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MXAN V1.0

A technical introduction to MXAN code and running environment

Nico Sanna

Sept 25th, 2019

MXAN: Three Dimensional Structures for Metal Sites in Condensed Phases and in Catalysts
SLAC/Stanford, 25 Sept 2015.

Summary

- MXAN workflow
- Intro to docker technology
- Docker runtime installation
- How is made? Details about our MXAN V1.0
- Test runs
- Q & A

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MXAN workflow

- A new F90 code
- Based on Intel compiler
- and libraries (MKL)
- Uses MINUIT from CERN
- Parallel w/ OpenMP
- Pre-release
- Molecular Dynamics

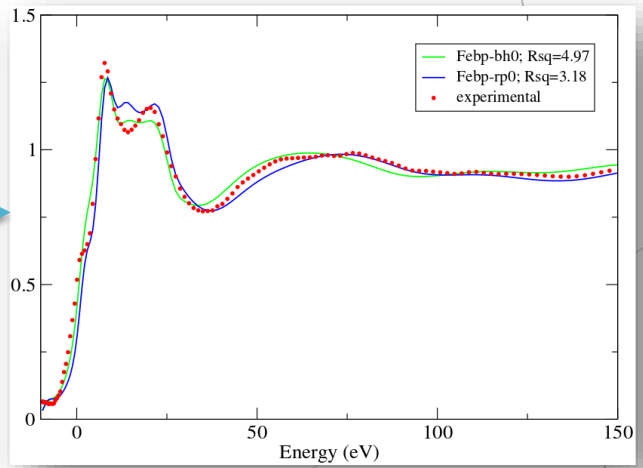
MXAN workflow

Exp.
X spectrum

INPUT

Molecular geometry

Theoretical Spectrum & Best Fit (MINUIT)



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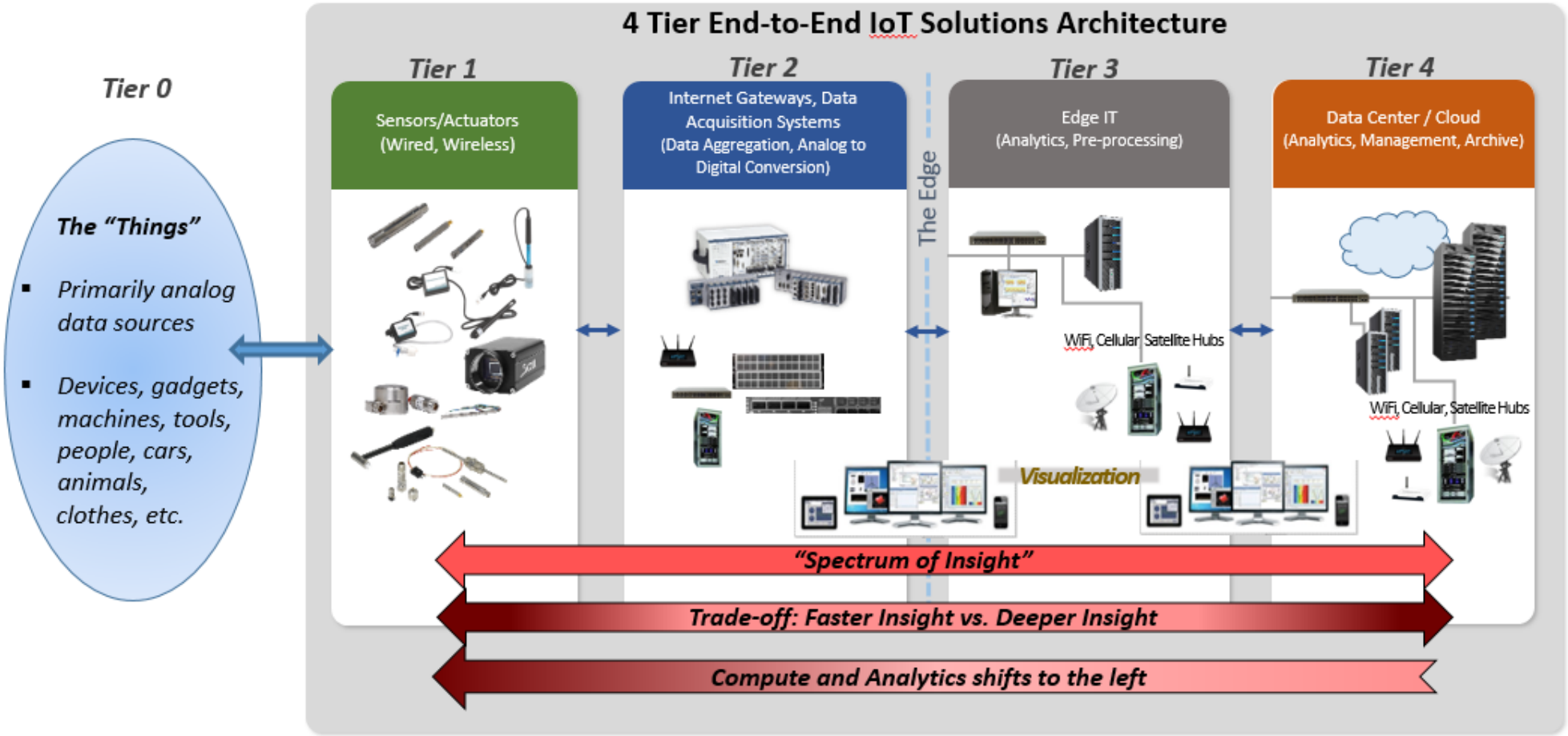
HPC+BDA+AI model



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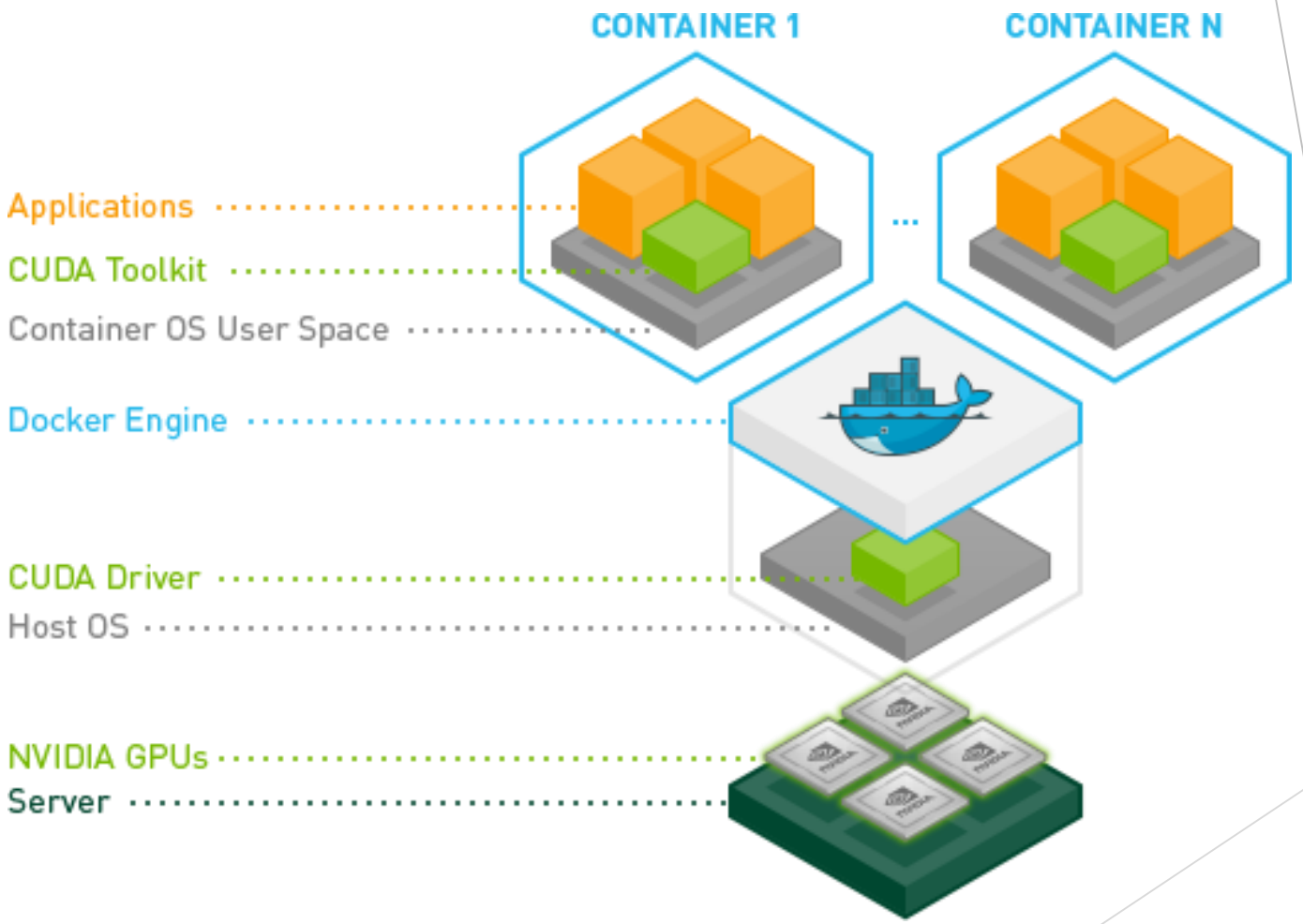

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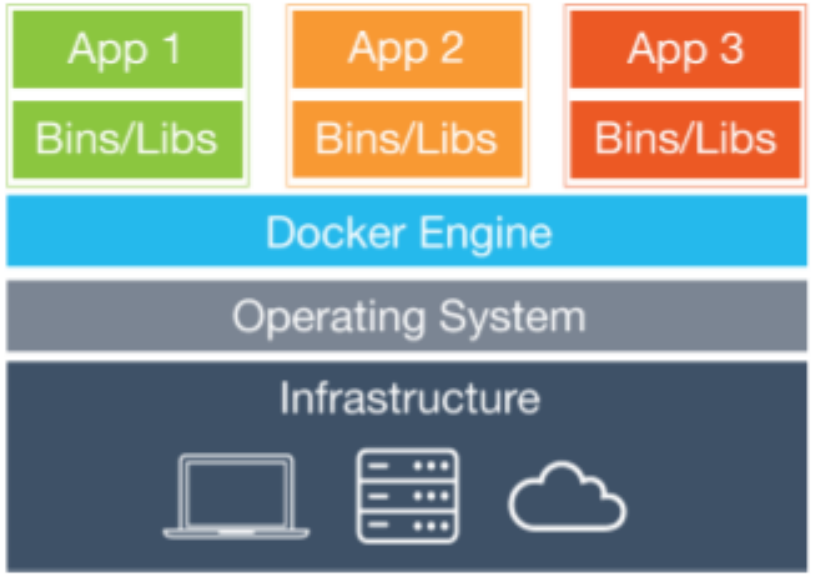
http://www.dibaf.unitus.it/

Case study: Docker

- Lightweight, open and secure container-based virtualization
  - Containers include the application and all of its dependencies, but share the kernel with other containers
  - Containers run as an isolated process in userspace on the host operating system
  - Containers are also not tied to any specific infrastructure



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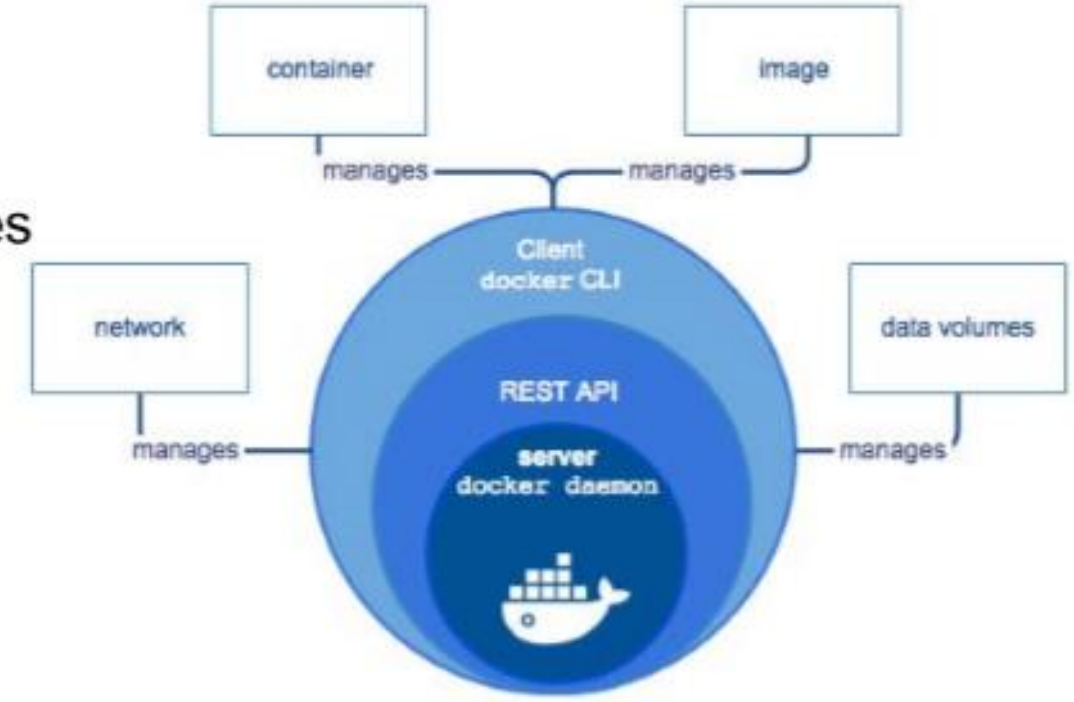
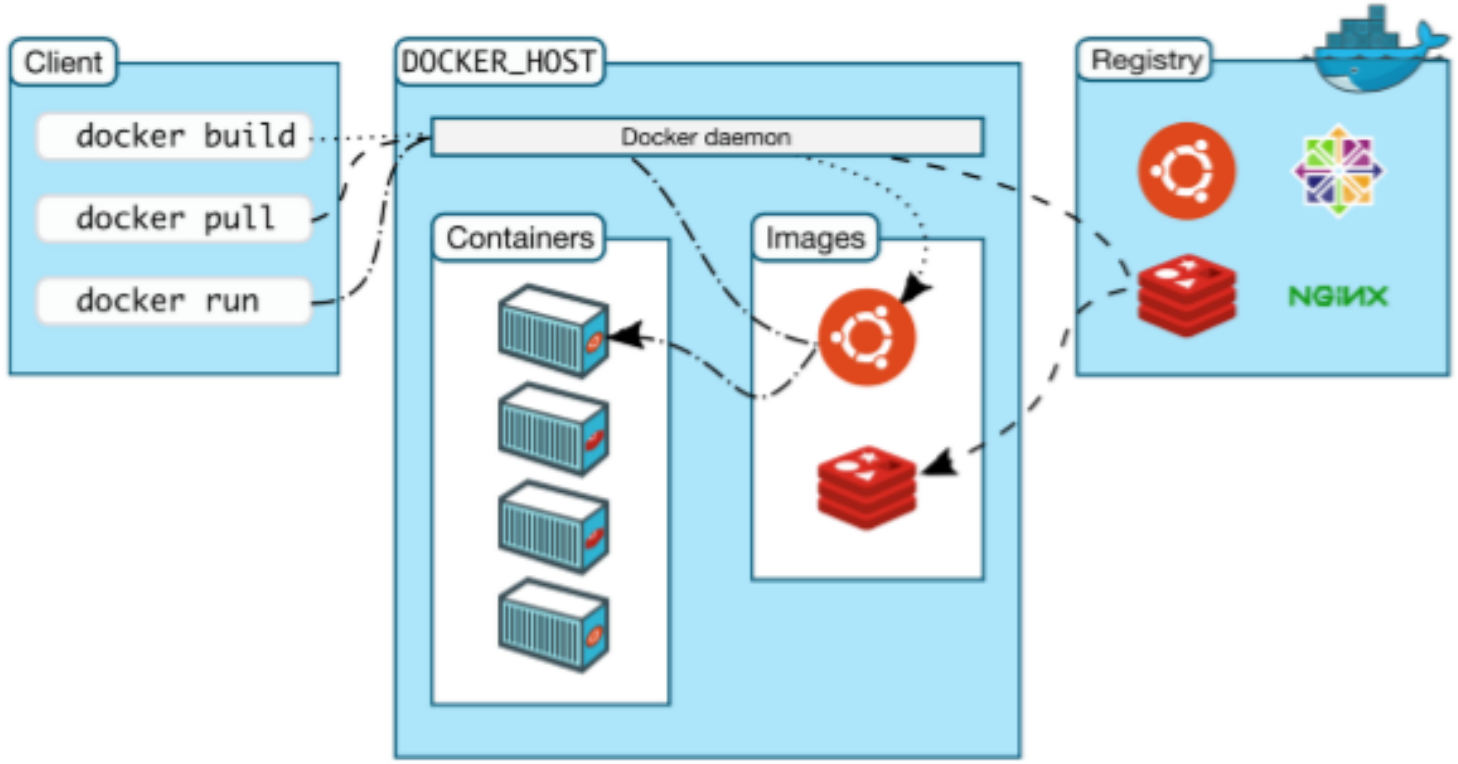
Docker engine

- *Docker Engine:* client-server application composed by:
  - A server, called daemon process
  - A REST API which specifies interfaces that programs can use to control and interact with the daemon
  - A command line interface (CLI) client



Docker architecture

- Docker uses a client-server architecture
  - The Docker *client* talks to the Docker *daemon*, which builds, runs, and distributes Docker containers
  - Client and daemon communicate via sockets or REST API



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Docker image

- Layered image
  - Each image consists of a *series of layers*
  - Docker uses *union file systems* to combine these layers into a single unified view
    - Layers are stacked on top of each other to form a base for a container's root file system
    - Based on the *copy-on-write* (COW) principle
- Layering pros
  - Enable layer reuse, installing common layers only once and saving bandwidth and storage space
  - Manage dependencies and separate concerns
  - Facilitate software specializations

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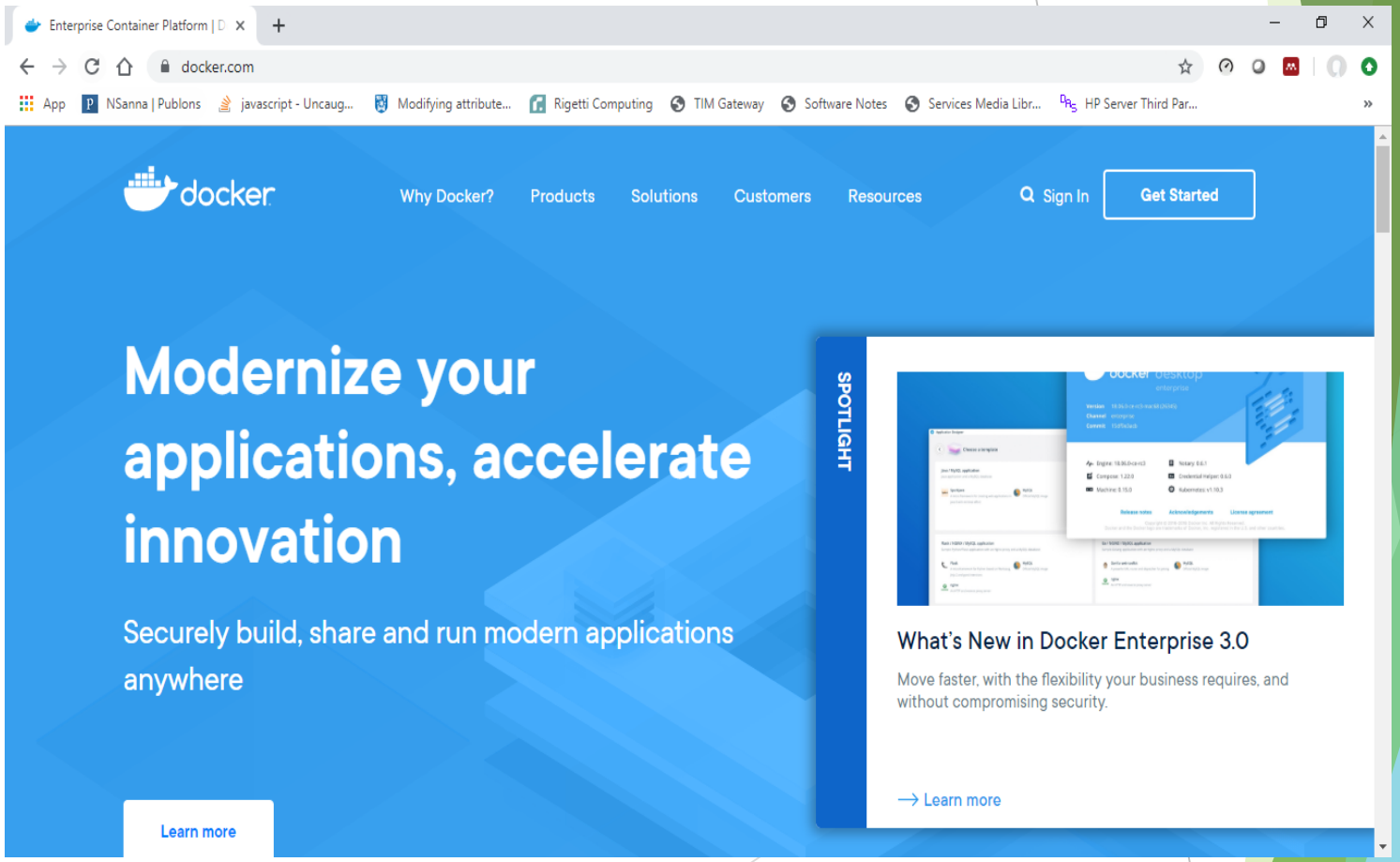
How to? Let's start and install DOCKER runtime on your PC or Mac

- Go to Docker Hub

  www.docker.com

  - Register
  - Download installer
  - Install it
  - Setup
  - READY!



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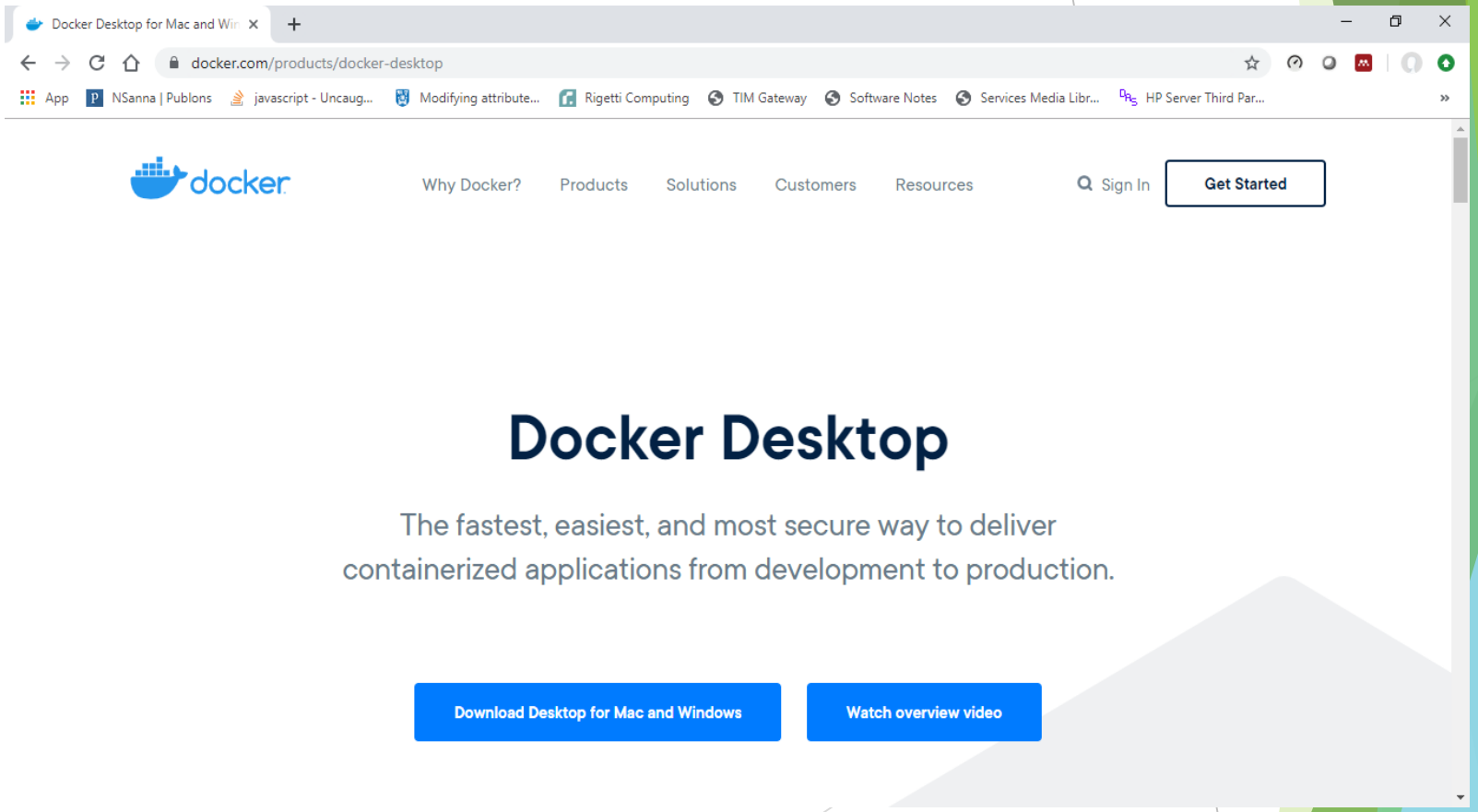

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NOTE: Set Intel VT to ON on your BIOS. Hyper-V virtualization will be set ON (Windows 10 - all versions but home - needed).

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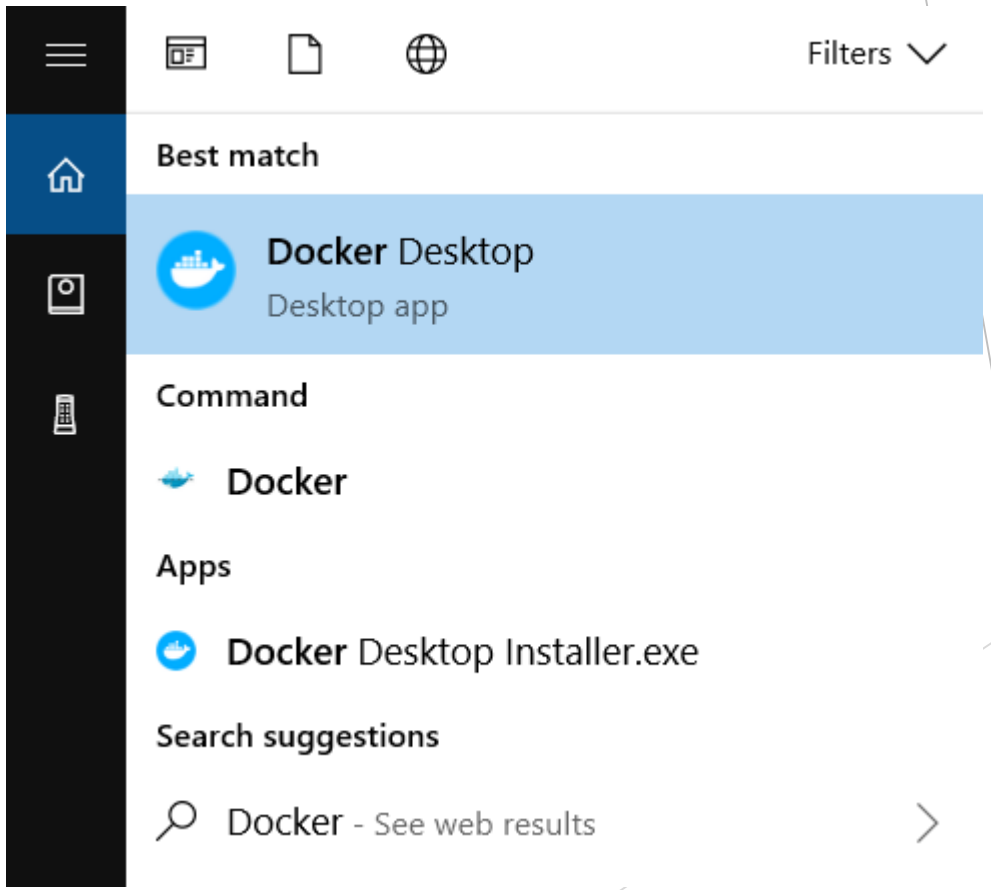

NOTE: When installing select LINUX containers.

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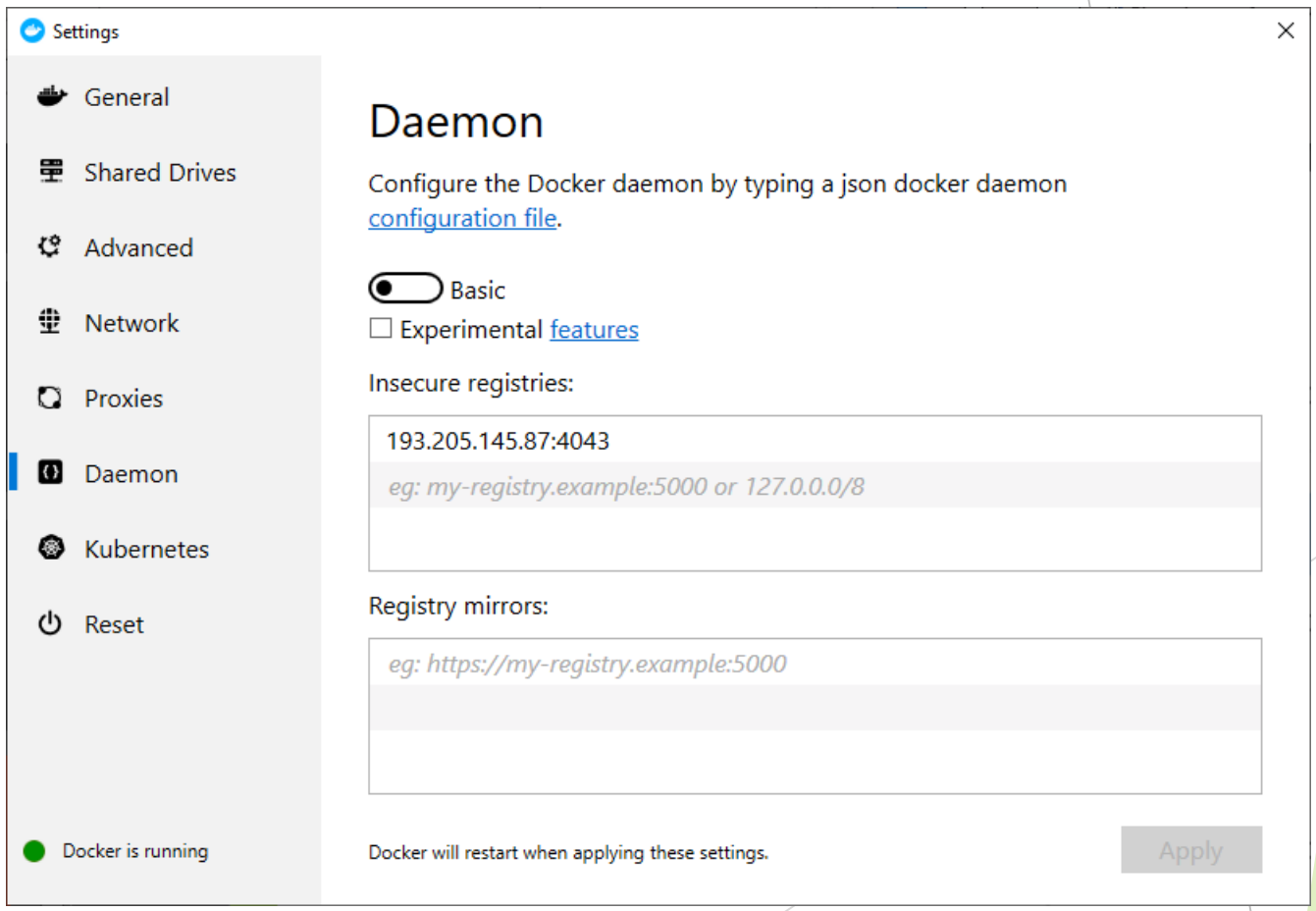

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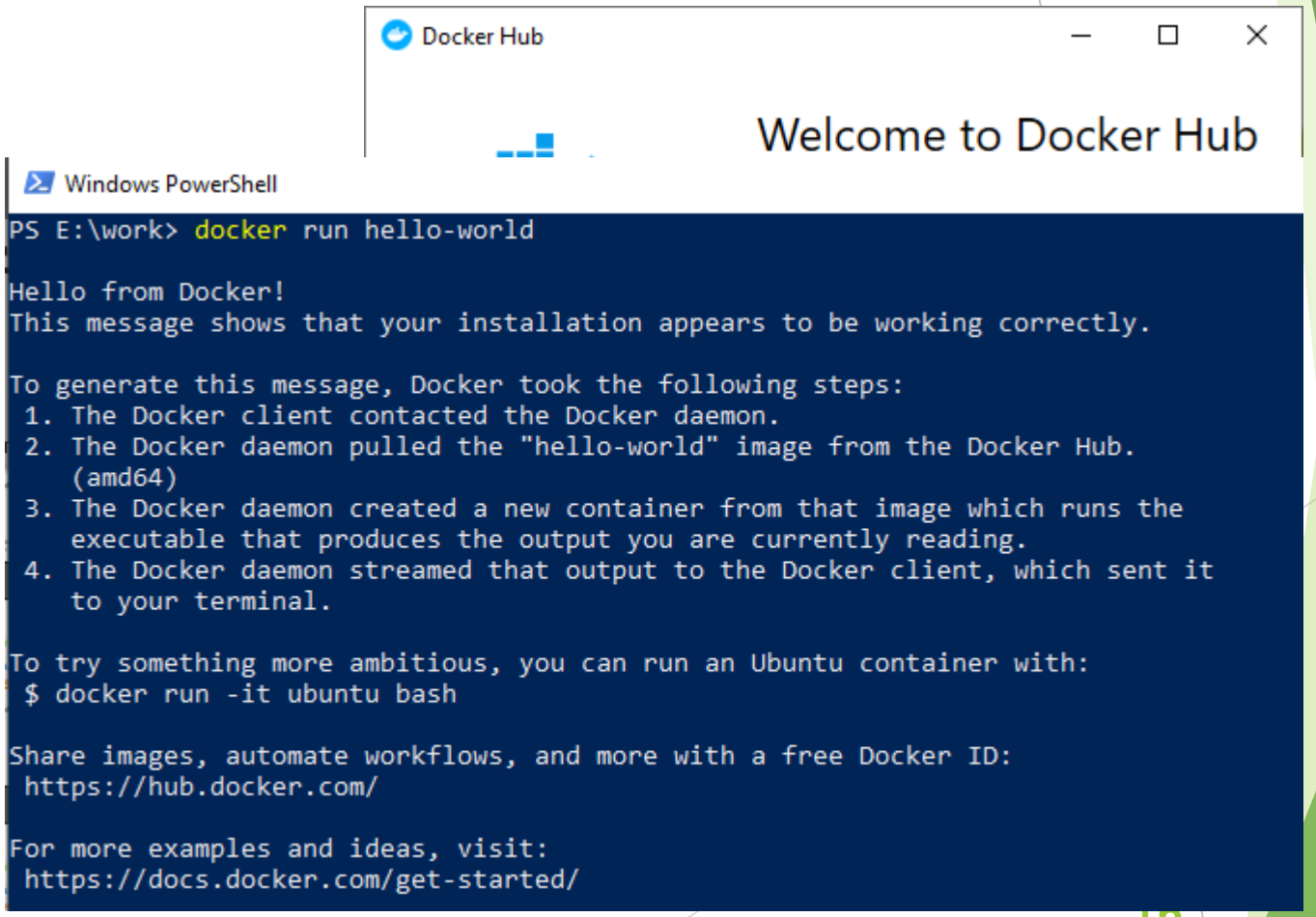

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LET'S
START!

How to run MXAN container on your PC or Mac

docker pull 193.205.145.87:4043/mxan2018:b2

Windows

docker run --rm -v"E:\work":/work 193.205.145.87:4043/mxan2018:b2 mxan_run Ni 2

Linux or Mac

docker run --rm –v$PWD:/work 193.205.145.87:4043/mxan2018:b2 mxan_run Ni 2

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MXAN script output

```
PS E:\work> docker run --rm -v"E:\work":/work 193.205.145.87:4043/mxan2018:b2 mxan_run Ni 2
... MXAN2018 JOB START @ Tue Sep 24 15:38:48 UTC 2019
================================================================================
Running your job with inputs from /work/Ni
total 28
drwxrwxrwx 2 root root 4096 Sep 24 15:28 .
drwxrwxrwx 2 root root 4096 Sep 24 15:29 ..
-rwxr-xr-x 1 root root 4682 Sep  2 13:29 COMMAND.MIN
-rwxr-xr-x 1 root root  844 Sep  2 13:29 DATA.Ni22
-rwxr-xr-x 1 root root 5852 Sep  2 13:29 ni_exp.dat
--------------------------------------------------------------------------------
Node        : a88e01189002
Job name    : Ni
Scratch dir :
Output in   : Ni.out.a88e01189002
No. threads : 2

MXAN2018 script is run with this command line:

/MXAN_2018R3105/mxan2018_intel


real    30m6.695s
user    28m41.770s
sys     0m12.580s
... MXAN2018 JOB STOP @ Tue Sep 24 16:08:55 UTC 2019
================================================================================
```


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Docker CLI useful commands at runtime

Docker process status

docker ps -a

REMOVE a stopped container

docker rm <CONTAINER ID>

STOP a running container

docker stop <CONTAINER ID>

LOGIN into a running container

docker exec -ti <CONTAINER ID> /bin/bash

```
Amministratore: Windows PowerShell
PS E:\work> docker ps -a
CONTAINER ID        IMAGE                                COMMAND             CREATED             STATUS              PORTS               NAMES
0e3d8a43081b        193.205.145.87:4043/mxan2018:b2      "mxan_run Ni 2"     7 minutes ago       Up 7 minutes                            determined_leavitt
PS E:\work> docker exec -ti 0e3d8a43081b /bin/bash
root@0e3d8a43081b:/work# ps auxw | grep mxan
root         1  0.0  0.1  18372  3200 ?        Ss   13:52   0:00 /bin/bash /MXAN_2018R3105/mxan_run Ni 2
root        11 96.5  0.8 537080 17852 ?        R    13:52   7:23 /MXAN_2018R3105/mxan2018_intel
root        81  0.0  0.0  11460  1144 pts/0    S+   14:00   0:00 grep --color=auto mxan
root@0e3d8a43081b:/work# exit
exit
PS E:\work> docker stop 0e3d8a43081b
0e3d8a43081b
PS E:\work> docker rm 0e3d8a43081b
Error: No such container: 0e3d8a43081b
PS E:\work> docker ps -a
CONTAINER ID        IMAGE               COMMAND             CREATED             STATUS              PORTS               NAMES
PS E:\work>
```

Thank you!
Grazie!

Maurizio Benfatto
Elisabetta Pace
Nico Sanna
Giovanni Chillemi
Cristiano Padrin

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