International Center for Computational Sciences

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WELCOME

Second **ICCS** Workshop on

Manycore and Accelerator-based High-performance Scientific Computing

January 24 – 28, 2011

The Challenges

Scientific Data Deluge

LSST	0.5 PB/month
JGI	5 TB/yr *
LOFAR	500 GB/s
SKA	100 x LOFAR

Roadmap to Exascale

Multicore
Manycore/Embedded
GPU/Accelerator

Programming Models

Energy Efficiency

1000x Performance enhancement with 10x energy consumption

* Jeff Broughton (NERSC) and JGI

To Do…

Horst Simon -- December 2, 2009

Community Building

Center

IJHPCA Issue

GPUcomputing.net
(FFT, Physics and Astronomy)

Education and Outreach

Tutorials

Workshops

NERSC test-bed cluster
(Dirac)

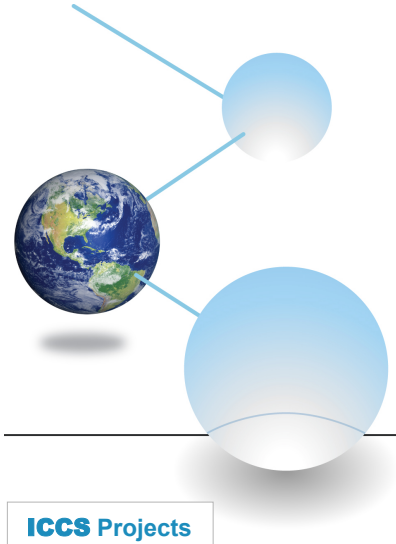
Benchmarking

N-body code

GAMER

Mellanox

…



ICCS

International Center for Computational Science

Three continents, three institutions

UC Berkeley/LBNL/NERSC
University of Heidelberg and
National Astronomical Observatories (CAS)

Founders

Horst Simon
Hemant Shukla
John Shalf
Rainer Spurzem

ICCS Projects

ISAAC

Infrastructure for Astrophysics Applications Computing

ISAAC is a three-year (2010-2013) NSF funded project to focus on research and development of infrastructure for accelerating physics and astronomy applications using and manycore architectures.

Goal is to successfully harness the power of the parallel architectures for compute-intensive scientific problems and open doors for new discovery and revolutionize the growth of science via, **Simulations**, **Instrumentations** and **Data processing / analysis**

GRACE II

SILK ROAD

ICCS Activities

Summer School Aug 2 – 6, 2010

Proven Algorithmic Techniques for Many-core Processors

Wen-Mei Hwu (UIUC) and David Kirk (NVIDIA)

Workshop Nov 30 – Dec 2, 2009

Many-core and Accelerator-based Computing for Physics and Astronomy Applications

Visit us – http://iccs.lbl.gov

ICCS Vision

R&D of Scientific HPC Solutions

Deliver Science Driven Solutions in Hardware, Programming Models, Algorithms, Infrastructure

Enabling Scientific Growth

Simulations, Remote Location Real-time Feedback, Energy Efficiency

Building International Community

Multi-discipline Scientific Communities, Industry Leaders, International Partnerships

Education and Outreach

Curriculum, Training, Publications, Software/Hardware Dissemination, Workshops, Conferences

ICCS Growth

LBNL Projects

ISAAC
Astrophysics

FPGA Hybrid-core
Geophysics, Bio-informatics, Astrophysics

Smart Grid
Energy Efficiency

Cloud Modeling
Climate science

ALS Software HUB
Advanced Light Source

International Projects

GRACE II
Astrophysics

SILK ROAD
Astrophysics

ICCS Collaboration

International

University of Heidelberg (Germany)
National Astronomy Observatories/Chinese Academy of Sciences (China)
Center de Physique des Particules (France)
Commonwealth Scientific and Industrial Research Organization (Australia)
Eidgenössische Technische Hochschule (Switzerland)
Inter University Center for Astronomy & Astrophysics (India)
National Center for Radio Astronomy (India)
...

Domestic

University of California
Lawrence Berkeley Laboratory
University of Illinois
California Institute of Technology
...

Industry

Intel
Apple
NVIDIA
AMD
...

ISAAC Focus

Simulations

IFU Spectrograph / Grism

PSF Modeling

Phase Retrieval

N-Body

21 cm EOR

Instrumentation

Real-time Radio Imaging

Image Fidelity

Software correlator

Wavefront correction

Computed Tomography

Data Processing / Analysis

Low-frequency radio pipeline

Wide field image subtraction

Cosmological statistics

Gravitational / hydrodynamic evolution

Infrastructure

Python based compiler, Profiling tools, Libraries, Autotuning, Motifs, Libraries, Algorithms (FFT, Gerchberg-Saxton, FDK, N-point correlation, …)

ISAAC projects in the works

Multi-dimensional double precision self-sorting in-place FFT
W. Petersen, H. Shukla, and D. Bailey

WELL & SPRNG series Random Number Generators (Monte Carlo application)
Maximum Entropy Method for deconvolution
Decorrelation (Liu et al.)
W. Petersen, and H. Shukla

Cosmological Statistics
H. Shukla, and A. Buluc

Fourier Optics
H. Shukla, A. Bonissent, and M. Sholl

JWST, LOFAR, Pan-STARRS, SKA, IUCAA/TMT …

Adaptive Optics Instrumentation (Richard Dekany)
Adaptive Real-time Imaging (Melvyn Wright)
21 CM EOR Simulations (Ilian Iliev)
Large N-body Simulations (Salman Habib)
GPU Interconnect and Framework (Franz-Josef Pfreundt)

NERSC

NERSC serves a large population

Approximately 3000 users, 400 projects, 500 codes

Focus on "unique" resources

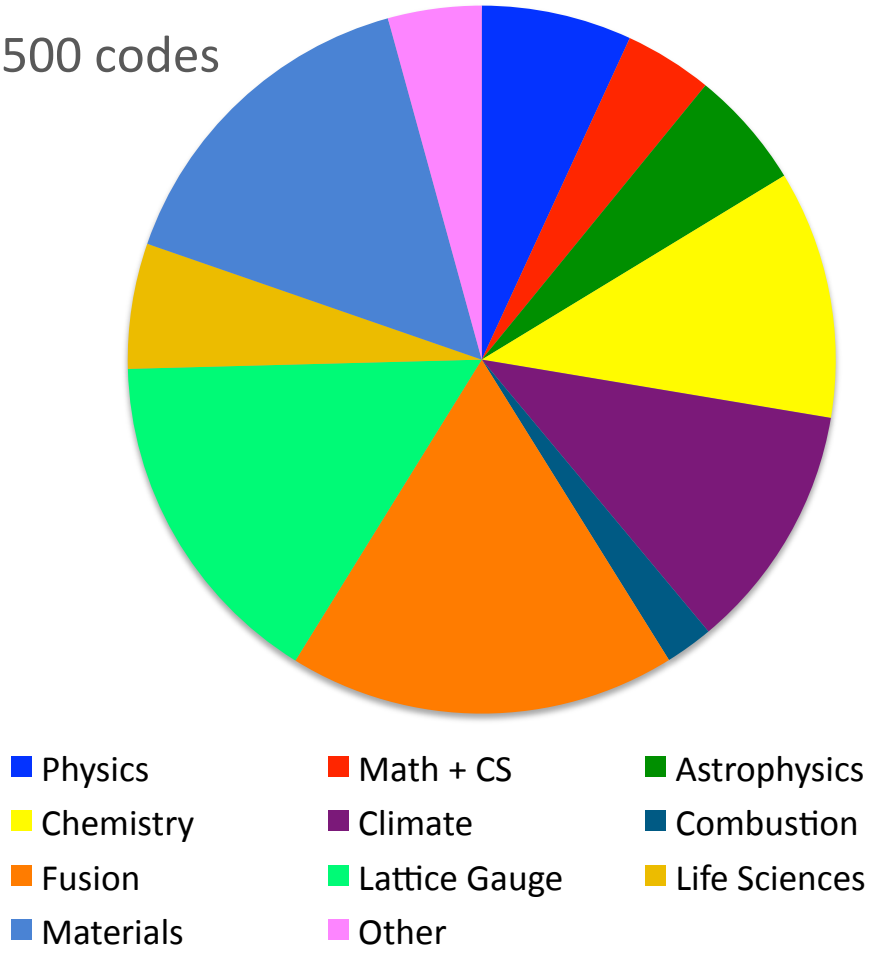
- Expert consulting and other services
- High end computing systems
- High end storage systems

NERSC is known for

- Outstanding services
- Large and diverse user workload

"NERSC continues to be a gold standard of a scientific High Performance Computational Facility."

– HPCOA Review August 2008



NERSC SYSTEMS

Large-Scale Computing Systems

Franklin (NERSC-5): Cray XT4

- 9,532 compute nodes; 38,128 cores
- ~25 Tflop/s on applications; 356 Tflop/s peak

Hopper (NERSC-6): Cray XT

- Phase 1: Cray XT5, 668 nodes, 5344 cores
- Phase 2: > 1 Pflop/s peak (late 2010 delivery)

Clusters

105 Tflops combined

Carver

- IBM iDataplex cluster

Magellan cloud testbed

- IBM iDataplex cluster

PDSF (HEP/NP)

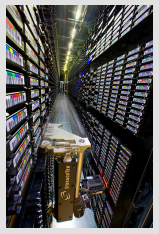
- Linux cluster (~1K cores)

NERSC Global File system (NGF)

Uses IBM's GPFS

1.5 PB; 20 GB/s

HPSS Tape Archive



- 40 PB capacity
- 4 Tape libraries
- 150 TB disk cache

Analytics

Euclid

- 512 GB
- (shared memory)

Dirac

- GPU testbed
- (48 nodes)

DIRAC

Hardware

44 Nodes

Software

Linux
CUDA 3.1
PGI compilers
GPU Direct

Node

CPU

2 Nehalem Quad Core
24 GB DDR3

GPU

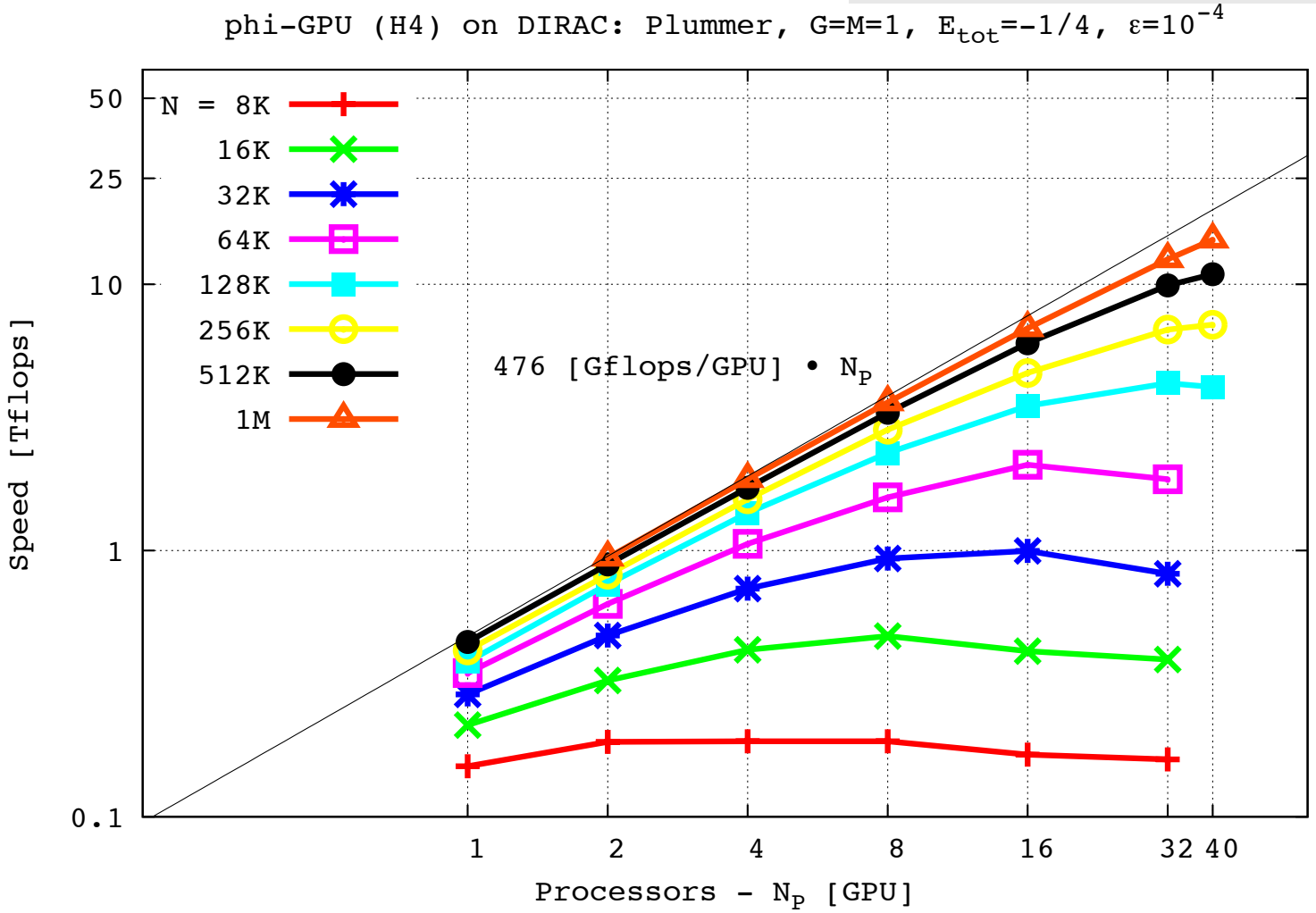
Tesla C2050
3 GB GDDR5
448 computing cores

Currently a testbed

Dirac Benchmark Results

Φ-GPU benchmarks

J. Fiestas, P. Berczik, R. Spurzem, T. Hamada
National Astronomical Observatories of China, CAS
Zentrum für Astronomie Univ. Heidelberg
Nagasaki University



Dirac Benchmark Results

Dirac vs Laohu

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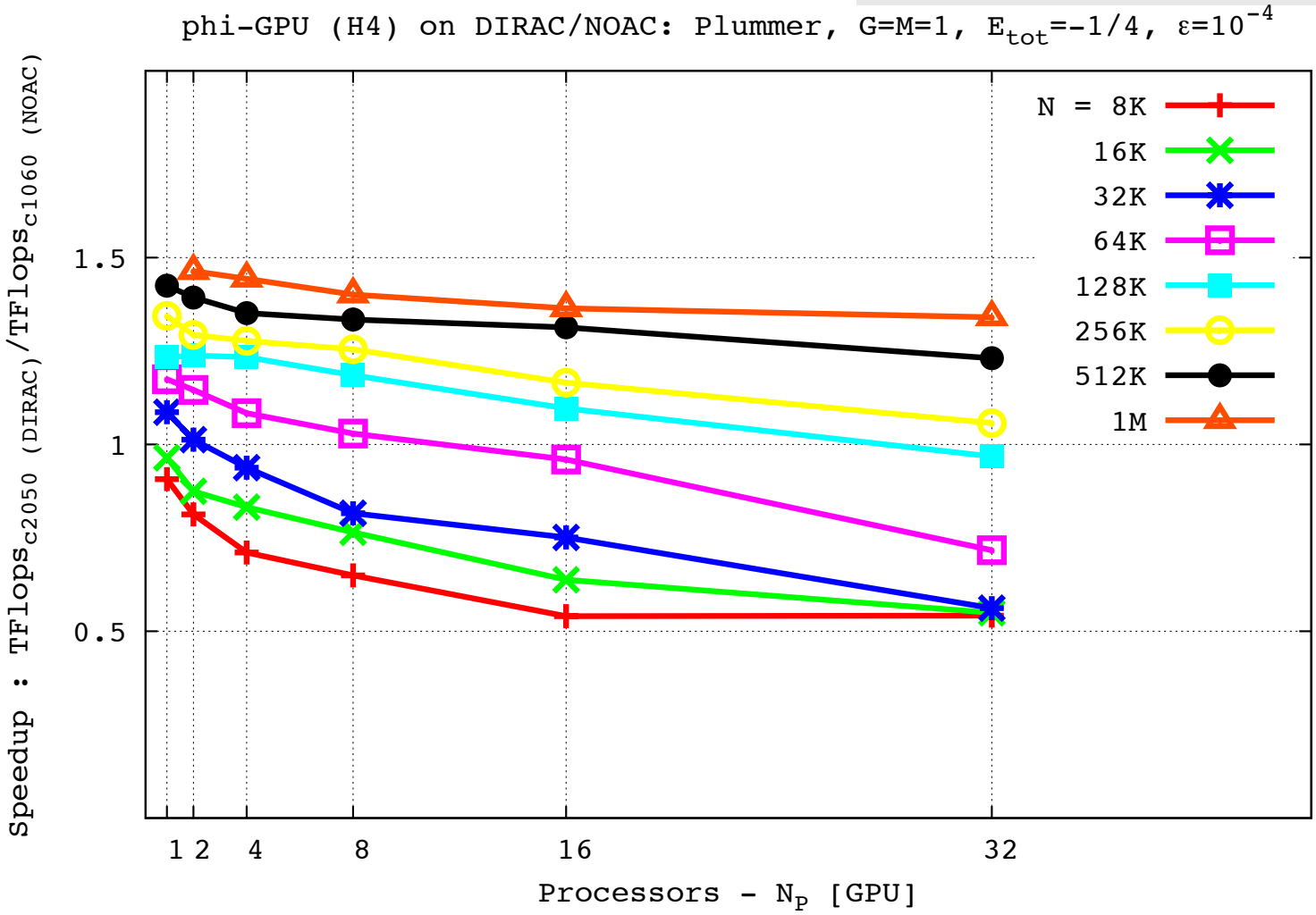
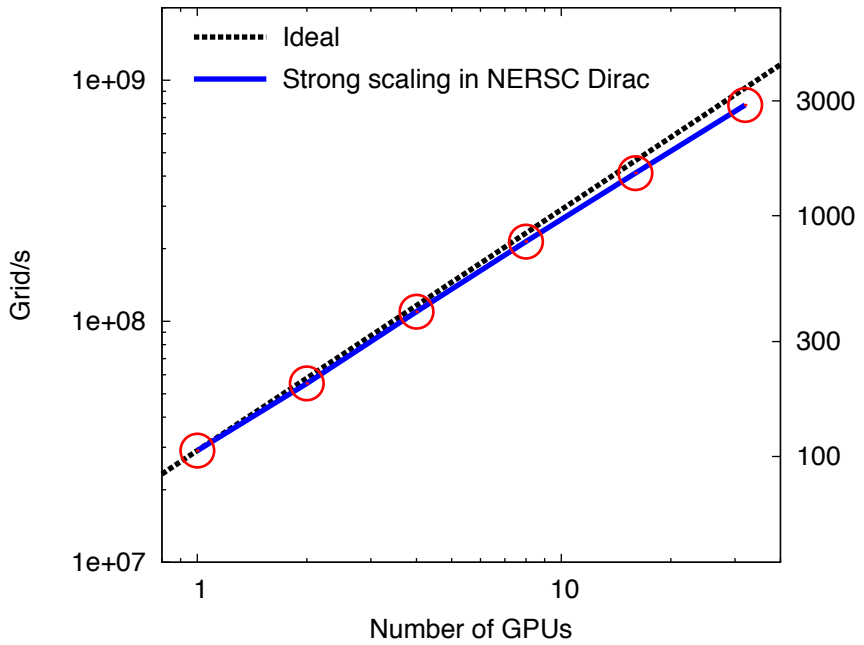
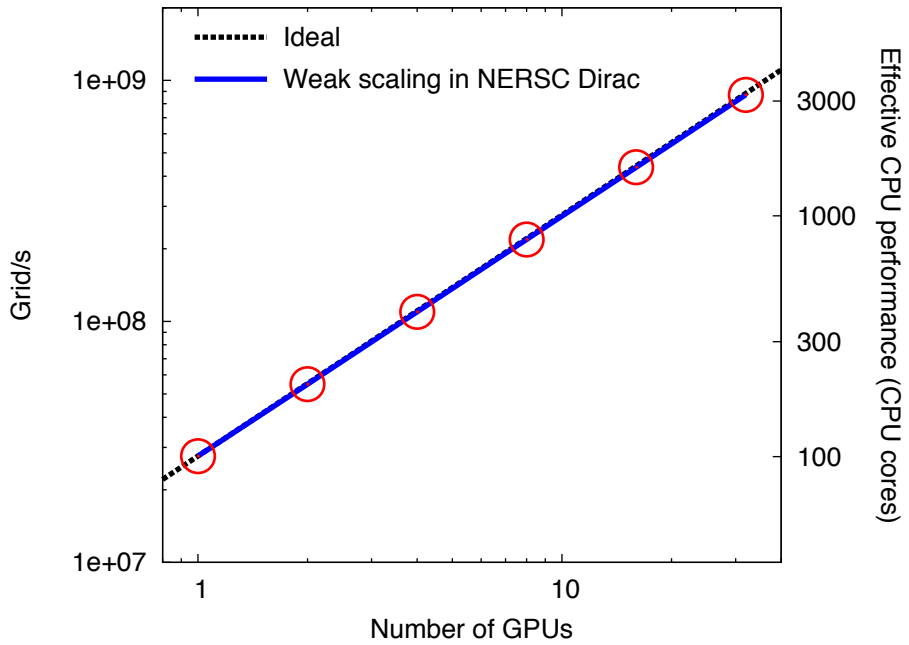


Dirac Benchmark Results

GAMER benchmarks
Hsi-Yu Schive





Hydrodynamics simulations without grid refinement

Moving Ahead

Recognize That The Road to Exascale Is Difficult

Multicore, Manycore/Embedded, Accelerator/GPUs

Future HPC Is Focused On

Energy efficiency
Programmability

Cross Discipline Efforts Should Feed The Collective Eco-system

New Scientific Programming Models
Standardizations
Common Frameworks
General Purpose Libraries

Old Code Won't Always Work

Re-imagine Algorithms

Workshop Details

International Journal of High Performance Computing Applications (IJHPCA) has announced a special issue for the ICCS workshop publications

If you are registered you can submit your paper. For details go to,

http://iccs.lbl.gov/workshops/submission.html

If you are a speaker please give your bio blurb to you session chair John Shalf, Rainer Spurzem or Hemant Shukla

Poster Session Wednesday January 26, 2011 4:30 – 5:30 PM