LUND UNIVERSITY

Scientific Computing in Python and Fortran

COMPUTE HT/2022

About me – Jonas Lindemann

- Programmed Computers since 1980
  - ABC 80 (Swedish school computer)
  - ABC 800/806
  - Texas TI99/4A (Failed 16-bit home computer)
  - Commodore 64/128
  - Commodore Amiga
  - PC
- Worked at the university since 1998
- Graduated as a Civil Engineer
- PhD in Structural Mechanics
- Worked at LUNARC
  - 2004 - Systems engineer
  - 2009 - Technical Director
  - 2012 – Director

”Scientific Computing Nerd”

Programming languages

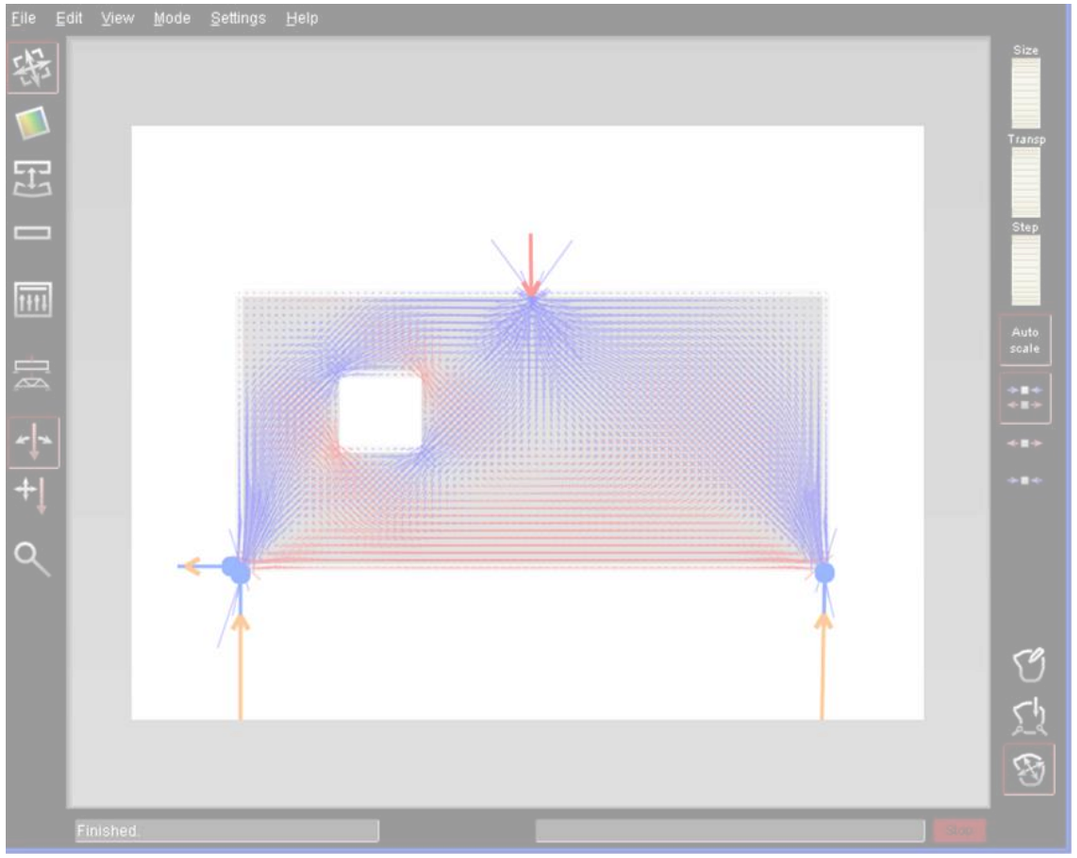
- Object Pascal – Since early 1990.
- C++ - since 1990 and forward.
- Fortran – Since 1998
- Java – Since 2002 (Not fulltime)
- Python 2.x and 3.x since 2003
- Processing
- Javascript

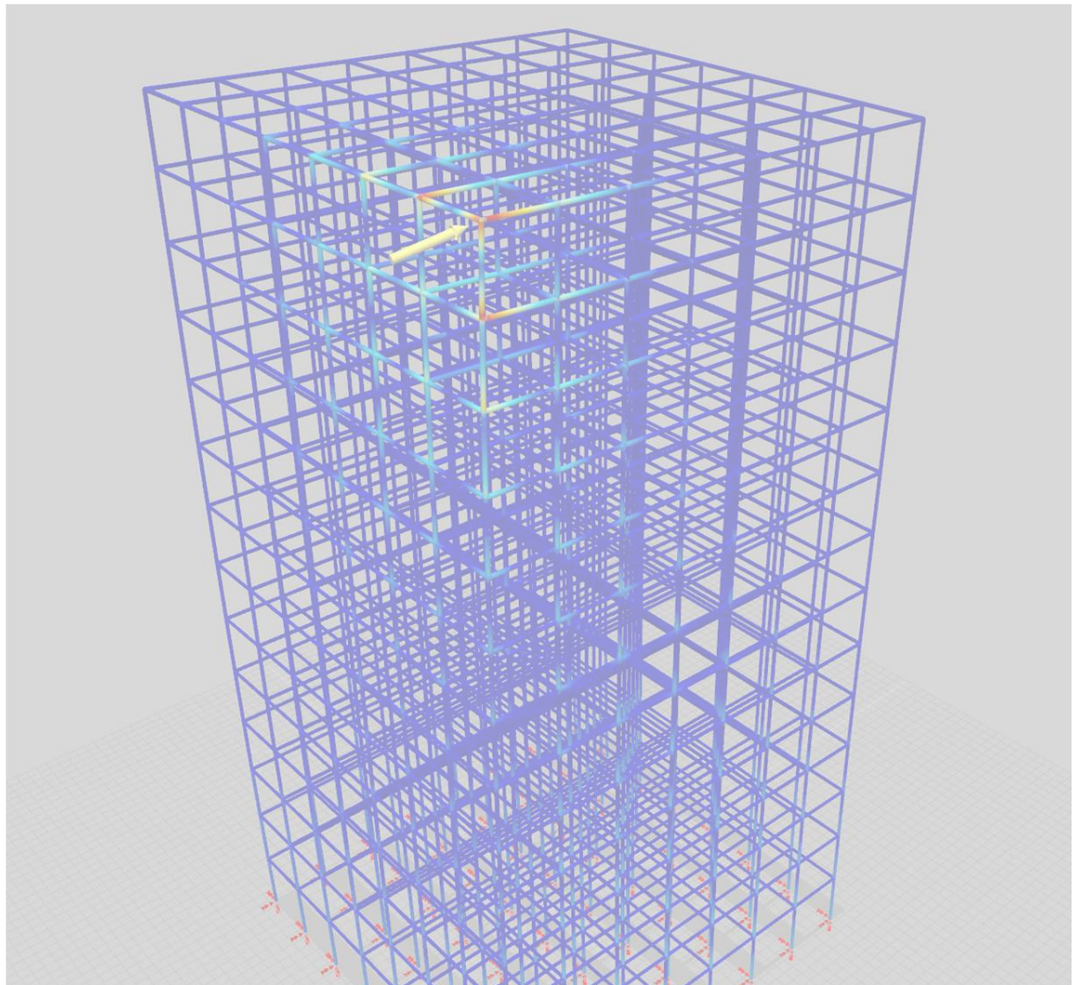




Developed software / libraries

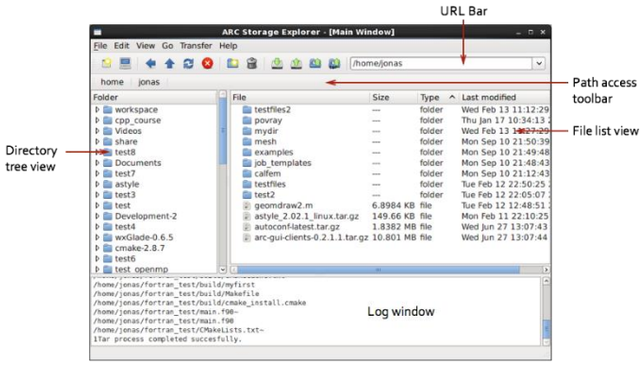
- ForcePAD and ForcePAD/R educational software, https://github.com/jonaslindemann/forcepad, Division of Structural Mechanics, Lund University, 2005-
- ObjectiveFrame educational software, https://github.com/jonaslindemann/objectiveframe, Division of Structural Mechacnis, Lund University, 2005
- Fortran Interface Wizard – Pascal / Fortran interrface generator, http://www.byggmek.lth.se/resources/fiwizard/fiwizard.htm, Division of Structural Mechanics, Lund University, 2005
- Interactive Visualisation Framework Ivf++ - OpenGL based visualisation library, https://github.com/jonaslindemann/ivfplusplus, Division of Structural Mechanics, Lund University, 2005

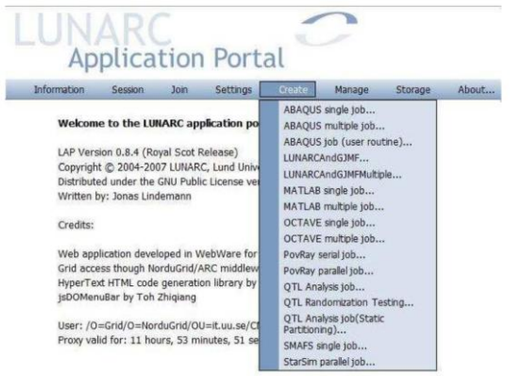


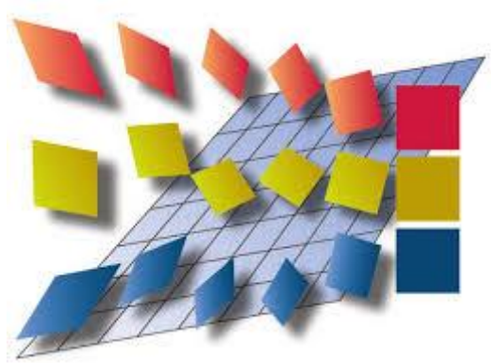


Developed software / libraries

- CALFEM - A Finite Element Toolbox, version 3.4, https://github.com/CALFEM, Division of Structural Mechanics and Solid Mechanics, 2005
- Lunarc Application Portal, https://github.com/lunarc/laportal, Lunarc, Lund University, 2003-
- FreeDev – A development environment for Python/Fortran integration, Division of Structural Mechanics, Lund University, 2005-
- ARC Graphical Clients, https://github.com/jonaslindemann/arc-gui-clients, Lunarc, Lund University, 2010-
- Python implementation of CALFEM, https://github.com/CALFEM/calfem-python, Division of Structural Mechanics, Lund University, 2009-

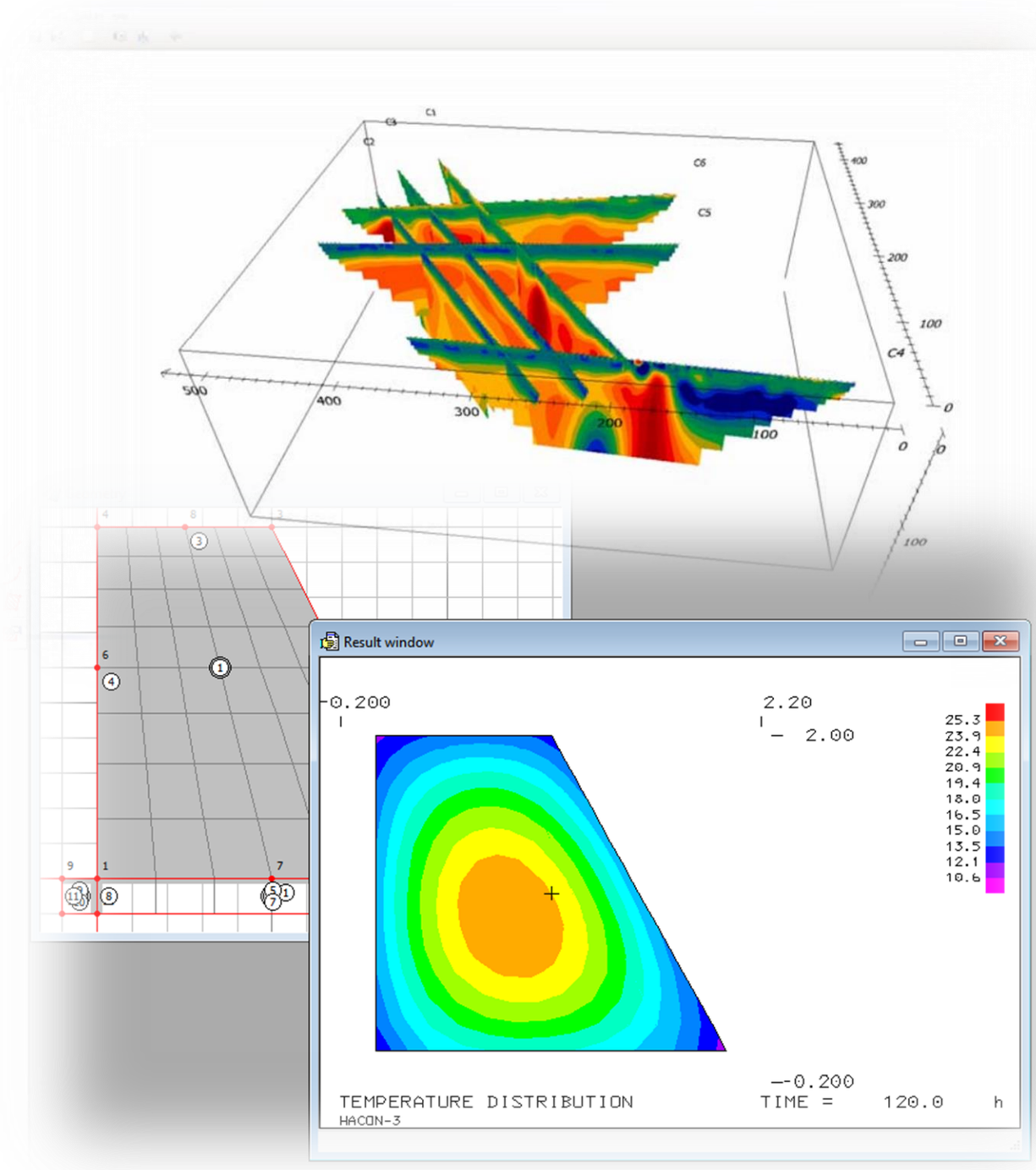






Developed software / libraries

- ***EriViz – Application for viewing pseudo section in 3D***, Zoom Media, 2010
- ***GfxLauncher – An Interactive application launcher for SLURM***, Lunarc, 2015-
- ***ml-browser – An interactive module browser for LMOD***, Lunarc, 2019-
- ***Hacon – Simulation software for hardening Concrete,*** Division of Structural Mechanics, 1997-



Developed software / libraries

- ***Qt Creator Fortran Extensions***, https://github.com/jonaslindemann/qtcreator-fortran, Lunarc, 2019-
- ***SteadyPitch – Pitch application for iPhone,*** **Zoom Media**, 2015
- ***MxDisplay – Software for electronic display for use in Motocross***, Open Source, 2018
- **Weather station with Particle IoT integrating with Google services,** 2020
- ***CadCanvas – Delphi components for generating CAD drawings***, Zoom Media, 2012
- ***eTool – A Java application for lamination simulation for TetraPak***, Division of Structural Mechanics, 2009

Course modules

- Introduction to Python
- Matrix computing with Python
- Plotting with Matplotlib
- Built-in functions and I/O
- Object-oriented programming in Python
- Data processing and visualisation
- User interfaces in Qt
- Fortran
- Mixed Language Programming

- Short assignments for each module
- Project assignment at the end
  - PhD related or given
- Lectures Mondays, see Canvas
- Tutorials Thursdays, see Canvas

Course administraton

- All course communication through Canvas
- Assignments turned in through Canvas
- I will try to answer comments through Canvas as soon as possible

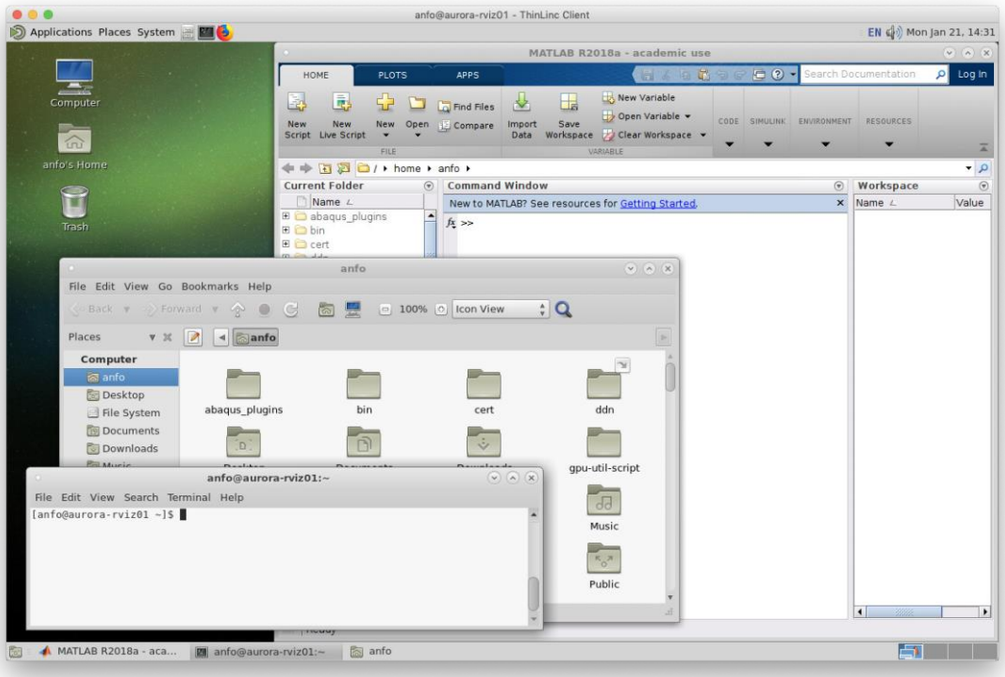
Course literature

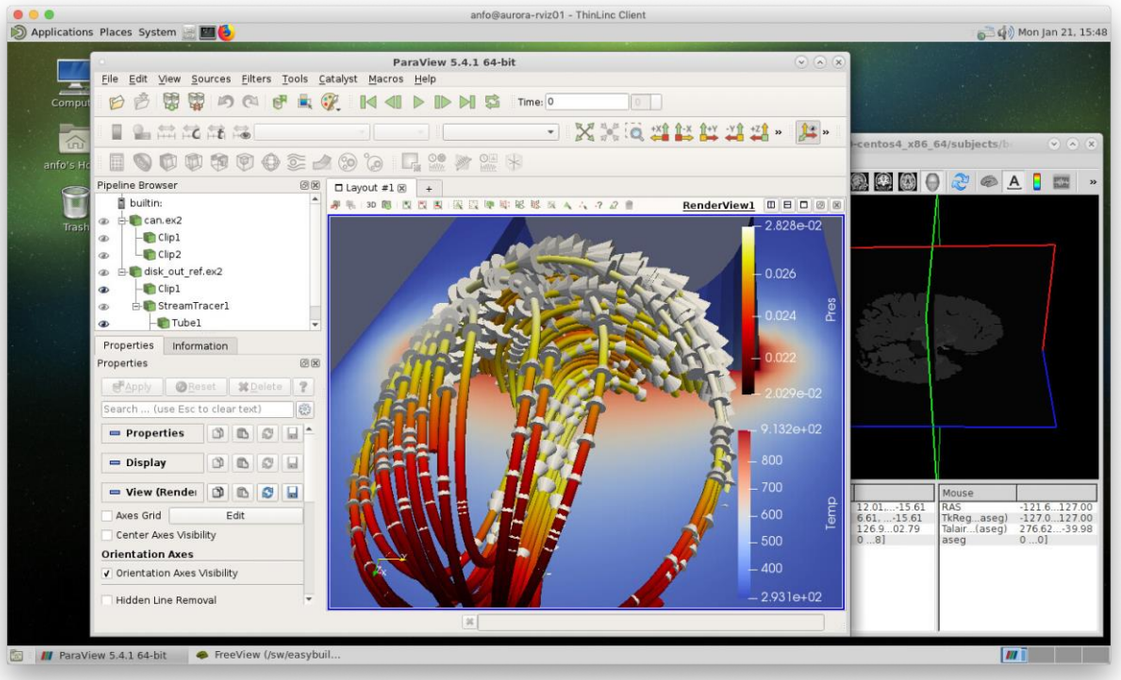
- Web based material
  - How To Think Like a Computer Scientist (Links to an external site.)
  - Kurs i Python (Links to an external site.)
  - Numpy guide
- Books
  - Ingenjörens Guide till Python, Jonas Lindemann, Studentlitteratur (Links to an external site.) (Links to an external site.)
  - Learning Python (Links to an external site.), Mark Lutz, David Ascher, O'Reilly
  - Programming Python Second Edition (Links to an external site.), Mark Lutz, O'Reilly
  - Python Scripting for Computational Science (Links to an external site.), Langtangen, Hans P, Springer

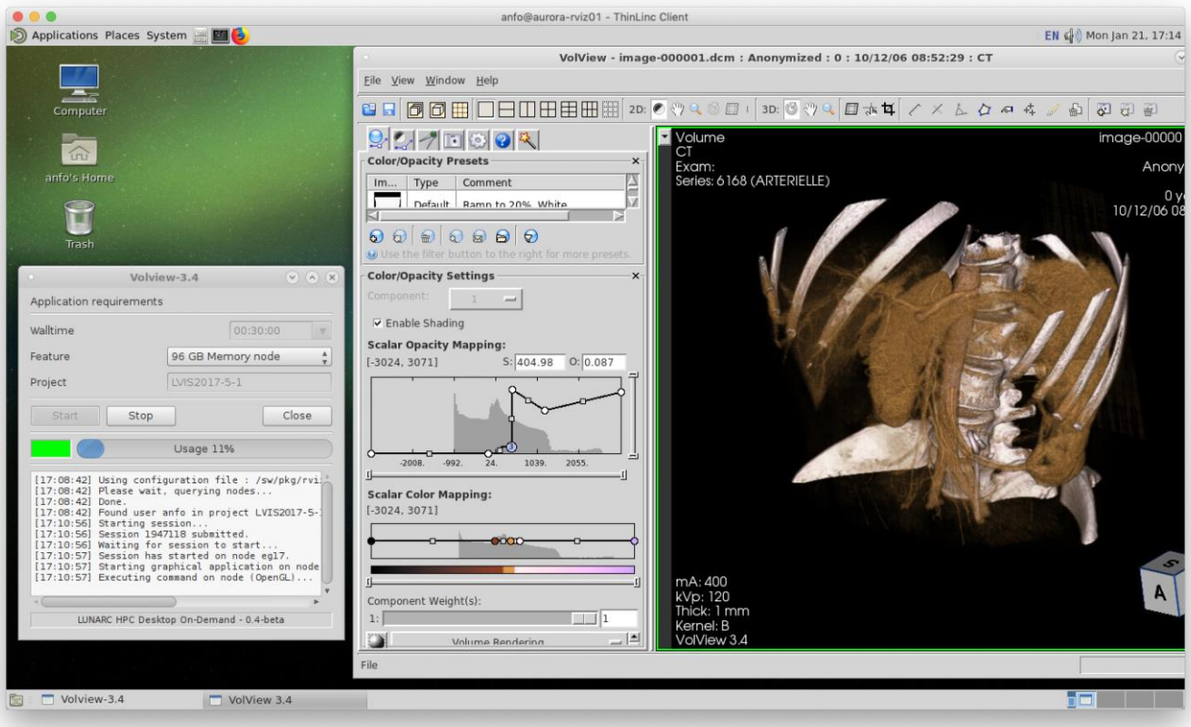
LUNARC

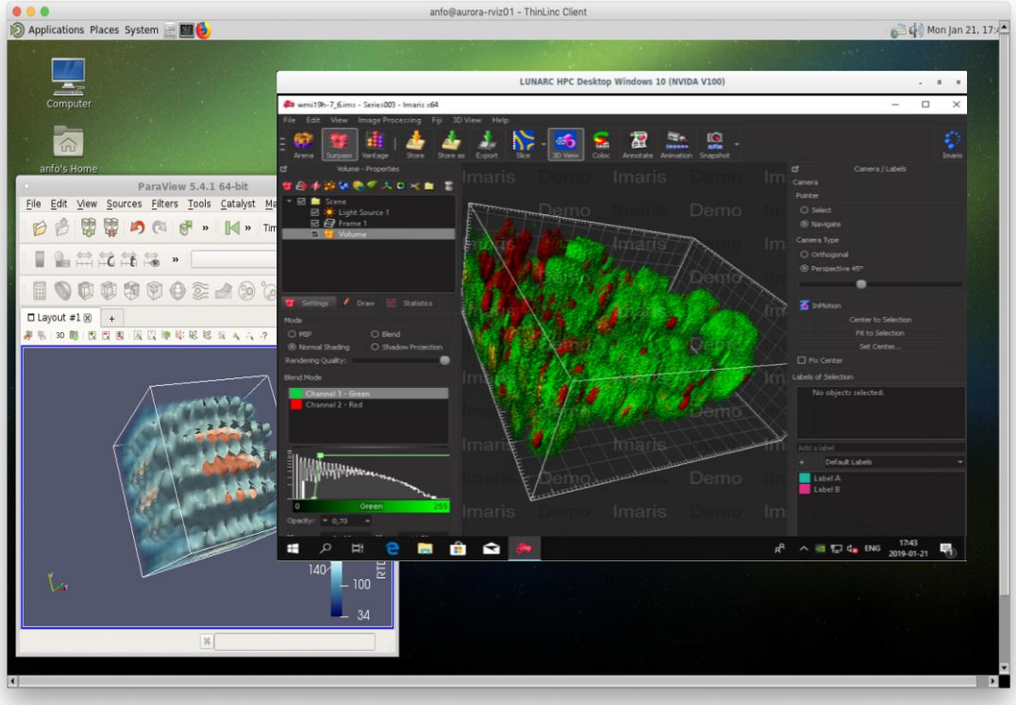
- Center for Scientific and Technical Computing
- High Performance Computing (HPC) resources at LU
- Training and education in using HPC resources
- Environment for performing scientific computing
  - Interactive HPC environment with hardware accelerated graphics
  - 300 computing nodes for running scientific codes
  - ~700 software scientific packages available
- For more information see
  - www.lunarc.lu.se

LUNARC HPC Desktop










SETTING UP A PYTHON
ENVIRONMENT

Installing Anaconda Python

Installing Anaconda

- Anaconda Python is prepackaged Python distribution for Scientific Computing
- Download from https://www.anaconda.com
- **Windows:** Creates shortcuts for starting an Anaconda Prompt on Windows. ”Anaconda Prompt”
- **macOS:** Modifies environment to replace the default Python with Anaconda Python-environment.
- **Linux:** Modifies environment to replace the default Python with Anaconda Python-environment.

Different ways of running Python