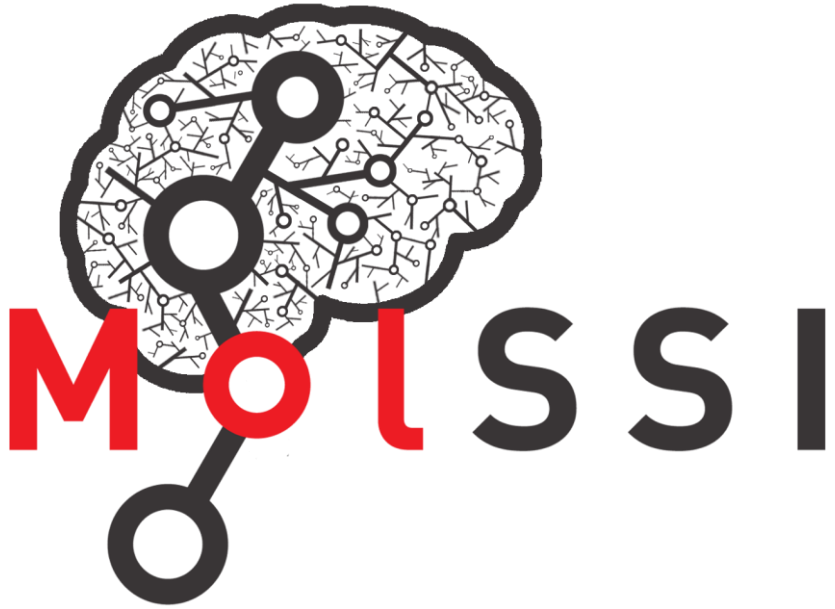


Industrial Training Program

Sina Mostafanejad

ACT-CMS Faculty Fellows Bootcamp
June 2024

MolSSI Industrial Training Program

- **Advanced Certified Workshops, Bootcamps, Learning Paths Hackathons, University Courses in**
  - **AI & ML**
  - **High-Performance Computing**
  - **Data Science**
  - **Software Engineering**
  - **Applied Mathematics**

https://molssi.org/industrial-training-workshops

Industrial Training

The MolSSI Industrial Training Program offers a wide range of comprehensive hands-on workshops and university curricula in Software Engineering, Artificial Intelligence, Machine Learning, Data Science and High-Performance Computing. With more than 5 years of experience in serving researchers and engineers across all domains of STEM, we strive to promote and lead our community best practices according to the latest technological and industrial advancements and the highest scientific standards.

In collaboration with our industrial partners, we have trained and certified a national and international community of hundreds of scientists and researchers comprised of undergraduate and graduate students, postdocs and faculty from academia, national labs and industry. Our MolSSI, Intel and NVIDIA certifications will boost your resume and give you the confidence you need for your dream job interview. Read our past trainees' testimonials!

In order to continue our commitment and services to the community, we offer a series of our certified courses for free, mostly in major national technological and scientific events and venues such as American Chemical Society. If you are interested to make these trainings available to your employees or students, please contact us.

MolSSI

The MolSSI's Python Data and Scripting Workshop course gives you a comprehensive hands-on experience and solid background in Python programming which prepares you for the everyday challenges in your current or future job in industry and academia. Our Best Practices workshop will complement these practical skills with key software development concepts to improve the productivity, reproducibility, portability, and interoperability of your scientific codes.

+ Read more about the MolSSI workshops

NVIDIA DEEP LEARNING INSTITUTE

In collaboration with NVIDIA Deep Learning Institute (NVIDIA-DLI), MolSSI offers the following instructor-led hands-on workshops in High-Performance Computing, Data Science, Artificial Intelligence and Machine Learning.

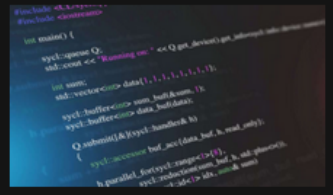
+ Read more about NVIDIA workshops provided by the MolSSI

intel

Armed with Intel oneAPI Toolkits and various accelerator architectures such as CPUs, GPUs and FPGAs on Intel DevCloud, we present a wide range of training courses in high-performance computing and artificial intelligence.

+ Read more about Intel workshops provided by the MolSSI

Basics of Accelerated Computing with Intel OpenMP GPU Offload



Fundamentals of Data-Parallel C++ and SYCL

MolSSI/NVIDIA Certified Hands-on Workshops in HPC and ML

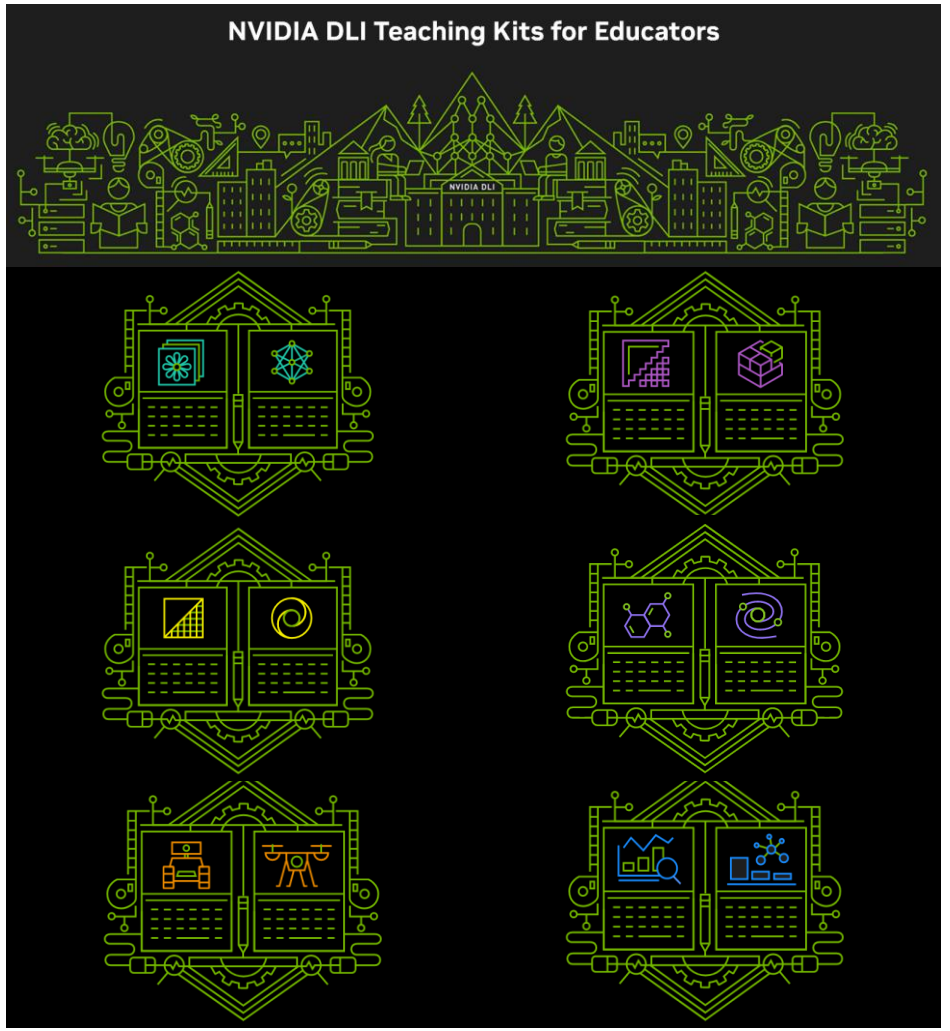
Collaboration with Academia & Industry

- **Provided Hardware and Software Resources**
  - **NVIDIA DLI**
    - 6 for-credit curricula and teaching kits
    - Delivery Platform
    - On-demand cloud resources
    - Travel support
    - Career advertisement
  - **Intel**
    - Access to teaching kits and course materials
    - Free Intel Developer Cloud account
    - Support from the CI team

Collaboration with Academia & Industry

- **Provided Hardware and Software Resources**
  - **Oracle Academy**
    - Full access to Oracle software stack
    - Free and full access to OCI
    - Access to teaching kits and course materials
    - Promotional support
    - Classroom delivery platform
  - **Wolfram U**
    - Access to teaching kits and course materials
    - Access to cloud resources
    - Limited free licenses for all attendees
    - Support from CI team
    - Promotional support

University Curricula



- **Data Science**
- **Deep Learning**
- **Accelerated Computing**
- **Science and Engineering (new)**
- **Edge AI and Robotics**
- **Graphics and Omniverse**

- https://www.nvidia.com/en-us/training/educator-programs/university-ambassador-program/
- https://molssi.org/industrial-training-workshops

Industrial Workshops

- Deep Learning
  - Fundamentals of Deep Learning
  - Data Parallelism: How to Train Deep Learning Models on Multiple GPUs (new)
  - Applications of AI for Anomaly Detection
  - Generative AI with Diffusion Models (new)
- Data Science
  - Accelerating Data Engineering Pipelines
  - Fundamentals of Accelerated Data Science with RAPIDS (Coming Soon)
- Accelerated Computing
  - Fundamentals of Accelerated Computing with CUDA C++
  - Accelerating CUDA C++ Applications with Multiple GPUs
  - Scaling CUDA C++ Applications to Multiple Nodes
  - Fundamentals of Accelerated Computing with CUDA Python
- Conversational Artificial Intelligence
  - Building Transformer-Based Natural Language Processing Applications (Coming Soon)
  - Building Intelligent Recommender Systems (Coming Soon)

- https://molssi.org/industrial-training-workshops
- https://www.nvidia.com/en-us/training/instructor-led-workshops

Industrial Workshops

- Machine Learning
  - Machine Learning using oneAPI
  - Accelerated Data Science with Optimized NumPy and SciPy
- Accelerated Computing
  - Essentials of C++ SYCL
  - Basics of OpenMP GPU Offload

- https://molssi.org/industrial-training-workshops
- https://www.intel.com/content/www/us/en/developer/learn/overview.html
- https://www.intel.com/content/www/us/en/developer/tools/oneapi/training/academic-program/educators/overview.html

Industrial Workshops

- Applied Mathematics
  - Wolfram Language Programming Fundamentals
- Chemistry and Cheminformatics
  - Wolfram Notebooks for Chemistry Research
  - Wolfram Notebooks for Teaching Chemistry

WOLFRAM U

WOLFRAM

- https://molssi.org/industrial-training-workshops
- https://www.wolfram.com/wolfram-u

Industrial Workshops

- Full Curriculum
  - Database Foundations (90 hours)
  - AI & ML in Java (40 hours)
- Education Bytes
  - Database: Hands-on Labs (< 16 hours)
  - Cloud Compute: Hands-on Labs (< 16 hours)
- Workshops
  - Getting Started with Java (< 16 hours)
  - Solve it with SQL (< 16 hours)
- Learning Paths

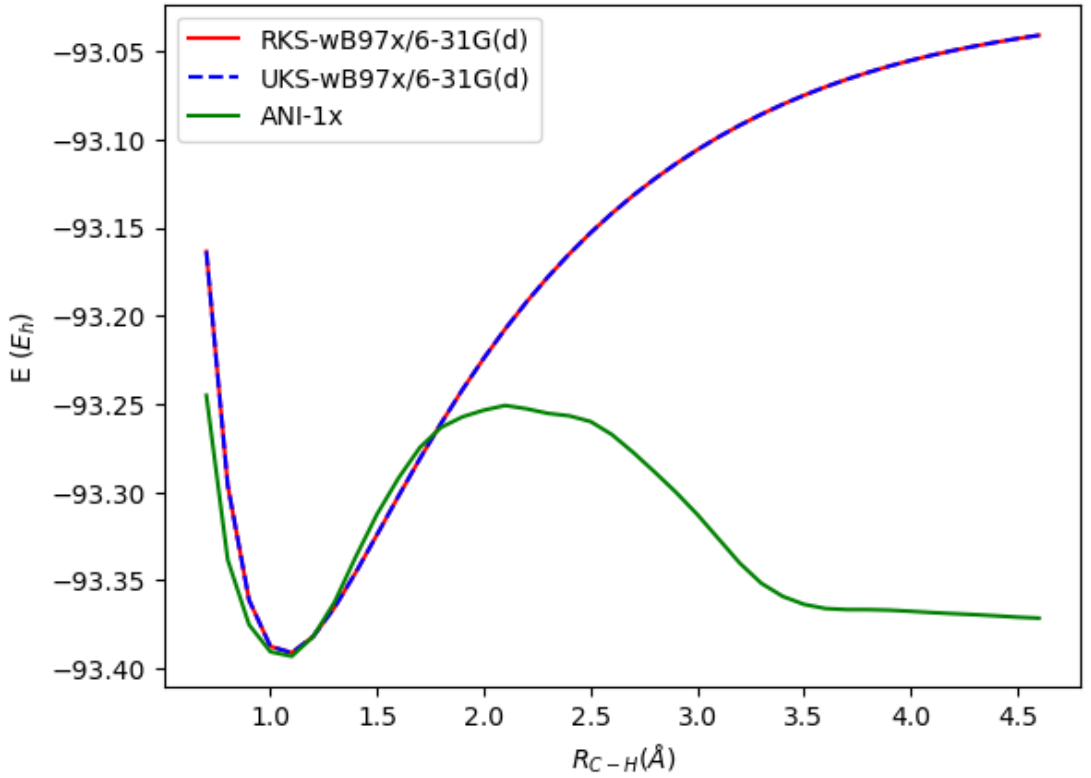
ORACLE Academy

ORACLE

- https://molssi.org/industrial-training-workshops
- https://academy.oracle.com/en/solutions-curriculum.html

New MolSSI Workshops

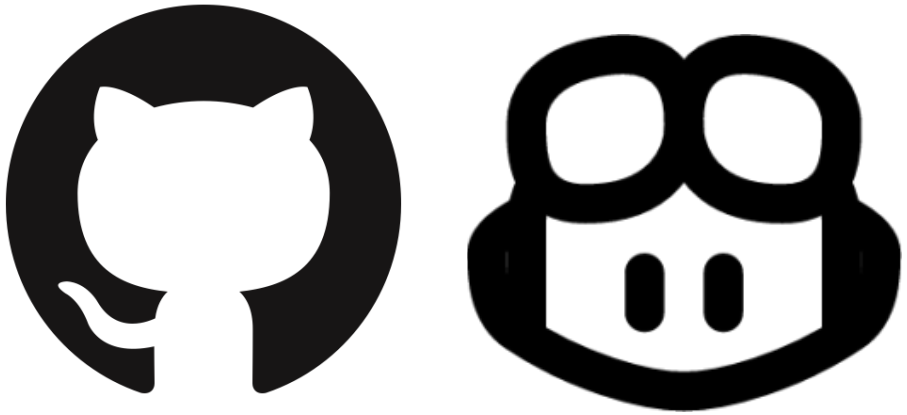
- **Machine Learning Potentials in Chemistry**
  - Foundations of Deep Learning
  - Intro to NNPs
  - Training NNPs
  - Inference
  - Applications



https://molssi.org/industrial-training-workshops

New MolSSI Workshops

- **A Practical Guide to GitHub Copilot**
  - Supported IDEs & languages
  - Tips and tricks
  - Best Practices
  - Context variables
  - Agents
  - Slash commands



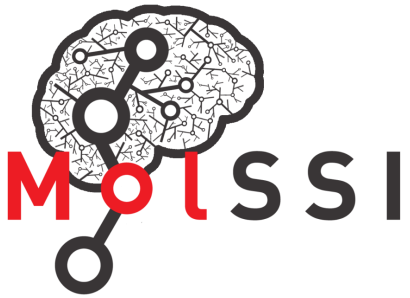
https://github.com/molssi-ai/industrial-training-program/tree/main/copilot

Highlights

- **Fundamentals of Accelerated Computing with CUDA C++**
  - NVIDIA's Higher Education Workshop Series for North America and Latin America, NVIDIA Deep Learning Institute, (June 22, 2022; November 10, 2023)
- **Fundamentals of Deep Learning**
  - American Chemical Society (ACS) National Meeting and Exposition, Indianapolis, IN, & Chicago, IL (Aug. 20, 2022 & Mar. 23, 2023)
- **Fundamentals of Data-Parallel C++ and SYCL**
  - Intel Certified Instructor Program and Molecular Sciences Software Institute, Blacksburg, Virginia, (Sep. 29 & 30, 2022)
- **NVIDIA GTC Conference in 2024**
  - Prime your University's Students and Researchers for the AI and Accelerated Computing Future through Self-Sustaining Training and Educator Programs, San Jose, CA (Mar. 18-21, 2024)

Testimonials

- **Fundamentals of Deep Learning**
  - "Excellent for learning the resource and gaining hands-on experience of how to apply deep learning to research."
  - "As a newcomer to Machine Learning, this workshop was eye opening."
- **Scaling CUDA C++ Applications to Multiple Nodes**
  - "Have greatly enjoyed the MoISSI workshops on GPU accelerated computing and find it a helpful training resource for my data science fellowship at CDC working in viral genomics"
  - "The workshop covers some cutting-edge and new technologies about GPU programming that is barely found on the internet. Much appreciate it, great job!"



Testimonials

- **Fundamentals of Accelerated Computing with CUDA C++**
  - "The MolSSI-NVIDIA workshop provided me with an excellent introduction to the topic of deep learning and accelerated computing using CUDA. Instructors are highly knowledgeable and prepared!"
  - "I feel as though I'm getting a peek under the hood of how my codes work. It makes me feel more confident in my work and excited for new material to learn."
- **Fundamentals of Data Parallel C++ and SYCL**
  - "The direct ties to the CUDA programming paradigms were vital for understanding the equivalent behavior in DPC++ and SYCL. Overall, it provided the insight to truly appreciate how DPC++ has simplified the procedure for high-performance computing."

International Outreach

- **Fundamentals of Deep Learning**
- **Fundamentals of Accelerated Computing with CUDA C/C++**
- **Accelerating CUDA C++ Applications with Multiple GPUs**

KAI SABANCI

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President

Kourosh Sharifi
Vice President

Sadiq Qara
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Kutluhan Ayguzel
Head of Sponsorship

Arya Hassibi
Head of Design and Marketting

ITP Web Page Statistics

(Jun. 20 - Aug. 19, 2023)

ITP Web Page Statistics

(Jun. 20 - Aug. 19, 2023)

Page Title	Views	Total Users	New Users	User Engagement
Main Page	152	92	14	1h 19m
Testimonials	9	8	4	2m 10s
Intel Workshop	13	14	0	4m 31s
NVIDIA Workshop	9	8	0	2m 38s
Total	**183**	**122**	**18**	**1h 28m 19s**