

# Pre-workshop activities: be ready for the hands-on session



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# STEP 1: Signing up for a nanoHUB account

The top screenshot shows the nanoHUB homepage. The navigation bar includes 'Login Sign Up Help Search'. The main heading is 'Serving Students, Researchers & Instructors'. Below this, statistics show '1.9 Million Annual Visitors' and '17,000 Simulation Users'. Four main service areas are listed: 'Model & Simulate', 'Learn & Teach', 'Develop Software', and 'Share & Publish'. The 'Sign Up' button in the navigation bar is highlighted with a red box, and an arrow points to the registration page below.

The bottom screenshot shows the 'Create New Account' page. It features a 'CONNECT WITH' section with four options: 'With an affiliated institution', 'Sign in with Facebook', 'Sign in with Google', and 'Sign in with LinkedIn'. A blue box on the right contains the text: 'You can choose to log in via one of these services, and we'll help you fill in the info below!'. Below this, it says 'Already have an account? Log in here.'



## STEP 2: Make sure you can launch a tool

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From your browser go to link: <https://nanohub.org/tools/matdatarepo/>

### Querying Data Repositories

By [Zachary D McClure<sup>1</sup>](#), [Alejandro Strachan<sup>1</sup>](#)

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Query database repositories using Python based APIs and tips for managing data

 Edit

Launch Tool

Version 1.0 - published on 03 Apr 2020

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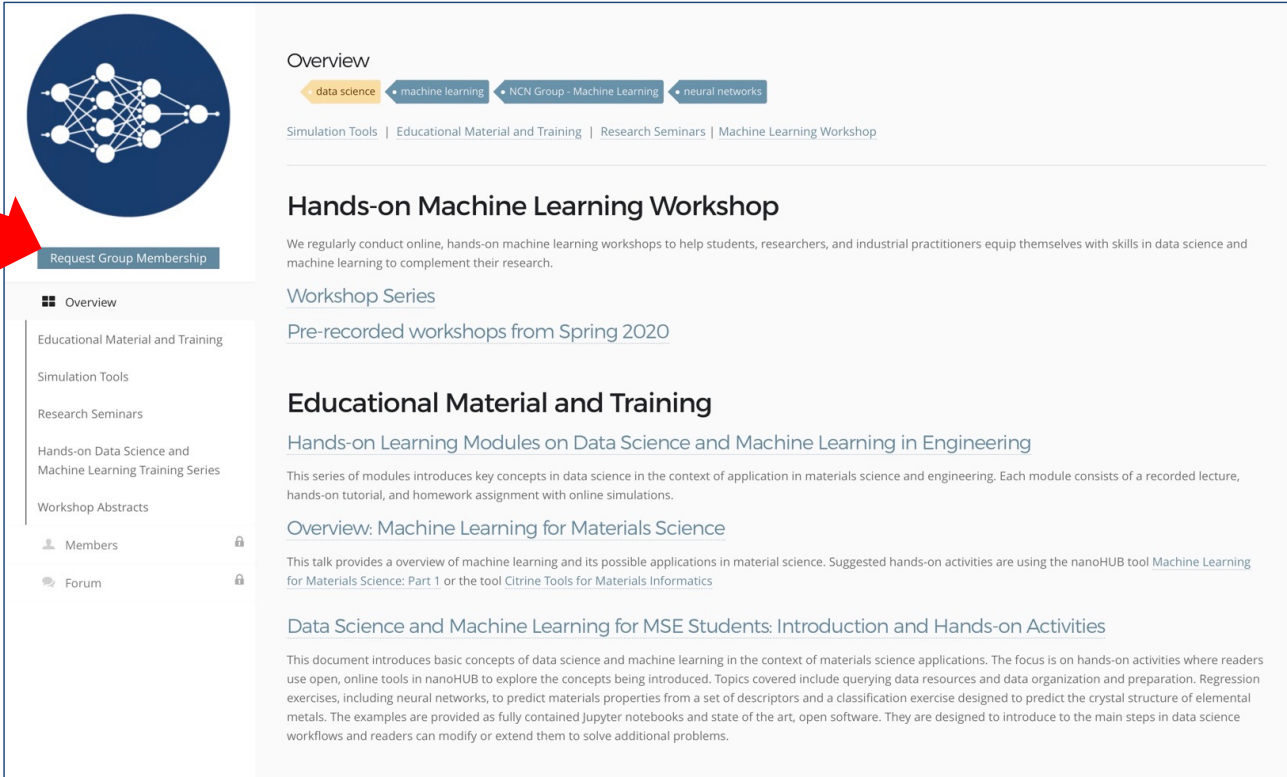
Click on Launch Tool to begin

Once Jupyter starts you will be able to run example notebooks

# STEP 3: join the ML group in nanoHUB for Q&A

<https://nanohub.org/groups/ml>

Request membership



The screenshot shows the nanoHUB group page for Machine Learning (ML). At the top left is a circular logo with a neural network diagram. Below it is a blue button labeled "Request Group Membership", which is highlighted by a red arrow and the text "Request membership". To the right of the logo is an "Overview" section with a breadcrumb trail: "data science" > "machine learning" > "NCN Group - Machine Learning" > "neural networks". Below the breadcrumb are links for "Simulation Tools", "Educational Material and Training", "Research Seminars", and "Machine Learning Workshop". The main content area features a section titled "Hands-on Machine Learning Workshop" with a description: "We regularly conduct online, hands-on machine learning workshops to help students, researchers, and industrial practitioners equip themselves with skills in data science and machine learning to complement their research." Below this is a "Workshop Series" section with a link to "Pre-recorded workshops from Spring 2020". The next section is "Educational Material and Training", containing a link to "Hands-on Learning Modules on Data Science and Machine Learning in Engineering" and a description: "This series of modules introduces key concepts in data science in the context of application in materials science and engineering. Each module consists of a recorded lecture, hands-on tutorial, and homework assignment with online simulations." Below that is an "Overview: Machine Learning for Materials Science" section with a description: "This talk provides an overview of machine learning and its possible applications in material science. Suggested hands-on activities are using the nanoHUB tool Machine Learning for Materials Science: Part 1 or the tool Citrine Tools for Materials Informatics." The final section is "Data Science and Machine Learning for MSE Students: Introduction and Hands-on Activities" with a description: "This document introduces basic concepts of data science and machine learning in the context of materials science applications. The focus is on hands-on activities where readers use open, online tools in nanoHUB to explore the concepts being introduced. Topics covered include querying data resources and data organization and preparation. Regression exercises, including neural networks, to predict materials properties from a set of descriptors and a classification exercise designed to predict the crystal structure of elemental metals. The examples are provided as fully contained Jupyter notebooks and state of the art, open software. They are designed to introduce to the main steps in data science workflows and readers can modify or extend them to solve additional problems." On the left side of the page is a navigation menu with items: "Overview", "Educational Material and Training", "Simulation Tools", "Research Seminars", "Hands-on Data Science and Machine Learning Training Series", "Workshop Abstracts", "Members" (with a lock icon), and "Forum" (with a lock icon).

# Go to the forum for Q&A during and after the session

The screenshot displays the nanoHUB interface for the 'Data Science and Machine Learning' group. The top navigation bar includes links for RESOURCES, EXPLORE, NANOHUB-U, PARTNERS, COMMUNITY, ABOUT, SUPPORT, DONATE, and TAKE A POLL. The user is logged in. The main content area is divided into three columns: a left sidebar with navigation options, a central forum listing, and a right sidebar with statistics and settings.

**Left Sidebar:**

- Overview
- Educational Material and Training
- Simulation Tools
- Research Seminars
- Hands-on Data Science and Machine Learning Training Series
- Workshop Abstracts
- Members (16)
- Forum (10)**

**Central Forum Listing:**

- FALL 2021 SERIES**
- 24. Autonomous Neutron Diffraction Experiments with ANDiE (0 Discussions, 0 Posts)
- SUMMER 2021 SERIES**
- 20. Batch Reification Fusion Optimization (BAREFOOT) Framework (0 Discussions, 0 Posts)
- 21. Active Learning via Bayesian Optimization for Materials Discovery (0 Discussions, 0 Posts)
- 22. A Machine Learning aided hierarchical screening strategy for materials discovery (0 Discussions, 0 Posts)
- 23. Debugging Neural Networks (10 Discussions, 13 Posts)
- SPRING 2021 SERIES**
- 12. Unsupervised clustering methods for image segmentation: application to scanning electron microscopy images of graphene (0 Discussions, 0 Posts)

**Right Sidebar:**

- Statistics:** Categories (24), Discussions (10), Posts (13)
- Email Settings:**  Email forum posts, Save
- Last Post:** For beginners, there is a great set of instructional machine learning and data science tutorial modules in nanoHUB... by Tanya Faltens on 10 Oct 2021 at 8:48 pm

Go to the forum for Q&A

