

Bringing Visualization to National HPC Infrastructure: A Prologue

Tim Gerrits, NHR4CES

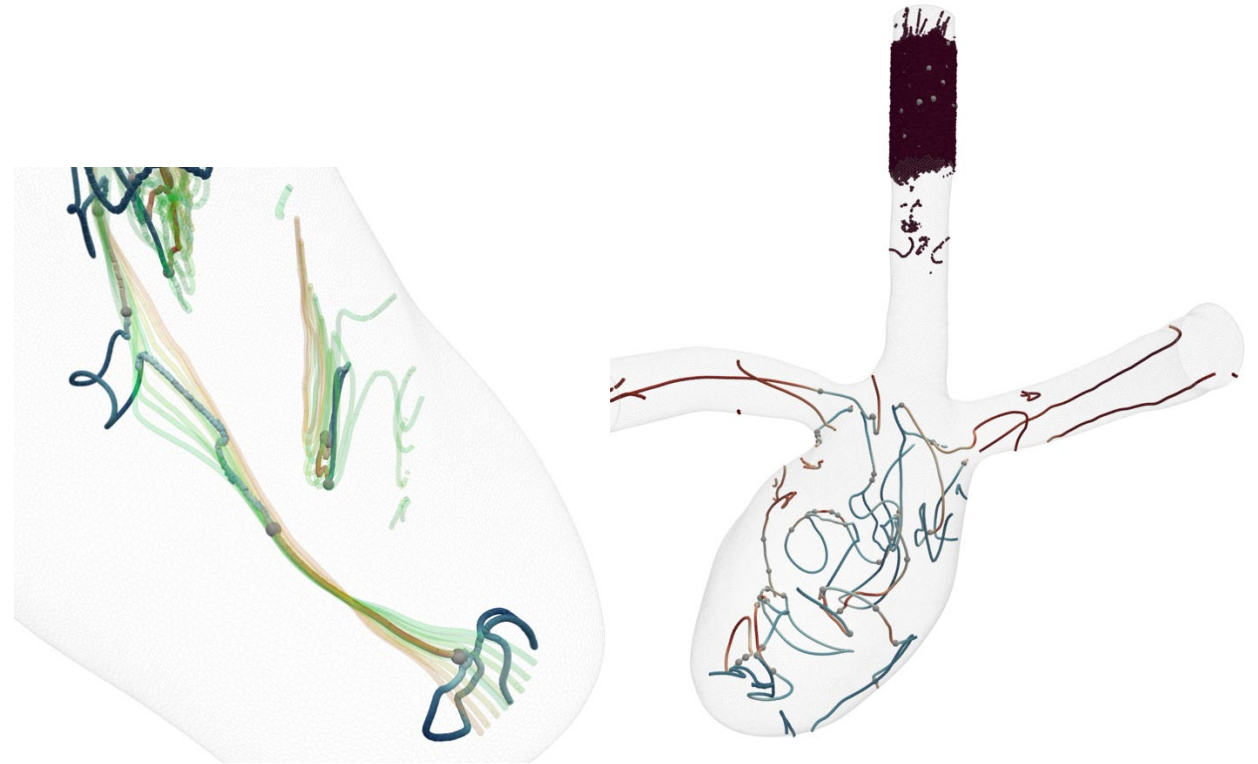
02.06.2022

Workshop on In-Situ Visualization @ISC '22

Keynote

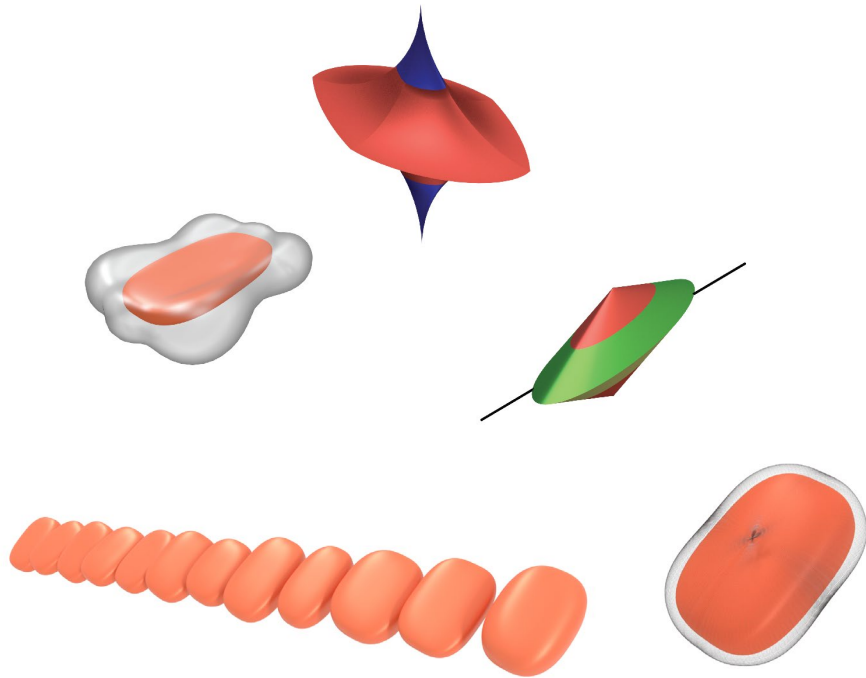
Scientific Visualization

Scientific Visualization

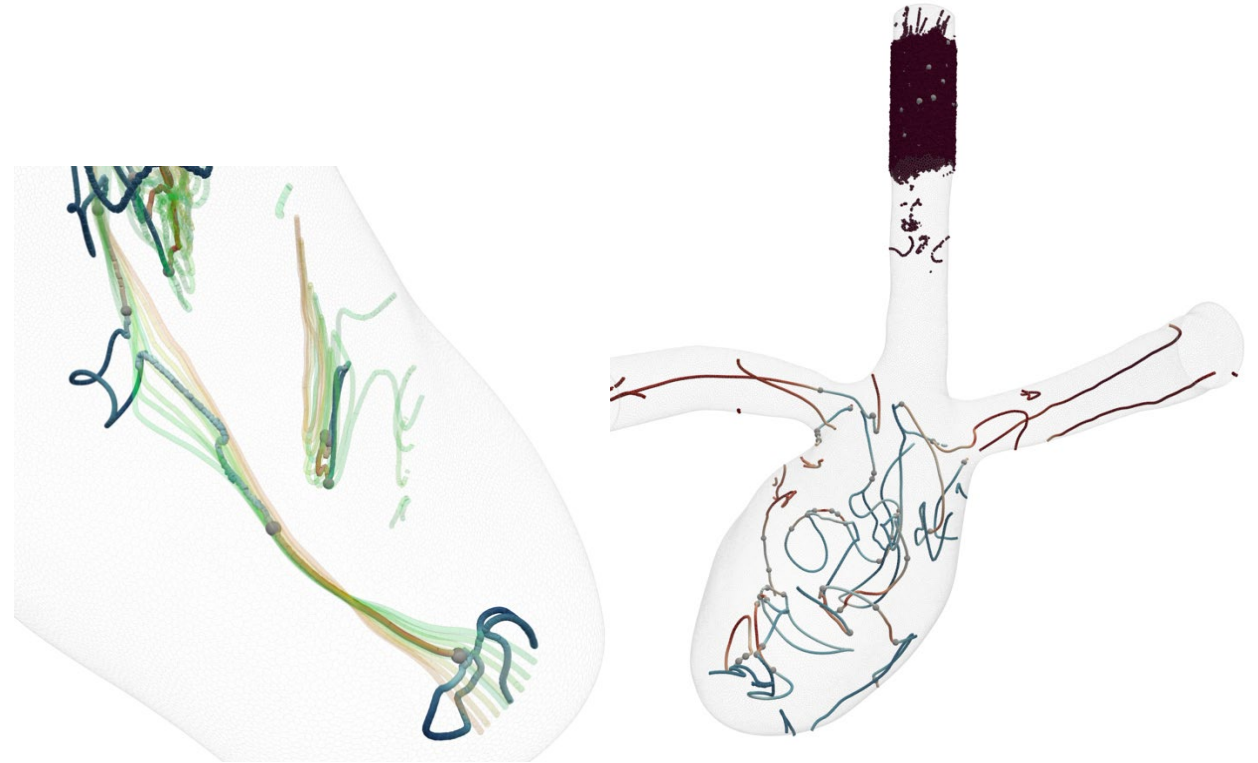


Tensor Field Ensemble Data

Scientific Visualization

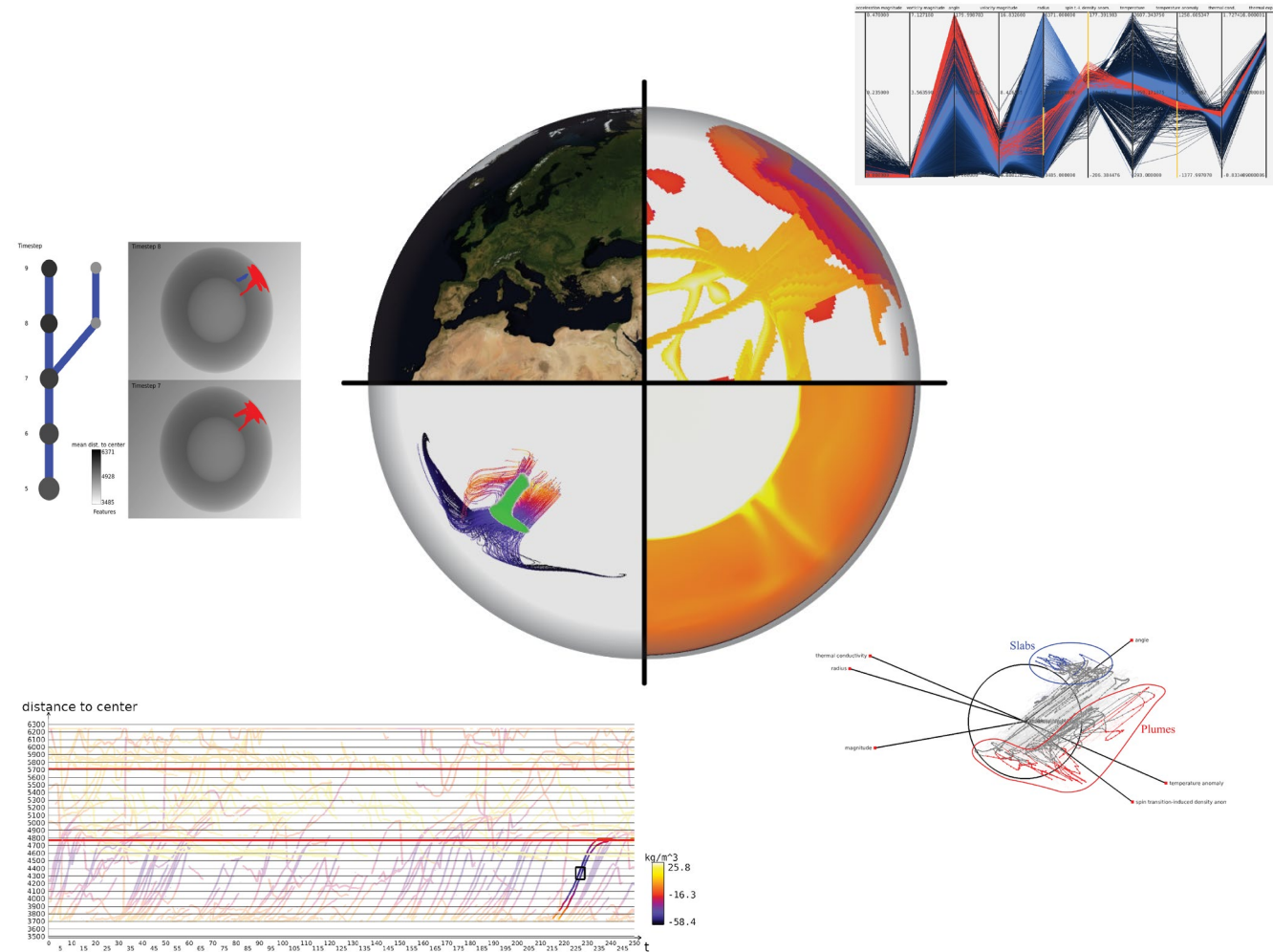
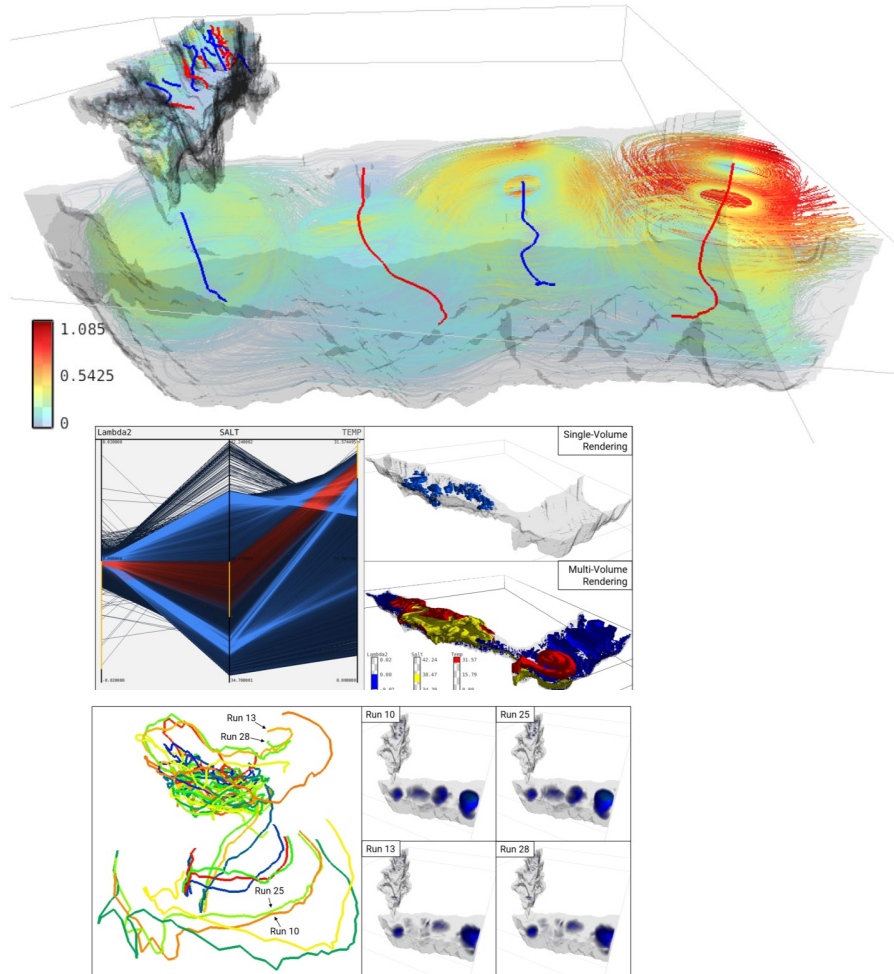


Second-Order Tensor Data



Tensor Field Ensemble Data

Scientific Visualization



Visualization Group at RWTH Aachen



Marcel Krüger



Ali Demiralp



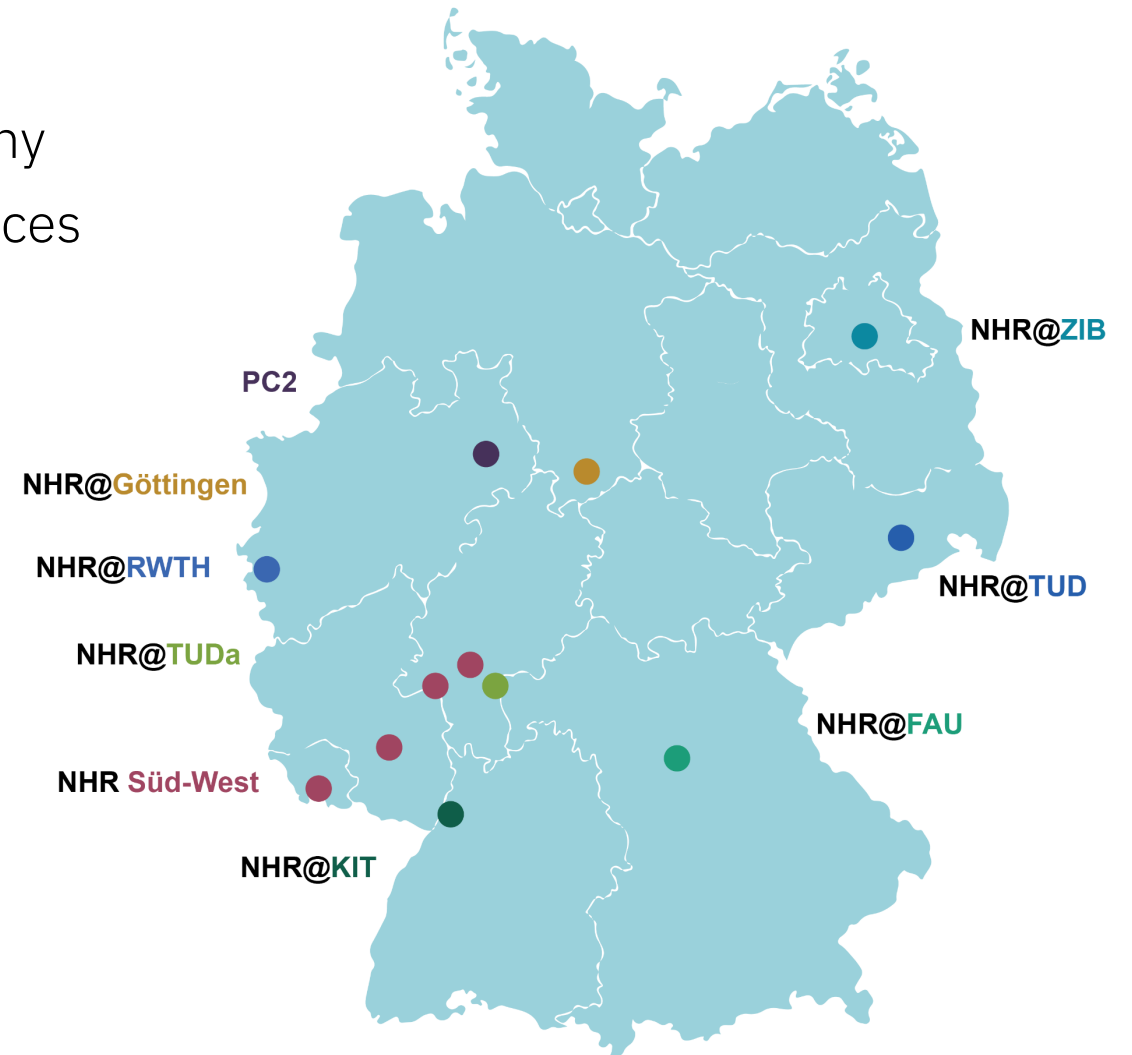
[Fb.com/itcenter.rwth](https://www.facebook.com/itcenter.rwth)

NHR4
CES

NHR for
Computational
Engineering
Science

Nationales Hochleistungsrechnen (NHR)

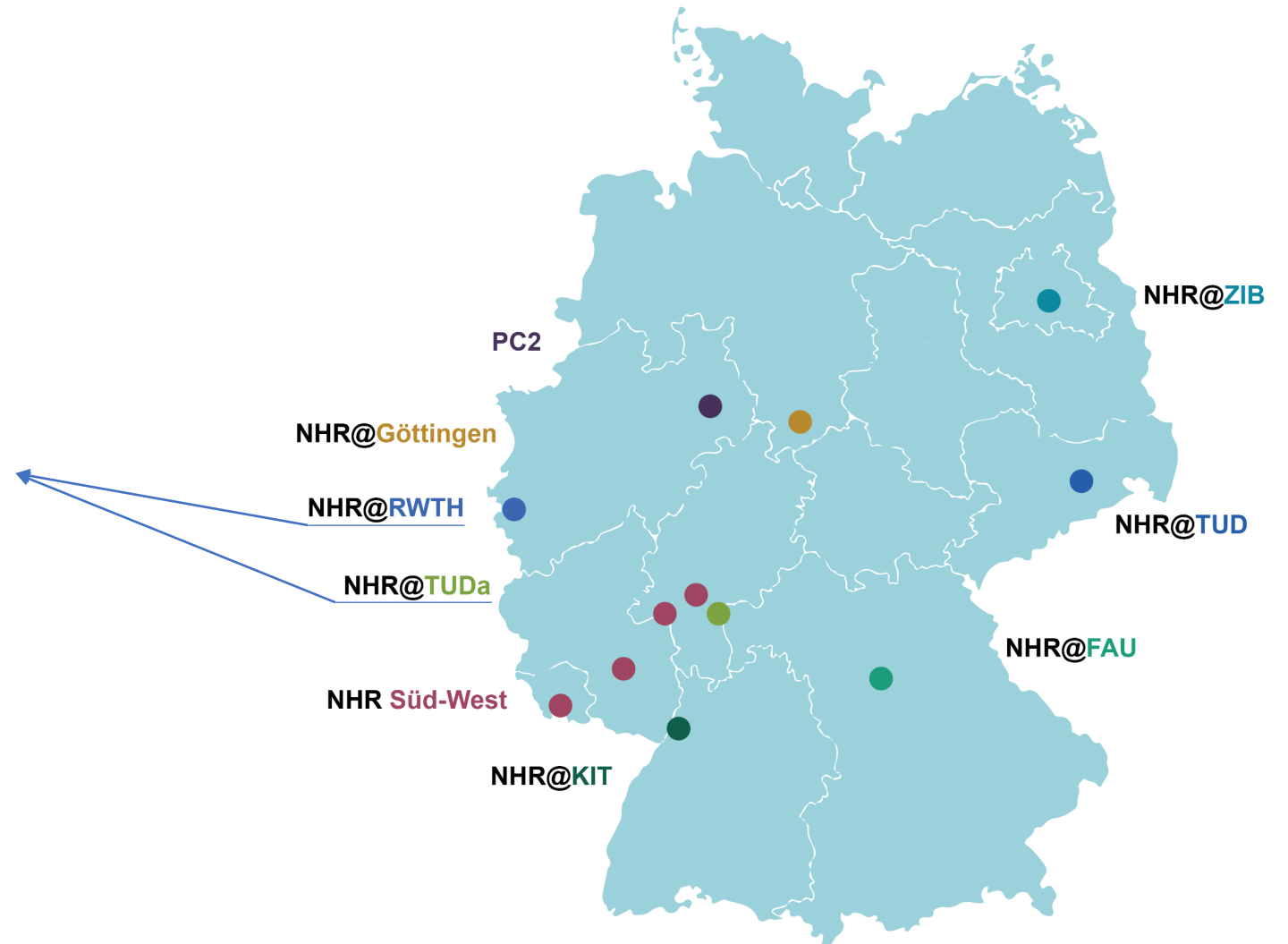
- Centralized infrastructure for HPC in Germany
- Offer training, support, expertise and resources
- 9 dedicated university computing centers
- Focus on communication for efficiency
- Annually 63 million € funded by GWK
- 10 years (extendible)



Nationales Hochleistungsrechnen (NHR)

NHR4
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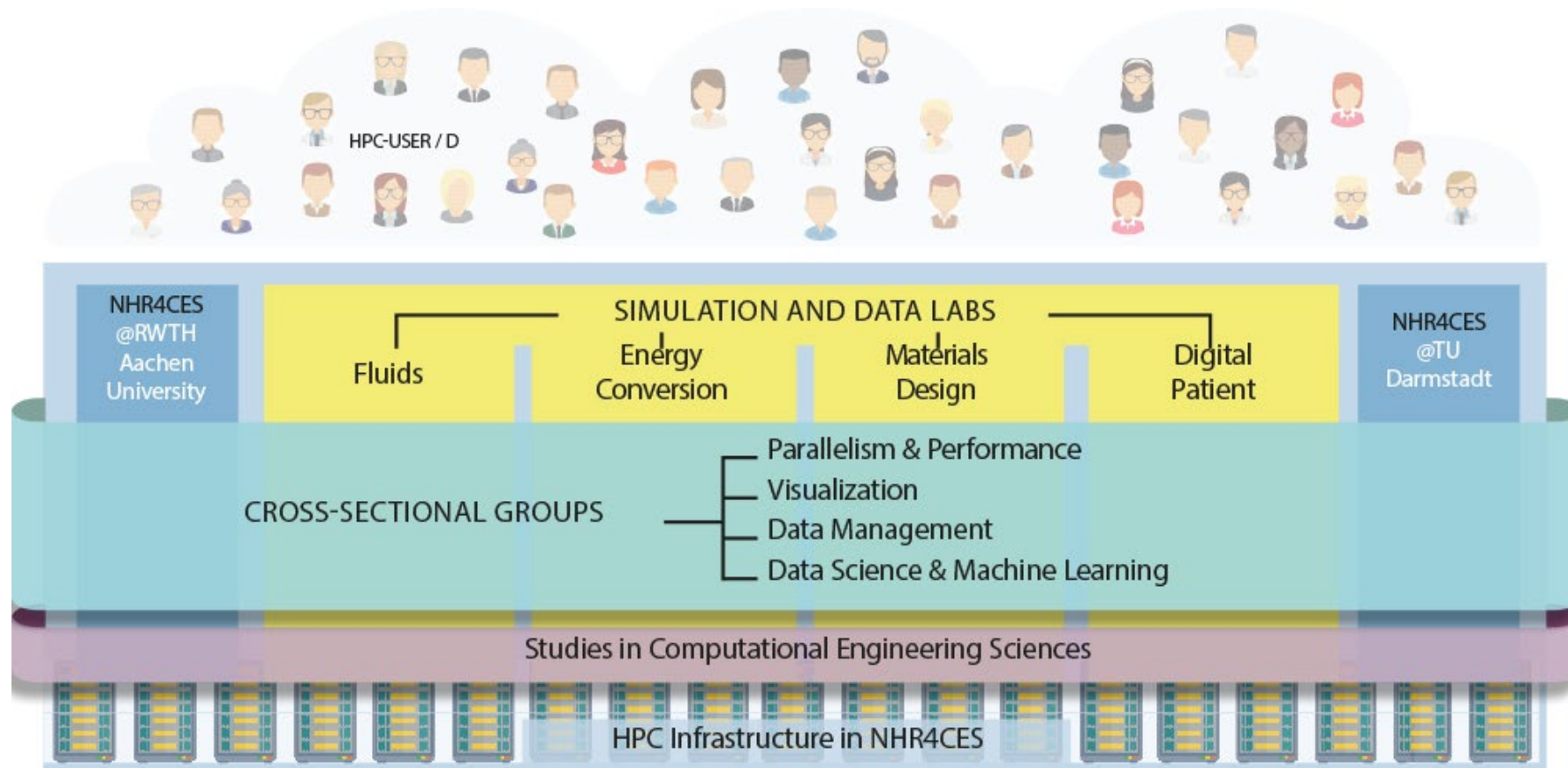


NHR4CES

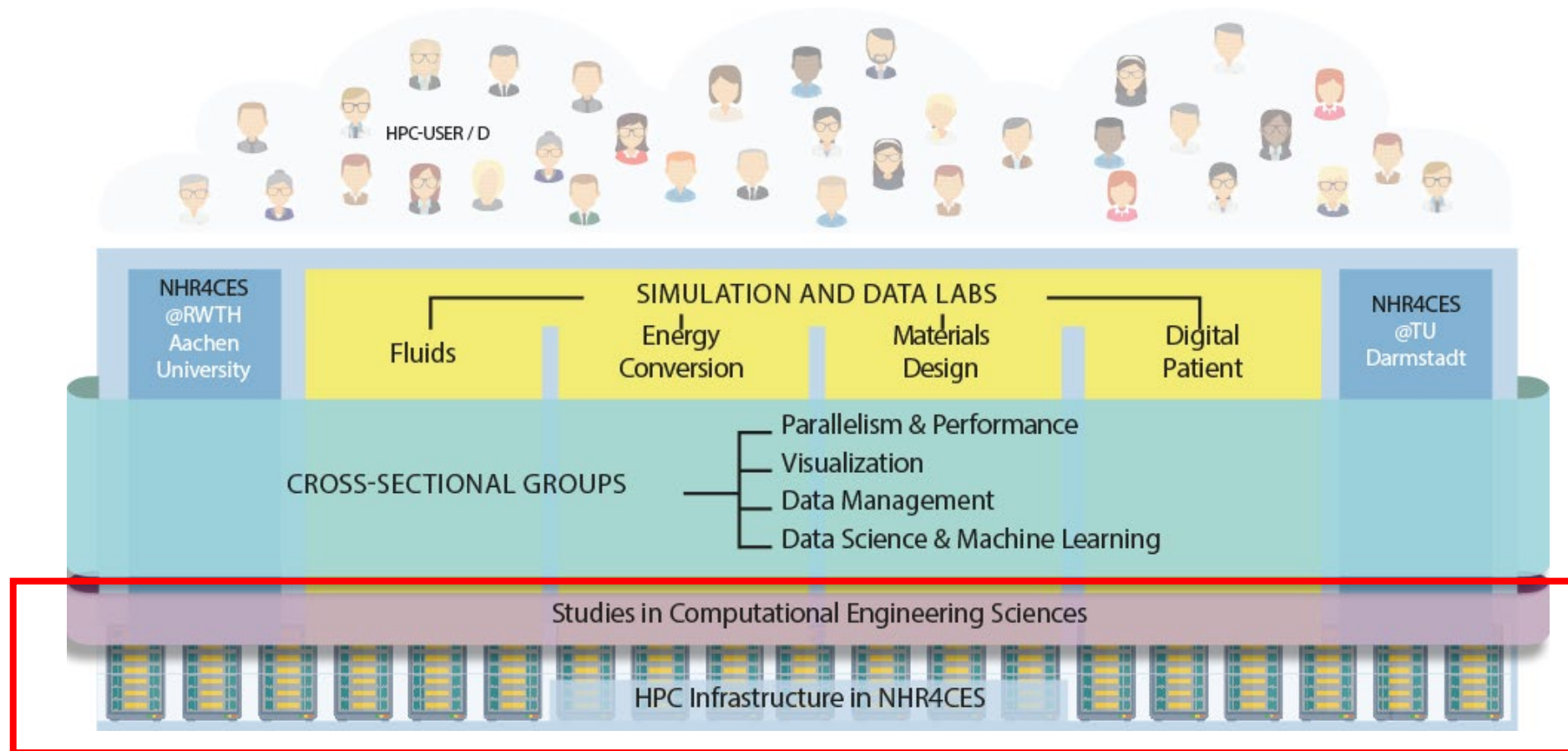
NHR4CES NHR for Computational Engineering Science



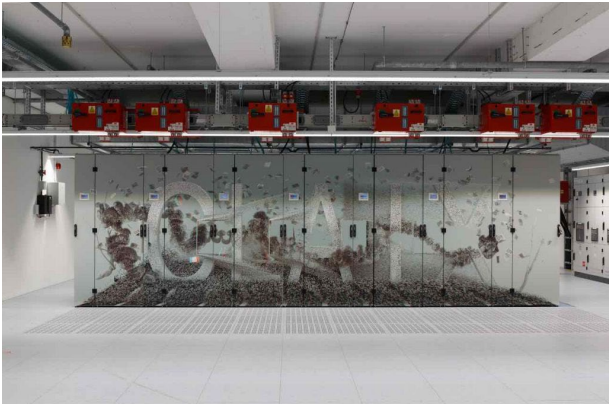
NHR4CES



NHR4CES



Creating Infrastructure



compute nodes for projects

Processor type

cores per node

Main memory per node [GB]

Capacity of HPC filesystem

Bandwidth of HPC filesystem

Theoretical peak performance

LINPACK performance

CLAIX-2018
RWTH Aachen

1080 standard nodes
+ 221 Tier-3 std. nodes

Intel Xeon Platinum 8160
(Skylake)

48

192

10 PB

150 GB/s

3.55 Pflops

2.04 Pflops on 2014 nodes

Lichtenberg II
TU Darmstadt

630 standard nodes
+ 10 special nodes

Intel Xeon Platinum 9242
(Cascade Lake AP)

96

384

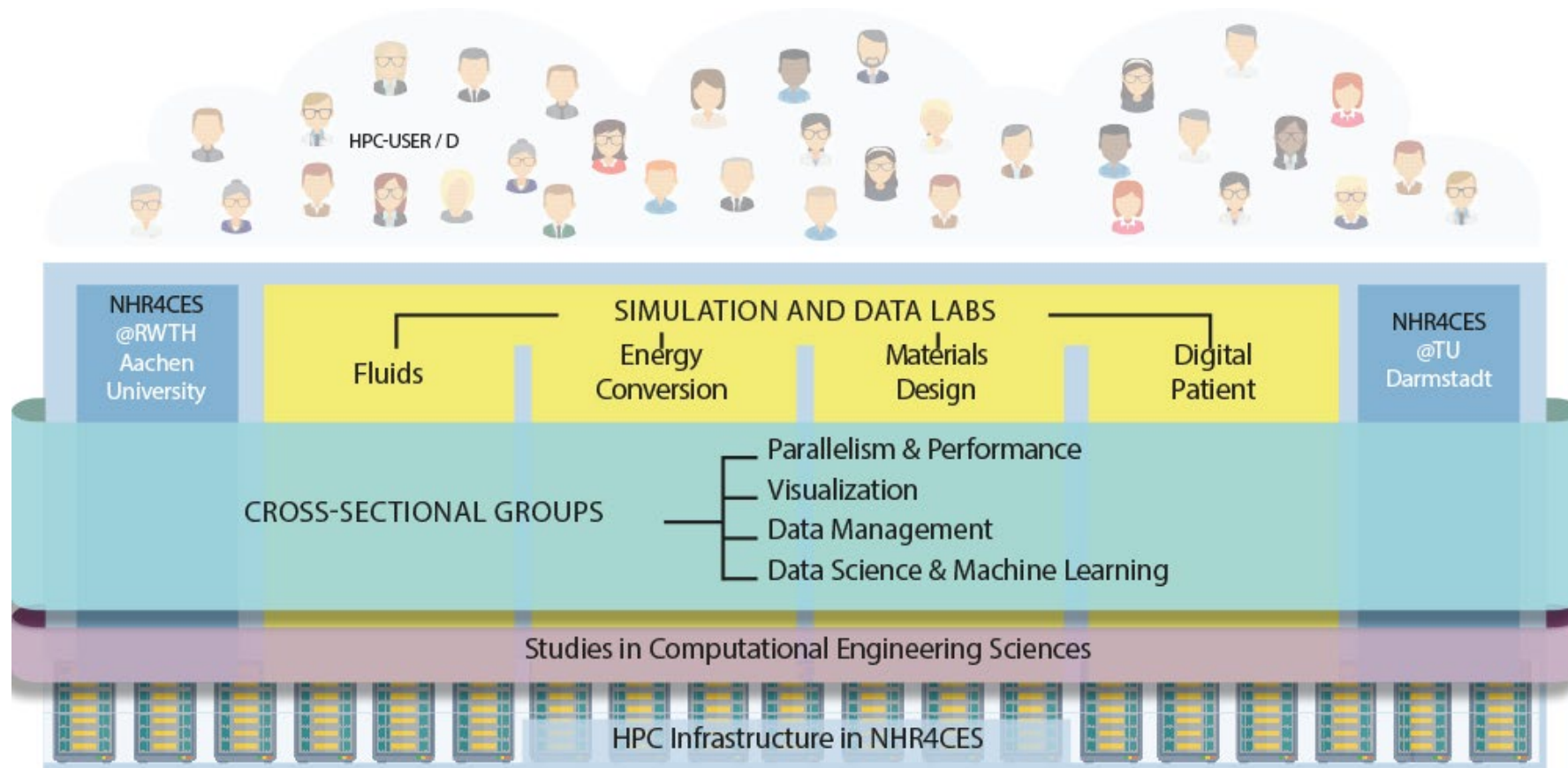
4 PB

120 GB/s

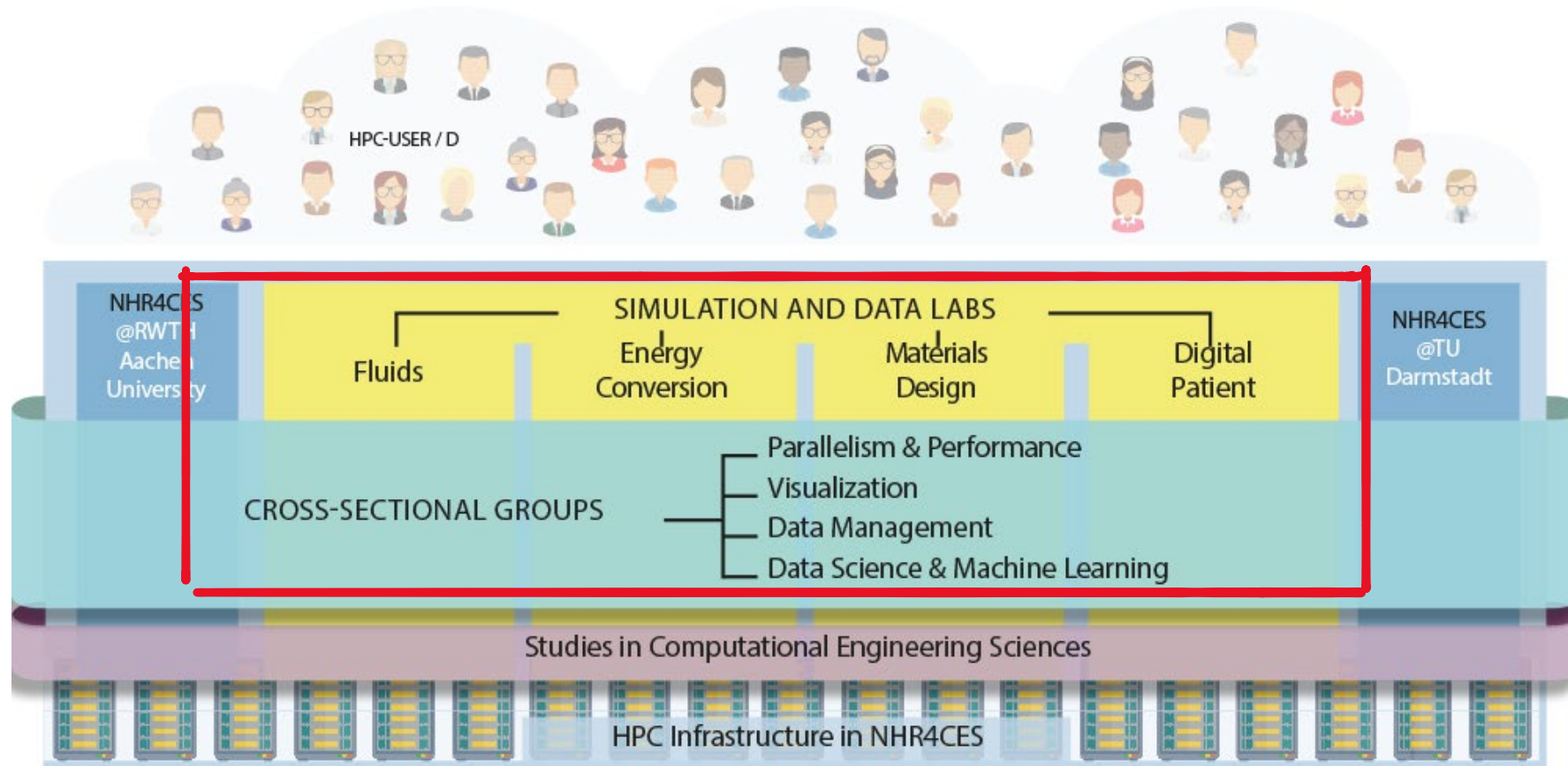
4.35 PFlop/s

3.15 PFlops

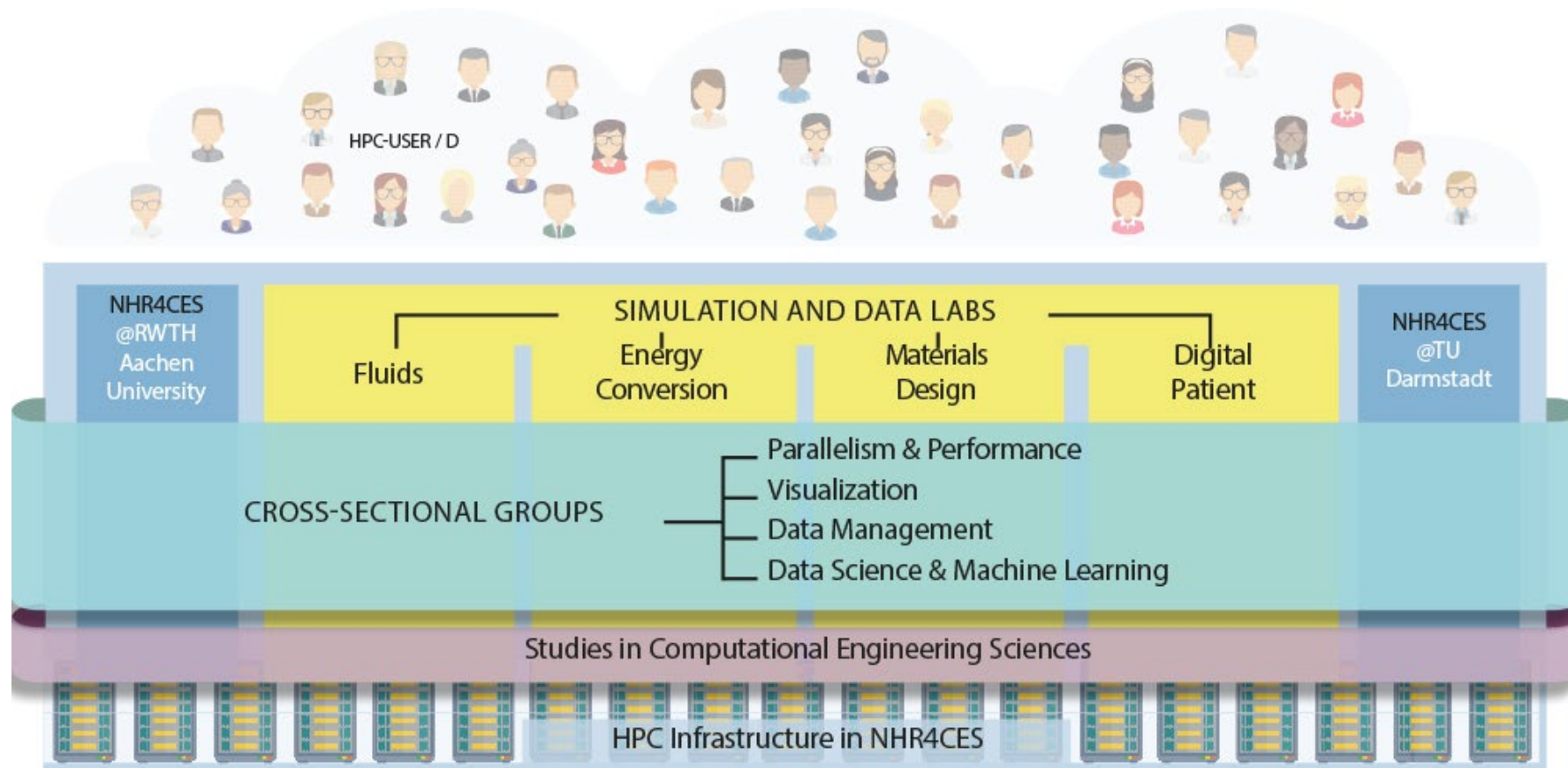
NHR4CES



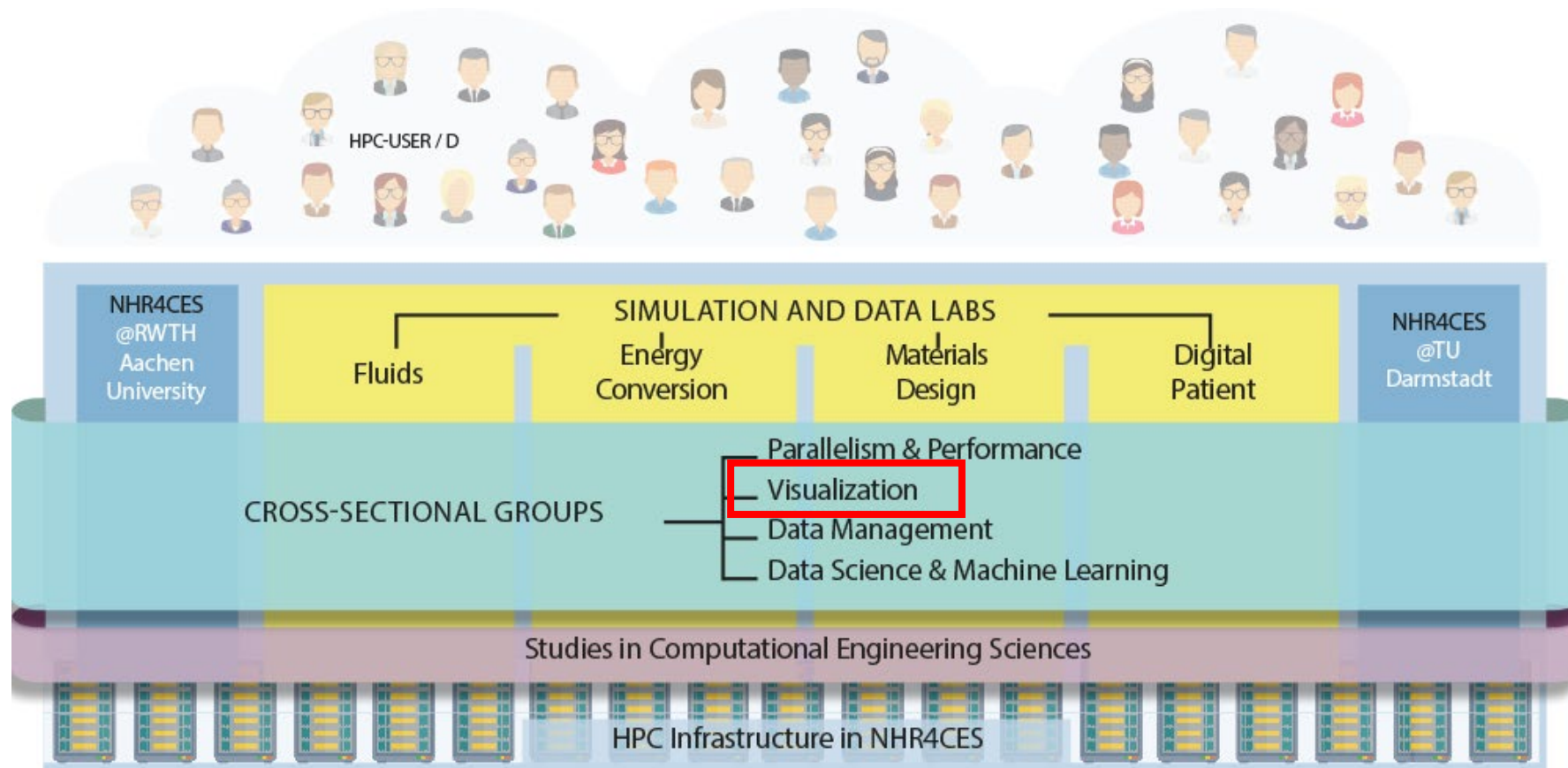
NHR4CES



NHR4CES



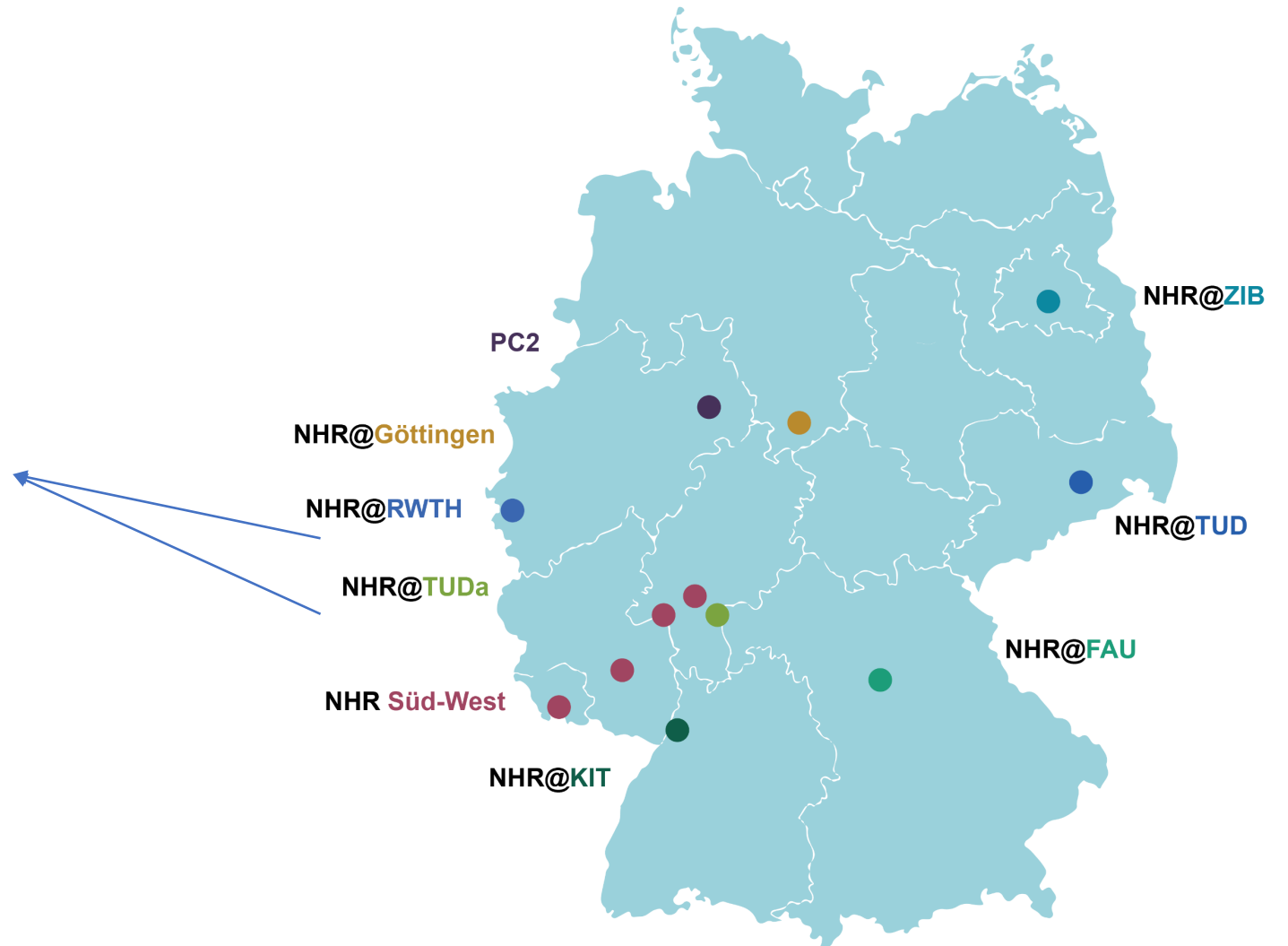
NHR4CES



Nationales Hochleistungsrechnen (NHR)

NHR4
CES

NHR for
Computational
Engineering
Science



What's the Story?

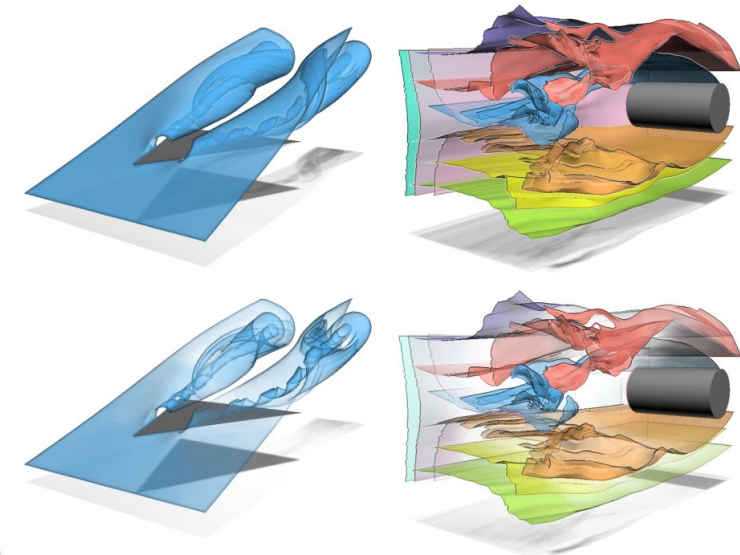
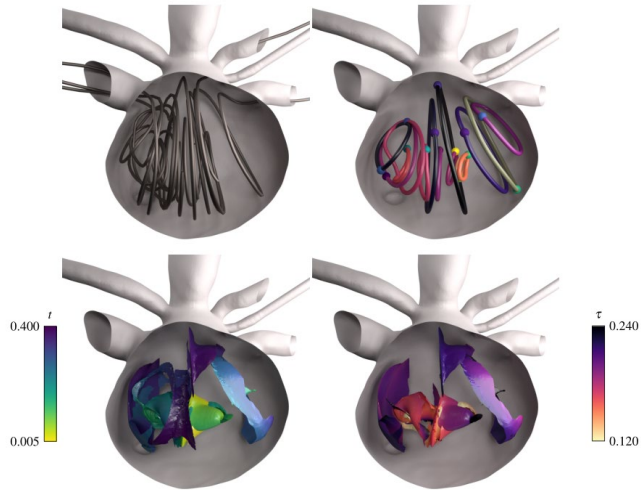
- Make visualization an essential part of NHR
- Support HPC users in visualization
 - SDLs
 - Community
 - New researchers / users
- Where to begin?

Visualization for Simulation and Data Labs

- Provide State-of-the-Art Visualization Methods
 - Classic 2D/3D applications
 - Immersive 3D environments
 - Interactive Analysis tools
- Develop new Methods for Specific Needs
 - Complex data types
 - Large data
 - Uncertain data
 - ...

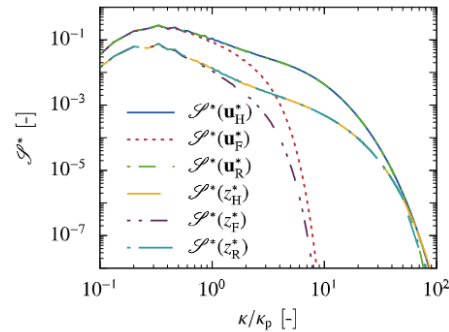
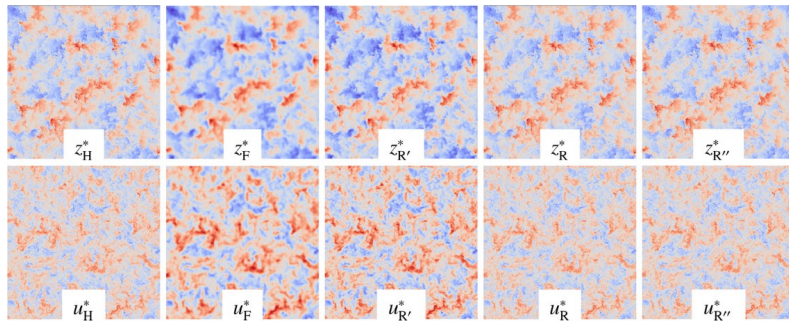
Visualization in HPC Context (Expectation)

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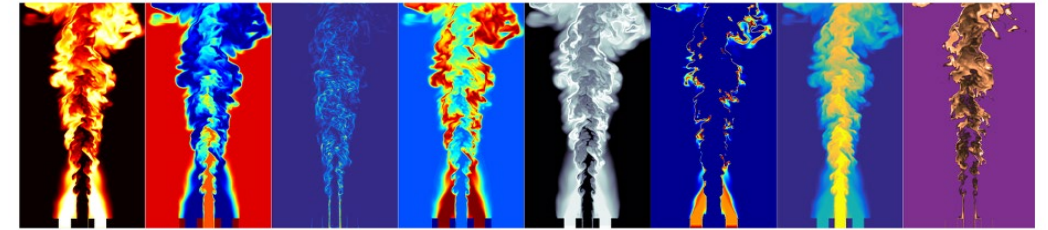


Visualization in HPC Context (Reality)

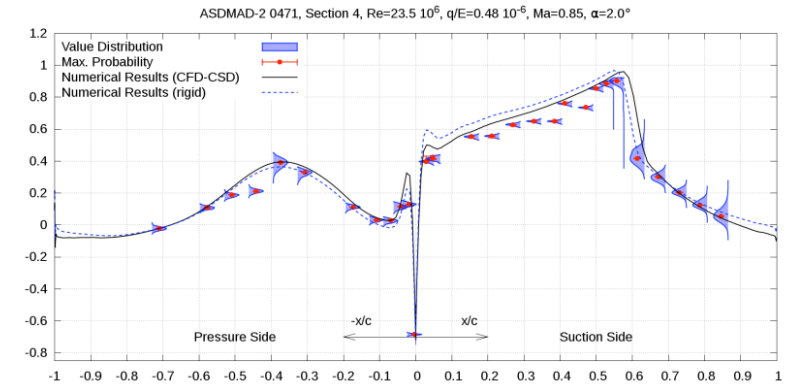
Visualization in HPC Context (Reality)



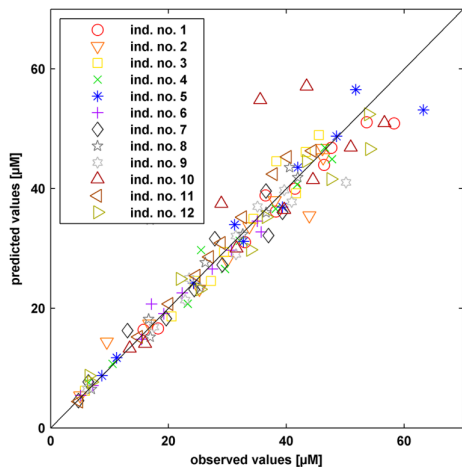
M. Bode et al.



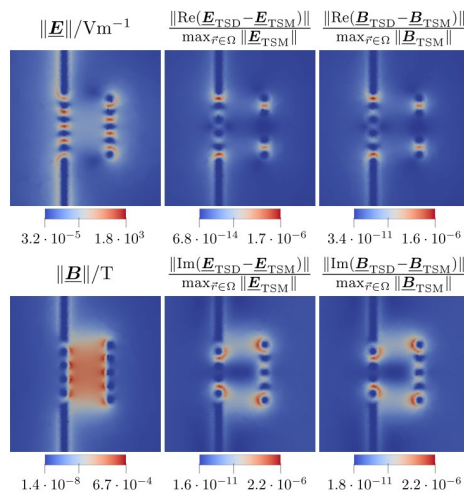
<https://www.itv.rwth-aachen.de/>



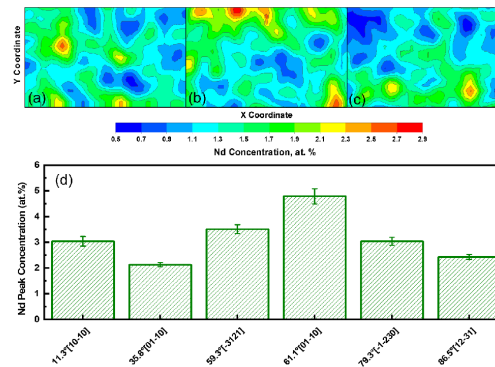
M. Brüderlin et al.



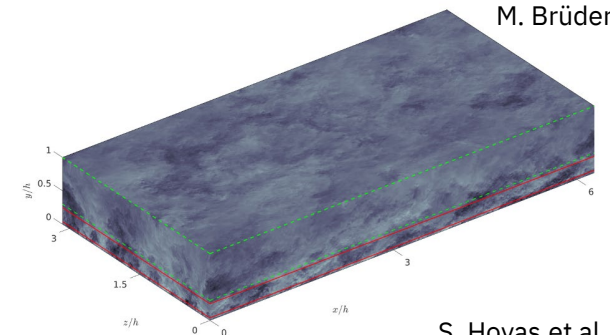
M. Krauss et al.



M. Clemens et al.



R. Pei et al.



S. Hoyas et al.

Open Questions for Visualization

- What does the HPC community actually need from visualization
- How can we bring visualization research into the HPC community
- How do we measure success?

State of Visualization in NHR4CES

- Domain / Data type / Research question
 - Workflow / Challenges
 - Visualization
 - What do they know
 - What do they use
 - What do they need
 - What do they want
 - In-Situ visualization
 - Who do they ask?
-
- Some more...
 - Personal meetings with groups

Visualization in Computational Engineering Sciences

Dear participant,
my name is Tim Gerrits and I am a visualization researcher working at the RWTH Aachen University.
I am currently leading the Crosssectional Group Visualization within the National High Performance Computing Center for Computational Engineering Sciences (<https://www.nhr4ces.de/>).

To better understand how visualization can support other research groups concerned with engineering sciences in their work, we want to get an idea on how visualization is already being used right now.
This includes assessing the current state in different groups, finding out which techniques, software packages and resources are typically known, implemented or relied upon and which techniques are not well known or even disregarded.

This survey takes approximately 10 - 15 minutes to complete but will help me and hopefully the visualization community to better support domain experts.

If there are any further questions or you are interested in discussing this topic in more detail with me, feel free to contact me via gerrits@vis.rwth-aachen.de

Thanks a lot for your time and participation
Tim Gerrits

Nach Abschnitt 1 Weiter zum nächsten Abschnitt

Abschnitt 2 von 10

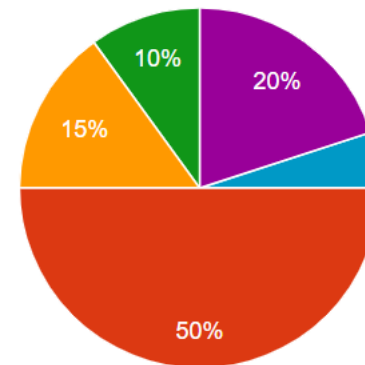
Research Background

First I would like to gather a coarse idea on the research background including the field of research and data challenges. This is used to better connect visualization tools and approaches to a specific domain.

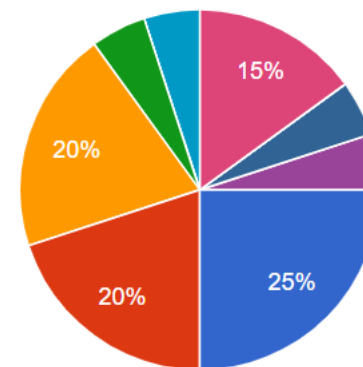
Who are we Providing Visualizations for?

- Young team
- Less experienced
- Long-term cooperation
- Highly variable domains

- Most of them:
Implement simulation
Refine models
Explore data
Scalar /multifield / vector data



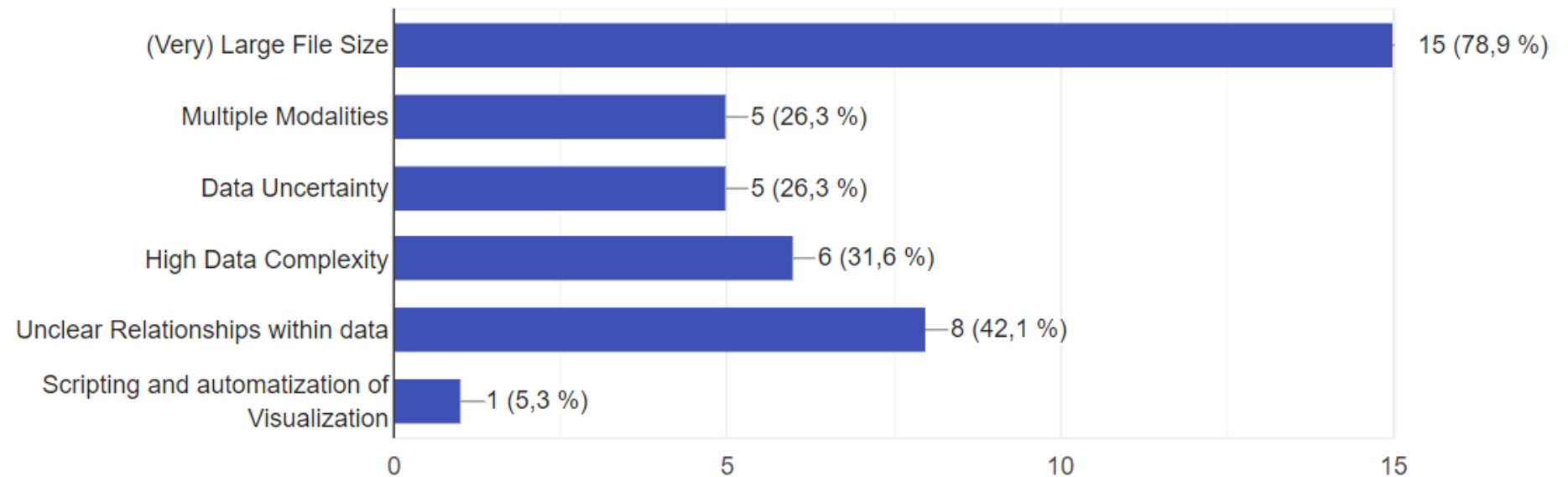
- Bachelor's / Master's Program
- PhD Student
- PostDoc Researcher
- Research Group Lead
- (Assistant / Junior) Professor
- Full Professor



- Fluid Dynamics
- Energy Conversion
- Material Sciences / Material Design
- Medicial Sciences / Digital Patient
- Artificial Intelligence / Machine Learning
- Data Science
- Data Management
- Physics

Data Challenge

- Large data
- Unclear relationships

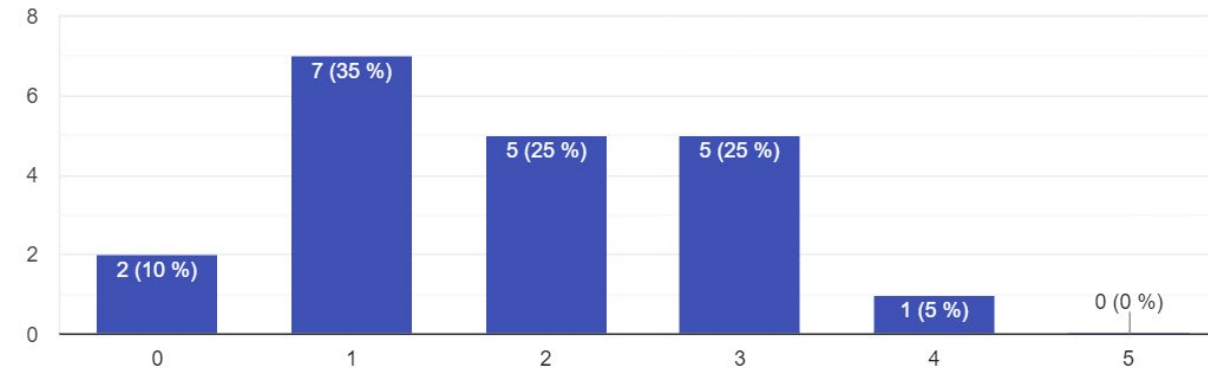
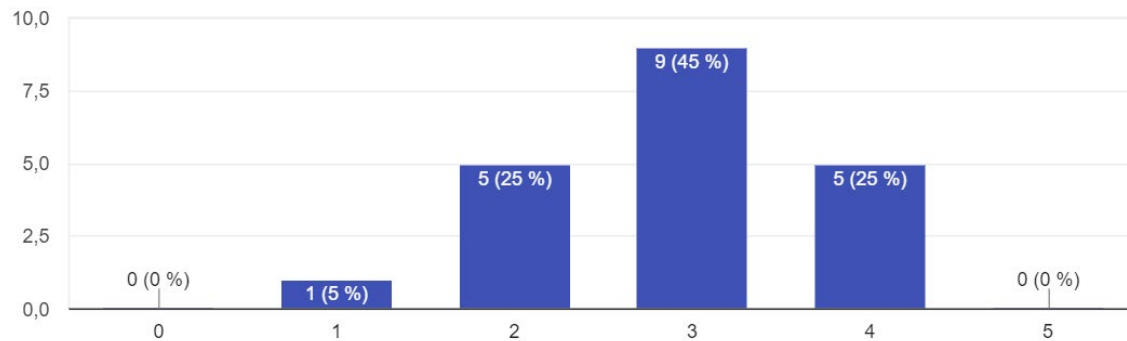


Cumbersome

- Converting data
- Robust workflow
- In-Situ visualization
- Not familiar with visualizations
- Overview of plots (ensemble)
- High complexity

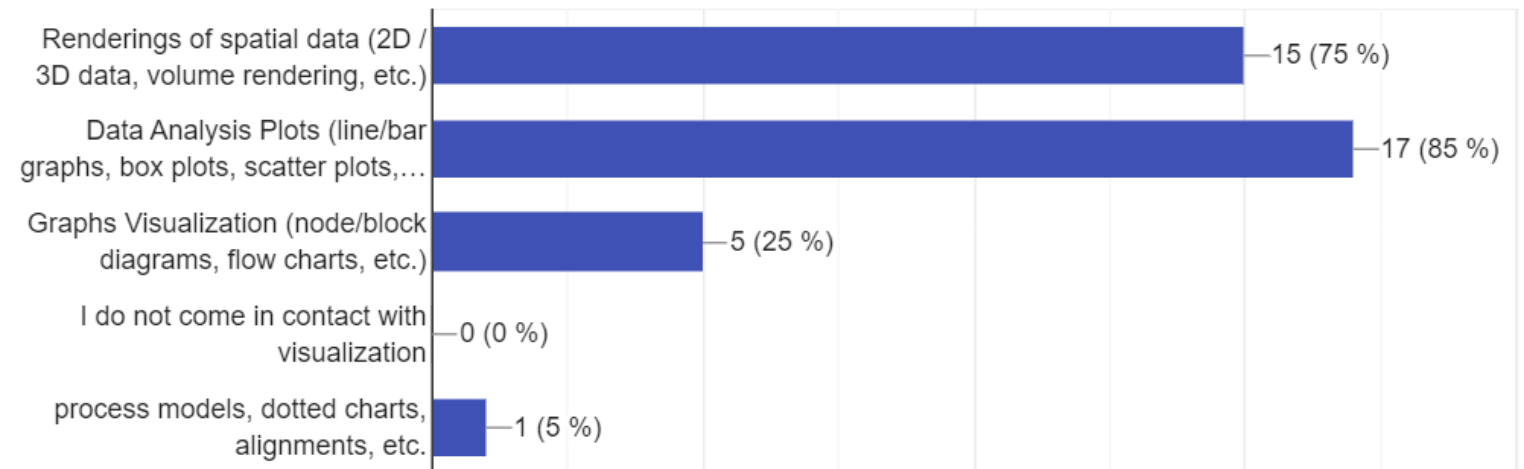
Using Visualization

- Most researchers consider their experience level low to middle
- Only few well informed about current visualization approaches within their domain



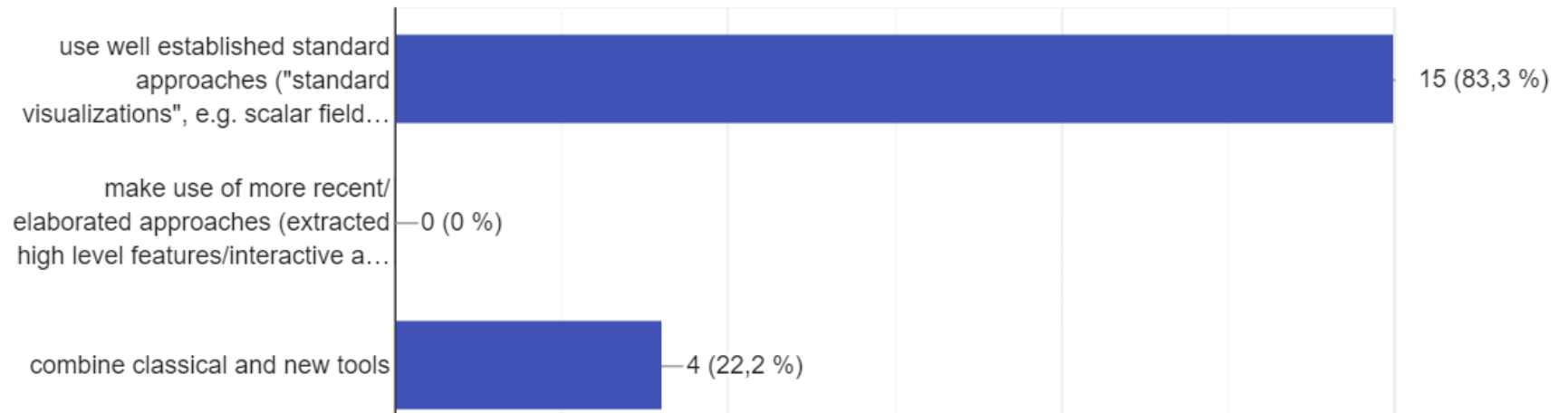
Using Visualization

- Create figures for publications
- Evaluation of results (General Plausibility / Error Check)
- Get overview and explore data

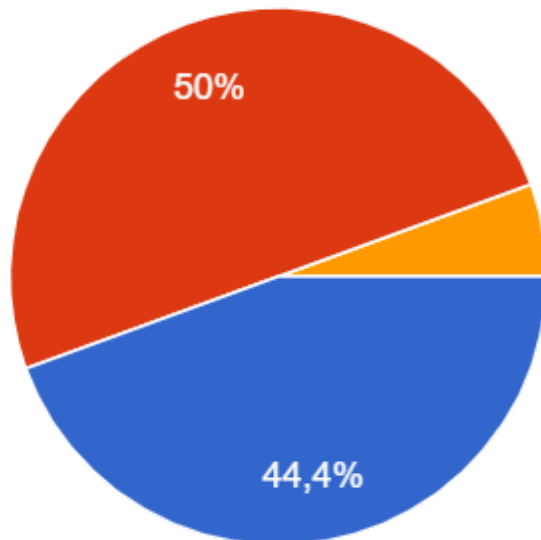


Using Visualization

- Opensource software ~75%
- 10% is custom written code
- Standard over advanced tools



Visualization Tools



- use whatever tool I know to get the job done fastest
- use a tool that is standardized within our research group
- contact a designated person/group who provides such graphics for me
- do not use visualization at all

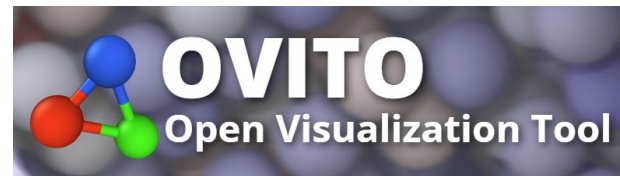
What They Use

- Line plots, line plots, line plots
- 2D slices of spatial data with standard color mapping
- Easy 1-2 click solutions

matplotlib



What They Use Sometimes



What They don't Use / don't Know

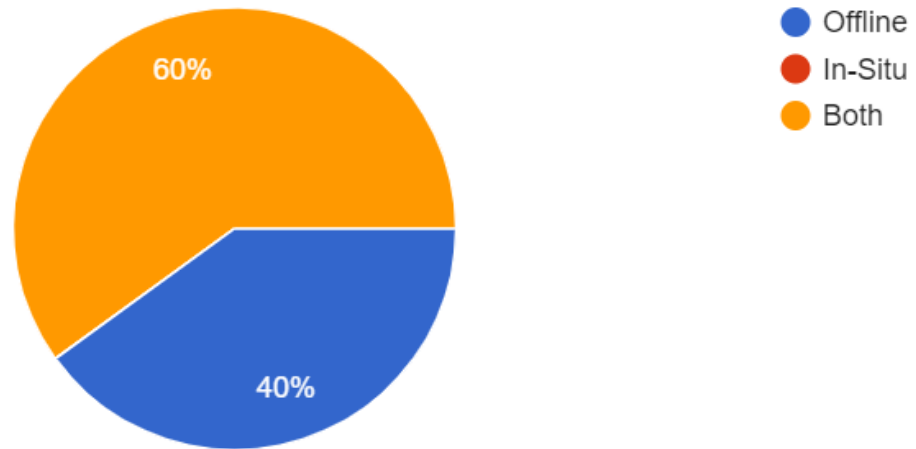
Catalyst,
Amira,
Ensignt,
Tableau,
D3.js,
Voreen,
Fiji,
ImageVis3D,
Imaris,
Inviwo,
Met.3D,
MeVisLab,
VAPOR,
VisTrails,
tomviz,
MeshLab

...

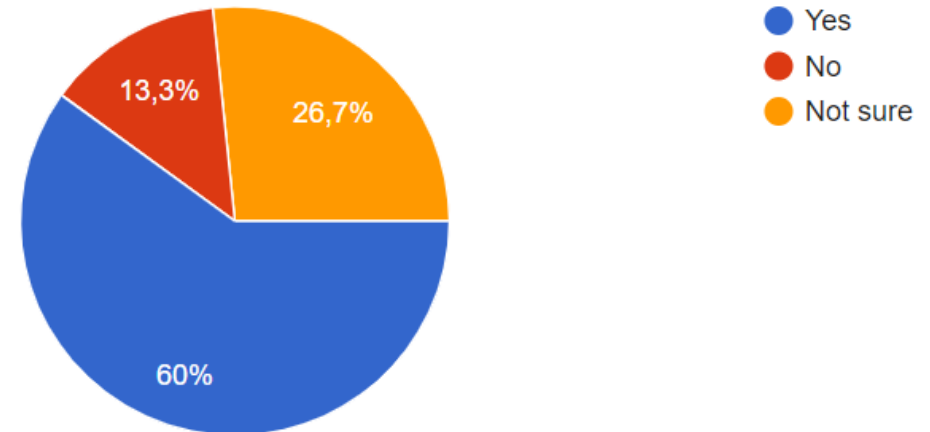
What They Wish for

- First of all: Easy of use, real-time response and easy integration into current workflow
- Interactive Analysis
- In-Situ visualization
- Ensemble visualization
- High-Dimensional data visualization
- Virtual Reality
- Often they don't know

In-Situ Visualization

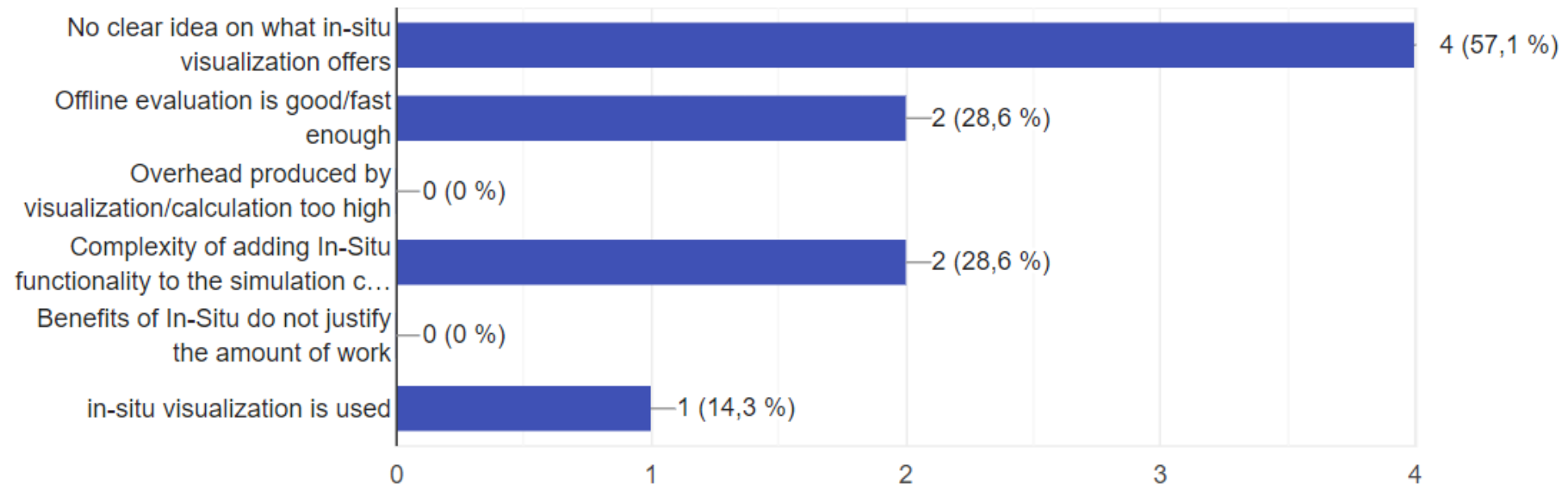


Offline vs In-Situ Vis

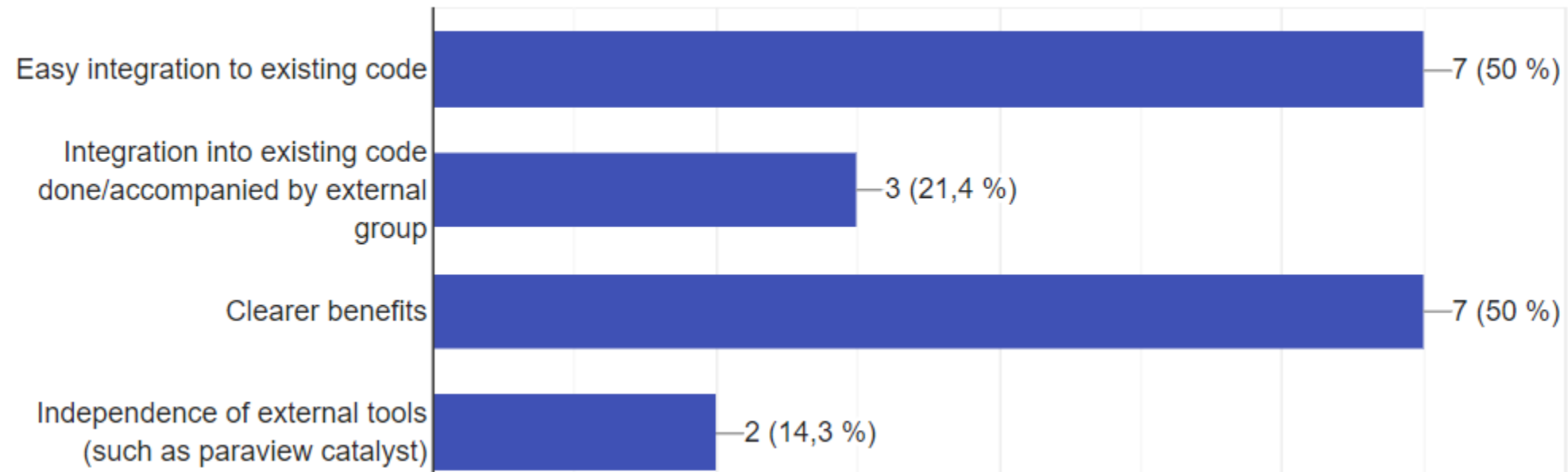


Is In-Situ Vis Useful?

Why no In-Situ Visualization



How to Make Them Use In-Situ



What They Wish for

Which services by the visualization group would you find most useful for your work?

9 Antworten

problems for specific applications (e.g., 3D spatial data) or file formats. 2. Provide an overview of the current state of art.

Checking publication figures and providing orientation

Provide expertise on current visualization tools for specific data types

Advice on useful tools for better visualizations in papers

List of possibilities and links to API documentation for C++ implementation. Support if needed.

Advise / guidance in what tools there are, to specific problems. Some help with the code if it makes sense, but I don't expect to just "order" the full solution.

In process mining, there are plenty of opportunities to co-develop new visualization. However, thus far the group was not interested in this.

Provide expertise on the subject. Provide updates on the latest vis tech that could be relevant for our group. Provide support for improving our vis workflows.

What I Learned from Asking

- All groups use only very basic visualization
- All groups want more and more advanced visualization (especially explorative tools)
- All groups don't really know what is out there, what can be done, what tools can offer
- Large gap between visualization community and HPC community

- Visualization needs to better communicate what they are capable of
- Increase ease of use for advanced vis methods (guidance, catalogue, ...)
- No general one-fits-all solution

What I Learned About Their In-Situ Vis Needs

- Benefit not clear
- Easy integration needed also for existing code
- No “fits it all” solution

So... What Now?

Creating the Outline

- Bring visualization closer to the users (knowledge and techniques)
 - Integrate into Workflow (from user view and from technical side)
 - Show advanced methods
 - Communicate current progress
 - Build a strong network
- Close the gap

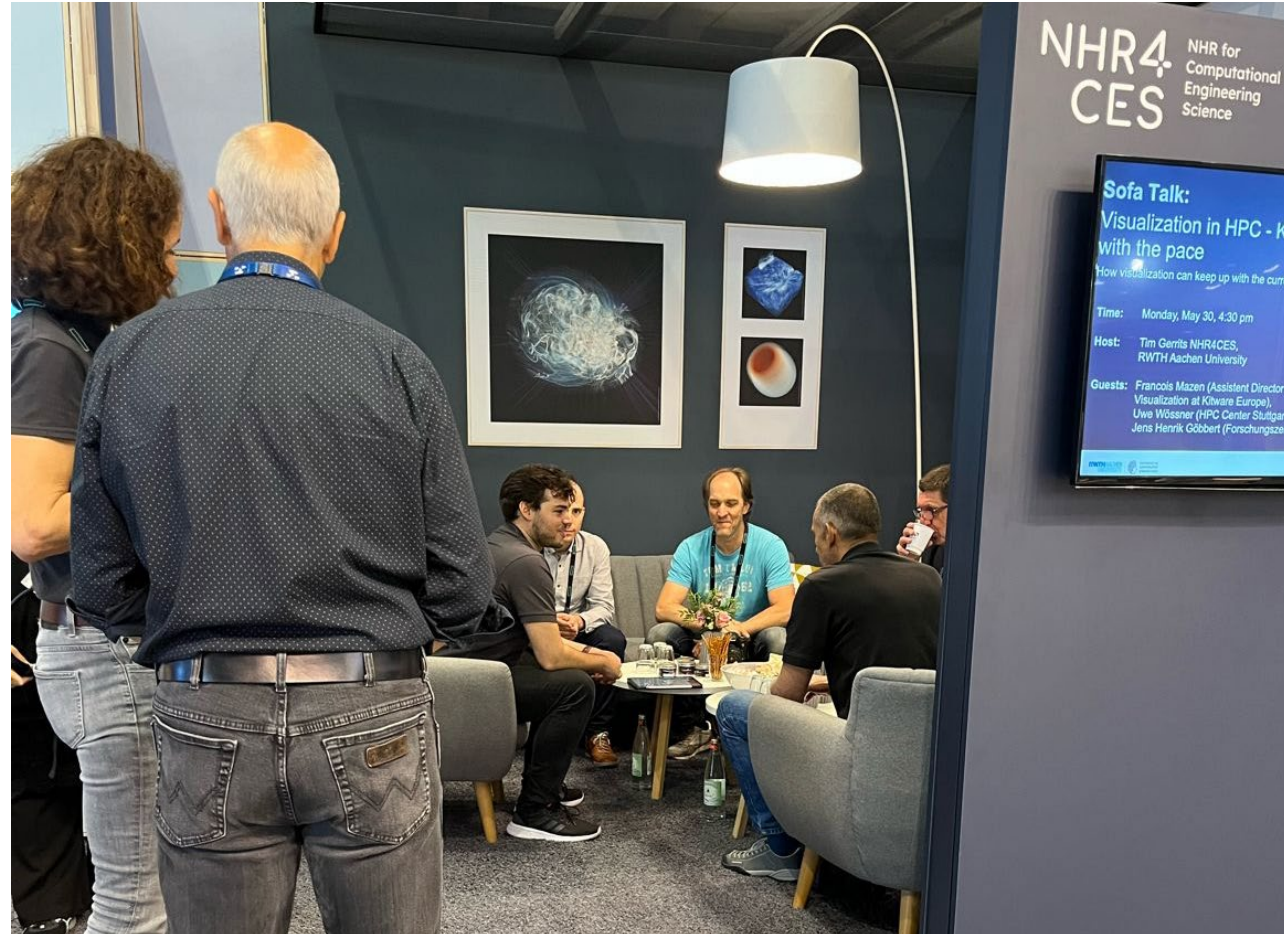
Creating the Outline

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With NHR, we have time and funding to create this culture and infrastructure

Writing the First Chapter

Writing the First Chapter



Training

Veranstaltungen

Nähere Informationen zu HPC-Veranstaltungen finden Sie im [Kalender der Gauß-Allianz](#).

Informationen über NHR-Veranstaltungen abonnieren Sie über diesen Verteiler:

<https://www.listserv.dfn.de/sympa/subscribe/nhr-announcements>

	Veranstalter	Organisator	
2022			
12.-23. Sept.	PC2, TU Clausthal	PC2, TU Clausthal	Kurs: Hands-on course on density-functional calculations - International CP-PAW Autumn School https://events.uni-paderborn.de/event/177/
19.-21. Jul. 9:00-16:30	PC2	PC2	Training: Julia for High-Performance Scientific Computing https://events.uni-paderborn.de/event/383/
19.+20. Jul. 9:00-18:00	PC2	PC2	Kurs: Performance Engineering course https://events.uni-paderborn.de/event/174/
11.-15. Jul.	NHR@TUD	NHR@TUD	Summerschool: 8th International ScaDS.AI Summerschool https://scads.ai/education/summer-schools/scads-ai-summer-school-2022/
11. Jul. 10:00-15:00	NHR@TUD	NHR@TUD	Tutorial: R on HPC - Introduction https://event.zih.tu-dresden.de/nhr/r-hpc
5.+6. Juli	NHR@Göttingen	NHR@Göttingen	Live-Veranstaltung: Proud and Strong in Computing Conference https://psc.gwdg.de/
4.+5. Jul.	NHR@Göttingen, NHR@ZIB	NHR@Göttingen, NHR@ZIB	Live-Veranstaltung: HLRN Open User Conference <i>Bitte die Timelines beachten!</i> https://events.gwdg.de/event/150/
20.+21. Jun.	NHR4CES@RWTH, NHR4CES@TUDa	NHR4CES@RWTH, NHR4CES@TUDa	Workshop: The Role of High-Performance Computing in Computational Engineering Science https://www.nhr4ces.de/index.php/nhr4ces-community-workshop/
15.+16. Jun. 9:30-16:00	NHR@Göttingen	NHR@Göttingen	Kurs: High Performance Data Analytics - Part 2 https://www.gwdg.de/academy/course?course=1398
15. Jun. 9:00-13:00	NHR@TUD	NHR@TUD	Tutorial: Analyzing Deep Learning APIs and Applications with HPC performance tools https://event.zih.tu-dresden.de/nhr/deepl-hpc
10. Jun.	NHR@TUD	NHR@TUD	Tutorial: HPC Cluster Administration mit xCAT

NHR4CES Community Workshop

NHR4CES Community Workshop

We at the National High Performance Computing Center for Computational Engineering Science (NHR4CES) are happy to announce the first:

NHR4CES Community Workshop:

The Role of High-Performance Computing in Computational Engineering Science

June 20, 1.45 pm – 5.45 pm and June 21, 2022, 8.45 am – 12.45 pm

With this, we hope to connect with our research community, encourage exchange, strengthen our network and create new connections.

During this two-day online workshop, participants have the opportunity to learn about the importance of High-Performance Computing (HPC) in various fields of Computational Engineering Science.

The event will comprise presentations by distinguished researchers from different domains and participants are invited to get involved in subsequent panel discussions.

The sessions cover topics from Computational Fluid Mechanics, Numerical Combustion, Material Science and Medical Science as well as Parallelism and Performance, Data Science & Machine Learning, Data Management, and Visualization.

The Workshop is aimed toward researchers who are already an active part or are planning to be part of these research communities as well everybody interested in collaborations or information on the available HPC resources and services offered by NHR4CES

Writing the First Chapter

WOIV'22
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[Timeline](#)
[People](#)
[Previous Editions](#)

WOIV'22

6th International Workshop on In Situ Visualization

Thursday, June 2, 2022 · 2pm to 6pm, CEST · Hamburg, Germany
Held in conjunction with [ISC High Performance 2022](#).

Register

Registration is open. Early-bird deadline: April 26, 2022.
Organized by [Peter Messmer](#), [Tom Vierjahn](#), and the [WOIV team](#).

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02.06.2022

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Keynote