CHANGING WHAT'S POSSIBLE

DIFFERENTIATE Working Group: Physics-Informed Machine Learning (PIML)

22 July 2020

Agenda

Time (EDT)	Speaker	Topic
1:00 – 1:10	David Tew	Introduction
1:10 – 1:40	Maziar Raissi	Hidden Physics Models
1:40 – 2:10	Christopher Rackauckas	Automated Discovery and Acceleration of Physical Equations with Julia's SciML Ecosystem
2:10 – 2:40	Karthik Duraisamy	Physics-constrained Machine Learning for Industrial Applications
2:40 – 2:50	All	Lessons Learned and Implications for D’
2:50 – 3:00	ARPA-E	External Developments

D’ Program Objective

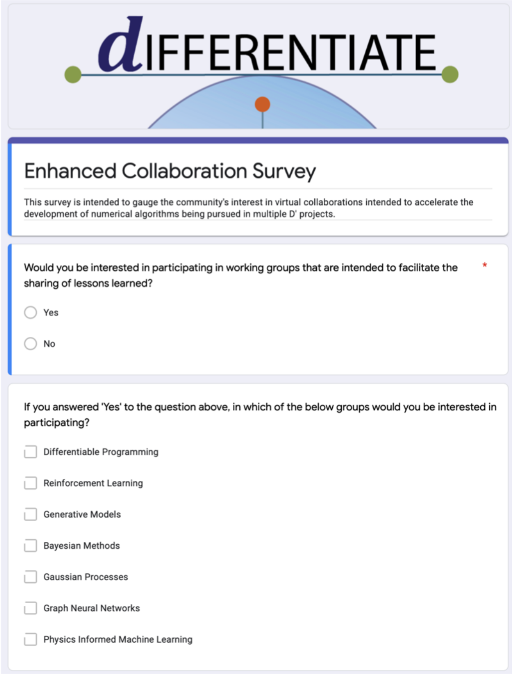
$30M

ML-Enhanced Design Tools → More Creative & Productive Engineers → Better Energy Products → Accelerated ARPA-E Mission

Enhanced Collaboration Proposal

- Objective
  - Accelerate progress by sharing (non-proprietary) lessons learned
  - Build strong community for future commercialization and technical efforts

- Approach
  - Open to all D’ community members but <u>NOT</u> required
  - Numerical algorithm-based organizational framework
  - Quarterly virtual technical working groups
  - Response solicited in survey after KO meeting


dIFFERENTIATE

Enhanced Collaboration Survey

This survey is intended to gauge the community's interest in virtual collaborations intended to accelerate the development of numerical algorithms being pursued in multiple D' projects.

Would you be interested in participating in working groups that are intended to facilitate the sharing of lessons learned? *

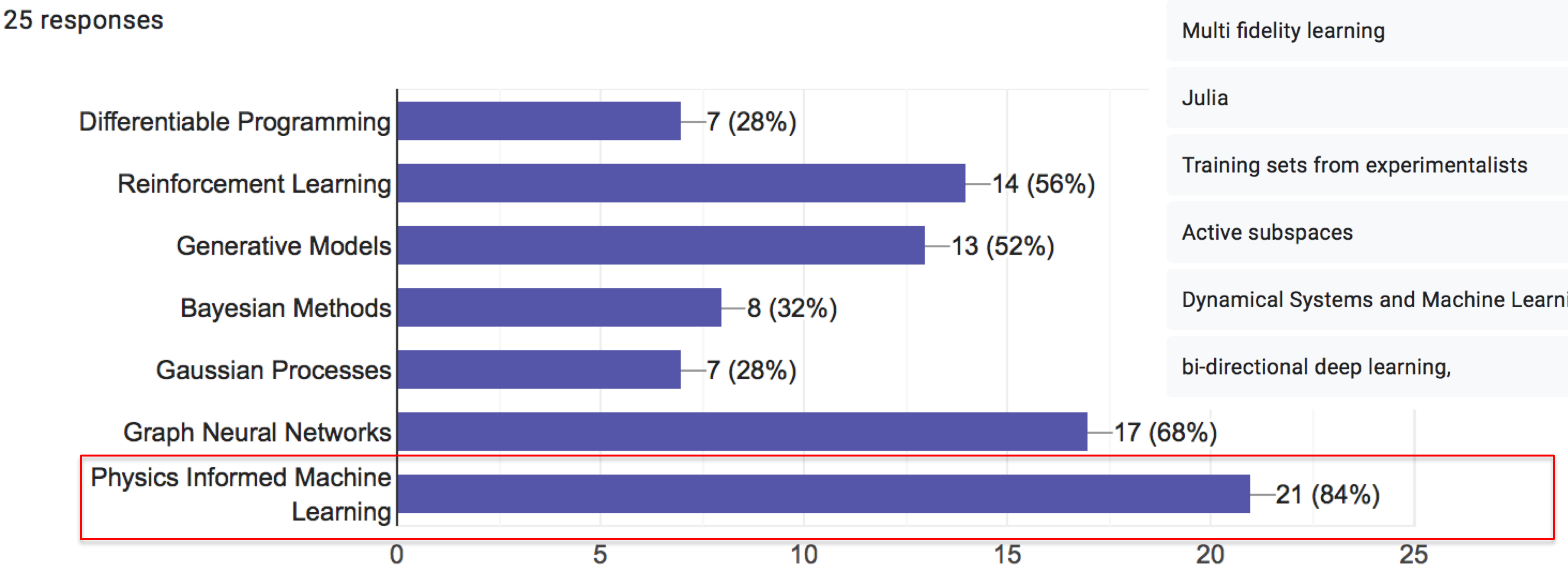
- Yes
- No

If you answered 'Yes' to the question above, in which of the below groups would you be interested in participating?

- Differentiable Programming
- Reinforcement Learning
- Generative Models
- Bayesian Methods
- Gaussian Processes
- Graph Neural Networks
- Physics Informed Machine Learning

Kick-Off Meeting Survey Responses

Potential Working Group Topics



What additional groups should we consider?

6 responses

- Multi fidelity learning
- Julia
- Training sets from experimentalists
- Active subspaces
- Dynamical Systems and Machine Learning
- bi-directional deep learning,

PIML: What?, Why? How?

(Dave's pre-workshop draft answers)

- **What?**
  - Leverage data and ML algorithms to evaluate, enhance or even discover physics-based models (e.g., differential equations) of physical systems
- **Why?**
  - Develop computationally-efficient & higher-fidelity models faster
  - Use models to design better performing engineering systems at lower cost

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2:40 – 2:50	All	Lessons Learned and Implications for D’
2:50 – 3:00	ARPA-E	External Developments **(Where do we learn more?)**

How?

CHANGING WHAT'S POSSIBLE

Physics-Informed Machine Learning/Scientific Machine Learning

External Developments

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D' Enhanced Team Collaboration Workshop

July 22, 2020

Total articles retrieved: 704

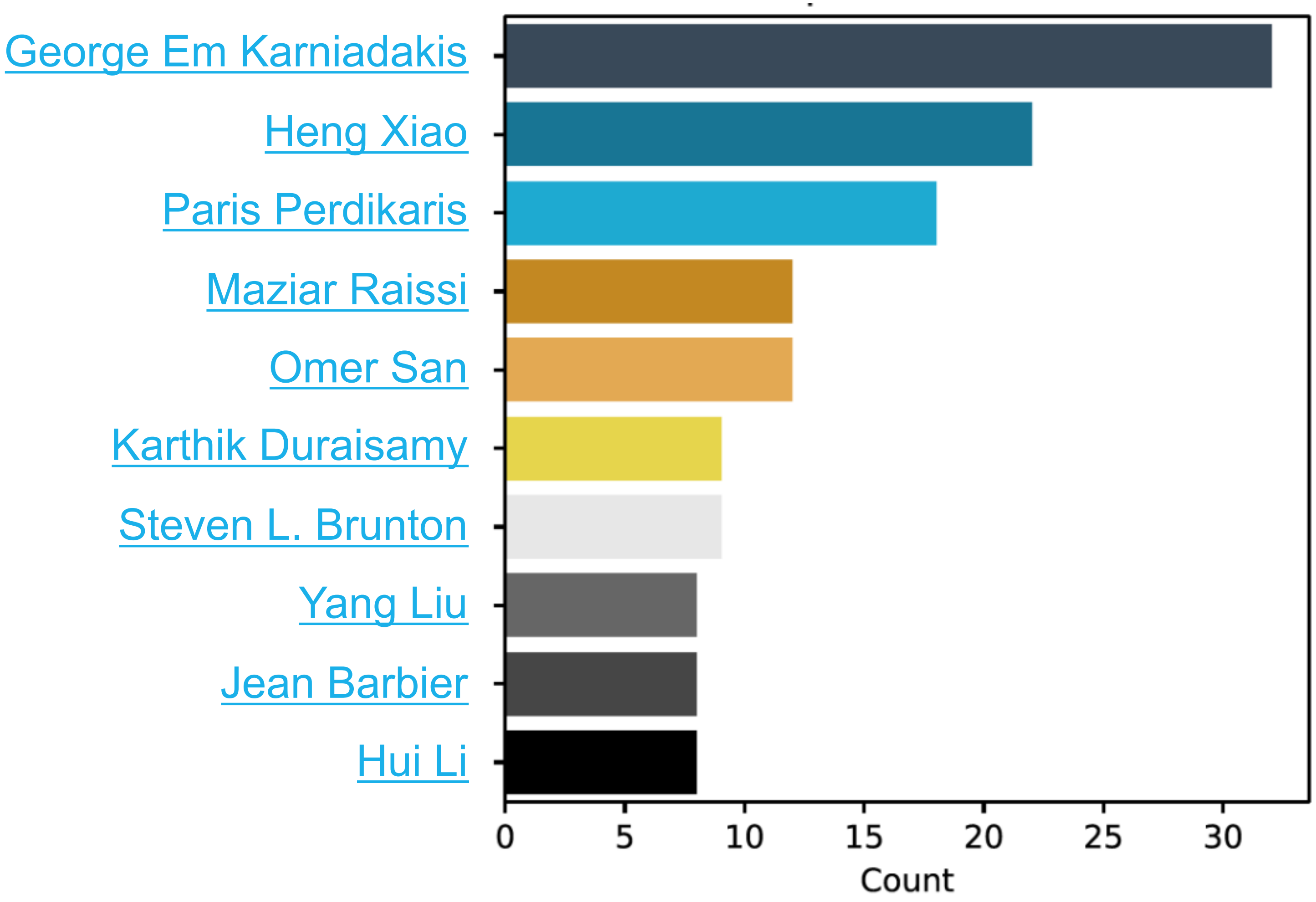
	2004	2005	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020
Scopus		1	1				1		1			5	21	41	226	209
Arxiv	1			3	1	2	1	1		1	3	2	14	29	56	84

<u>arXiv:</u> 198 articles

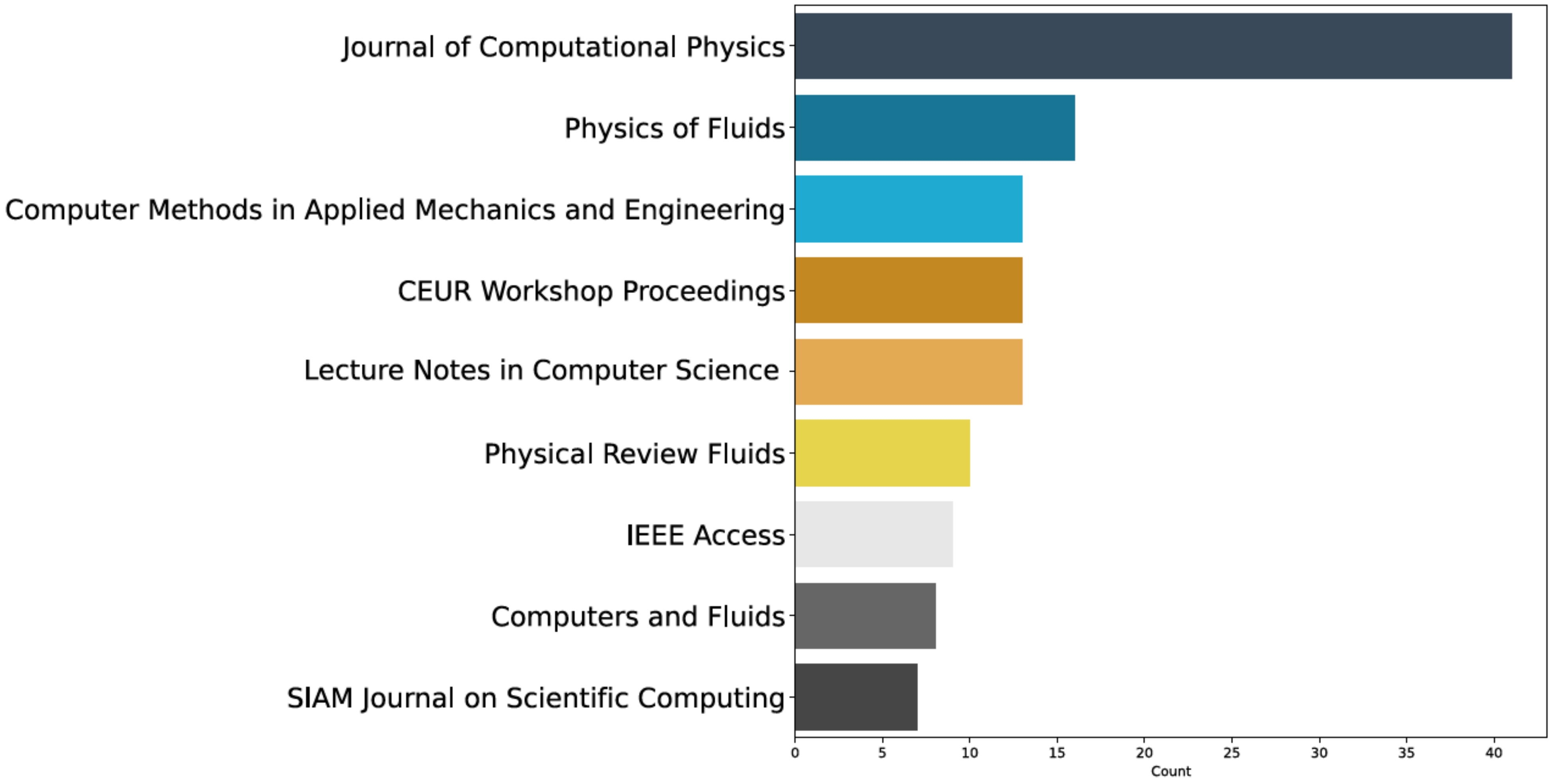
<u>Scopus:</u> 506 articles

<u>Search terms included</u>
"physics informed"
"scientific machine learning"
"SciML" along with
"machine learning"
"deep learning"
"neural networks"

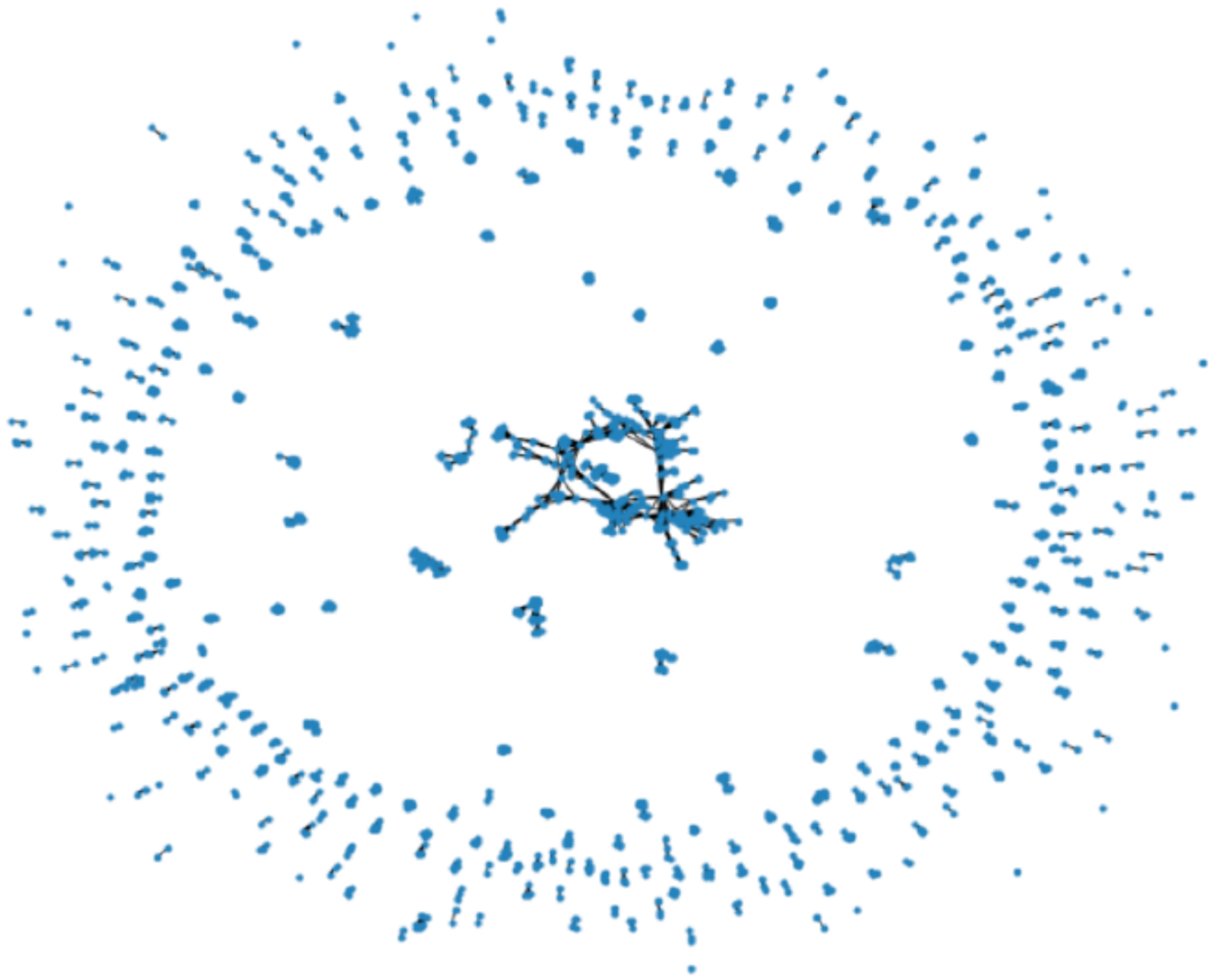
Top authors by article count



Top journals/proceedings by article count

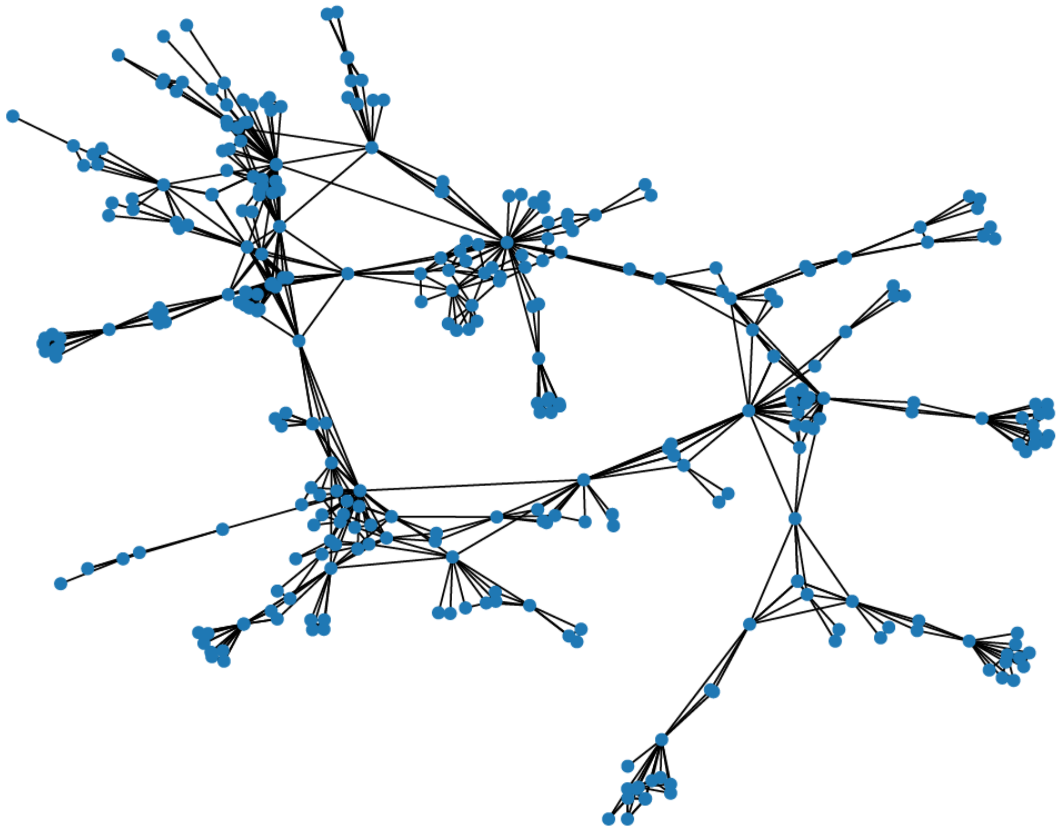


Co-authorship Network



- 704 articles
- 2035 authors
- 364 subgraphs of connected components

Top authors by number of connections



The largest subgraph of connected components
- 325 authors
- 990 connections

- George Em Karniadakis
- Paris Perdikaris
- Adama Tandia
- Roger H. French
- Steven L. Brunton
- Heng Xiao
- Satish Karra
- Shriram Srinivasan
- Rick Weber

Most cited articles by top connected authors

George Em Karniadakis (Publication years: 2018 and later)

Authors	Title
Raissi, M., Perdikaris, P., Karniadakis, G.E.	Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations
Raissi, M., Karniadakis, G.E.	Hidden physics models: Machine learning of nonlinear partial differential equations
Raissi, M., Perdikaris, P., Karniadakis, G.E.	Numerical Gaussian processes for time-dependent and nonlinear partial differential equations
Zhiping, M.A.O., Karniadakis, G.E.	A spectral method (of exponential convergence) for singular solutions of the diffusion equation with general two-sided fractional derivative
Li, Z., Bian, X., Tang, Y.-H., Karniadakis, G.E.	A dissipative particle dynamics method for arbitrarily complex geometries
Raissi, M., Wang, Z., Triantafyllou, M.S., Karniadakis, G.E.	Deep learning of vortex-induced vibrations
Zhang, K., Li, Z., Maxey, M., Chen, S., Karniadakis, G.E.	Self-Cleaning of Hydrophobic Rough Surfaces by Coalescence-Induced Wetting Transition
Perakakis, N., Yazdani, A., Karniadakis, G.E., Mantzoros, C.	Omics, big data and machine learning as tools to propel understanding of biological mechanisms and to discover novel diagnostics and therapeutics
Li, H., Lu, L., Li, X., Buffet, P.A., Dao, M., Karniadakis, G.E., Suresh, S.	Mechanics of diseased red blood cells in human spleen and consequences for hereditary blood disorders
Papageorgiou, D.P., Abidi, S.Z., Chang, H.-Y., Li, X., Kato, G.J., Karniadakis, G.E., Suresh, S., Dao, M.	Simultaneous polymerization and adhesion under hypoxia in sickle cell disease

Most cited articles by top connected authors

Paris Perdikaris (Publication years: 2018 and later)

Authors	Title
Raissi, M., Perdikaris, P., Karniadakis, G.E.	Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations
Raissi, M., Perdikaris, P., Karniadakis, G.E.	Numerical Gaussian processes for time-dependent and nonlinear partial differential equations
Zhu, Y., Zabaras, N., Koutsourelakis, P.-S., Perdikaris, P.	Physics-constrained deep learning for high-dimensional surrogate modeling and uncertainty quantification without labeled data
Sahli Costabal, F., Matsuno, K., Yao, J., Perdikaris, P., Kuhl, E.	Machine learning in drug development: Characterizing the effect of 30 drugs on the QT interval using Gaussian process regression, sensitivity analysis, and uncertainty quantification
Yang, Y., Perdikaris, P.	Adversarial uncertainty quantification in physics-informed neural networks
Bonfiglio, L., Perdikaris, P., Vernengo, G., De Medeiros, J.S., Karniadakis, G.	Improving SWATH seakeeping performance using multi-fidelity Gaussian process and Bayesian optimization
Bonfiglio, L., Perdikaris, P., Brizzolara, S., Karniadakis, G.E.	Multi-fidelity optimization of super-cavitating hydrofoils
Kissas, G., Yang, Y., Hwuang, E., Witschey, W.R., Detre, J.A., Perdikaris, P.	Machine learning in cardiovascular flows modeling: Predicting arterial blood pressure from non-invasive 4D flow MRI data using physics-informed neural networks
Sahli Costabal, F., Perdikaris, P., Kuhl, E., Hurtado, D.E.	Multi-fidelity classification using Gaussian processes: Accelerating the prediction of large-scale computational models
Bonfiglio, L., Perdikaris, P., del Águila, J., Karniadakis, G.E.	A probabilistic framework for multidisciplinary design: Application to the hydrostructural optimization of supercavitating hydrofoils

Most cited articles by top connected authors

Heng Xiao (Publication years: 2018 and later)

Authors	Title
Duraisamy, K., Iaccarino, G., Xiao, H.	Turbulence modeling in the age of data
Wu, J.-L., Xiao, H., Paterson, E.	Physics-informed machine learning approach for augmenting turbulence models: A comprehensive framework
Xiao, H., Cinnella, P.	Quantification of model uncertainty in RANS simulations: A review
Wu, J., Yin, X., Xiao, H.	Seeing permeability from images: fast prediction with convolutional neural networks
Sun, R., Xiao, H., Sun, H.	Investigating the settling dynamics of cohesive silt particles with particle-resolving simulations
Wu, J., Xiao, H., Sun, R., Wang, Q.	Reynolds-averaged Navier-Stokes equations with explicit data-driven Reynolds stress closure can be ill-conditioned
Wu, J.-L., Sun, R., Laizet, S., Xiao, H.	Representation of stress tensor perturbations with application in machine-learning-assisted turbulence modeling
Wang, J.-X., Roy, C.J., Xiao, H.	Propagation of input uncertainty in presence of model-form uncertainty: A multifidelity approach for computational fluid dynamics applications
Wang, J.-X., Huang, J., Duan, L., Xiao, H.	Prediction of Reynolds stresses in high-Mach-number turbulent boundary layers using physics-informed machine learning
Tang, H., Wang, J., Weiss, R., Xiao, H.	TSUFLIND-EnKF: Inversion of tsunami flow depth and flow speed from deposits with quantified uncertainties