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Survey

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HPCNano's Modeling Capability, System Scalability, and Applicability

Information about Research Institutions/Agencies/Companies

West Virginia University, Physics, Prof. Martina E. Bachlechner

Material Type (Example: CNT, Nano-wire,...)

Interfaces

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Mechanical, structural

Scale (Number of atoms)

Millions

Brief Summary type of Models (Example: DFT, MD, QM, ...)

MD

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Semiconductor, Ceramics

Computing Capacity (Example: Number of processors, data storage, centralized/distributed system, etc...)

16 CPU, 1800+AMD, 1GB Ram Beowulf-like PC cluster

Information about Research Institutions/Agencies/Companies

Lawrence Berkeley National Lab, Dr. Lin Wang

Material Type (Example: CNT, Nano-wire,...)

Quantum dot, Quantum wire, CMOS

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical and Optical

Scale (Number of atoms)

4000-10000

Brief Summary type of Models (Example: DFT, MD, QM,...)

DFT, QM

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Semiconductor

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

>1000 processors

Information about Research Institutions/Agencies/Companies

IBM, Dr. Alessandru Curioni

Material Type (Example: CNT, Nano-wire,...)

CNT, Gateoxides, Polymer

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electronic, defects, stability

Scale (Number of atoms)

100-10,000,000

Brief Summary Type of Models (Example: DFT, MD, QM,...)

DFT, MD, QM

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Semiconductor, Pharma, etc

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

296 nodes Linux cluster, 256 SMP cluster system (PURS), 2BG/LRACHS (4096 proc)

Information about Research Institutions/Agencies/Companies

PSC, Research Institute, Dr. Ying Wang

Material Type (Example: CNT, Nano-wire,...)

Nano-particles

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electronic, magnetic, and mechanical

Scale (Number of atoms)

10,000-100,000 on Teraflops computers

Brief Summary Type of Models (Example: DFT, MD, QM,...)

DFT

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Information technology

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

>10,000 CPUs, 100GB memory

Information about Research Institutions/Agencies/Companies

RIST, Dr. Atsushi Miyauchi

Material Type (Example: CNT, Nano-wire,...)

DNA

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Dynamics

Scale (Number of atoms)

2000+

Brief Summary type of Models (Example: DFT, MD, QM,...)

QM

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Medical

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

8~5120 Processors

Information about Research Institutions/Agencies/Companies

Dept. of EEE, Okayama Univ. Japan, Prof. Kenji Tsuruta

Material Type (Example: CNT, Nano-wire,...)

Nanophase, nanocomposite, nano-wire, CNT, C₆₀/Graphite

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Everything

Scale (Number of atoms)

DFT<200, TB<10⁶, Hybrid<10⁸, Classical<10⁹

Brief Summary Type of Models (Example: DFT, MD, QM,...)

DFT, TB, DFT and/or TB/MD, MD

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Semiconductor, Ceramics

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

~100 cpu, Grid-connected ~300cpu (3 Univs.)

Information about Research Institutions/Agencies/Companies

Argonne National Lab, ANL, Dr. Raymond A Bair, Director, Argonne Leadership Computing Facility

Material Type (Example: CNT, Nano-wire,...)

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Scale (Number of atoms)

100,000 and up

Brief Summary Type of Models (Example: DFT, MD, QM,...)

PQM, CPMD, DFT

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Energy systems

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

100,000+ processors (2008) mpp, 4+ petabytes storage

Information about Research Institutions/Agencies/Companies

Fundamental and Environment Research Labs, NEC, Dr. Yoshiyuki Miyamoto

Material Type (Example: CNT, Nano-wire,...)

CNT, Solid surfaces

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, optical, defectk impurity

Scale (Number of atoms)

100 and up

Brief Summary Type of Models (Example: DFT, MD, QM,...)

DFT, MD

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Semiconductor, photochemical

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

~100 processors (vector)

Information about Research Institutions/Agencies/Companies

Florida ACM University, Dept. of Physics, Prof. Mark, A. Jack

Material Type (Example: CNT, Nano-wire,...)

CNT, graphene

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, optical, magnetic (response to

Scale (Number of atoms)

1800 atoms or more

Brief Summary Type of Models (Example: DFT, MD, QM,...)

Quantum transport within Green functions

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Sensors, ahwonov-bolum osillators, nanoscale electronic devices

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

128 node MAC cluster, NNIN computer cluster (Harvard, CNS, Cornell CNF) user access

Information about Research Institutions/Agencies/Companies

LBNL, Juan Meza

Material Type (Example: CNT, Nano-wire,...)

Quantum Dot, Wires etc

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, optical, interface

Scale (Number of atoms)

100-1,000,000

Brief Summary Type of Models (Example: DFT, MD, QM,...)

DFT

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Basic Research

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

Nersc --- 6000 Processors

Information about Research Institutions/Agencies/Companies

Kyushu University, Dr. Toshiya Takami

Material Type (Example: CNT, Nano-wire,...)

Peptide, protein

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, optical, interface

Scale (Number of atoms)

100-1,000,000

Brief Summary Type of Models (Example: DFT, MD, QM,...)

DFT

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Basic Research

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

Nersc --- 6000 Processors

Information about Research Institutions/Agencies/Companies

LBNL, Zhengji Zhao

Material Type (Example: CNT, Nano-wire,...)

Any type of nano-structure (semiconductor)

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, optical, interface

Scale (Number of atoms)

O(N), million of atoms, and

Brief Summary Type of Models (Example: DFT, MD, QM,...)

DFT

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Semiconductor

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

1,000,000 of processors

Information about Research Institutions/Agencies/Companies

NCSA, Sudhakar Panidighanitam

Material Type (Example: CNT, Nano-wire,...)

Nano, sub molecular

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical properties

Scale (Number of atoms)

100 of atoms

Brief Summary Type of Models (Example: DFT, MD, QM,...)

QM, MD, and DFT

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Chemical, electrical, physical

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

100's processors

Information about Research Institutions/Agencies/Companies

Computational research lab, Sateesh Awade

Material Type (Example: CNT, Nano-wire,...)

Nano and electronic structure

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, and mechanical

Scale (Number of atoms)

Brief Summary Type of Models (Example: DFT, MD, QM,...)

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

64 Processors, 50 TF

Information about Research Institutions/Agencies/Companies

Core Technology Research Center, Ricoh Co. Ltd, Yoshio Watanabe

Material Type (Example: CNT, Nano-wire,...)

Organic electronic materials, power under electrostatic and and magnetic force

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, mechanical, interfacial

Scale (Number of atoms)

Brief Summary Type of Models (Example: DFT, MD, QM,...)

MD (Power Behavior simulation is simulator to MD with dissipation)

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

Electrophotography, organic electronic devices

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

Rico only has small computer cluster and want to use ES.

Information about Research Institutions/Agencies/Companies

Purdue Univ., Gerhard Klimeck

Material Type (Example: CNT, Nano-wire,...)

CNT, Nanowire, quantum dots

Property (Electrical, thermal, defect, impurity, mechanical, interfacial)

Electrical, mechanical, interfacial

Scale (Number of atoms)

21 millions atoms

Brief Summary Type of Models (Example: DFT, MD, QM,...)

Empirical tight binding

Application Area (Example: Semiconductor, Pharma, Aerospace, Chemical, ...)

semiconductor

Computing Capacity (Example: Number of processors, data storage, centralized/distributed systems, ...)

NCN 1000, CPUs