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FORSCHUNGSZENTRUM

Scientific Visualization at Jülich Supercomputing Centre

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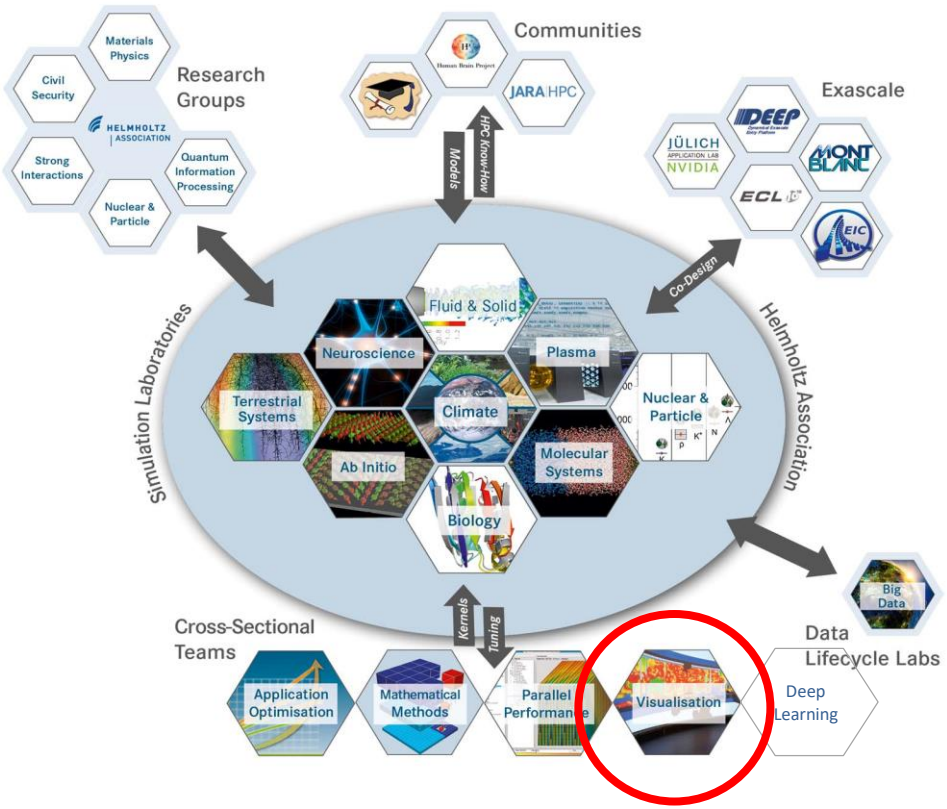
Visualization at JSC

Cross-Sectional Team “Visualization”

- **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

Domain-specific User Support and Research at JSC



http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Visualization/_node.html

Visualization at JSC

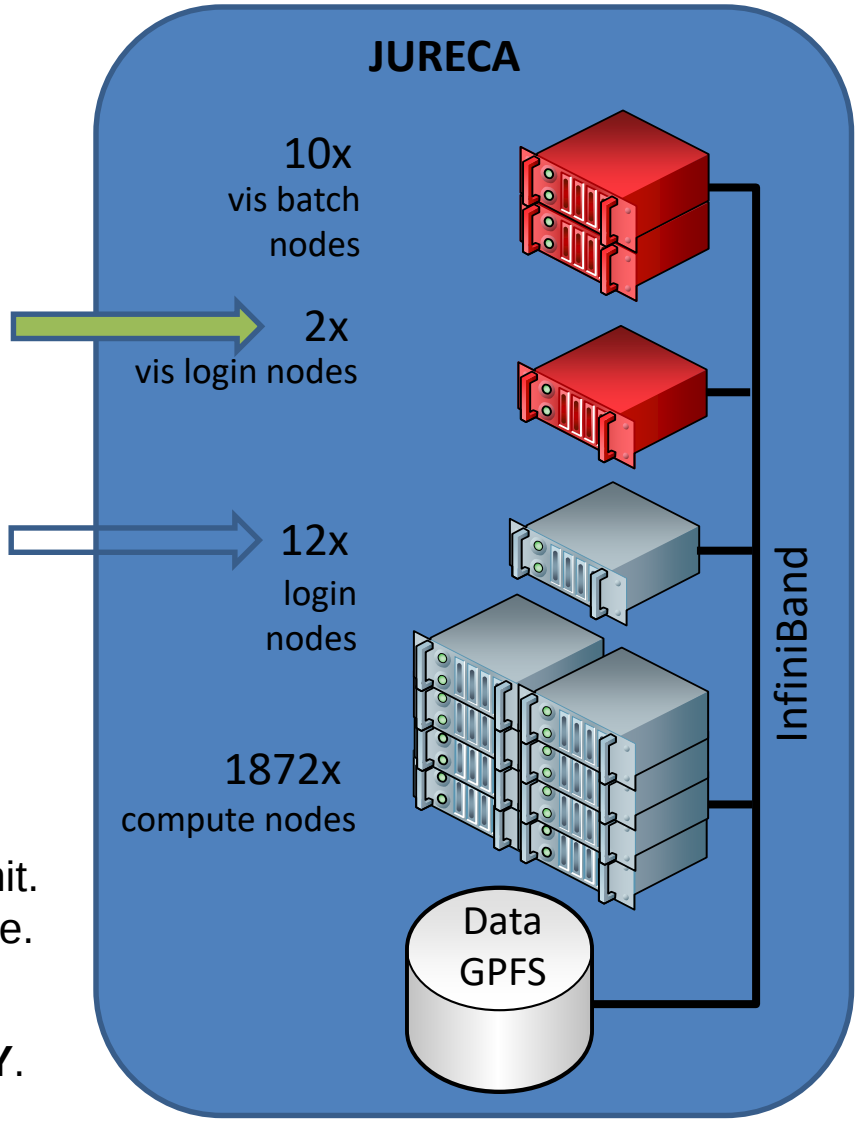
General Hardware Setup

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

Visualization at JSC

Usage Model for Vis Nodes

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

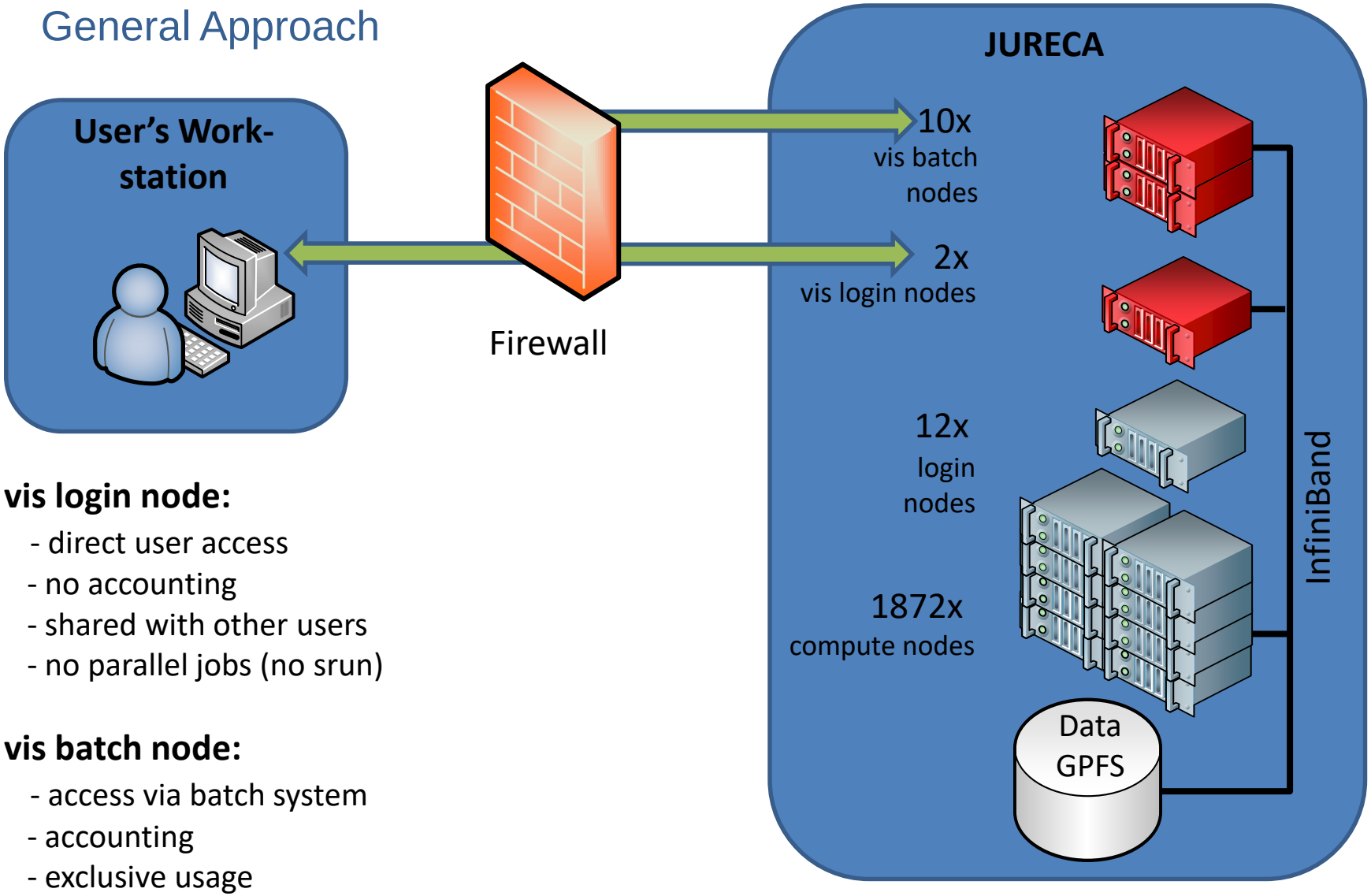
Non HPC-Project Users:

- 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

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Traditional Approach (X forwarding + Indirect Rendering)

ssh –X <USERID>@<SERVER>

- uses GLX extension to X Window System
- X display runs on user workstation
- OpenGL command are encaplusated 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 be error prone (OpenGL version mismatch, …)

Try to AVOID for 3D visualization.

Remote 3D Visualization

with VNC (Virtual Network Computing) + VirtualGL

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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.

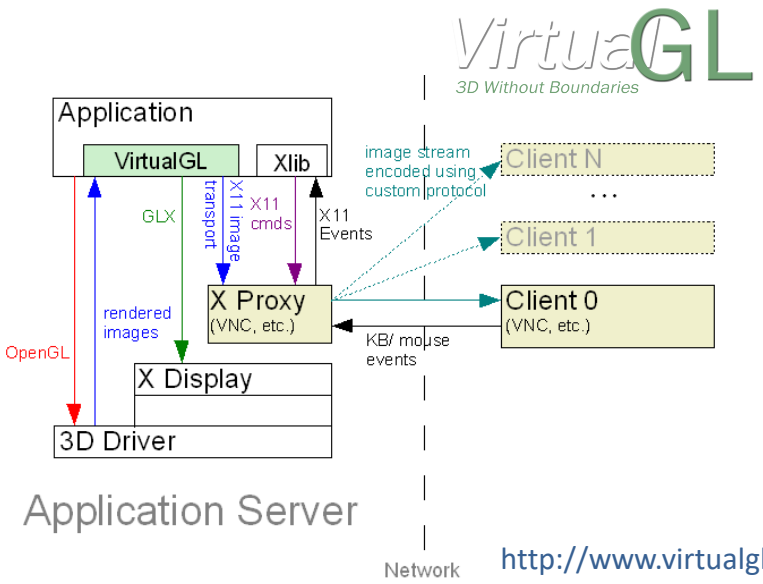
Remote 3D Visualization

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.



http://www.virtualgl.org

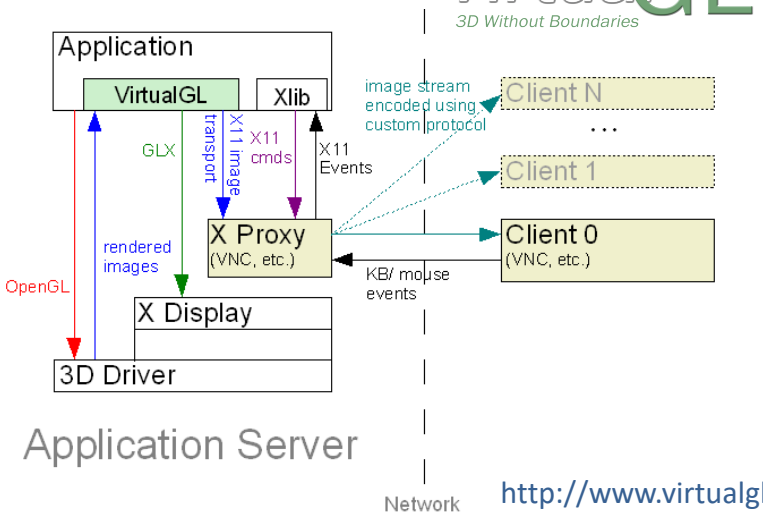
Remote 3D Visualization

with VNC (Virtual Network Computing) + VirtualGL

VNC + VirtualGL

vglrun <application>

- 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, …)

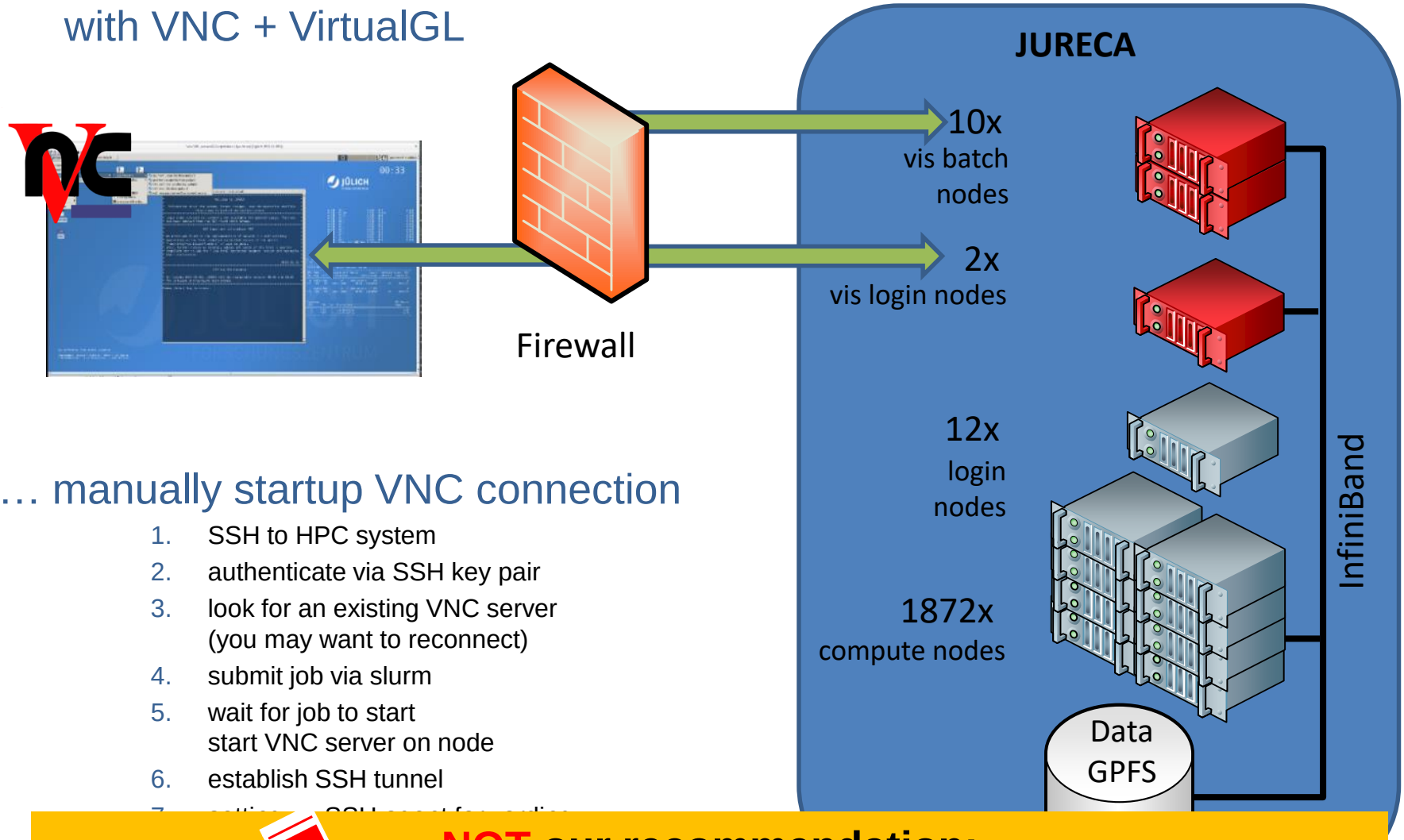


http://www.virtualgl.org

Our recommendation:
Use VNC for remote rendering on JURECA.

Remote 3D Visualization

with VNC + VirtualGL



… manually startup VNC connection

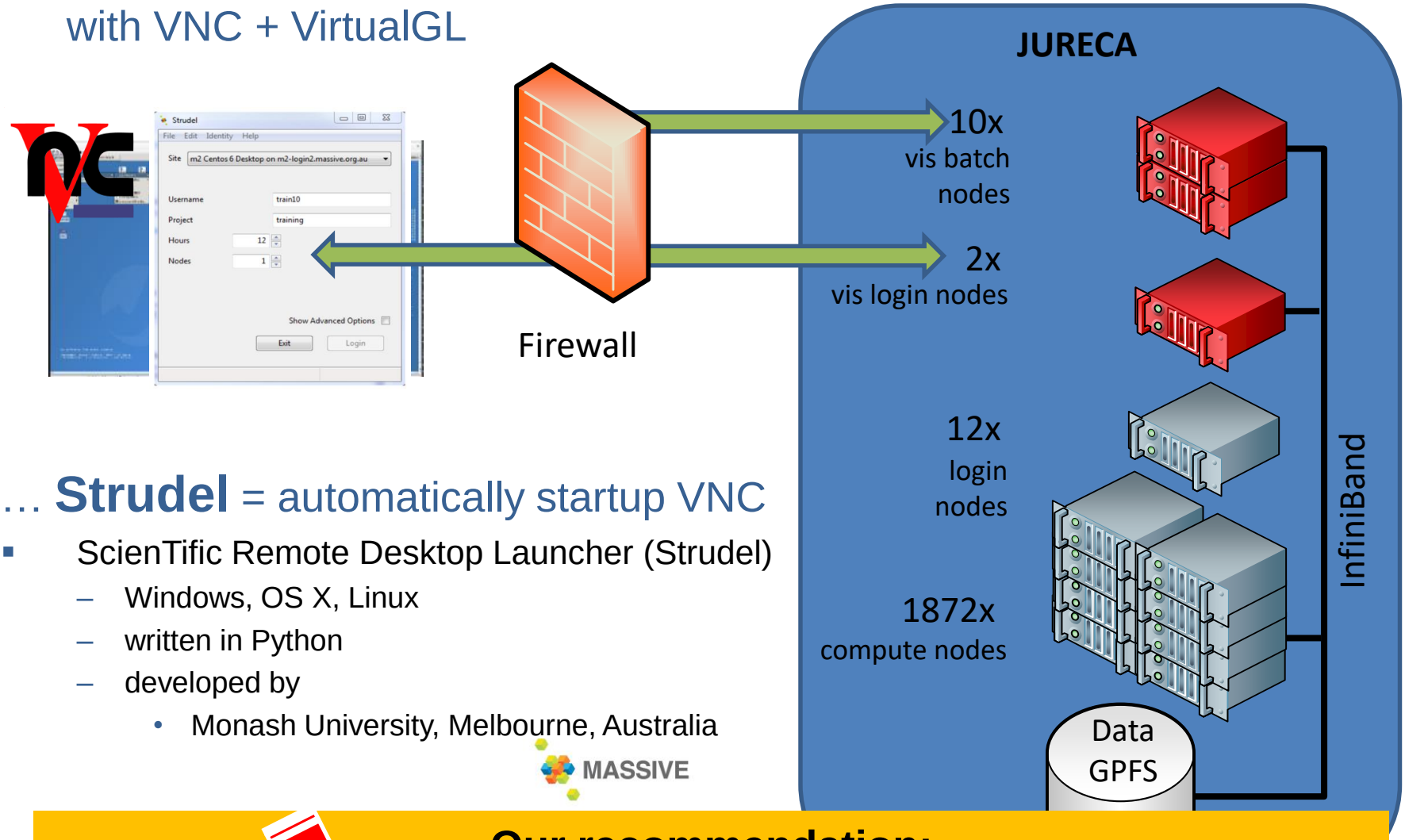
1. SSH to HPC system
2. authenticate via SSH key pair
3. look for an existing VNC server
   (you may want to reconnect)
4. submit job via slurm
5. wait for job to start
   start VNC server on node
6. establish SSH tunnel

NOT our recommendation:
This is far too time consuming.

https://trac.version.fz-juelich.de/vis/wiki/vnc3d/manual

Remote 3D Visualization

with VNC + VirtualGL



… **Strudel** = automatically startup VNC

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

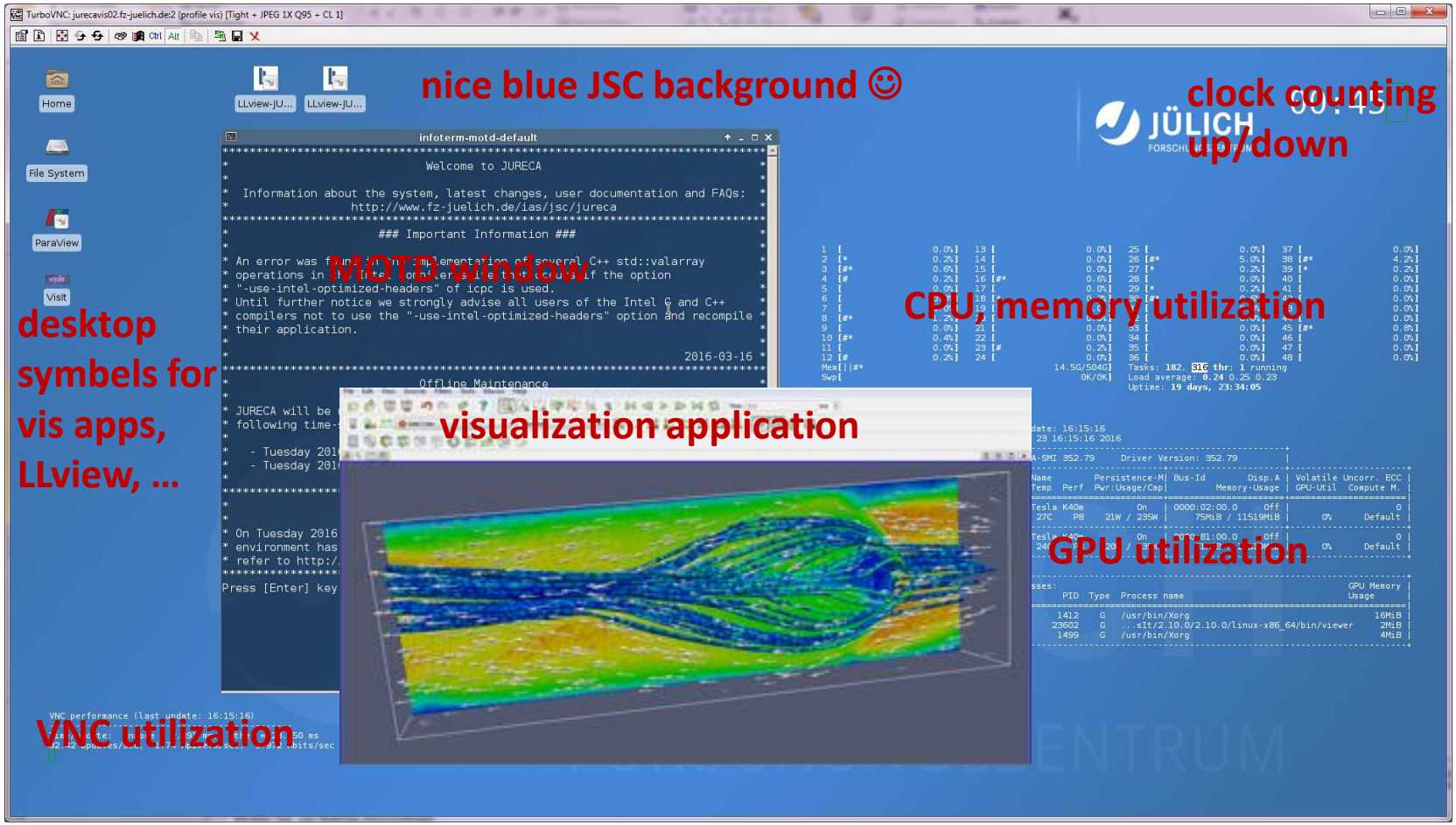
MASSIVE

Our recommendation:
Use ‘Strudel’ to start a VNC session.

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

Remote 3D Visualization

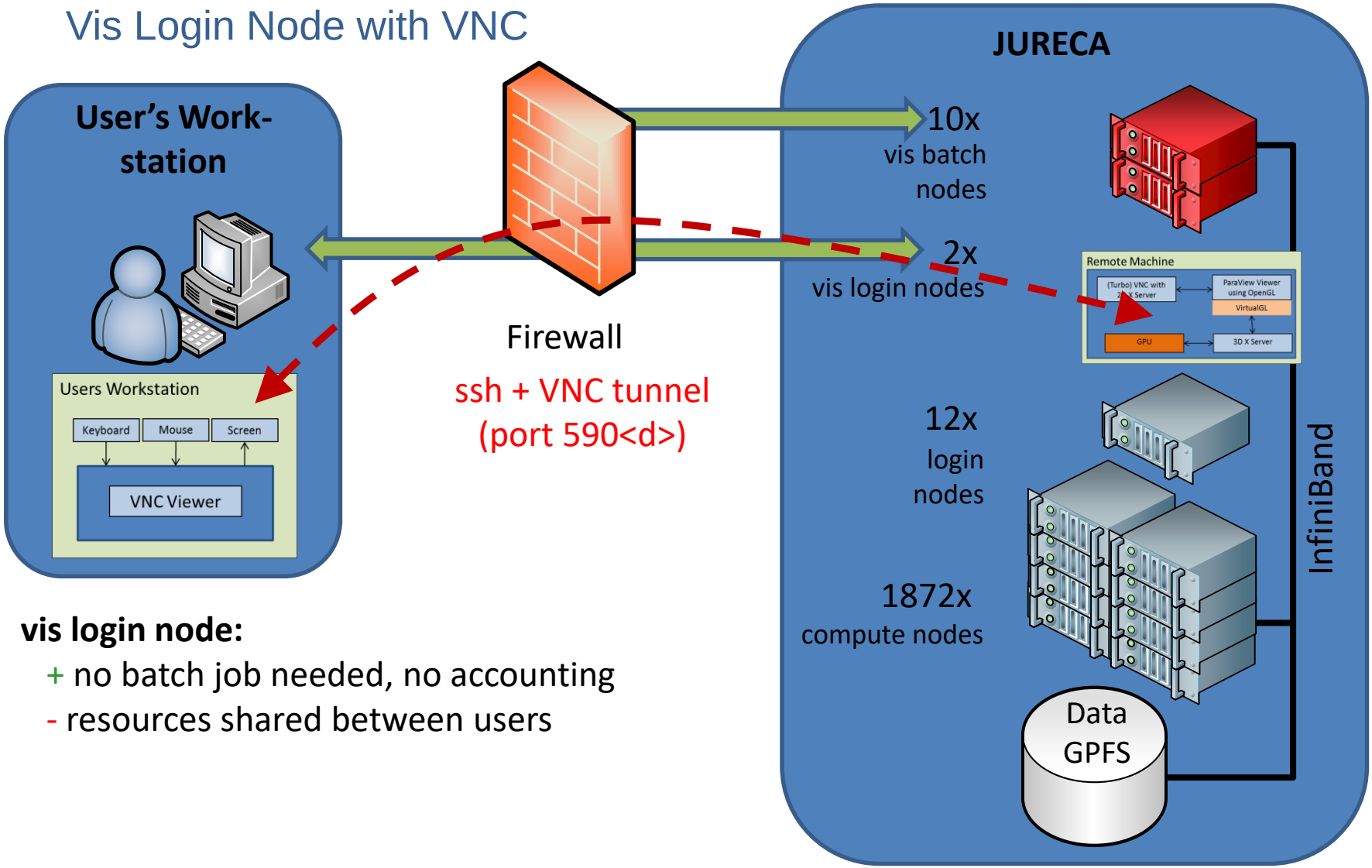
Desktop Profiles with VNC + VirtualGL



Remote 3D Visualization (possible scenarios)

Visualization Scenario 1:

Vis Login Node with VNC

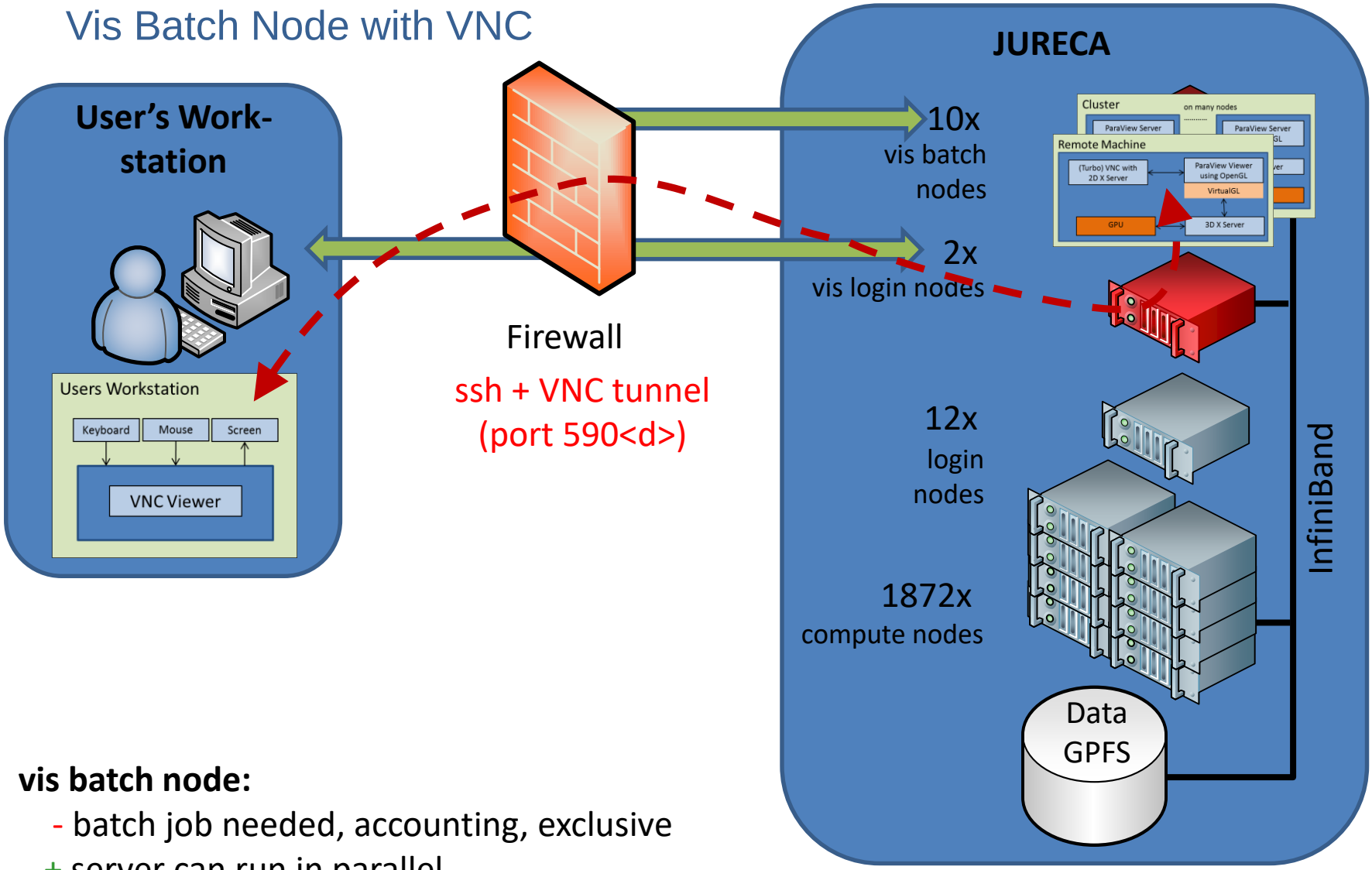


vis login node:

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

Visualization Scenario 2:

Vis Batch Node with VNC

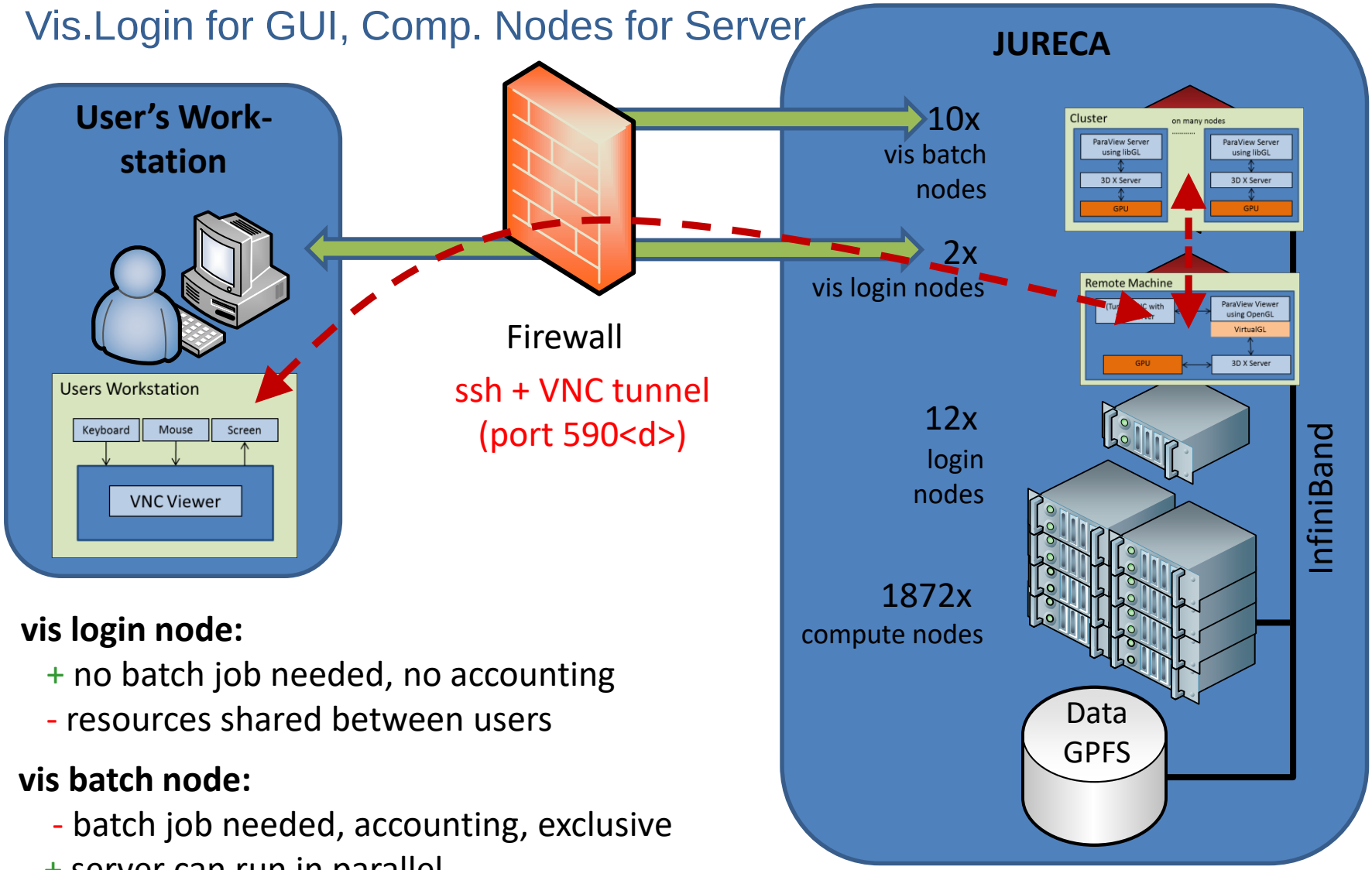


vis batch node:

- \- 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:

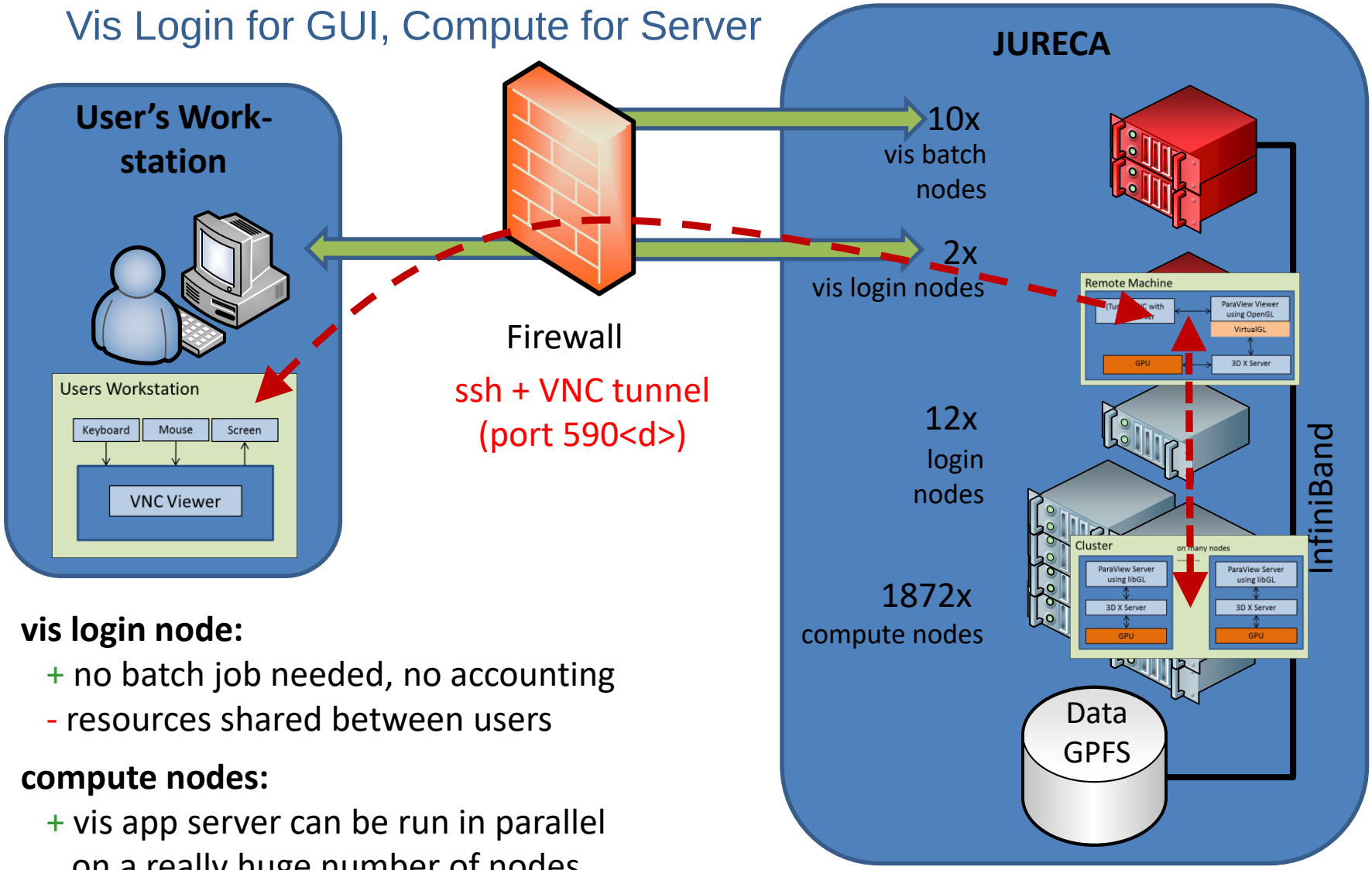
+ no batch job needed, no accounting
- resources shared between users

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:

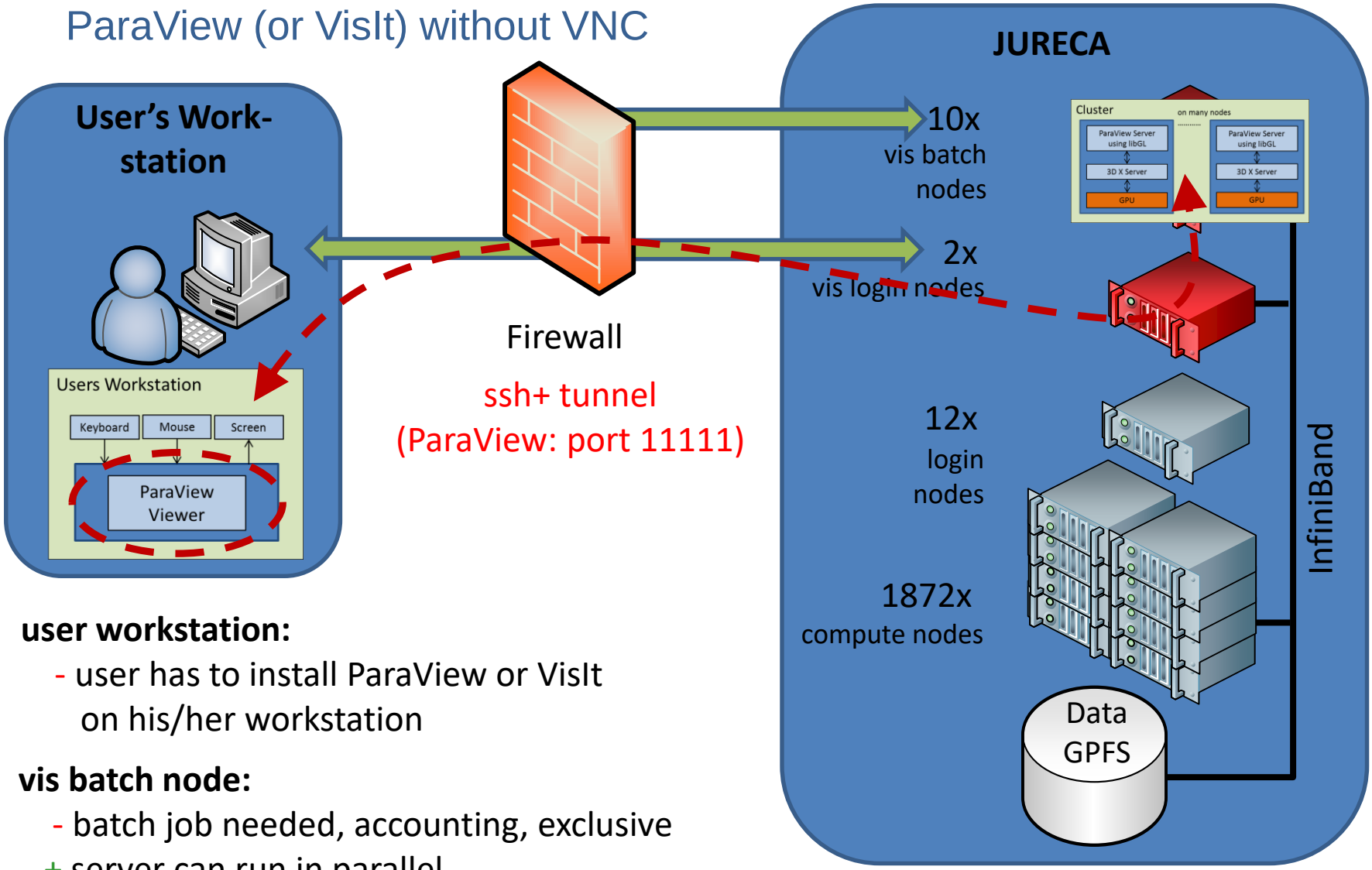
+ no batch job needed, no accounting
- resources shared between users

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.

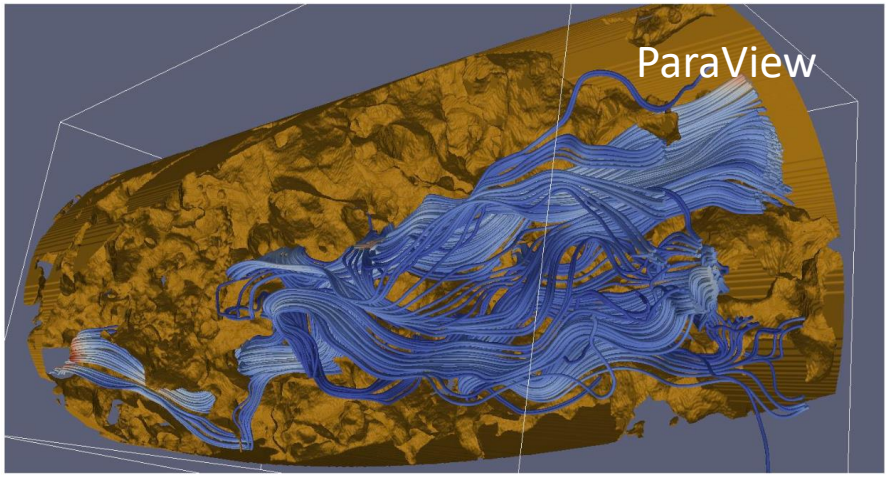
Our recommendation:
Use 'Xpra' as 'ssh –X' replacement.

https://xpra.org/

Nice To Know

Nice to know:

OSPRay



CPU ray tracing framework for scientific vis. rendering

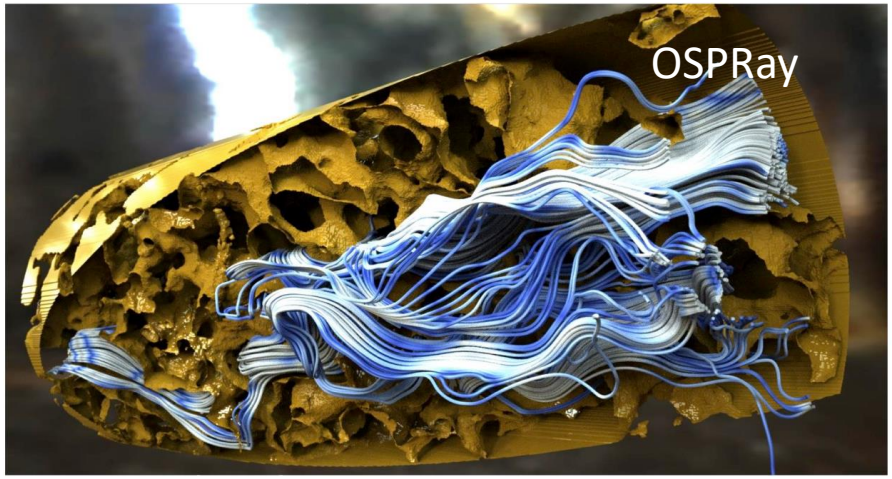
- efficient rendering on CPUs
- ray tracing / high fidelity rendering
- made for scientific visualization

Built on top of

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

Integrated into

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

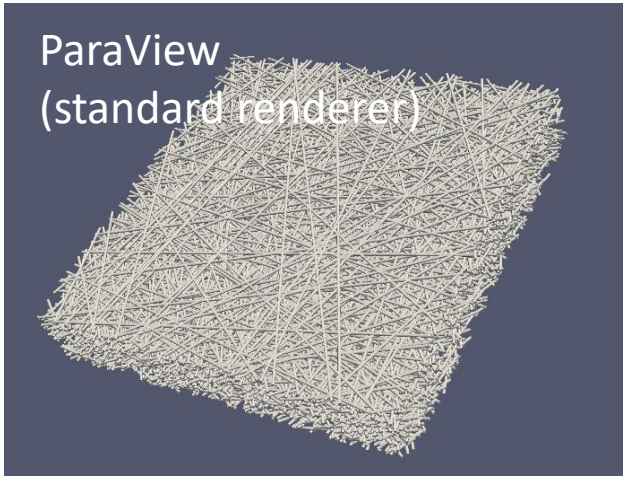


"FIU" Ground Water Simulation
Texas Advanced Computing Center (TACC) and Florida International University

http://www.ospray.org/
http://www.sdvis.org/ospray/download/talks/IEEEVis2016_OSPRay_talk.pdf

Nice to know:

OSPRay with ParaView

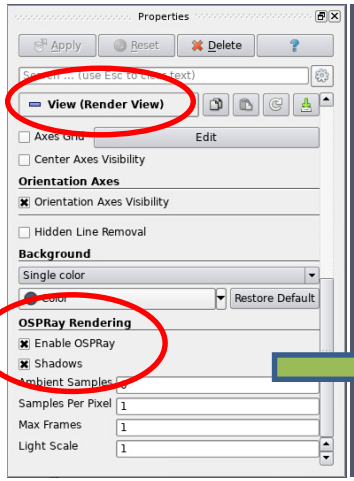


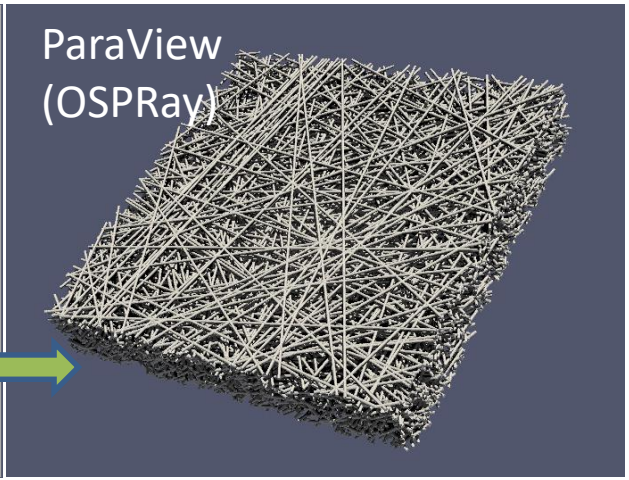
Ray tracing within ParaView

- 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

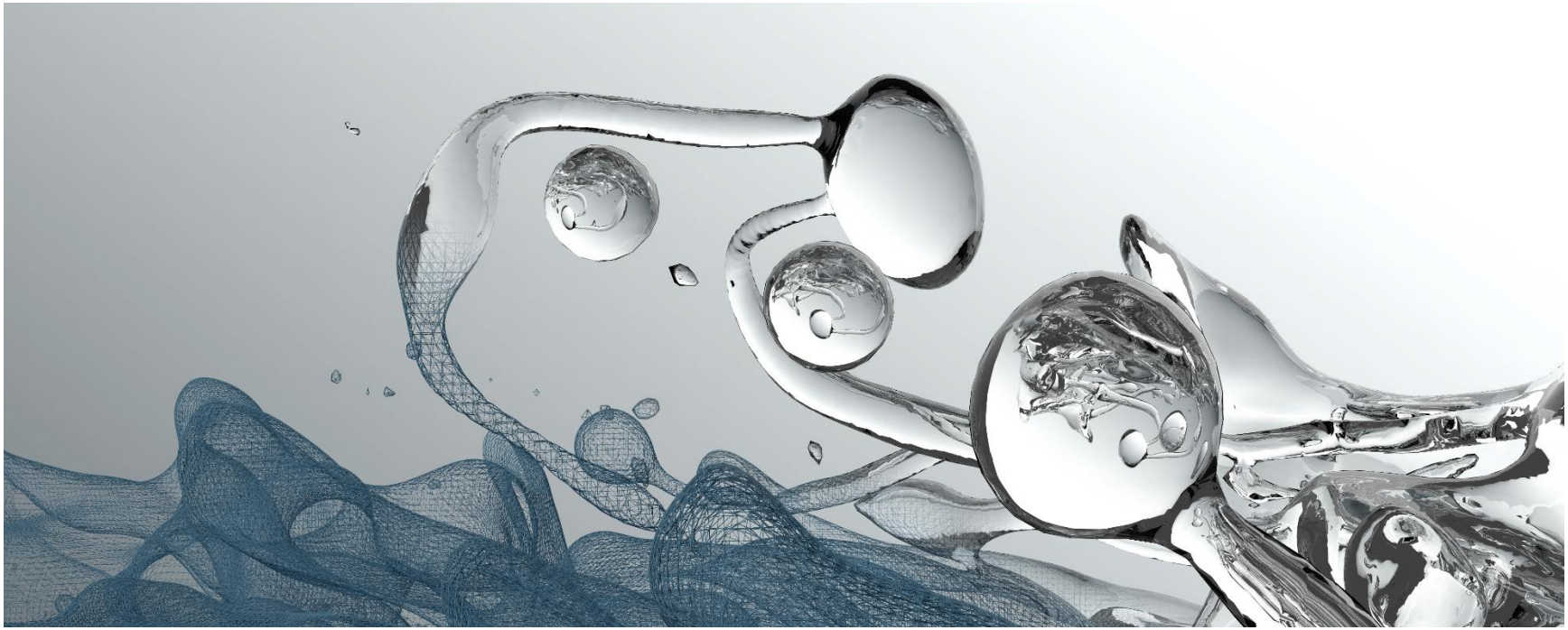
Please visit

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

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Interactive Supercomputing at Jülich Supercomputing Centre

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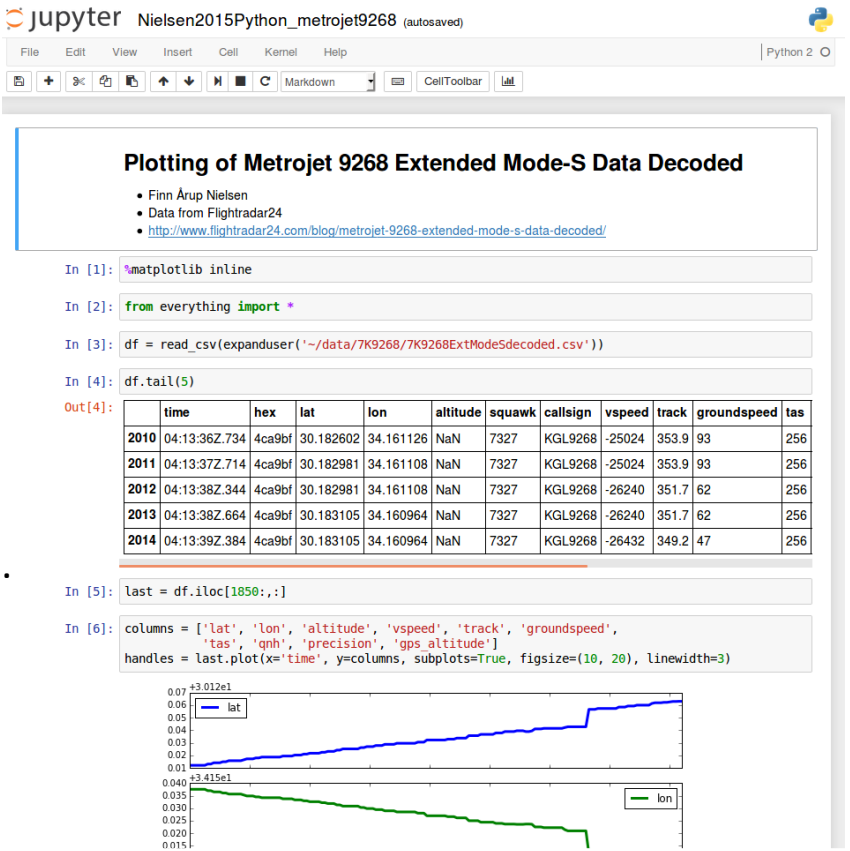
Interactive Supercomputing

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



https://trac.version.fz-juelich.de/vis/wiki/Jupyter

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.

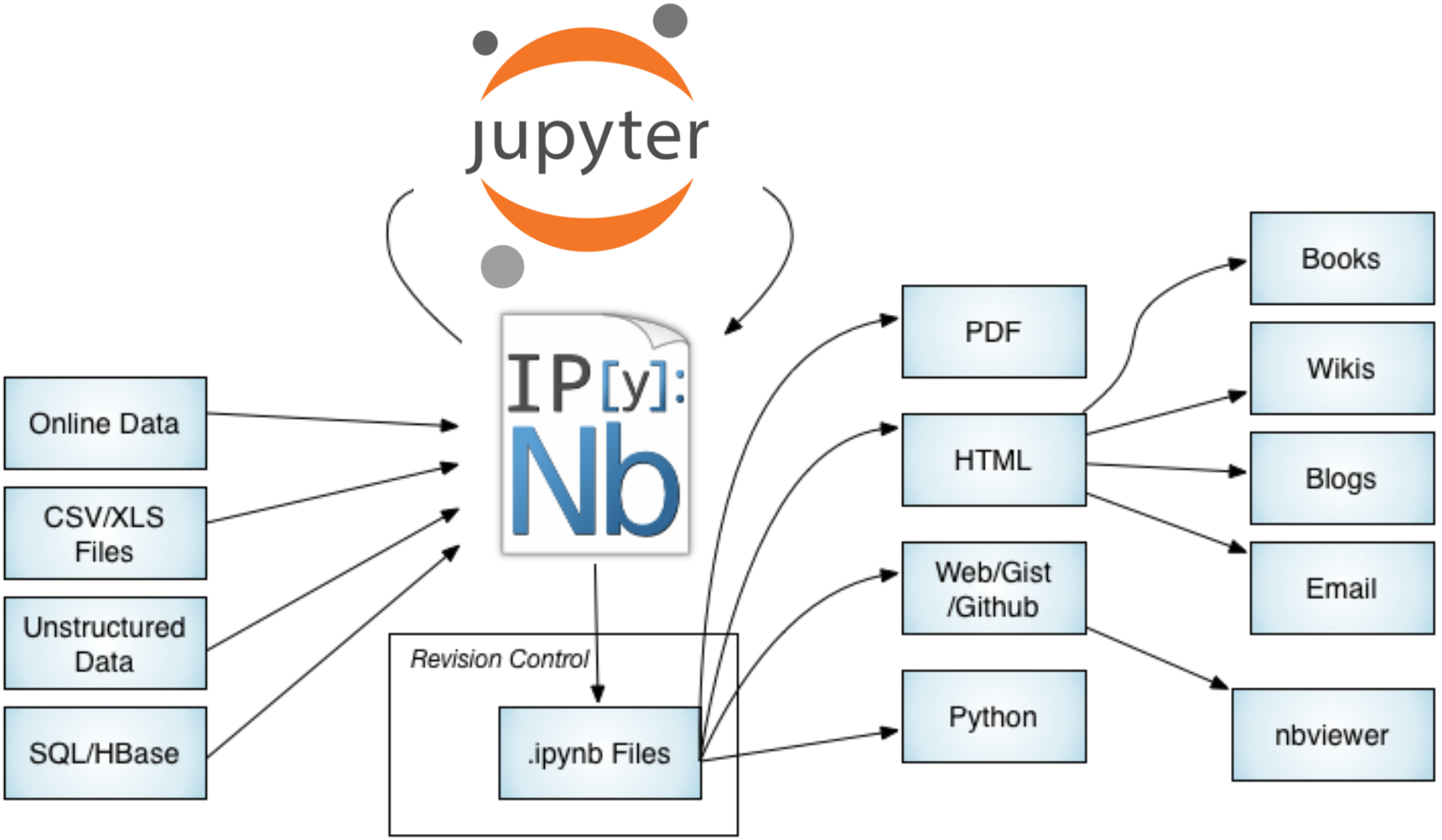
Even if the widely applicable libraries and tools for this are often open source projects (such as NumPy, TensorFlow, …), the specific code researchers write for a particular piece of work is often **left unpublished, hindering reproducibility**.

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

https://trac.version.fz-juelich.de/vis/wiki/Jupyter

Interactive Supercomputing

Why you should use Jupyter



https://trac.version.fz-juelich.de/vis/wiki/Jupyter

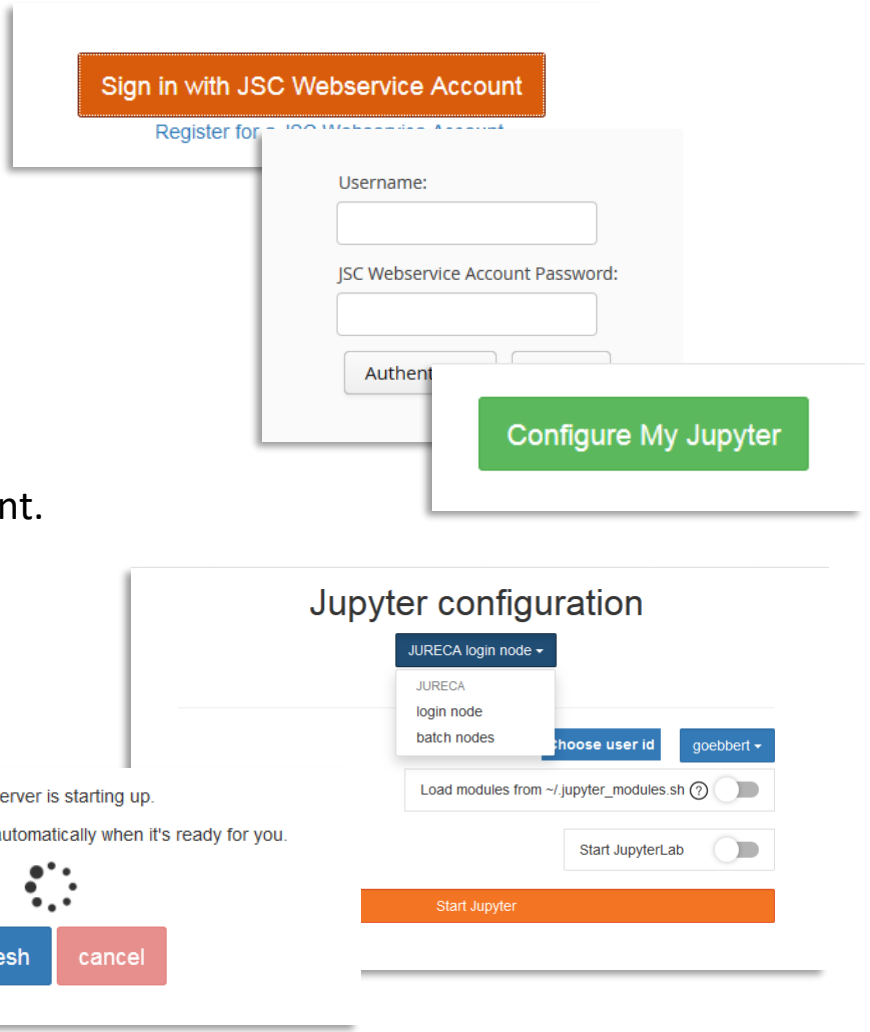
Interactive Supercomputing

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.

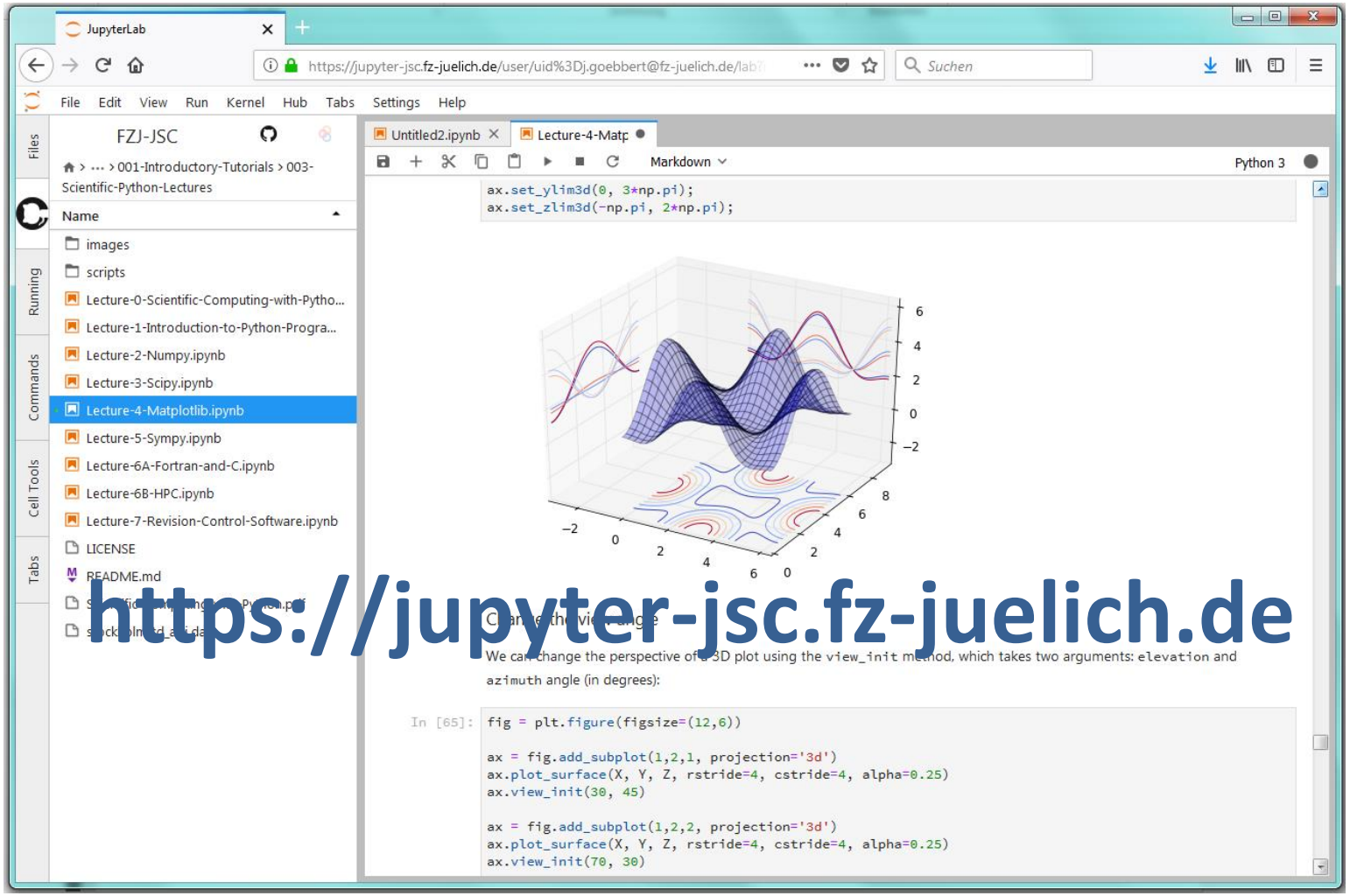
... and you are ready to start with Jupyter.



https://trac.version.fz-juelich.de/vis/wiki/Jupyter

Interactive Supercomputing

JupyterLab



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

https://trac.version.fz-juelich.de/vis/wiki/Jupyter