OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

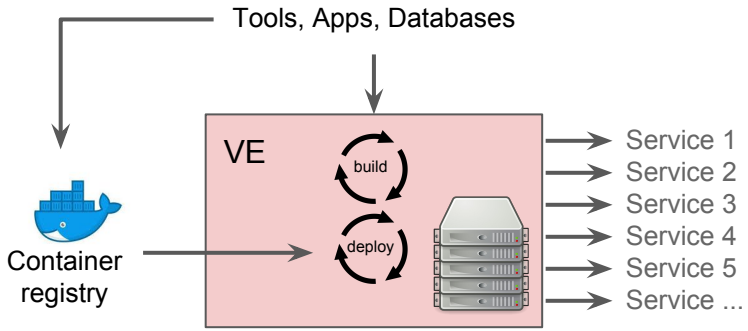
Introduction to OpenRiskNet e-infrastructure

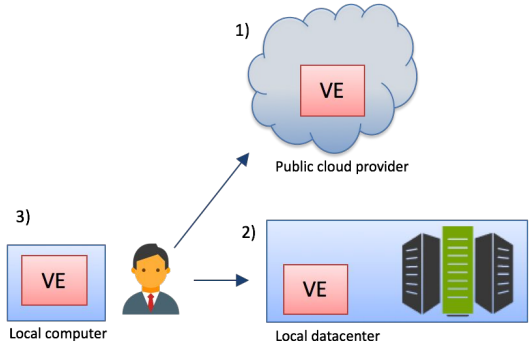
The OpenRiskNet Consortium

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:

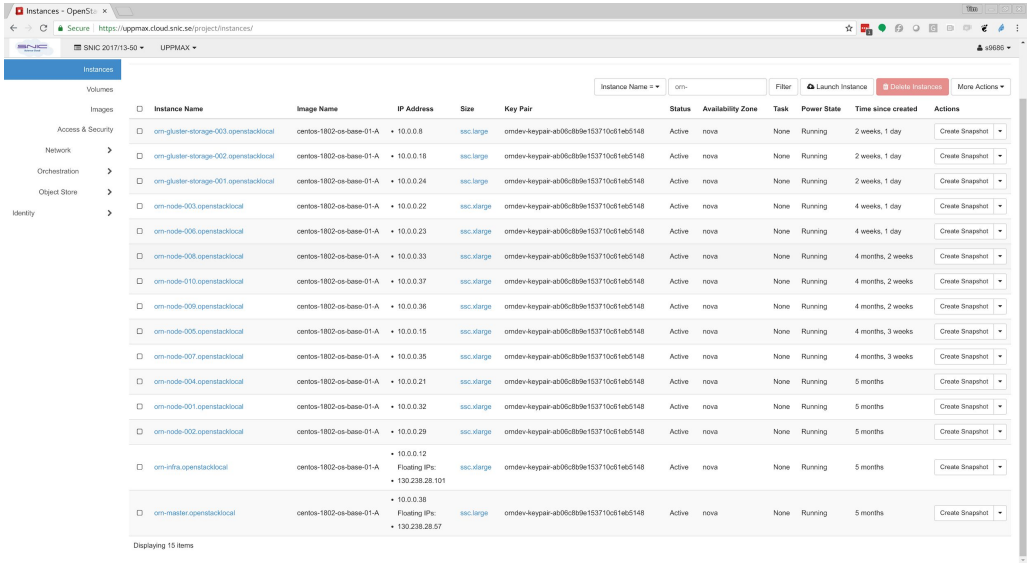
- Instructions and materials for deploying an ORN VE
  - https://github.com/OpenRiskNet/home/tree/master/openshift
  - We aim to support a number of cloud providers and deployment scenarios
- A reference site where you can test the currently deployed tools
  - https://home.prod.openrisknet.org/
  - Intended 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

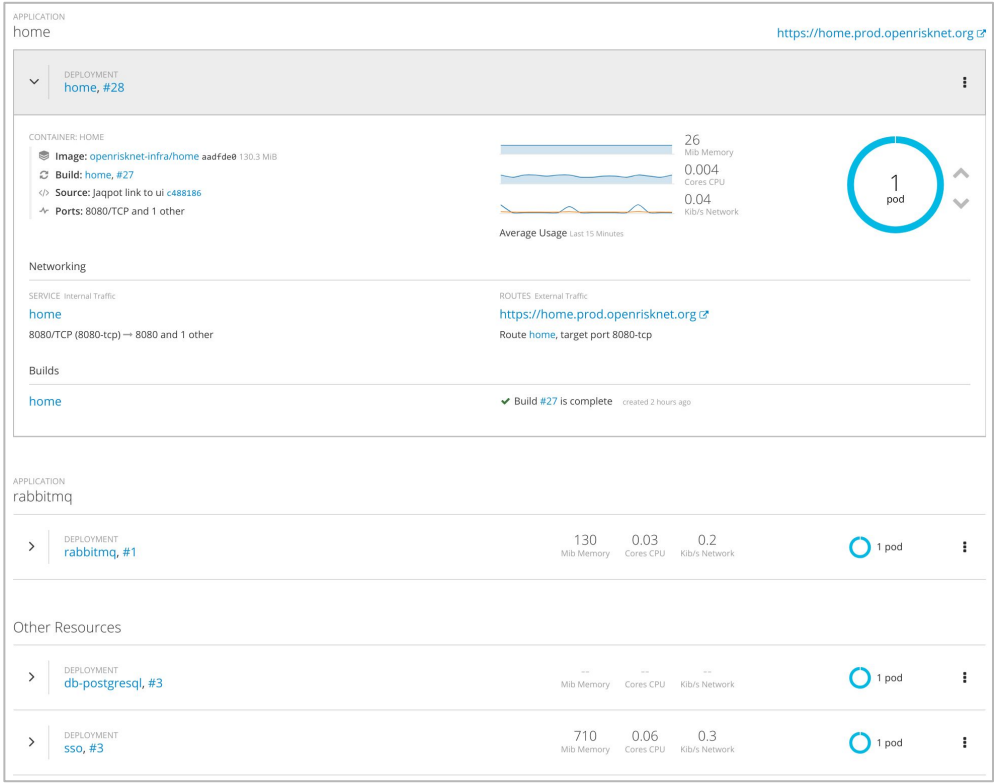
ORN Reference Site

- 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



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/

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