Container platform Kubernetes

Lukáš Hejtmánek

CERIT-SC

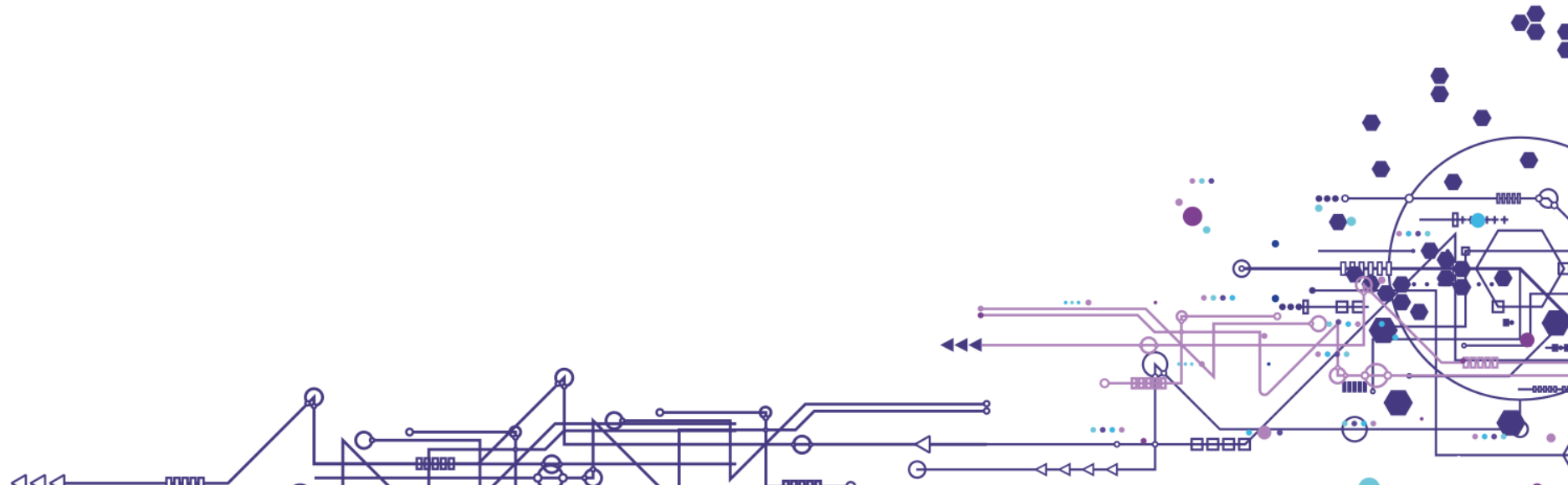cesnet MUNI CERIT-SC VŠB TECHNICKÁ UNIVERZITA OSTRAVA | IT4INNOVATIONS NÁRODNÍ SUPERPOČÍTAČOVÉ CENTRUM
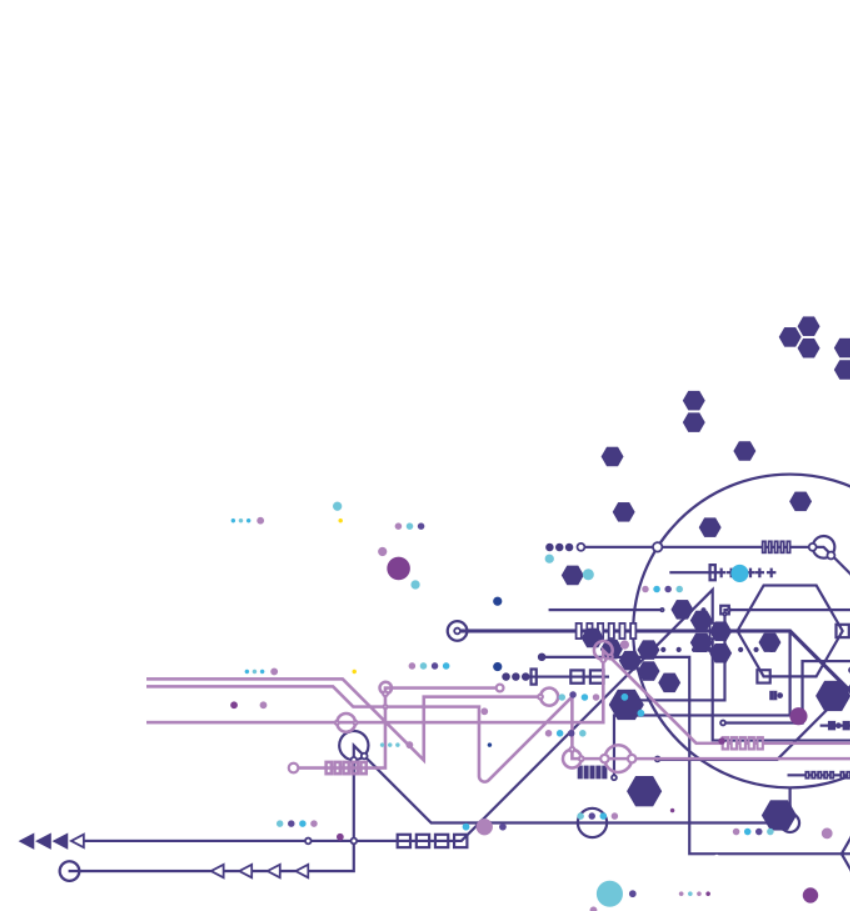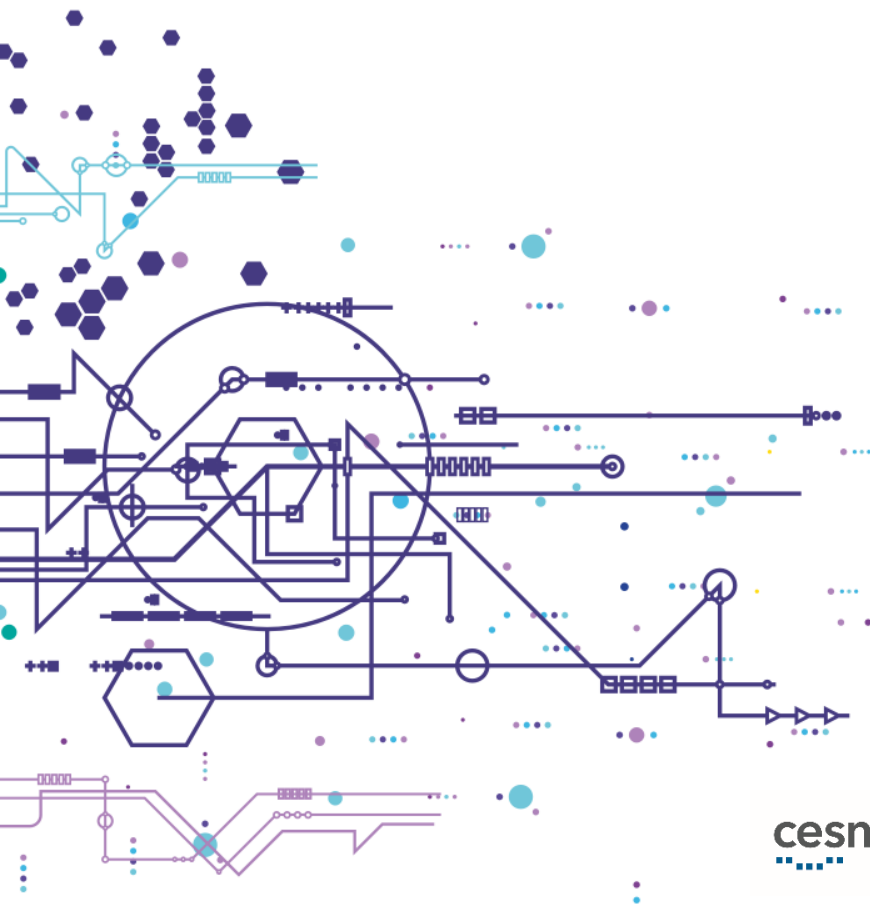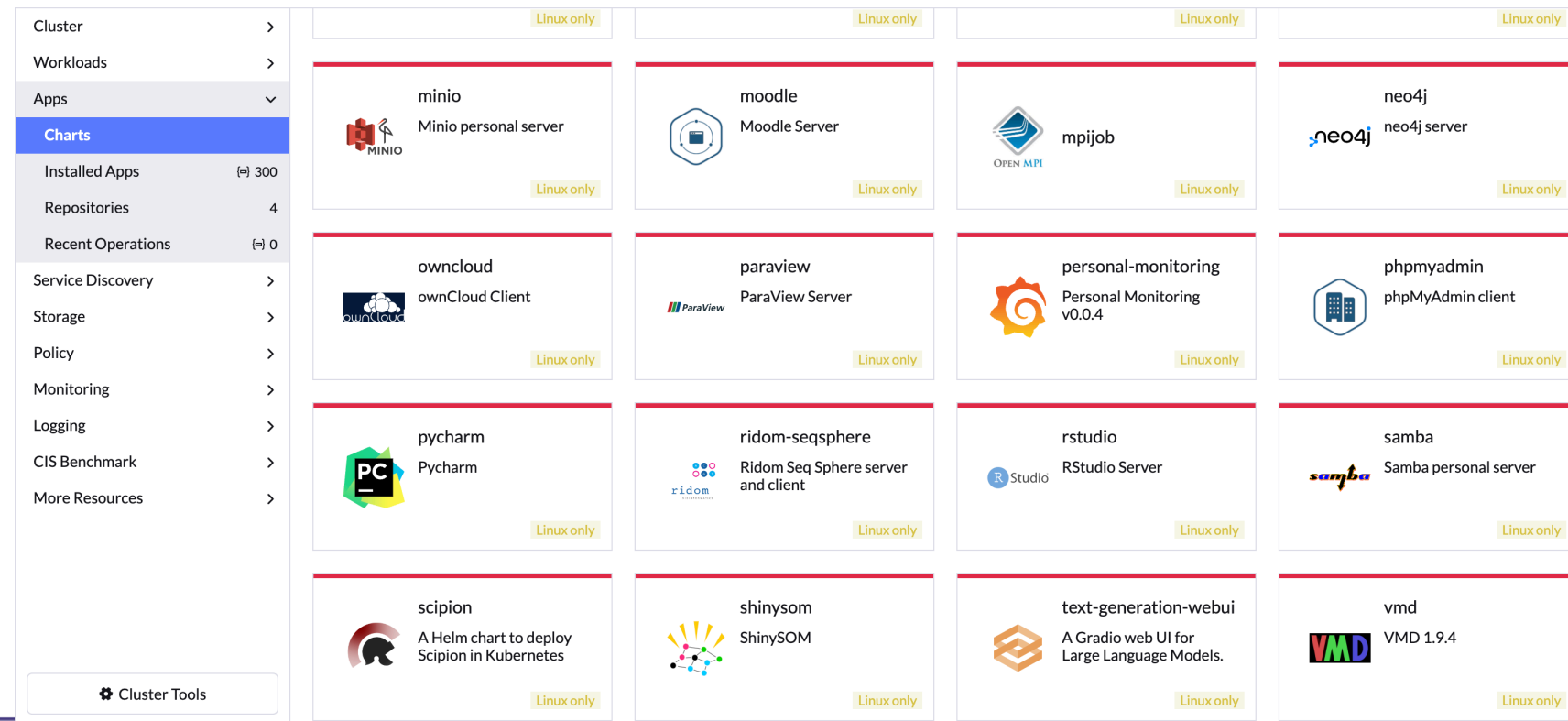
Kubernetes Platform Services

- Rancher application catalogue

- Web applications

- Native Kubernetes API

Rancher Applications

- Catalogue of applications — mostly remote GUI
  - Ansys, Matlab, Rstudio, Generic Desktop, VMD
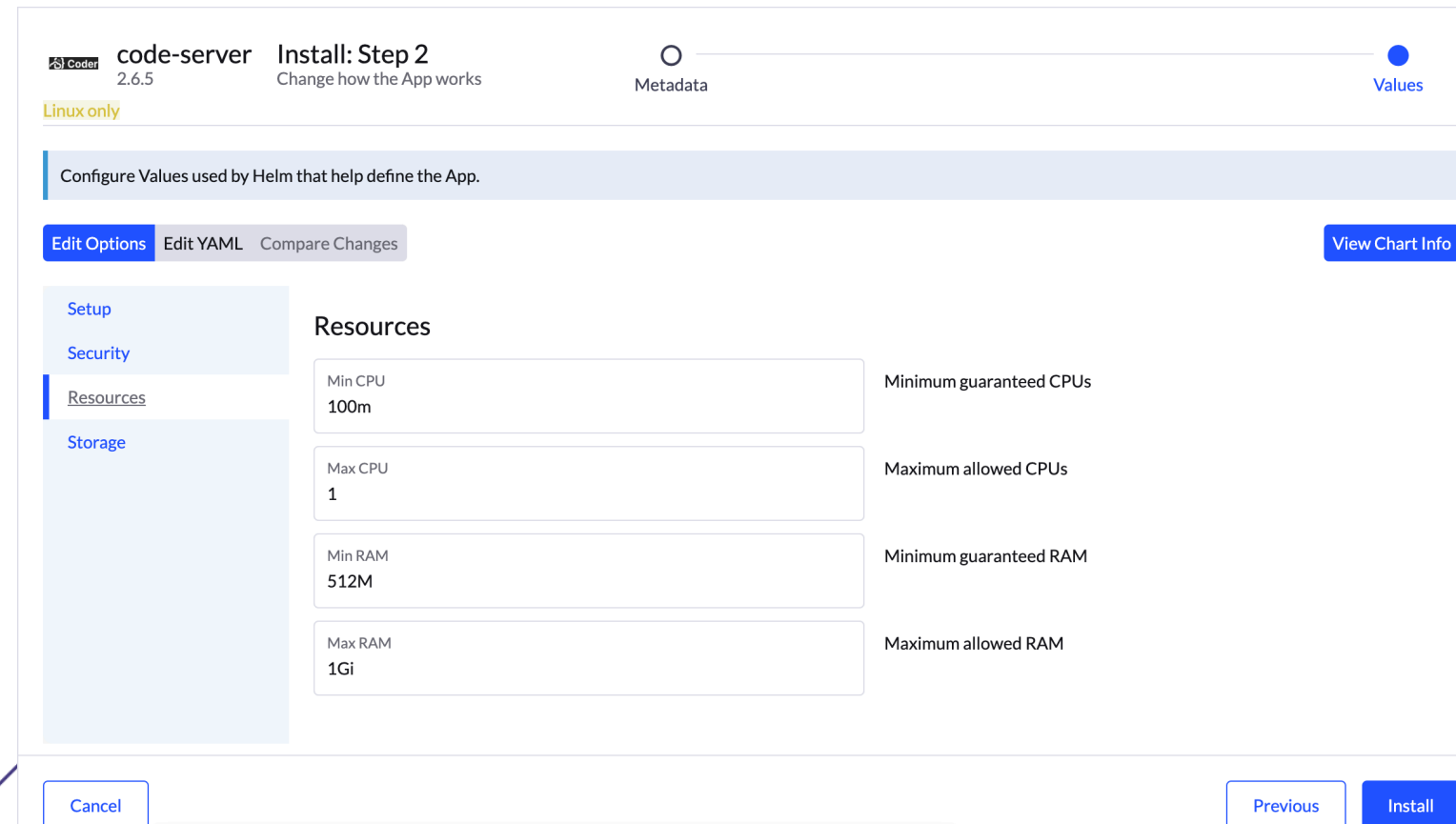 - Code-Server, Pycharm
  - UI for LLM

Rancher Applications — How to Use?

- Log to rancher: https://rancher.cloud.e-infra.cz
- Select cluster, Apps, Charts
- Fill option form (go through all options)
- Application should be running
- Navigate to Service
- See https://docs.cerit.io

Rancher Applications — Missing One?

I want **YOU** to request!
Requesting station:
k8s@ics.muni.cz
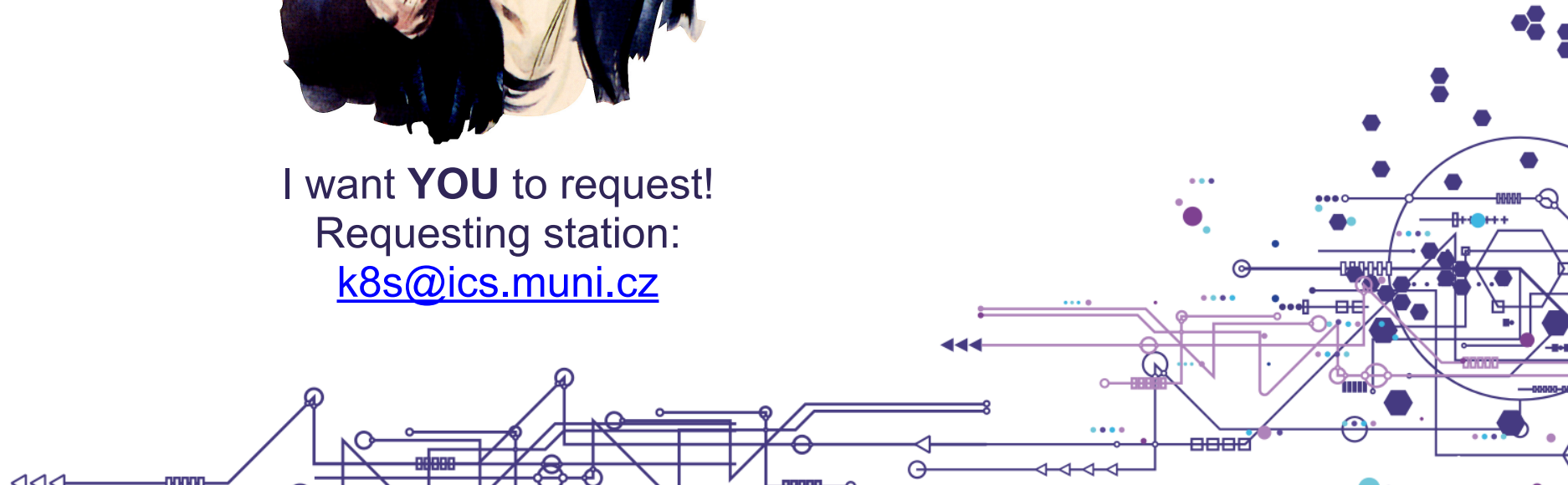
Web Applications
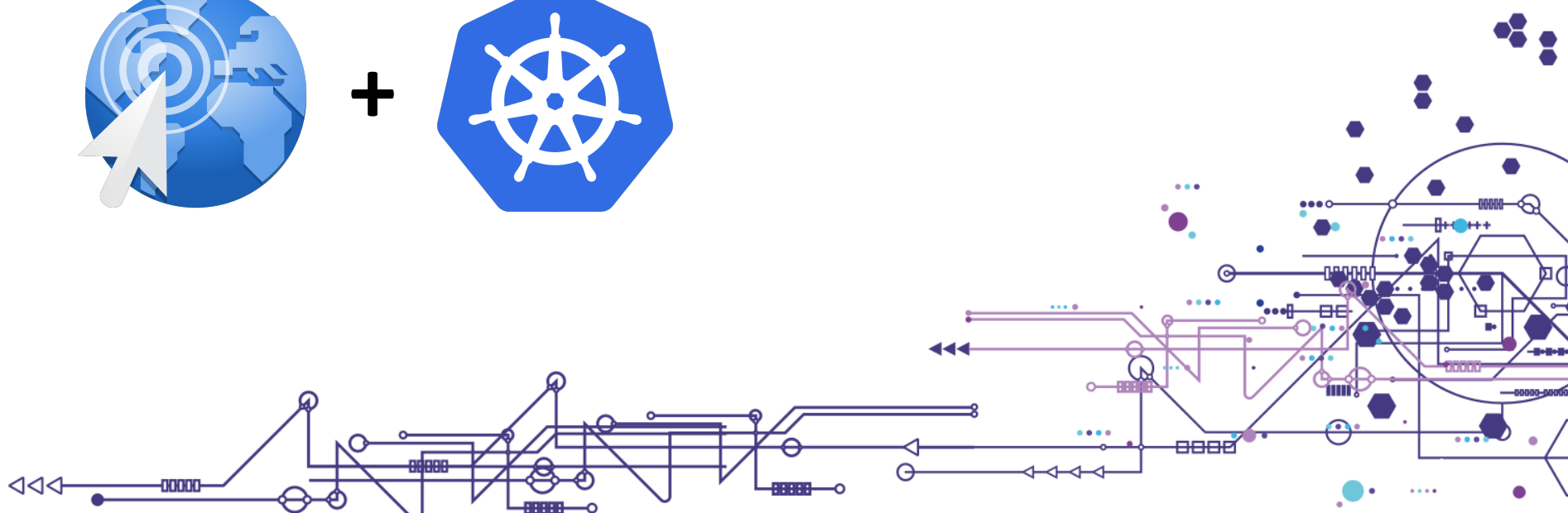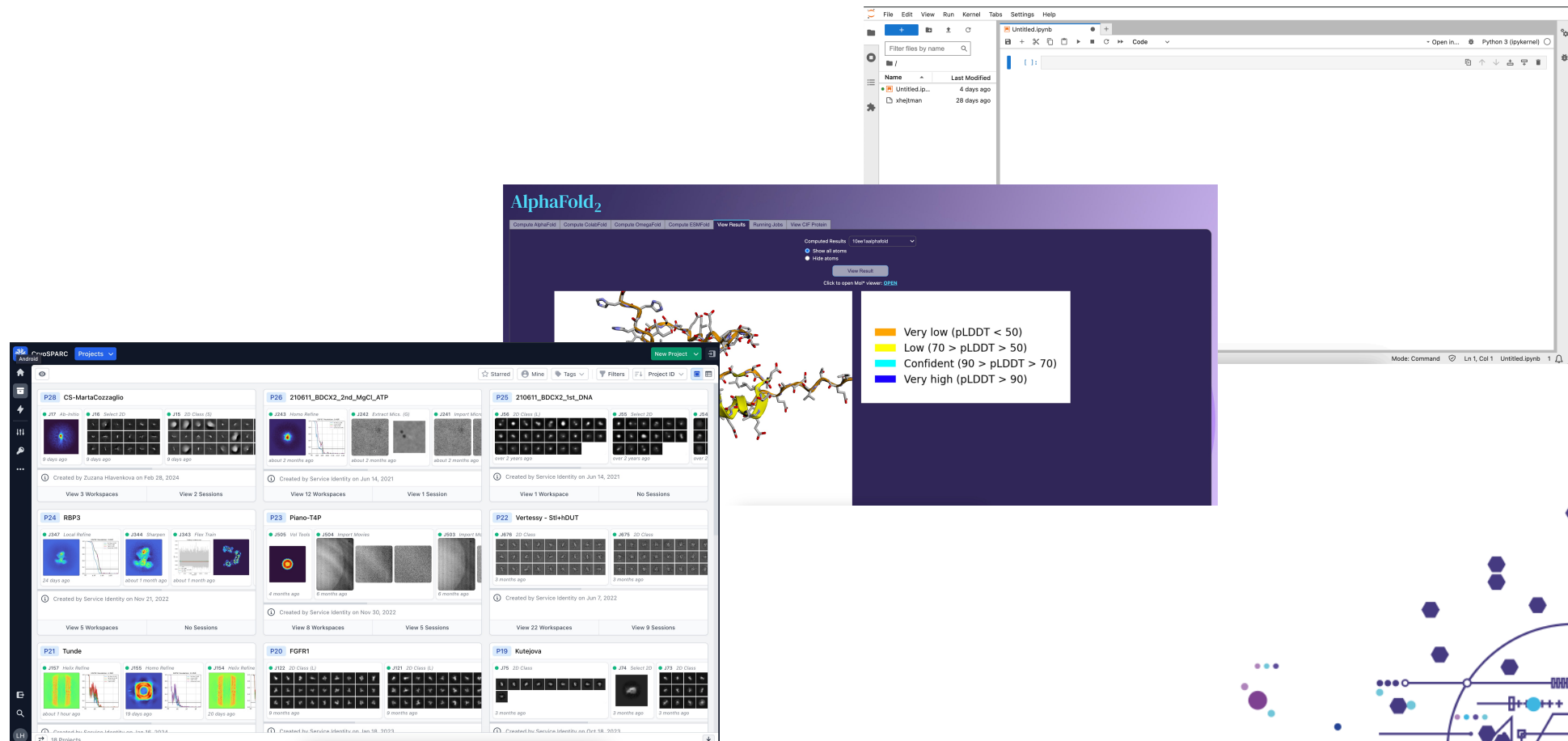
Web Applications

- Jupterhub

- Alphafold

- Cryosparc

Jupyterhub

- https://hub.cloud.e-infra.cz
- Integrated with e-INFRA CZ storages
    - Integration with Onedata datasets in progress
- Without explicit run-time limit
- Number of prepared images — ask if you need more k8s@ics.muni.cz
    - Rstudio, Matlab, RSAT images
- Allows to spawn additional jobs from the notebook
- Notebooks for advanced users
    - https://binderhub.cloud.e-infra.cz
    - Builds notebook image from source
    - Possible to request resources
        - CPU, GPU, Memory

Jupyterhub

jupyterhub　Home　Token
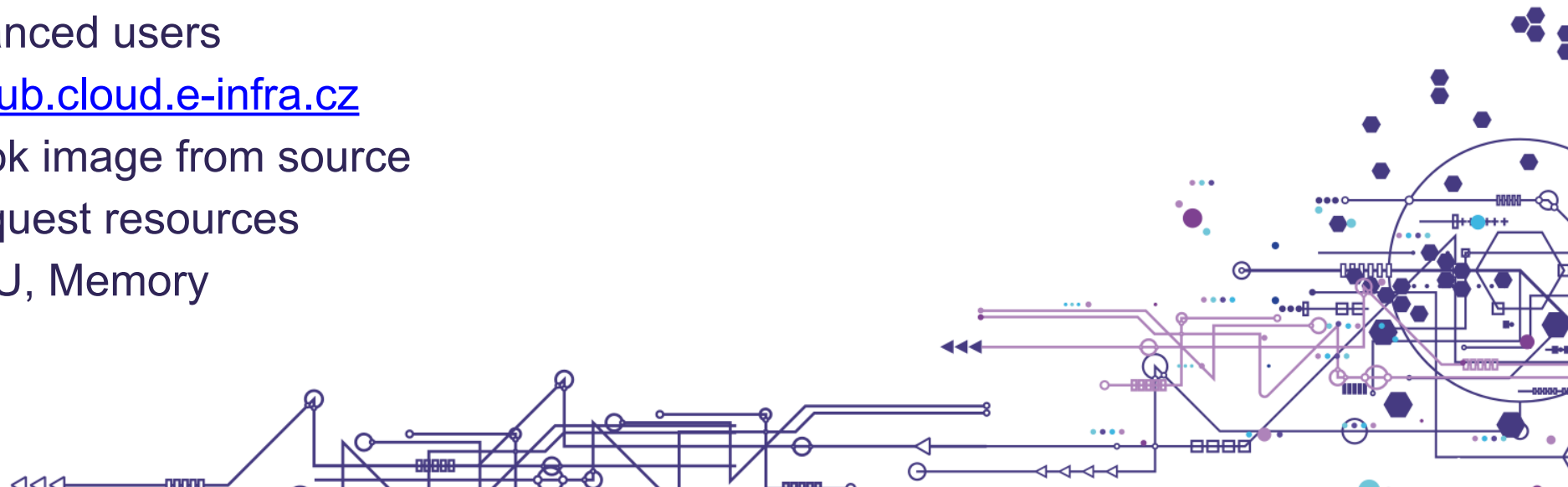
Server Options

Choosing image

Predefined Jupyter Notebook images are:

- Minimal NB - Jupyter minimal notebook
- Datascience NB - Jupyter datascience NB (Python, R, Julia)
- Scipy NB - Jupyter scipy NB (minimal NB + interactive visualizations and plots in Python)
- Tensorflow NB - Jupyter TensorFlow NB (scipy NB + tensorflow and keras)
- Tensorflow GPU NB - Jupyter TensorFlow NB on GPU (Jupyter Notebooks with the power of GPU, perform GPU calculations using Tensorflow and Pytorch in collaborative notebooks. Diplayed device is XLA_GPU)
- RationAI with GPU, TF, TB - Jupyter TensorFlow NB on GPU (Image for specific team)
- RStudio - RStudio via Jupyterhub
- Alphapose - Alphapose AI framework

Apart from Jupyter Notebook images, you can also spawn RStudio instance with *R 4.2.1*. GPU is not supported in the image, all other features are support (including conda). If you seek another version of R with RStudio, GPU support or have other requirements send your inquiry to our IT Service desk.

If you want to run custom image, write its name into the text field in format *repo/image_name:tag* or *repo/image_name*. Images with no tag will be treated as latest, default image is set to Minimal NB.

Select an image: [Minimal NB ▾]

Choosing storage

The notebook will spawn with chosen persistent volume which will be mounted into */home/jovyan*. Persistent home means that even when notebook gets deleted, the data will persist and can be used again. You can choose from mounting a **new** home for the spawned notebook or mounting an **existing** one. If you choose to mount a new home and home's name would be the same as the name of notebook being spawned, you must explicitly check the checkbox stating *Erase if home exists*. Otherwise, new home will not be created and already existing home will be mounted!

Select persistent home type: [New ▾]

9

Jupyterhub
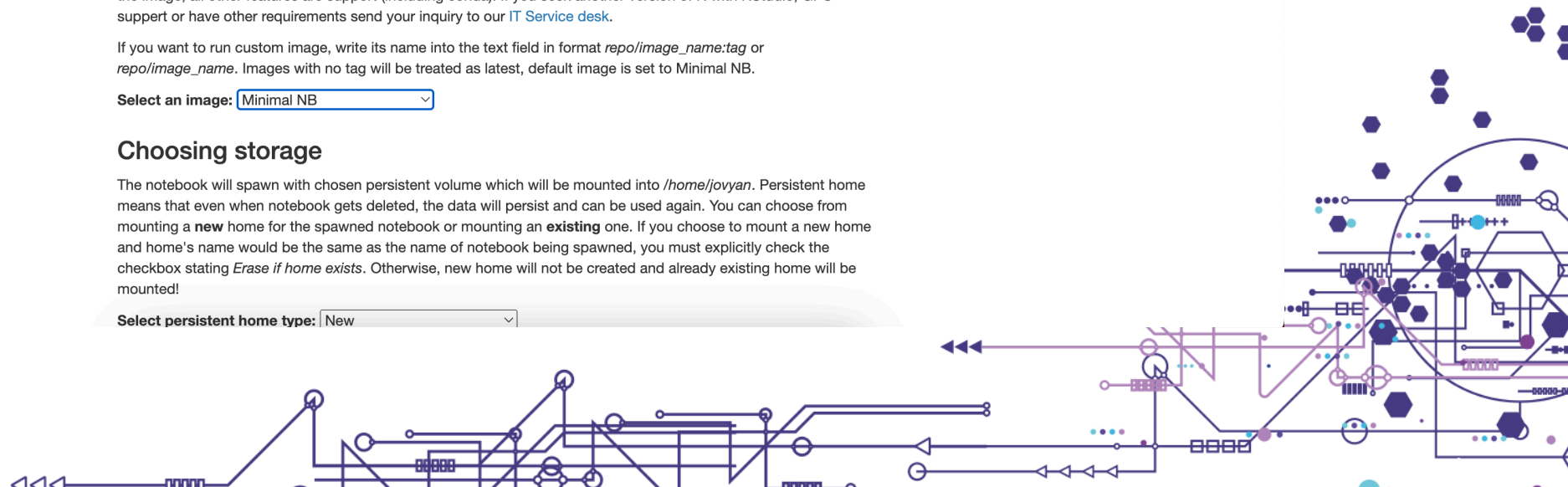
- You can request to deploy a custom instance
  - Access limited to a Perun group
  - Custom start form and images
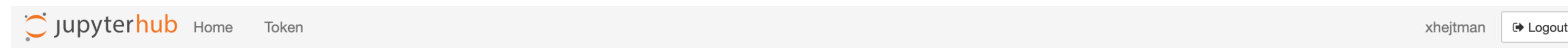
Alphafold

- Web UI for Alphafold tools
- Supports several different tools
  - Alphafold, Colabfold, Omegaold, Esmfold
- Colabfold
  - Running our mmseqs server (no rate limit)
  - Added possibility to limit number of models
- Integrated Mol* viewer and e-INFRA CZ storage (brno12)
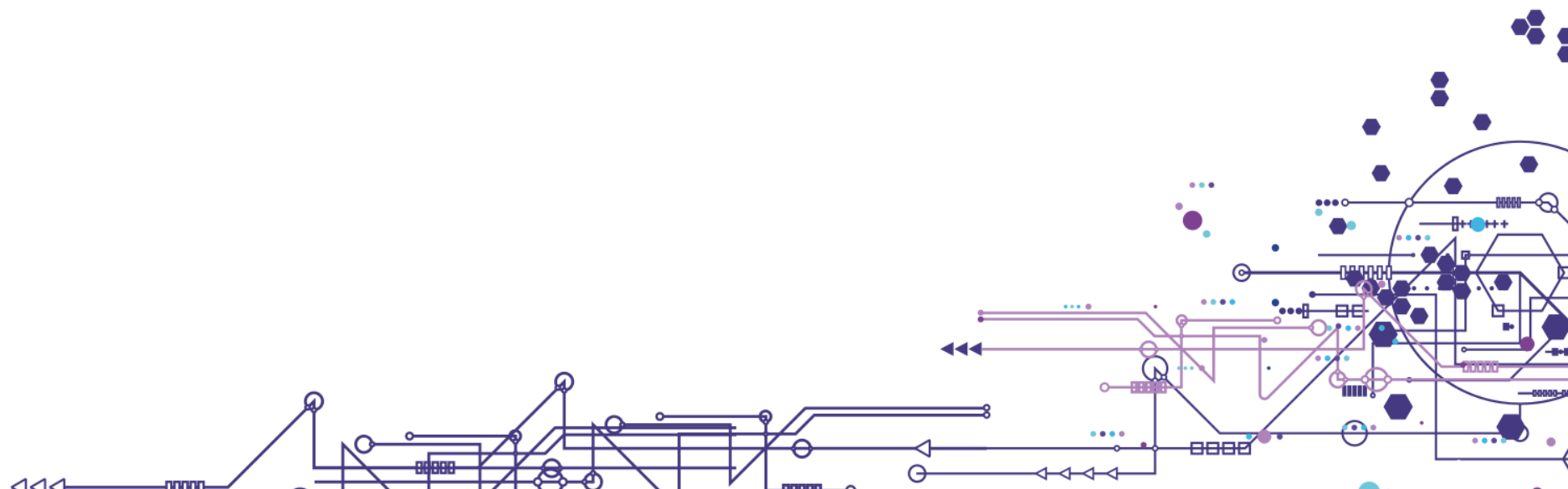
Alphafold

AlphaFold₂

Compute AlphaFold | Compute ColabFold | Compute OmegaFold | Compute ESMFold | View Results | Running Jobs | View CIF Protein

Protein name	adventurous-frank
Proteins	>Sequence1
Max template date	default
DB Preset	full_dbs
Model Preset	monomer
Precomp MSAS	☐
Predictions per model	5
Run Relax	☑
Make results public	☑
E-mail	xhejtman@ics.muni.cz
Force computation	☐
Version of Alphafold	Alphafold 2.3.1

✔ Run

Operated by CERIT-SC, ICS MUNI, support: k8s@ics.muni.cz

Documentation | Terms of use

Alphafold
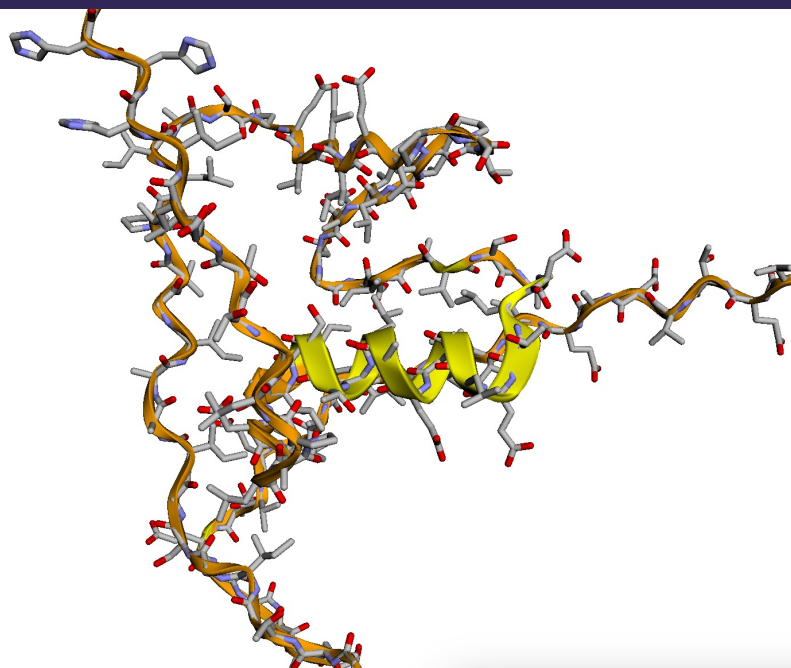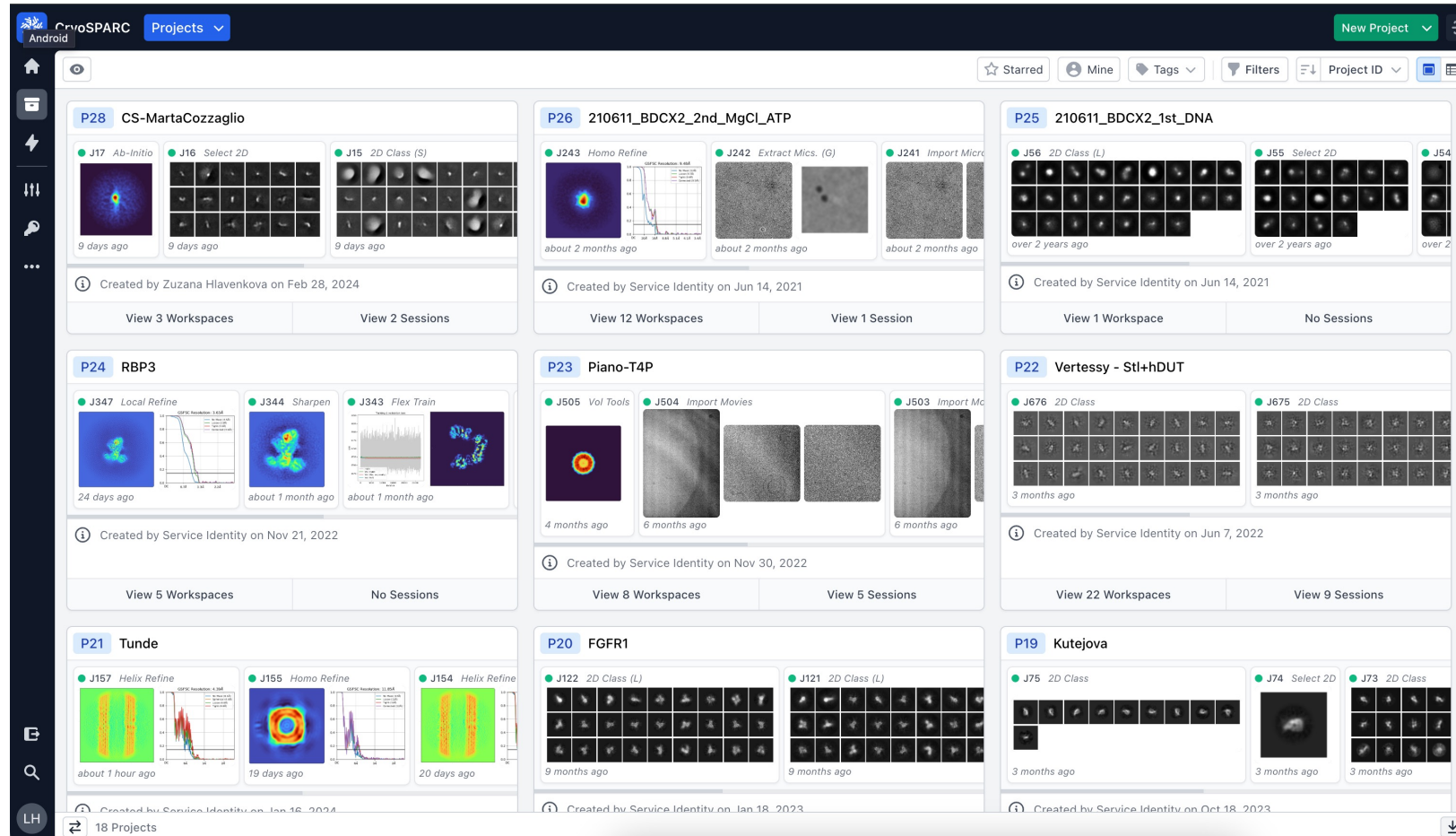
Cryosparc

- Web UI running in K8s

- Jobs can run in both K8s and PBS

- Easy deployment of new instances

  - Own licence required
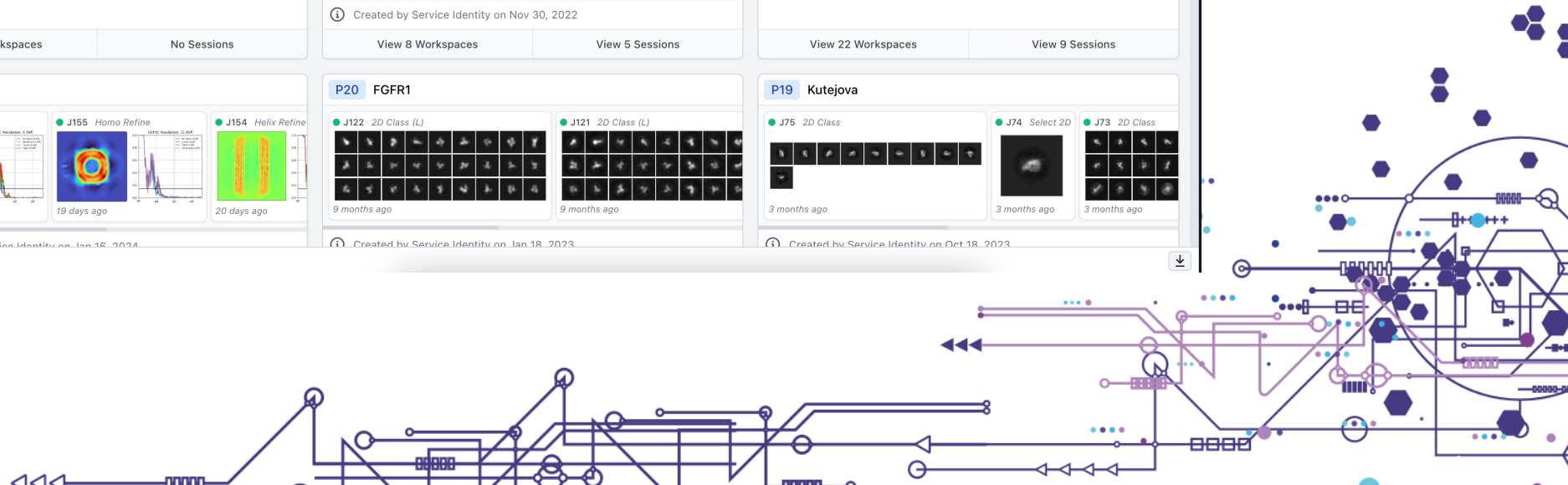
Cryosparc

Native Kubernetes API

Native Kubernetes API Use Cases

- Get kubeconfig from Rancher
- Deploy **helm** package
  - Pre-packaged application to run in Kubernetes
  - Form of a template
  - Need to fill custom values
  - Examples:
    - `helm install --namespace logging logging-operator oci://ghcr.io/kube-logging/helm-charts/logging-operator -f values.yaml`
    - `helm install -n my_namespace my_application . -f values.yaml`
- Deploy **Docker** image
  - Find or create the docker image
  - Create **Deployment** manifest
  - Create **Service** manifest (LoadBalancer or ClusterIP)
    - Create **Ingress** manifest
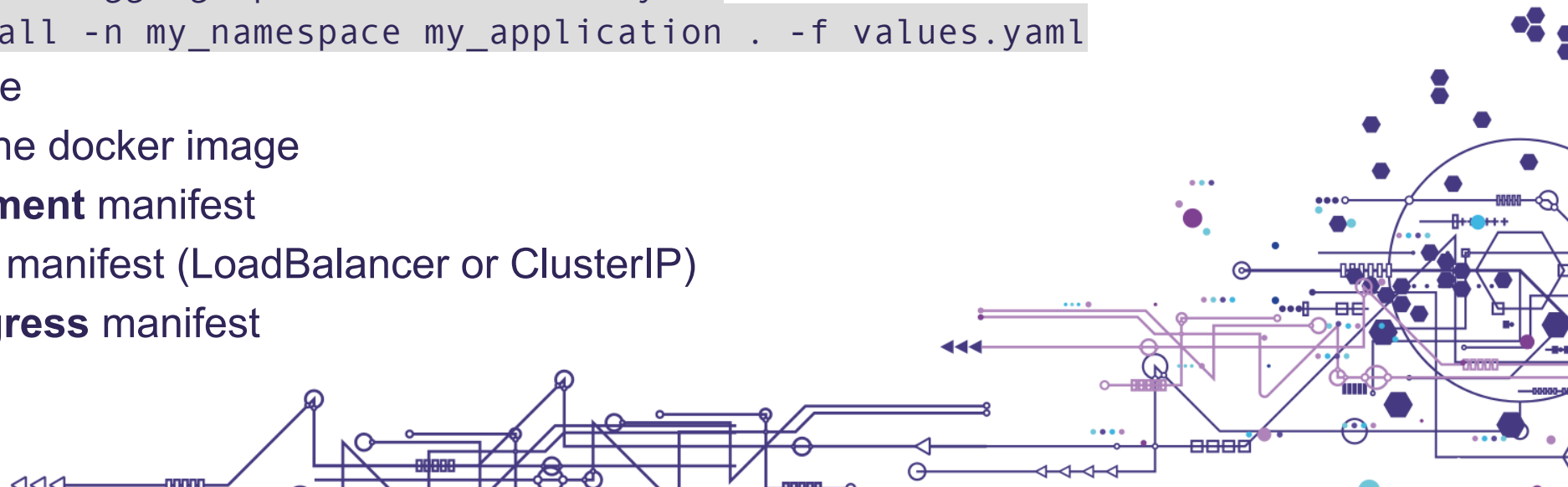
Native Kubernetes API — Tips

- Exposing Web application to the Internet
    - Deployment + Service + Ingress
    - Let's encrypt certificate can be requested
- Exposing raw application to the Internet
    - Deployment + Service (LoadBalancer type)
    - Exposed at particular IP, can get ad-hoc name .dyn.cloud.e-infra.cz
    - Let's encrypt certificate can be requested
    - Can be used for, e.g., opening ssh connection to the container

Native Kubernetes API — Tips

- How to run Docker image that expects to be run as root
  - Mostly root privileges are not necessary
  - Mount `emptyDir` volume where write access is needed (e.g. logs)
  - Rebuild image
    - ```
      FROM original_image AS src
      FROM scratch
   COPY --chown=1000:1000 --from=src / /
      USER 1000
      ```
    - Does not work with Kaniko builder
    - Does not inherit `ENV, WORKDIR, CMD` settings
- How to allow additional packages to be installed?
  - Rebuild image as above
  - Install `fakeroot` (for deb based distros)
  - `ln -s /usr/bin/fakeroot /usr/bin/sudo`

# Native Kubernetes API — Common Problems

- `would violate PodSecurity "restricted:latest": allowPrivilegeEscalation != false (container "demo" must set securityContext.allowPrivilegeEscalation=false), runAsNonRoot != true (pod or container "demo" must set securityContext.runAsNonRoot=true)`
  - Deployment is missing proper `securityContext`
  - [https://docs.cerit.io/docs/securitycontext.html](https://docs.cerit.io/docs/securitycontext.html)
- `Error: container has runAsNonRoot and image will run as root`
  - Deployment or image is missing run user definition
    - Deployment: `runAsUser: 1000`
    - Image: `USER 1000`
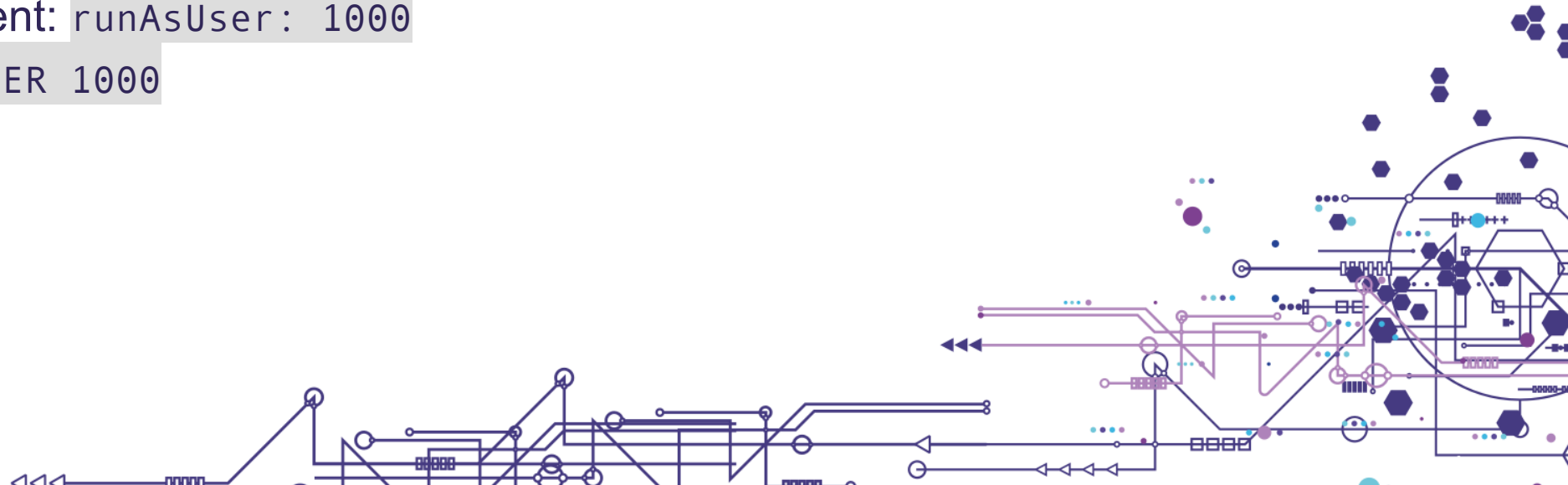
e-INFRA cz

Questions?

k8s@ics.muni.cz

e-infra.cz