

OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

OpenRiskNet e-infrastructure Deployment

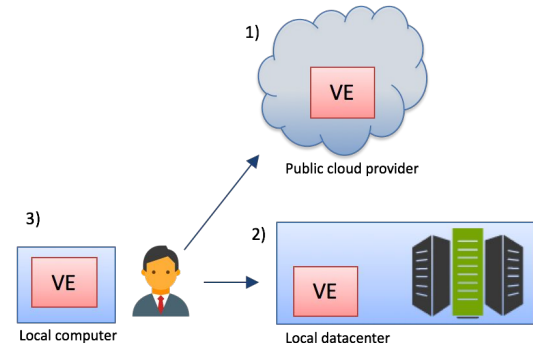
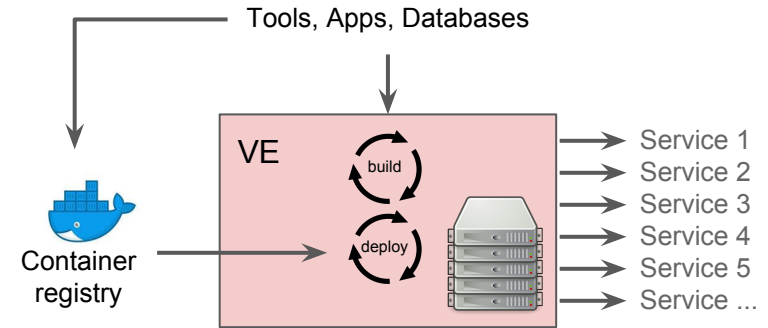
The OpenRiskNet Consortium

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

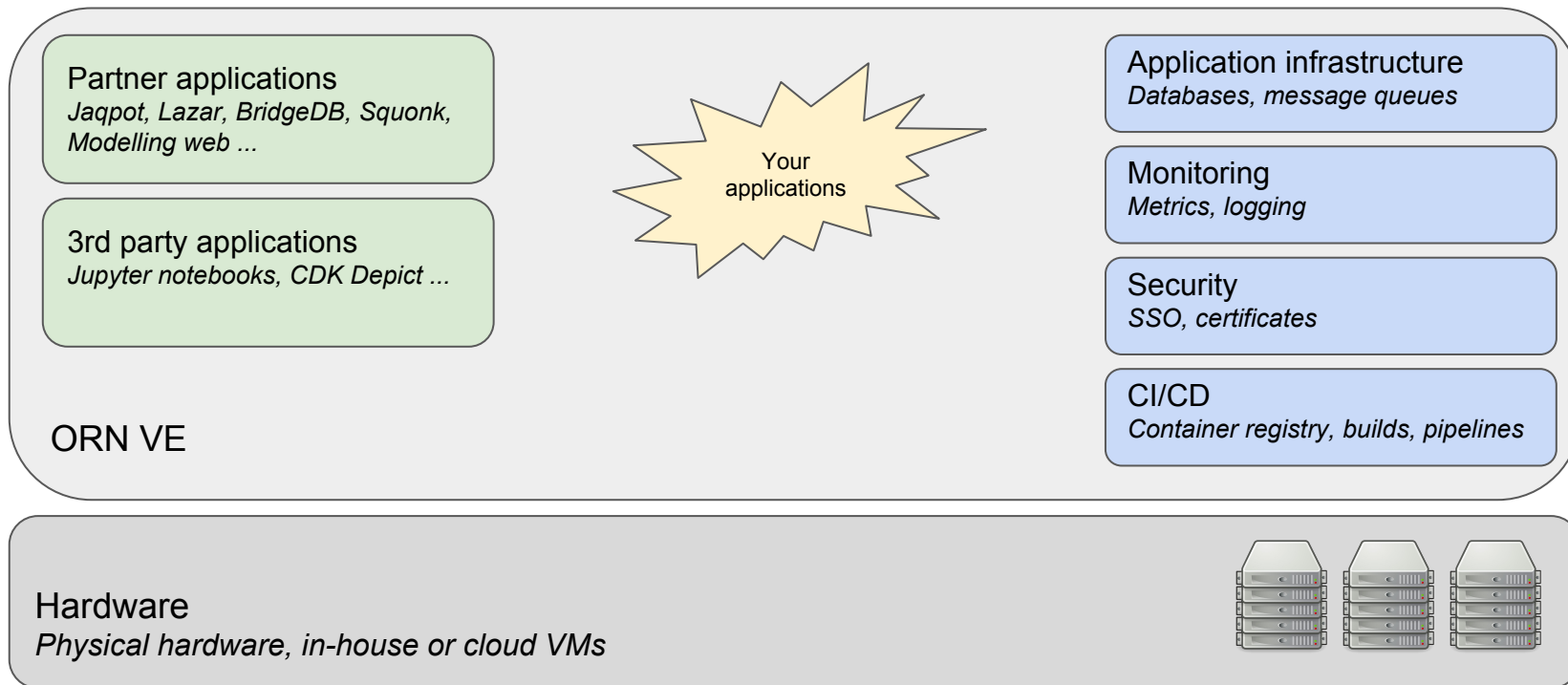


OpenRiskNet Virtual Environment (VE)

- 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



VE Architecture



Example OpenRiskNet VEs

ORN Reference site ([link](#))

ORN Development site

Sites run by ORN partners

Diamond Light Source ([link](#))

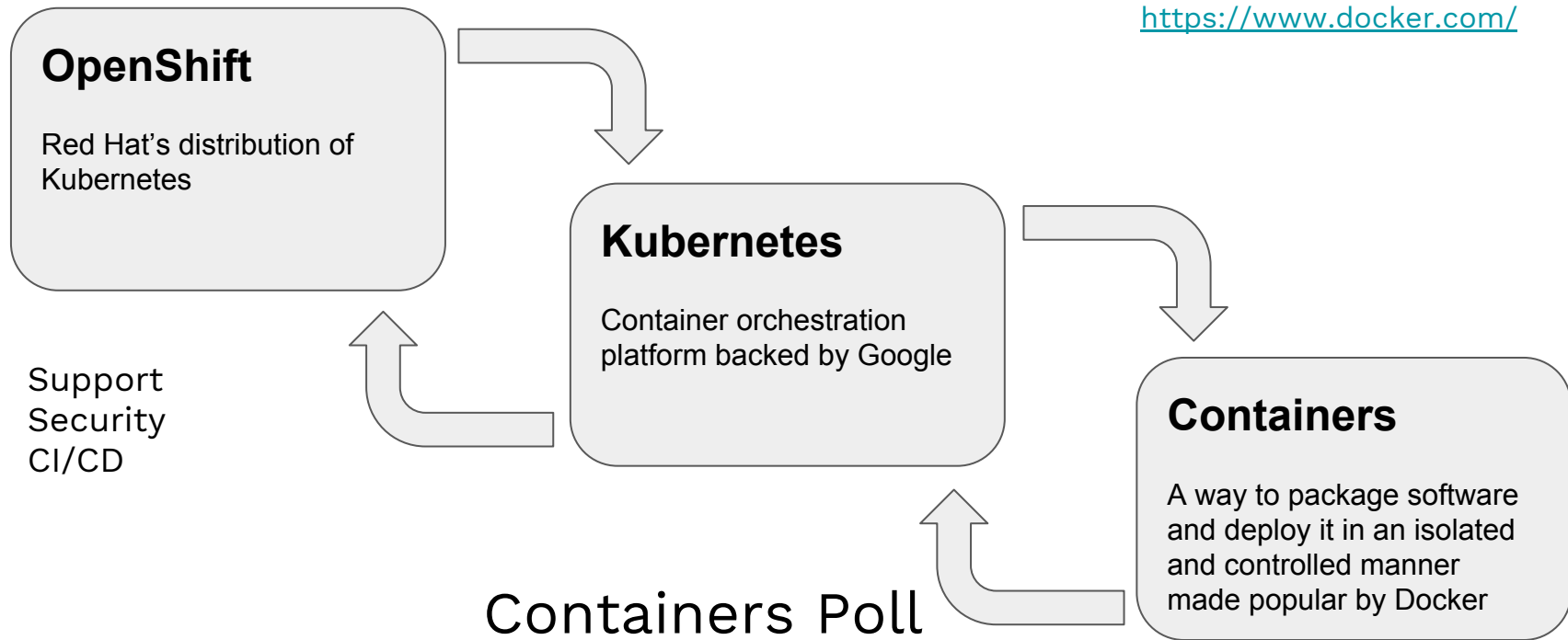
The screenshot displays the Fragalysis web interface. At the top, there are navigation buttons: 'Log in', 'Save Session', 'Save Session As', 'Share Snapshot', and 'Download MJD structures'. Below these, a status bar indicates 'Currently no active session.' The main content area is divided into two panels. The left panel, titled 'Molecule Cluster Selector', shows 'On 1 of a total of 1' and includes 'Previous' and 'Next' buttons. Below this, there is a grid of four molecular clusters, each with a chemical structure and a 'Ligand' button. The right panel shows a 3D molecular model of a protein structure (red ribbons) with a ligand (orange and blue spheres) bound to it. A 'Viewer controls' section at the bottom of the right panel includes a 'Change background colour' button. On the far right, there is a sidebar with statistics: 'Number picked: 0', 'Number vectors explored: 0', 'Number series explored: 0', and 'Estimated cost: 0'. Below these are buttons for 'Download CSV (Chroms)' and 'Download Yankuplus', and a note that 'Selected interaction: Not selected'.

What forms a VE

<https://www.openshift.com/>

<https://kubernetes.io/>

<https://www.docker.com/>



History of Orchestration Tools

- [KubeNow](#) from UU allows to deploy K8S or Openshift
- OKD Orchestrator described here builds on principles from KubeNow to provide an orchestrator specific for OpenShift and targeted towards deploying an OpenRiskNet VE
- Orchestration tools coming with OpenShift 4 look much improved and may supersede these other tools

Steps to deployment:

1. Plan the hardware needs (Servers, CPUs, memory, availability ...)
2. Set up public IP addresses and hostnames
3. Run Orchestrator
 - a. Stage 1: Define configuration based on #1 and #2
 - b. Stage 2: Compile machine images (not needed if using bare metal)
 - c. Stage 3: Provision VMs (not needed if using bare metal)
 - d. Stage 4: Deploy OpenShift
4. Run “day 2” operations
5. Deploy applications

Supported platforms and setups

		Platform			
		Bare metal	OpenStack	AWS	GCE
Setup	Compact	+++	+	+++	+
	Standard	+++	+	+++	+++
	High Availability	-	-	-	-

- +++ Tested
- + Should work but not much tested
- Planned

Other potential platforms:

- Azure
- Digital Ocean
- Others?



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- P11 Institut National De L'environnement Et Des Risques INERIS, France (INERIS)
- P12 Vrije Universiteit Amsterdam, Netherlands (VU)



Links

These slides and videos: <https://openrisknet.org/events/57/>

OKD Orchestrator Github: <https://github.com/InformaticsMatters/okd-orchestrator>

OKD Orchestrator Docs: <https://docs.informaticsmatters.com/build/html/index.html>

Red Hat OpenShift (OKD): <https://www.okd.io/>

OKD Documentation: <https://docs.okd.io/latest/welcome/index.html>

Red Hat OpenShift (OCP): <https://www.openshift.com/products/container-platform/>

OpenRiskNet website: <https://openrisknet.org/>

OpenRiskNet reference site: <https://home.prod.openrisknet.org/>