Joint Institute for Computational Sciences

- State funded, UT institute on the Oak Ridge campus advancing shared objectives in computational science research, education, workforce development, and national leadership
  - About $110M in external funding
- Internationally recognized research and faculty in computational and computer science, chemistry and materials science, mathematics, and molecular biology
- Operate national facilities and support campus communities
  - National Institute of Computational Science: Kraken, (Athena), Nautilus, Keeneland
  - XSEDE
Joint Institute for Computational Sciences

- Provide resources and support for UT researchers and educators
  - Training, education, consulting, curriculum development
  - Kraken, (Athena), Nautilus, Keeneland, and ties to ORNL facilities
- Support program development in computational science
  - Collaboration on proposal development and execution; deployment and operation of advanced resources
  - Bridge between UT and ORNL staff and programs
- Educate new generations of scientists in all aspects of computation
  - AACE Application Acceleration Center of Excellence
  - Graduate and undergraduate internships, REU, work experience
  - IGMCS
First academic petaflop
Delivers 65% of all NSF compute cycles

Awarded the NSF Track 2B ($65M) plus $10M from UT
Phased deployment of Cray XT systems
Staffed with ~30 FTEs and growing rapidly
Total funding ~$100M
Kraken

#3 Fastest machine in the world (Top500 11/09)

9,408 dual socket, 16GB memory nodes
2.6 GHz 6-core AMD Istanbul processor per socket
1.17 Petaflops peak performance (112,986 cores)
Cray Seastar 2 3-D Torus interconnect
3.3 Petabytes DDN disk (raw)
147 Terabytes memory
100 cabinets
~2,200 sq ft
Lightweight kernel
Kraken Allocations by Discipline

- Physics - 130; 26%
- Astronomical Sciences - 120; 21%
- Atmospheric Sciences - 510; 15%
- Molecular Biosciences - 410; 10%
- Chemistry - 140; 6%
- Chemical, Thermal Systems - 610; 5%
- Staff Accounts - 940; 4%
- Materials Research - 150; 4%
- Earth Sciences - 520; 3%
- Advanced Scientific Computing - 340; 3%
- Cross-Disciplinary Activities - 360
### TOP 10 Sites for November 2010

For more information about the sites and systems in the list, click on the links or view the complete list.

<table>
<thead>
<tr>
<th>Rank</th>
<th>Site</th>
<th>Computer</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>National Supercomputing Center in Tianjin, China</td>
<td>Tianhe-1A - NUDT TH MPP, X5670 2.93GHz 6C, NVIDIA GPU, FT-1000 8C NUDT</td>
</tr>
<tr>
<td>2</td>
<td>DOE/SC/Oak Ridge National Laboratory, United States</td>
<td>Jaguar - Cray XT5-HE Opteron 6-core 2.6 GHz Cray Inc.</td>
</tr>
<tr>
<td>3</td>
<td>National Supercomputing Centre in Shenzhen (NSCS), China</td>
<td>Nebulae - Dawning TC3600 Blade, Intel X5650, Nvidia Tesla C2050 GPU Dawning</td>
</tr>
<tr>
<td>4</td>
<td>GSIC Center, Tokyo Institute of Technology, Japan</td>
<td>TSUBAME 2.0 - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows NEC/HP</td>
</tr>
<tr>
<td>5</td>
<td>DOE/SC/LBNL/NERSC, United States</td>
<td>Hopper - Cray XE6 12-core 2.1 GHz Cray Inc.</td>
</tr>
<tr>
<td>6</td>
<td>Commissariat a l’Energie Atomique (CEA), France</td>
<td>Tera-100 - Bull bullx super-node S6010/S6030 Bull SA</td>
</tr>
<tr>
<td>7</td>
<td>DOE/NNSA/LANL, United States</td>
<td>Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband IBM</td>
</tr>
<tr>
<td>8</td>
<td>National Institute for Computational Sciences/University of Tennessee, United States</td>
<td>Kraken XT5 - Cray XT5-HE Opteron 6-core 2.6 GHz Cray Inc.</td>
</tr>
<tr>
<td>9</td>
<td>Forschungszentrum Juelich (FZJ), Germany</td>
<td>JUGENE - Blue Gene/P Solution IBM</td>
</tr>
<tr>
<td>10</td>
<td>DOE/NNSA/LANL/SNL, United States</td>
<td>Cielo - Cray XE6 8-core 2.4 GHz Cray Inc.</td>
</tr>
</tbody>
</table>
O(1) programmers
O(100,000) nodes
O(1,000,000) cores
O(10,000,000) threads … and more are coming

- Complexity kills our ambitions in HPC
- How do we write code for computers that do not yet exist?
- Why are our equations are ~100 lines but the program is ~1,000,000 lines & growing
  - This is the semantic gap – how to shrink it?
Multiresolution Adaptive Numerical Scientific Simulation

George I. Fann\textsuperscript{1}, Diego Galindo\textsuperscript{1}, Robert J. Harrison\textsuperscript{1,2}, Rebecca Hartman-Baker\textsuperscript{1}, Judy Hill\textsuperscript{1}, and Jun Jia

\textsuperscript{1}Oak Ridge National Laboratory
\textsuperscript{2}University of Tennessee, Knoxville

In collaboration with

Gregory Beylkin\textsuperscript{4}, Lucas Monzon\textsuperscript{4}, Hideo Sekino\textsuperscript{5} and Edward Valeev\textsuperscript{6}

\textsuperscript{4}University of Colorado
\textsuperscript{5}Toyohashi Technical University, Japan
\textsuperscript{6}Virginia Tech

robert.harrison@utk.edu
What is MADNESS?

- A general purpose numerical environment for reliable and fast scientific simulation
  - Chemistry, nuclear physics, atomic physics, material science, nanoscience, climate, fusion, ...
- A general purpose parallel programming environment designed for the peta/exa-scales
- Addresses many of the sources of complexity that constrain our HPC ambitions

http://code.google.com/p/m-a-d-n-e-s-s
http://harrison2.chem.utk.edu/~rjh/madness/
Molecular Electronic Structure

- Energy and gradients

- ECPs coming (Sekino, Kato)

- Response properties (Vasquez and Sekino)

- Still not as functional as previous Python version

Spin density of solvated electron
Nuclear physics

J. Pei, G.I. Fann, Y. Ou, W. Nazarewicz
UT/ORNL

- DOE UNDEF
- Nuclei & neutron matter
- ASLDA
- Hartree-Fock Bogliobulov
- Spinors
- Gamov states

Imaginary part of the seventh eigen function
two-well Wood-Saxon potential
Solid-state electronic structure

- Thornton, Eguiluz and Harrison (UT/ORNL)
  - NSF OCI-0904972: Computational chemistry and physics beyond the petascale
- Full band structure with LDA and HF for periodic systems
- In development: hybrid functionals, response theory, post-DFT methods such as GW and model many-body Hamiltonians via Wannier functions

Coulomb potential isosurface in LiF
Time-dependent electronic structure

Vence, Krstic, Harrison
UT/ORNL

$H_2^+$ molecule in laser field (fixed nuclei)
Nanoscale photonics
(Reuter, Northwestern; Hill, Harrison ORNL)

Diffuse domain approximation for interior boundary value problem; long-wavelength Maxwell equations; Poisson equation; Micron-scale Au tip 2 nm above Si surface with H2 molecule in gap – $10^7$ difference between shortest and longest length scales.
The math behind the MADNESS

- Multiresolution

\[ V_0 \subset V_1 \subset \cdots \subset V_n \]

\[ V_n = V_0 + (V_1 - V_0) + \cdots + (V_n - V_{n-1}) \]

- Low-separation rank

\[ f(x_1, \ldots, x_n) = \sum_{l=1}^{M} \sigma_l \prod_{i=1}^{d} f_i^{(l)}(x_i) + O(\epsilon) \]

\[ \| f_i^{(l)} \|_2 = 1 \quad \sigma_l > 0 \]

- Low-operator rank

\[ A = \sum_{\mu=1}^{r} u_\mu \sigma_\mu v_\mu^T + O(\epsilon) \]

\[ \sigma_\mu > 0 \quad v_\mu^T v_\lambda = u_\mu^T u_\lambda = \delta_{\mu\lambda} \]
JICS and NICS contacts

- JICS  http://www.jics.tennessee.edu
- NICS  http://www.nics.tennessee.edu

Campus contacts
- Christian Halloy  halloy@jics.utk.edu
- Kwai Wong  wong@jics.utk.edu

NICS outreach
- James Ferguson  jwf@utk.edu

JICS director
- Robert J. Harrison  robert.harrison@utk.edu