PACIFIC SYMPOSIUM ON BIOCOMPUTING 2022

2022 marks the 27th Pacific Symposium on Biocomputing (PSB). At the time of this writing, we expect to be on the Big Island in person with a recognizable "normal" PSB. In 2021 we conducted a control experiment of having an entirely virtual "zoom" PSB. As expected, the scientific papers and the talks were still excellent—we learned during the pandemic that formal scientific presentations can work well in a virtual format. However, the meeting undeniably lost critical elements—the personal, professional and scientific conversations at the sessions, conference meals, at the pool, at the beach and *in the ocean* (!) were lost. We were reminded how much we depend on this annual face-to-face interaction with colleagues in Hawaii as a source of news, ideas and collaborations. Some were also reminded how therapeutic a week of warm sunshine can be at the onset of what is deep winter for many in the northern hemisphere.

So we are now back with a new appreciation of all that this meeting means to us personally and professionally. The world has changed greatly since we last gathered together in January of 2020. SARS-CoV-2 and Covid-19 continue to cause suffering and death, the role and importance of science in public health and public policy is under great debate, and the twin revolutions of biology and computation (especially AI, as well as data science and informatics) continue to raise important ethical issues of privacy, security, justice, bias, equity and access. Many institutions are finally focused seriously on ensuring justice, equity, diversity and inclusion for all the underrepresented and underserved—particularly for Black and Indigenous people. These issues influence the day-to-day work we do in biocomputation (the scientific projects we pursue, the people we work with, the goals of our work) and must be confronted directly and with an understanding of how our work impacts the world.

In addition to being published by World Scientific and indexed in PubMed, the proceedings from all PSB meetings are available online at <u>http://psb.stanford.edu/psb-online/</u>. PSB has 1227 papers listed in PubMed (as of today). These papers are routinely cited in archival journal articles and often represent important early contributions in new subfields—many times before there is an established literature in more traditional journals; for this reason, many papers have garnered hundreds of citations.

The Twitter handle PSB 2022 is @PacSymBiocomp and the hashtag this year will be #psb22.

The efforts of a dedicated group of session organizers have produced an outstanding program. The sessions of PSB 2022 and their hard-working organizers are as follows:

AI-driven Advances in Modeling of Protein Structure

Session Chairs: Krzysztof Fidelis, Sergei Grudinin

Big Data Imaging Genomics: Reproducible Findings, Individual Predictions, and Clinical Decisions

Session Chairs: Peter Kochunov, Li Shen, John Darrell Van Horn, Paul M. Thompson

Human Intrigue: Meta-Analysis Approaches for Big Questions with Big Data

Session Chairs: Carly A. Bobak, Meghan E. Muse, Kristine A. Giffin, Derek A. Williamson, Dennis P. Wall, Casey S. Greene, Jason Moore

Precision Medicine: Using Artificial Intelligence to Improve Diagnostics and Healthcare

Session Chairs: Steven E. Brenner, Martha L. Bulyk, Jonathan Chen, Dana C. Crawford, Roxana Daneshjou, Samuel G. Finlayson, Łukasz Kidziński

We are also pleased to present five workshops in which investigators with a common interest come together to exchange results and new ideas in a format that is more informal than the peer-reviewed sessions. For this year, the workshops and their organizers are:

Emerging Topics in Cancer Evolution

Organizers: Mohammed El-Kebir, Quaid Morris, Layla Oesper, Cenk Sahinalp

Genomic and Synthetic Biology Digital Biosecurity

Organizers: Corey M. Hudson, Nina Alli, Ravishankar K. Iyer, Zbigniew T. Kalbarczyk, Nicholas D. Pattengale

Image-based profiling: a powerful and challenging new data type

Organizers: Gregory P. Way, Hannah Spitzer, Philip Burnham, Arjun Raj, Fabian Theis, Anne E. Carpenter

Packaging Biocomputing Software to Maximize Distribution and Reuse

Organizers: William S. Bush, Brett Beaulieu-Jones, Christian Darabos, Nicholas Wheeler

Social, Technical, and Ethical Challenges in Biomedical Data Privacy

Organizers: Gamze Gursoy, Steven Brenner, Bradley Malin, Barbara Koenig

The PSB 2022 keynote speakers are Olga Troyanskaya (Science keynote) and Rob Reich (Ethical, Legal and Social Implications keynote).

Tiffany Murray has managed the peer review process and assembly of the proceedings since 2001 and plays a key role in many aspects of the meeting. We are grateful for the support of the National Institutes of Health¹, ISCB, Cleveland Institute for Computational Biology, Cipherome, and Penn Medicine, Penn Center for Precision Medicine. The Research Parasite Awards benefit from support from GigaScience, Jeff Stibel, Mr. and Mrs. Stephen Canon, and Drs. Casey and Anna Greene. The Research Symbiont Awards benefit from support from the Wellcome Trust and the DragonMaster Foundation.

We are particularly grateful to the PSB staff Al Conde, Paul Murray, Ryan Whaley, Mark Woon, BJ Morrison-McKay, Cynthia Paulazzo, Jackson Miller, Heather Miller, and Nicholas Murray for their assistance. We also acknowledge the many busy researchers who reviewed the submitted manuscripts on a very tight schedule. The partial list following this preface does not include many who wished to remain anonymous, and of course we apologize to any who may have been left out by mistake.

We (Altman, Hunter, Klein & Ritchie) acknowledge the many scientific and administrative contributions of our PSB Co-Chair, Dr. A. Keith Dunker for 26 years. While Keith has taken a step back from some of his PSB Co-Chair duties, his participation, at whatever level he wishes, will always be welcomed and valued. Thank you Keith for everything you have done for PSB.

We look forward to a great meeting and to seeing you on the Big Island. Aloha!

Pacific Symposium on Biocomputing Co-Chairs, October 8, 2021

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Thanks to the reviewers...

Finally, we wish to thank the scores of reviewers. PSB aims for every paper in this volume to be reviewed by three independent referees. Since there is a large volume of submitted papers, paper reviews require a great deal of work from many people. We are grateful to all of you listed below and to anyone whose name we may have accidentally omitted or who wished to remain anonymous.

Rocky Aikens Anna Antoniak Peniel Argaw Suzan Arslanturk Thibault Asselborn Omid Azizi Max Bluestone Carly Bobak Wouter Boomsma Soren Brunak Patrick Bryant Ljubomir Buturovic Christopher Cassa Pablo Chacon Chao Cheng Jianlin Cheng Brianna Chrisman Conor Corbin Heather Cordell Bruno Correia Tristan Cragnolini Roxana Daneshjou Charlotte Deane Dennis Della Corte James Diao Grant Duffy Arne Elofsson Barbara Engelhardt Ruogu Fang Amy Farnham Gilbert Feng Nick Fowler Jason Fries Kiran Garimella Olivier Gevaert Kristine Giffin Benjamin Glicksberg Dominik Glodzik Casper Goverde Algirdas Grybauskas John Gullet Ariana Haidari Yehudit Hassin Kathrin Hatch

Bryan He Shan He Andrew Hederman Edward Hollox Junzhou Huang Possu Huang Trey Ideker Zach Izzo Max Jansen Hyun-Hwan Jeong Raehoon Jeong Dokyoon Kim Sebastian Kmiecik Peter Kochunov David Koes Ilya Korsunsky Preethi Krishnan Wan-Ping Lee Damien Lekkas Joshua Levy Binglan Li Guangyuan "Frank" Li Wei Vivian Li Zilin Li Kresten Lindorff-Larsen Jinze Liu Xinghua Lu Almut Luetge Chong Liang Luo Michael Mariani Carla Marquez Luna Kaia Mattioli Matthew McDermott Lauren McDonnell Brett McKinney Lauren Mogil Ananda Mondal Meghan Muse Minh Nguyen Quang Nguyen Morteza Noshad Kliment Olechnovic David Ouyang Sergey Ovchinnikov

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