Precision Convergence Webinar Series

Towards Sustainable Software
For Research and Societal Impact at Scale

By Dr. Daniel S. Katz

With High-Level Panel of Leaders in Science, Technology, On-the-Ground Action, and Policy

Thursday, December 02, 2021 | 11 AM to 1 PM EST (2 hours in duration)

Please Register HERE

ABSTRACT: Humanity has a mix of overlapping goals that relate to science (and more broadly, wissenschaft). We seek new knowledge for its own purpose as well as for its potential solution to both detailed and general problems, situations, and crises. And we want to be able to verify (or disprove) such knowledge (reproducibility), then build on it (reuse), as simply and as cost-effectively as possible. This knowledge can be captured in text, images, data, software, etc. In this talk, I will focus on knowledge captured in research software, which can be both read, executed, and extended. However, software, unlike data, requires ongoing human activity to fix bugs and to adapt to frequent changes in the software and hardware environment on which it depends, as well as changing user needs. This required human activity leads to different models of software sustainability, including a mix of open source communities, industrial or government support, and commercialization, some of which are also tied to different distribution mechanisms, such as source code, executables, containers, and services. This leads to a number of overlapping challenges and corresponding efforts, including making research software FAIR (findable, accessible, interoperable, and reusable), publishable, and citable, as well as considering how to support the human effort needed to maintain and sustain the software, including incentives and career paths. This talk will highlight some recent activities in these areas, including FAIR for research software principles, software citation, the Journal of Open Source Software, and software career paths.

PRESENTER: Daniel S. Katz is Chief Scientist at the National Center for Supercomputing Applications (NCSA), Research Associate Professor in Computer Science, Electrical and Computer Engineering, and the School of Information Sciences at the University of Illinois Urbana-Champaign. He is also a Better Scientific Software (BSSw) Fellow. He was previously a Senior Fellow in the Computation Institute at the University of Chicago and Argonne National Laboratory, a Program Director in the Division of Advanced Cyberinfrastructure at the National Science Foundation, Director for Cyberinfrastructure Development at the Center for Computation & Technology, Louisiana State University, Principal Member of the Information Systems and Computer Science Staff and Supervisor of the Parallel Applications Technologies group at the Jet Propulsion Laboratory, and a Computational Scientist at Cray Research. Dan's interest is in the development and use of advanced cyberinfrastructure to solve challenging problems at multiple scales, including in applications, algorithms, fault tolerance, and programming in parallel and distributed computing, and in policy issues, such as citation and credit mechanisms and practices associated with software and data, organization and community practices for collaboration, and career paths for computing researchers. He is a senior member of the IEEE and ACM, a founding editor and current Associate Editor-in-Chief of the Journal of Open Source Software, and Steering Committee Chair of the Research Software Alliance (ReSA).

About the series: The precision convergence series is launched to catalyze unique synergy between, on the one hand, novel partnerships across sciences, sectors and jurisdictions around targeted domains of real-world solutions, and on the other hand, a next generation convergence of AI with advanced research computing and other data and digital architectures such as PSC's Bridges-2, and supporting data sharing frameworks such as HuBMAP, informing in a real time as possible the design, deployment and monitoring of solutions for adaptive real-world behavior and context.

The McGill Centre for the Convergence of Health and Economics (MCCHE) is a virtual world network of scientist, action and policy leaders promoting the weaving of digital-powered interdisciplinary science into person-centered domain-specific solutions at scale to global challenges faced by traditional and modern economy and society worldwide. The MCCHE stimulates lasting collaborations that bridge the many divides in the market, economy, and society that are at the root of these most pressing modern challenges through collaborative of modular convergence innovation platforms.

The Pittsburgh Supercomputing Center is a joint computational research center between Carnegie Mellon University and the University of Pittsburgh. Established in 1986, PSC is supported by several federal agencies, the Commonwealth of Pennsylvania and private industry. PSC provides university, government, and industrial researchers with access to several of the most powerful systems for high-performance computing, communications, and data-handling available to scientists and engineers nationwide for unclassified research. PSC advances the state-of-the-art in high-performance computing, communications and informatics and offers a flexible environment for solving the largest and most challenging problems in computational science.

Co-Chairs:

Laurette Dubé, PhD is the founding Chair and Scientific Director of the McGill Centre for the Convergence of Health Economics. She holds the James McGill Chair of Consumer and Life-style Psychology and Marketing. Her work has been published in top disciplinary journals in Psychology, Management and Medicine as well as in multidisciplinary journals. She holds an MBA in finance, and a PhD in behavioural decision making and consumer psychology. During her 2020-2021 sabbatical, she is a visiting scholar at the National Research Council of Canada and at the Pittsburgh Supercomputing Center, Carnegie Mellon, USA. https:// thefutureeconomy.ca/interviews/ laurette-dube

Shawn Brown, PhD is Vice Chancellor for Research Computing at the University of Pittsburgh and the Director of Pittsburgh Supercomputing Center at the Carnegie Mellon University/ University of Pittsburgh and. Prior to his appointment, Dr. Brown served as the Associate Direc-tor of Research Software Development at the McGill Centre of Integrative Neuroscience at the McGill Neurological Institute. Dr. Brown is an expert on high - performance computing and computational simulation. He has over 25 years of experience in developing software to support the use of high-performance computing for research in areas such as chemistry, bioinformatics, and public health. his research interests are ALSO in how agent-based modeling and other com-putational techniques can be used to provide decision support in public health and chronic dis-ease.

Panellists:

Dr Patricia P. Silveira, MD, PhD is the Scientific director of the Genomics and Epigenetics pillar of the Ludmer Centre for Neuroinformatics & Mental Health, based at the Douglas Re-search Centre, an associate professor at the Department of Psychiatry at McGill University, and a core member of the U.S. based National Scientific Council on the Developing Child. A pedia-trician and neuroscientist, Dr Silveira's research focuses on how perinatal and early-childhood environments shape and modulate both health and disease across the lifespan, into old age. Her aim is to identify genetic/ epigenetic and peripheral markers that interact with environmental adversities in childhood, modifying endophenotypes (impulsivity, sensitivity to reward, food choices) that ultimately affect healthy growth and neurodevelopment, increasing an individual's risk for developing chronic diseases and mental illnesses across their lifespan. Her lab is focused on understanding child development and long-term risk for disease from a gene network-environment interaction perspective, using a life-course approach, deploying and applying novel methodologies to integrate multilevel data using big data.

Dr. Yaroslav O. Halchenko is a Research Associate Professor leading the http:// centerforopenneuroscience.org at the Department of Psychological and Brain Sciences of Dart-mouth College. The center's mission is to promote, develop, and contribute to Open software, data, and standards to improve efficiency, sharing, and reproducibility in Neuroscience and other fields. Dr. Halchenko is a Debian developer and a lead and/or active contributor to a number of free and open source projects such as NeuroDebian (http://neuro.debian.net), DataLad (https:// datalad.org), DANDI archive (https://dandiarchive.org), BIDS standard (https:// bids.neuroimaging.io), etc.

Dr. Morag Park is a Professor in the Departments of Oncology and Biochemistry and joined McGill in 1989. She is a Fellow of the Royal Society of Canada, Fellow of the Canadian Academy of Health Sci-ences, James McGill Professor and holds the Diane and Sal Guerrera Chair in Cancer Genetics at McGill University. Dr. Park received a B.Sc. with first class honors from the University of Glasgow, a Ph.D. in Viral carcinogenesis at the Medical Research Council Virology Institute in Scotland and completed post-doctoral training at the National Institutes for Cancer Research in Washington DC, US. She joined McGill University in 1989. She was the Director of the Molecular Oncology Group at the McGill University Hos-pital Centre (2006-8), Scientific Director of the Institute of Cancer Research for the CIHR (2008-13), co-chair of the Canadian Cancer Research Alliance (2008-2010) and is now Director of the Goodman Cancer Research Centre (2013-present). She is a recipient of a Canadian Cancer Research Alliance Award (2015) for Exceptional Leadership in Cancer Research, and also a recipient of the Canadian Society for Molecular Biosciences Arthur Wynne Gold Medal Prize (2016) for having made major contributions to biochemistry, molecular and cell biology in Canada, Most recently she is a recipient of the Canadian Cancer Society's 2017 Robert L. Noble Prize. Dr. Park is a research leader in the field of receptor tyrosine kinases (RTK) and mechanisms of oncogenic activation of RTKs in human cancers. She cloned the Met RTK, which is now a key therapeutic target in oncology. She established the Breast Cancer Functional Genomics Group at McGill. She has pioneered studies of the breast tumour and immune microenvironment in triple negative breast cancer (TNBC). She has established animal models as well as patient derived xenografts to study heterogeneity, tumor progression and drug response in TNBC. She was the elected chair of the Tumour Microenvironment Network of the American Association for Cancer Research (2015-2017). She has more than 200 publications.

Fabio Galbusera, PhD, is the director of the Laboratory of Biological Structures Mechanics at IRCCS Istituto Ortopedico Galeazzi. His main research interests are the biomechanics of the spine, the use of numerical models for its investigation as well as spinal imaging, about which he published more than 130 papers in international peer-reviewed journals. He is member of the International Society for the Study of the Lumbar Spine (ISSLS), of the Spine Society of Europe (Eurospine), of AO Spine and of the European Society of Biomechanics, and is currently part of the Editorial Boards of Journal of Biomechanics, European Spine Journal, European Radiology Experimental and Frontiers in Bioengineering and Biotechnology. Dr. Galbusera graduated in Biomedical Engineering at the Politecnico di Milano, Italy and received the PhD at the Institute of Orthopaedic Research and Biomechanics, Ulm University, Germany. He has recently published a book about the biomechanics of the human spine, covering its basic principles as well as spinal disorders and treatments.

Petra Ritter is a full professor for Brain Simulation. She heads the Brain Simulation Section with an interdisciplinary team of developers and medical doctors at the Berlin Institute of Health and the Dept. of Neurology, Charité University Medicine Berlin. Her research focuses on integrating multi-level data in computational models of the brain to discover multi-scale mechanisms of brain function and dysfunction. She is leading the development of a Virtual Research Environment. Petra Ritter serves as the lead of the German national research infrastructure initiative neuroscience (NFDI-Neuroscience) as well as lead of a European Open Science Cloud (EOSC) Project - "The Virtual Brain Cloud". In her role as the lead of the Co-design Project The Virtual Brain she has directed the implementation of General Data Protection Regulation (GDPR) compliant simulation and processing workflows in the Human Brain Project's e-infrastructure EBRAINS. She is presently leading the development of the "Health Data Cloud" - EBRAINS' service for sensitive data. Petra Ritter co-leads the open-source The Virtual Brain simulation platform. She is a member of the INCF governance board and of the INCF Council for Training, Science, and Infrastructure (CTSI). Petra Ritter is working with the Brain Imaging Data Structure (BIDS) community to develop FAIR data standards and has contributed the extension proposal "BIDS Computational Model Specification".