23,000 annual simulation users

nanoHUB:
getting started guide to tool developers

Develop and publish tools in nanoHUB

Make your research reproducible and your workflows and data FAIR

Tanya Faltens, Daniel Mejia, Steven Clark, Juan Carlos Verduzco & Ale Strachan*
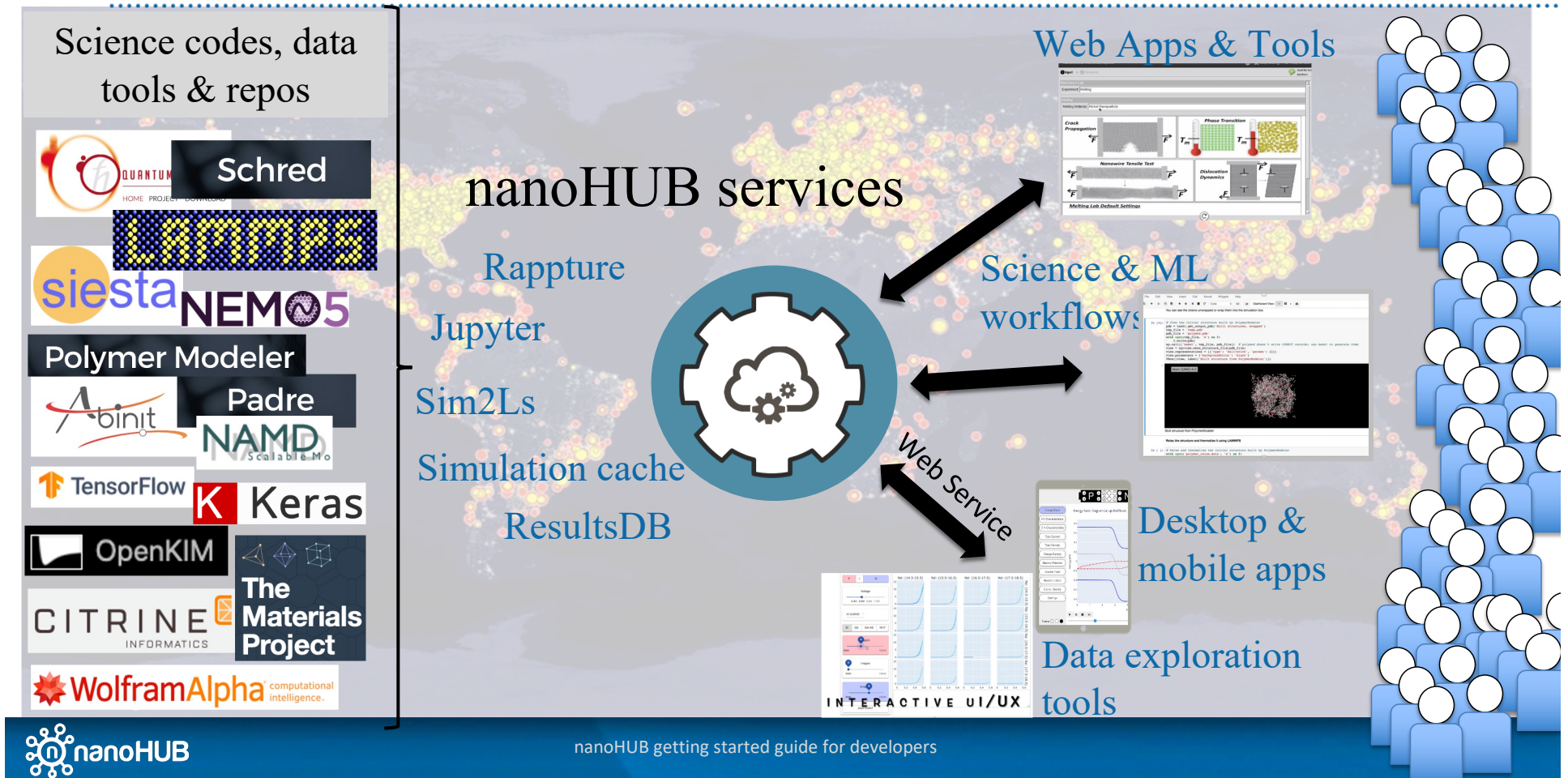
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nanoHUB

nanoHUB: online apps, tools, & data

Science codes, data tools & repos

nanoHUB services

- Rappture
- Jupyter
- Sim2Ls
- Simulation cache
- ResultsDB

Web Apps & Tools

Science & ML workflows

Web Service

Desktop & mobile apps

**Data exploration tools**

INTERACTIVE UI/UX

Overview

1. Why publish tools & apps in nanoHUB?
   - Tools are publications (DOIs and indexed by Web of Science)
   - Share your work with your community (22,000+ annual sim users)
2. Various tool and app types
   - Apps, workflows, Jupyter notebooks, commercial codes, X11 GUIs
3. Sim2Ls, FAIR workflows and data
   - Develop and publish Sim2Ls
4. Developing Apps
   - Connecting Sim2Ls to Jupyter and Web Apps
5. Tool Publication process
   - Register, deploy, test, and publish
6. Development environment
   - A Unix development environment (Jupyter or Linux desktop)
7. Simulation and data as a service
   - Launching tools and querying the ResultsDB

Why publish in nanoHUB?

Share your code/workflow with your community & make it:

1. Findable

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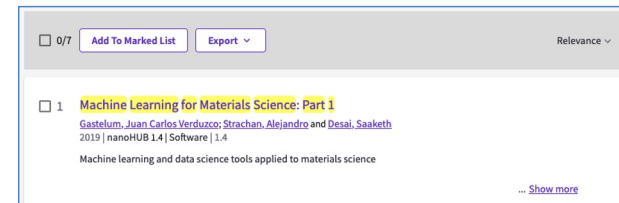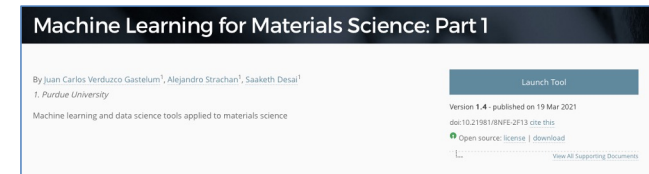
2. Accessible

- Online using a web browser
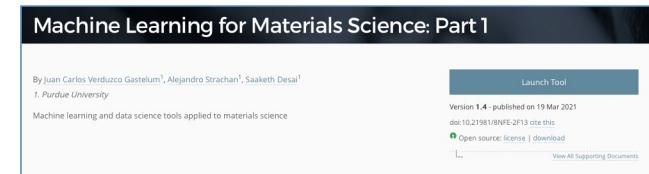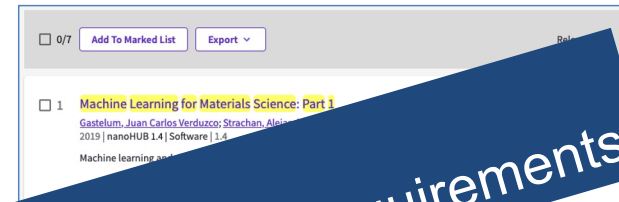- Using standard web services

2. Interoperable

- Publish complete workflows & use metadata to make services and requirements discoverable

4. Reusable

- Full workflows and data are open and accessible

5. Reproducible

- Apps, tools, & workflows are containerized with their compute environment

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Get credit for sharing your work
Satisfy or exceed funding agencies and publishers' data requirements

Machine Learning for Materials Science: Part 1

By Juan Carlos Verduzco Gastelum[1], Alejandro Strachan[1], Saaketh Desai[1]
1. Purdue University
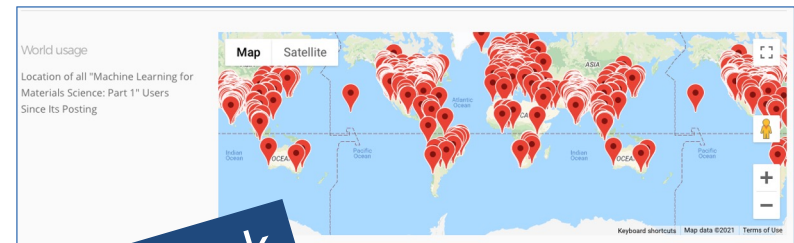Machine learning and data science tools applied to materials science

Version 1.4 - published on 19 Mar 2021
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Launch Tool

Why publish in nanoHUB? (cont'd)

4. Track your impact with detailed user metrics

https://nanohub.org/tools/mseml

Assess the impact of your work
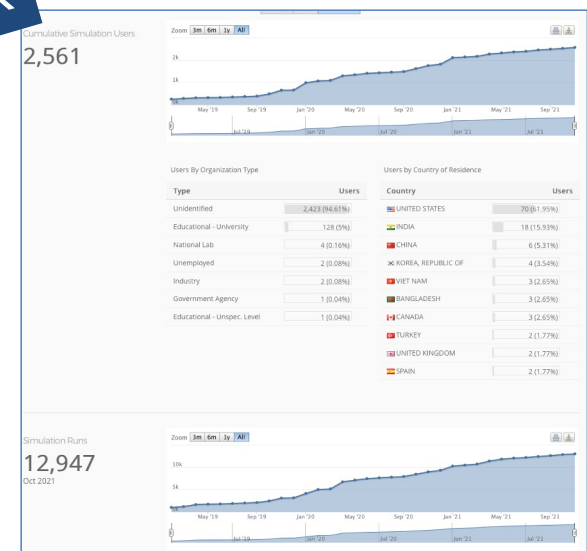
5. For certain tools outputs and results are automatically saved

- **Simulation cache** provides fast results for previously run simulations
- **Results database** enables querying all prior results