



Deep Learning on the LRZ AI Systems

An High Level Overview of Some LRZ Resources









The LRZ AI System

Deep Learning On the LRZ AI Infrastructure | 23.07.22 | PD. Dr. Juan J. Durillo

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Who can access?

- User requirements to get the access:
 - 1. Own a Linux Cluster account,
 - 2. Send a request through a service request ticket explaining the intended use.
- Upon approval, you will be invited to a DSS container - You need to accept this invitation before being able to access the Al systems!
- This DSS container will be used as your \$HOME (although this is going to change in the future.)



Resources Overview



	Slurm Partition	Number of nodes	CPUs per node	Memory per node	GPUs per node	Memory per GPU
DGX A100 Architecture	lrz-dgx-a100-80x8	4	256	2 TB	8 NVIDIA A100	80 GB
	lrz-dgx-a100-40x8	1	256	1 TB	8 NVIDIA A100	40 GB
DGX-1 V100 Architecture	lrz-dgx-1-v100x8	1	80	512 GB	8 NVIDIA Tesla V100	16 GB
DGX-1 P100 Architecture	lrz-dgx-1-p100x8	1	80	512 GB	8 NVIDIA Tesla P100	16 GB
HPE Intel Skylake + NVIDIA Node	lrz-hpe-p100x4	1	64	256 GB	4 NVIDIA Tesla P100	16 GB
V100 GPU Nodes	lrz-v100x2 (default)	4	20	368 GB	2 NVIDIA Tesla V100	16 GB

Using the Cluster

- SLURM: Simple Linux Utility for Resource Management
 - open source
 - fault-tolerant
 - highly scalable
- Cluster management and job scheduling
- (Three) main tasks
 - allocates exclusive and/or non-exclusive access to resources (compute nodes)
 - provides a framework for starting, executing, and monitoring work on the allocated nodes
 - arbitrates contention for resources by managing a queue of pending work.



workload manager

LRZ AI System Configuration







Accessing the LRZ System



• Login node <u>datalab2.srv.lrz.de</u> accessible via ssh

ssh -Y datalab2.srv.lrz.de -l xxyyyzz

- From the login node, jobs are submitted to the hardware described at the beginning of this course using SLURM
- A couple of handy SLURM commands



Allocating and Starting Jobs Interactively

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• Get resources allocated



• Submit start job in the allocated resources

\$ srun --pty bash

\$ srun hostname



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- Batch jobs are the preferred way of using the LRZ AI Systems.
- The **sbatch** command submits jobs described in a *sbatch script* file.
- Two additional arguments required in sbatch scripts: *output* and *error messages* file.
- After the preamble, the job to be executed is described.

|--|

\$ sbatch test.sbatch

User Defined Software Stack: Container Technologies





User Defined Software Stack: Container Images





- Typically, a single compressed file
 - It contains a complete Linux File System + Metadata
- Different container technologies might:
 - use different formats
 - e.g., OCI format is a specification for container images based on the Docker Image Manifest Version 2, Schema 2 format
 - hide images to users
- Are meant to be static
- Not to be confused with a docker file

User Defined Software Stack: Container



Typical Linux File System

- A running instance of a container image
 - A complete Linux File System within a Linux File System
 - Libraries might be different (versions)
 - Provided programs might be different
- Specific program in charge of unpacking the image and storing it within the proper folder
 - Docker, Podman, Enroot, etc.
- More than one container can
 - Exist at any point in time
 - Be generated from a single image

Understanding Containers: Container



Typical Linux File System

- It is possible to "run a process within a container"
 - Confine the process to the content of the container File System
 - Specific program in charge for confining and running the process within the container
 - docker run/start, enroot start

\$ Idd /bin/program linux-vdso.so.1 (0x00007fff204e8000) libselinux.so.1 => /lib/x86_64-linux-gnu/libselinux.so.1 (0x00007f411cc6a000) libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6 (0x00007f411ca78000) libpcre2-8.so.0 => /usr/lib/x86_64-linux-gnu/libpcre2-8.so.0 (0x00007f411c9e8000) libdl.so.2 => /lib/x86_64-linux-gnu/libdl.so.2 (0x00007f411c9e2000) /lib64/ld-linux-x86-64.so.2 (0x00007f411ccd0000) libpthread.so.0 => /lib/x86_64-linux-gnu/libpthread.so.0 (0x00007f411c9bf000)

Process run within Running Container 2

The Enroot Container Technology

- Containerized applications with enroot, a rootless container runtime by Nvidia
- Slightly different workflow than with Docker



 It should be noticed than the workflow in the AI System consist in submitting jobs that run containerized within an enroot defined container

Nvidia NGC: Container Images Repository





Setup Generate API Key Install NGC CLI My Account Settings > -Setup Terms of Use Generate your own API key in order to use the NGC service through the The NGC command line interface (NGC CLI) can run deep learning jobs on NVIDIA Docker containers. Docker client or through NGC CLI. Privacy Policy Get API Key Documentation Downloads Sign Out

Setup > API Key

API

API Information

Generate your own API key to use the NGC service through the Docker client. Anyone with this API Key has access to all services, actions, and resources on your behalf.

Click Generate API Key to create your own API Key. If you have forgotten or lost your API Key, you can come back to this page to create a new one at any time.

Usage

Use your API key to log in to the NGC registry by entering the following command and following the prompts:

NGC CLI

Docker™ 🖙

\$ ngc config set

For the username, enter '\$oauthtoken' exactly as shown. It is a special authentication token for all users.

\$ docker login nvcr.io Username: \$oauthtoken Password: <Your Key>

Docker™ 🖙

For the username, enter '\$oauthtoken' exactly as shown. It is a special authentication token for all users.

\$ docker	login nvcr.io
Username Password	: \$oauthtoken OHBodjU6NGE4NWM1NzUtZDE1ZS8
Do not	y generated successfully. This is the only time your API Key will be displayed. Keep your API Key secret. share it or store it in a place where others can see or copy it.
APT Kev	HRAd I UKNG FANIM I NYI I Y 7D F1 7 SA

Key (partially shown here for security reasons)

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Beyond Existing NGC: Creating Custom Enroot Image

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- Get resources / get an allocation of resources
 - salloc -p test-v100x2 -q testing --gres=gpu:1
- Open a terminal on the allocated resources
 - srun --pty bash
- (Optional) Create a base container image (e.g., pulling from NGC)
 - enroot import -o pytorch_base.sqsh docker://nvcr.io#nvidia/pytorch:22.06-py3
- Create a container out of an image
 - enroot create --name pytorch_container pytorch_base.sqsh



Beyond Existing NGC: Creating Custom Enroot Image

- Start a terminal your recently created container
 - enroot start pytorch_container bash
- Modify your container accordingly
- Leave your container
- Export the created container as an image
 - enroot export --output hugging_face.sqsh pytorch_container

Using the Cluster with Enroot Containers



• Get resources allocated





• Meet the pyxis plugin: container creating and job submission in a single step

\$ srun --container-mounts=./<u>data-test:/mnt/data-test</u> --container-name=horovod --container-image='horovod/horovod+0.16.4-tf1.12.0-torch1.1.0-mxnet1.4.1py3.5' bash

Open On Demand: Web Frontend for the LRZ AI System

- Interactive web service for AI systems where Jupyter Notebook, JupyterLab and RStudio Server environments are available, at <u>https://datalab3.srv.lrz.de</u>.
- Given that requested resources are available, the status of the session will change from "Queued" to "Starting" and finally "Running".
- <u>https://doku.lrz.de/display/PUBLIC/LRZ+AI</u>
 <u>+Systems</u>





The Compute Cloud

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Cloud Computing Characteristics



A consumer can request and receive access to a service offering without an administrator or some sort of support staff having to fulfil the request manually.	on demand
Cloud services should be easy to access. Ideally only a basic network connection should be required.	broad network access
Ability to grow with user demand. If the system is well defined it should be relatively easy for the provider to add more	flexible
Cloud services must have the ability to measured usage. Usage can be quantified using various metrics, such as time, bandwidth used, and data used. This ability to measure allow what is known as pay as you go model.	measurable
A user will not need all the resources available to her. When resources are not used, they should be released, and other users can benefit of it or they can be simply not used (not consuming energy.)	resource pooling

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Cloud Services



- SaaS Fully developed software solution to be used
 - e.g., Google Drive
- PaaS Provides a framework on top of which is possible to build, deploy, and manage software products
 - e.g., Heroku
- IaaS Provides a completely virtualized computing infrastructure provisioned and managed over the internet
 - e.g., LRZ Compute Cloud

OpenStack: The Engine of the LRZ Compute Cloud

- What do we need for transforming a set of resources (data center) into a cloud?
 - to manage/admin the hardware
 - to provision machines to users
 - to allow users to authenticate

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to manage the network across resources

OpenStack is a cloud operating system that controls large pools of compute, storage, and networking resources throughout a datacenter, all managed and provisioned through APIs with common

 OpenStack bundles together a bunch of different technologies, addressing the different needs transforming resources into a Cloud Service

The LRZ Compute Cloud at a Glance





OpenStack - Terminology



Image

A single file which contains a virtual disk with a bootable operating system installed on it. Images are like a template of a computer's root drive. They contain the operating system and can also include software and layers of your application, such as database servers, web servers, and so on.





OpenStack - Terminology



Instance

A copy of an image running as a virtual server the cloud. We will also call it server.

Flavor

Flavors define the compute, memory, and storage capacity of instances. To put it simply, a flavor is an available hardware configuration for a server.

Name	vCPUs	RAM	Remarks	Access
tiny	1	512 MB	for testing purposes only, most Operating Systems will not boot due to restricted resources	public
nvidia-v100.2	40	700 GiB	use 2 GPUs on a GPU node (use entire GPU node)	restricted, contact us
nvidia-v100.1	20	350 GiB	use 1 GPU on a GPU node	restricted, contact us
lrz.xlarge	10	47.5 GiB	use 1/4 compute node	public
lrz.xhuge	48	1488 GiB	use 1/4 of the hugemem node	restricted, contact us
Irz.small	1	4.75 GiB	use 1/40 compute node	public
Irz.medium	2	9.5 GiB	use 1/20 compute node	public
lrz.large	4	19 GiB	use 1/10 compute node	public
lrz.huge	24	744 GiB	use 1/8 of the hugemem node	restricted, contact us
lrz.4xlarge	40	190 GiB	use entire compute node	restricted, contact us
lrz.4xhuge	192	5952 GiB	use entire hugemem node	restricted, contact us
lrz.2xlarge	20	95 GiB	use 1/2 compute node	restricted, contact us
lrz.2xhuge	96	2976 GiB	use 1/2 of the hugemem node	restricted, contact us

The LRZ Compute Cloud at a Glance





OpenStack - Terminology



Volume

A volume is a detachable block storage device, similar to a USB hard drive. You can attach a volume to only one instance. But an instance can attach several volumes

The LRZ Compute Cloud at a Glance





OpenStack - Terminology



Networking

OpenStack provides networks, subnets, and routers as object abstractions. Each abstraction has functionality that mimics its physical counterpart: networks contain subnets, and routers route traffic between different subnets and networks. Instances are created within internal private networks. These networks can be routed to external networks (e.g., Internet or or MWN) via a virtual router.

Private and Floating IP

Each instance has a fixed IP within its private Network. That IP can be associated to an IP of the external network that network is connected by means of what it is called *floating IP address*. The floating IP address will allow addressing the instance from the outside.

Security group

A security group acts as a virtual firewall for servers and other resources on a network. It is a container for rules for allowing different types of network traffic to and from an instance.



called MWN-pool

A server on the Compute Cloud



- De-facto operation is no Graphical Interface on the provided images
 - Although it is possible (e.g., <u>https://rv.lrz.de</u> ← only accessible from within MWN)
- Accessing instances via ssh
 - No login based on password by default (public and private keys!)
- OpenStack must be aware of your public key(s) to add it(them) to newly created instances (otherwise you will not be able to login)
 - You can import a public key of a keypair generated using your method of preference
 - You can generate a keypair using OpenStack
 - the private key will be downloaded to your computer
 - the public will be recorded by OpenStack

















Project	Access	Project / Volumes / Volumes									
Compute	>	Volumes									
Volumes	✓ /olumes						Filter	Q. + C	reate Volume	≓ Accept Transfer	🗊 Delete Volu
Sn	apshots	Displaying 8 items									
Network	>	Name	Description	Size	Status	Туре	Attached To	Availability Zone	Bootable	Encrypted	Actions
Orchestration	>	3896da63-2f67-4417-91bb-6a7d32d35cc8		30GiB	In-use	ceph	/dev/vda on test	nova	Yes	No	Edit Volume
Identity	>	C 0c5b5550-947b-44c5-a20a-46ba298a5d97	-	30GiB	Available	ceph		nova	Yes	No	Edit Volume
		D 10a34d24-1d7b-46a4-bd3e-f1558a1d3918		30GiB	Available	ceph		nova	Yes	No	Edit Volume
		tensorflow-gpu-volume		25GiB	Available	ceph		nova	Yes	No	Edit Volume
		C706810c-dcd3-4fea-9214-aedc8ecfc901	-	20GiB	Available	ceph		nova	Yes	No	Edit Volume
		G3e9cb82-3bb5-44d3-be13-7421d12ff5a2		20GiB	Available	ceph		nova	Yes	No	Edit Volume
		O data	data for isc 2019 demo	80GiB	Reserved	ceph	nova	nova	No	No	Update Metad
		15bbb9b3-ce0c-4c0f-a79a-b398ee8a72d0		20GiB	Reserved	ceph		nova	Yes	No	Update Metad
		Displaying 8 items									



TASK : Create a Ubuntu-based server for running Jupyter Notebooks

- On the Compute Cloud Web Interface
 - Generate a new keypair (follow along the live demo)
- On your computer
 - A file with the extension .pem will be downloaded to your machine (the private key) from previous step
 - In Linux/UNIX: change the permission of that file to 600 (\$ chmod 600 ...)
 - In Windows with WLS: copy the downloaded file to inside the WSL (/mnt/c/ allows you accessing C:\ in windows from WSL,)
 - Once copied, change the permissions as in the Linux/UNIX case
 - In Windows with Putty: import it using PuttyGen
 - check <u>https://stackoverflow.com/questions/3190667/convert-pem-to-ppk-file-format</u> if you need help



- On the Compute Cloud Web Interface
 - Create an instance (next steps are documented with screen shots in successive slides)
 - Choose Ubuntu as image
 - CPU only flavor (preferably a small one)
 - Should be accessible from Internet
 - Place the instance on the private network called internet
 - Once the instance is created assign it a floating IP from the Internet pool



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	Volumes	Key Pairs	Instance Nar	Network Ports Security Groups	Availability Zone	1 Current Usage 1 Added 2 Remaining	Time since created Actions	
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					> CentOS-6	5/22/19 12:07 AM	8.00 GB	raw	Public	•			
					> CentOS-7	5/21/19 5:58 PM	8.00 GB	raw	Public	•			
					> cirros	5/21/19 5:59 PM	44.00 MB	raw	Public	•			
					> Debian-10-buster	7/31/19 6:57 PM	2.00 GB	raw	Public	•			
					> Debian-8-jessie	3/22/19 3:35 AM	2.00 GB	raw	Public	•			
					> Debian-9-stretch	5/21/19 5:58 PM	2.00 GB	raw	Public	•			
					> Fedora-29	5/21/19 5:53 PM	4.00 GB	raw	Public	•			
					> Fedora-30	7/31/19 6:55 PM	4.00 GB	raw	Public	•			
					> FreeBSD-11.2	5/21/19 5:58 PM	31.00 GB	raw	Public	•			



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Identity		>		Server Groups	> Irz.medium	2	9 GB	20 GB	20 GB	0 GB	No	•			
				Scheduler Hints	> tiny	1	▲ 512 MB	1 GB	🛕 1 GB	0 GB	No	•			
				Metadata	> Irz.large	4	18 GB	20 GB	20 GB	0 GB	No	*			
					> Irz.small	1	4.5 GB	20 GB	20 GB	0 GB	No	*			
					 nvidia-v100. 1 	20	368 GB	20 GB	20 GB	0 GB	No	•			
					> Irz.xlarge	10	45 GB	20 GB	20 GB	0 GB	No	•			
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 ✓ Select at least one network Instance Na Network Ports Key Pairs Time since created Actions Q Click here for filters. ж Security Groups Network Subnets Associate Shared Admin State Status 4 months 3 weeks Key Pair Test Active > test No Up 4 Displaving 1 iter Configuration > MWN MWN_subnet Yes Up Active 4 Server Groups > internet internet_subnet Active 4 Yes Up Scheduler Hints Metadata × Cancel < Back Next >











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Project V API Access	Project / Network / Security Groups				
Compute >	Security Groups				
Volumes >					
Network 🗸				Filter Q + Create Security Group	Delete Security Group
Network Topology	Displaying 8 items				
Networks	Name	Security Group ID	Description		Actions
Routers	InHPC-DE.rv.security_group	d1cdda6d-60b9-4d97-ab6b-1736b3595e80	Security group used for the testing insta	ance containing the remote visualization stack.	Manage Rules
Security Groups	 JupyterHUB 	8474f2ab-1c1c-4477-aa24-cb4f6f848ef8			Manage Rules
Floating IPs	default	2a0b66d5-7a9f-49ae-8d30-f11ddea6f968	Default security group		Manage Rules
Orchestration >	example	d926448f-7830-4ec0-8888-a056ff9d4a1a	example		Manage Rules
Identity >	novnc	65143f52-5536-4e8b-b977-8d0e36f2e056	novnc		Manage Rules
	□ ssh	f4ec8f5f-8797-488a-9cd3-3da12a068cd5			Manage Rules
	□ web	189b2ecd-d0bf-4b9c-a3fc-3f734d57dbe3	web servers		Manage Rules
	x11vnc-connections	fb86cef1-828e-4172-a3f5-4346bb75e1e2	Allows direct connections to x11vnc from	m the client machines	Manage Rules
	Displaying 8 items				



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Project 🗸	Project / Network / Security Groups	Create Security Group	2		
Compute > Volumes >	Security Groups	Name *	Description: Security groups are sets of IP filter rules that are applied to network interfaces of a VM. After the security group is		
Network V Network Topology Networks	Displaying 8 Items Name Name		created, you can add rules to the security group.	Create Security Group	Actions
Houters Security Groups	JupyterHUB		Cancel Create Security Group		Manage Rules
Load Balancers Floating IPs	default	2a0b66d5-7a9f-49ae-8d30-f11ddea6f968	Default security group		Manage Rules
Orchestration >	example	d926448f-7830-4ec0-8888-a056ff9d4a1a	example		Manage Rules -
Identity >	novnc	65143f52-5536-4e8b-b977-8d0e36f2e056	novnc		Manage Rules
	🗆 ssh	f4ec8f5f-8797-488a-9cd3-3da12a068cd5			Manage Rules
	O web	189b2ecd-d0bf-4b9c-a3fc-3f734d57dbe3	web servers		Manage Rules
	x11vnc-connections	fb86cef1-828e-4172-a3f5-4346bb75e1e2	Allows direct connections to x11vnc from the client man	chines	Manage Rules
	Displaying 8 Items				



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Project	Project / Network / Security Groups / Manage Security Group Rul						
Compute > Volumes >	Manage Security Group Rules: InHPC-DE.rv.security_group (d1cdda6d-60b9-4d97-ab6b-1736b3595e80)						
Network 🗸 🗸	Displaying 7 items						+ Add Rule Delete Rules
Networks	Direction	Ether Type	IP Protocol	Port Range	Remote IP Prefix	Remote Security Group	Actions
Routers Security Groups	Egress	IPv4	Any	Any	0.0.0/0	-	Delete Rule
Load Balancers	Egress	IPv4	TCP	4000	0.0.0/0	-	Delete Rule
Floating IPs	Egress	IPv4	UDP	4001	0.0.0/0	-	Delete Rule
Identity	Egress	IPv6	Any	Any	::/0	-	Delete Rule
	□ Ingress	IPv4	TCP	22 (SSH)	0.0.0/0	-	Delete Rule
		IPv4	TCP	4000	0.0.0/0	-	Delete Rule
	Ingress	IPv4	UDP	4001	0.0.0/0	-	Delete Rule
	Displaying 7 items						



Subtask: Access the created instance via SSH

- On the Computer Cloud Web Interface
 - Create a security group that allow ingress connections to port 22!
 - Add this security group to the instance
- On your computer
 - Open a terminal application

ssh _i <path_to_the_pem_file> ubuntu@<floating-ip>

After this step, the rest of slides assume everyone is connected via ssh to the created instance

Install pip

A Guided Example

ullet



Install jupyterlab using pip



• Run jupyter-lab to listen on the private IP of the machine



You can check the IP using ifconfig (you need to install net-tools)



• Connect to she showed URL with a browser. Why is not working?



- On the Compute Cloud Web Interface
 - Create a security group that allow ingress connections to port 8888!
 - Add this security group to the instance



• Connect to she showed URL with a browser. Why is still not working?



- The showed URL is relative to the Compute Cloud instance private network.
 - Substitute in that URL the IP with the floating IP of the instance and try accessing the instance now



• Not done: A few libraries are missing for executing our Jupyter Notebook Example



Summary



- Overview of the LRZ Resources for ML/DL Workloads
- Focus session on the LRZ AI System, a scenario intended for ML/DL training
- Focus session on the LRZ Compute Cloud, a scenario intended for ML/DL development and inference