

# Cloud-basierte Web-Anwendungen und Jupyter Notebooks im Zusammenhang mit globalen Luftqualitätsdaten

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With a lot of material from

## **JUPYTERLAB - SUPERCOMPUTING IN YOUR BROWSER**

Training course "Introduction to the usage and programming of supercomputer resources in Jülich"

2022-05-16 | JENS H. GÖBBERT (J.GOEBBERT@FZ-JUELICH.DE)

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## Tropospheric Ozone Assessment Report (TOAR)

*Global metrics for climate change, human health and crop/ecosystem research*



### Mission:

To provide the research community with an up-to-date scientific assessment of tropospheric ozone's global distribution and trends from the surface to the tropopause.

### Deliverables:

- 1) The first tropospheric ozone assessment report based on all available surface observations, the peer-reviewed literature and new analyses.
- 2) A database containing ozone exposure metrics at thousands of measurement sites around the world, freely accessible for research on the global-scale impact of ozone on climate, human health and crop/ecosystem productivity.

### Stakeholders:

Member of the Heimholtz A:



Task Force on Hemispheric  
Transport of Air Pollution



**JÜLICH**  
Forschungszentrum

# TOAR-I publications in Elementa

<https://collections.elementascience.org/toar>



**ELEMENTA**  
Wang, P. et al. 2018. Tropospheric Ozone Assessment Report: Assessment of global-scale model performance for global and regional ozone distributions, variability, and trends. *Elem Sci Ann* 9: 10. DOI: <https://doi.org/10.1525/elementa.2018.09.001>

**REVIEW**  
**Tropospheric Ozone Assessment Report: Assessment of global-scale model performance for global and regional ozone distributions, variability, and trends**  
P. J. Young<sup>1,2,3</sup>, V. Naik<sup>4</sup>, A. M. Fiore<sup>5</sup>, A. Gaudel<sup>6,7</sup>, J. Guo<sup>8</sup>, M. Y. Lin<sup>9,10</sup>, J. L. Neel<sup>11</sup>, D. D. Parrish<sup>12</sup>, H. E. Rieber<sup>13</sup>, J. L. Schaeff<sup>14</sup>, S. Timmes<sup>15</sup>, O. Wild<sup>16</sup>, L. Zhang<sup>17</sup>, J. Ziemke<sup>18,19</sup>, J. Brandt<sup>20</sup>, A. Delic<sup>21</sup>, R. M. Doherty<sup>22</sup>, C. Germon<sup>23</sup>, M. I. Heggli<sup>24</sup>, L. Hu<sup>25</sup>, U. Irm<sup>26</sup>, R. Kumar<sup>27</sup>, A. Lohar<sup>28</sup>, L. Murray<sup>29</sup>, D. Plummer<sup>30</sup>, J. Rodriguez<sup>31</sup>, A. Salas-Lopez<sup>32</sup>, M. G. Schultz<sup>33,34</sup>, M. T. Woodhouse<sup>35</sup> and G. Zeng<sup>36</sup>

**ELEMENTA**  
Schult, M.G. et al. 2017. Tropospheric Ozone Assessment Report: Database and metrics data of global surface ozone observations. *Elem Sci Ann* 8: 5. DOI: <https://doi.org/10.1525/elementa.2017.08.005>

**RESEARCH ARTICLE**  
**Tropospheric Ozone Assessment Report: Database and metrics data of global surface ozone observations**  
Martin G. Schultz<sup>1,2</sup>, Sabine Schroder<sup>1</sup>, Olga Lyapina<sup>1</sup>, Owen R. Cooper<sup>3,4</sup>, Ian Galbally<sup>5</sup>, Irina Petropavlovskikh<sup>6,7</sup>, Erika von Schneidmesser<sup>8</sup>, Hiroshi Tanimoto<sup>9</sup>, Yassin Eshorabany<sup>10</sup>, Manish Naja<sup>11</sup>, Rodrigo J. Seguel<sup>12</sup>, Ute Damer<sup>13</sup>, Paul Eckhardt<sup>14</sup>, Stefan Feigenson<sup>15</sup>, Markus Fliebig<sup>16</sup>, Anne-Gunn Hjeltnes<sup>17</sup>, You-Doog Hong<sup>18</sup>, Peter Christian Kjaer<sup>19</sup>, Hiroaki Kohda<sup>20</sup>, Gary Lear<sup>21</sup>, David Tarasick<sup>22</sup>, Mikko Ueno<sup>23</sup>, Markus Walksch<sup>24</sup>, Darrel Boumgarner<sup>25</sup>, Ming-Tung Chung<sup>26</sup>, Robert Gillett<sup>27</sup>, Meehye Lee<sup>28</sup>, Suzie Molloy<sup>29</sup>, Raeesa Moolali<sup>30</sup>, Tao Wang<sup>31</sup>, Katrina Sharps<sup>32</sup>, Jose A. Adams<sup>33</sup>, Gerard Ancellet<sup>34</sup>, Francesco Apolloni<sup>35</sup>, Paulo Artaxo<sup>36</sup>, Maria E. Barreira<sup>37</sup>, Magdalena Bogucka<sup>38</sup>, Paolo Bonasoni<sup>39</sup>, Limsook Chung<sup>40</sup>

**ELEMENTA**  
Archibald, A. T. et al. 2020. Tropospheric Ozone Assessment Report: A critical review of changes in the tropospheric ozone burden and budget from 1850 to 2100. *Elem Sci Ann* 11: 1. DOI: <https://doi.org/10.1525/elementa.2020.11.001>

**RESEARCH ARTICLE**  
**Tropospheric Ozone Assessment Report: A critical review of changes in the tropospheric ozone burden and budget from 1850 to 2100**  
A. T. Archibald<sup>1,2,3,4</sup>, J. L. Neel<sup>5,6</sup>, Y. F. Eshorabany<sup>7</sup>, O. R. Cooper<sup>8,9</sup>, P. J. Young<sup>10,11</sup>, H. Akiyoshi<sup>12</sup>, R. A. Cox<sup>13</sup>, M. Coyle<sup>14,15</sup>, R. G. Derwent<sup>16</sup>, M. Dutsch<sup>17</sup>, A. Finco<sup>18</sup>, G. J. Frost<sup>19</sup>, I. E. Galbally<sup>20,21</sup>, G. Gerost<sup>22</sup>, C. Granje<sup>23,24</sup>, P. T. Griffiths<sup>25</sup>, J. R. Hossain<sup>26</sup>, L. Hu<sup>27</sup>, P. Jöckel<sup>28</sup>, B. Josse<sup>29</sup>, M. Y. Lin<sup>30</sup>, M. Mertes<sup>31</sup>, D. Morgenstern<sup>32</sup>, M. Naja<sup>33</sup>, V. Naik<sup>34</sup>, S. Ohtsuna<sup>35</sup>, D. A. Plummer<sup>36</sup>, L. L. Revelle<sup>37</sup>, A. Salas-Lopez<sup>38</sup>, P. Savijärvi<sup>39</sup>, Y. M. Shin<sup>40</sup>, I. Shalunov<sup>41</sup>, D. Shalunov<sup>42</sup>, S. Timmes<sup>43</sup>, T. Trick<sup>44</sup>, T. J. Wallington<sup>45</sup>, T. Wang<sup>46</sup>, H. M. Worden<sup>47</sup>, and G. Zeng<sup>48</sup>

**ELEMENTA**  
Lefohn, A.L. et al. 2018. Tropospheric ozone assessment report: Present-day metrics for climate change, human health, and ecosystem research. *Elem Sci Ann* 9: 26. DOI: <https://doi.org/10.1525/elementa.2018.09.026>

**RESEARCH ARTICLE**  
**Tropospheric ozone assessment report: Global ozone metrics for climate change, human health, and crop/ecosystem research**  
Allen S. Lefohn<sup>1</sup>, Christopher S. Malley<sup>2,3,4</sup>, Luther Smith<sup>5</sup>, Benjamin Wells<sup>6</sup>, Milan Habuch<sup>7</sup>, Heather Simon<sup>8</sup>, Vaishali Nair<sup>9</sup>, Gina Mills<sup>10</sup>, Martin G. Schultz<sup>11</sup>, Elena Paoletti<sup>12</sup>, Alessandra De Marco<sup>13</sup>, Xiaobin Xu<sup>14</sup>, Li Zhang<sup>15</sup>, Tao Wang<sup>16</sup>, Howard S. Neufeld<sup>17</sup>, Robert C. Musselman<sup>18</sup>, David Tarasick<sup>19</sup>, Michael Brauer<sup>20</sup>, Zhaozhong Feng<sup>21</sup>, Haoye Tang<sup>22</sup>, Kazuhiko Kobayashi<sup>23</sup>, Pierre Sicard<sup>24</sup>, Sverre Solberg<sup>25</sup> and Giacomo Gerost<sup>26</sup>

**ELEMENTA**  
Mills, G. et al. 2018. Tropospheric Ozone Assessment Report: Present-day tropospheric ozone distribution and trends relevant to vegetation. *Elem Sci Ann* 9: 38. DOI: <https://doi.org/10.1525/elementa.2018.09.038>

**RESEARCH ARTICLE**  
**Tropospheric Ozone Assessment Report: Present-day distribution and trends of tropospheric ozone relevant to climate and global atmospheric chemistry model evaluation**  
A. Gaudel<sup>1,2</sup>, O. R. Cooper<sup>3,4</sup>, G. Ancellet<sup>5</sup>, B. Barret<sup>6</sup>, A. Boyard<sup>7</sup>, J. P. Burrows<sup>8</sup>, C. Clerbaux<sup>9</sup>, P.-F. Coheur<sup>10</sup>, J. Cuesta<sup>11</sup>, E. Cuevas<sup>12</sup>, S. Donkai<sup>13</sup>, F. Ebojite<sup>14</sup>, G. Foret<sup>15</sup>, O. Garcia<sup>16</sup>, M. J. Granados-Muñoz<sup>17,18</sup>, J. W. Hansigan<sup>19</sup>, F. Hase<sup>20</sup>, B. Hassler<sup>21,22</sup>, G. Huang<sup>23</sup>, D. Harman<sup>24</sup>, D. Jeffery<sup>25</sup>, N. Jones<sup>26</sup>, P. Kalabokidis<sup>27</sup>, B. Kerridge<sup>28</sup>, S. Kulshwick<sup>29</sup>, B. Laster<sup>30</sup>, T. Leblanc<sup>31</sup>, E. Le Flochort<sup>32</sup>, W. Lin<sup>33</sup>, J. Liu<sup>34</sup>, X. Liu<sup>35</sup>, E. Mahieu<sup>36</sup>, A. McClure-Begley<sup>37</sup>, J. L. Neel<sup>38</sup>, M. Osman<sup>39</sup>, M. Palmi<sup>40</sup>, H. Petetin<sup>41</sup>, I. Petropavlovskikh<sup>42</sup>, R. Quenne<sup>43</sup>, N. Rahn<sup>44</sup>, A. Rozanov<sup>45</sup>, M. G. Schultz<sup>46</sup>, J. Schwab<sup>47</sup>, S. Siddons<sup>48</sup>, D. Smeets<sup>49</sup>, M. Steinbacher<sup>50</sup>, T. Tamoto<sup>51</sup>, D. W. Tarasick<sup>52</sup>, U. Thouret<sup>53</sup>, A. M. Thompson<sup>54</sup>, T. Trick<sup>55</sup>, E. Weatherhead<sup>56</sup>, C. Wespes<sup>57</sup>, H. M. Worden<sup>58</sup>, C. Vigouroux<sup>59</sup>, X. Xu<sup>60</sup>, G. Zeng<sup>61</sup>, J. Ziemke<sup>62</sup>

**ELEMENTA**  
Tarasick, D. et al. 2010. Tropospheric Ozone Assessment Report: Trends in surface ozone from 1877 to 2010, observed levels, trends and uncertainties. *Elem Sci Ann* 1: 36. DOI: <https://doi.org/10.1525/elementa.2010.01.036>

**REVIEW**  
**Tropospheric Ozone Assessment Report: Tropospheric ozone from 1877 to 2016, observed levels, trends and uncertainties**  
David Tarasick<sup>1</sup>, Ian E. Galbally<sup>2</sup>, Owen R. Cooper<sup>3,4</sup>, Martin G. Schultz<sup>5</sup>, Gerard Ancellet<sup>6</sup>, Thierry Leblanc<sup>7</sup>, Timothy J. Wallington<sup>8</sup>, Jerry Ziemke<sup>9</sup>, Xiong L. Martin Steinbacher<sup>10</sup>, Johannes Staehelin<sup>11</sup>, Corinne Vigouroux<sup>12</sup>, James W. Hannigan<sup>13</sup>, Omaira Garcia<sup>14</sup>, Gilles Foret<sup>15</sup>, Prodroomos Zanis<sup>16</sup>, Elizabeth Weatherhead<sup>17</sup>, Irina Petropavlovskikh<sup>18</sup>, Kai-Lan Chang<sup>19</sup>, Ali A. Wahneema<sup>20</sup>, Jane Liu<sup>21</sup>, Juan Cuesta<sup>22</sup>, Gaelle Dufour<sup>23</sup>, Valerie Thouret<sup>24</sup>, George Stachurski<sup>25</sup>, Thomas Trick<sup>26</sup> and Jessica L. Neu<sup>27</sup>

**ELEMENTA**  
Fleming, S.J. et al. 2018. Tropospheric Ozone Assessment Report: Present-day ozone distribution and trends relevant to human health. *Elem Sci Ann* 9: 7. DOI: <https://doi.org/10.1525/elementa.2018.09.007>

**RESEARCH ARTICLE**  
**Tropospheric Ozone Assessment Report: Present-day ozone distribution and trends relevant to human health**  
Zoe L. Fleming<sup>1</sup>, Ruth M. Doherty<sup>2</sup>, Erika von Schneidmesser<sup>3</sup>, Christopher S. Malley<sup>4,5,6</sup>, Owen R. Cooper<sup>7,8</sup>, Joseph P. Pinto<sup>9</sup>, Augustin Colette<sup>10</sup>, Xiaobin Xu<sup>11</sup>, David Simmonds<sup>12</sup>, Martin G. Schultz<sup>13,14</sup>, Allen S. Lefohn<sup>15</sup>, Samira Homad<sup>16</sup>, Raeesa Moolali<sup>17</sup>, Sverre Solberg<sup>18</sup> and Zhaozhong Feng<sup>19</sup>

**ELEMENTA**  
Mills, G. et al. 2018. Tropospheric Ozone Assessment Report: Present-day tropospheric ozone distribution and trends relevant to vegetation. *Elem Sci Ann* 9: 38. DOI: <https://doi.org/10.1525/elementa.2018.09.038>

**RESEARCH ARTICLE**  
**Tropospheric Ozone Assessment Report: Present-day tropospheric ozone distribution and trends relevant to vegetation**  
Gina Mills<sup>1</sup>, Håkan Pleijel<sup>2</sup>, Christopher S. Malley<sup>3,4</sup>, Baerbel Sinha<sup>5</sup>, Owen R. Cooper<sup>6</sup>, Martin G. Schultz<sup>7</sup>, Howard S. Neufeld<sup>8</sup>, David Simmonds<sup>9</sup>, Katrina Sharps<sup>10</sup>, Zhaozhong Feng<sup>11</sup>, Giacomo Gerost<sup>12</sup>, Harry Harman<sup>13</sup>, Kazuhiko Kobayashi<sup>14</sup>, Pallavi Savanna<sup>15</sup>, Elena Paoletti<sup>16</sup>, Vinayak Sinha<sup>17</sup> and Xiaobin Xu<sup>18</sup>

**ELEMENTA**  
Chang, K.-L. et al. 2017. Regional trend analysis of surface ozone observations from monitoring networks in eastern North America, Europe and East Asia. *Elem Sci Ann* 8: 9. DOI: <https://doi.org/10.1525/elementa.2017.08.009>

**RESEARCH ARTICLE**  
**Regional trend analysis of surface ozone observations from monitoring networks in eastern North America, Europe and East Asia**  
Kai-Lan Chang<sup>1</sup>, Irina Petropavlovskikh<sup>2</sup>, Owen R. Cooper<sup>3</sup>, Martin G. Schultz<sup>4</sup> and Tao Wang<sup>5</sup>

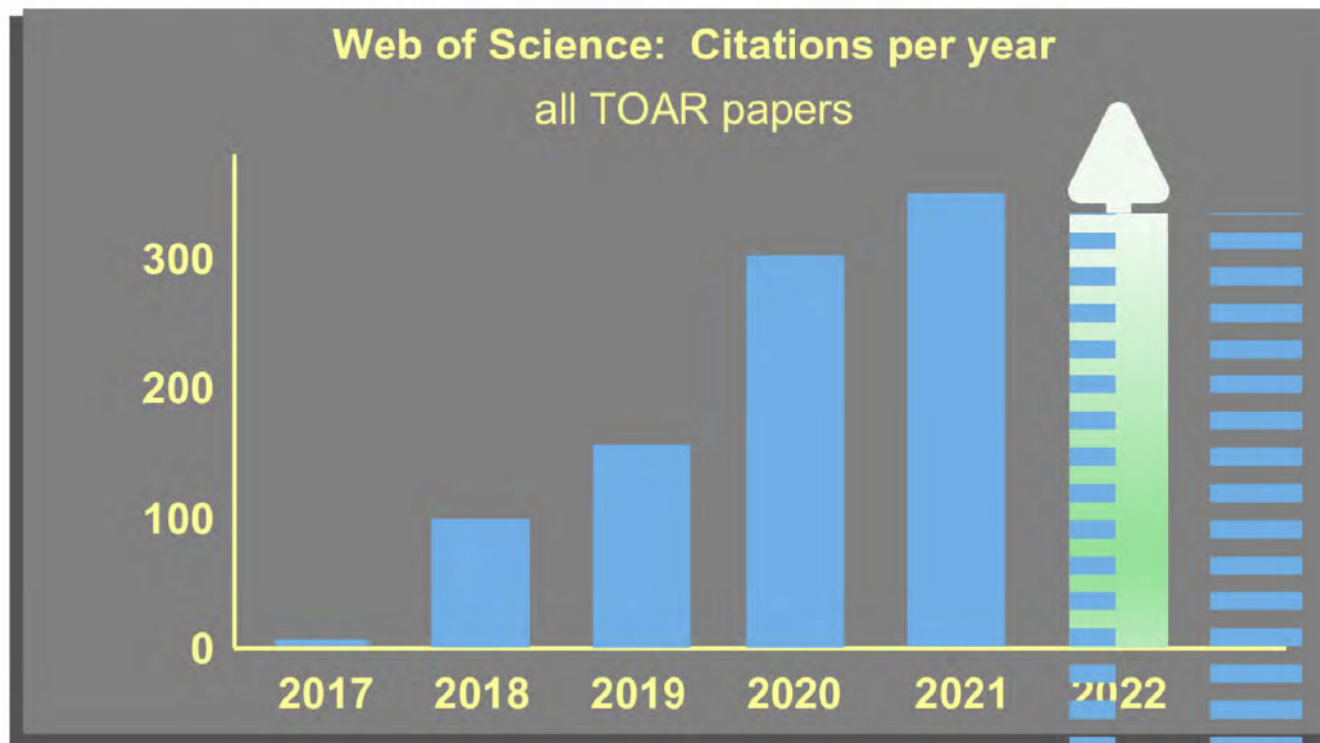
**ELEMENTA**  
Surface ozone is a greenhouse gas and pollutant detrimental to human health and crop and ecosystem productivity. The Tropospheric Ozone Assessment Report (TOAR) is designed to provide the research community with an up-to-date observation-based overview of tropospheric ozone's global distribution and trends. The TOAR Surface Ozone Database contains ozone metrics at thousands of monitoring sites.

**ELEMENTA**  
Xu, X. et al. 2020. Long-term changes of regional ozone in China: implications for human health and ecosystem impacts. *Elem Sci Ann* 11: 13. DOI: <https://doi.org/10.1525/elementa.2020.11.013>

**RESEARCH ARTICLE**  
**Long-term changes of regional ozone in China: implications for human health and ecosystem impacts**  
Xiaobin Xu<sup>1</sup>, Weili Lin<sup>2</sup>, Wanyun Xu<sup>3</sup>, Junli Jin<sup>4</sup>, Ying Wang<sup>5</sup>, Gen Zhang<sup>6</sup>, Xiaochun Zhang<sup>7</sup>, Zhiqiang Mal<sup>8</sup>, Yuanzhen Dong<sup>9</sup>, Qianli Ma<sup>10</sup>, Dajiang Yu<sup>11</sup>, Zou Li<sup>12</sup>, Dingding Wang<sup>13</sup> and Huarong Zhao<sup>14</sup>



## TOAR-I publications are highly cited





## TOAR-II Primary Goal and Scientific Scope

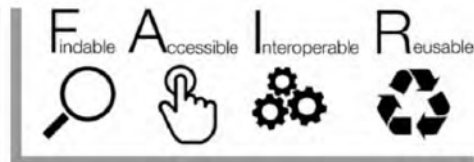


**Final Product:** An observation-based, up-to-date assessment of tropospheric ozone's distribution and trends on regional, hemispheric and global scales.

TOAR-II will assess the physical science basis for tropospheric ozone's global distribution and trends (*similar to IPCC Working Group I*)

TOAR-II will also explore and quantify the **impacts** of tropospheric ozone on human health, crop and ecosystem productivity and climate change (*similar to IPCC Working Group II*)

**Foundation:** An enhanced data infrastructure based on open data and FAIR principles





## **Purpose of TOAR data:**

To provide globally consistent metrics for analyses of health, vegetation, and climate impacts from ozone air pollution



We provide data + analysis services

# The TOAR Data Infrastructure

... comprises of



The TOAR database of global ground-level air quality observations



Web services for accessing and processing of TOAR data and metadata



Publication services for original TOAR datasets



Tools, source code, and documentation

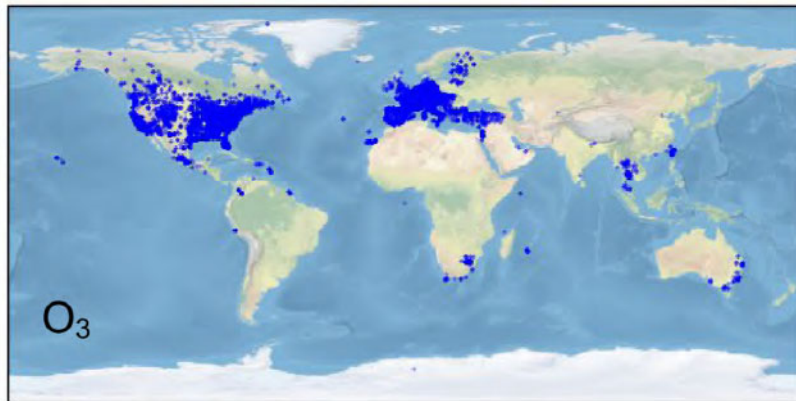




# The TOAR Database

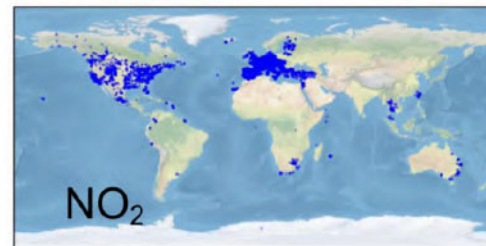
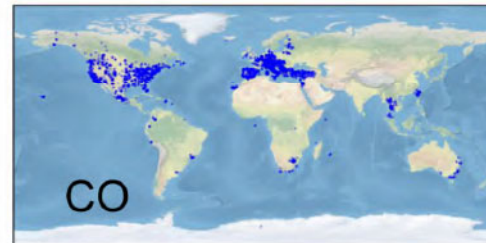
## Current status as of 01 Sept 2022

stations: 20,100; time series: 81,231;  
data records: 3,403,601,152



You can also find and submit data of PM<sub>x</sub>, NO, BC, various VOCs and meteorological variables.

Member of the Helmholtz Association



# The TOAR Data Commitment

TOAR is fully committed to

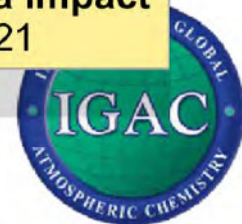


**Open Data:** all data collected in TOAR must be freely available with no use constraints  
☾ CC-BY 4 license; citations&acknowledgements

We won a 2<sup>nd</sup> price in the German  
**Open Data Impact Award 2021**



**FAIRness:** make it easy to find, access, interoperate and re-use TOAR data, also in other contexts  
☾ elaborated metadata schema; REST-API; coordination with other data centres



**Reproducibility:** TOAR analyses shall be fully reproducible, even when the database grows  
☾ use of PIDs, versioning, QC flags, FDOs



# The TOAR Data REST API

<https://toar-data.fz-juelich.de/api/v2>

## 2.6 Search (combined endpoint of stations and timeseries)

This endpoint enables queries that filter for a combination of metadata of stations and timeseries. Any combination of query options (except for id) from both [2.4 Stationmeta](#) and [2.5 Timeseries](#) is possible here.

Example from the [TOAR Quick Start Guide](#):

[https://toar-data.fz-juelich.de/api/v2/search/?bounding\\_box=49,7,50,8&variable\\_id=5,4&limit=None](https://toar-data.fz-juelich.de/api/v2/search/?bounding_box=49,7,50,8&variable_id=5,4&limit=None)

The above command will get you all the time series within an area between 49°N 7°E and 50°N 8°E that record ozone or pm1.



```
JSON Raw Data Headers
Save Copy Collapse All Expand All (slow) Filter JSON
0:
  id: 18776
  label: ""
  order: 1
  sampling_frequency: "hourly"
  aggregation: "mean of two values"
  data_start_date: "1990-01-01T01:00:00+00:00"
  data_end_date: "2021-11-30T14:00:00+00:00"
  data_origin: "instrument"
  data_origin_type: "measurement"
  provider_version: "N/A"
  sampling_height: 2
```

# Summary of TOAR data resources



**Data portal:** <https://toar-data.org>



**Access to data & documentation:**  
<https://toar-data.fz-juelich.de>




**Training material:**  
<https://go.fzj.de/toar-data-training>  
<https://go.fzj.de/toar-user-git>







# Jupyter notebooks for TOAR analyses

<https://go.fzj.de/toar-user-git>


esde > toar-public > TOAR Data User Workshop 2022



**T** TOAR Data User Workshop 2022  ☆ Star 1



Project ID: 4766 

← 31 Commits  1 Branch  0 Tags  4.3 MB Project Storage

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main  toar-data-user-workshop-2022 Find file ↓ Clone ↓

 updated the map plot of all stations  
Niklas Selke authored 6 days ago 2137cb51 

 README  No license. All rights reserved

Name	Last commit	Last update
contributed	Add new directory	2 months ago
pdf_exports	updated the map plot of all stations	6 days ago
.gitignore	added a .gitignore file and made some chan...	2 months ago
2022-02-Logo-TOAR-DataBase.p...	Upload New File	3 months ago
GettingStarted.ipynb	added saving to file to GettingStarted.ipynb ...	2 months ago

**TOAR**  
tropospheric  
ozone  
assessment  
report  
*Phase II*



# BENEFITS

## Why Jupyter is so popular among Data Scientists

Some of the reasons ...

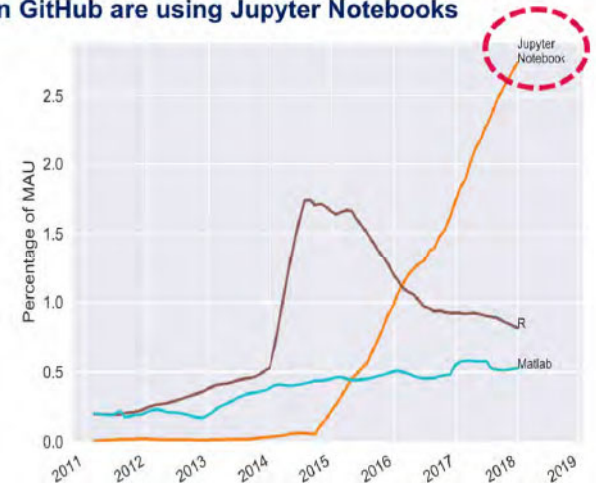
- Jupyter allows to **view the results of the code in-line** without the dependency of other parts of the code.
- Jupyter mixes easy for users who extend their code **line-by-line with feedback** attached all along the way
- Jupyter Notebooks support visualization and include rendering data in **live-graphics and charts**.
- Jupyter is maintaining the **state of execution of each cell** automatically.
- Supports IPyWidget packages, which provide **standard user interface** for exploring code and data interactively.
- Platform and language **independent** because of its representation in JSON format.

# MOTIVATION

## Rise of Jupyter's popularity

- In 2007, Fernando Pérez and Brian Granger announced „**ipython**: a system for interactive scientific computing“ [1]
- In 2014, Fernando Pérez announced a spin-off project from IPython called **Project Jupyter**.
  - IPython continued to exist as a Python shell and a kernel for Jupyter, while the Jupyter notebook moved under the Jupyter name.
- In 2015, GitHub and the Jupyter Project announced native rendering of Jupyter notebooks file format (.ipynb files) on the **GitHub**
- In 2017, the **first JupyterCon** was organized by O'Reilly in New York City. Fernando Pérez opened the conference with an inspiring talk. [2]
- In 2018, **JupyterLab** was announced as the next-generation web-based interface for Project Jupyter.
- In 2019, JupyterLab 1.0 ...  
In 2020, JupyterLab 2.0 ...  
In 2021, JupyterLab 3.0 ...

Counting how many Monthly Active Users (MAU) on GitHub are using Jupyter Notebooks



<https://www.benfrederickson.com/ranking-programming-languages-by-github-users/>  
<https://github.com/benfred/github-analysis>

[1] Pérez F, Granger BE (2007) Ipython: a system for interactive scientific computing. Comput Sci Eng 9(3):21–29

[2] Pérez F, Project Jupyter: From interactive Python to open science -> <https://www.youtube.com/watch?v=xuNj5paMucw>

# JUPYTER NOTEBOOK

creating reproducible computational narratives

Markdown Cells

Code Cells

Fourier transform

Fourier transforms are one of the universal tools in computational physics, which appear over and over again in different contexts. SciPy provides functions for accessing the classic `FFTPACK` library from NetLib, which is an efficient and well tested FFT library written in FORTRAN. The SciPy API has a few additional convenience functions, but overall the API is closely related to the original FORTRAN library.

To use the `fftpack` module in a python program, include it using:

```
[1]: from numpy.fft import fftfreq
from scipy.fftpack import *
```

To demonstrate how to do a fast Fourier transform with SciPy, let's look at the FFT of the solution to the damped oscillator:

$$\frac{d^2 x}{dt^2} + 2\zeta\omega_0 \frac{dx}{dt} + \omega_0^2 x = 0$$

where  $x$  is the position of the oscillator,  $\omega_0$  is the frequency, and  $\zeta$  is the damping ratio. To write this second-order ODE on standard form we introduce  $p = \frac{dx}{dt}$ :

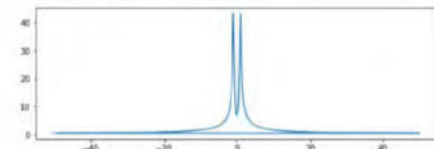
```
[2]: N = len(t)
dt = t[1]-t[0]
dt

[3]: 0.01001001001001001
```

```
[4]: # calculate the fast fourier transform
# y2 is the solution to the under-damped oscillator from the previous section
F = fft(y2[:,0])

# calculate the frequencies for the components in F
w = fftfreq(N, dt)

[5]: fig, ax = plt.subplots(figsize=(9,3))
ax.plot(w, abs(F));
```



Output

Output



# TERMINOLOGY

## What is JupyterLab

### JupyterLab

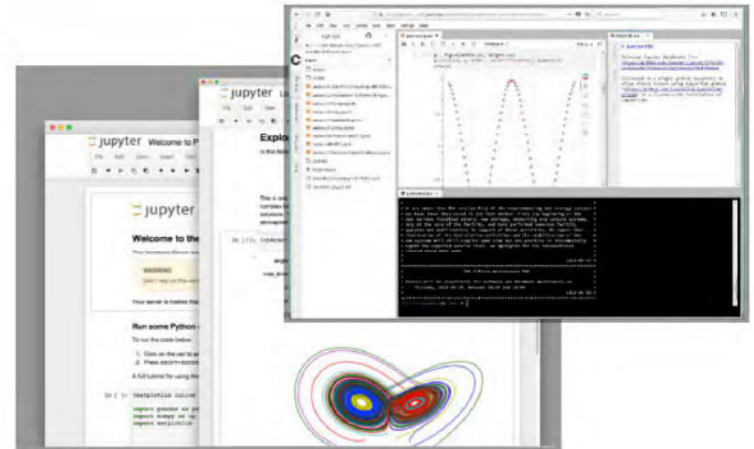
- **Interactive** working environment in the web browser
- For the creation of **reproducible** computer-aided narratives
- Very **popular** with researchers from all fields
- Jupyter = Julia + Python + R

### Multi-purpose working environment

- Language agnostic
- Supports execution environments (“*kernels*”)
  - For dozens of languages: Python, R, Julia, C++, ...
- Extensible software design („*extensions*”)
  - many server/client plug-ins available
  - Eg. in-browser-terminal and file-browsing

### Document-Centered Computing (“*notebooks*”)

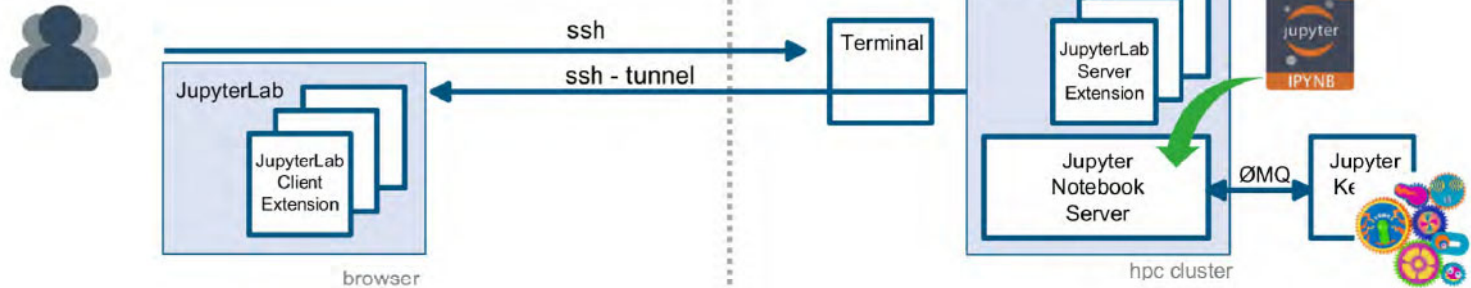
- Combines code execution, rich text, math, plots and rich media.
- All-in-one document called Jupyter Notebook



<https://jupyterlab.readthedocs.io>

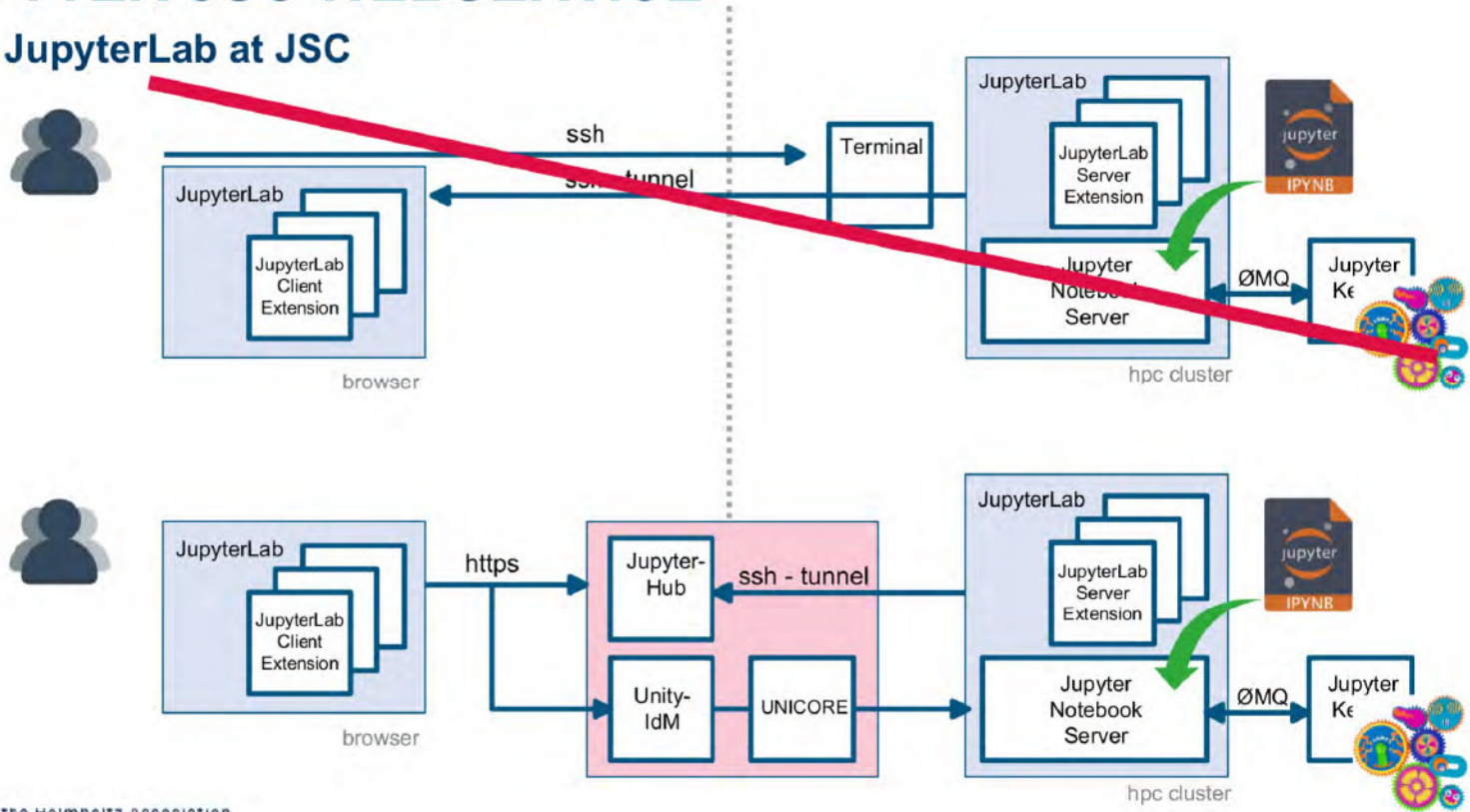
# JUPYTER-JSC WEBSERVICE

## Start your JupyterLab



# JUPYTER-JSC WEBSERVICE

## Start JupyterLab at JSC

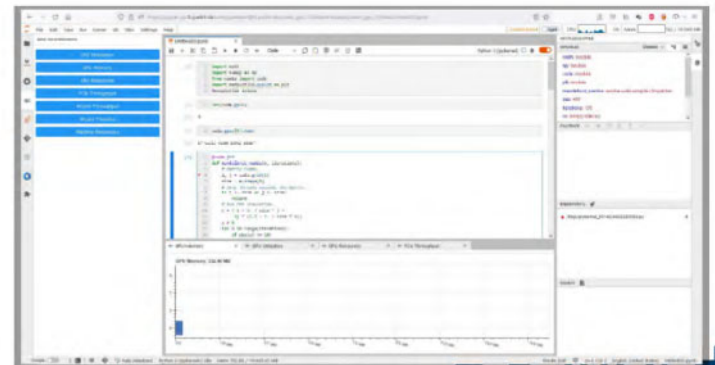
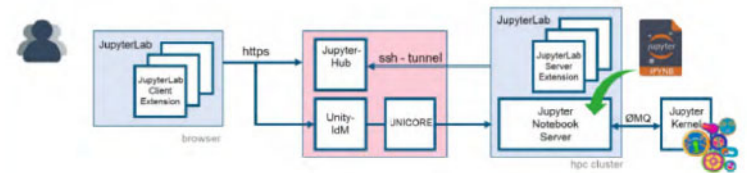


# JUPYTER-JSC WEBSERVICE

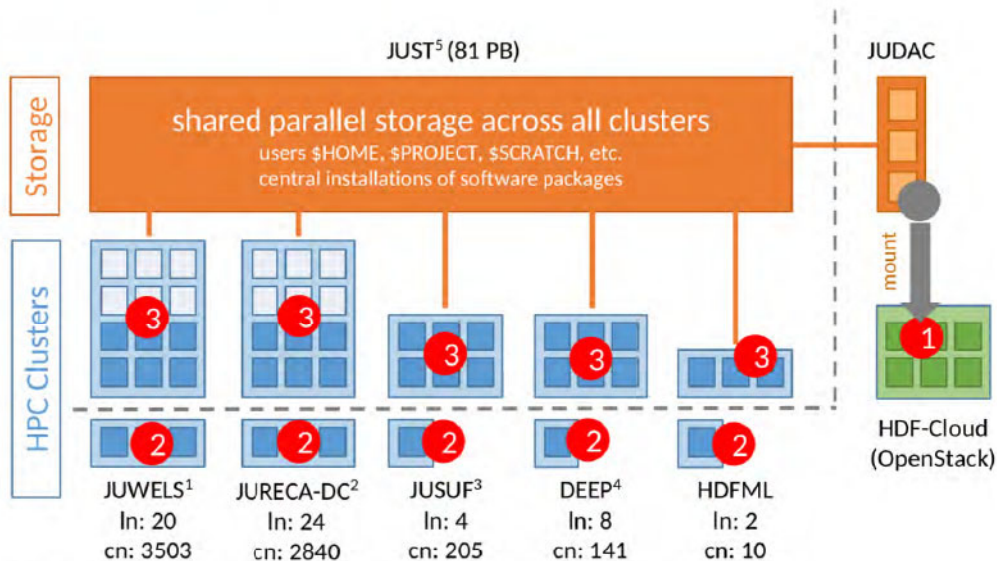
## Start JupyterLab at JSC



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# JUPYTERLAB EVERYWHERE



no. login nodes = ln  
no. compute nodes = cn

[1] <https://apps.fz-juelich.de/jsc/hps/juwels/configuration.html>

[2] <https://apps.fz-juelich.de/jsc/hps/jureca/configuration.html>

[3] <https://apps.fz-juelich.de/jsc/hps/jusuf/cluster/configuration.html>

[4] [https://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/DEEP-EST/\\_node.html](https://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/DEEP-EST/_node.html)

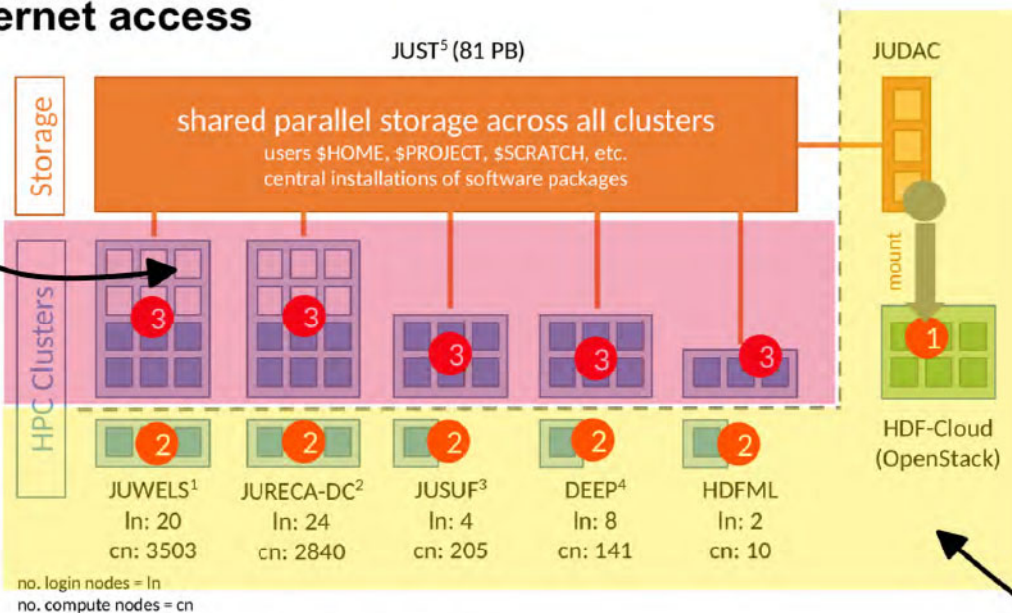
[5] [https://www.fz-juelich.de/ias/jsc/EN/Expertise/Datamanagement/OnlineStorage/JUST/Configuration/Configuration\\_node.html](https://www.fz-juelich.de/ias/jsc/EN/Expertise/Datamanagement/OnlineStorage/JUST/Configuration/Configuration_node.html)

## JupyterLab everywhere

- 1 JupyterLab on HDF-Cloud
- 2 JupyterLab on login nodes
- 3 JupyterLab on compute nodes

# JUPYTERLAB EVERYWHERE

## NO internet access



## JupyterLab everywhere

- 1 JupyterLab on HDF-Cloud
- 2 JupyterLab on login nodes
- 3 JupyterLab on compute nodes

## internet access

[1] <https://apps.fz-juelich.de/jsc/hps/juwels/configuration.html>

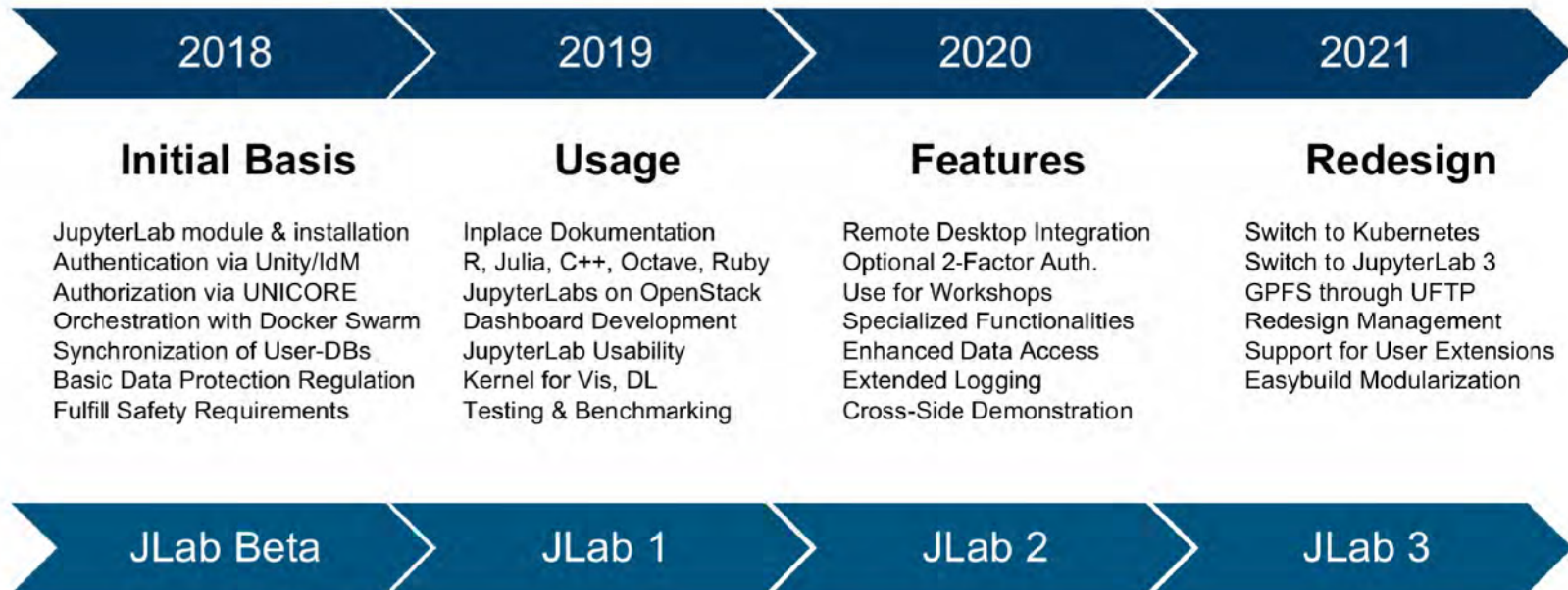
[2] <https://apps.fz-juelich.de/jsc/hps/jureca/configuration.html>

[3] <https://apps.fz-juelich.de/jsc/hps/jusuf/cluster/configuration.html>

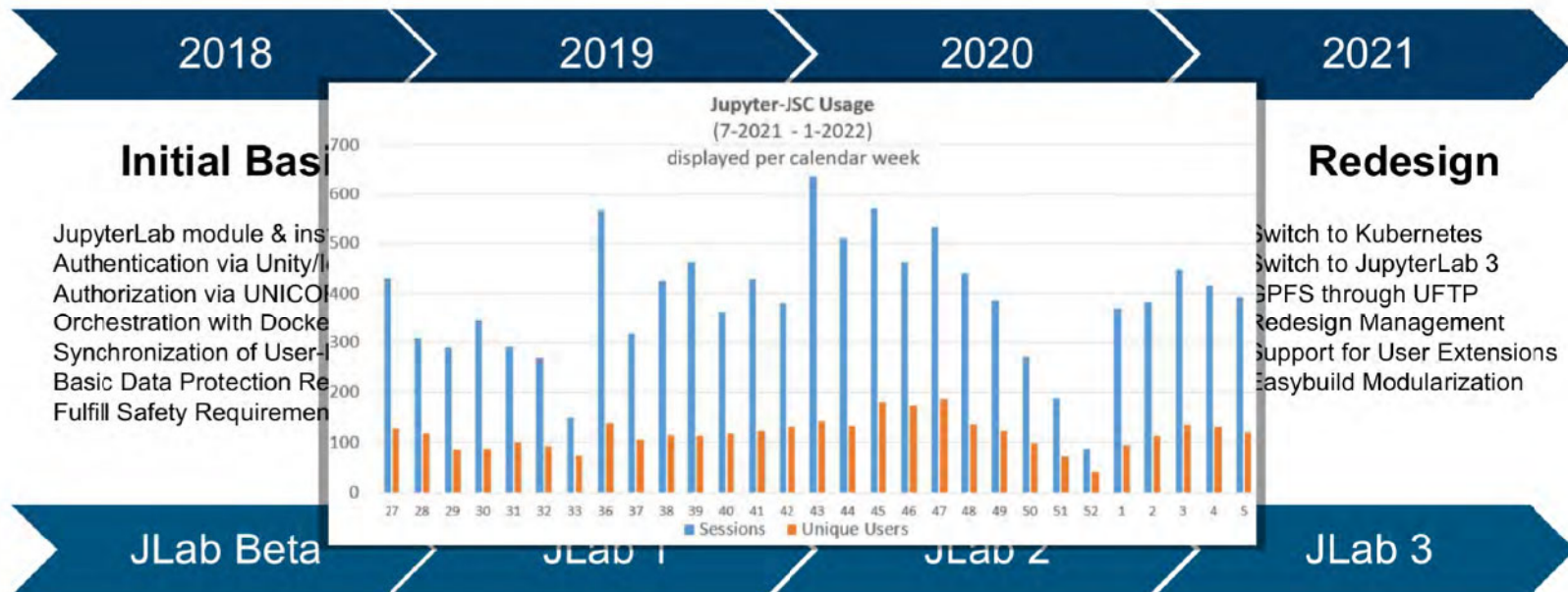
[4] [https://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/DEEP-EST/\\_node.html](https://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/DEEP-EST/_node.html)

[5] [https://www.fz-juelich.de/ias/jsc/EN/Expertise/Datamanagement/OnlineStorage/JUST/Configuration/Configuration\\_node.html](https://www.fz-juelich.de/ias/jsc/EN/Expertise/Datamanagement/OnlineStorage/JUST/Configuration/Configuration_node.html)

# HISTORY OF JUPYTERLAB AT JSC



# HISTORY OF JUPYTERLAB AT JSC





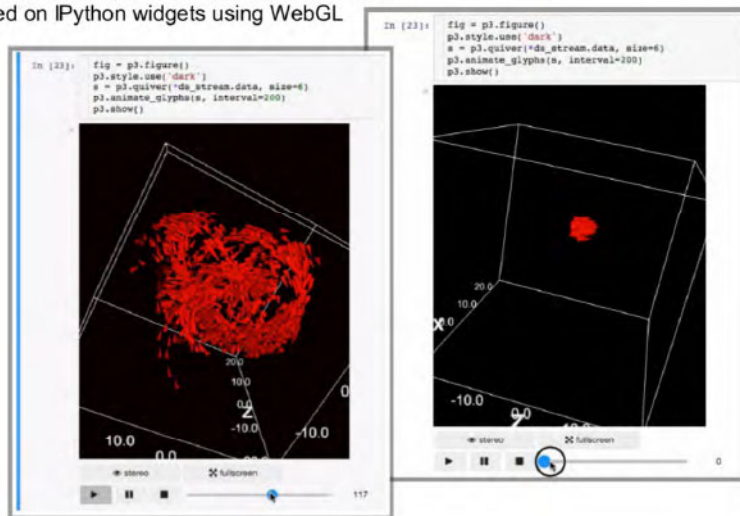


# JUPYTER-JSC EXTENSIONS

## Installed by default

### IPyVolume

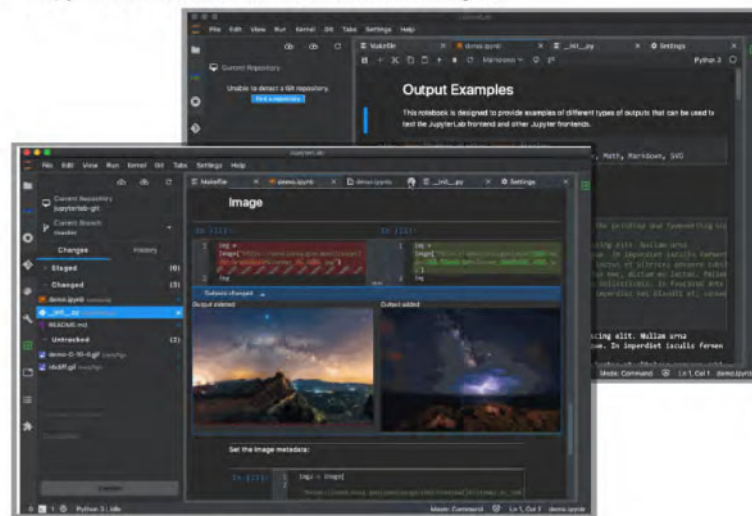
3d plotting for Python in the Jupyter notebook  
based on IPython widgets using WebGL



<https://github.com/maartenbreddels/ipyvolume>

### JupyterLab-Git

JupyterLab extension for version control using Git



<https://github.com/jupyterlab/jupyterlab-git>

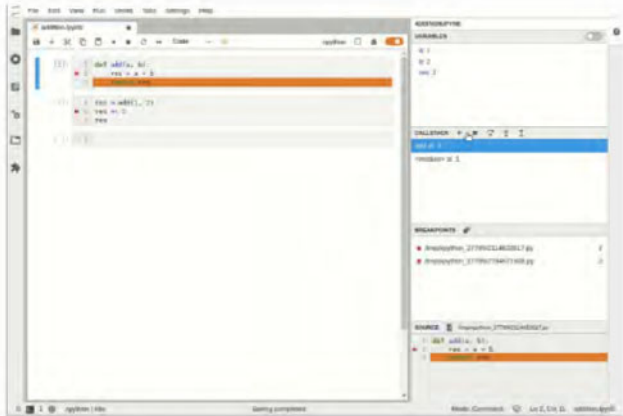
# JUPYTER-JSC EXTENSIONS

## Installed by default

### JupyterLab - Visual Debugger

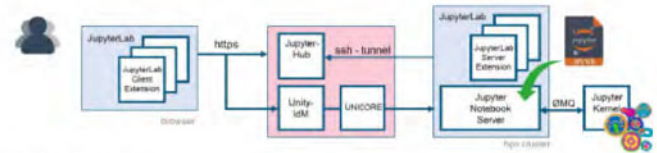
JupyterLab 3.0 now ships with a Debugger front-end by default.

This means that notebooks, code consoles and files can now be debugged from JupyterLab directly! For the debugger to be enabled and visible, a kernel with support for debugging is required.



<https://jupyterlab.readthedocs.io/en/stable/user/debugger.html>

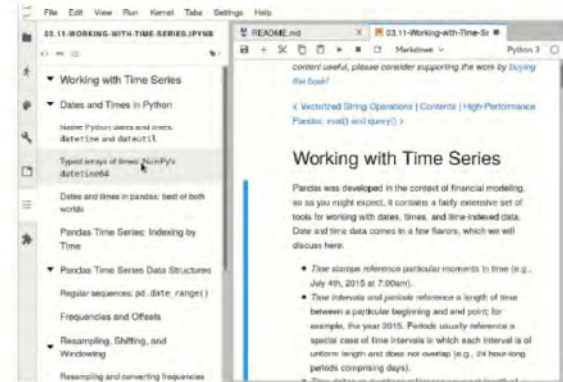
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### JupyterLab-toc

A Table of Contents extension for JupyterLab.

This auto-generates a table of contents in the left area when you have a notebook or markdown document open. The entries are clickable, and scroll the document to the heading in question.

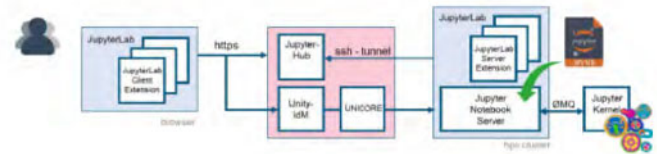


<https://github.com/jupyterlab/jupyterlab-toc>



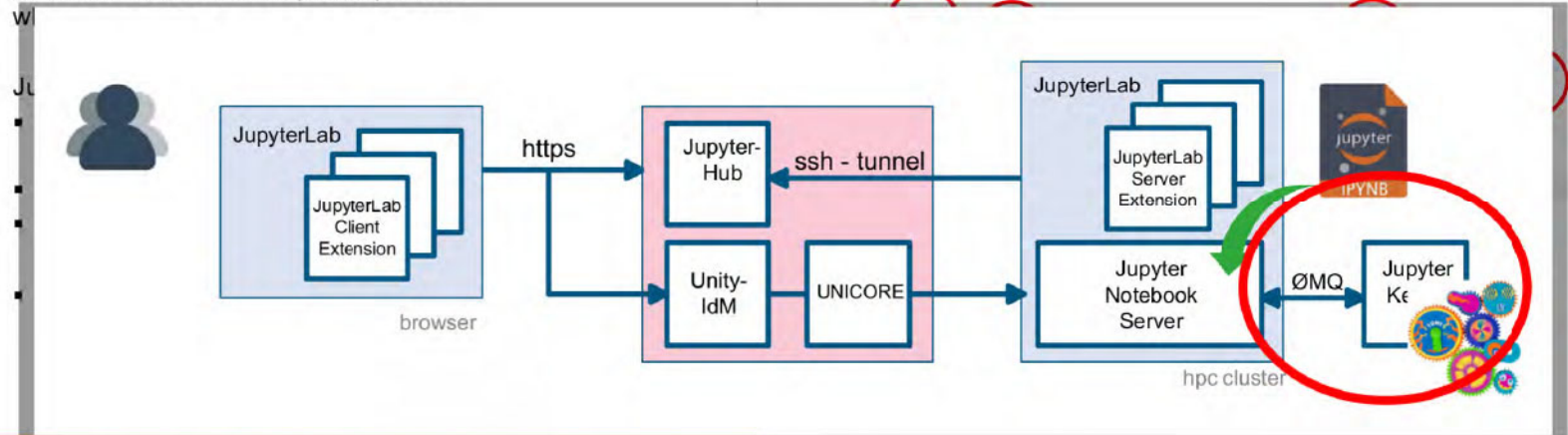
# JUPYTER KERNEL

## How to create your own Jupyter Kernel



### Jupyter Kernel

A "kernel" refers to the separate process

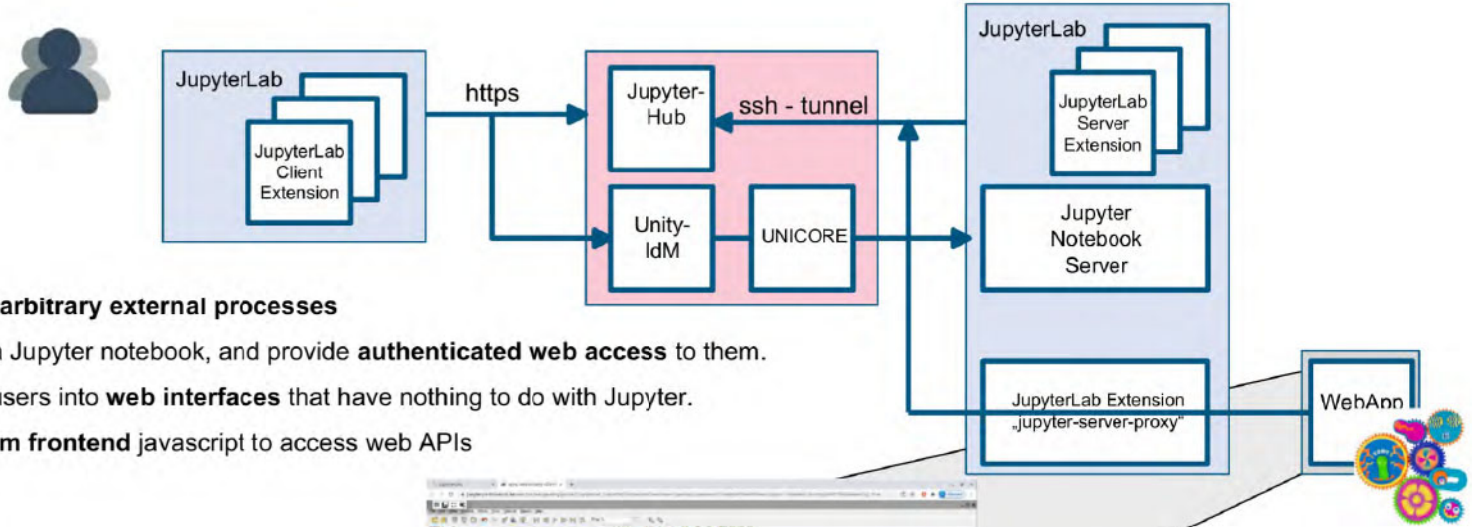


You can easily **create your own kernel** which for example runs your specialized virtual Python environment.

<https://github.com/jupyter/jupyter/wiki/Jupyter-kernels>

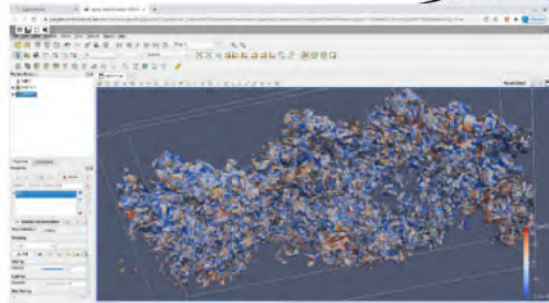
# JUPYTERLAB – WEBSERVICE PROXY

## Extension: jupyter-server-proxy



Allows to run **arbitrary external processes**

- alongside a Jupyter notebook, and provide **authenticated web access** to them.
- launching users into **web interfaces** that have nothing to do with Jupyter.
- **access from frontend javascript** to access web APIs



Turbulent mixing with variable density, subset of 1939x600x3584 grid points, Michael Gauding, CORIA

<https://github.com/jupyterhub/jupyter-server-proxy>

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# QUESTIONS?

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



JUPYTER  
**Jsc**

SUPERCOMPUTING IN YOUR BROWSER