## 2021 3rd Annual Workshop on Extreme-scale Experiment-in-the-Loop Computing (XLOOP 2021)

St. Louis, Missouri, USA 19 November 2021



IEEE Catalog Number: CFP21W37-POD ISBN: 978-1-6654-1123-3

### Copyright © 2021 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:
 CFP21W37-POD

 ISBN (Print-On-Demand):
 978-1-6654-1123-3

 ISBN (Online):
 978-1-6654-1122-6

#### **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



# 2021 3rd Annual Workshop on Extreme-scale Experiment-in-the-Loop Computing (XLOOP) XLOOP 2021

### **Table of Contents**

Message from the Workshop Chairs
Session 1
ALS Share, a Lightweight Data Sharing Service for a Synchrotron Radiation Facility
Designing a Streaming Data Coalescing Architecture for Scientific Detector ASICs with  Variable Data Velocity
Bridging Data Center AI Systems with Edge Computing for Actionable Information Retrieval

### **Session 2**

High-Performance Hybrid-Global-Deflated-Local Optimization with Applications to Active Learning	24
Marcus Michael Noack (Lawrence Berkeley National Laboratory, USA), David Perryman (The University of Tennessee at Knoxville, USA), Harinarayan Krishnan (Lawrence Berkeley National Laboratory, USA), and Petrus H.Zwart (Lawrence Berkeley National Laboratory, USA)	24
Adversarial Attacks Against AI-Driven Experimental Peptide Design Workflows	. 30
Optimizing High-Throughput Capabilities by Leveraging Reinforcement Learning Methods with the Bluesky Suite	36
Daniel Olds (Brookhaven National Laboratory, USA), Daniel B. Allan	
(Brookhaven National Laboratory, USA), Thomas A. Caswell (Brookhaven National Laboratory, USA), Joshua Lynch (Brookhaven National	
Laboratory, USA), Phillip M. Maffettone (Brookhaven National	
Laboratory, USA), and Stuart I. Campbell (Brookhaven National	
Laboratory, USA)	
Author Index	43