

# OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

## Introduction to OpenRiskNet e-infrastructure

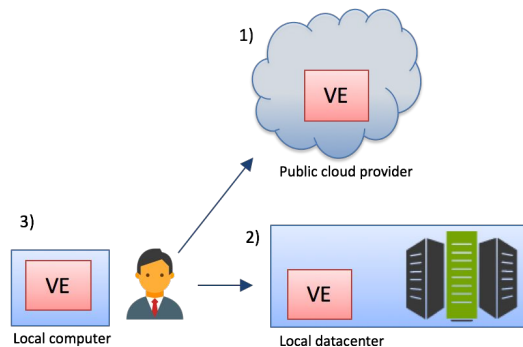
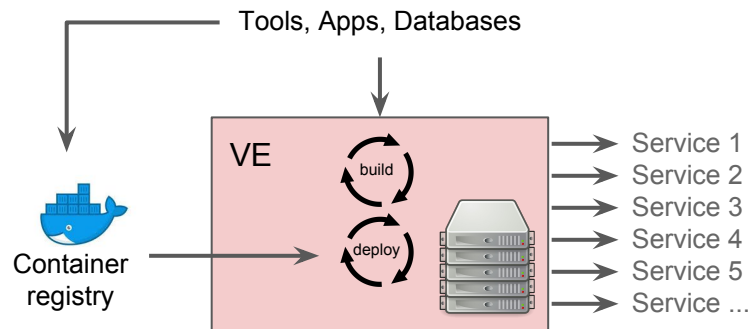
### The OpenRiskNet Consortium

OpenRiskNet: Open e-Infrastructure to Support Data Sharing, Knowledge Integration and *in silico* Analysis and Modelling in Risk Assessment  
Project Number 731075



# OpenRiskNet Virtual Environment (VE)

- Computational infrastructure into which applications can be deployed
- Includes environment for building and testing those applications
- Includes compute, security, storage, monitoring ...
- Can be deployed to range of infrastructures



# The ORN Project Provides:

- Instructions and materials for deploying an ORN VE
  - <https://github.com/OpenRiskNet/home/tree/master/openshift>
  - We aim to support a number of cloud providers and deployment scenarios
- A reference site where you can test the currently deployed tools
  - <https://home.prod.openrisknet.org/>
  - Intended for evaluation and testing - not production use

# VE Architecture



- Based on OpenShift Container Platform (<https://www.openshift.com/>)
  - Red Hat's distribution of Kubernetes
  - Designed for large scale, but can be run on a laptop
  - Adds important capabilities such as CI/CD, security, monitoring
  - Open Source, but with option of commercial support
  - Red Hat are a technology partner for the project
- If your tool/service is already containerised it should be relatively simple to deploy it to an ORN VE
- Containerising applications is relatively simple, but may need some refactoring in some cases



# ORN Reference Site



- Running on Swedish Science Cloud (SSC)
- OpenStack Cloud environment
- Currently uses
  - 15 VMs
  - 100 CPU cores
  - 200GB RAM
- Compute and storage can be expanded as needed

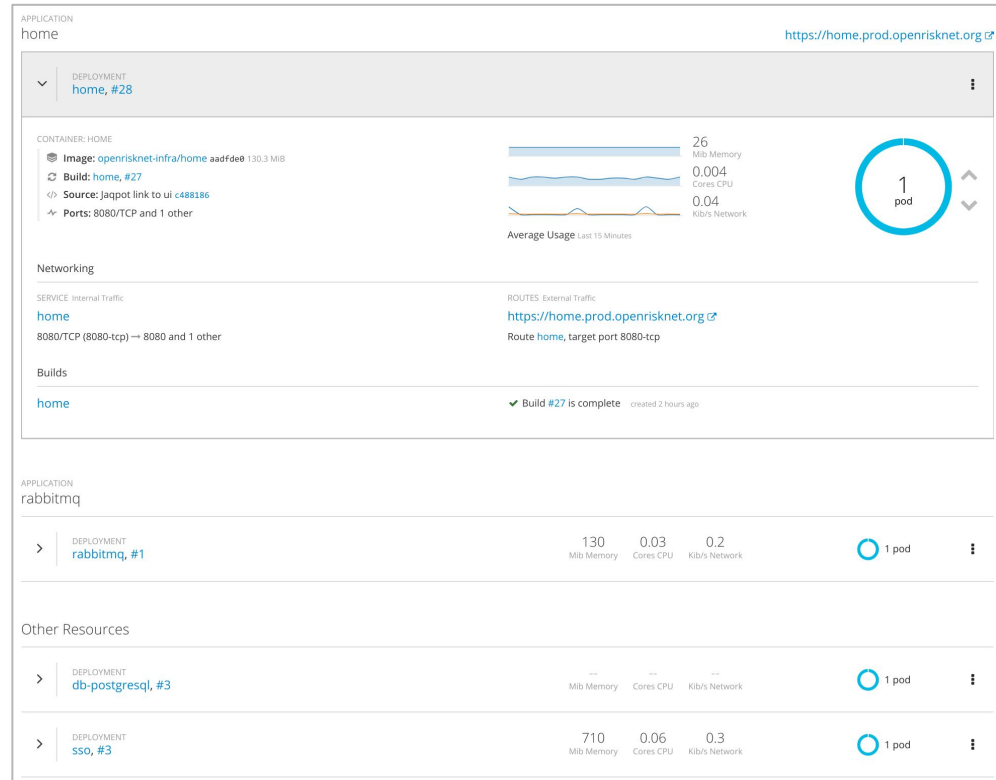
A screenshot of the OpenStack dashboard interface. The browser address bar shows "https://uppmax.cloud.snic.se/project/instances/". The page title is "Instances - OpenStack". On the left, there is a navigation menu with categories like "Volumes", "Images", "Access & Security", "Network", "Orchestration", "Object Store", and "Identity". The main content area displays a table of instances. The table has columns for Instance Name, Image Name, IP Address, Size, Key Pair, Status, Availability Zone, Task, Power State, Time since created, and Actions. There are 15 items displayed, all in a "Running" state. The instances are named "om-gluiter-storage-003" through "om-master".

Instance Name	Image Name	IP Address	Size	Key Pair	Status	Availability Zone	Task	Power State	Time since created	Actions
om-gluiter-storage-003.openstacklocal	centos-1802-os-base-01-A	10.0.0.8	ssc.large	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	2 weeks, 1 day	Create Snapshot
om-gluiter-storage-002.openstacklocal	centos-1802-os-base-01-A	10.0.0.18	ssc.large	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	2 weeks, 1 day	Create Snapshot
om-gluiter-storage-001.openstacklocal	centos-1802-os-base-01-A	10.0.0.24	ssc.large	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	2 weeks, 1 day	Create Snapshot
om-node-003.openstacklocal	centos-1802-os-base-01-A	10.0.0.22	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	4 weeks, 1 day	Create Snapshot
om-node-006.openstacklocal	centos-1802-os-base-01-A	10.0.0.23	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	4 weeks, 1 day	Create Snapshot
om-node-008.openstacklocal	centos-1802-os-base-01-A	10.0.0.33	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	4 months, 2 weeks	Create Snapshot
om-node-010.openstacklocal	centos-1802-os-base-01-A	10.0.0.37	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	4 months, 2 weeks	Create Snapshot
om-node-009.openstacklocal	centos-1802-os-base-01-A	10.0.0.36	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	4 months, 2 weeks	Create Snapshot
om-node-005.openstacklocal	centos-1802-os-base-01-A	10.0.0.15	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	4 months, 3 weeks	Create Snapshot
om-node-007.openstacklocal	centos-1802-os-base-01-A	10.0.0.35	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	4 months, 3 weeks	Create Snapshot
om-node-004.openstacklocal	centos-1802-os-base-01-A	10.0.0.21	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	5 months	Create Snapshot
om-node-001.openstacklocal	centos-1802-os-base-01-A	10.0.0.32	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	5 months	Create Snapshot
om-node-002.openstacklocal	centos-1802-os-base-01-A	10.0.0.29	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	5 months	Create Snapshot
om-virta.openstacklocal	centos-1802-os-base-01-A	10.0.0.12 Floating IP: 130.238.28.101	ssc.xlarge	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	5 months	Create Snapshot
om-master.openstacklocal	centos-1802-os-base-01-A	10.0.0.38 Floating IP: 130.238.28.57	ssc.large	omdev-keypair-ab05c8b9e153710d61e05148	Active	nova	None	Running	5 months	Create Snapshot



# OpenShift

- Deployed as part of the VE
- Provides the ability to build, deploy, scale and monitor containerised applications
- Accessible through web console, CLI and API
- Main point of access for the application developer/deployer



# Deployment Examples

- Deployments for partner apps defined in GitHub:
  - <https://github.com/OpenRiskNet/home/tree/master/openshift/deployments>
- A simple example: BridgeDB
  - <https://github.com/OpenRiskNet/home/tree/master/openshift/deployments/bridgedb>
  - Singe Docker container
- More complex examples:
  - JupyterHub:  
<https://github.com/OpenRiskNet/home/tree/master/openshift/deployments/jupyter>
  - Squonk Computational Notebook:  
<https://github.com/InformaticsMatters/squonk/tree/master/openshift/templates>

# Interoperability

- Having a range of tools and services available is useful, but it's much more useful if they can be made to be interoperable
- OpenShift Services are annotated so that they become discoverable
- A service's REST API is semantically described with JSON-LD definitions within OpenAPI (Swagger)
- ORN registry provides ability to query for services
  - *Give me all services that can predict a LogP from a SMILES*
  - *Give me all services that can convert an InChi to a SMILES*
- Registry: <http://orn-registry-openrisknet-registry.prod.openrisknet.org/>
- Query tool: <https://orn-query-test.cloud.douglasconnect.com/>
- Ontology: <https://docs.google.com/spreadsheets/d/1-IrUj8htx5ipsly1f-bv8-BuALVnRR3zxbChchx9QMo>
- Guide: <https://docs.google.com/document/d/1a9Wndz5nqBzO2Km93lSpHjvftLLHufTo6Do3UpqyliE>



# Example: Lazar - toxicity prediction using read across

- Annotate the OpenShift service definition to make it discoverable:

```
76 - kind: Service
77   apiVersion: v1
78   metadata:
79     name: lazar-rest
80     namespace: lazar
81     annotations:
82     openrisknet-static-services: http://lazar-rest.lazar.svc.cluster.local:8088/api/api.json
```

See:

<https://github.com/OpenRiskNet/home/blob/master/openshift/deployments/lazar/lazar-rest-template.yaml>

- Annotate the OpenAPI definition with x-orn-\* extensions:

```
{
  "openapi": "3.0.0",
  "x-orn-@id": "https://lazar.prod.openrisknet.org",
  "x-orn-@type": "x-orn:Service",
  "x-orn-@context": {
    "@vocab": "http://openrisknet.org/schema#",
    "x-orn": "http://openrisknet.org/schema#",
    "x-orn-@id": "@id",
    "x-orn-@type": "@type"
  },
```

See:

<https://lazar.prod.openrisknet.org/api/api.json>

# Demos

OpenStack on SSC: <https://uppmax.cloud.snic.se/project/>

OpenShift Console: <https://prod.openrisknet.org/console/>

Landing Page: <https://home.prod.openrisknet.org/>

# Acknowledgements

**OpenRiskNet** (Grant Agreement 731075) is a project funded by the European Commission within Horizon2020 Programme

## Project partners:

P1 Douglas Connect GmbH, Switzerland (DC)

P2 Johannes Gutenberg-Universität Mainz, Germany (JGU)

P3 Fundacio Centre De Regulacio Genomica, Spain (CRG)

P4 Universiteit Maastricht, Netherlands (UM)

P5 The University Of Birmingham, United Kingdom (UoB)

P6 National Technical University Of Athens, Greece (NTUA)

P7 Fraunhofer Gesellschaft Zur Foerderung Der Angewandten Forschung E.V., Germany (Fraunhofer)

P8 Uppsala Universitet, Sweden (UU)

P9 Medizinische Universität Innsbruck, Austria (MUI)

P10 Informatics Matters Limited, United Kingdom (IM)

P11 Institut National De L'environnement Et Des Risques INERIS, France (INERIS)

P12 Vrije Universiteit Amsterdam, Netherlands (VU)