VIRTUAL OPEN SCIENCE
COLLABORATION ENVIRONMENT

ViCE:
From desktop to cloud or HPC – Virtualized Research Environments

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Structure of the talk

- Virtualization – paradigm shift for researchers and university computer centers
- Motivation: Virtualized teaching and learning environments for computer pools / desktop virtualization
- HPC, bwCloud and hybrid cluster operations
- Virtual Research Environments and how to create them
- Outlook

Challenges of CC operations

- Today‘s challenges of computer centers
  - Very diverse scientific communities and broad set of software, tool demands
  - Different, contradicting demands regarding software environments
  - Short notice demands for hardware to be used at least for five years (but often for much shorter projects)
  - Personnel to operate all the (small, diverse) hardware servers expensive
  - Most resources underutilized most of the time; Save on money and hardware resources
  - Save on rackspace, power and cooling – computer centers generate significant energy bills

eScience and CC operations

- History of applied CC operations research by the attached professorship and the eScience dept.
- Where it began:

  → *Optimize operation of computer pools*

  - Very diverse user base requiring very different software environments for different courses: Lecturers, students
  - No real common denominator
    - Windows OS for „standard“ software packages like text processing, spreadsheets or interactive statistics, web publishing, …
    - Linux OS for software development, many open source packages like R, GIS, ...
  - Very different ideas on how even a common software base should be configured (modules, examples installed or not, preconfiguration of packages, …)

Pre-Virt: Make everyone unhappy

- Lecturers expect the computer center to comply to their expectations on installed software
  - Should be available in 20 minutes time (when the course starts) on 20+ machines
  - Works for me, should work in the PC pools too (where is the problem??)
  - Install some evaluation software which is only valid for 20 days (even a month would be to short for decent planning)
  - Why didn‘t you install the exhaustive example collection?
  - Why did you changed/updated the software base; when it was fine in my last course!?
- Traditional software deployment doesn‘t work that way
- Not all software and versions easily live together in a single installation

Pre-Virt: Make everyone unhappy

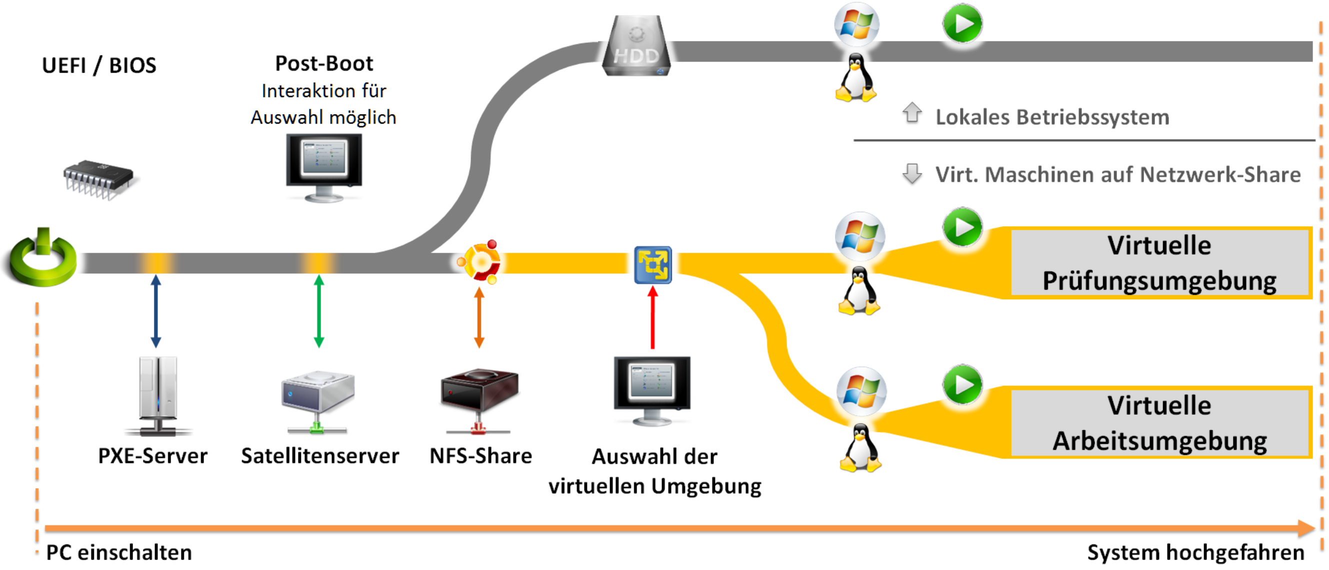
- Pool admins annoyed by ever changing expectations of different lecturers
  - Often not available in the right time
  - PC pools never free during normal working hours or at least not long enough for proper software roll-out and testing
- Utilization of computer pools suboptimal
  - Software environment for the morning course might significantly differ from the one for afternoon and evening again and again for the week to follow
  - Difficult to schedule courses to pools
  - Software installation in one pool is completely different to the one in the other (no option to change the room if a particular one not available)

Pre-Virt: Make everyone unhappy

- Students are unhappy not to find the software environment of the course they are attending
  - Might be only available in the pool booked by some other course
  - Might just got removed because of conflicting demands of some other course
- Tight hardware – software coupling introduces inflexibility in time and space
  - Inflexibility increases operational costs

Optimize operation of PC pools

- Virtualization comes into play: Break the tight link between software and hardware
- Developed a new form of Desktop virtualization
- Only PXE boot a Linux system on the PC (without the need of locally installed software at all)
- Even allows to maintain local installation


UEFI / BIOS
Post-Boot
Interaktion für Auswahl möglich
HDD
Lokales Betriebssystem
Virt. Maschinen auf Netzwerk-Share
Virtuelle Prüfungsumgebung
Virtuelle Arbeitsumgebung
PXE-Server
Satellitenserver
NFS-Share
Auswahl der virtuellen Umgebung
PC einschalten
System hochgefahren

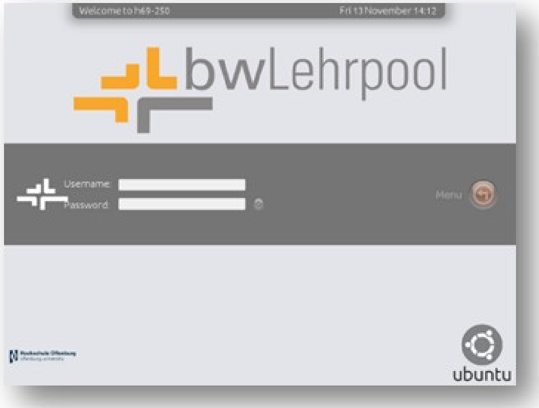
Optimize operation of PC pools

- Let the user choose from a wide selection of different environments (which are actually made available as images from a network share)
- Then configure a hypervisor (or container) to run selected environment
- Linux base system tries to handle all locally relevant stuff
  - Configuring of hardware including drivers
  - Authentication of users
  - Mounting home directory and further shares if desired
  - Provide printing services

→ Trying to avoid any site dependencies within the virtual teaching and learning environment

Selection of teaching environment

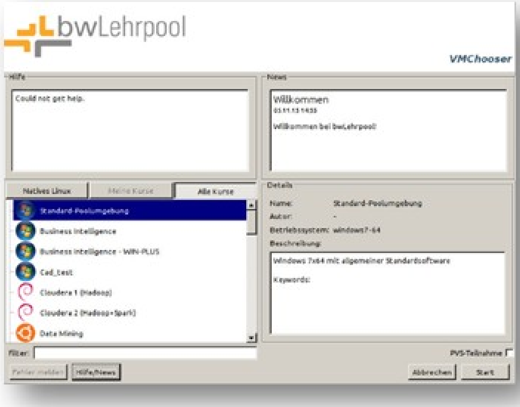
- Hypervisor runs locally on the PC with selected virtual environment
- Excellent for class rooms
- Change rapidly from Programming C in Linux to Desktop Publishing in Windows without „leftovers“



Username:
Password:

Loginmaske

Login



Could not get help.

Willkommen
03.11.15 14:55
Willkommen bei bwLehrpool!

- Standard-Poolumgebung
- Business Intelligence
- Business Intelligence - WIN-PLUS
- Cad_test
- Cloudera 1 (Hadoop)
- Cloudera 2 (Hadoop+Spark)
- Data Mining

Name: Standard-Poolumgebung
Autor: -
Betriebssystem: windows7-64
Beschreibung:
Windows 7x64 mit allgemeiner Standardsoftware

Keywords:

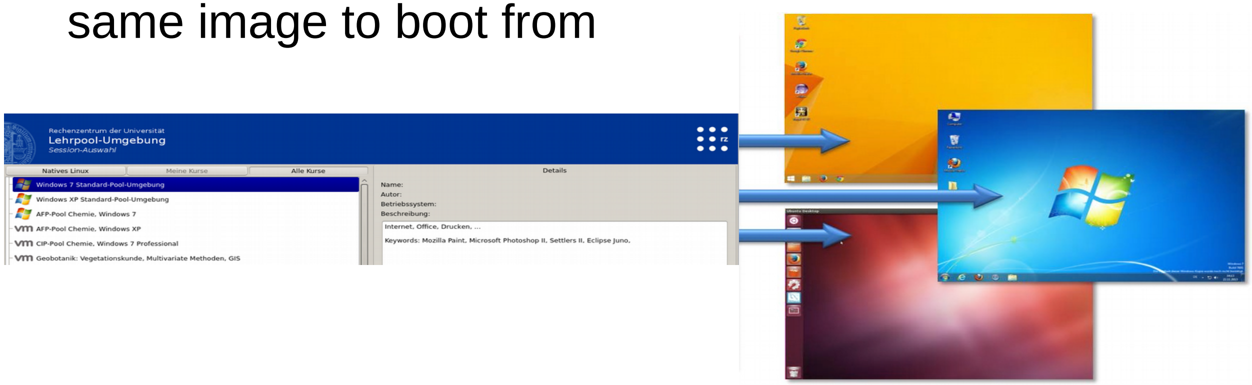
VMChooser

Auswahl

Virtuelle Maschine

bwLehrpool: Separation of tasks

- Administration of hardware is independent of the administration of the netbooted base Linux
- Software environment and configuration is absolutely up to the lecturer who wants to teach a certain course
  - No time and physical dependencies for installations
  - Lecturer receives just a base image and extends it to his/her needs
  - All booted systems are exactly the same as using the same image to boot from



Rechenzentrum der Universität
Lehrpool-Umgebung
Session-Auswahl

- Windows 7 Standard-Pool-Umgebung
- Windows XP Standard-Pool-Umgebung
- AFP-Pool Chemie, Windows 7
- AFP-Pool Chemie, Windows XP
- CIP-Pool Chemie, Windows 7 Professional
- Geobotanik: Vegetationskunde, Multivariate Methoden, GIS

Details

Name:
Autor:
Betriebssystem:
Beschreibung:

Internet, Office, Drucken, ...

Keywords: Mozilla Paint, Microsoft Photoshop II, Settlers II, Eclipse Juno,

New ways of cooperation & application

- Courses / images of virtual teaching and learning environments could get exchanged statewide offering cooperation between different entities
- Next step: community provided environments e.g. created by students of a certain semester or faculty

- Successful model of task separation between users, lecturers and computer centers
- Plus: Adding to the drive in resource virtualization

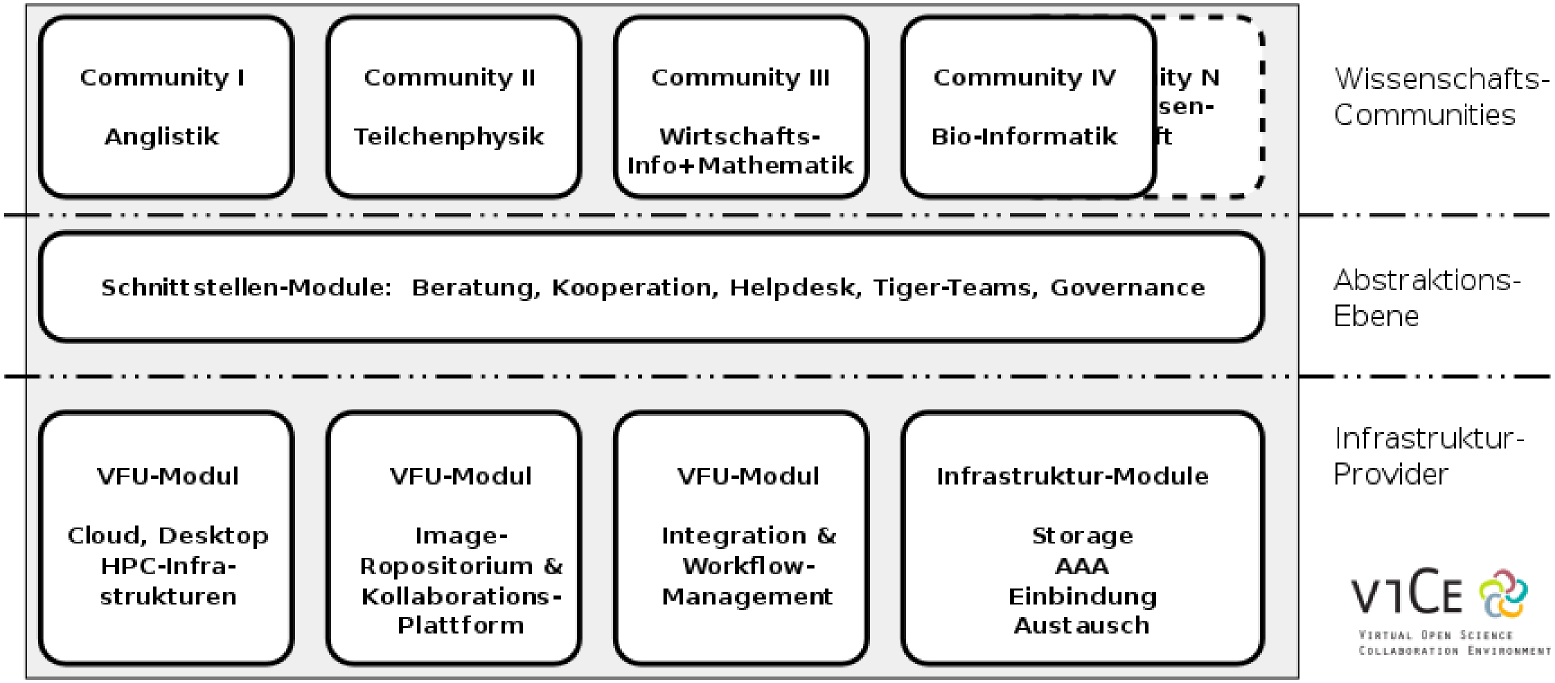
→ Concept established – now widen it‘s application to further domains

Virtual science – how far we got?

- Challenge: convince science that virtualization approach is beneficial
  - If only for convenience and reliability of results
- Virtual(ized) research environments (VRE) for various scientific communities
  - Build virtual machines which suit a whole discipline → at least for their research interest
  - Bio-informatics: virtual Galaxy workflow engine
  - Long term usage and reproducibility
  - Long term archive (create some kind of “electronic lab book” as a side effect)
  - Right from the outset
- CERN already uses „standard virtual machines“
  - Some disciplines are on the right track

Bridging worlds

- ViCE – state sponsored cooperation project of multiple disciplines and computer centers
- Separate infrastructure / provider from core scientific tasks



Community I
Anglistik

Community II
Teilchenphysik

Community III
Wirtschafts-
Info+Mathematik

Community IV
Bio-Informatik

ity N
sen-
ft

Wissenschafts-
Communities

Schnittstellen-Module: Beratung, Kooperation, Helpdesk, Tiger-Teams, Governance

Abstraktions-
Ebene

VFU-Modul
Cloud, Desktop
HPC-Infra-
strukturen

VFU-Modul
Image-
Ropositorium &
Kollaborations-
Plattform

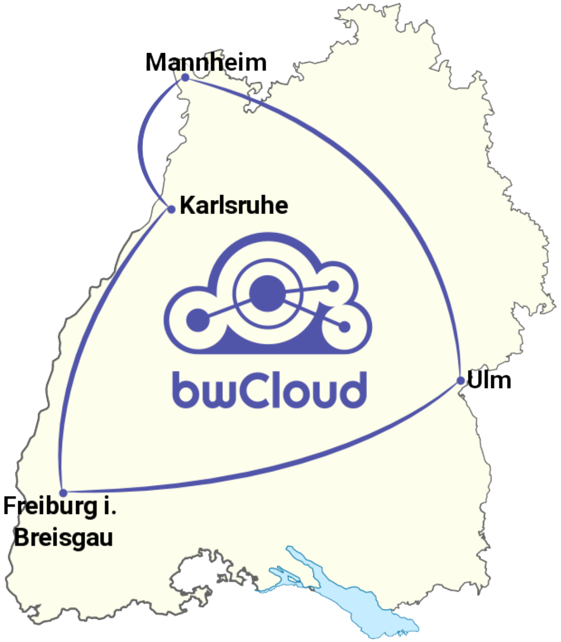
VFU-Modul
Integration &
Workflow-
Management

Infrastruktur-Module
Storage
AAA
Einbindung
Austausch

Infrastruktur-
Provider

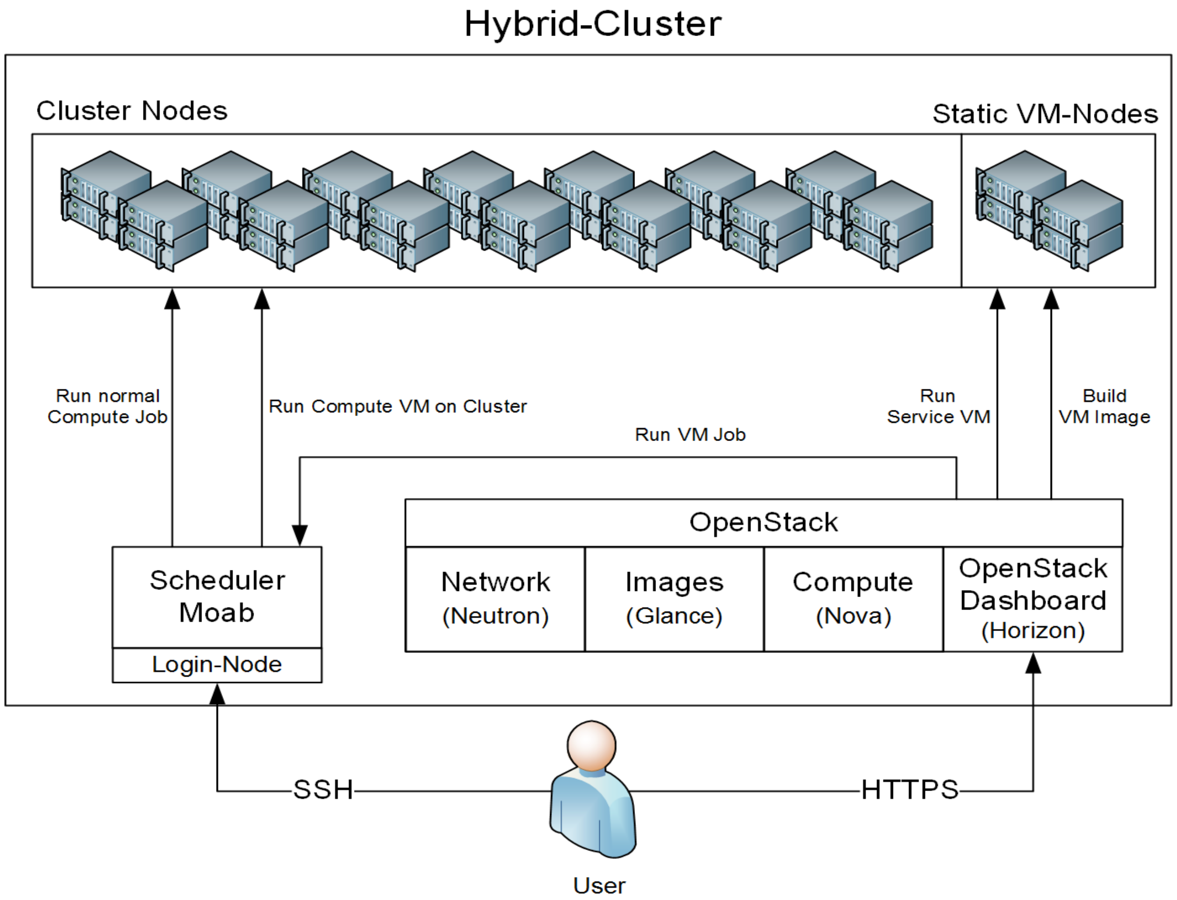
Research infrastructures

- bwCloud and NEMO significant compute infrastructures in Freiburg well above 1000 nodes in a flexible boot and deployment environment
- Both state wide cooperation of university computer centers in various constellations



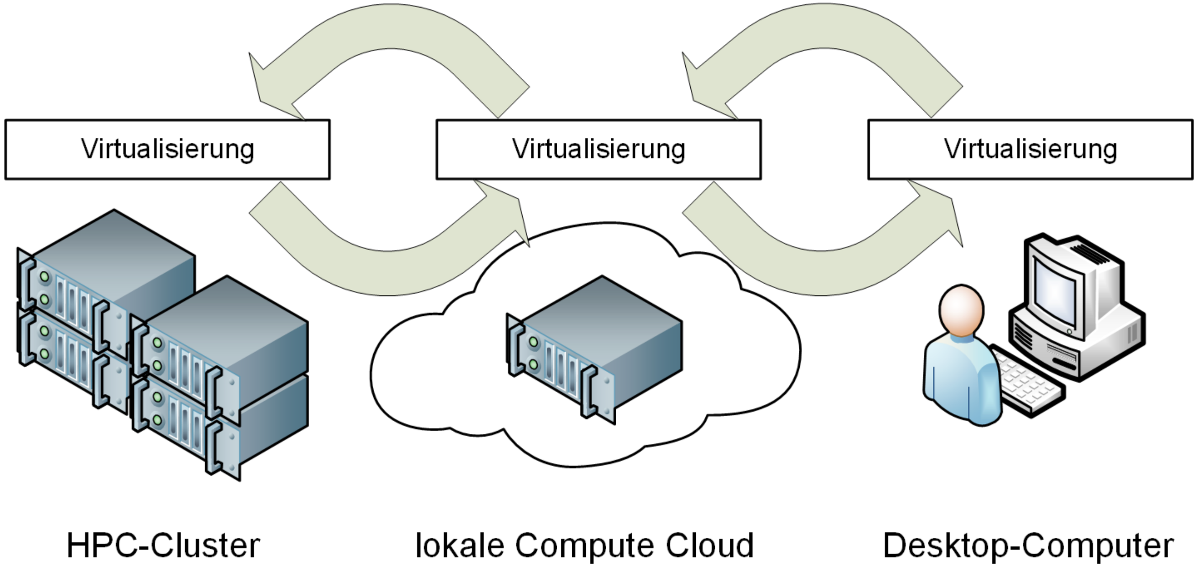
HPC and virtualization and cloud

- Same hardware, different usecases: Create flexibility by abstracting hardware and software (again)



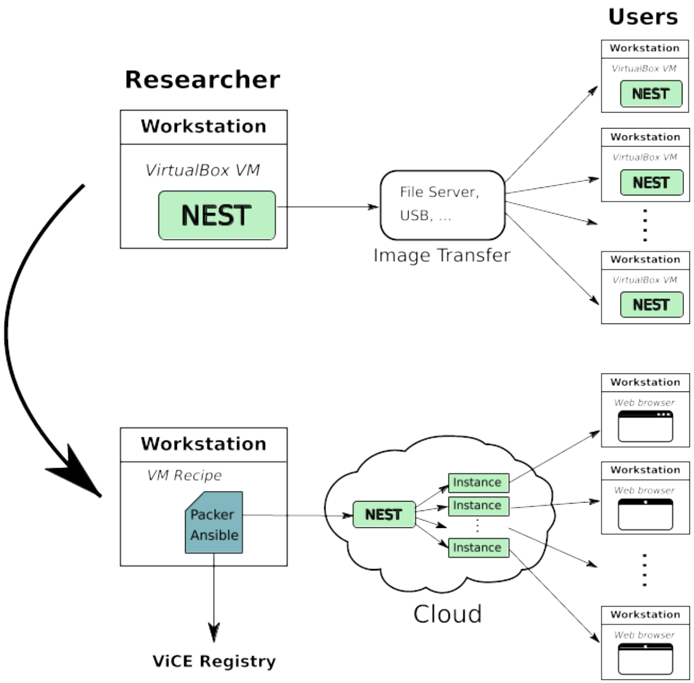
HPC and virtualization

- Optimally: Allow flexibility over the different domains
  - Start to create and test a scientific workflow interactively on your desktop
  - Move it into the cloud in long running and not dependent on massive resources
  - Move it to the cluster if larger resources required or massive parallelization possible



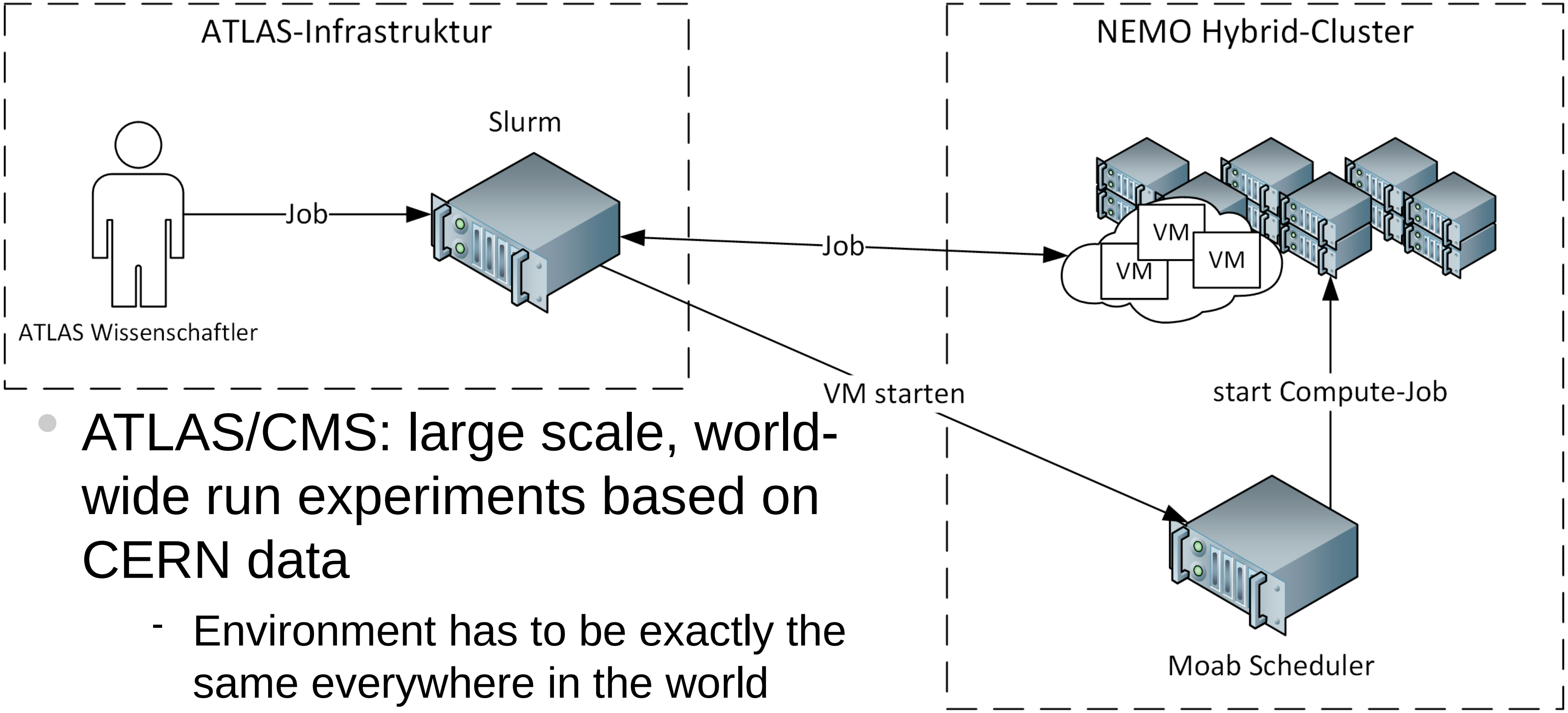
Usecases explored in ViCE

- Bioinformatics: Galaxy workflows in VMs and containers
- Computer linguistic and English language studies – provide a state-wide common environment for teaching, learning and research



- Microsystems technology: Remote visualization to view large data sets (without copying them; ongoing experiments)
- Economics: Dealing with large scale data and researching into secure environments
- Neuroscience: From fast setup of interactive course environment to non-interactive use in HPC

Usecases in Particle Physics



Phd thesis of K. Meier

- ATLAS/CMS: large scale, world-wide run experiments based on CERN data
  - Environment has to be exactly the same everywhere in the world
  - Software updates are slow because of exhaustive regression tests
  - Software environment can not easily be reproduced directly on the NEMO cluster

HPC and virtualization

- Additional benefits: VREs could get suspended and resumed (to be operationalized though)
- Plenty of new options for scheduling / to improve scheduling
  - Offer long running jobs on a cluster with a standard 4 days walltime
  - Suspend (expensive, because of long running) jobs before cluster maintanance
  - Create a „fast lane“ and let certain jobs overtaking long running ones (which otherwise would clog the cluster)

Steps to define VREs

- Depends on the scientific application and scaling factor (e.g. desktop interactive vs. massively parallel)
- Audience: per scientist, per scientific workgroup or even per scientific field
- Options of authentication depend on the actual users to log-on to the machine, if any
- Resources for scientific workflows might differ significantly for e.g. grid systems, resource brokers, portals, knowledge systems or (large) data collections
- Technical environment: The origin technical platforms may include desktop, cloud or HPC resources

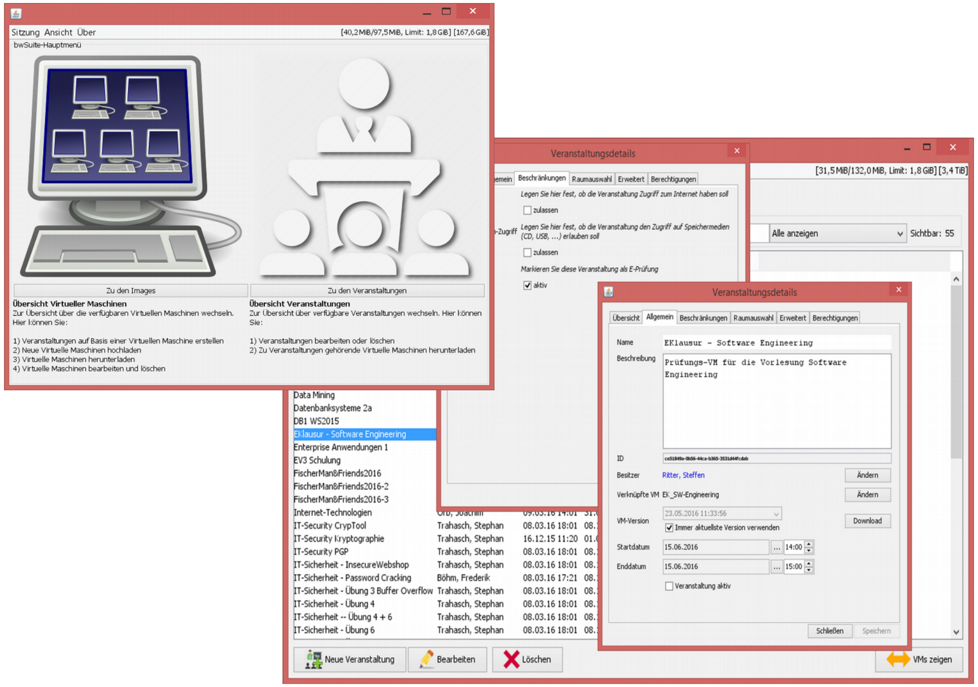
Steps to define & create VREs

- External dependencies of filesystems, identity management systems or if required of license servers
- How to deal, manage, describe and provide access to large collections of VRE (versions)

- Planning of setup and maintenance: Optimally, instances can be created by automatic procedures like *Packer*, *Ansible* and alike or cloned from templates
- Long running VREs might require updates and older versions need to be stored for reproducibility

Manage VREs

- Primarily: Interactive tool to manage Vms/VREs in bwLehrpool
- Additionally: Created a prototypical ViCE registry which can exchange meta data with bwCloud/OpenStack and bwLehrpool



Sitzung Ansicht Über [40,2MiB/97,5MiB, Limit: 1,8GiB] [167,6GiB]

bwSuite-Hauptmenü

Zu den Images

Übersicht Virtueller Maschinen
Zur Übersicht über die verfügbaren Virtuellen Maschinen wechseln. Hier können Sie:

1) Veranstaltungen auf Basis einer Virtuellen Maschine erstellen
2) Neue Virtuelle Maschinen hochladen
3) Virtuelle Maschinen herunterladen
4) Virtuelle Maschinen bearbeiten und löschen

Zu den Veranstaltungen

Übersicht Veranstaltungen
Zur Übersicht über verfügbare Veranstaltungen wechseln. Hier können Sie:

1) Veranstaltungen bearbeiten oder löschen
2) Zu Veranstaltungen gehörende Virtuelle Maschinen herunterladen

Veranstaltungsdetails

Beschränkungen | Raumauswahl | Erweitert | Berechtigungen

Legen Sie hier fest, ob die Veranstaltung Zugriff zum Internet haben soll
☐ zulassen

-Zugriff Legen Sie hier fest, ob die Veranstaltung den Zugriff auf Speichermedien (CD, USB, ...) erlauben soll
☐ zulassen

Markieren Sie diese Veranstaltung als E-Prüfung
☑ aktiv

[31,5MiB/132,0MiB, Limit: 1,8GiB] [3,4TiB]

Alle anzeigen Sichtbar: 55

Data Mining			
Datenbanksysteme 2a			
DB1 WS2015			
EKlausur - Software Engineering			
Enterprise Anwendungen 1			
EV3 Schulung			
FischerMan&Friends2016			
FischerMan&Friends2016-2			
FischerMan&Friends2016-3			
Internet-Technologien	Orb, Joachim	09.03.16 14:01	31.
IT-Security CrypTool	Trahasch, Stephan	08.03.16 18:01	08.
IT-Security Kryptographie	Trahasch, Stephan	16.12.15 11:20	01.
IT-Security PGP	Trahasch, Stephan	08.03.16 18:01	08.
IT-Sicherheit - InsecureWebshop	Trahasch, Stephan	08.03.16 18:01	08.
IT-Sicherheit - Password Cracking	Böhm, Frederik	08.03.16 17:21	08.
IT-Sicherheit - Übung 3 Buffer Overflow	Trahasch, Stephan	08.03.16 18:01	08.
IT-Sicherheit - Übung 4	Trahasch, Stephan	08.03.16 18:01	08.
IT-Sicherheit -- Übung 4 + 6	Trahasch, Stephan	08.03.16 18:01	08.
IT-Sicherheit - Übung 6	Trahasch, Stephan	08.03.16 18:01	08.

Neue Veranstaltung | Bearbeiten | Löschen | VMs zeigen

Veranstaltungsdetails

Übersicht | Allgemein | Beschränkungen | Raumauswahl | Erweitert | Berechtigungen

Name: EKlausur - Software Engineering

Beschreibung: Prüfungs-VM für die Vorlesung Software Engineering

ID: ce51849a-0b56-44ca-b365-3531d44fcdab

Besitzer: Ritter, Steffen [Ändern]

Verknüpfte VM: EK_SW-Engineering [Ändern]

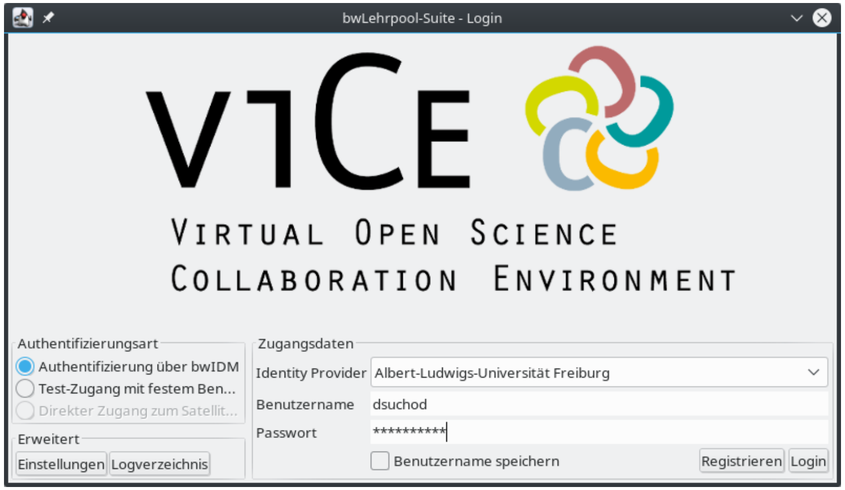
VM-Version: 23.05.2016 11:33:56 [Download]
☑ Immer aktuellste Version verwenden

Startdatum: 15.06.2016 14:00

Enddatum: 15.06.2016 15:00

☐ Veranstaltung aktiv

Schließen | Speichern



bwLehrpool-Suite - Login

ViCE
Virtual Open Science
Collaboration Environment

Authentifizierungsart
● Authentifizierung über bwIDM
○ Test-Zugang mit festem Ben...
○ Direkter Zugang zum Satellit...

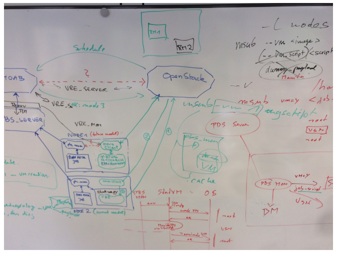
Erweitert
Einstellungen | Logverzeichnis

Zugangsdaten
Identity Provider: Albert-Ludwigs-Universität Freiburg
Benutzername: dsuchod
Passwort: **********
☐ Benutzername speichern

Registrieren | Login

Challenges / Research Questions

- How to properly describe scientific software and/or complete VREs?
  - Which meta data, schema to use?
  - E.g. suggestion of a very abstract schema definition (dataset), http://schema.org/Dataset or discussion on data publishing: http://blog.wolfram.com/2017/04/20/launching-the-wolfram-data-repository-data-publishing-that-really-works/#the-data-curation-hierarchy
- Scheduling challenge
  - Hybrid clusters generate nice „scheduling nightmares“
  - Running non-interactive batch jobs for a rather wide selection of different computations and simulations
  - Batch scheduler tries to allocate appropriate resources and optimally fill the cluster



Consequence: Virtual workflows

- 180° turn:
  - Provide a virtual machine to the computer (instead of using it bare metal)
  - With all necessary drivers, connectors, etc before the environment is used for research
  - Then it becomes easy to archive the complete environment
- Only approved images will be used
  - Higher reliability in research
  - Reduced complexity – all computers run the same environment; same artefacts
  - Coexistence with local environments and environments of other users
  - Saves time – no need to install software
  - Talk about science rather than setup + configuration problems

Creating electronic „lab books“

- Digital science often a „good“ example for fire & forget principle
  - Results created/generated by computer program(s) which are heavily dependent on a certain environment
- Status Quo in digital science
  - Data, results become worthless without proper context
  - „inherit“ the data and worry about how it was produced
  - Not everything is known, although promised
  - Some inter-dependencies forgotten
  - Exact state of the original computer environment is unkown
  - Updates, modification to the system, twists imposed by manufacturers of research hardware
  - Malicious modifications of the computing environment?
    - By accident – or intentionally?
    - i.e. make the mistake and worry later

Thank you / Questions!?

- Further information: ViCE people
  - ATLAS / physics: F. Bühler, A. Gamel
  - Bio informatics: B. Grüning, H. Rasche
  - Computer center FR: J. Bauer, M. Janczyk, B. Wiebelt, O. Zharkow, D. v. Suchodoletz

- Project descriptions:
  - https://www.alwr-bw.de/kooperationen/vice
  - http://www.bwlehrpool.de
  - https://www.bw-cloud.org/en