SPPEXA – Software for Exascale Computing
SPPEXA Workshop in Japan
## *April 6, 2017*

SPPEXA

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

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

H.-J. Bungartz
W.E. Nagel
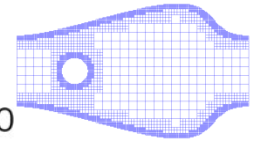**B. Uekermann**
P. Neumann

CSE & HPC
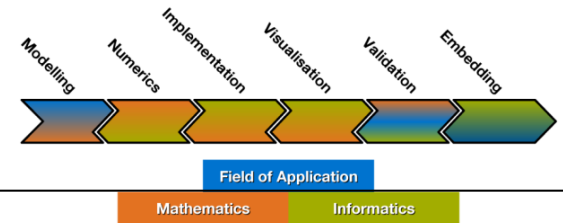
Mathematical model

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{\rho}\nabla p - \nu \Delta \mathbf{u} = 0$$

Discretization & solver

$$\nabla \cdot \mathbf{u} = 0$$

$$A\dot{\mathbf{u}}_h + D\mathbf{u}_h + C(\mathbf{u}_h)\mathbf{u}_h - M^T p_h/\rho = \mathbf{0}$$
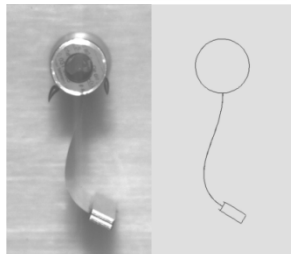
$$M\mathbf{u}_h = 0$$

Impact of each step on all other steps!
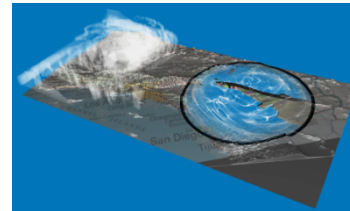*Hence #1: no pipeline any more, no cycle, but a complete graph*
Hence #2: no isolated considerations, but co-design!
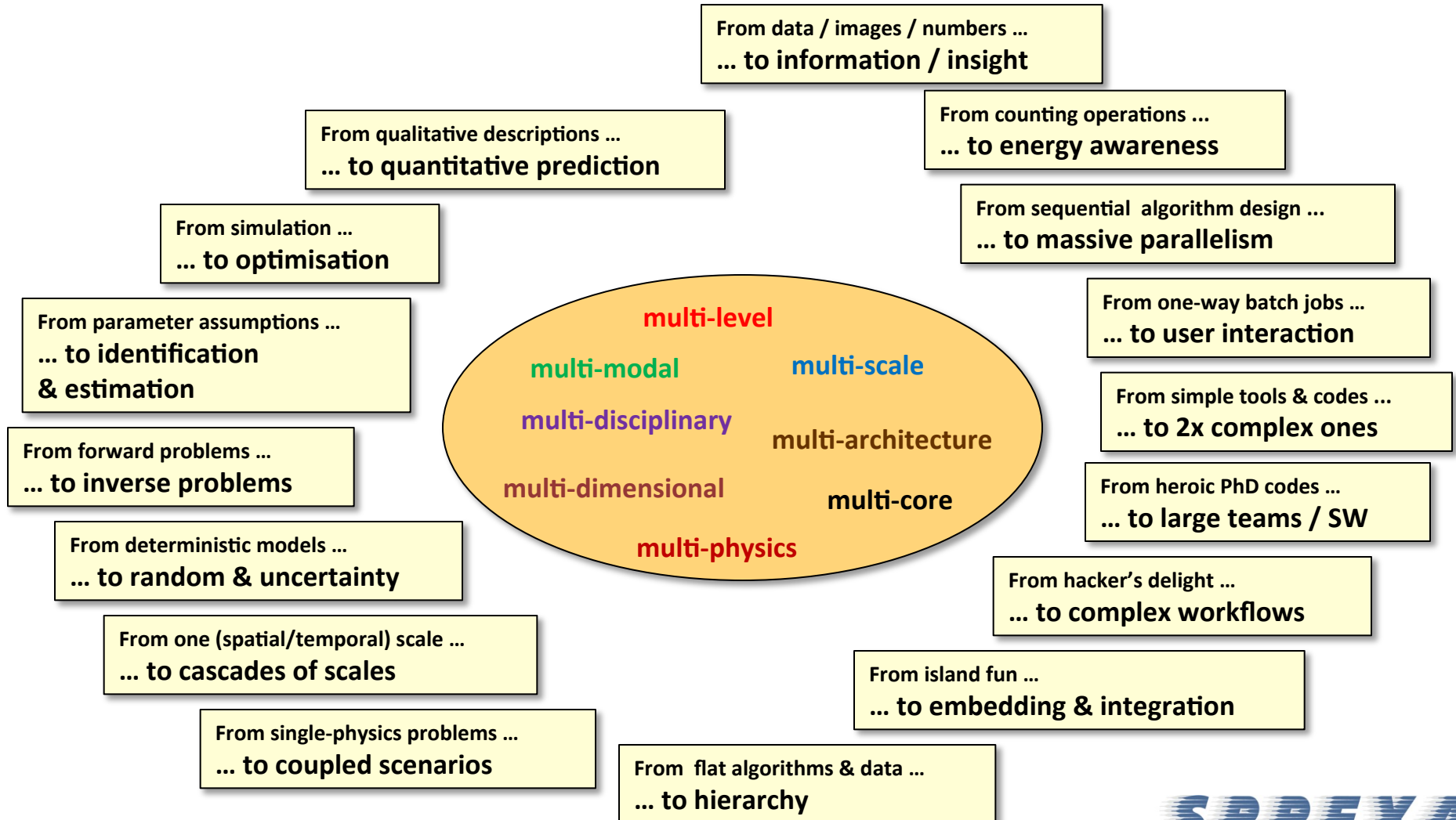
Parallel implementation, HPC

Insight, Design

Validation

Exploration

Software

SPPEXA

2

CSE&HPC Challenges

From data / images / numbers ...
... to information / insight

From counting operations ...
... to energy awareness

From qualitative descriptions ...
... to quantitative prediction

From sequential algorithm design ...
... to massive parallelism

From simulation ...
... to optimisation

From parameter assumptions ...
... to identification & estimation

From one-way batch jobs ...
... to user interaction

From simple tools & codes ...
... to 2x complex ones

multi-level

multi-modal   **multi-scale**

multi-disciplinary

multi-architecture

From forward problems ...
... to inverse problems

multi-dimensional   **multi-core**

From heroic PhD codes ...
... to large teams / SW

From deterministic models ...
... to random & uncertainty

multi-physics

From hacker's delight ...
... to complex workflows

From one (spatial/temporal) scale ...
... to cascades of scales

From island fun ...
... to embedding & integration

From single-physics problems ...
... to coupled scenarios

From flat algorithms & data ...
... to hierarchy

SPPEXA

Exascale – An International Hot Topic

"The Exascale Computing Initiative has also identified the need for innovations in applications and algorithms to address fundamental challenges in extreme-scale systems related to concurrency, data movement, energy efficiency and resilience. Innovative solutions to these challenges will jointly benefit analysis and computational algorithms for both data-intensive science and exascale computing. Finally, advances in networking facilities, as projected for future generations of ESNet [9], will also benefit both data-intensive science and exascale computing."

…

"There is a need to increase the pool of computer and computational scientists trained in both exascale and data-intensive computing."

Synergistic Challenges in Data-Intensive Science and Exascale Computing,
DOE ASCAC Data Subcommittee Report, 2013

"An intensive co-design effort is essential for success, where computer scientists, applied mathematicians, and application scientists work closely together to produce a computational science discovery environment able to exploit the computational resources that will be available at the exascale."

Applied Mathematics Research for Exascale
DOE/ASCR Report, March 2014

Exascale – An International Hot Topic

- **USA**
  - Exascale Initiative: FastForward, DesignForward
  - XSEDE (supported by NSF)
  - Exascale Co-Design Centers (ExMatEx, CESAR, ExaCT)
  - DOE SciDAC/ASCR

    ASCR Call "Exploratory Research for Extreme-Scale Science"
    $\rightarrow$ released in December 2014!

  - …
- **Europe**
  - EU: EXA2CT, CRESTA, DEEP(-ER), MONT BLANC (2), EPIGRAM, NUMEXAS, EESI
  - France: ExaSE, C2S@Exa, …
  - **Germany: SPPEXA,…**
- **Japan**
  - CREST Post-Peta Scale
  - …

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 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 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

SPPEXA

ADA-FS: Advanced Data Placement via Ad-hoc File Systems at Extreme Scales

- **Consortium:**
  - Wolfgang E. Nagel, TU Dresden
  - André Brinkmann, U Mainz
  - Achim Streit, KIT

- **Perspective:**
  - Improve I/O performance by central I/O planning and ad-hoc overlay file system
  - Use idle shares to boost effective I/O bandwidth and reduce latency
  - Provide design, proof-of-concept software infrastructure, and highly scalable demonstrations thereof

AIMES: Advanced Computation and I/O Methods for Earth-System Simulations

- **Consortium:**
  - Thomas Ludwig, U Hamburg
  - Thomas Dubos, U Versailles
  - Naoya Maruyama, RIKEN
  - Takayuki Aoki, Tokyo Tech

- **Perspective:**
  - Derive high-level DSL for icosahedral earth-system models
  - Develop a concept and tool to translate high-level representation into variety of existing languages
  - Investigate suitable formats for icosahedral data
  - Advance lossy data compression strategies

ExaDG: Higher-Order Discontinuous Galerkin for the Exa-scale

- **Consortium:**
  - Guido Kanschat, U Heidelberg
  - Katharina Kormann, TU München
  - Martin Kronbichler/ Wolfgang A. Wall, TU München

- **Perspective:**
  - Develop generic exa-scale DG algorithms
  - Improve and allow for efficient data-reuse
  - Tensor-aware multigrid solvers and preconditioners
  - Application in benchmark problems from engineering (e.g., CFD)

MYX: MUST Correction Checking for YML and XMP Programs

- **Consortium:**
  - Matthias S. Müller, RWTH Aachen
  - Serge Petiton/ Nahid Emad, Maison de la Simulation
  - Taisuke Boku, U Tsukuba
  - Hitoshi Murai, RIKEN AICS

- **Perspective:**
  - Scalable methods to perform run-time correctness checking of YML- and XMP-parallel applications
  - Integration of these methods into MUST

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
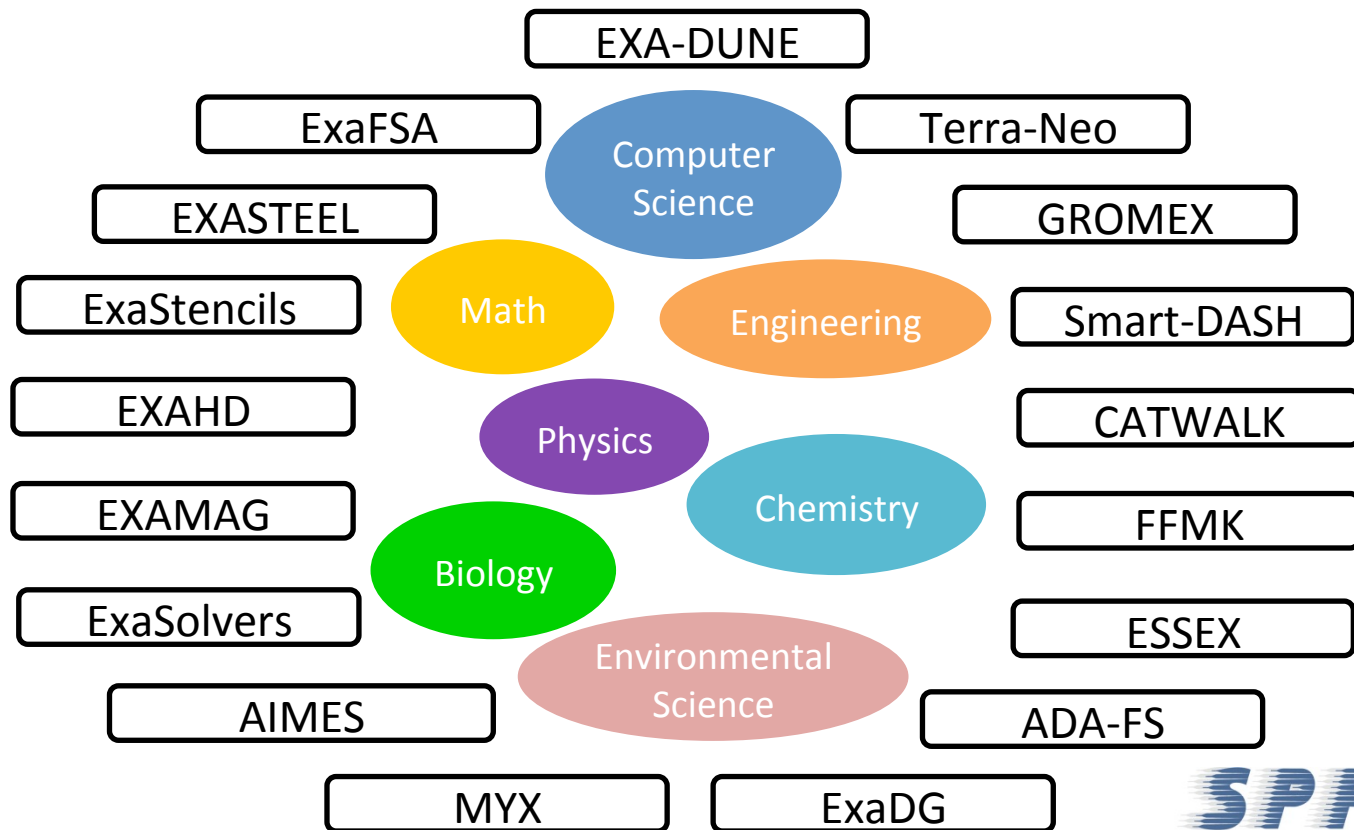
A Really International Endeavor: Partner Institutions from…

- **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
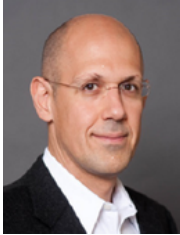 - Hebrew University Jerusalem, Israel

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 Sternel (TU Darmstadt)
    - Takayuki Aoki (Tokyo Tech)
    - Nahid Emad (Maison de la Simulation/U Versailles)

- Scientific Programme 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 Directory, 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 March 2017: funding for 28 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)

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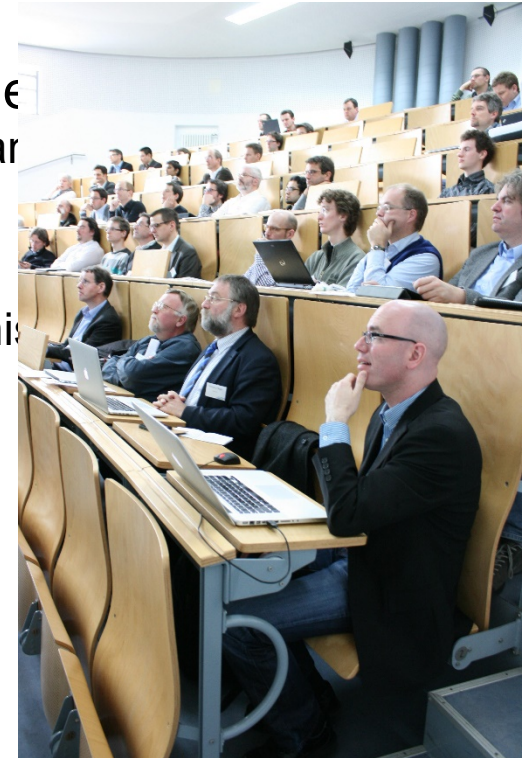# Recent & Upcoming Project-Specific Workshops

- Sep 14-15, 2016:   Application Interfaces for an Exascale OS (Jerusalem)
- Dec 14-16, 2016:   First International Workshop on Data Locality in Modern Computing Systems (Granada)
- Feb 20-22, 2017:   Fast High Order DG Methods for Future Architectures (Heidelberg)
- Mar 23-24, 2017:   Understanding I/O Performance Behavior (UIOP) (Hamburg)
- Apr 6, 2017:   Parallel Programming Models – Productivity and Applications (Tokyo)
- May 25-28, 2017:   Exascale Data Generation and Analysis for MD Simulation (Göttingen)
- June 26-28, 2017:   Exascale Solver for Application-Driven Science (@PASC) (Lugano)
- Sept 26-27, 2017:   Exascale I/O for Unstructured Grids (Hamburg)

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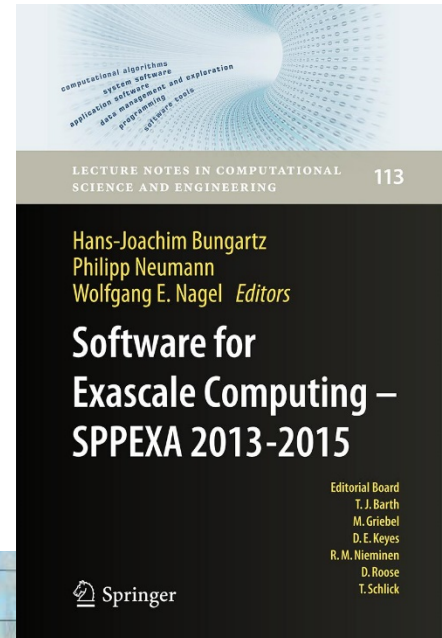 - Report on scientific and strategic achievements

eks
researchers
nD theses

s
der community
funding

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

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Doctoral Retreat and Coding Week

- Sep 16-20, 2013:   Applications & Algorithms
                        TU Darmstadt, Roller/Sternel
- 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

Thank You for Your Attention!

German Priority Programme 1648
Software for Exascale Computing

SPPEXA

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

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 +++ HLRS 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 +++ HLRS 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

Coordinators

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Benjamin Uekermann
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