Erlangen Regional Computing Center

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

High Performance Computing an der Friedrich-Alexander-Universität Erlangen-Nürnberg

Prof. Gerhard Wellein

Department Informatik und Regionales Rechenzentrum Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg

Gegründet am 4. November 1743 durch Markgraf Friedrich von Brandenburg-Bayreuth

1769 ausgebaut durch Markgraf Alexander von Brandenburg-Ansbach und Brandenburg-Bayreuth

Structure of FAU

5 Faculties with 23 Departments
University Hospital with 43 Departments / 7 Institutes

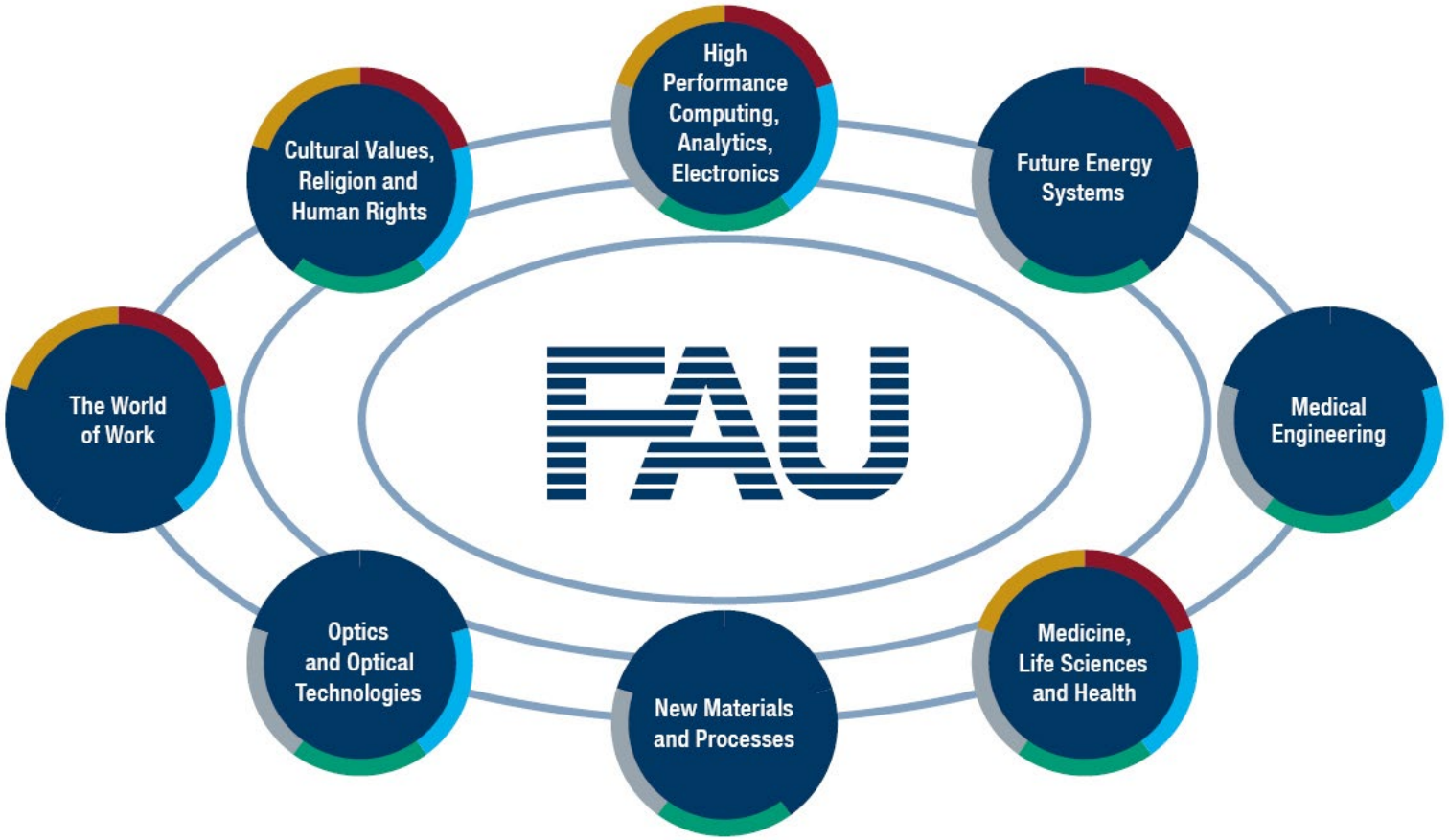
Humanities, Social Sciences, and Theology	Business, Economics, and Law	Medicine	Sciences	Engineering

- 39.000 Students (50% female, 13% international)
- 261 Degree Programmes (of which 77 Bachelor, 93 Master)

- 585 Professors
- 3.500 Research Employees
- 2.300 Non-research Employess

- 211 Mio. € Third-Party Funding (2019)
- Ranked No 3 in Europe in the Reuters Innovation Ranking 2019

FAU Key Research Priorities



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Das Regionale Rechenzentrum Erlangen

1968: Einrichtung des Universitätsrechenzentrums Erlangen

1979: Erweiterung zum Regionalen Rechenzentrum Erlangen

High Performance Computing

RRZE: Versorgungsauftrag

- Dienstleister der verteiltesten Universität Deutschlands
  - FAU bewirtschaftet 220 Gebäude
  - in fünf Städten: Erlangen, Nürnberg, Fürth, Bamberg und Pleinfeld (Wassersportzentrum)

- Regionales Rechenzentrum Erlangen
  - Universität Bayreuth und Otto-Friedrich-Universität Bamberg
  - Technische Hochschule Nürnberg, Evangelische Hochschule Nürnberg, Hochschulen Ansbach, Coburg und Hof
  - Aktuelle Aufgaben: Software-Beschaffung, Sync&Share Dienste,…
  - Betrieb zentraler Infrastrukturen wie HPC

RRZE: Zahlen

65.000	aktive Nutzer
61.000	Netzanschlüsse
190.000	Anzahl der verwalteten IP-Adressen
1 PB	Datenumsatz / Monat zum Internet
1.500	Subnetze
1.800	WLAN Access Points
360.000	E-Mail-Einlieferungsversuche / Tag
87.000	angenommene E-Mails / Tag
4.300.000	Zugriffe / Tag auf die zentralen FAU-Webserver
1.162	vom RRZE betreute Webauftritte an der FAU
609	vom RRZE betreute Serversysteme
4.194 TB	Datensicherung
Zahlen / High Performance Computing (HPC)	
> 100 TB	Hauptspeicher
> 800 TF/s	Rechenleistung (FP64)
> 32.000	Prozessorkerne

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High Performance Computing at RRZE

Systems, Infrastructure, Research and Teaching/Training

High Performance Computing

HPC@RRZE: Who are we?

- **HPC center**

- 2 main and 4 special purpose systems
- In total 1656 nodes and 134 GPGPUs
- User support & training: 3 people
- Systems & software: 3 people

- Associated **computer science research group**
  - Performance Engineering
  - Performance Modeling
  - Tool development
  - Sparse and stencil solvers

LIKWID TOOLS

KERNCRAFT

OSACA

- 1 professor
- 1 senior researcher
- 6 PHD students

https://github.com/RRZE-HPC

https://hpc.fau.de

HPC@RRZE: HPC Clusters

Node type	#nodes	cores/ node	#cores	price	peak perf.	TOP500	year
2 x Intel Xeon 2.66 GHz; 2 GB	77	2	154	0.35 M€	0.8 TFlop/s	315	2003
2 x Intel Xeon 3.0 GHz; 8 GB	182	4	728	1.0 M€	8.7 TFlop/s	124	2006
2 x Intel Xeon 2.66 GHz; 24 GB	500	12	6.000	2.3 M€	64 TFlop/s	130	2010
2 x Intel Xeon 2.2 GHz; 64 GB	**560**	**20**	**11.200**	**2.5 M€**	**200 TFlop/s**	**210**	**2013**
2 x Intel Xeon 2.2 GHz; 64 GB	**728**	**20**	**14.560**	**2.5 M€**	**513 TFlop/s**	**346**	**2016**

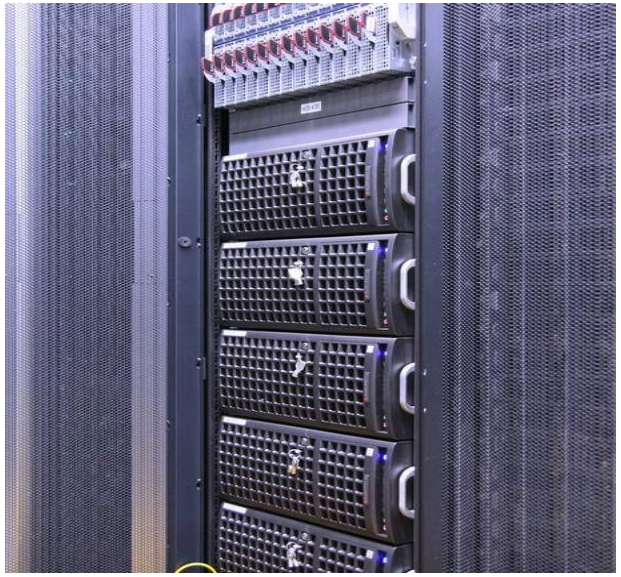
Basic strategy: **3-year investment cycles** → 2 systems in operation
Funding: Art. 91b

HPC-networks: Infiniband / Omnipath
Local parallel filesystems

New system
in 2021: 4.5 M€+

HPC@RRZE: GPUs

7 nodes:	2x “Nehalem” @2.66 GHz +	2x GTX980
7 nodes:	2x “Broadwell” @2.2 GHz +	4x GTX1080
10 nodes:	2x “Broadwell” @2.2 GHz +	4x GTX1080Ti
12 nodes:	2x “Skylake” @3.2 GHz +	4x RTX2080Ti
4 nodes:	2x “Skylake” @3.2 GHz +	4x Tesla V100



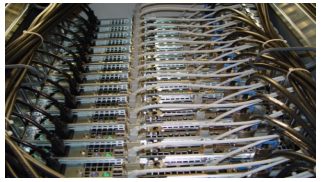
- Most nodes funded by individual users or research groups
- Major applications:
  - AMBER
  - GROMACS
- Some load from AI/ML
- Approx. 1.5 PF (FP32)

HPC@RRZE: Storage

- 6.5 PB central HPC storage (incl. backup & snapshots) IBM Spectrum Scale / NFS
- Tape Library with > 3000 slots & 8 LTO8 drives

HPC storage

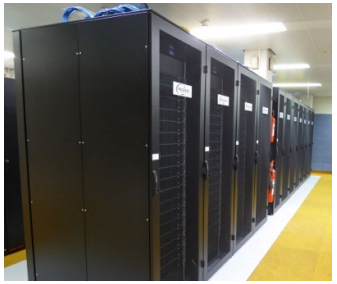
throughput cluster



“fat” nodes

40/100 GBit Backbone

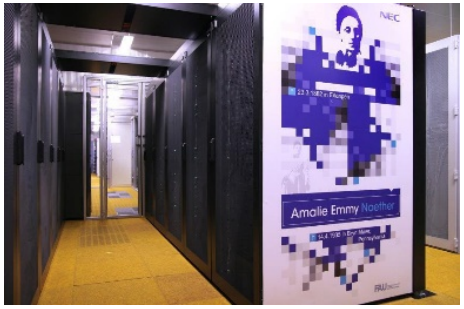
GPU cluster



HPC@RRZE: Infrastructure

- RRZE computer room / cooling
  - 400 m^2 – elevated floor
  - Max. capacity: 3360 U(nits) / 2500 U (used)

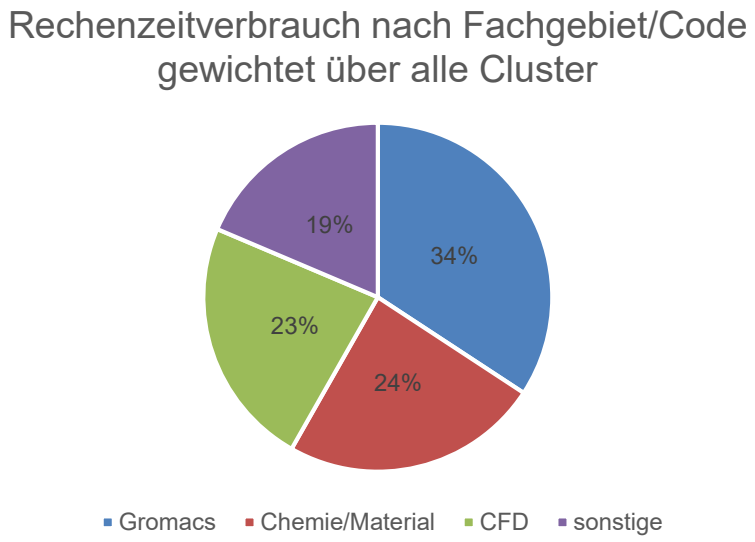
- Power consumption
  - Non-HPC: 200 KW
  - HPC: 400 KW



- HPC: back-door cooling

- Cold-water supply (TechFak):
  "Combined heat and power unit (CHE)
  with absorption chiller,
  compression chillers and free-air cooling"

HPC@RRZE: Users

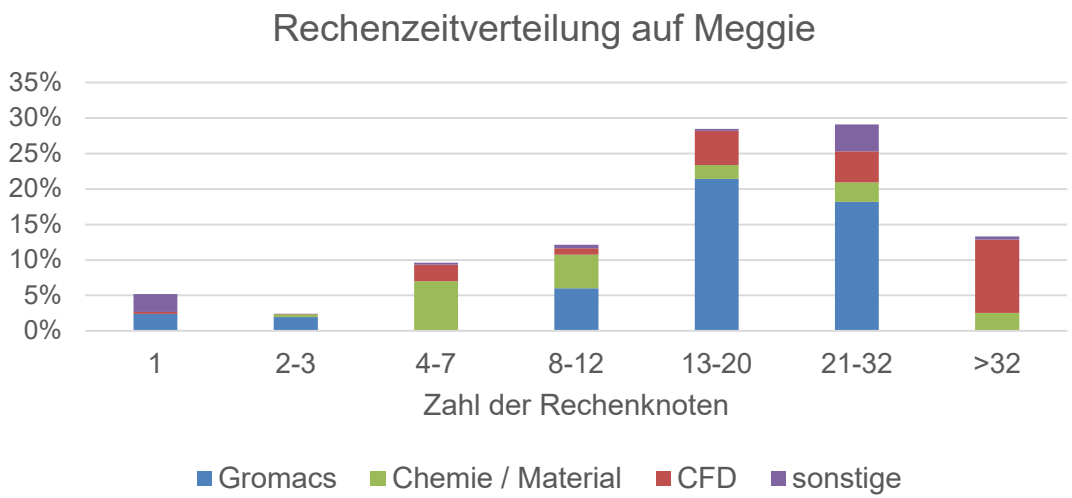


2019 (Alle HPC-Systeme):

- 535 aktive Accounts
- 65 unterschiedlichen Gruppen
- ca. 215 Millionen core-hrs
- 1,2 Millionen Jobs

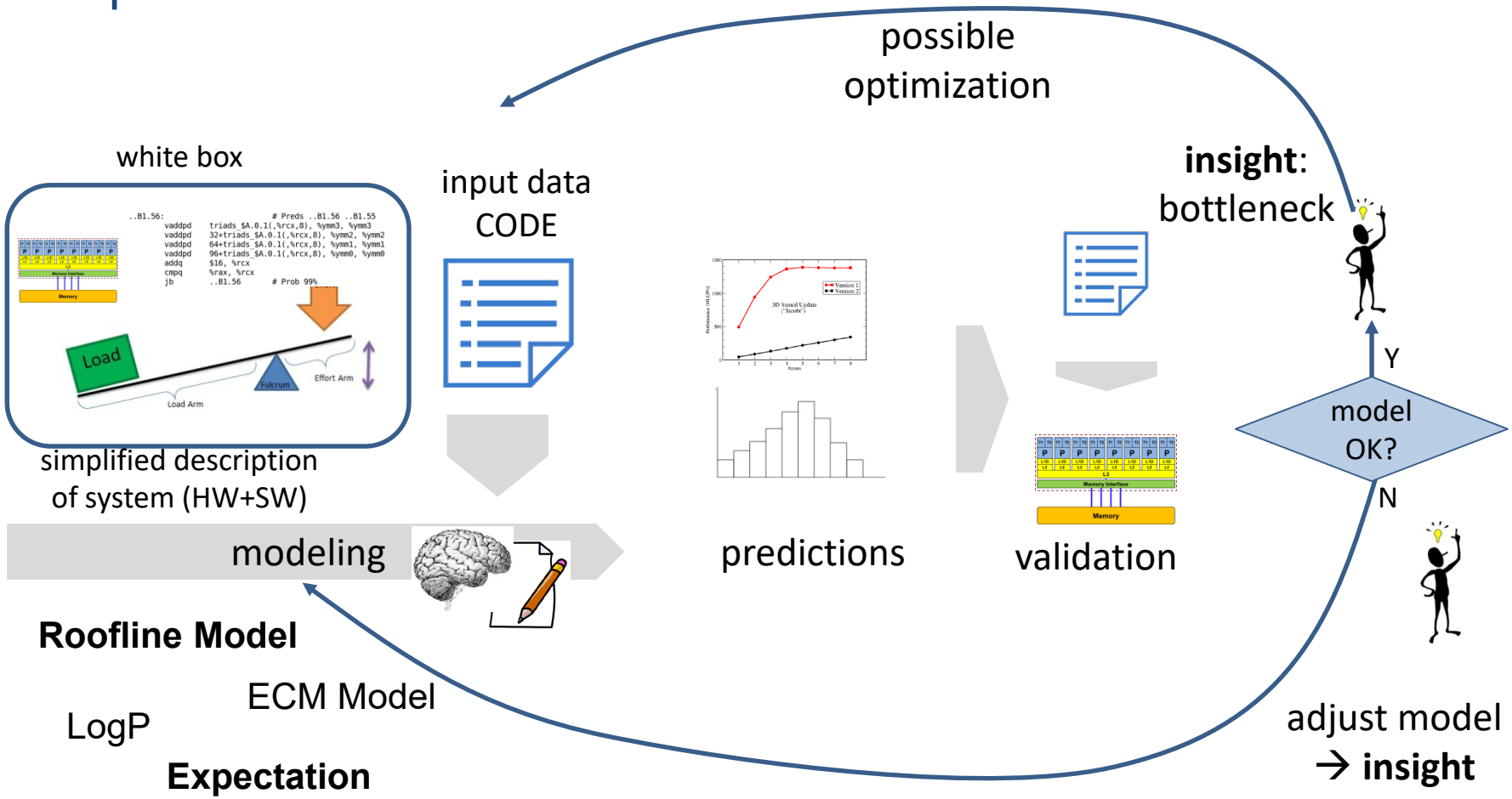
Trends:

- Community Codes an Stelle von Eigenentwicklungen
- Verbesserte GPU Unterstützung in Community Codes
- “Unexpected“ Power-Users



HPC@RRZE: Performance Engineering

PE: Identification and solution of performance issues by applying a well-defined process based on performance models and patterns.



HPC@RRZE: Recent Research Projects

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

ProPE

Performance Engineering@Tier-2
FAU/RRZE+RWTH/ITC+TU Dresden/ZIH

SPPEXA

DFG Priority Programme1648
ESSEX-II / EXASTEEL-II
(see www.sppexa.de)

DFG Deutsche Forschungsgemeinschaft

Performance Engineering

Performance Modelling

Performance Tools

Sparse and Stencil Solvers

SKAMPY
(FAU / KIT)

Meta X a

METACCA
(FAU / U. Saarland / DFKI / U. Mainz)

SEASITE
(FAU / U. Bayreuth / TU Chemnitz)

HPC-Software für skalierbare Parallelrechner
gefördert durch das
Bundesministerium für Bildung und Forschung

KONWIHR

Energy Oriented Center of Excellence: toward exascale for energy

EoCoE

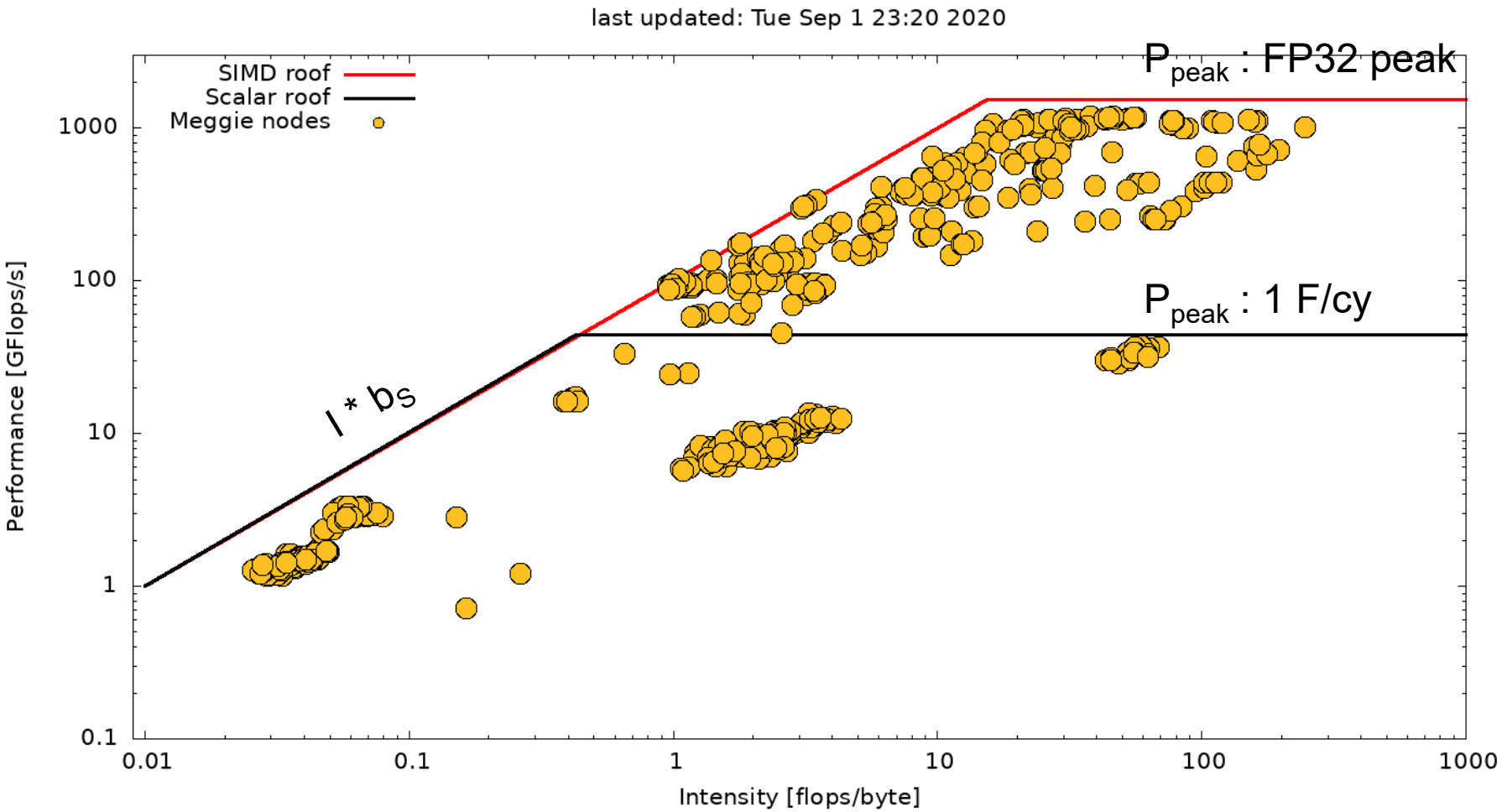
HPC@RRZE: Performance Monitoring

- PE applied to performance monitoring of RRZE's cluster
- Idea: Use roofline model to detect "badly performing jobs"
- Doing:
  - Continuously measure FLOP-rate [F/s] and memory bandwidth [B/s] using LIKWID → Measured "Computational Intensity" I [F/B]
  - Performance limit of hardware (node):

$$P = \min(P_{peak}, I * b_S)$$

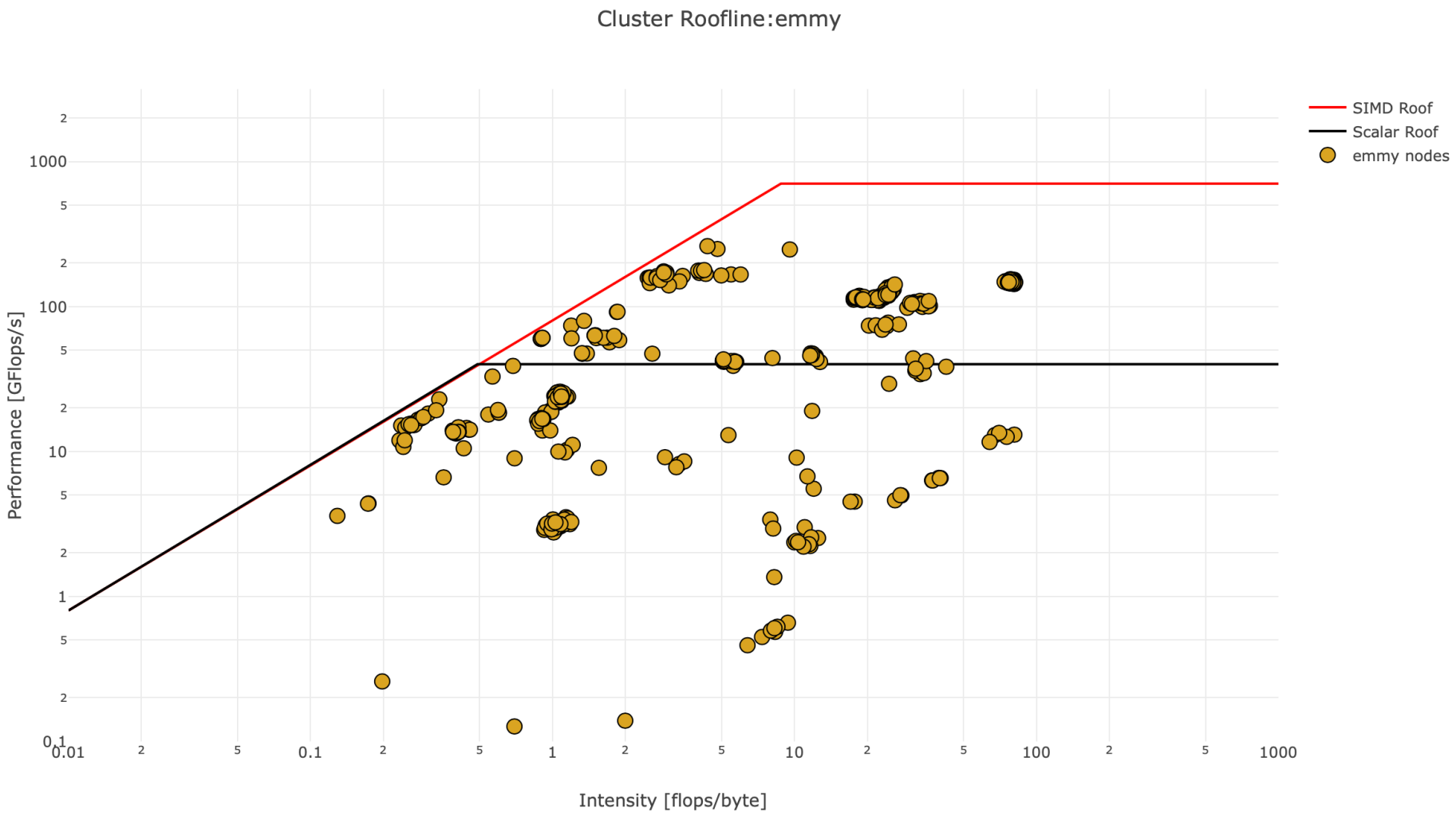
(with P_{peak} :peak performance and b_S :main memory bandwidth)

HPC@RRZE: Roofline model monitoring



Meggie Cluster: Only (larger) parallel jobs of experienced users

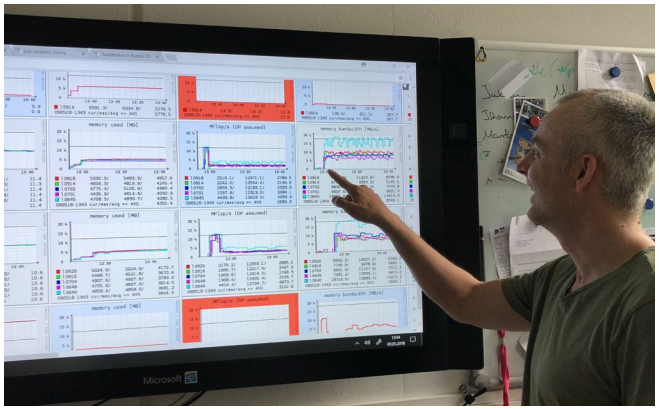
HPC@RRZE: Roofline model monitoring

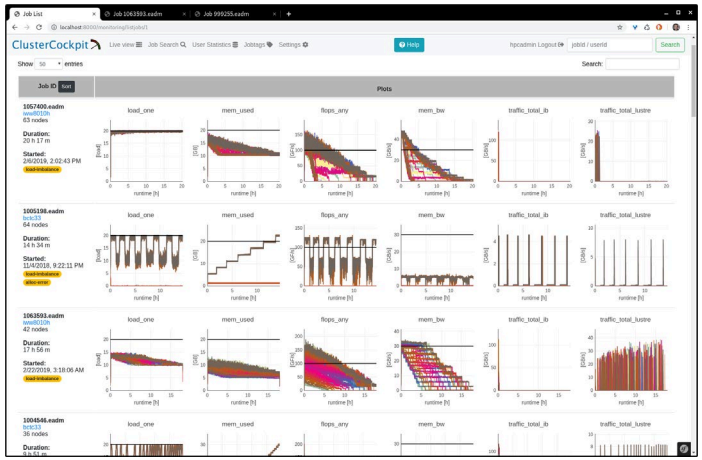


Emmy Cluster: No access restrictions

HPC@RRZE: Job-specific Performance Monitoring

- Continuous monitoring of hardware utilization and performance metrics
- Homegrown solution + development of ClusterCockpit





- Frequent “performance“ problems detected
  - Over-/undersubscription of allocated nodes
  - Pinning ←→ SMT
  - Massive work (a.k.a. load) imbalances
- Users have acces to their own performance data

HPC@RRZE: Support and Training

- Classic **helpdesk** support
- In-depth **performance projects**, as **KONWIHR** project with funding
- Annual **HPC course** (1 week) together with LRZ Garching
- Monthly **HPC-Café** as informal user meeting
- Invited **Tutorials** at conferences, for HPC projects and at HPC centers (12 – 15 events per year; international)

HPC@RRZE: Success story – HPC Café

Informal support channel to complement traditional points of contact!

- Monthly event providing free coffee and cake (currently online only)
- Focus on a specific topic, either as a short talk or a discussion
- Opportunity for questions and feedback
- Accompanied crash-course for HPC beginners with focus on RRZE systems

- First event: 10.9.2019
- 15-25 participants each
- High demand for HPC Crash course!

https://hpc.fau.de/services/hpc-cafe/

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

HPC activities at FAU

Research groups, Institutions and beyond

High Performance Computing

FAU‘s institution and embedding

- ZISC: FAU‘s central institution to foster scientific computing (Speaker: Stingl)
- CCC: Competence center for computational chemistry with applications from chemistry, life sciences, and materials science (Speaker: Imhof)

HPC@RRZE

- KONWIHR: Competence Network for High Performance Computing in Bavaria (Speaker: Bungartz/Wellein)
- Gauß-Alliance: Associated founding member

Perf-Lab: Bundling HPC Methodology

Professorship for High Performance Computing

Prof. Gerhard Wellein

Dr. Jan Eitzinger

Chair for Computer Science 10: System Simulation

Prof. Ulrich Rüde

Prof. Christoph Pflaum

Prof. Harald Köstler

HPC division at Erlangen Regional Computing Center

Prof. Gerhard Wellein

Dr. Georg Hager

Dr. Thomas Zeiser

Chair for Computer Science 2: Programming Systems

Prof. Michael Philippsen

Chair for Computer Science 3: Computer Architecture

Prof. Dietmar Fey

Dr. Johannes Hofmann

Chair for Computer Science 12: Hardware-Software Co-Design

Prof. Jürgen Teich

PD Dr. Frank Hannig

Chair for Computer Science 14: Machine Learning and Data Analytics

Prof. Björn Eskofier

Prof. Anne Koelewijn

Dr. Felix Kluge

ZISC

KONWIHR

- Competence center for HPC-related science within ZISC
- Members cover aspects from:
  - HPC
  - Automatic code generation
  - DSL
  - Scientific computing
  - Novel hardware architectures
  - Parallel programming systems
  - Data driven science
  - Machine learning applications.

https://www.perf-lab.hpc.fau.de

Atomistic structure simulation Lab

Theoretical Chemistry

Department of Chemistry and Pharmacy

Prof. Andreas Görling

Prof. Dirk Zahn

Computer Chemistry Center

Computer Chemie Centrum

Prof. Petra Imhof

Prof. Tim Clark

Prof. Bernd Meyer

Computational Biology

Department BIOLOGIE

Prof. Rainer Böckmann

Bioinformatics

FAU Medizinische Fakultät Institut für Biochemie

Prof. Heinrich Sticht

Materials Science

INSTITUTE I MATERIALS SCIENCE AND ENGINEERING

Prof. Erik Bitzek

HPC @ FAU

High Performance Computing

Prof. Gerhard Wellein

- Interdisciplinary competence center within ZISC
- Supports users in the selection and use of atomistic simulation methods in HPC environments
- Actively accompanies and coordinates the development of high-performance simulation codes

https://www.atomistic-simlab.hpc.fau.de/

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RRZE and FAU

Developments and directions

High Performance Computing

FAU: High-Tech Agenda (HTA) Bayern

Mind. 50 neue Professuren für FAU

Hightech Agenda
Bayern

8 KI
Department for AI in Biomedical Engineering

4 weitere KI im Verbund

42 Professuren zur strategischen Allokation

Aktuell FAU-intern in Ausschreibung

FAU kann im Rahmen weiterer Ausschreibungen weitere Professuren erhalten

HPC@RRZE: NHR Center Proposal

- Germany establishes national HPC centers (Tier-2) at universities (NHR Alliance)

- Tasks of NHR Alliance:
  - Operation of HPC system with nation wide access
  - User support and training
  - Provide expertise in application fields, methods and HPC techniques

- DFG call (Jan 7, 2020):
  Admission of Computing Centres to the NHR Alliance
- Review by DFG and „GWK-Startegieausschuss“

- Final announcement by GWK: November, 2020
- Start: January, 2021

HPC@RRZE: NHR Center Proposal

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

NHR Proposal: Waiting for final decision…..

- Applications: Atomistic simulations of chemical and biomolecular structures (Chemistry, Life Sciences, Materials Science)
- Methods: Scalable Iterative Solvers
- HPC techniques: Performance Engineering (incl. code generation)
- 3-year investment cycles: HPC cluster with GPUs (tailored to applications)
- Strong focus on user support, training and teaching

Principal Investigators

Name	Department
Prof. Dr. Erik Bitzek	Department of Materials Science and Engineering, FAU
Prof. Dr. Rainer Böckmann	Department of Biology, FAU
Prof. Dr. Andreas Görling	Department of Chemistry and Pharmacy, FAU
Prof. Dr. Petra Imhof	CCC and Department of Chemistry and Pharmacy, FAU
Prof. Dr. Ulrich Rüde	ZISC and Department of Computer Science, FAU
Prof. Dr. Heinrich Sticht	Institute of Biochemistry, FAU
Prof. Dr. Gerhard Wellein	RRZE and Department of Computer Science, FAU

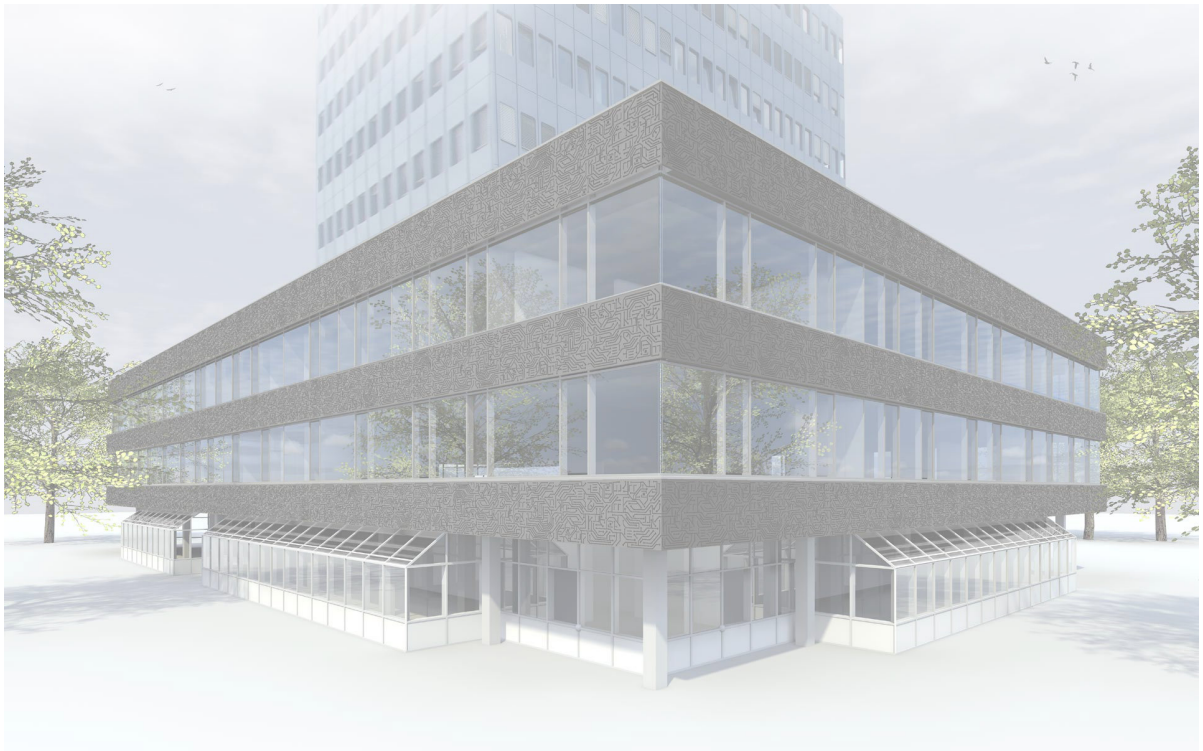
RRZE: Future directions

- Kabinettssitzung der Staatsregierung vom 17.12.2019

• Regionales Rechenzentrum Nordbayern in Erlangen (RRZE)
Das Rechenzentrum wird zu einem IT-Kompetenz- und Innovationszentrum für den Wissenschaftsraum Nürnberg-Erlangen-Fürth weiterentwickelt und umgestaltet. Dafür gibt es enge Abstimmungen mit dem renommierten Leibniz-Rechenzentrum (LRZ). Von der gebündelten Rechenkapazität und dem konzentrierten Know-how werden alle Hochschulen Nordbayerns profitieren. Darüber hinaus stärkt die Region damit ihr Profil als bedeutendes Zentrum der Informatik und des wissenschaftlichen Hochleistungsrechnens.

- Aktuelle Diskussionen (RRZE2030)
  - IT-Versorgung der TU Nürnberg
  - Ausbau der regionalen Aufgaben
  - Neubau eines energieeffizienten Rechenzentrums am TechFak-Campus der FAU

- 2028: 60 Jahre RRZE….



Vielen Dank für Ihre Aufmerksamkeit!

High Performance
Computing

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