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Autore	Bungartz H.-J (Hans-Joachim)
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Electrostatics and Dynamic Protonation for Realistic Biomolecular Simulations on the Exascale -- ExaStencils: Advanced Stencil-Code Engineering -- ExaFSA: Exascale Simulation of Fluid-Structure-Acoustics Interactions -- EXAHD: An Exa-Scalable Two-Level Sparse Grid Approach for Higher-Dimensional Problems in Plasma Physics and Beyond -- EXAMAG: Exascale Simulations of the Magnetic Universe -- FFMK: A Fast and Fault Tolerant Microkernel-based System for Exascale Computing -- ESSEX-II: Equipping Sparse Solvers for Exascale -- EXASOLVERS: Extreme Scale Solvers for Coupled Problems -- ADA-FS: Advanced Data Placement via Ad-hoc File Systems at Extreme Scales -- AIMES: Advanced Computation and I/O Methods for Earth-System Simulations. ExaDG: High-Order Discontinuous Galerkin for the Exa-Scale. MYX-MUST Correctness Checking for YML and XMP Programs -- ExtraPeak: Automatic Performance Modeling of HPC Applications with Multiple Model Parameters.

Sommario/riassunto

This open access book summarizes the research done and results obtained in the second funding phase of the Priority Program 1648 "Software for Exascale Computing" (SPPEXA) of the German Research Foundation (DFG) presented at the SPPEXA Symposium in Dresden during October 21-23, 2019. In that respect, it both represents a continuation of Vol. 113 in Springer’s series Lecture Notes in Computational Science and Engineering, the corresponding report of SPPEXA’s first funding phase, and provides an overview of SPPEXA’s contributions towards exascale computing in today's sumpercomputer technology. The individual chapters address one or more of the research directions (1) computational algorithms, (2) system software, (3) application software, (4) data management and exploration, (5) programming, and (6) software tools. The book has an interdisciplinary appeal: scholars from computational sub-fields in computer science, mathematics, physics, or engineering will find itof particular interest. .