

# Docker Workshop

## UberCloud HPC Application Containers

Frankfurt, June 23, 2016

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# UberCloud Overview

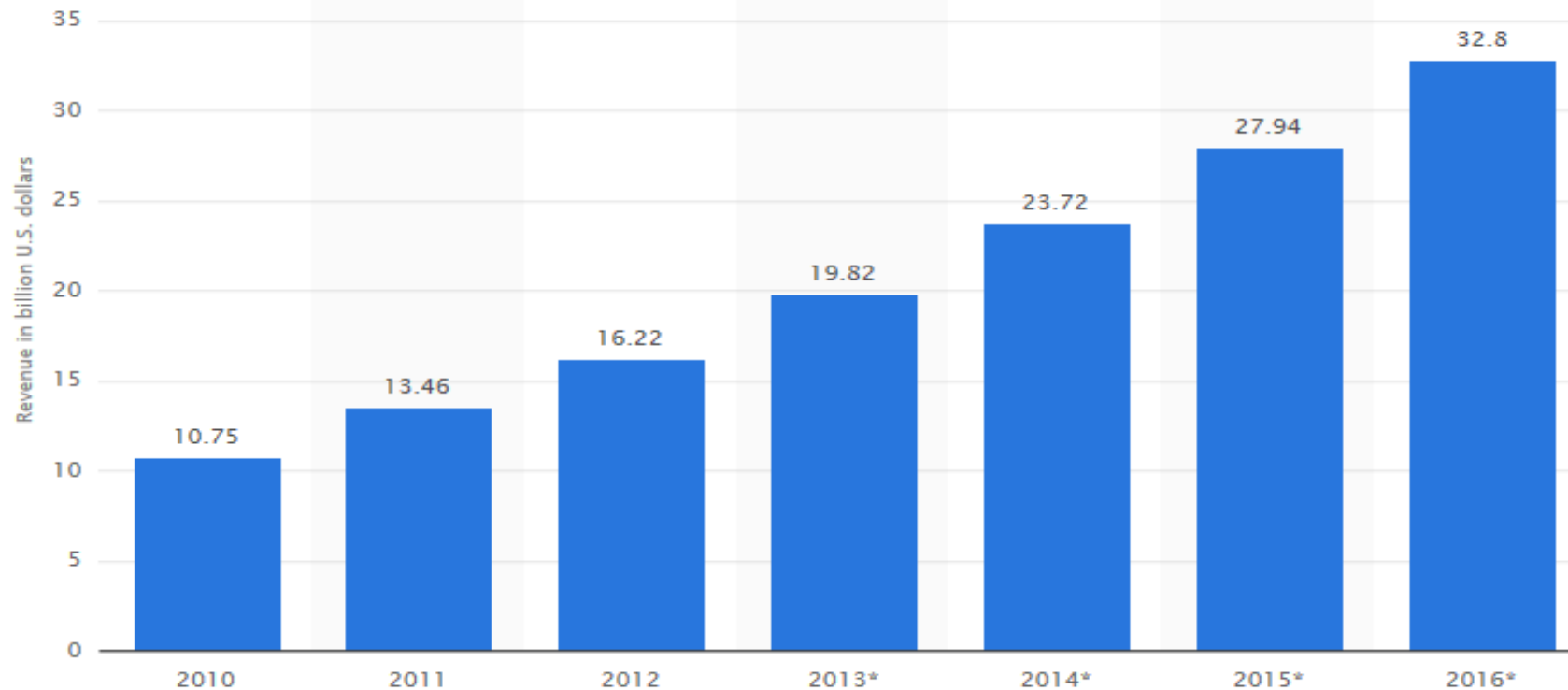
- + **July 2012:** Building user **community** around 'cloud experiments' (176 so far), feedback, measuring traction and cloud roadblocks
- + **March 2013:** Starting Docker HPC **technology** development for technical computing => Packageable, portable, accessible, usable, scalable, with low overhead
- + **November 2014:** Opening online **marketplace** with currently 34 stores & established provider ecosystem (resources, software, expertise)
- + **September 2015: Freemium Model:** Pragmatic blend of free open source HPC Containers with commercial closed source IP

# The market for HPC computing services

- + Today: 20+million engineers, scientists and their service providers in a very fragmented market:**
  - + CAE, Biotech, Pharma, Oil & Gas, Finance, Chemistry, Environment, Big Data Analytics, Government, Research**
  - + But, all have one thing in common: they need computing**
- + Tomorrow: plus 30+ million 'makers' (3D printing), plus big data analytics, plus digital natives, plus . . .**

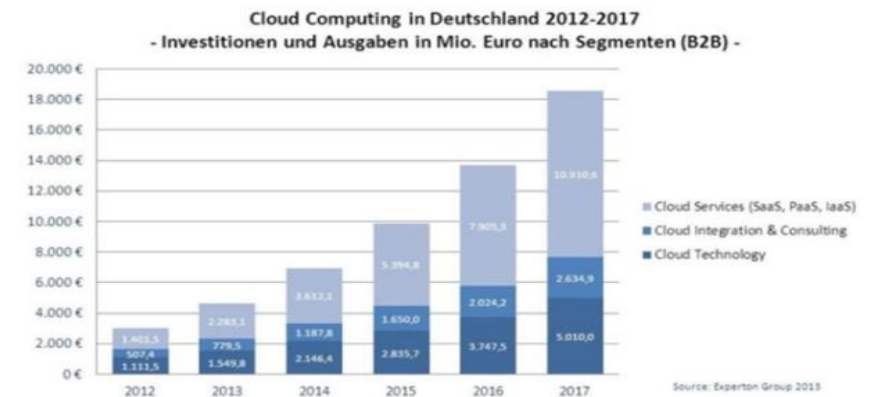
# SaaS – Software as a Service

## SaaS Market Growth for Enterprise Applications



# Key HPC Cloud Market Drivers

- + Enterprise use of cloud drives R&D use of Cloud
- + Engineers' growing **awareness** about **benefits**
- + Engineers' experience with **consumer** cloud = "work imitates life" \*)
- + The large guys\*\*) expect **suppliers** to do better, faster, cheaper



\*) CDW 2013 State of the Cloud Report

\*\*) The "Boeings"



# Key HPC cloud market drivers



ISVs are moving to the cloud



Massive Online Open Courses  
are sitting in the cloud



Big Data analytics needs  
massive computing

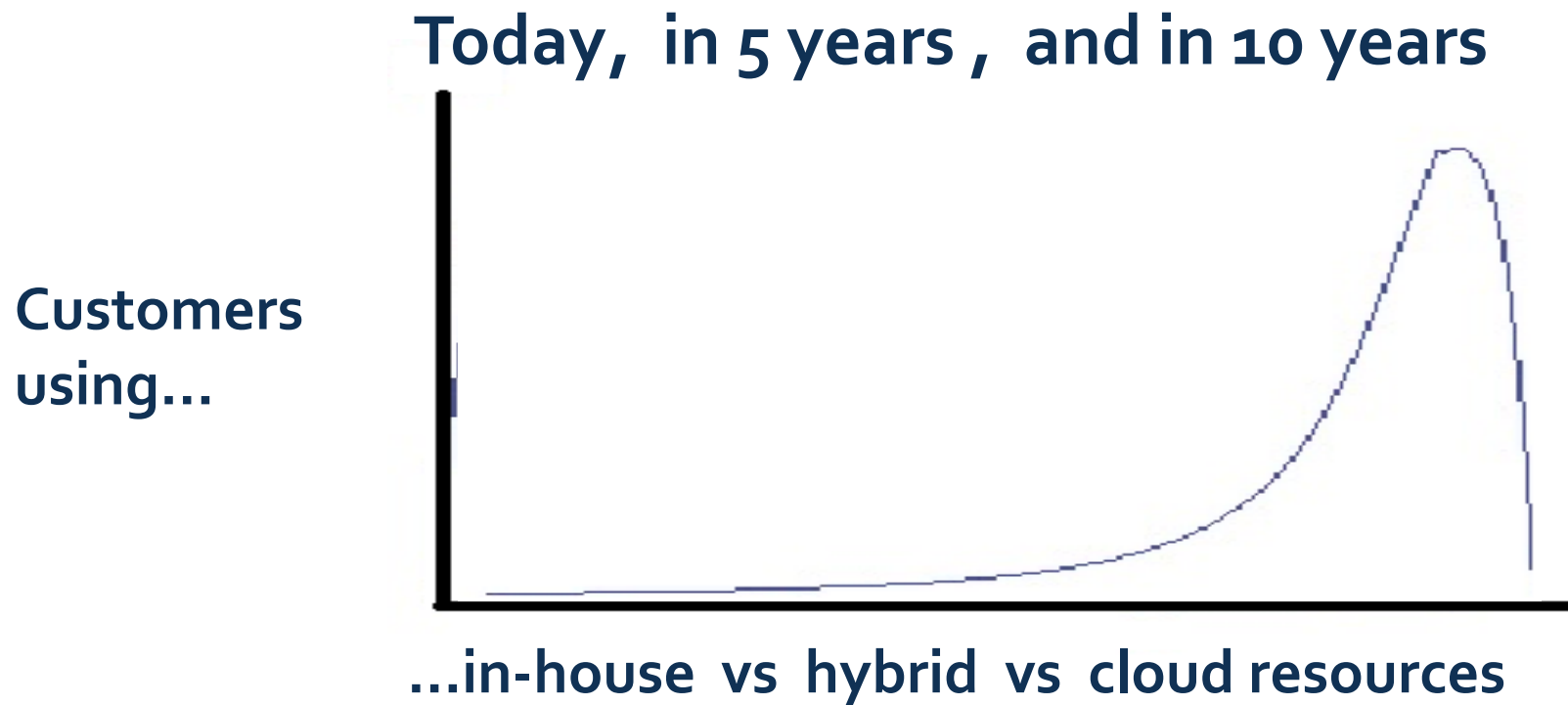
30 mio 'makers'



Our digital natives 'live'  
in the cloud



# Adoption of Cloud Computing \*)



\*) For engineering and scientific applications

# Challenges to move to the HPC Cloud

- + **The end-user:** engineers & scientists are reluctant to use cloud
- + **The software provider:** concern to disrupt their traditional licensing model
- + **The cloud resource provider:** HPC apps are architecture dependent
- + **The HPC market:** 16 verticals with very different requirements
- + **Roadblocks: real:** data transfer, licensing, no standards, cloud access, cloud lock-in/portability, losing control
- + **Roadblocks: perceived:** security, compliance, cost, cloud expertise
- + **Solution: HPC Containers**



# Security

## + Information security, privacy:

- + protecting the users intellectual property
- + guarding raw data (physics, geometry, results)

## + Recommendation:

- + document your security requirements
- + select a suitable provider
- + Encryption, VPN, dedicated cloud server, TRUST, etc.

## + Comment:

- + Security in the cloud is at the same standard level as any other IT infrastructure. It's more a mental issue.

# Data Transfer

- + **Internet too slow for heavy data transfer:**

- + Often GBytes of results
- + Especially last mile problem

- + **Recommendation:**

- + Don't ship every byte, just important ones (VCollab)
- + Use remote visualization (NICE DCV)
- + if necessary, fedex the data over-night

- + **Comment:**

- + Clouds can't solve your last mile problem

# Cloud Cost

## + **Cost of Cloud is often hidden:**

- + Server versus Cloud cost is often unclear
- + pay-per-use billing can result in unpredictable cost
- + project can easily run out of budget

## + **Recommendation:**

- + Cost estimation upfront (UberCloud paper [www..../cost](http://www.theubercloud.com/cost) \*)
- + Automated, policy driven monitoring of usage & billing

## + **Comment:**

- + Replacement and bursting are 2 different questions

\*) <https://www.TheUberCloud.com/cost/>

# Software licensing

## + Incompatible software licensing models:

- + ISVs often stick to their annual, perpetual licensing

## + Recommendation:

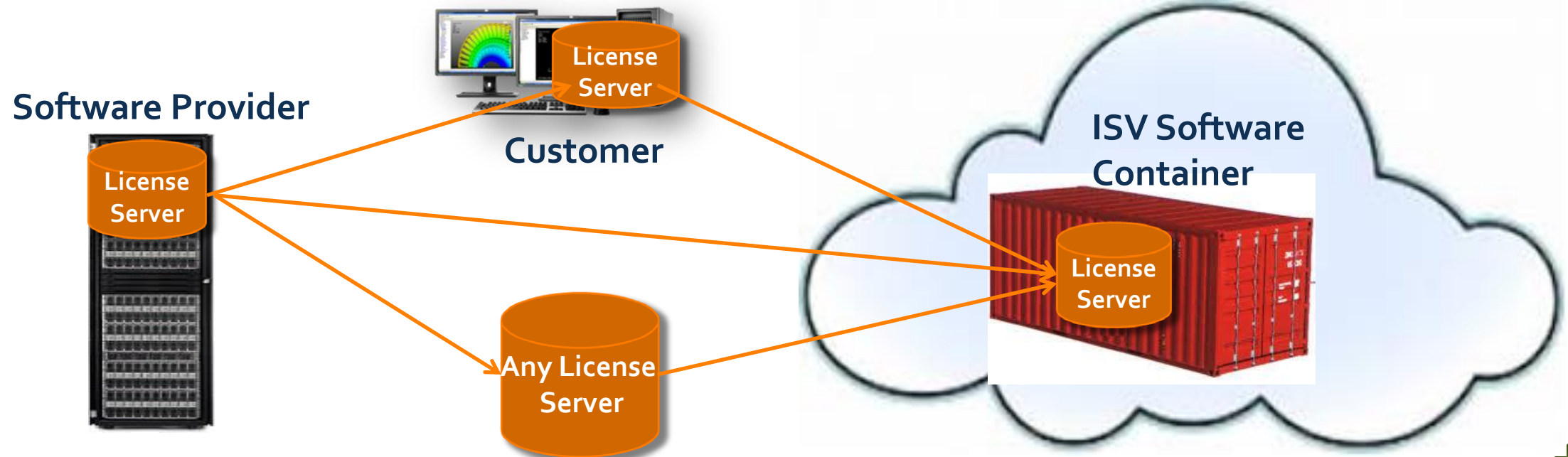
- + Check CAE software stack on UberCloud Marketplace
- + Talk to your ISV
- + ISVs should develop on-demand or short-term software licensing

## + Comment:

- + Some ISVs have cloud licensing (CD-adapco, COMSOL, ANSYS coming soon,...)
- + Many ISVs are developing cloud licensing
- + Engineers need **pay-per-project** (week, month)

# How does UberCloud resolve software licensing issue

- + 200+ experiments led to an excellent network of ISV relationships with 120+ ISVs
- + Solution: UberCloud including a license server into every container



## UberCloud Marketplace

Ready for Computing as a Service, for your professional engineering and scientific simulation projects? Need software licenses, computing resources, storage capacity and expert consulting, packaged into one solution stack, available at your fingertips? The UberCloud Marketplace is your one-stop shopping mall to get access to these resources, on-demand, when you need them. And, stay tuned, currently we are working on opening 20+ more marketplace stores; and one could be yours.



### Software Providers:

#### ANSYS

ANSYS has pioneered the development and application of simulation methods to solve the most challenging engineering problems. [Show 4 products](#)

#### ANSYS on OzenCloud

Ozen Engineering - the ANSYS Partner & Distributor in California - provides software, training, technical support and consulting services. [Show 4 products](#)

#### Autodesk

A360 project collaboration software helps design, engineering, and project teams work together efficiently on a centralized platform. [Show 3 products](#)

#### CADFEM

The CADFEM Engineering Simulation Cloud provides an easily accessible high-performance CAE environment for ANSYS Workbench. [Show 8 products](#)

#### CAE Fidesys

CAE Fidesys is an easy-to-use and effective next-generation CAE tool for performing a full cycle of engineering-strength analysis. [Show 9 products](#)

#### CD-adapco

STAR-CCM+ is an entirely integrated engineering process for solving problems involving flow (of fluids or solids), heat transfer and stress. [Show 5 products](#)

#### COMSOL - Coming Soon

COMSOL is the developer of COMSOL Multiphysics, an interactive environment for engineering & scientific modeling and simulation. [Show 2 products](#)

#### CST - Computer Simulation Technology

CST offers accurate, efficient computational solutions for 3D electromagnetic design & analysis, operating in a wide range of frequencies. [Show 8 products](#)

#### DYNAmore - Coming Soon

Dynamore supports engineers to solve non-linear mechanical problems with FE solver LS-DYNA and LS-OPT for optimization. [Show 2 products](#)

#### ESI OpenFOAM - Demo Store

World-leading provider in Virtual Product Engineering, leveraging the physics of materials and eliminating the need for physical prototypes. [Show 3 products](#)

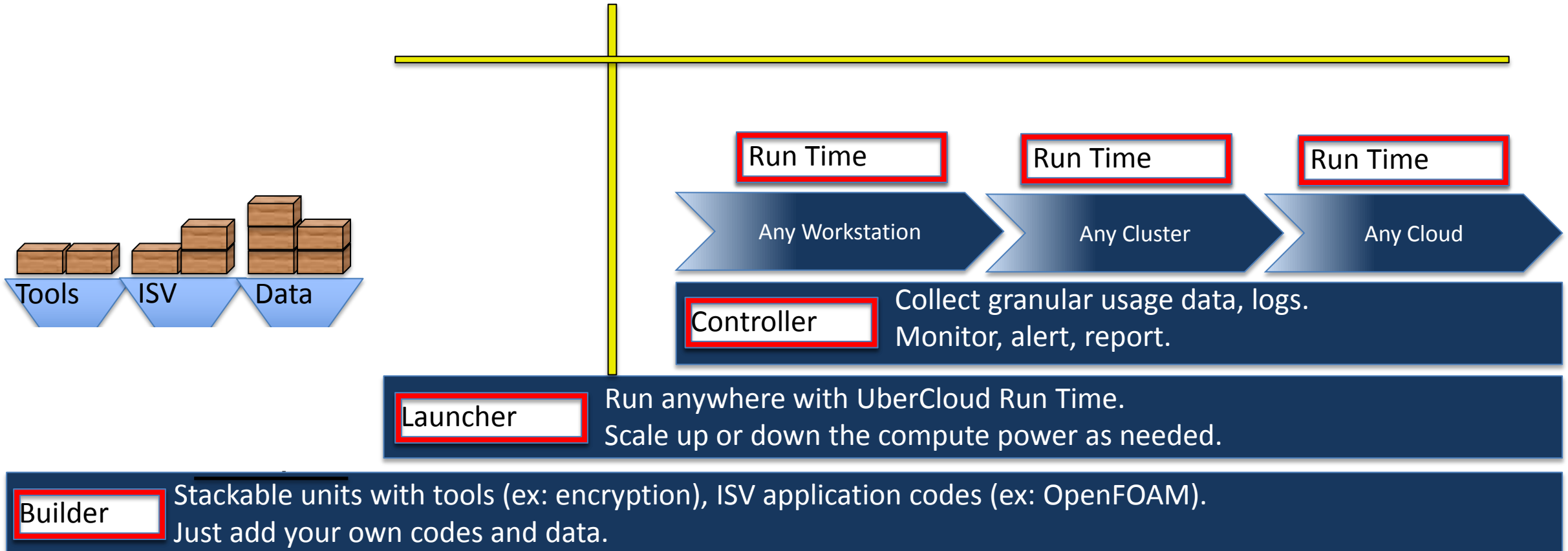




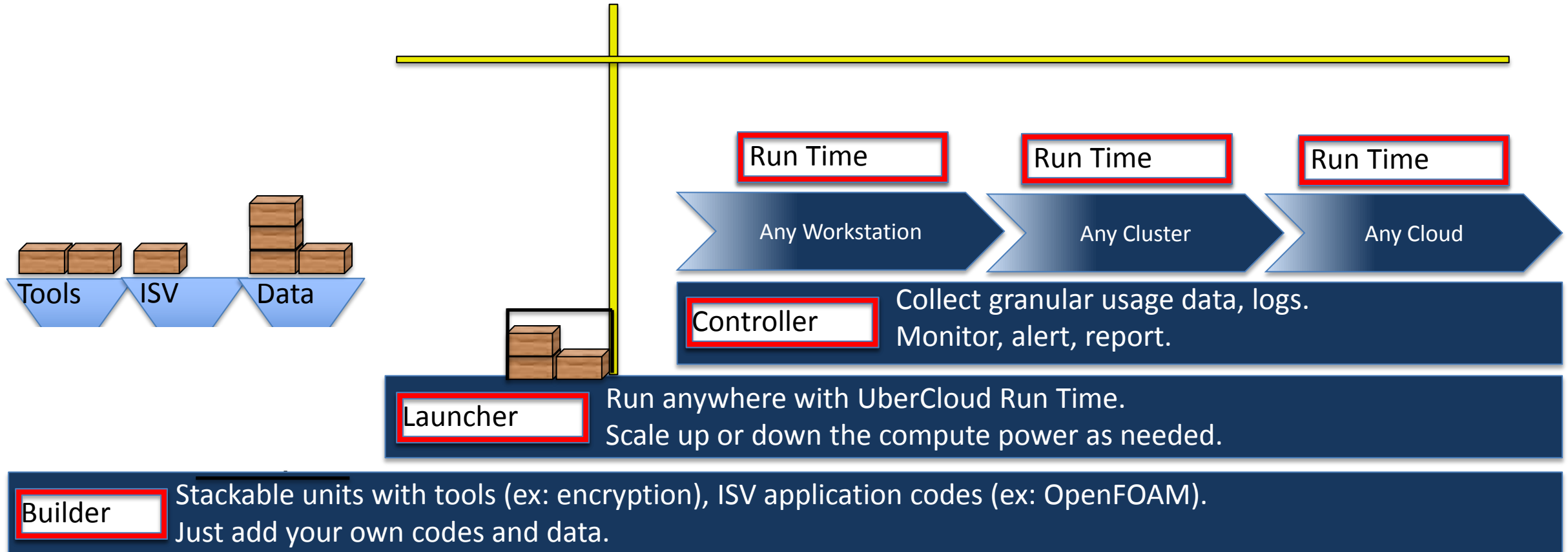
# UberCloud application containers

- + Based on Docker, enhanced for engineering & scientific applications
- + Software packages designed to deliver the tools that an engineer needs
- + Ready to execute, in an instant. No need to install software, deal with complex OS commands, or configure.
- + Software is pre-installed, configured, and tested, and running on bare metal, without loss of performance.
- + ANSYS, CD-adapco, Numeca, OpenFOAM, Gromacs, Scilab, and more

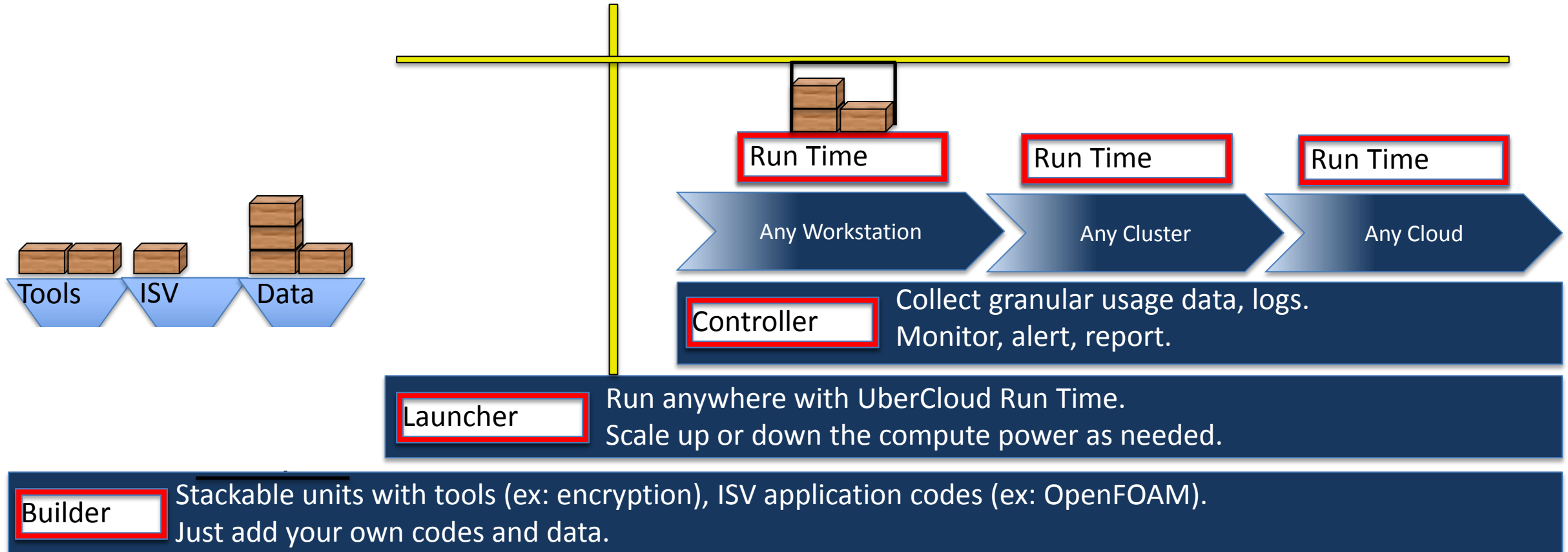
# Containers: Build once, run anywhere



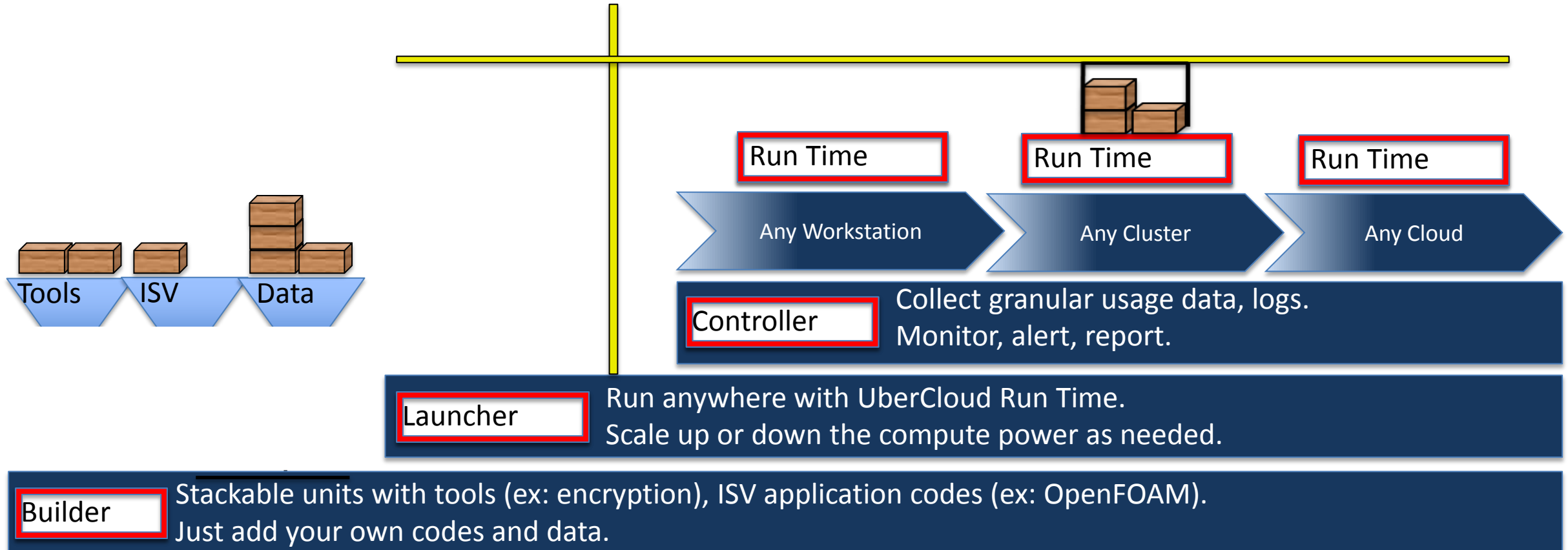
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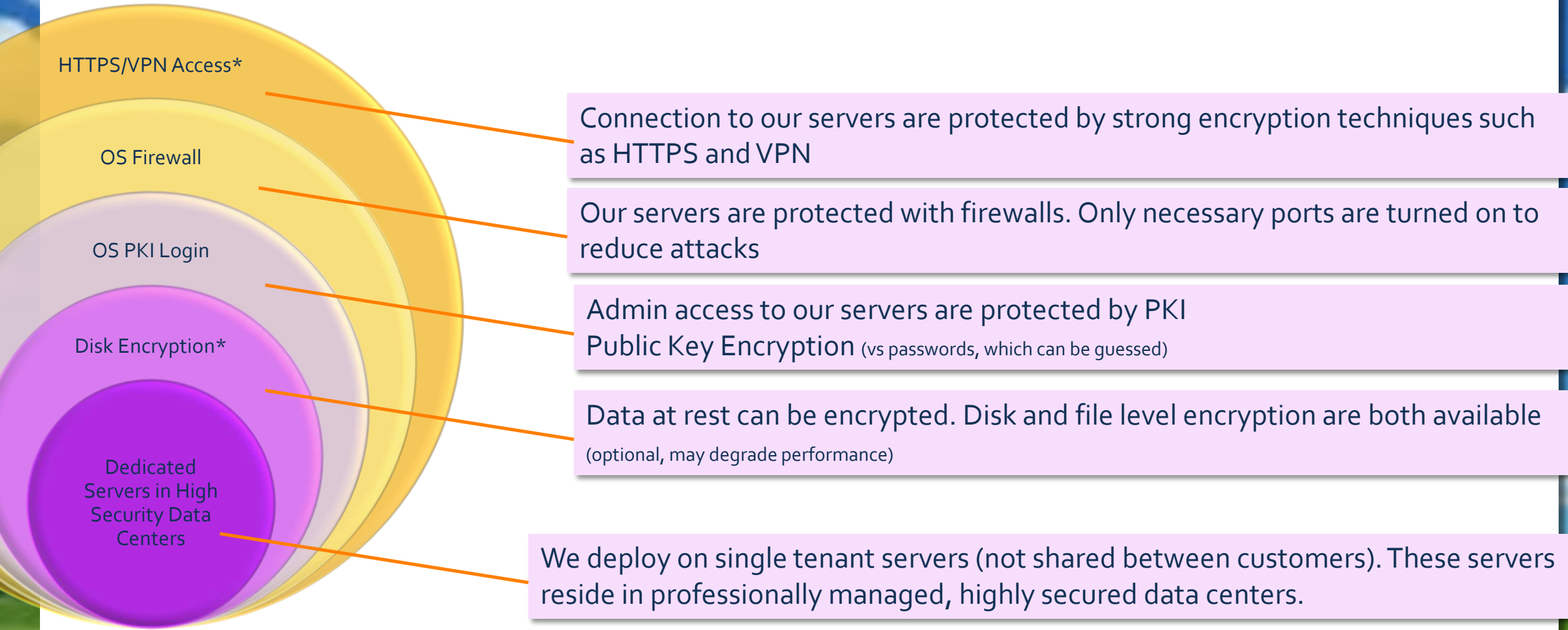
Containers remove Portability & Standard related challenges.  
By integrating 3<sup>rd</sup> party tools we tackle the following:

CAE Cloud Challenges	UberCloud
Security	√
Portability	√
Compliance	√
Data Transfer	√
Standardization	√
Software Licenses	√
Resource Availability	√
Transparency of Market	√
Cost & ROI Transparency	√
No Cloud Expertise Needed	√



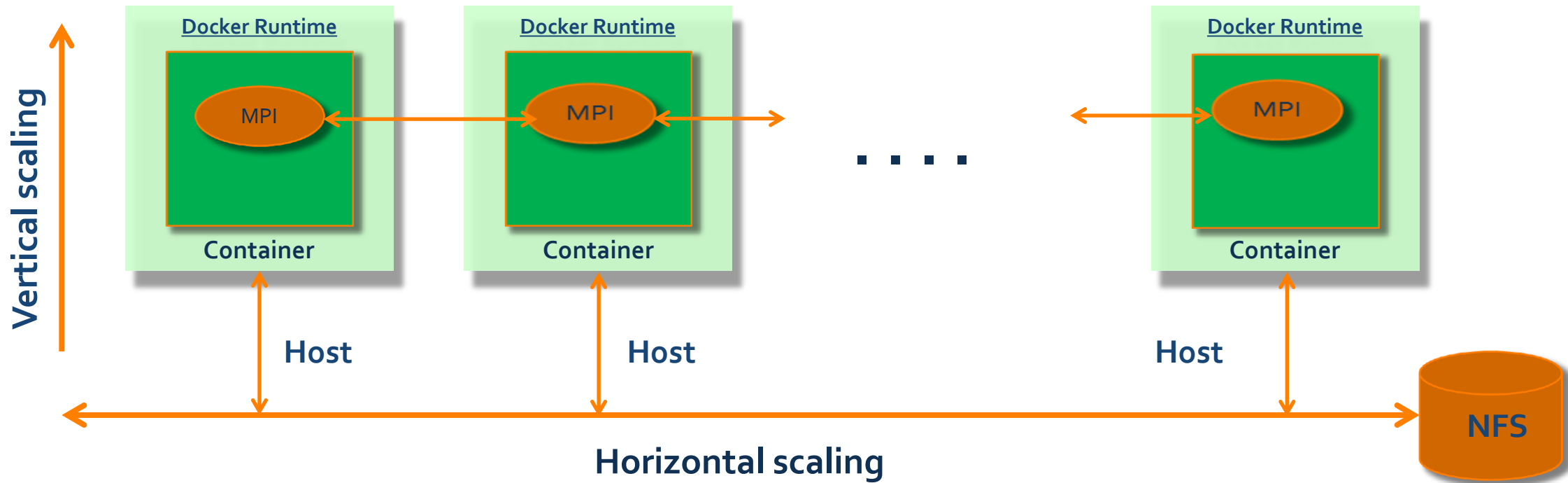


# UberCloud Security Layers



\* HTTPS/VPN access and Disk Encryption are optional

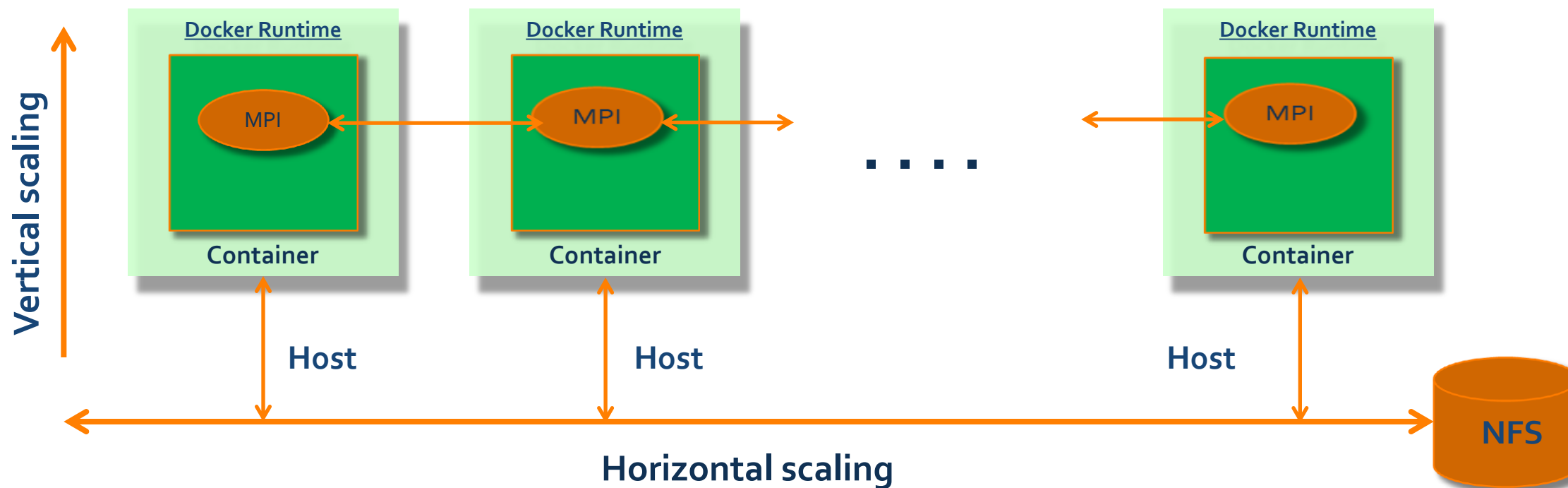
# UberCloud multi-container environment



Dramatically simplifying



# UberCloud multi-container environment



**Packaging, Porting, Access, Use, Scaling, with Low Overhead**



# OpenFOAM Test: Bare Metal vs Docker

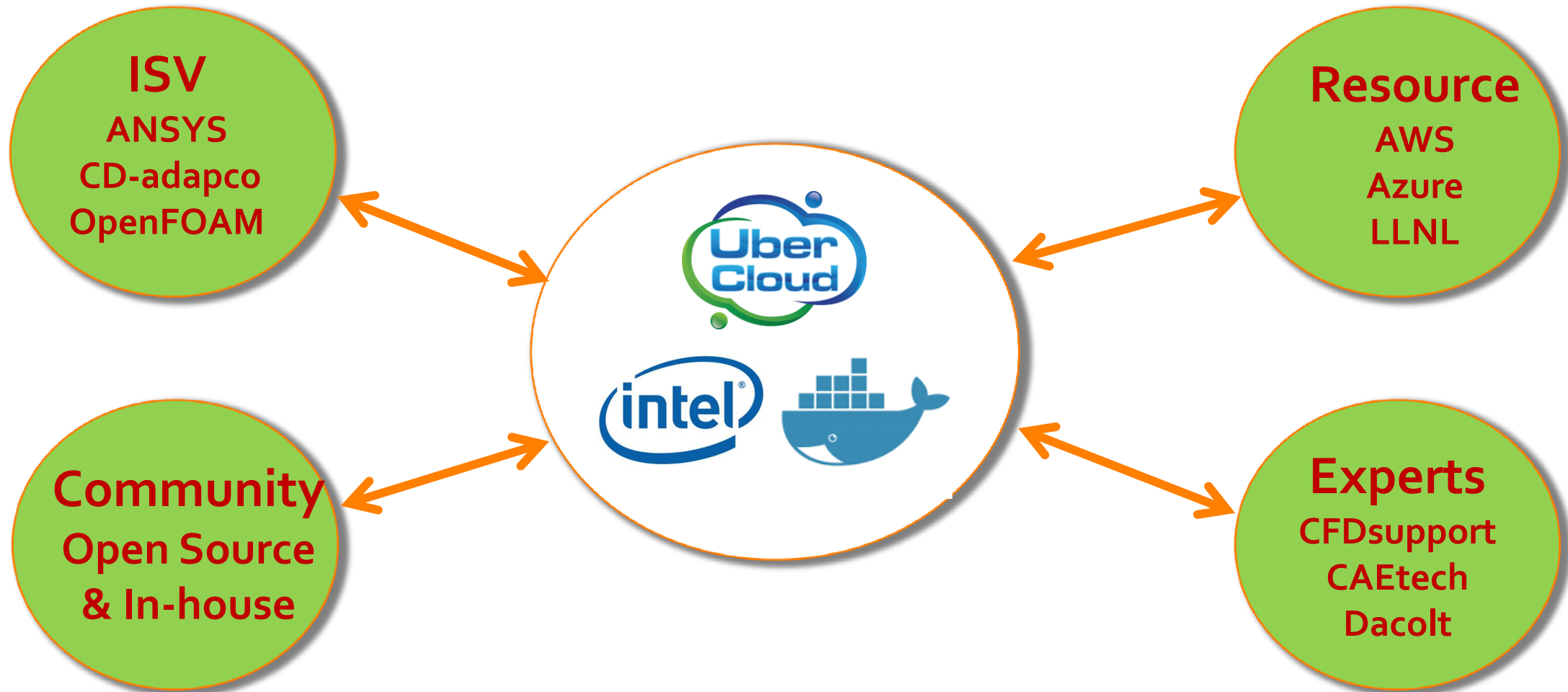
**Simple Average of the 3 runs and comparison between Bare Metal and Container**

	<b>Serial (1 Host x 1 CPU) = 1 Core Total</b>	<b>1 Host Parallel (4 Host x 1 CPU) = 4 Core Total</b>	<b>2 Host Parallel (2 Host x 2 CPU) = 4 Core total</b>
Bare Metal	10,847	2,040	1,842
Container	10,869	1,851	1,852
<b>Overhead</b>	<b>0.20%</b>	<b>-9.30%</b>	<b>0.51%</b>

OpenFOAM with 1.4 million cells on bare metal and in UberCloud Docker container



# Dockerized Technical Computing Ecosystem





# UberCloud multi-container environment

- + Intel MPI libraries pre-setup for multi-node high performance
- + Intel compilers achieve architecture specific high performance
- + Networking between containers
- + Setting up shared file system access (NFS)
- + Secure communication (ssh) between containers
- + Benefits from single-node transferred to multi-node containers:
  - + No setup of the environment
  - + Portability and packaging
  - + Easy access and use
  - + Low overhead



+





# UberCloud Containers – The last 9 months

- + DCV in container for Remote Desktop with HD quality
- + Encrypted connections for data transmissions
- + OpenHPC compatible
- + Resource Manager capabilities for complex, multi-host deployments
- + Multi-host networking over low latency networking stacks (IB and RDMA)
- + Support for multiple OS distributions
- + Support for multiple MPI distributions
- + Dozens of ISV codes supported
- + Complex workflows such as optimization supported
- + Integrated into Cloud Marketplaces like Azure

# At last Docker Workshop: Demo

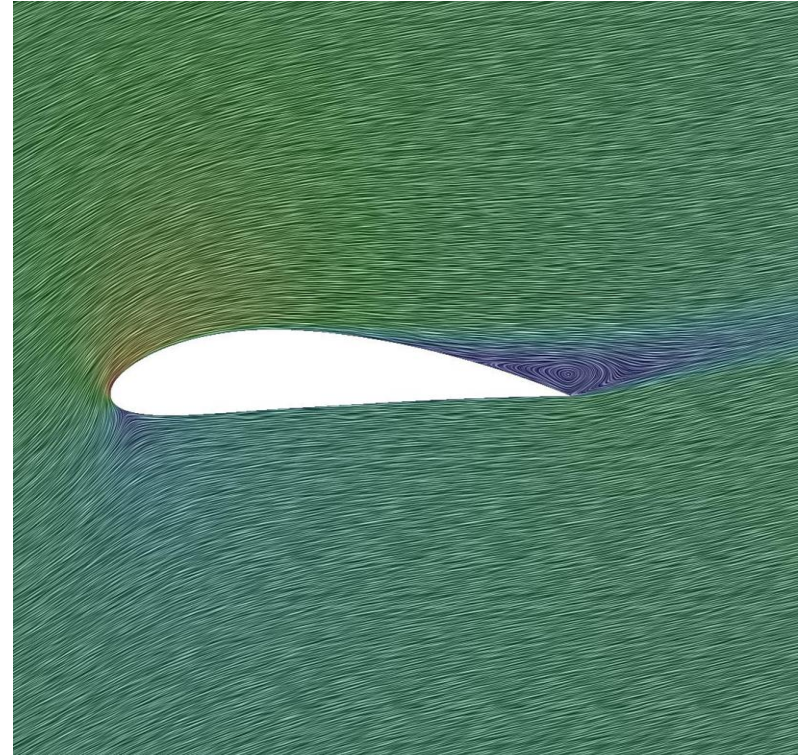
## Taking an OpenFOAM Application to the Cloud

We won't repeat it here



# What do we do now?

Connect to the cloud  
Run OpenFOAM  
*NACA4412*



# 1. Get the Internet connection to your container

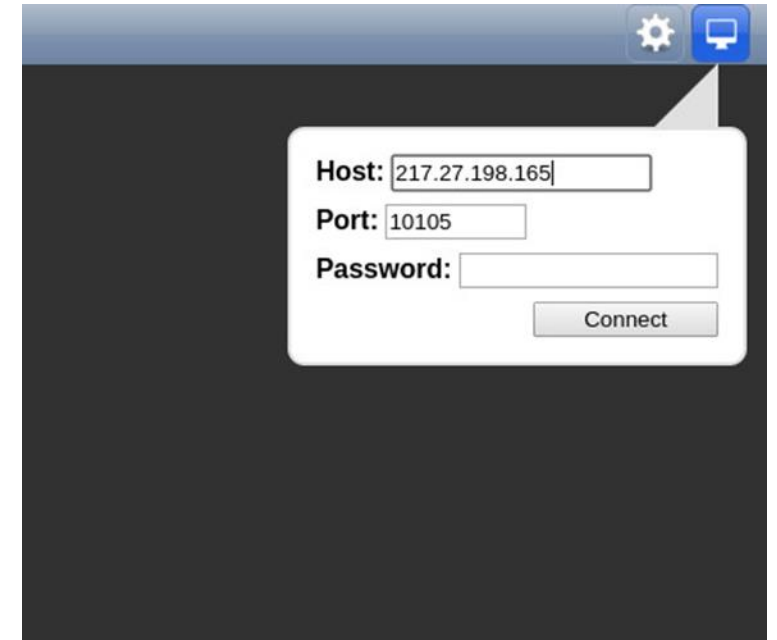
Wifi

Open your web browser

Container URL:

<http://217.27.198.165:10201/vnc.html>

Password: 1l258ZqG....



HPC ON DEMAND



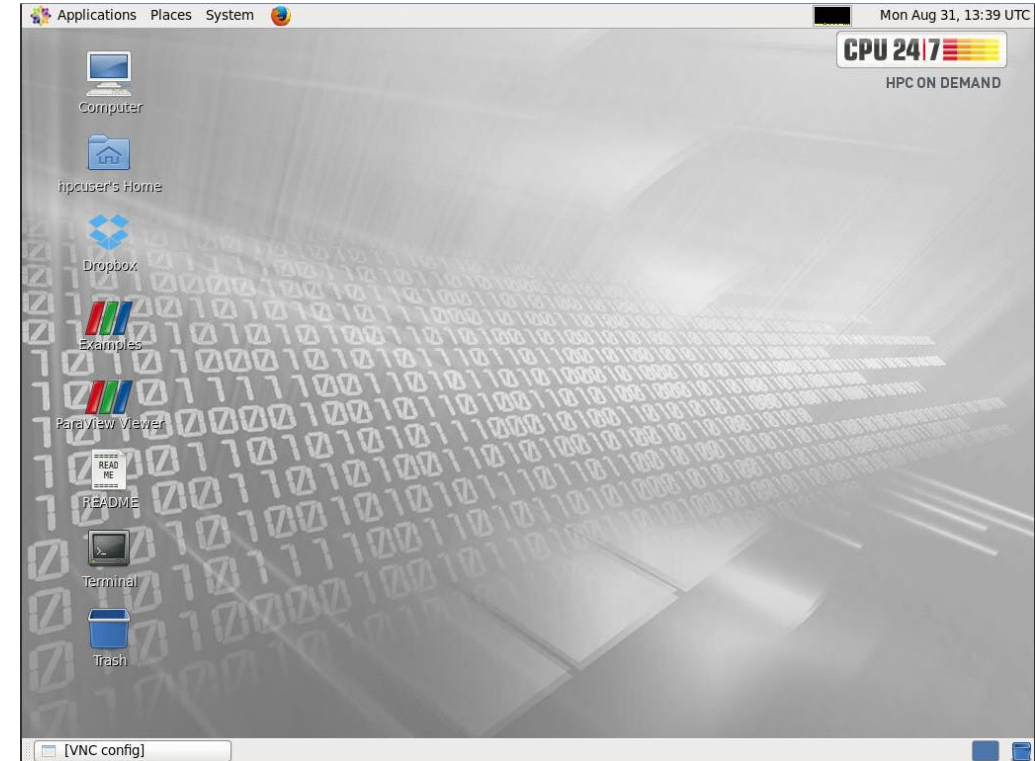
## 2. Run the NACA case & play around

Open Terminal

In the NACA4412 directory run:

\$

\$ ./Allrun &



### 3. Useful commands

midnight commander: `$ mc`

text editor: `$ gedit`

what processes are running?: `$ top`

plot convergence: `$ gnuplot residuals.gp`

`$ gnuplot probesP.gp`

`$ gnuplot plotFinalResults.gp`

view results in ParaView: `$ paraFoam`







# Thank You !

Please register at

<http://www.TheUberCloud.com>

It's free