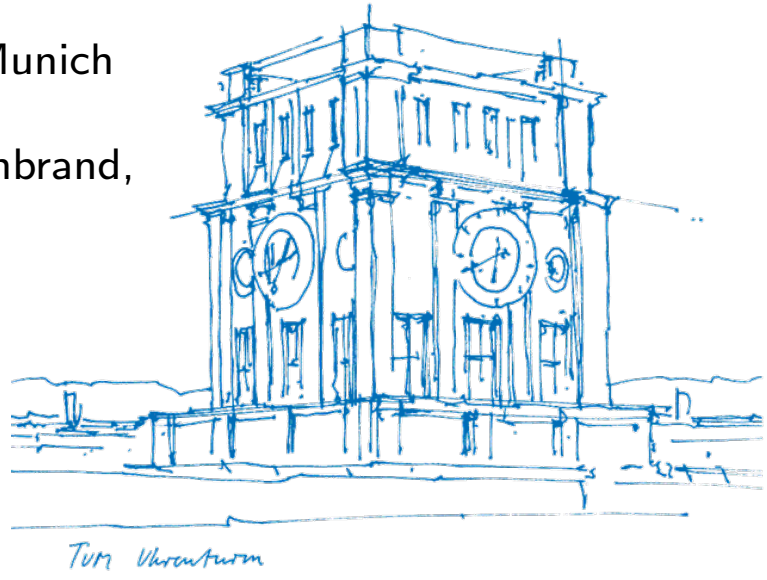
Seminar Efficient Programming of HPC Systems – Frameworks and Algorithms – Kick-off

Erwin Laure

Max Planck Computing and Data Facility & Chair of Computer Architecture and Parallel Systems
Faculty of Informatics Technical University of Munich

with Material from Alexis Engelke, David Hildenbrand, Michael Petter, and Josef Weidendorfer

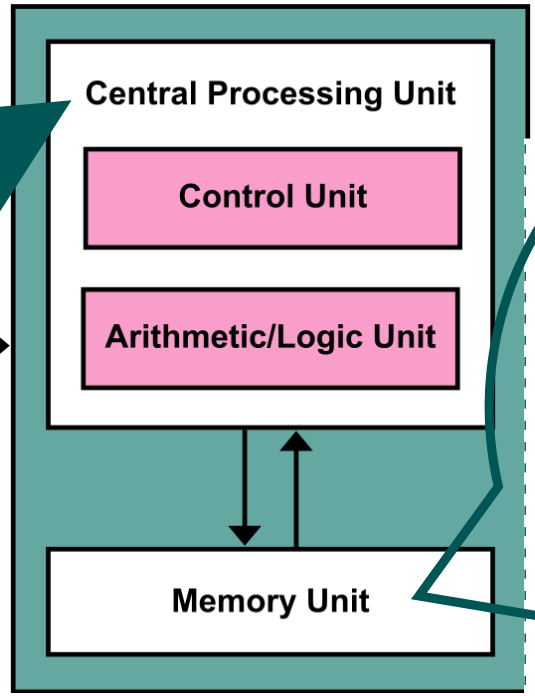
6.05.2025

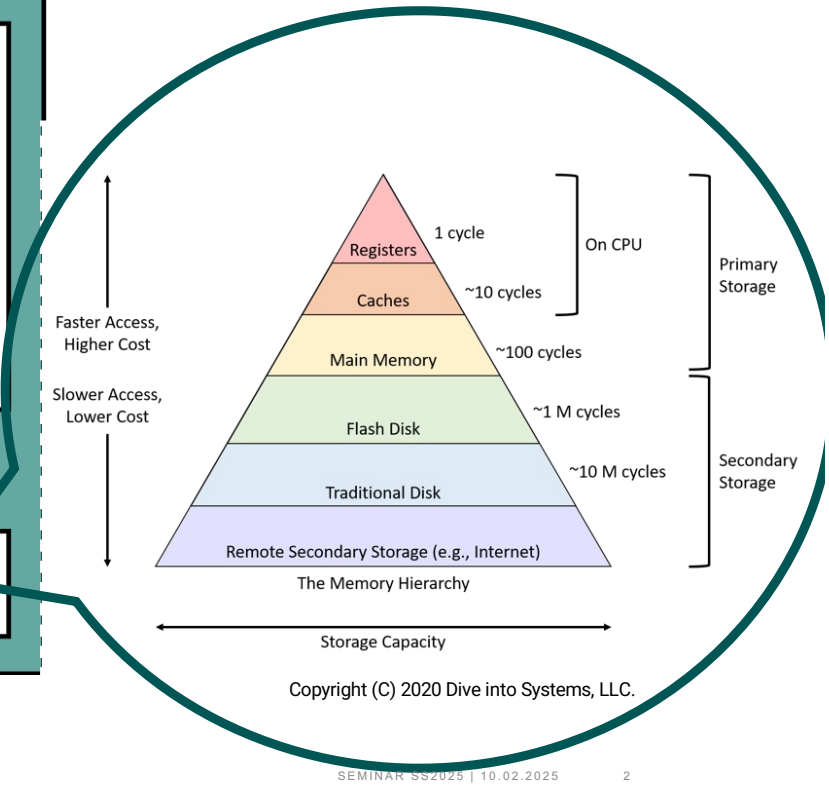


Background

FROM SIMPLE VON NEUMANN ARCHITECTURES TO MODERN HPC SYSTEMS

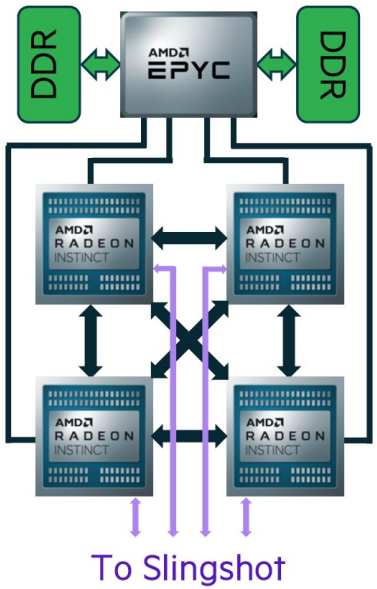
- Multi-Core
  - E.g. 128-core AMD
- Lots of Optimizations
  - Pre-fetch
  - Branch prediction
  - FMA
  - Vector
  - Etc.
- Other features
  - Encryption
  - Viz
  - Etc.





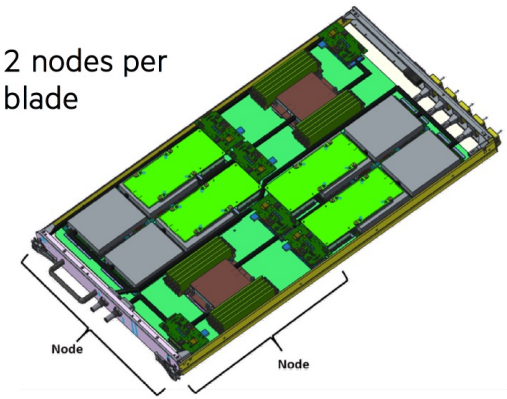
Background

AND THEN WE ALSO ADD ACCELERATORS (GPUS)



AMD GPU (ORNL)

2 nodes per blade



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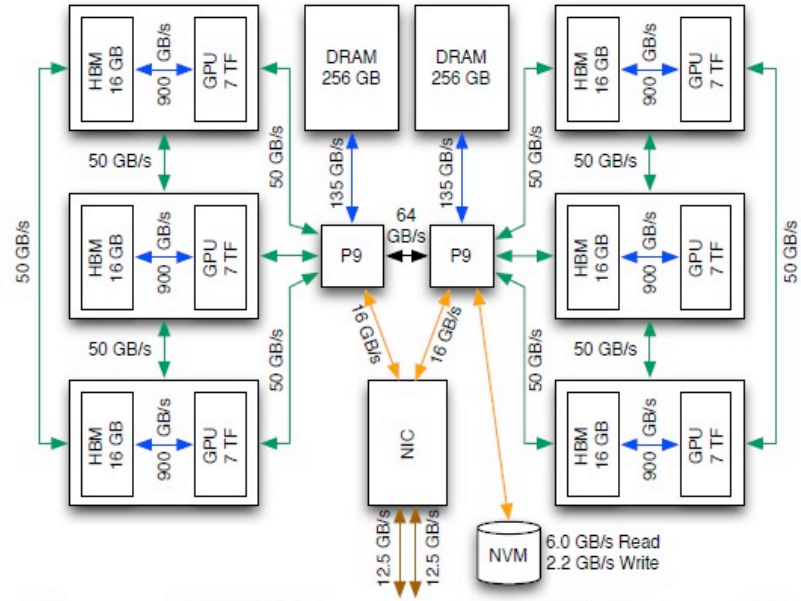


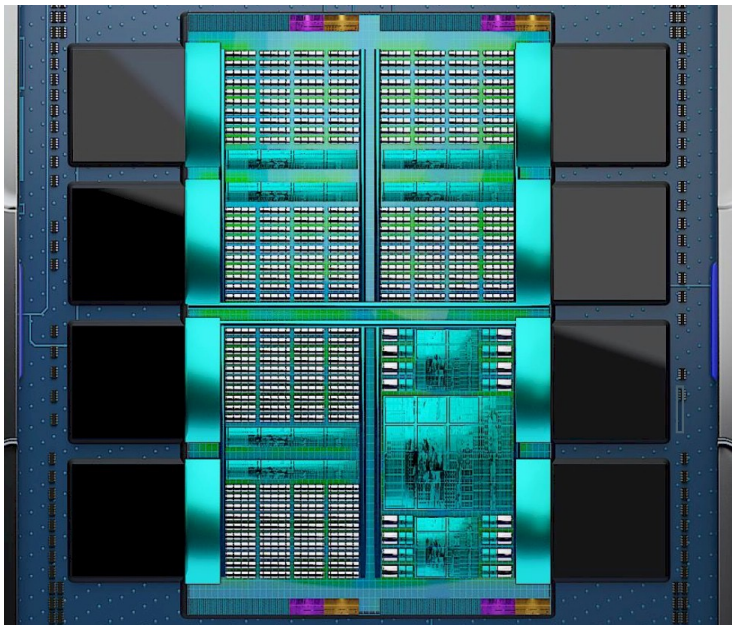
TF	42 TF (6x7 TF)
HBM	96 GB (6x16 GB)
DRAM	512 GB (2x16x16 GB)
NET	25 GB/s (2x12.5 GB/s)
MMsg/s	83

HBM/DRAM Bus (aggregate B/W)
NVLINK
X-Bus (SMP)
PCIe Gen4
EDR IB

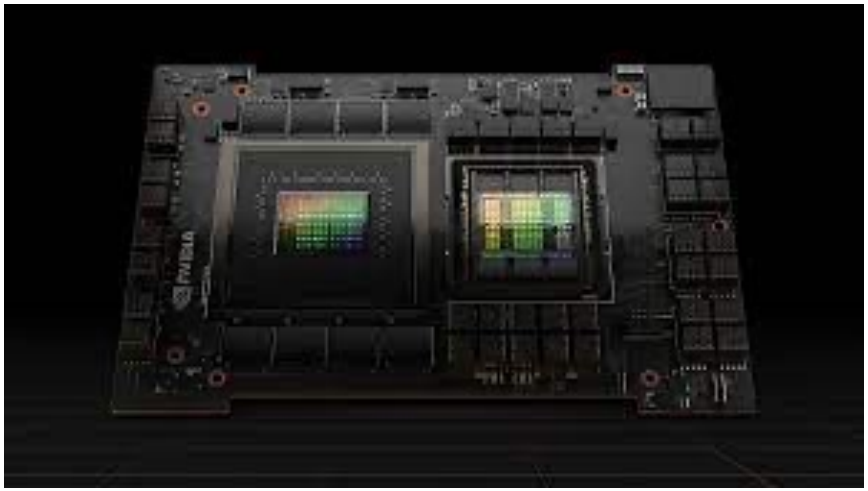
HBM & DRAM speeds are aggregate (Read+Write).
All other speeds (X-Bus, NVLink, PCIe, IB) are bi-directional.

Background

NEW GPU-CONCEPTS MIGHT BE EASIER TO USE (CACHE COHERENT DESIGN)



AMD MI300A



Nvidia Grace-Hopper

AND USE MANY, REALLY MANY OF THESE NODES

- **El Capitan Supercomputer @ LLNL:**
  - 11.136 nodes
  - 1,74 EF performance
  - 30 MW power consumption
  - in total over 11 M cores (mostly GPU – MI300A)

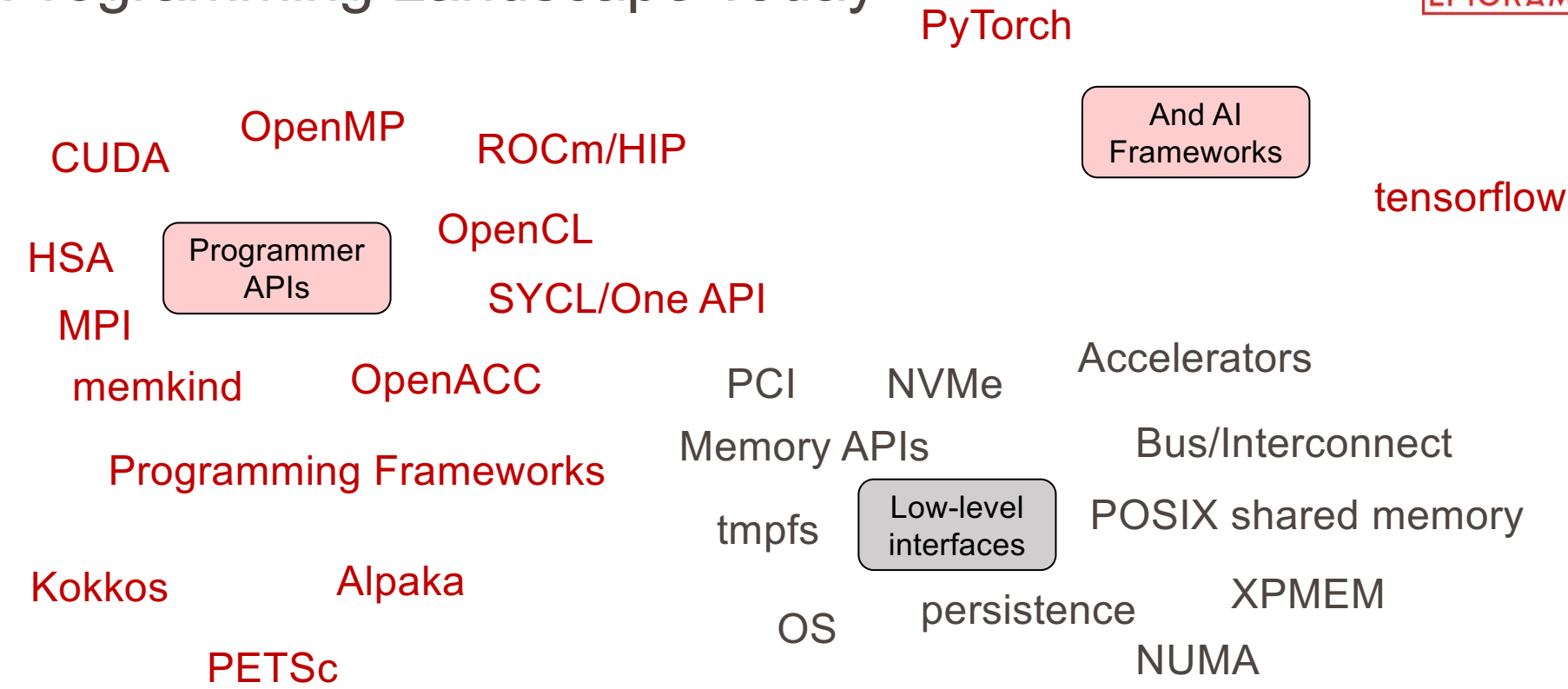
(SOME) CHALLENGES IN PROGRAMMING THESE SYSTEMS

- **Level of parallelism**
  - O(10^9) FPUs
- **Hardware heterogeneity**
  - CPUs, GPUs, other
  - HBM, NVMe, object store
- **Programming/Performance Portability**
- **Impact of AI**
  - Low precision hardware (GPUs)
  - “AI for Science”
- **Novel numerical/methodological approaches**
  - How to deal with low precision hardware (mixed precision, emulation, etc.)

THE GOOD OLD TIMES

- Programms written in Fortran (or C/C++)
- MPI (Message Passing Interface) for moving data across distributed memory
- OpenMP for expressing parallelism on shared memory

Programming Landscape Today



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Goals & Topics

- **Investigate techniques, frameworks, algorithms to efficiently program such systems**
  - Focus on heterogeneous architectures (GPUs, shared/distributed memory)

- Topics
  - High-level frameworks (Kokkos, Alpaka, Cabana, PETSc, etc.)
  - Numerical libraries (SLATE, Ginkgo, heFFTe, etc.)
  - Data Formats (Mixed-precision, non-IEEE data formats, data compression)
  - Data Structures and Layouts (AoS-SoA-AoSoA)
  - Adaptive Mesh Refinement (AMReX, p4est, etc.)
  - Adaptive (task) Parallelism (HPX, StarPU, OpenMP, etc.)
  - In-Situ Approaches (ADIOS, etc.)
  - Frameworks for AI (pytorch, tensorflow, etc.)

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  - Frameworks for AI (pytorch, tensorflow, etc.)
  - Bring your own topic

Specific Goals

- Find 3-4 suitable publications & suitable websites
- Describe briefly how the mentioned approach works and helps with achieving efficiency
- Does the mentioned approach enable a code to be portable across architectures?
- Show and discuss performance numbers (from papers)
- Discuss advantages and drawbacks

Organization

- Kick-off meeting (today)

- Select a topic (send 3 choices via email) - assignment early next week
- Literature research + derive article structure
- Discuss structure with advisor
- Write draft paper – deadline 2025-06-30

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- Incorporate feedback from peers and advisor
- Final submission + presentation – July 16, 2025

Scientific Writing and Presentation

- Literature and sources
  - Finding literature and citable sources/references
- Writing a seminar paper
  - Structure, style, citing
- Presentation techniques
  - Structure, slide design, presentation style

Citable Literature

Good to use

- Books, book chapters
- Papers (conf./journal)
- Published articles
- Manuals

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Try to avoid

- Wikipedia
- Facebook, etc.
- Advertisements
- Lecture slides
- Source code
- **ChatGPT**

Finding literature

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- Starting points: IEEExplore, ACM DL, Google Scholar, arxiv.org, ChatGPT, ...
  - Select appropriate keywords
  - Many papers/books accessible freely via the library

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- Other starting point: your advisor
- Graph algorithms
  - Publications of the same author(s)
  - Publications at the same venue
  - Cites ... (listed references)
  - Cited by ...

Structure

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- Abstract: Brief summary of area, problem, approach, result
- Introduction: introduce area, problem, key results, contributions, outline
- Background: if needed, describe prerequisites

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- (*In a paper:* Related Work)
- Summary & outlook

Writing style

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- Factual, precise, focused
  - Stay on topic, no story telling, ...
  - Limit to important and necessary topics
  - Don't omit necessary prerequisites

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- Factual, precise, focused
  - Stay on topic, no story telling, ...
  - Limit to important and necessary topics
  - Don't omit necessary prerequisites
- Avoid forward references
- Avoid *I*, prefer *we* (or passive voice)
- *We* only describes the authors, not the reader

Citing

- All work that is not yours **must** be cited
  - Clearly describe source
  - But: no wrong/inaccurate attributions
- Citing styles:
  - Literal (direct) quote
  - indirect quote (rephrase) ←strongly preferred
- Exception: foundations can be assumed (generally first few Bachelor semesters)

Citing: Examples

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The x86 architecture defines the register CR2 [1].

```
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register CR2~\cite{intel2019man}.
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```

Other approaches [1,2,3] ...

```
Other approaches~\cite{foo,bar,baz}
\dots
```

Presentation: Content Selection

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Presentation for the **audience**!

Presentation: Content Selection

Presentation for the **audience**!

- What do you want the audience to take away?
  (Not: what can I talk about!)
- What are the key points?
- How much content fits into the time slot?

Structure

- Motivation
  - Why is the topic relevant?
- Background
  - Consider referencing information from previous talks
- Concept
- Evaluation
  - How good is the described concept?
- Conclusions and outlook

Structure

- Important: topics build upon each other!
  (avoid forward references)
- Only give important details
- Use good/helpful examples
- Critical discussion of the topic

Media

- Slides (Beamer)
  - For use during the talk
  - Good to prepare
  - *Backup-Folien* as preparation for questions
- Whiteboard, blackboard
  - Permanently needed information
  - Answering questions
- Hardware, demonstrators, etc.

- Check possibilities in advance

Before the Talk

- Prepare slides, etc.
- Do a dry-run
  - Always recommended
  - Helps with uncertainity and time estimation
- Prepare on-site
  - Laptop, Beamer, laser pointer, clock, etc.

Talking Style

- Speak freely
- Don't go too fast/slow
- Stay in contact with the audience
  - Eye contact, position, etc.
- Usually at least 1 minute per slide
- Explain charts
- Stay in time limit
  - Optional slides can fill time
  - Regularly consult a watch

- **Stay calm**

Slides: Content

- One topic per slide
- Avoid text
  - ≤ 8 points
- Prefer graphics/illustrations

Slides: Content

- One topic per slide
- Avoid text
  - ≤ 8 points
- Prefer graphics/illustrations
- No unused points
  - Cover everything on the slides in your talk

Slides: Content

- Title page
  - Title, name, institution, date, location

Slides: Content

- Title page
  - Title, name, institution, date, location
- On every other slide: number and title

Slides: Content

- Title page
  - Title, name, institution, date, location
- On every other slide: number and title
- Conclusion
  - Alle important points on one slide

Slides: Colors

- **Black on white**

Slides: Colors

- **Black on white**
- **Black on white**

Slides: Colors

- **Black on white**
- **Black on white**

- Sufficient contrast
- Use colors sparingly, but systematically
- Be careful with gradients
- No annoying backgrounds (wave textures, etc.)

- **Animations only with sufficiently added value**

Slides: Text and Graphics

- Double-check text for typos, etc.
- Use a readable, sans-serif font
- Prefer vector graphics (or images with a high resolution)
- Avoid screenshots/scans
- Important: citations

- Listings only with a sufficiently large value

Negative Example

Alignments in brief

>1bl8_A mol:protein length:97 Potassium Channel Protein
ALHWRAAGAATVLLVIVLLAGSYLAVLAERGAPGAQLIT
YPRALWWSVETATTVGYGDLYPVTLWGRCVAVVVMVA
GITSFGLVTAALATWFVGREQ

>1orq_C mol:protein length:223 Potassium Channel
IGDVMEHPLVELGVSYAALLSVIVVVVECTMQLSGEYLV
RLYLVDLILVIILWADYAYRAYKSGDPAGYVKKTLYEI
PALVPAGLLALIEGHLAGLGLFRLVRLLRFLRILLIISRG
SKFLSAIADAADKIRFYHLFGAVMLTVLYGAFAIYIVEY
PDPNSSIKSVFDALWWAVVTATTVGYGDVVPATPIGKV
IGIAVMLTGISALTLLIGTVSNMFQKILV

Query= 1bl8_A mol:protein length:97 **Potassium Channel Protein**
(97 letters)

>1orq_C mol:protein length:223 **Potassium Channel**
Length = 223

Scoring matrix
Algorithm to optimize score

Score = 58.5 bits (140), Expect = 4e-14
Identities = 26/72 (36%), Positives = 43/72 (59%)

```
Query: 21  GSYLAVLAERGAPGAQLITYPRALWWSVETATTVGYGDLYPVTLWGRCVAVVVMVAGITS 80
           G++   + E   P + +  +  ALWW+V TATTVGYGD+ P T  G+ + + VM+ GI++
Sbjct: 147 GAFAIYIVEYPDPNSSIKSVFDALWWAVVTATTVGYGDVVPATPIGKVIGIAVMLTGISA 206

Query: 81  FGLVTAALATWF 92
             L+   ++  F
Sbjct: 207 LTLLIGTVSNMF 218
```

[redacted]

Negative Example

Negative Example

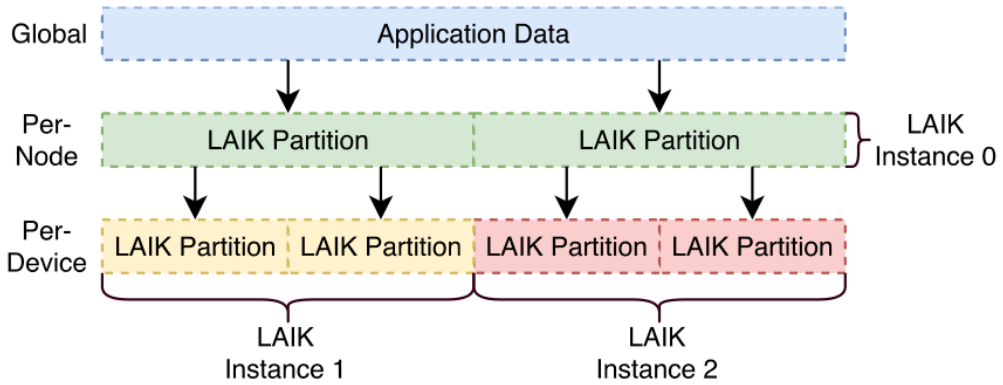
```
\begin{frame}
\frametitle{Die Anti-Folie}
\begin{figure} [ht]
  \centering
  \includegraphics[width=0.95\textwidth]{pictures/antifolie.jpg}
    \caption{Werbe-Folie. Foto von Flickr-Benutzer niallkennedy
      (https://www.flickr.com/photos/niallkennedy/58697220/sizes/l/)}
  \label{fig:gliederung}
\end{figure}
\end{frame}
```

Abbildung: Screenshot of code with insufficient resultion

LAIK (5) – Hierarchische Partitionierung

- multiple Partitionierung auf verschiedenen Ebenen
- Beispiel: inter/intra-node
- sinnvoll für Exascale, heterogene Systeme

- Veränderung des Indexraums muss möglich sein!



End of Presentation

- Summary slide with main take-away points

End of Presentation

- Summary slide with main take-away points
- NO *Questions* slide!

Summary

- Bring your point to the audience – written or spoken
- Good literature as starting point
- Logical structure for paper and presentation
- Presentation: good preparation is important

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- Chance to learn ☺

Summary

- Paper 6-8 pages
- Presentation about 15 Minutes plus questions (5 minutes)

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- Grading
  - 40% paper
  - 40% presentation
  - 20% review
  - all needs to be positive
- start literature search now and get in contact with your tutor

Questions

Questions

Summary

- Paper 6-8 pages
- Presentation about 15 Minutes plus questions (5 minutes)

- Grading
  - 40% paper
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  - all needs to be positive

- communicate **three (3)** topics until May 9
- final topics and tutor will be assigned next week
- start literature search now and get in contact with your tutor