

SPPEXA - Software for Exascale Computing



computational algorithms
system software
application software
data management and exploration
programming
software tools

A strategic Priority Program by
DFG - German Research Foundation/Germany
ANR - Agence Nationale de la Recherche/France
JST - Japan Science and Technology Agency/Japan

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SPPEXA Characteristics

- **Strategic initiative of DFG to fund HPC SW in Germany**
 - Fundamental research
 - Establish collaborative, interdisciplinary co-design of HPC applications and HPC methods through several research consortia
- **Aims of SPPEXA's central coordination**
 - Central SPPEXA events, establish and foster international collaboration, doctoral retreats & coding weeks
 - Support project-specific activities, dynamically distributed network funds, educational impact, gender incentives
- **SPPEXA research is ...**
 - ... driven by domain sciences / CSE applications
 - ... powered by scientific computing & informatics / CSE methodology
 - ... in parts smooth/evolutionary, in parts radical/revolutionary

SPPEXA's 6 Research Directions

- **Computational algorithms**
 - Large-scale machines
 - Efficient w.r.t. “modern” complexity measures
- **System software and runtime libraries**
 - Process scheduling
 - System health monitoring
 - Resilience handling
- **Software tools**
 - Compiling, running, verifying, testing, optimizing
- **Application software**
 - Key driver for exascale
 - Hardware-software co-design necessary
- **Programming**
 - Make traditional approaches exascale ready
 - New programming models
- **Data Management**
 - Process large data sets
 - Archive, make data available

SPPEXA - It Has Been a Long Way...

2006 - First discussions within DFG's Commission on IT Infrastructure (KfR)

- HPC SW runs into problems - lack of funding mechanisms; cf. international situation

2007/2008 - Memorandum initiated by the geosciences

- Title *Scientific Software in the PetaFlop Era*, Roundtable discussion in Tutzing, April 2008

2010 - Suggestion by German participants in the exascale initiatives

- Against the background of (1) massive investments in high-end systems world-wide and (2) massive investments in HPC software in the USA (DoE-SciDAC-1/2, NSF-OCI), e.g.

2010 - KfR takes responsibility

- Another strategic paper and a discussion with DFG's president, Prof. M. Kleiner (Nov. 2010)
- Outcome: suggestion of a flexible, strategically initiated SPP, financed via Strategy Funds

2011 - Increase of speed

- Roundtable expert meeting in MAY; DFG-internal discussions (MAY-JUL)
- Submission in AUG; international reviewing in SEP; decision in OCT; call in NOV

2012 - Review of proposals

- 68 sketches in JAN, first selection in MAR leading to 24 consortia invited for full proposals
- Submission of full proposals in MAY, review workshop in JUL

2013 - Launch of SPPEXA: 13 projects

2014 - Call for proposals SPPEXA-2, incl. international partner institutions

2016 - SPPEXA-2: 16 projects, > 50 institutions

- 16 projects, > 8 projects with international consortium
- > 50 institutions

SPPEXA Facts

- **17 research consortia funded**
 - Interdisciplinary, international research consortia
 - Involving 2-5 groups each
 - Addressing at least 2 out of the 6 SPPEXA topics
 - About 60 PIs and 60 PhD students/Postdocs per first/second phase
 - Overall budget of 3.8m € per year
- **Two three-year funding phases**
- **Launch of first phase in January 2013**
- **Second phase: Launch in January 2016**
 - Strong internationalization component: joint call with France and Japan
 - More than 8 international project consortia

EXA-DUNE

ExaFSA

Terra-Neo

EXASTEEL

GROMEX

ExaStencils

Smart-DASH

EXAHD

CATWALK

EXAMAG

FFMK

ESSEX

ExaSolvers

ADA-FS

AIMES

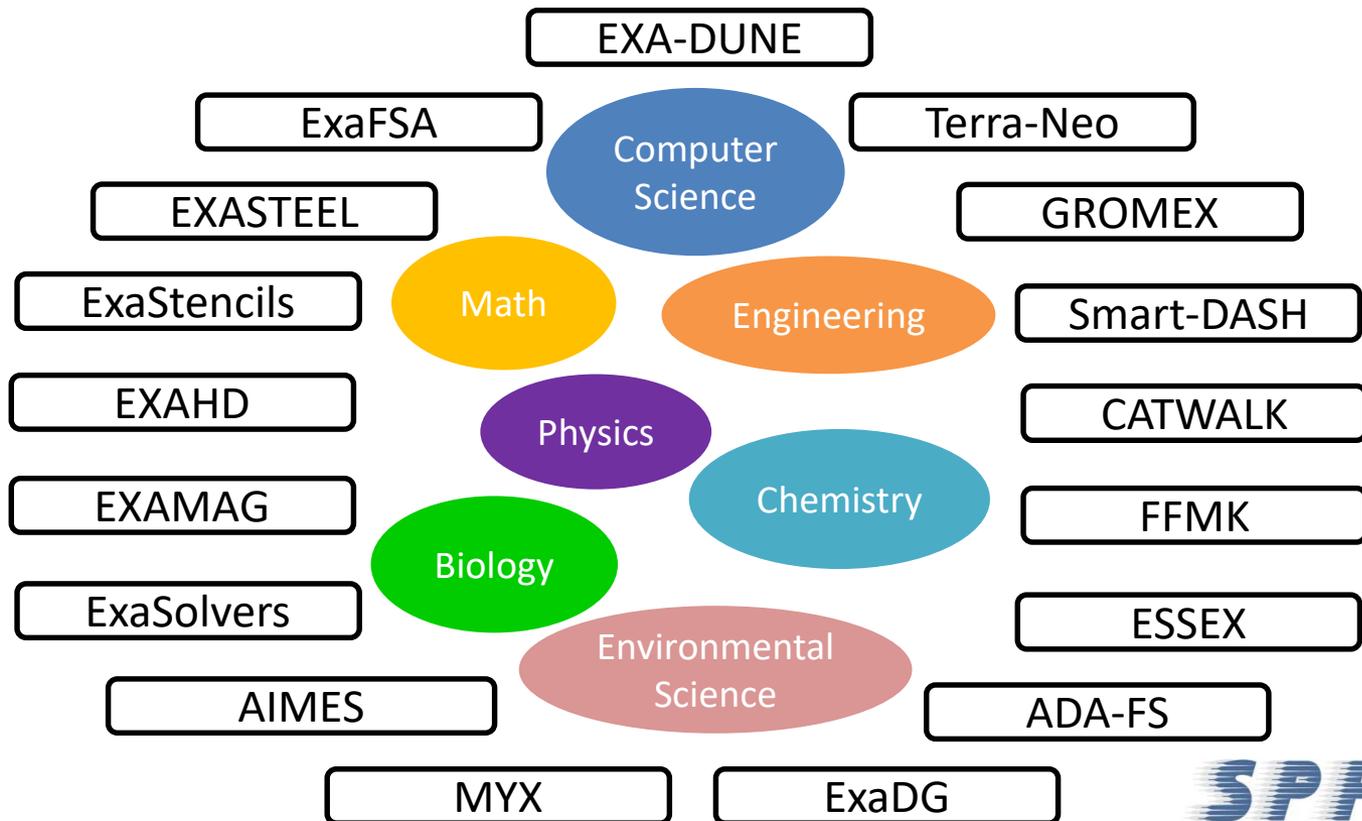
ExaDG

MYX



A Really Interdisciplinary Endeavor

- **Highly interdisciplinary projects and project consortia**
 - Requires close collaboration within and among SPPEXA consortia
 - The central coordination fosters synergistic effects within SPPEXA



A Really International Endeavor: Partner Institutions from...

- **Japan:**
 - RIKEN
 - Tokyo Tech
 - University of Tsukuba
 - University of Tokyo
 - Tohoku University
 - Tokyo University of Science
 - Toyo University
- **France:**
 - Université Versailles
 - Université de Strasbourg
 - Maison de la Simulation, Saclay
- **other Countries:**
 - TU Delft, Netherlands
 - USI Lugano, Switzerland
 - Royal Institute of Technology, Sweden
 - UCLA, USA
 - ANU, Australia
 - Hebrew University Jerusalem, Israel



Steering Committee & Project Management

- Steering Committee: 2 coordinators and 6 PIs
 - Coordinators:
 - Hans-Joachim Bungartz (TU München)
 - Wolfgang Nagel (TU Dresden)
 - 6 Project PIs, elected for 3 years on Plenary Meeting:
 - Sabine Roller (U Siegen)
 - Christian Lengauer (U Passau)
 - Hans-Peter Bunge (LMU)
 - Dörte Sternal (TU Darmstadt)
 - Takayuki Aoki (Tokyo Tech)
 - Nahid Emad (Maison de la Simulation/U Versailles)
- Scientific Program Manager
 - Philipp Neumann/ Benjamin Uekermann (TUM)
 - Project management on day-to-day basis



Advisory Board

- **George Biros (U Texas)**
Institute for Computational Engineering and Sciences
- **Rupak Biswas (NASA)**
Head, NASA Advanced Supercomputing (NAS) Division
- **Klaus Becker (Airbus)**
Industry
- **Rob Schreiber (HP Labs)**
Assistant Director, Exascale Computing Lab @HP Labs
- **Craig Stewart (Indiana University)**
Executive Director, Pervasive Technology Institute, Indiana U



Central Coordination: Responsibilities

- Strategic design of joint/central SPPEXA activities
 - Representation at conferences (SC, ISC, EuroPar and many more)
 - Representation at national and international level
- Funding for project-specific workshops
 - Until October 2017: funding for 33 workshops and minisymposia
- Organization of annual assemblies
 - Foster scientific exchange between projects
 - Report on scientific and strategic achievements
- Educational activities
 - Doctoral retreats and coding weeks
 - Foster exchange between young researchers
 - Prizes for outstanding student/PhD theses
- Public relations
 - Sharing/Publishing SPPEXA news
 - Presenting the projects to the wider community
- Gender activities and childcare funding

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Central Coordination: SPPEXA International

- 2013: Satellite Event@ISC
(International Supercomputing Conference)
- 2014: SPPEXA Workshop@Euro-Par
(International Conference on parallel processing)
- 2014: Female Researcher Meeting@WCCM
(World Congress of Computational Mechanics)
- 2014: Panel Discussion@SC
(Supercomputing Conference)
- 2016: SPPEXA Symposium
(Conference, 13 minisymposia, 60 talks)
- 2017: First French-German-Japanese Workshop on HPC
(At French Embassy in Tokyo)
- 2017: Female Researcher Meeting@ECCOMAS
(International Conference on Coupled Problems)

Central Coordination: Funding of Research Stays

- New in phase 2
- Specifically for F-G-J collaborations
- We fund research stays of PhD students (> 1 month)
- Approximately 1500€ per student
- Simple organization

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Recent & Upcoming Project-Specific Workshops

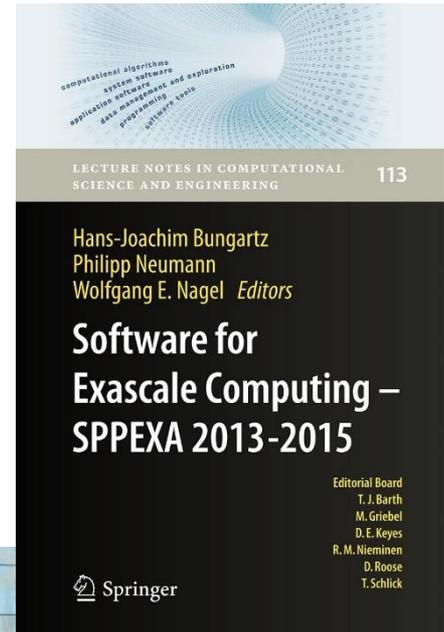
- Apr 6, 2017: Parallel Programming Models - Productivity and Applications (Tokyo)
- May 25-28, 2017: Exascale Data Generation and Analysis for MD Simulation (Göttingen)
- June 19-23, 2017: ISC2017: PhD Forum and Project Poster Session (Frankfurt)
- June 26-28, 2017: Exascale Solver for Application-Driven Science (@PASC) (Lugano)
- Sept 07-08, 2017: GAMM Applied Numerical Linear Algebra (Cologne)
- Sept 26-27, 2017: Exascale I/O for Unstructured Grids (Hamburg)
- Oct 18, 2017: Parallel Programming Models - Productivity and Applications (2nd Edition) (Tokyo)
- Oct 23-27, 2017: 6th Workshop on Parallel-in-Time Integration (Monte Verita, CH)
- **2nd Call for Workshops 2017: Deadline Nov 17, 2017**

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SPPEXA Symposium 2016

- Jan 25-27 2016 at LRZ, Garching/Munich
- 14 minisymposia, 153 participants
- Invited speakers:
 - George Biros, University Texas at Austin
 - Takayuki Aoki, Tokyo Tech
 - Craig Stewart, Indiana University
- Proceedings *Software for Exascale Computing* to appear in *Lecture Notes in Computational Science and Engineering*, Springer



Next Central SPPEXA Events

- Next Annual Plenary Meeting:
 - March 21 and 22, 2018 in Garching / Munich
 - Registration opens soon
 - International collaborators are welcome!
- Final Symposium
 - Spring 2019 in Dresden

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Doctoral Retreat and Coding Week

- Sep 16-20, 2013: Applications & Algorithms
TU Darmstadt
- Sep 21-Oct 3, 2014: The Fast and the Curious
Sarntal, Italy



- Sep 14-18, 2015: HPC Software
U Passau
- Sep 5-9, 2016: Accelerator Computing
Obernai, France
- Sep 4-8, 2017: Data Intensive Applications
TU Dresden

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Public Relations

- InSiDE Magazine
 - Popular scientific magazine of Gauss Centre of Supercomputing (managed by HLRS)
 - Short articles on all SPPEXA projects (one per volume)
 - E.g. ESSEX Fall 2015, DASH Fall 2017
 - Currently needed: Project for Spring 2018 volume
- Science Node
 - Successor of International Science Grid This Week
 - Free online publication of popular scientific articles about real world impact of advanced computing and networks
 - Since recently, SPPEXA is Gold Sponsor of Science Node
 - Quarterly articles on SPPEXA projects

Contact Information

German Priority Programme 1648 Software for Exascale Computing



About SPPEXA The Priority Programme *Software for Exascale Computing (SPPEXA)* of the German Research Foundation (DFG) addresses fundamental research on the various aspects of HPC software. SPPEXA runs 2013-2019, and it is implemented in two three-year phases, consisting of 13 (phase 1) and 16 (phase 2) project consortia and more than 50 institutions involved. With SPPEXA's second-phase projects funded by DFG as well as the French National Research Agency (ANR) and the Japan Science and Technology Agency (JST), SPPEXA strives for bi- and trinational research to pave the road towards exascale computing.

EXAMAG - Exascale Simulations of the Magnetic Universe
U Heidelberg +++ U Würzburg +++ U Tokyo +++
U Strasbourg

Smart-DASH - Smart Data Structures and Algorithms with Support for Hierarchical Locality
LMU München +++ U Stuttgart +++ HLR Stuttgart +++
TU Dresden +++ KIT Karlsruhe

EXASTEEL - From Micro to Macro Properties
U Köln +++ TU Bergakademie Freiberg +++ U Essen +++
TU Dresden +++ U Lugano +++ FAU Erlangen-Nürnberg

Terra-Neo - Integrated Co-Design of an Exascale Earth Mantle Modeling Framework
LMU München +++ FAU Erlangen-Nürnberg +++
TU München

AIMES - Advanced Computation and I/O Methods for Earth-System Simulations *new!*
U Hamburg +++ U Versailles +++ RIKEN +++ Tokyo Tech

ExaStencils - Advanced Stencil-Code Engineering
U Passau +++ FAU Erlangen-Nürnberg +++ U Kassel +++
U Tokyo

EXAHD - An Exa-Scalable Two-Level Sparse Grid Approach for Higher-Dimensional Problems in Plasma Physics
U Stuttgart +++ TU München +++ U Bonn +++
ANU Canberra +++ MPG Garching +++ UC Los Angeles

GROMEX - Unified Long-Range Electrostatics and Dynamic Protonation for Realistic Biomolecular Simulations on the Exascale
MPI BPC Göttingen +++ JSC Jülich +++ Stockholm U

EXA-DUNE - Flexible PDE Solvers, Numerical Methods, and Applications
U Heidelberg +++ U Münster +++ U Stuttgart +++
TU Kaiserslautern +++ TU Clausthal +++ TU Dortmund

CATWALK - A Quick Development Path for Performance Models
ETH Zürich +++ RWTH Aachen +++ JSC Jülich +++
TU Darmstadt +++ GU Frankfurt

ESSEX - Equipping Sparse Solvers for Exascale
FAU Erlangen-Nürnberg +++ DLR Köln +++ U Greifswald +++
U Wuppertal +++ U Tsukuba +++ U Tokyo

ExaSolvers - Extreme Scale Solvers for Coupled Problems
RWTH Aachen +++ Tokyo U of Science +++ U Lugano +++
HLR Stuttgart +++ U Trier +++ GU Frankfurt +++ Toyo U

ADA-FS - Advanced Data Placement via Ad-hoc File Systems at Extreme Scales *new!*
TU Dresden +++ JGU Mainz +++ KIT

ExaFSA - Exascale Simulation of Fluid-Structure-Acoustics Interactions
U Stuttgart +++ TU Delft +++ U Siegen +++
TU Darmstadt +++ Tohoku U

ExaDG - High-Order Discontinuous Galerkin for the Exa-Scale *new!*
U Heidelberg +++ TU München

FFMK - A Fast and Fault Tolerant Microkernel-Based System for Exascale Computing
TU Dresden +++ ZIB Berlin +++ Hebrew U Jerusalem

MYX - MUST Correctness Checking for YML and XMP Programs *new!*
RWTH Aachen +++ MDLS Saclay +++ U Tsukuba +++ RIKEN

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