

Scientific Visualization at Jülich Supercomputing Centre

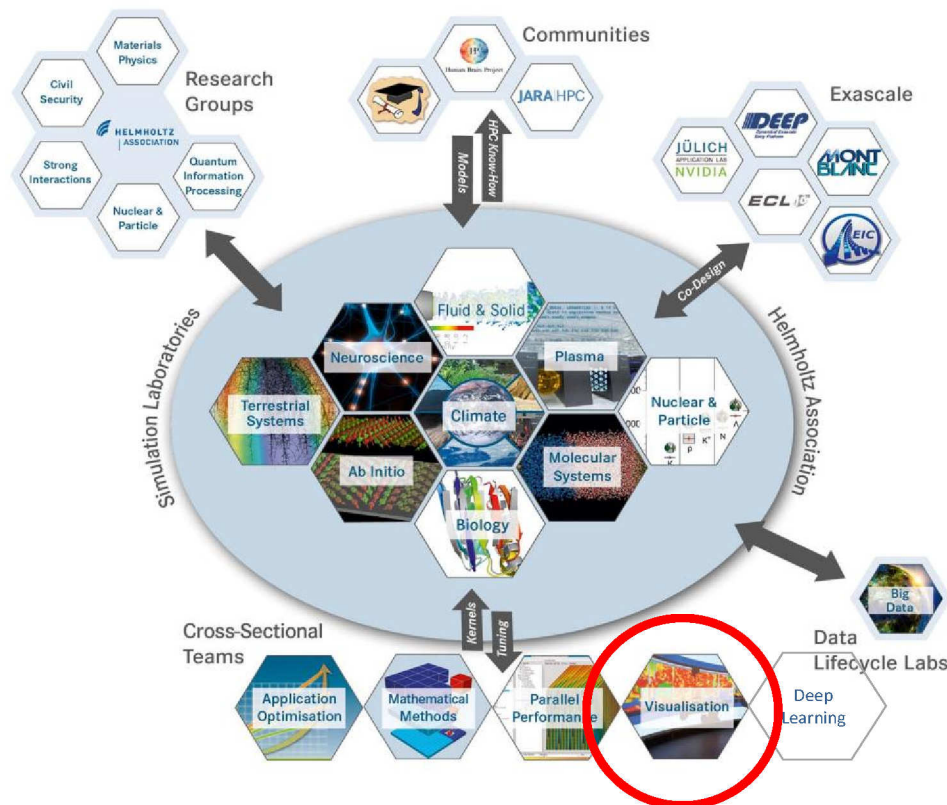
¹ Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, Germany
Cross-Sectional-Team „Visualization“
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Visualization at JSC

Cross-Sectional Team “Visualization”

Domain-specific User Support and Research at JSC

- **Scientific Visualization**
 - R&D + support for visualization of scientific data
- **Virtual Reality**
 - VR systems for the analysis and presentation
- **Multimedia**
 - multimedia productions for websites, presentations or on TV

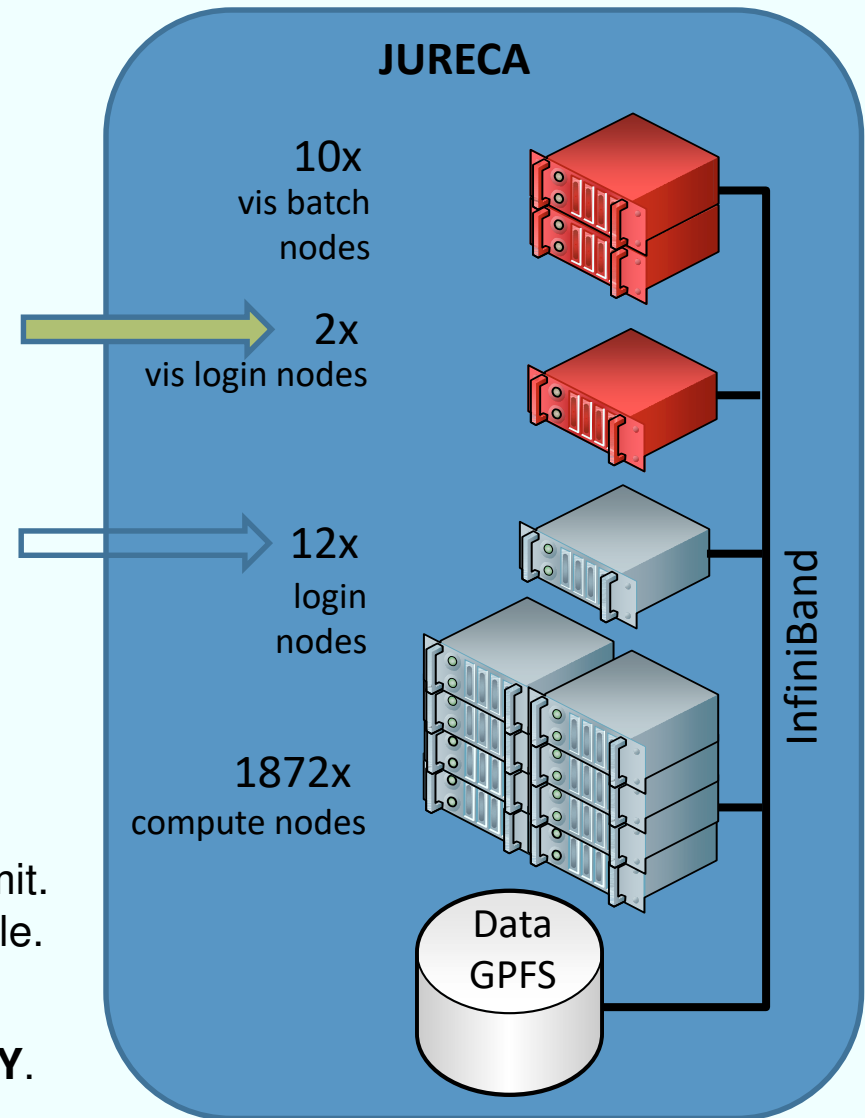


Visualization at JSC

General Hardware Setup

12x Visualization Nodes

- 2 GPUs Nvidia Tesla K40 per node
- 12 GB RAM on each GPU
- **2x Vis. Login Nodes**
 - jurecavis.fz-juelich.de
 - (*jurecavis01 or jurecavis02 in round-robin fashion*)
- **10x Vis. Batch Nodes**
 - 8 nodes with 512 GB RAM
 - 2 nodes with 1024 GB RAM
 - special partition: **vis**
 - Use vis. batch nodes via job submit. SSH to allocated resource possible.



Keep in mind:

Visualization is **NOT** limited to vis. nodes **ONLY**.
 (software rendering is possible on any node)

Visualization at JSC

General Software Setup

Special Software Stack on Vis Nodes:

Base Software:



X-Server, X-Client (Window-Manager)



OpenGL (libGL.so, libGLU.so, libglx.so), Nvidia

Middleware:



Virtual Network Computing: VNC-Server, VNC-Client



VirtualGL



Strudel

Parallel and Remote Rendering Apps, In-Situ Visualization:



ParaView



VisIt

Other Visualization Packages:

VMD, PyMol, Blender, GPicView, GIMP

JURECA projects, JUWELS projects:

- Every project gets a small contingent (1000 core h) for vis nodes in addition to project contingent
- Contingent is valid for partition “vis”
- If you need more compute time for visualization: send a request to sc@fz-juelich.de

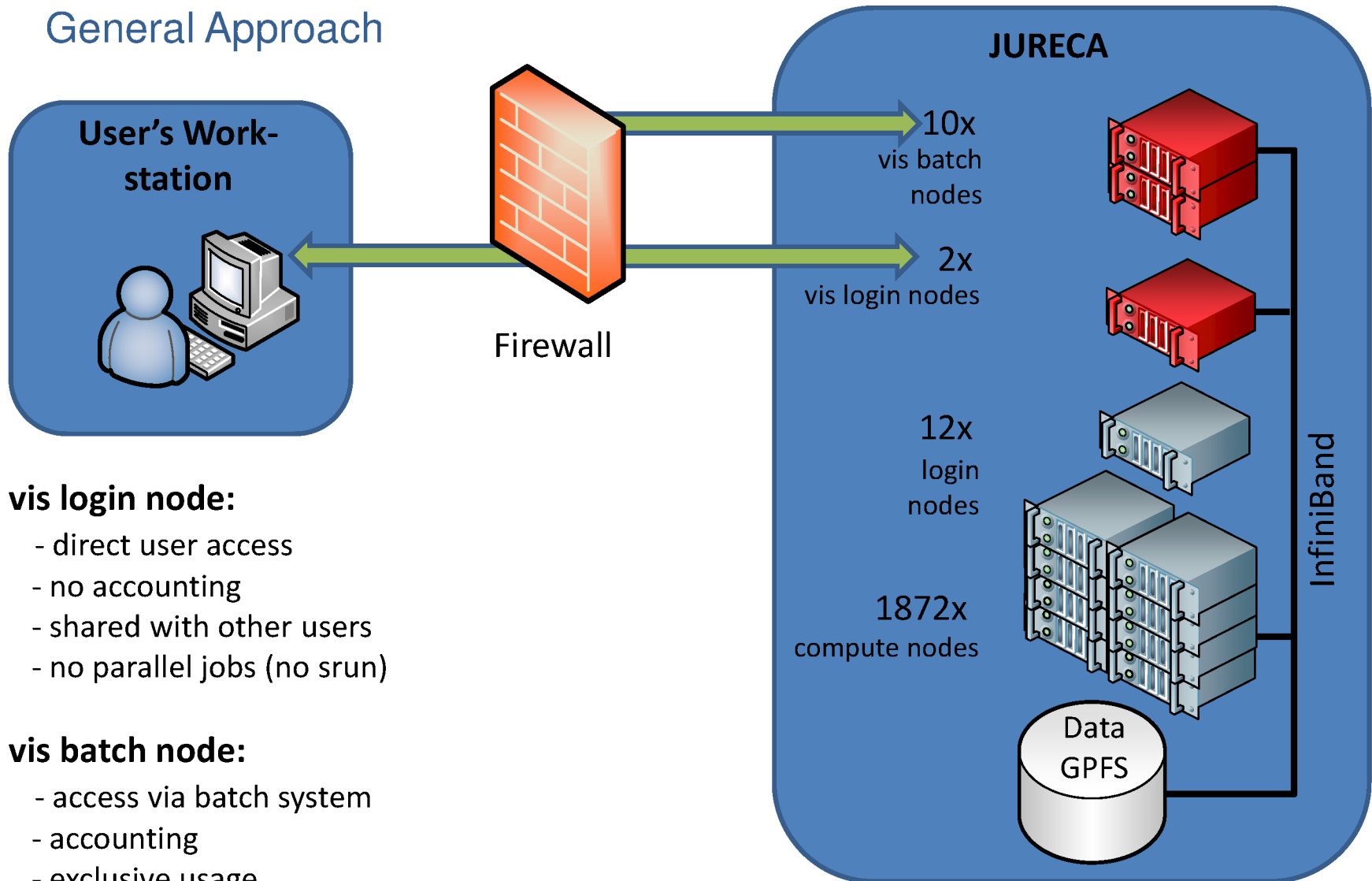
Non HPC-Project Users:

- apply for test project
- get a small contingent for vis nodes (1000 core h)

Remote 3D Visualization

Remote 3D Visualization

General Approach



vis login node:

- direct user access
- no accounting
- shared with other users
- no parallel jobs (no srun)

vis batch node:

- access via batch system
- accounting
- exclusive usage
- parallel jobs possible

Remote 3D Visualization

at Jülich Supercomputing Centre

- X forwarding + Indirect Rendering
slow, maybe incompatible → bad idea
- “remote aware” visualization apps (ParaView, VisIt)
application dependent error-prone setup
- VNC (Virtual Network Computing) + VirtualGL
our recommendation → good idea
- Xpra - stream application content with H.264 + VirtualGL
alternative recommendation → good idea

Remote 3D Visualization

with X forwarding + Indirect Rendering

Traditional Approach (X forwarding + Indirect Rendering)
ssh -X <USERID>@<SERVER>

- uses GLX extension to X Window System
- X display runs on user workstation
- OpenGL commands are encapsulated inside X11 protocol stream
- OpenGL commands are executed on user workstation
- **disadvantages**
 - User's workstation requires a running **X server**.
 - User's workstation requires a **graphic card** capable of the required OpenGL.
 - User's workstation defines the **quality and speed** of the visualization.
 - User's workstation requires **all data needed** to visualize the 3d scene.
 - This approach is known to be error prone (OpenGL version mismatch, ...)

Try to **AVOID** for 3D visualization.

Remote 3D Visualization

with VNC (Virtual Network Computing) + VirtualGL

State-of-the-Art Approach (VNC with VirtualGL)

vncserver, vncviewer



- platform independent
- application independent
- session sharing possible

- **advantages**
 - **No X is required** on user's workstation (X display on server, one per session).
 - **No OpenGL is required** on user's workstation (only images are send).
 - Quality of visualization does **not depend** on user's workstation.
 - Data size send is **independent** from data of 3d scene.
 - Disconnection and reconnection possible.

<http://www.virtualgl.org>

Try to **USE** for 3D visualization.

Remote 3D Visualization

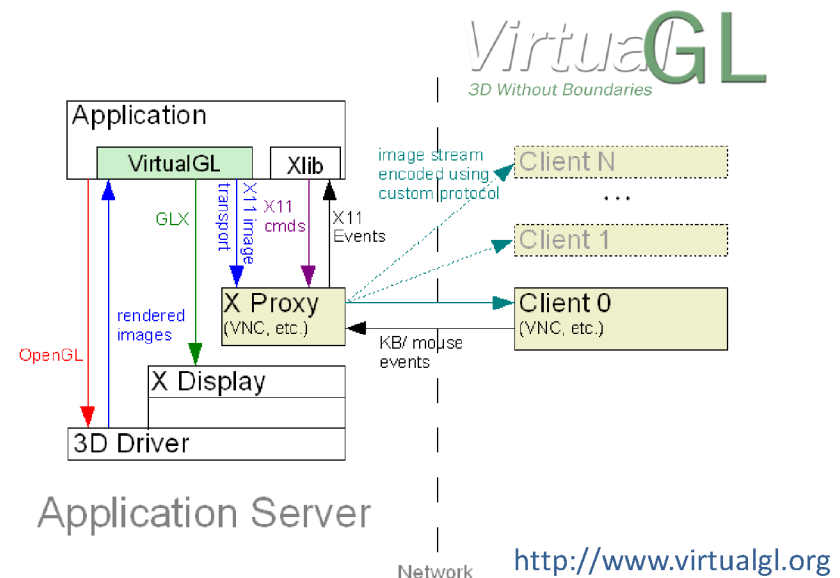
with VNC (Virtual Network Computing) + VirtualGL

VNC + VirtualGL

vglrun <application>



- OpenGL applications send both GLX and X11 commands to the same X display.
- Once **VirtualGL** is preloaded into an OpenGL application, it **intercepts the GLX** function calls from the application and **rewrites them**.
- The corresponding GLX commands are then sent to the X display of **the 3d X server**, which has a 3D hardware accelerator attached.



Remote 3D Visualization

with VNC (Virtual Network Computing) + VirtualGL

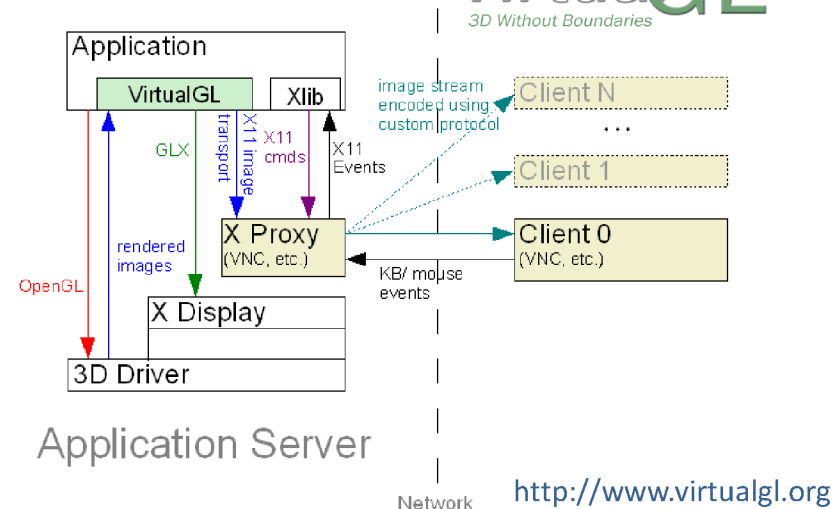
VNC + VirtualGL

vglrun <application>



VirtualGL
 3D Without Boundaries

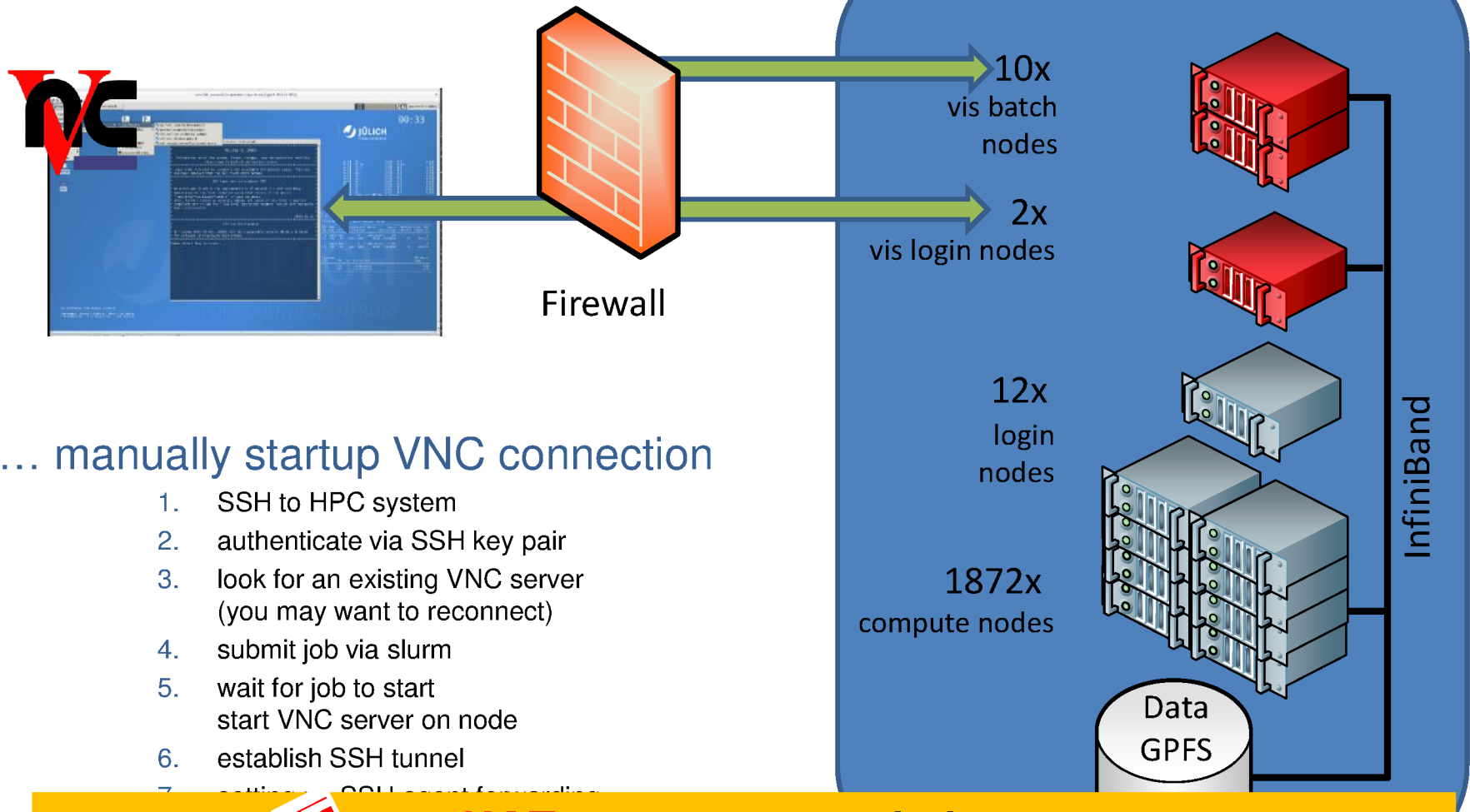
- Recommended solution for **any OpenGL application**
 e.g. ParaView, VisIt, IDL, VMD, PyMol, ...
- Allows fast and reliable **server-side hardware rendering**
 (GPU acceleration) with VirtualGL
- User only installs local VNC viewer.
- Desktop sharing possible
- Should also be used for the frontend
 of “remote aware” applications
 (e.g. for ParaView and VisIt, ...)



Our recommendation:
Use VNC for remote rendering on JURECA.

Remote 3D Visualization

with VNC + VirtualGL



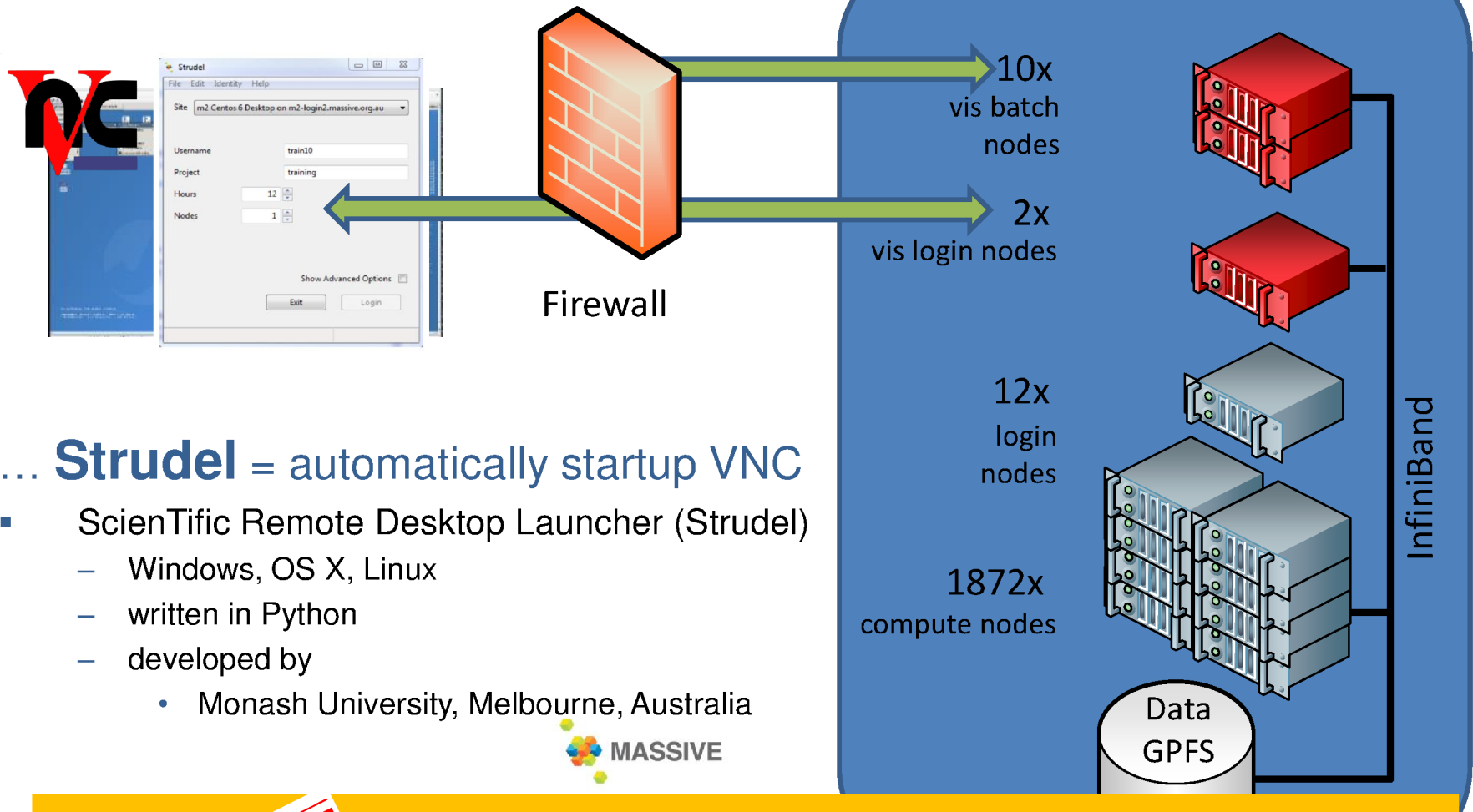
... manually startup VNC connection

1. SSH to HPC system
2. authenticate via SSH key pair
3. look for an existing VNC server (you may want to reconnect)
4. submit job via slurm
5. wait for job to start
start VNC server on node
6. establish SSH tunnel
7. settings SSH agent forwarding

NOT our recommendation:
 This is far too time consuming.

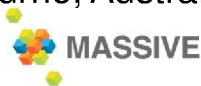
Remote 3D Visualization

with VNC + VirtualGL



... **Strudel** = automatically startup VNC

- SciencTific Remote Desktop Launcher (Strudel)
 - Windows, OS X, Linux
 - written in Python
 - developed by
 - Monash University, Melbourne, Australia

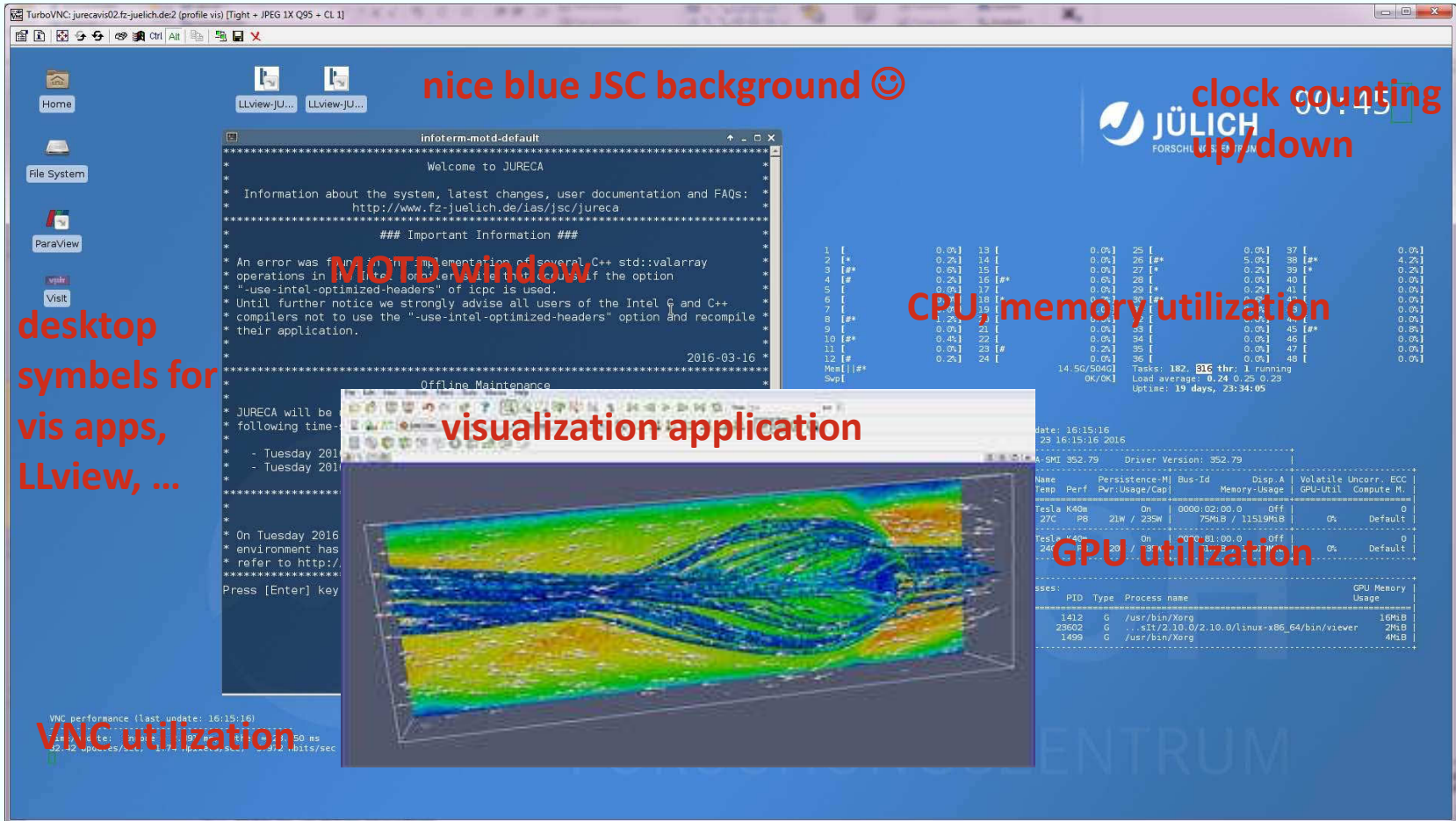


Our recommendation:
Use 'Strudel' to start a VNC session.

<https://trac.version.fz-juelich.de/vis/wiki/vnc3d/strudel>

Remote 3D Visualization

Desktop Profiles with VNC + VirtualGL



nice blue JSC background ☺

clock counting up/down

desktop symbols for vis apps, LLview, ...

MDT window

CPU memory utilization

visualization application

GPU utilization

VNC utilization

info:term-motd-default

```
*****
Welcome to JURECA

Information about the system, latest changes, user documentation and FAQs:
http://www.fz-juelich.de/ias/jsc/jureca
*****

### Important Information ###

An error was found in the implementation of several C++ std::valarray
operations in the Intel compiler. If the option
"-use-intel-optimized-headers" of icpc is used,
Until further notice we strongly advise all users of the Intel C and C++
compilers not to use the "-use-intel-optimized-headers" option and recompile
their application.

2016-03-16
*****

Offline Maintenance

JURECA will be
following time-
- Tuesday 201
- Tuesday 201

*****

On Tuesday 2016
environment has
refer to http://
*****
Press [Enter] key
```

GPU utilization

Name	Persistence-M	Bus-Id	Disp-A	Memory-Usage	GPU-Util	Compute M.
Tesla K40m	On	0000:02:00.0	Off	75MiB / 11519MiB	0%	Default
Tesla K40m	On	0000:01:00.0	Off	75MiB / 11519MiB	0%	Default

VNC utilization

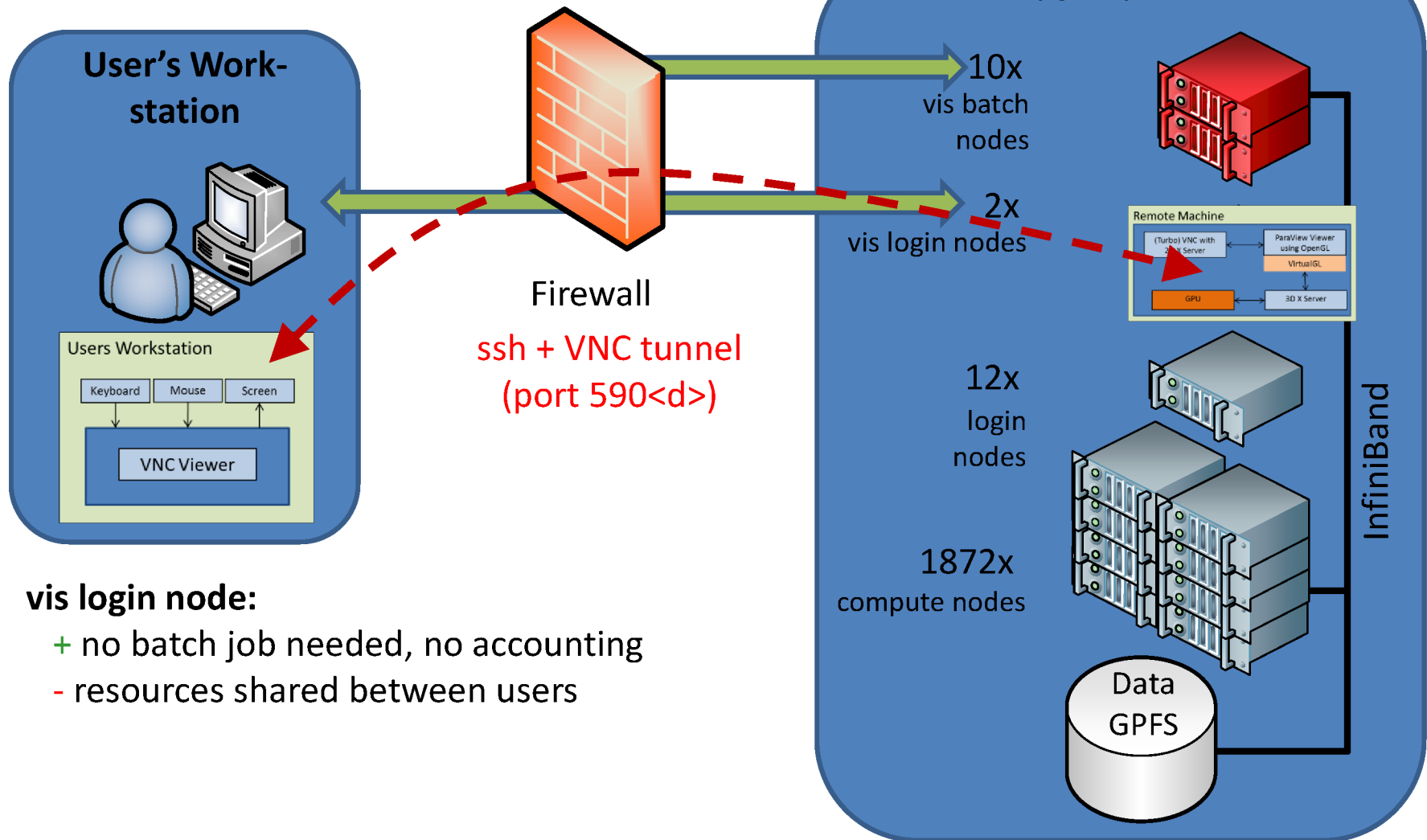
VNC performance (last update: 16:15:16)

Process	Usage	Time	Size	Speed
LLview	100%	100%	100%	100%
LLview	100%	100%	100%	100%
LLview	100%	100%	100%	100%

Remote 3D Visualization (possible scenarios)

Visualization Scenario 1:

Vis Login Node with VNC

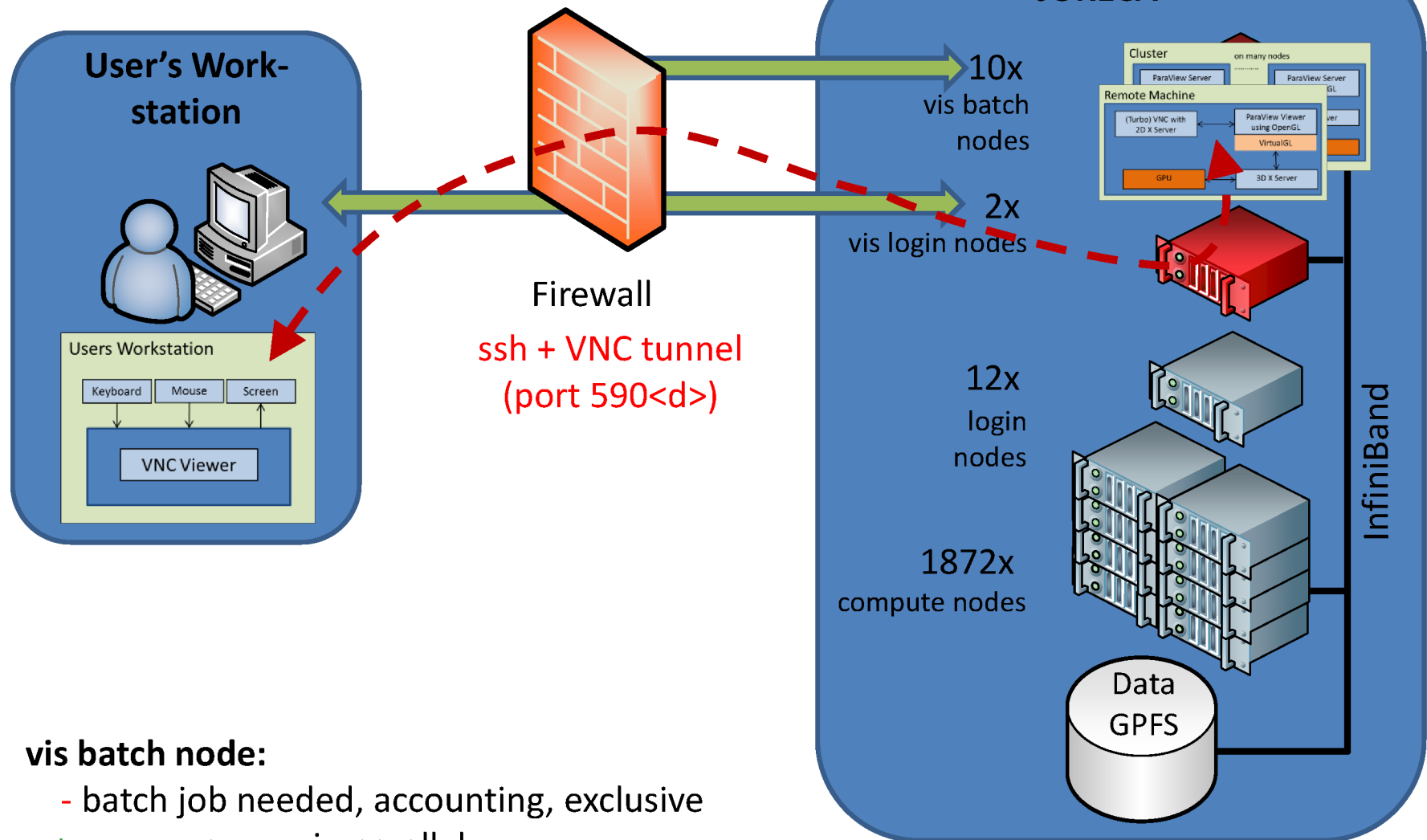


vis login node:

- + no batch job needed, no accounting
- resources shared between users

Visualization Scenario 2:

Vis Batch Node with VNC

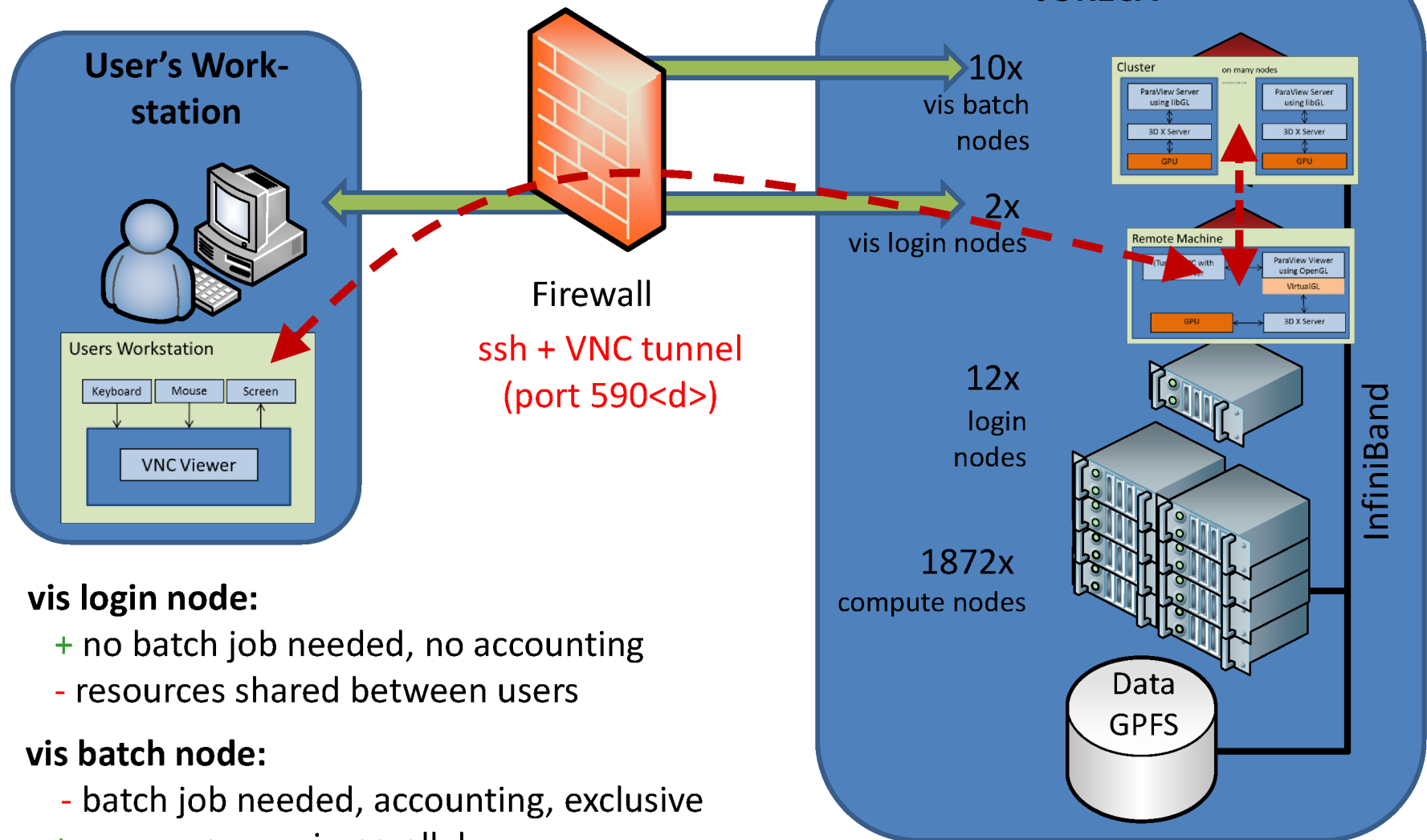


vis batch node:

- batch job needed, accounting, exclusive
- + server can run in parallel
- (but number of vis nodes limited to 4)

Visualization Scenario 3:

Vis.Login for GUI, Comp. Nodes for Server



vis login node:

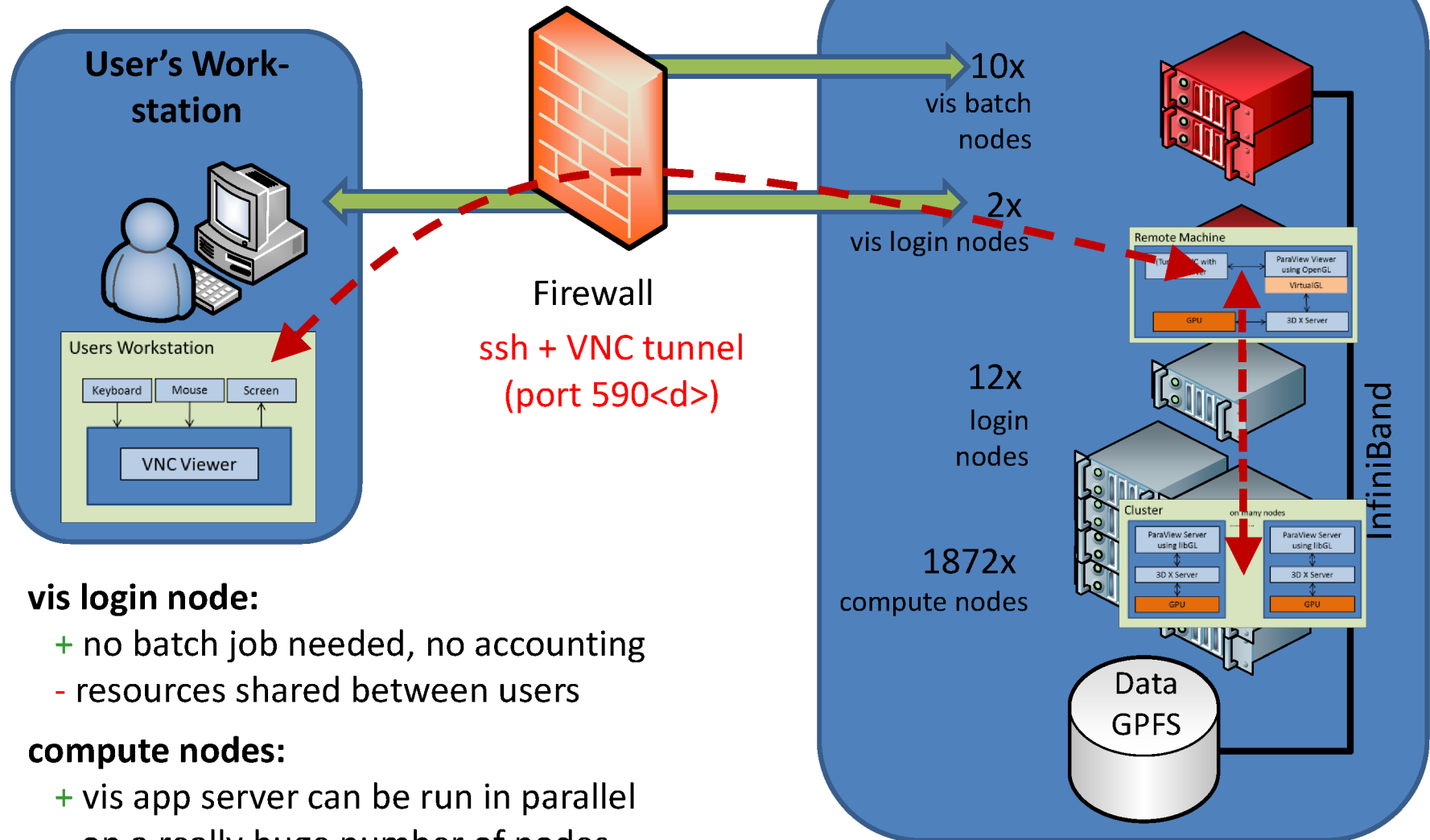
- + no batch job needed, no accounting
- resources shared between users

vis batch node:

- batch job needed, accounting, exclusive
- + server can run in parallel
(but number of vis nodes limited to 4)

Visualization Scenario 4:

Vis Login for GUI, Compute for Server



vis login node:

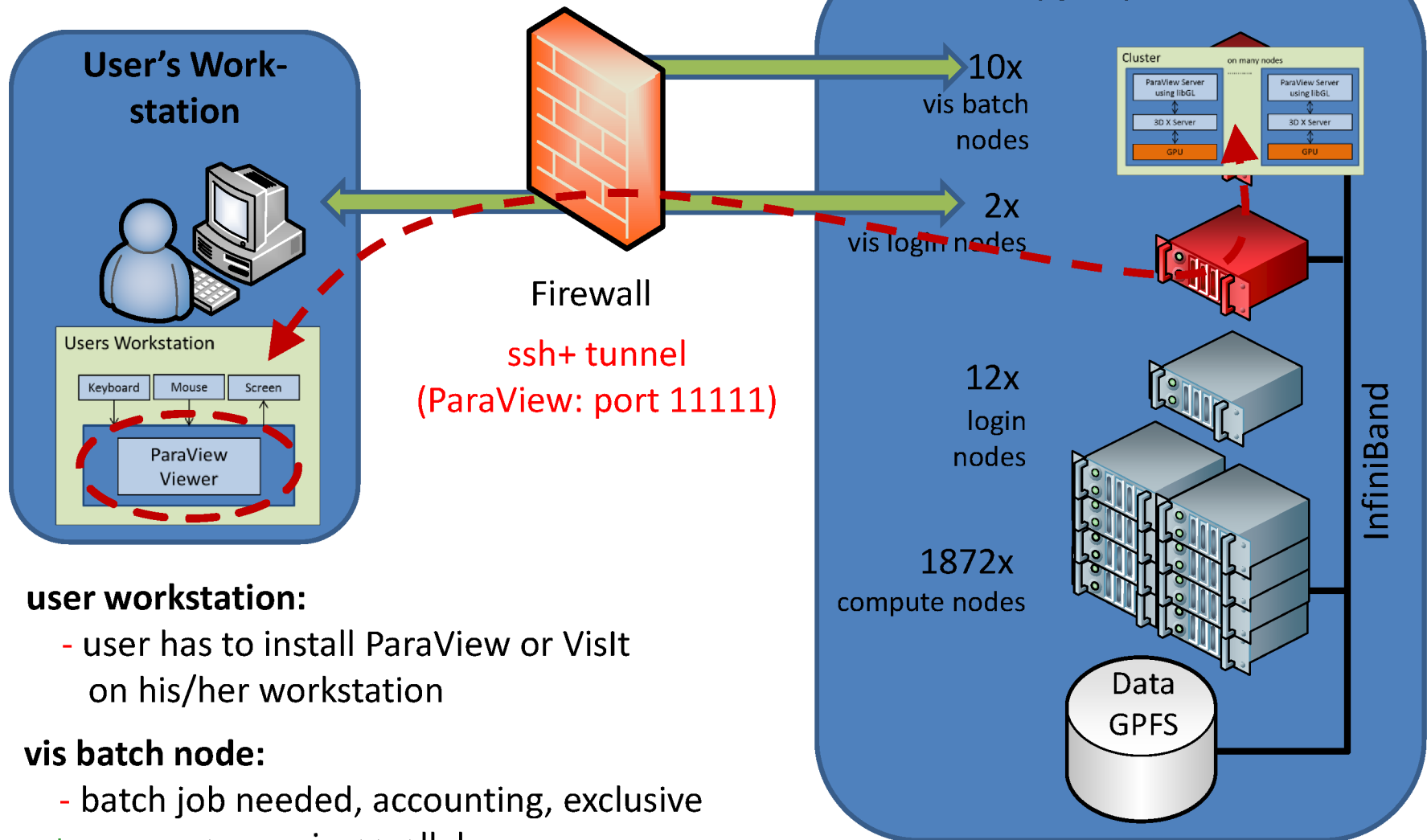
- + no batch job needed, no accounting
- resources shared between users

compute nodes:

- + vis app server can be run in parallel on a really huge number of nodes
- only software rendering

Visualization Scenario 5:

ParaView (or VisIt) without VNC



user workstation:

- user has to install ParaView or VisIt on his/her workstation

vis batch node:

- batch job needed, accounting, exclusive
- + server can run in parallel
(but number of vis nodes limited to 4)

Remote 3D Visualization (alternatives)

Remote 3D Visualization

with Xpra (X Persistent Remote Applications) + VirtualGL

"screen for X11,, (stream application content with H.264 + VirtualGL)

```
xpra start ssh:<SERVER>:<DISPLAY> \  
    --ssh-key=<PATH_TO_SSH-PRIVATE-KEY> \  
    --start-child=<XAPPLICATION>
```

- X-applications forwarded by Xpra appear on the local desktop as normal windows
- allows disconnection and reconnection without disrupting the forwarded application
- Xpra protocol is self-tuning and relatively latency-insensitive
- **advantages**
 - **No X is required** on user's workstation (X display on server).
 - **No OpenGL is required** on user's workstation (only images are send).
 - Quality of visualization does **not depend** on user's workstation.
 - Data size send is **independent** from data of 3d scene.
 - Disconnection and reconnection possible.



Our recommendation:
Use 'Xpra' as 'ssh -X' replacement.

<https://xpra.org/>

Nice To Know

Nice to know:

OSPRay

CPU ray tracing framework for scientific vis. rendering

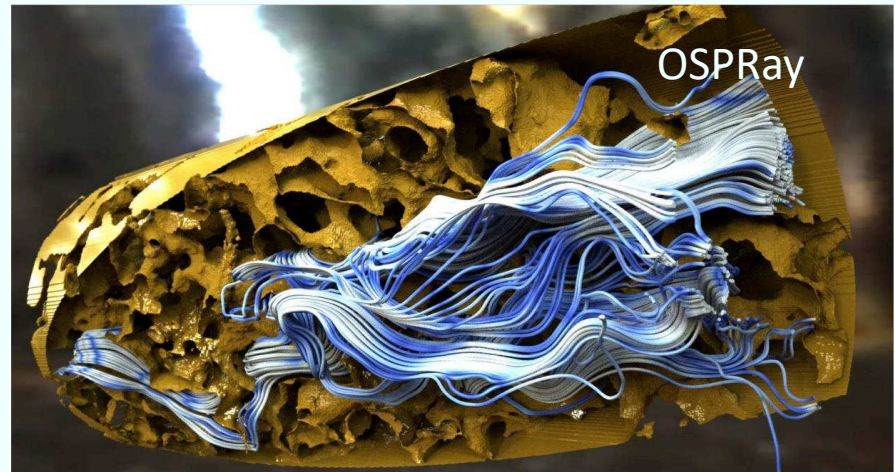
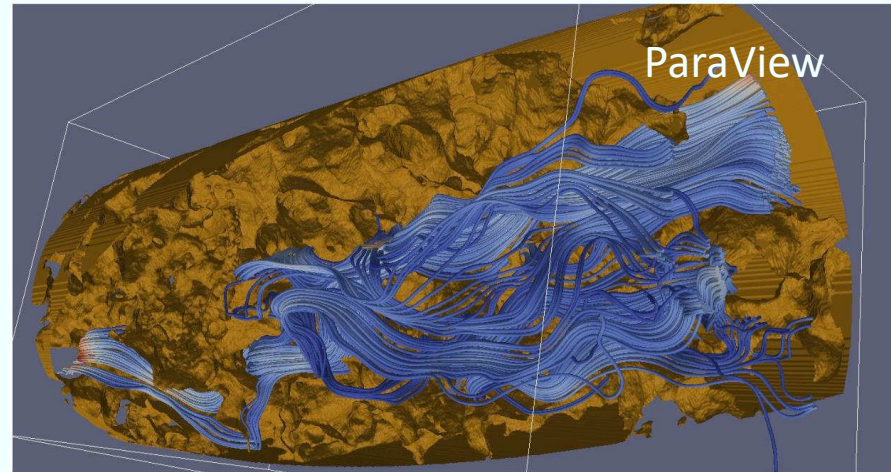
- efficient rendering on CPUs
- ray tracing / high fidelity rendering
- made for scientific visualization

Built on top of

- Embree (Intel ray tracing kernels)
- Intel SIMD Program Compiler

Integrated into

- ParaView, VMD, VisIt, VL3,
EasternGraphics,...



"FIU" Ground Water Simulation

Texas Advanced Computing Center (TACC) and Florida International University

<http://www.ospray.org/>

http://www.sdvis.org/ospray/download/talks/IEEEVis2016_OSPray_talk.pdf

Nice to know:

OSPRay with ParaView

Ray tracing within ParaView

- Build option in ParaView 5.2 by default

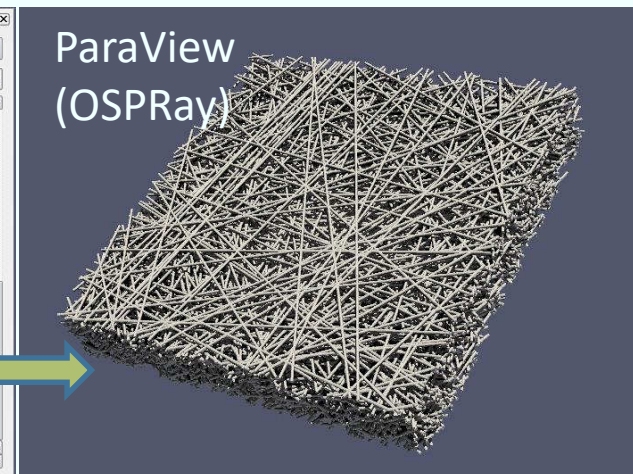
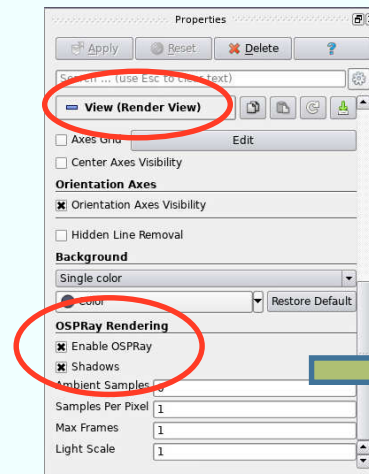
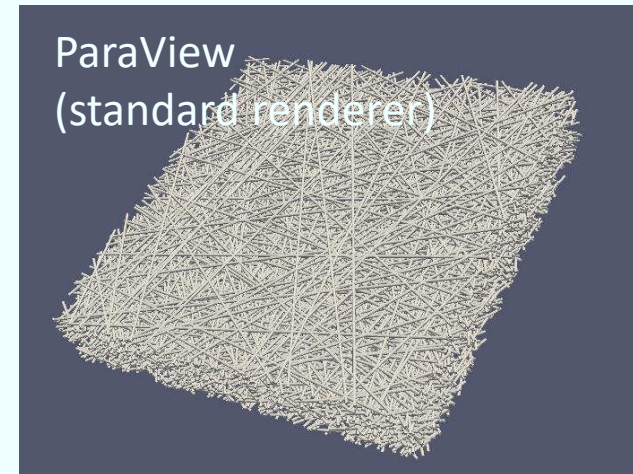
Why ray tracing?

- gives more realistic results
- adds “depth” to your image
- can be faster on large data

Requirement:

CPUs: Anything SSE4 and newer
 (in part, including Intel®
 Xeon Phi™ Knights Landing)

<http://www.ospray.org/>
http://www.sdvis.org/ospray/download/talks/IEEEVis2016_OSPray_talk.pdf



Cooperation with Electrochemical Process Engineering (IEK-3)
 Jülich Forschungszentrum GmbH, Germany

Documentation

JURECA Visualization Related Documentation

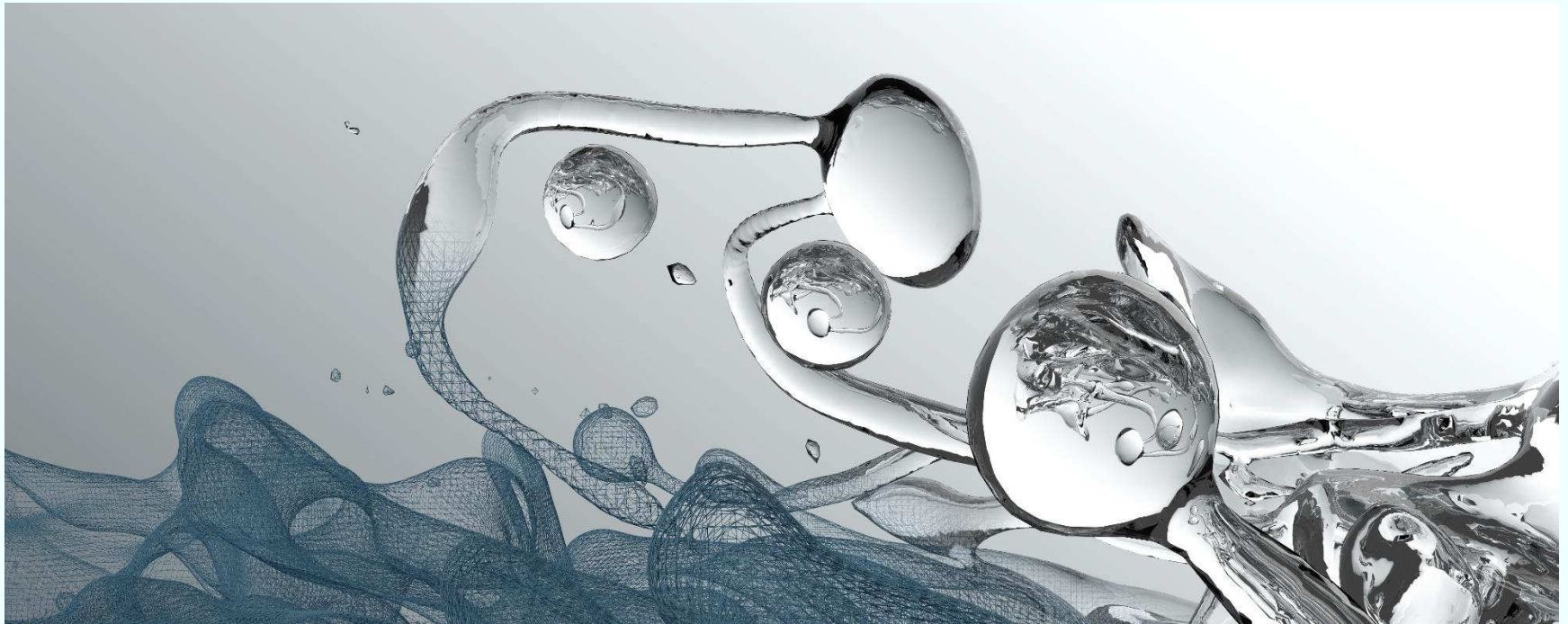
Please visit

<https://trac.version.fz-juelich.de/vis/>

Please send us your feedback.

h.zilken@fz-juelich.de j.goebbert@fz-juelich.de

Questions ... ?



rendered with Blender from a DNS of a diesel injection spray of ITV, RWTH Aachen University

Interactive Supercomputing at Jülich Supercomputing Centre

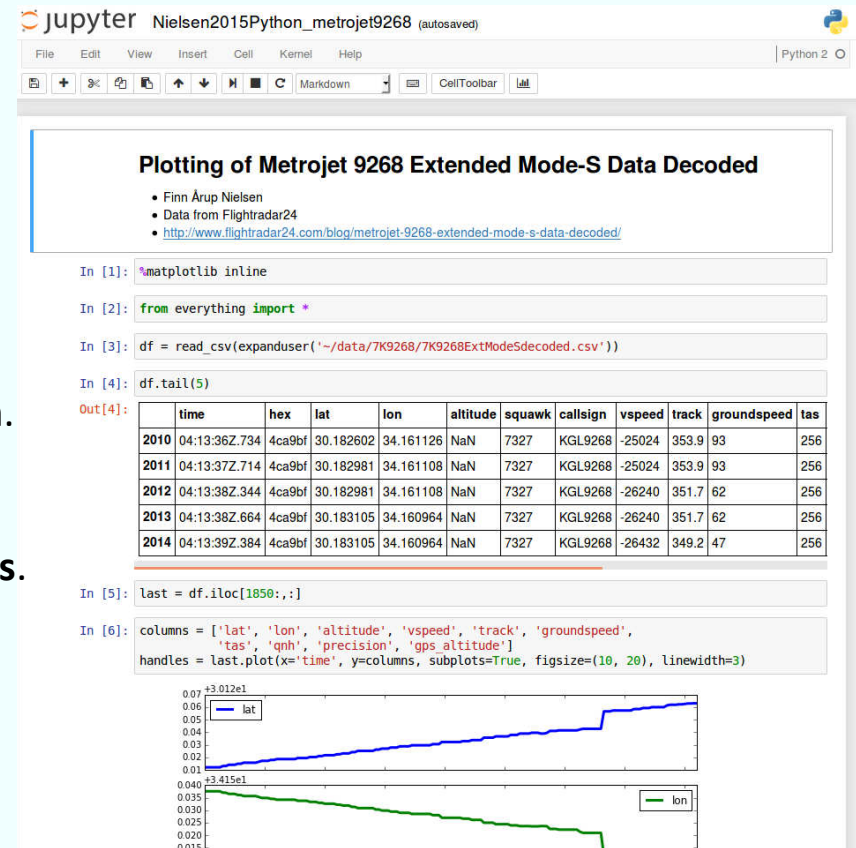
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Interactive Supercomputing

What is Jupyter

Jupyter ...

- ... is an interactive computational environment **in the web browser.**
- ... combines code execution, rich text, mathematics, plots and interactive visualization.
- ... is the interface to Jupyter Notebooks for **creating reproducible computational narratives.**
- ... supports multiple programming languages beside Python (C++, Julia, JavaScript, ...).
- ... was formerly called IPython notebook



Interactive Supercomputing

Why you should use Jupyter

Researchers today across all academic disciplines often need to **write computer code** in order to collect and process data, carry out statistical tests, run simulations or draw figures.

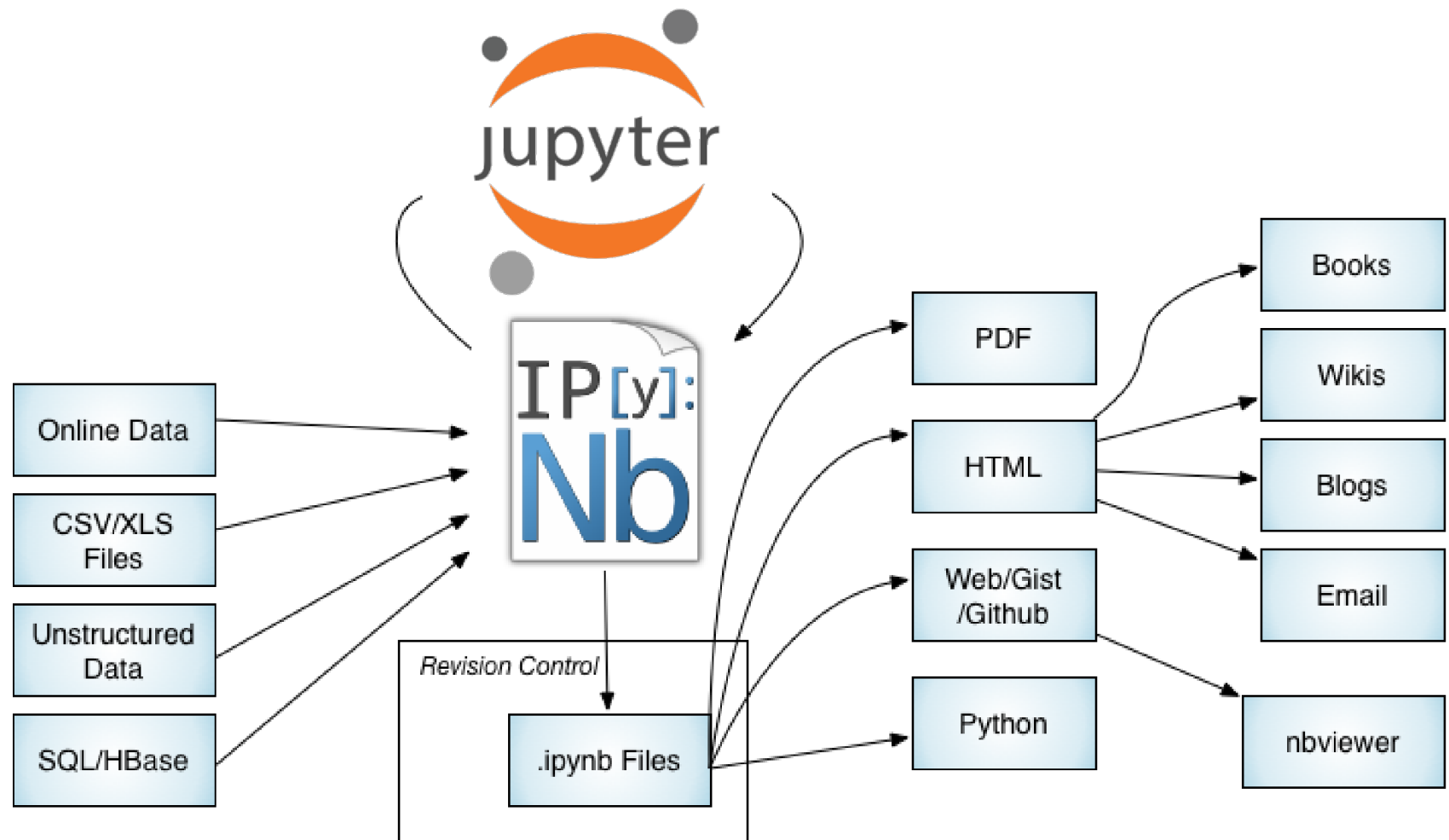
Even if the widely applicable libraries and tools for this are often open source projects (such as NumPy, TensorFlow, ...), the specific code researchers write for a particular piece of work is often **left unpublished, hindering reproducibility**.

Jupyter Notebooks integrating prose, code and results offer **a way to publish a computational method** which can be readily read and replicated.



Interactive Supercomputing

Why you should use Jupyter



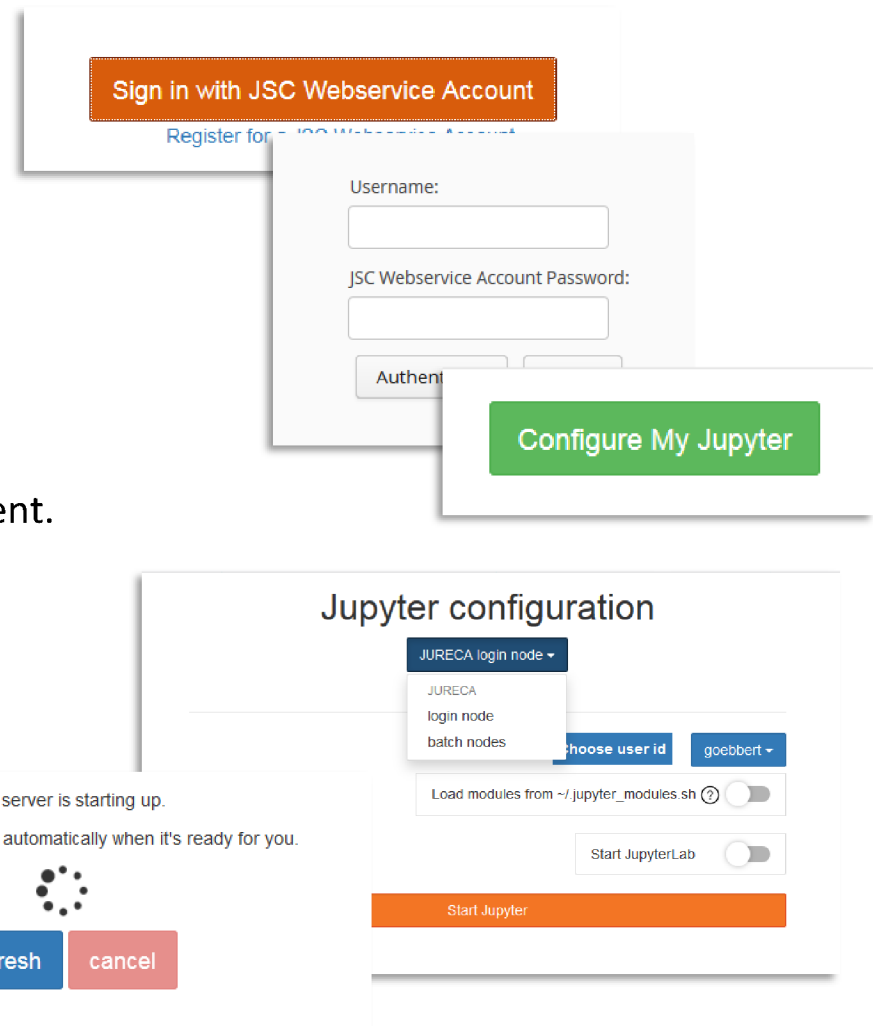
Interactive Supercomputing

How to use Jupyter

<https://jupyter-jsc.fz-juelich.de>

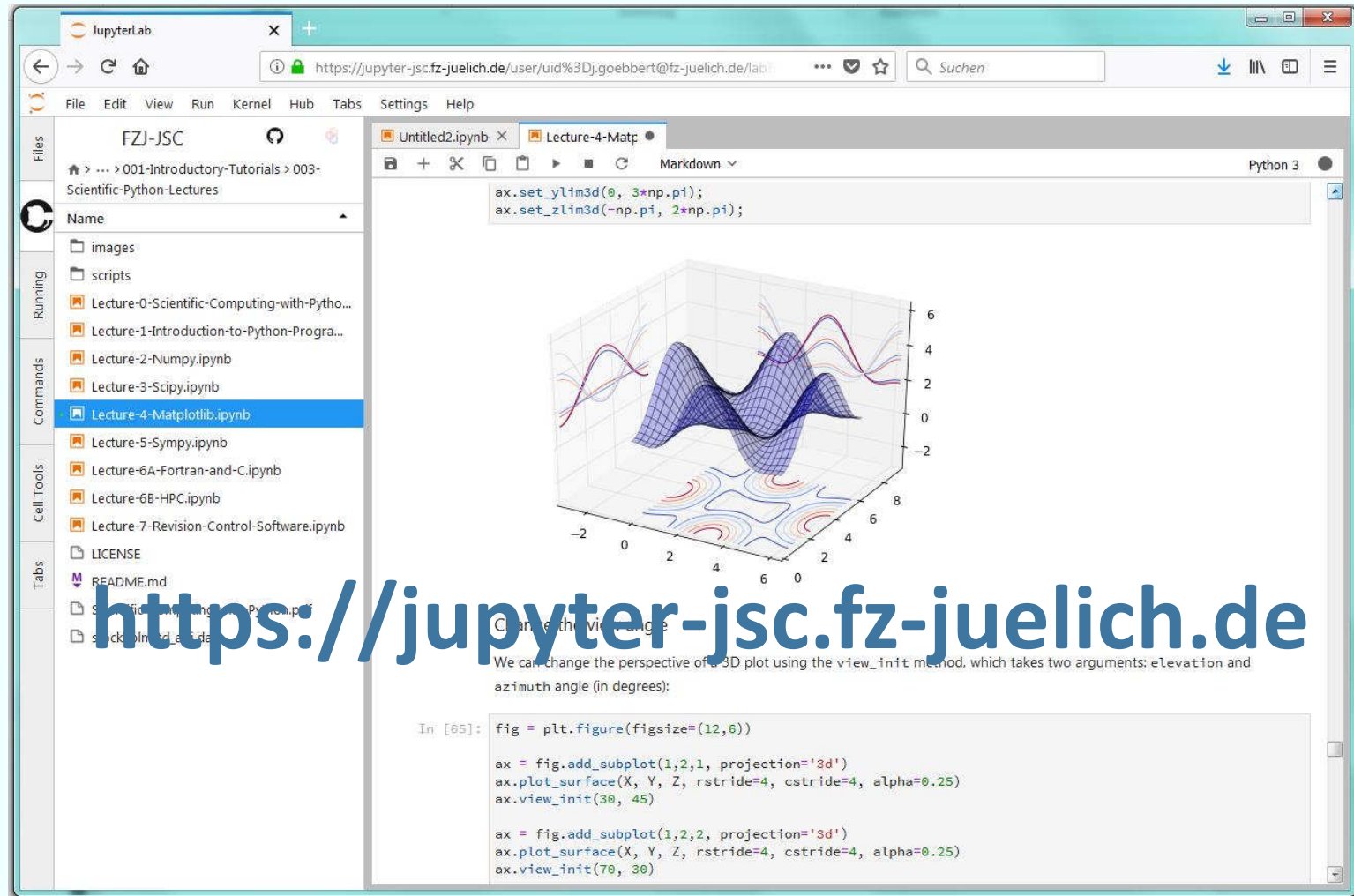
- Apply for a JSC Web Service Account
- Sign in with your JSC Web Service Account
- Accept the usage and data protection agreement.

... and you are ready to start with Jupyter.



Interactive Supercomputing

JupyterLab



The screenshot displays the JupyterLab web interface in a browser window. The address bar shows the URL <https://jupyter-jsc.fz-juelich.de/user/uid%3Dj.goebbert@fz-juelich.de/lab/>. The left sidebar shows a file explorer for the 'FZJ-JSC' directory, with 'Lecture-4-Matplotlib.ipynb' selected. The main area contains two code cells. The top cell, titled 'Untitled2.ipynb', contains the following Python code:

```
ax.set_ylim3d(0, 3*np.pi);  
ax.set_zlim3d(-np.pi, 2*np.pi);
```

Below the code is a 3D surface plot showing a complex, wavy surface in a 3D coordinate system. The axes are labeled with numerical values. The bottom cell contains the following Python code:

```
In [65]: fig = plt.figure(figsize=(12,6))  
  
ax = fig.add_subplot(1,2,1, projection='3d')  
ax.plot_surface(X, Y, Z, rstride=4, cstride=4, alpha=0.25)  
ax.view_init(30, 45)  
  
ax = fig.add_subplot(1,2,2, projection='3d')  
ax.plot_surface(X, Y, Z, rstride=4, cstride=4, alpha=0.25)  
ax.view_init(70, 30)
```

Below the code is a text block that reads: "Change the view range. We can change the perspective of a 3D plot using the `view_init` method, which takes two arguments: elevation and azimuth angle (in degrees):".

<https://jupyter-jsc.fz-juelich.de>