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Mundani, Ernst Rank, Andreas Springer, Boris Vexler -- Optimal Control of Partially Miscible Two-Phase Flow with Applications to Subsurface CO2 Sequestration: Moritz Simon and Michael Ulbrich -- A Newton-CG Method for Full-Waveform Inversion in a Coupled Solid-Fluid System: Christian Boehm and Michael Ulbrich -- Advances in the Parallelisation of Software for Quantum Chemistry Applications: Martin Roderus, Alexei Matveev, Hans-Joachim Bungartz and Notker Rösch -- Designing Spacecraft High Performance Computing Architectures: Fisnik Kraja, Georg Acher, Arndt Bode -- Requirements Engineering for Computational Seismology Software: Yang Li, Bernd Bruegge, Simon Stähler, Nitesh Narayan, and Heiner Igel -- A High-Performance Interactive Computing Framework for Engineering Applications: Jovana Kneževi´c, Ralf-Peter Mundani, Ernst Rank -- A Framework for the Interactive Handling of High-Dimensional Simulation Data in Complex Geometries: A. Benzina, G. Buse, D. Butnaru, A. Murarasu, M. Treib, V. Varduhn, R.-P. Mundani -- Experiences with a Flexibly Reconfigurable Visualization System on Software Development and Workplace Ergonomics: Marcus Tönnis, Amal Benzina, Gudrun Klinker.

Sommario/riassunto

This proceedings volume collects review articles that summarize research conducted at the Munich Centre of Advanced Computing (MAC) from 2008 to 2012. The articles address the increasing gap between what should be possible in Computational Science and Engineering due to recent advances in algorithms, hardware, and networks, and what can actually be achieved in practice; they also examine novel computing architectures, where computation itself is a multifaceted process, with hardware awareness or ubiquitous parallelism due to many-core systems being just two of the challenges faced. Topics cover both the methodological aspects of advanced computing (algorithms, parallel computing, data exploration, software engineering) and cutting-edge applications from the fields of chemistry, the geosciences, civil and mechanical engineering, etc., reflecting the highly interdisciplinary nature of the Munich Centre of Advanced Computing.