprakash (Argonne National Laboratory, USA), Subramanian Sankaranarayanan (Argonne National Laboratory, USA), and Tom Peterka (Argonne National Laboratory, USA) | 1  |
| Case Study on Coupling OpenFOAM with Different Machine Learning Frameworks  Fabian Orland (RWTH Aachen University, Germany), Kim Sebastian Brose (RWTH Aachen University, Germany), Julian Bissantz (Technical University Darmstadt, Germany), Federica Ferraro (Technical University Darmstadt, Germany), Christian Terboven (RWTH Aachen University, Germany), and Christian Hasse (Technical University Darmstadt, Germany)  | 7  |
| PhySRNet: Physics Informed Super-Resolution Network for Application in Computational Somethanics  |    |
| Determining HEDP Foams' Quality with Multi-View Deep Learning Classification  | 19 |

## **Session 2**

| Pattern-Based Autotuning of OpenMP Loops using Graph Neural Networks  Akash Dutta (Iowa State University, USA), Jordi Alcaraz (University of Oregon, USA), Ali TehraniJamsaz (Iowa State University, USA), Anna Sikora (Universitat Autonoma de Barcelona, Spain), Eduardo Cesar (Universitat Autonoma de Barcelona, Spain), and Ali Jannesari (Iowa State University, USA) | 26 |
|---|----|
| Ensuring AI For Science Is Science: Making Randomness Portable  Hana Ahmed (Sandia National Laboratories, USA), Roselyne Tchoua (DePaul University, USA), and Jay Lofstead (Sandia National Laboratories, USA)  | 32 |
| Practical Federated Learning Infrastructure for Privacy-Preserving Scientific Computing<br>Lesi Wang (University of Nevada, United States) and Dongfang Zhao<br>(University of Nevada, United States)   | 38 |
| Scalable Integration of Computational Physics Simulations with Machine Learning   | 44 |
| Author Index  | 51 |