



Quantifying the Impact of GPUs on Performance and Energy Efficiency in HPC Clusters

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National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign

Cast of Characters

- Jim Philips and John Stone: Theoretical and Computational Biophysics Group, Beckman Institute, UIUC
- Kenneth Esler: NCSA and UIUC Physics
- Joshi Fullop: NCSA Systems Monitoring
- Jeremy Enos, Volodymyr Kindratenko, Craig Steffen, Guochun Shi, Mike Showerman: NCSA Innovative Systems Laboratory

Overview

- AC GPU computing cluster
- Power monitoring
 - Search for power monitors
 - Roll our own--version 1: Tweet-A-Watt
 - Roll our own--version 2: Arduino-based power monitor
- Current power monitoring on real applications

AC cluster (Accelerator Cluster)

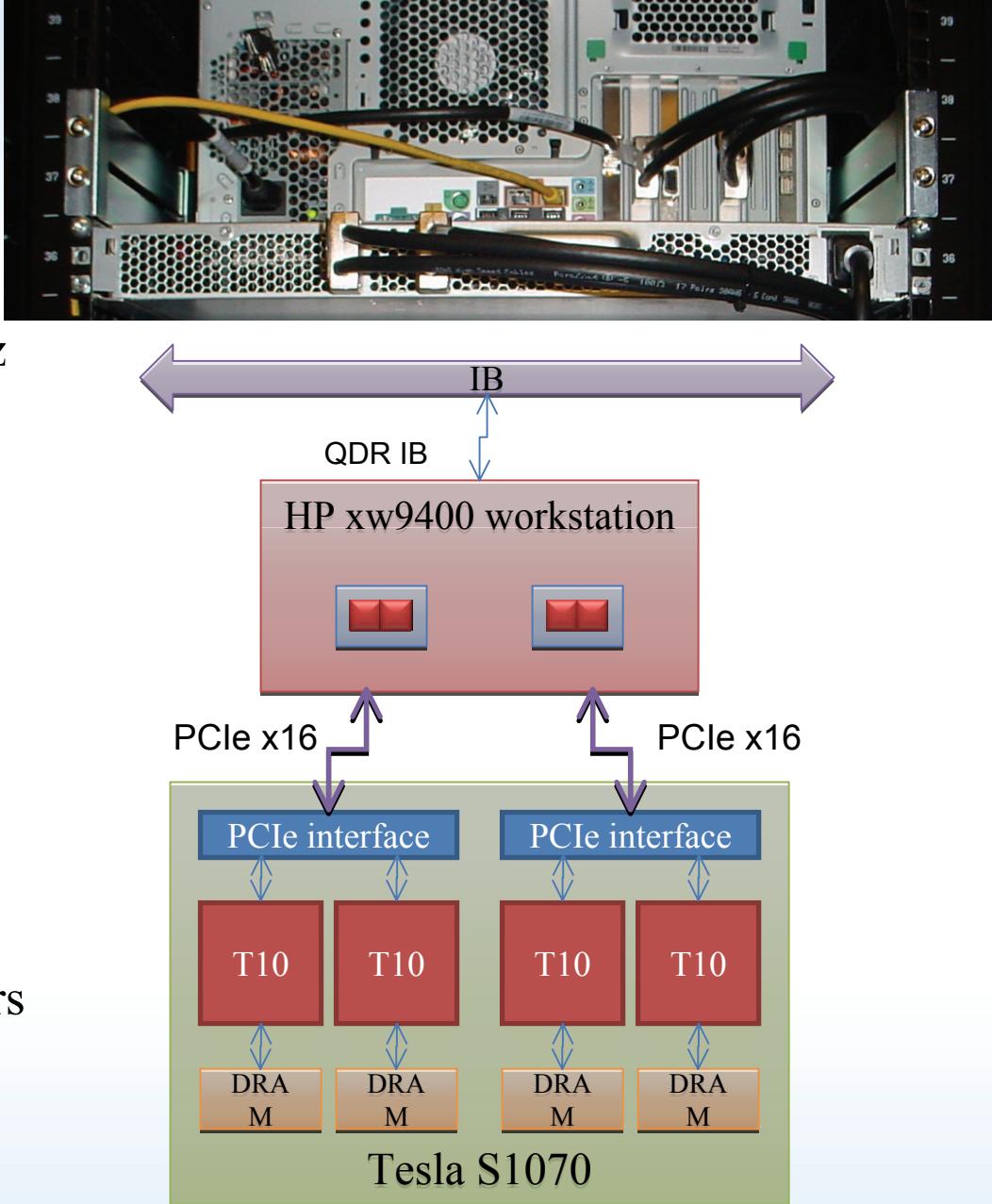
- Originally “QP” cluster for “Quadro Plex”
- 32 HP XW9400 nodes. Each node:
 - 2 dual-core 2.4 GHz Opteron 2216
 - 8 GB RAM per node
 - **NVIDIA Tesla S1070 each:**
 - **4 Tesla C1060 GPUs (128 total in cluster)**
- Interconnect network is QDR Infiniband
- CUDA 3.1 compiler/build stack
- Job control/scheduler Moab
 - **Specific resource management for jobs via Torque**
- QP first commissioned November 2007
- AC on-line since December 2008

AC Cluster



AC01-32 nodes

- **HP xw9400 workstation**
 - 2216 AMD Opteron 2.4 GHz dual socket dual core
 - 8GB DDR2 in ac04-ac32
 - 16GB DDR2 in ac01-03, “bigmem” on qsub line
 - PCI-E 1.0
 - Infiniband QDR
- **Tesla S1070 1U GPU Computing Server**
 - 1.3 GHz Tesla T10 processors
 - 4x4 GB GDDR3 SDRAM
 - 1 per host



AC cluster used for

- Virtual school for Science and Engineering (attached to the Great Lakes Consortium for Petascale Computing)
NVIDIA/CUDA August 2008,2009,2010
- Other classes in 2010:
 - “Intro to CUDA” Volodymyr Kindratenko, Singapore June 13-19
 - Barcelona Spain, Wen-Mei Hwu July 5-9
 - Thomas Scavo July 13-23
 - “Proven Algorithmic Techniques for Many-core Processors”
Thomas Scavo August 2-6
 - John Stone August 7-8

AC GPU Cluster Power Measurements

| State | Host Peak (Watt) | Tesla Peak (Watt) | Host power factor (pf) | Tesla power factor (pf) |
|--|---------------------|----------------------|------------------------------|----------------------------|
| power off | 4 | 10 | .19 | .31 |
| start-up | 310 | 182 | | |
| pre-GPU use idle | 173 | 178 | .98 | .96 |
| after NVIDIA driver module unload/reload ⁽¹⁾ | 173 | 178 | .98 | .96 |
| after deviceQuery ⁽²⁾ (idle) | 173 | 365 | .99 | .99 |
| GPU memtest #10 (stress) | 269 | 745 | .99 | .99 |
| after memtest kill (idle) | 172 | 367 | .99 | .99 |
| after NVIDIA module unload/reload ⁽³⁾ (idle) | 172 | 367 | .99 | .99 |
| VMD Madd | 268 | 598 | .99 | .99 |
| NAMD GPU STMV | 321 | 521 | .97-1.0 | .85-1.0 ⁽⁴⁾ |
| NAMD CPU only ApoA1 | 322 | 365 | .99 | .99 |
| NAMD CPU only STMV | 324 | 365 | .99 | .99 |

1. Kernel module unload/reload does not increase Tesla power
2. Any access to Tesla (e.g., deviceQuery) results in doubling power consumption after the application exits
3. Note that second kernel module unload/reload cycle does not return Tesla power to normal, only a complete reboot can
4. Power factor stays near one except while load transitions. Range varies with consumption swings

Search for Power Monitors: What questions do we want to answer?

- How much power do jobs use?
- How much do they use for pure CPU jobs vs. GPU-accelerated jobs?
- Do GPUs deliver a hoped-for improvement in power efficiency?

Hardware: Criteria for data-sampling device

- Cheap
- Easy to buy/produce
- Allows access to real data (database or USB, no CD-installed GUIs)
- Monitors 208V 16A power feed
- Scalable solution across machine room (one node can collect one-node's data)

Search for Good (and Cheap) Hardware Power Monitoring

- Laboratory units too expensive
- Commercial Units:
 - 1A granularity?
 - No direct data logging
 - No real-time data logging

Very capable

- PS3000 PowerSight Power Analyzer
\$ 2495.00

Capable; Closer but still too expensive

- [ElitePro™ Recording Poly-Phase Power Meter](#) Standard Version consists of:
 - US/No. America 110V 60 Hz Transformer
 - 128Kb Capacity
 - Serial Port Communications
 - Indoor Use with Crocodile Clips
 - Communications Package (Software) and Current Transformers sold separately.
- [More Information](#)

Price: \$965.00 Part Number: EP

Instrumented PDUs: poor power granularity

- 1A granularity
- 120V circuits



Watts-up integrated power monitor: CLOSE

- Smart Circuit 20 31298 \$194.95
- Outputs data to web page (how to efficiently harvest this data?)

Data Center Power—208 V, 20 or 30A



Power Monitoring Version 1: Tweet-a-Watt Receiver and Transmitter



<http://www.ladyada.net/make/tweetawatt/>

Kits available from www.adafruit.com

Tweet-a-Watt

- Kill-a-watt power meter
- Xbee wireless transmitter
- power, voltage, shunt sensing tapped from op amp
- Lower transmit rate to smooth power through large capacitor
- Readout software modified from available Python scripts to upload sample answers to local database
- We built 3 transmitter units and one Xbee receiver
- Currently integrated into AC cluster as power monitor



Evaluation of Tweet-a-Watt

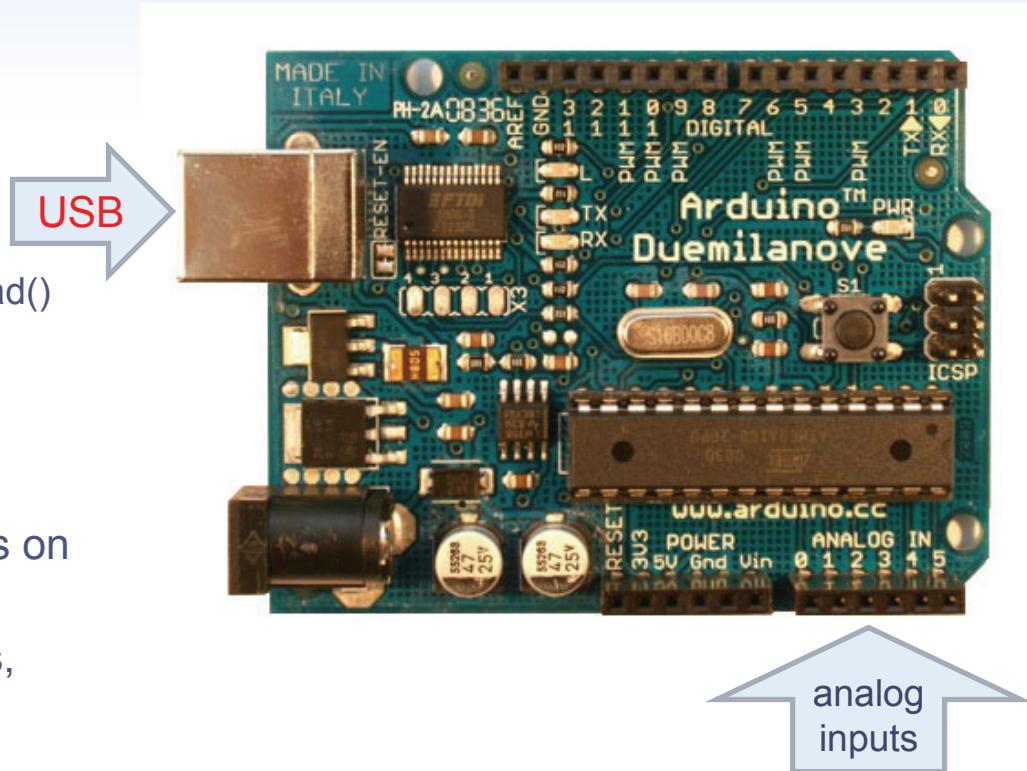
- Limited to Kill-a-Watt capability (**120V, 15A circuit**)
- Low sampling rate (report every 2 seconds, readout every 30 seconds)
- Either TWO XBEE units required or scaling issue
- Fixed but configurable program; one set, difficult to program (low sampling rate means unit is off most of the time)
- Correlated voltage and current (read power factor and true power usage)
- 50-foot plus range (through two interior walls)
- Currently tied to software infrastructure: **Application power studies done with Tweet-a-Watt**

Power Monitor version 2: One-off function Prototype Power Monitor

- Used chassis from existing (120 V) PDU for interior space
- Connectors, breaker, and wiring to carry 208V 16A power distribution
- Current sense transformers and Arduino microcontroller for current monitoring
- Prototyped (but not deployed) Python script to insert output into power monitor database

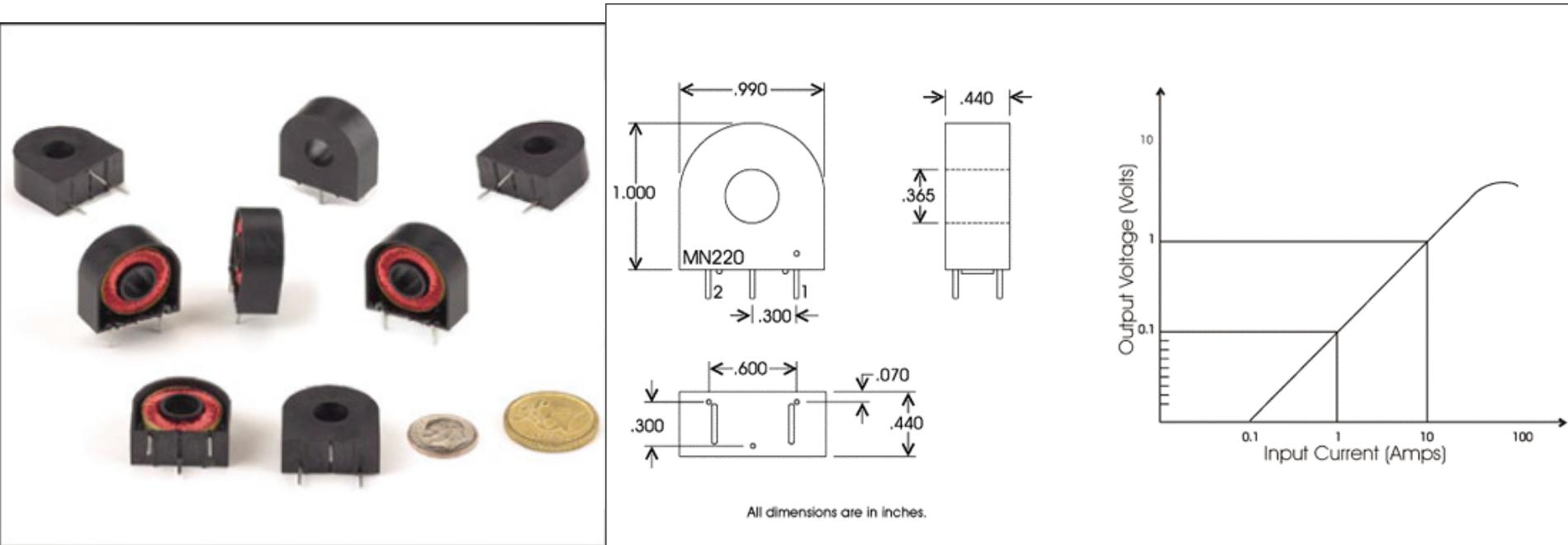
Arduino-based Power Monitor

- Based on Arduino Duemilanove
 - Runs at 16 MHz
 - has 6 **analog voltage-to-digital converters** (sampled explicitly by `read()` function)
 - Runs microcode when powered on (from non-volatile memory)
- Accumulates sample arrays for N samples per channel per report (N is on subsequent slides)
- Accumulates current measurements, computes RMS values, and outputs results in ASCII on USB connection
- Arduino is powered from the USB connection



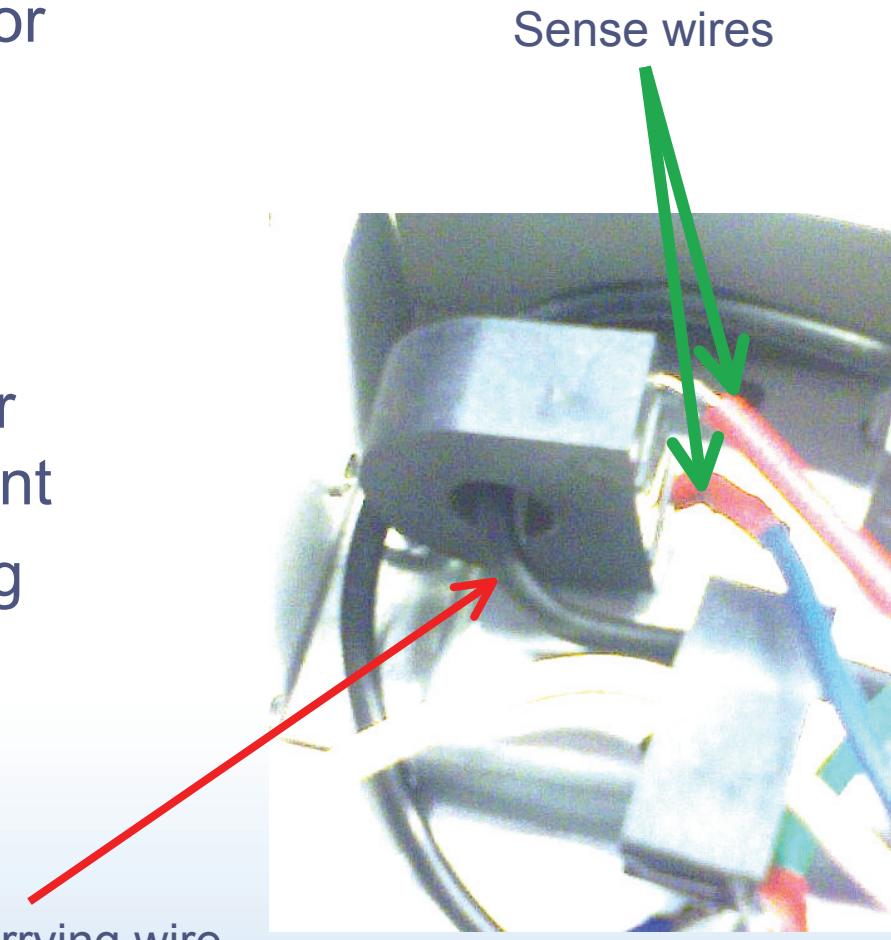
MN 220 picking transformer from Manutech

- Manutech.us
- 1000 to 1 voltage transformer; 1 to 1000 current transformer
- Suggested burden resistor: 100 Ohms.
- AC output voltage proportional to AC current input.
- Output at 100 Ohms: 100 mV/Amp.
- Various ranges of output are achievable by using different burden resistors.



Current Sense Transformer

- MN-220 current “transformer” designed for 1 to 20 amp primary
 - 1000-1 step-up current transformer
- Burden resistor sets the sensitivity; sets “volts per count” calibration constant
- Allows current monitoring without Arduino contact with high-voltage wires



Industrial Design

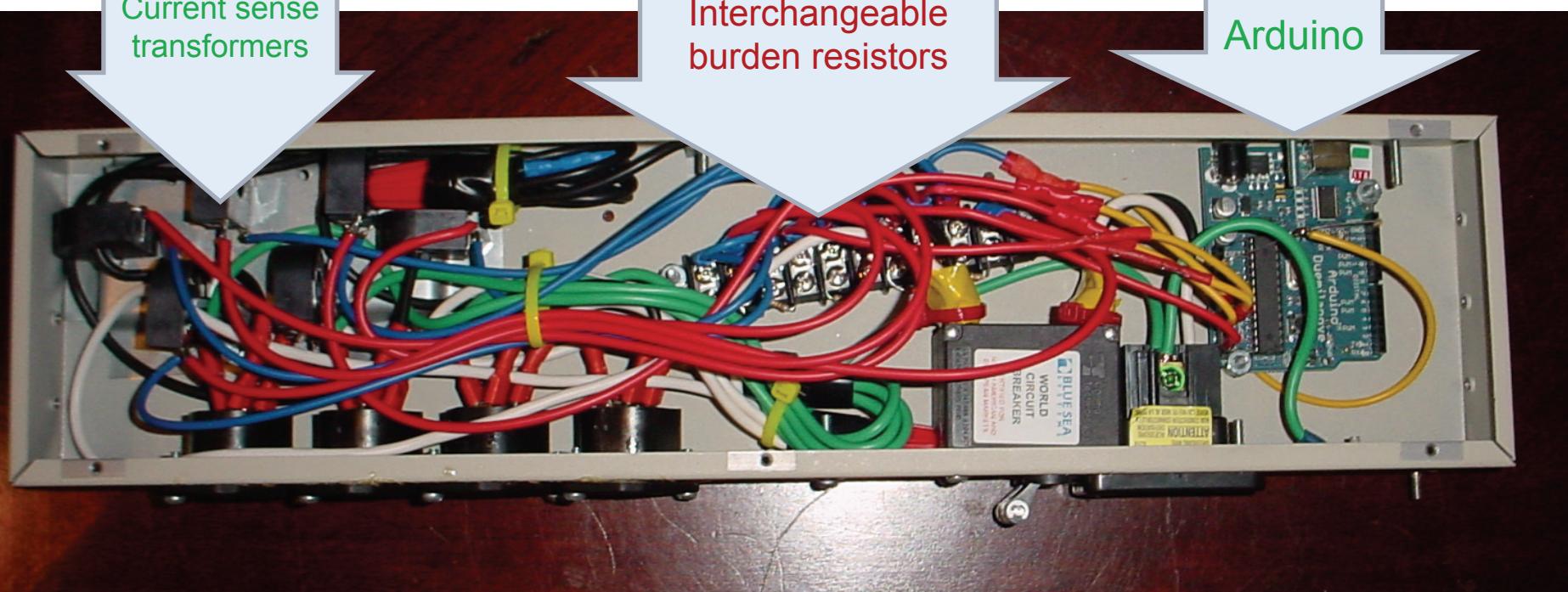
- 5 separate sense transformers for 4 power legs and opposite leg of input
- Current sense ONLY; Arduino is completely isolated from power conductors. No phase or power factor information, RMS current *only*



Current sense
transformers

Interchangeable
burden resistors

Arduino



Arduino development environment

- C-like language environment
 - #defines for calibration constants
 - Initial setup() function runs once
 - loop() function repeats forever

SPECIAL WARNING: Arduino INTs are 16 bits! Summing the squares of measured voltages (in the 200 to 400 range) will OVERFLOW the accumulator INT. (Convert to float before squaring)

```
File Edit Sketch Tools Help
[Icons]
work_voltmeter_doublefloat

#define AMPSPERCT0 (14.796)
#define AMPSPERCT1 (9.574)
#define AMPSPERCT2 (9.574)
#define AMPSPERCT3 (14.796)
#define AMPSPERCT4 (48.828)

// correction factors
#define CORRECO (1.0)
#define CORREC1 (1.249)
#define CORREC2 (1.193)
#define CORREC3 (1.043)
#define CORREC4 (0.967)

void setup(){
    analogReference(DEFAULT);
    pinMode(0, INPUT);
    Serial.begin(9600);
}

void loop(){
    float accum0 = 0.0, accum1 = 0.0, accum2 = 0.0, accum3 = 0.0, accum4 = 0.0, accum5 = 0.0;
    float total0=0.0, total4=0.0;
    float rmsCts = 0.0;
    int N=0;
    int relval;
```

Output Format (our implementation)

- Every sampling period outputs block of ASCII text to virtual console (accessed under Linux typically at /dev/ttyUSB0)
- No protocol or readers necessary; software can be checked with commands *tail* or *more*
- If ANY sample on a channel is within 10% of the hard limit, then the channel is flagged as “overflow” in the output stream
(note the \r \n double-line breaks)

File Edit View Terminal Help

(4)[]= 1335.24

analogzero=524.68 514.80

(0)[]= 1366.71

(1)[]= 7.87

(2)[]= 8.34

(3)[]= 13.22

(4)[]= 1329.58

analogzero=501.67 507.42

(0)[]= 1318.34

(1)[]= 8.02

(2)[]= 8.97

(3)[]= 9.76

(4)[]= 1315.29

analogzero=496.03 506.72

(0)[]= 1346.84

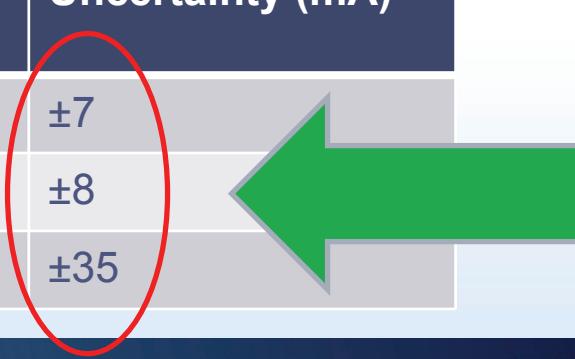
(1)[]= 8.46

(2)[]= 6.59

Calibration, Uncertainty and Readout Speed

- Arduino only does RMS summing; not synchronized with AC clock. Possible sampling errors from undersampling AC waveform (hopefully eliminated by enough samples)
- Samples-per-report is set high enough to minimize undersampling errors
- Uncertainty measured with idle node (upper uncertainty limit only)

| Measurements per report | Time between reports (s) | Uncertainty (mA) |
|-------------------------|--------------------------|------------------|
| 250 | .28 | ±7 |
| 125 | .2 | ±8 |
| 60 | .15 | ±35 |



Industrial design continued

- Interchangeable burden resistors to match pickup transformer output voltage to Arduino voltage sense
- Initially configured with two 600W channels, two 1000W channels, and main leg monitor is about 3300W for 16A at 208V
- Conclusion: **no advantage** to careful matching of burden resistors.
Uncertainty of 3300W channel vs. 600W:
 - 250 samples: 6 vs 7mA
 - 125 samples: 8 vs 8
 - 60 samples: 37 vs 35
- Advantage: eliminates a LOT of wiring from the prototype

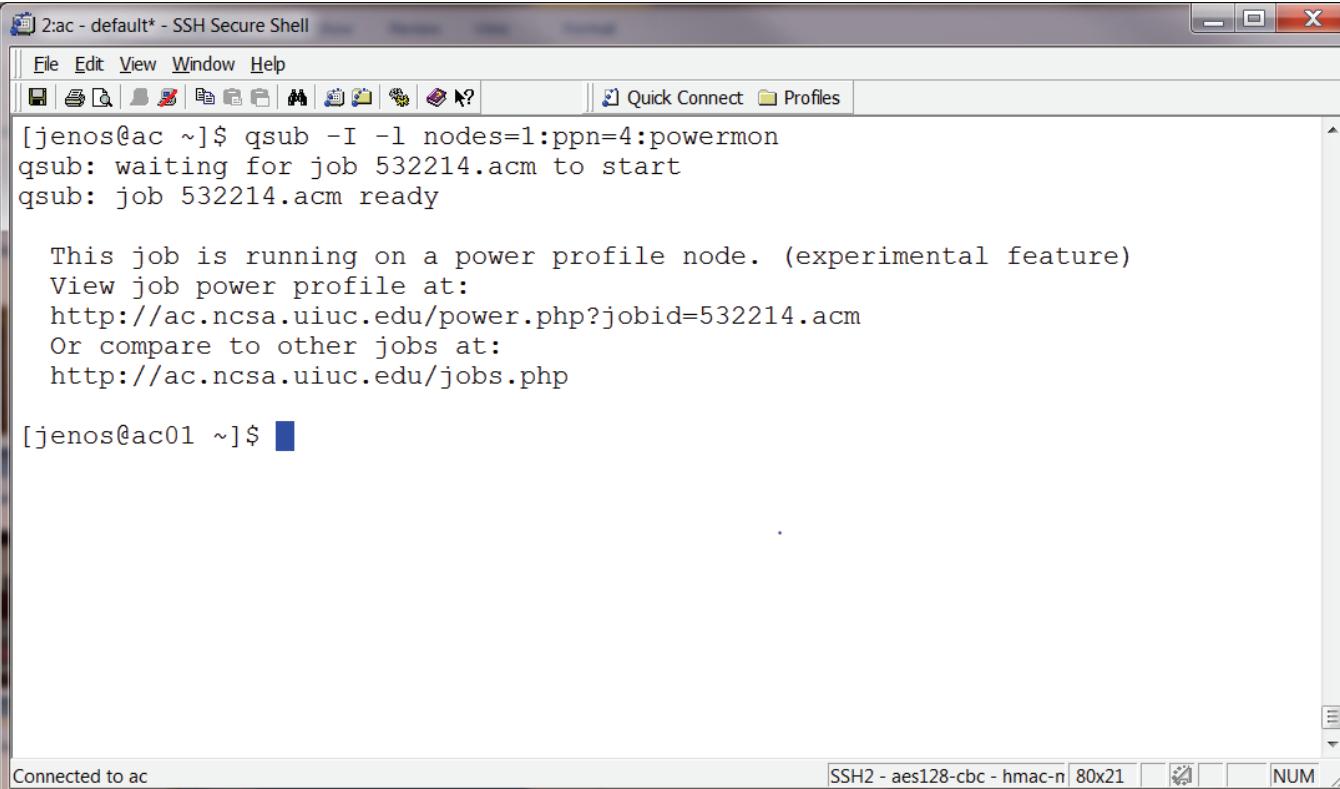


Data storage and calibration database

- Prolog scripts identify the (one) power monitored node (via Torque)
- Job history entry tags job to be attached to time window of power monitor data
- The job scripts create an automagic link to graphed output data per-sample and total usage summary

Power monitor data presentation

- <http://ac.ncsa.uiuc.edu/docs/power.readme>
- submit job with prescribed Torque resource (powermon)
- Run application as usual, follow link(s)



The screenshot shows a terminal window titled "2:ac - default* - SSH Secure Shell". The window contains the following text:

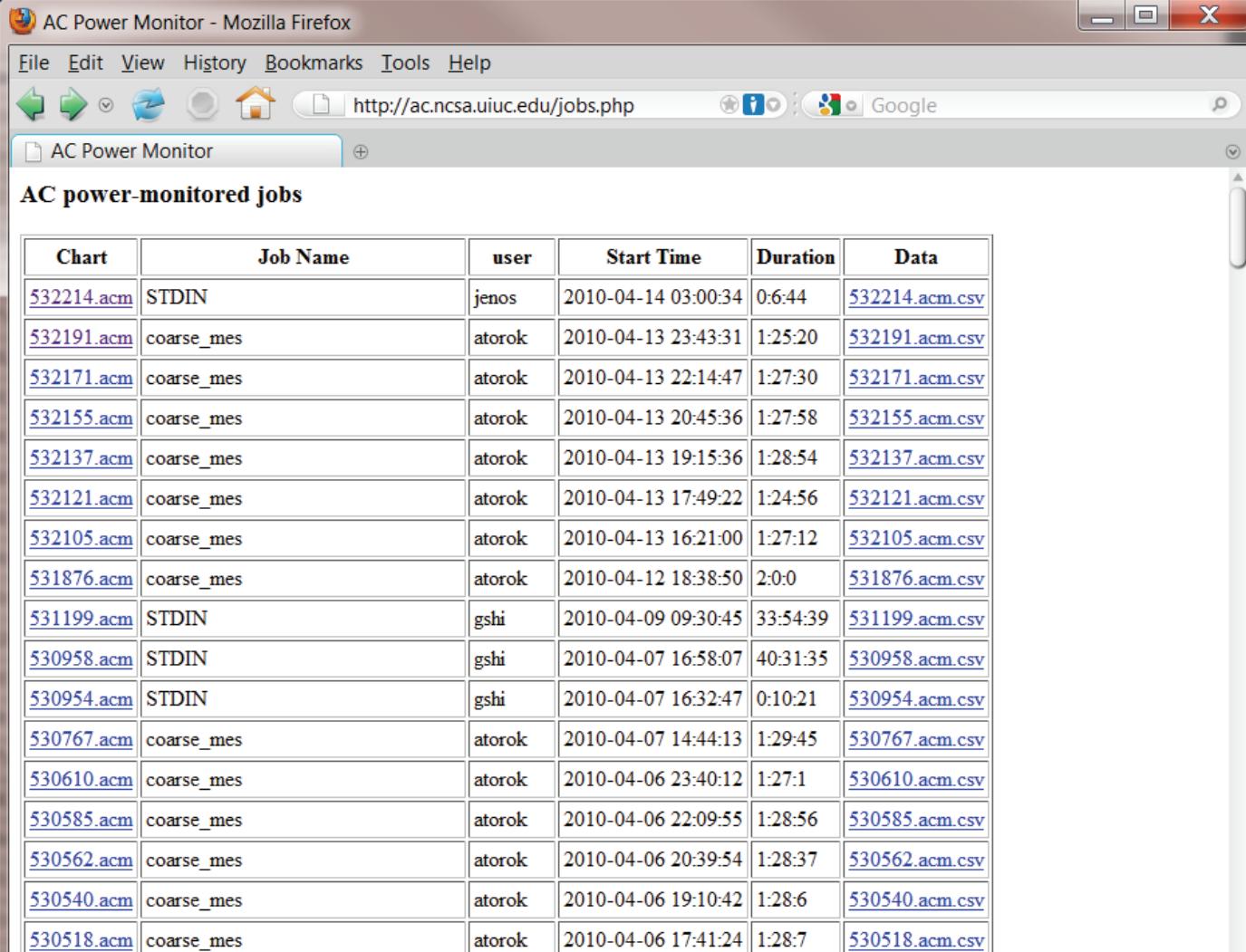
```
[jenos@ac ~]$ qsub -I -l nodes=1:ppn=4:powermon
qsub: waiting for job 532214.acm to start
qsub: job 532214.acm ready

This job is running on a power profile node. (experimental feature)
View job power profile at:
http://ac.ncsa.uiuc.edu/power.php?jobid=532214.acm
Or compare to other jobs at:
http://ac.ncsa.uiuc.edu/jobs.php

[jenos@ac01 ~]$
```

The status bar at the bottom of the window indicates "Connected to ac" and "SSH2 - aes128-cbc - hmac-n 80x21".

Each monitored job shows up as a link at <http://ac.ncsa.uiuc.edu/jobs.php>

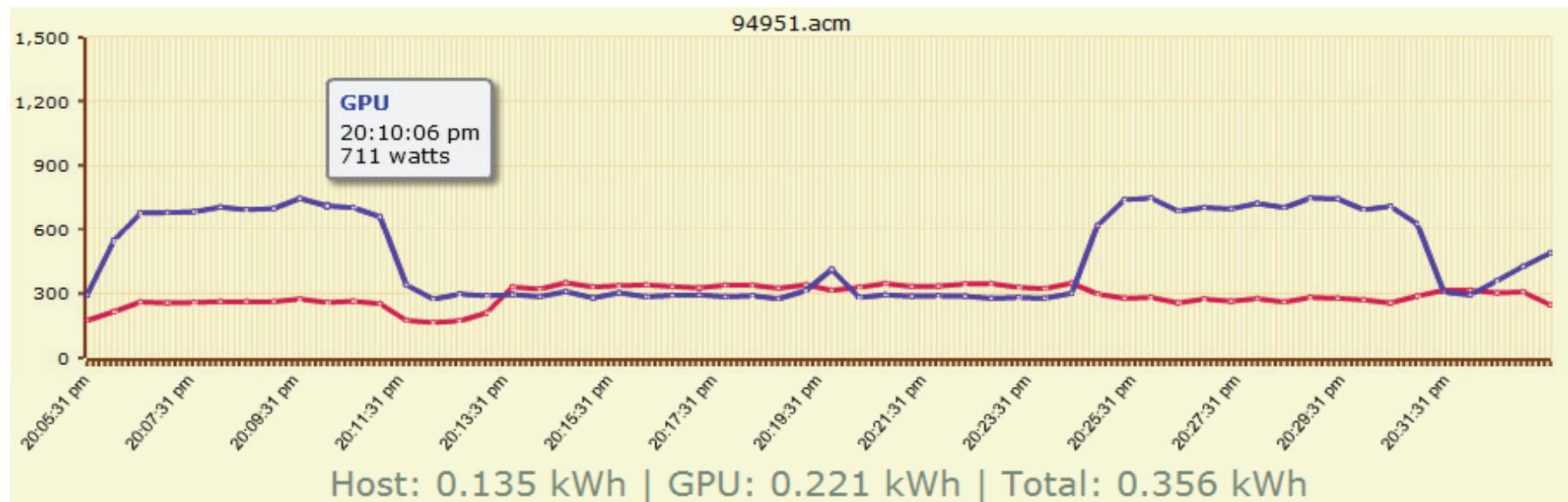


A screenshot of a Mozilla Firefox browser window titled "AC Power Monitor - Mozilla Firefox". The address bar shows the URL <http://ac.ncsa.uiuc.edu/jobs.php>. The page content is titled "AC power-monitored jobs" and displays a table with the following data:

| Chart | Job Name | user | Start Time | Duration | Data |
|----------------------------|------------|--------|---------------------|----------|--------------------------------|
| 532214.acm | STDIN | jenos | 2010-04-14 03:00:34 | 0:6:44 | 532214.acm.csv |
| 532191.acm | coarse_mes | atorok | 2010-04-13 23:43:31 | 1:25:20 | 532191.acm.csv |
| 532171.acm | coarse_mes | atorok | 2010-04-13 22:14:47 | 1:27:30 | 532171.acm.csv |
| 532155.acm | coarse_mes | atorok | 2010-04-13 20:45:36 | 1:27:58 | 532155.acm.csv |
| 532137.acm | coarse_mes | atorok | 2010-04-13 19:15:36 | 1:28:54 | 532137.acm.csv |
| 532121.acm | coarse_mes | atorok | 2010-04-13 17:49:22 | 1:24:56 | 532121.acm.csv |
| 532105.acm | coarse_mes | atorok | 2010-04-13 16:21:00 | 1:27:12 | 532105.acm.csv |
| 531876.acm | coarse_mes | atorok | 2010-04-12 18:38:50 | 2:0:0 | 531876.acm.csv |
| 531199.acm | STDIN | gshi | 2010-04-09 09:30:45 | 33:54:39 | 531199.acm.csv |
| 530958.acm | STDIN | gshi | 2010-04-07 16:58:07 | 40:31:35 | 530958.acm.csv |
| 530954.acm | STDIN | gshi | 2010-04-07 16:32:47 | 0:10:21 | 530954.acm.csv |
| 530767.acm | coarse_mes | atorok | 2010-04-07 14:44:13 | 1:29:45 | 530767.acm.csv |
| 530610.acm | coarse_mes | atorok | 2010-04-06 23:40:12 | 1:27:1 | 530610.acm.csv |
| 530585.acm | coarse_mes | atorok | 2010-04-06 22:09:55 | 1:28:56 | 530585.acm.csv |
| 530562.acm | coarse_mes | atorok | 2010-04-06 20:39:54 | 1:28:37 | 530562.acm.csv |
| 530540.acm | coarse_mes | atorok | 2010-04-06 19:10:42 | 1:28:6 | 530540.acm.csv |
| 530518.acm | coarse_mes | atorok | 2010-04-06 17:41:24 | 1:28:7 | 530518.acm.csv |

Power Profiling – Walk through

AC Power Utilization



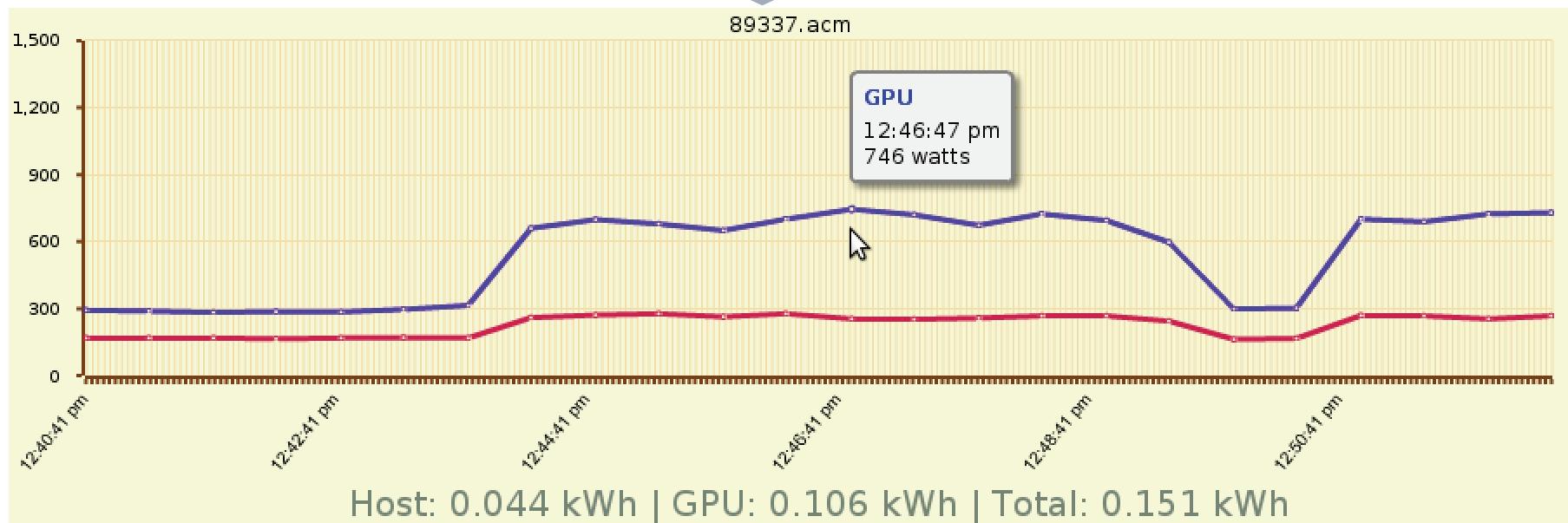
JSON Data

- Mouse-over value displays
- Under curve totals displayed
- If there is user interest, we may support calls to add custom tags from application

Output Graphs

Job ID

AC Power Utilization



Unique Features of this Hardware+Software Setup

- Hardware solution
 - Cheap
 - Scalable
- Presentation integrated with job software
- Simple to use with jobs.php link
- Not required; can be ignored by other users

Real Application Speed and Efficiency

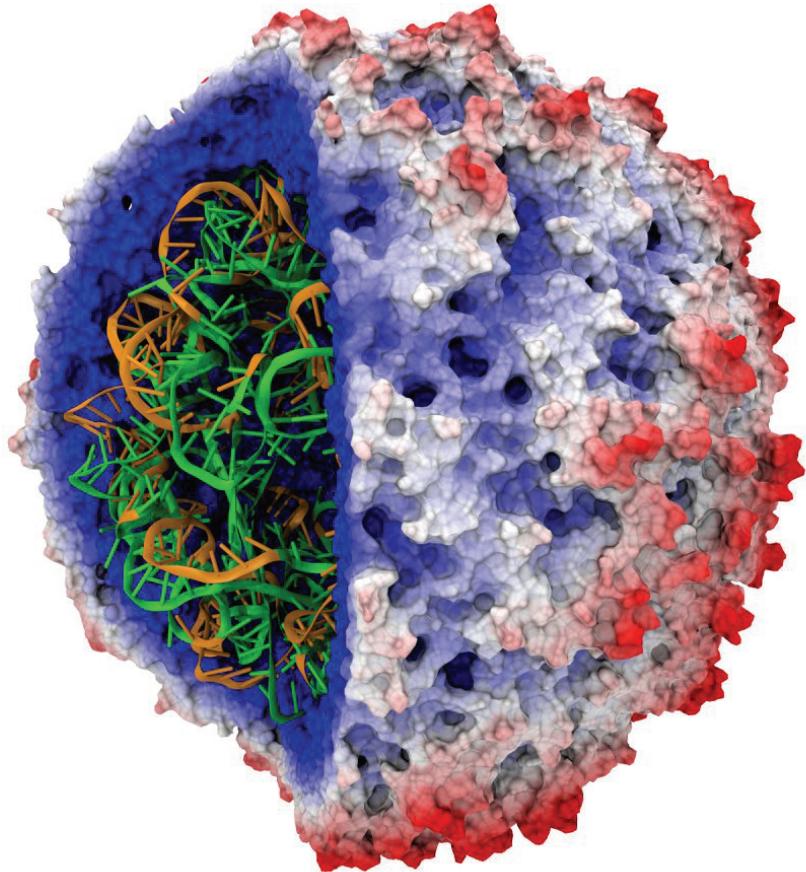
- Speedup measured in terms of **wall clock time** for whole application to run
- Power consumption measurements made over at least 20 sample runs
- Removed power measurements from startup and shutdown phases of applications

NOTE: The NVIDIA cards have internal power measuring.
We didn't use them because

- That leaves out the power supply of the Tesla
- We got inconsistent node-to-node results
- We wanted to understand the systematics of the data

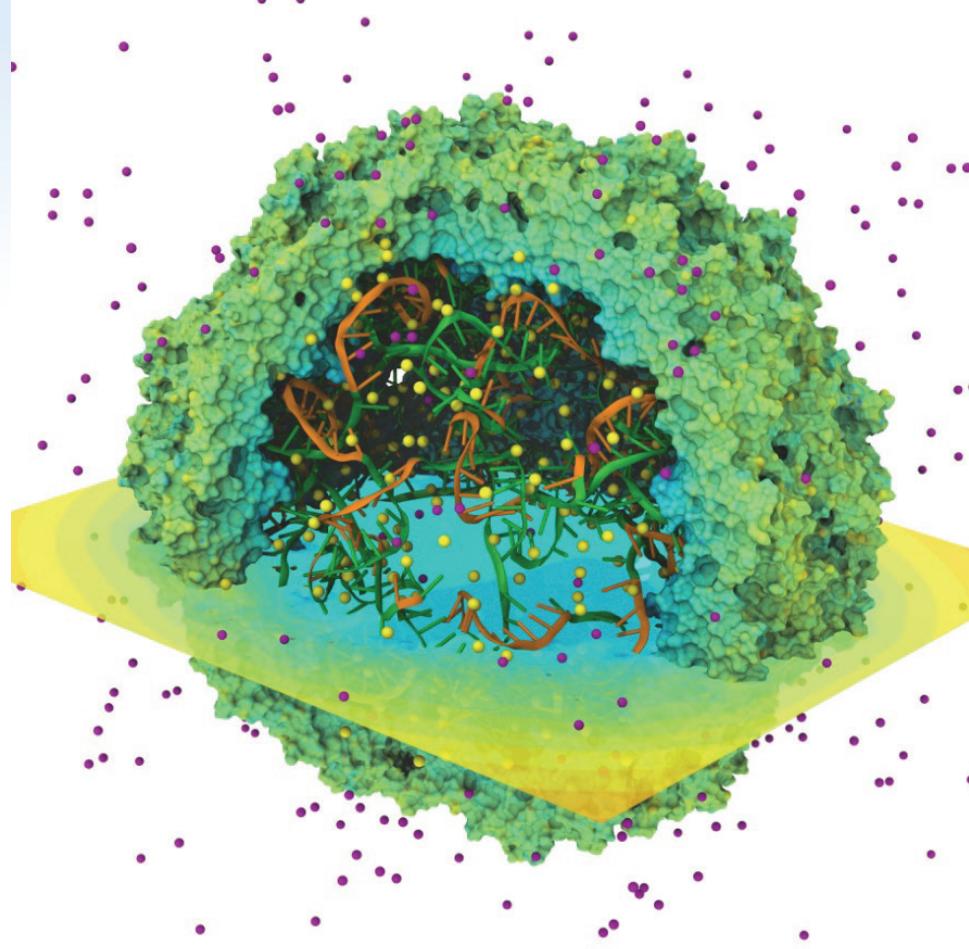
Case Study: NAMD

- Molecular Dynamics based on Charmm++ parallel programming environment; contains support for GPU codes
- Sample set was “STMV” 1 million atom virus simulation
 - Performance measure is simulation time step per wall clock time
- CPU-only: 6.6 seconds per timestep; 316 Watts
- CPU+GPU: 1.1 seconds per timestep; 681 Watts
- Speedup: 6
- **Speedup-per-watt: 2.8**



Case Study: VMD

- Molecular visualization and analysis tool
- Computes 3D electrostatic potential fields, forces, and electron orbitals
- Computation problem: 685,000 atom STMV trajectory using multilevel summation method
- CPU-only: t=1465 seconds; 300 watts
- CPU+GPU: t=58 seconds; 742 watts
- Speedup factor: 26
- **Speedup-per-watt: 10.5**



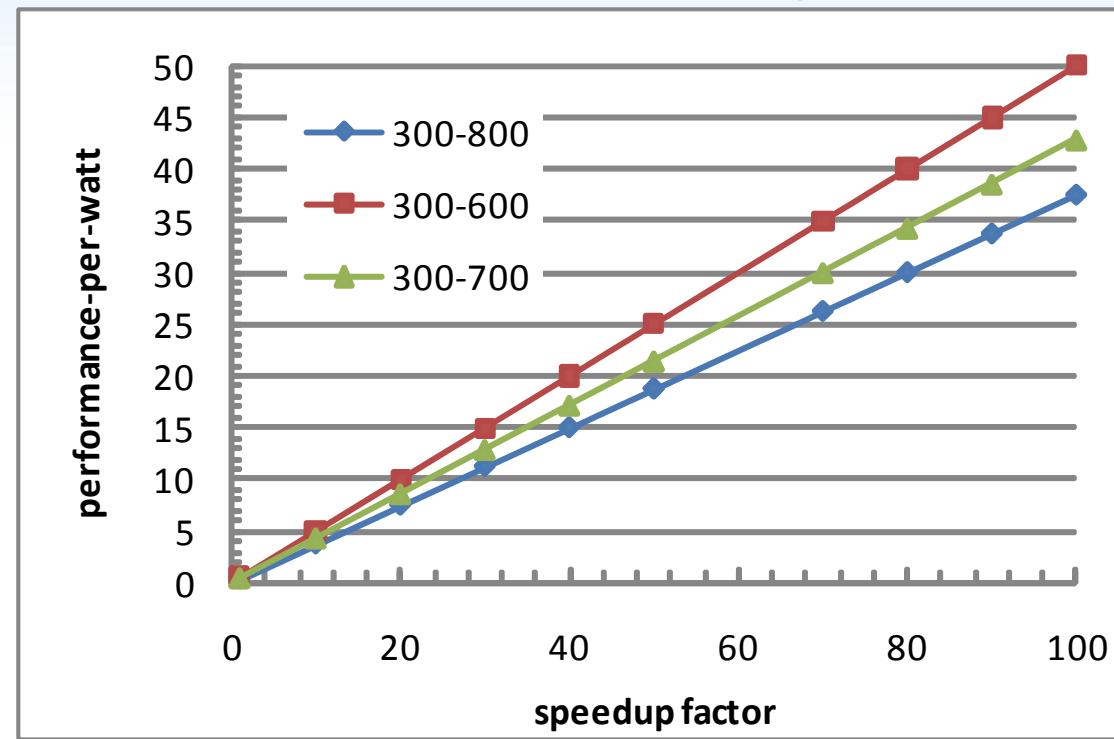
Case Study: QMCPACK

- Quantum Monte Carlo for tracking movement of interacting QM particles
- Simulating 128-atom simulation cell of bulk diamond, including 512 valence electrons
- Caviat:
 - CPU-only version uses double precision
 - CPU/GPU version uses mostly single-precision
 - Results are consistent within result uncertainty
- Results reported for Diffusion Monte Carlo; results for variational Monte Carlo are similar
- CPU-only: 1.16 walker generations per second
- CPU+GPU: 71.1 walker generations per second
- Speedup: 62
- **Speedup-per-watt:** 23

Application Case Study: MILC

- MIMD Lattice Computation of QCD
 - MILC calculations must now include electromagnetic effects in the calculations
- Problem set 28x28x28x96 lattice
- Single-core version only at this time
 - Computation on single-core vs. single-core+GPU
 - Power monitoring is for whole CPU node or CPU node+GPU
- CPU core: 77324 s
- CPU+GPU: 3881 s
- Speedup: 20
- Speedup-per-watt: 8

Current State: Speedup to Efficiency Correlation



- The GPU consumes roughly double the CPU power, so a 3x GPU is required to break even
- Performance-per-watt is asymptotically roughly half speedup factor or less

Future Work

- Arduino-based power monitor not yet commissioned
- Data-collection issues with higher granularity:
 - Only take data for jobs (no monitoring idle nodes)
 - User selects sampling rate (high-res power monitoring only when it will be used)
- Future: user tags application phases to refine data analysis (startup, shutdown, computation, communication)

HPRCTA 2010 (workshop at SC 2010 in New Orleans)

- **Fourth International Workshop on High-Performance Reconfigurable Computing Technology and Applications**
- All day Sunday, November 14
- The workshop is co-organized by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign, the George Washington University, OpenFPGA, and Xilinx
- Submissions due **September 3, 2010**
- <http://www.ncsa.illinois.edu/Conferences/HPRCTA10/>
- <http://tinyurl.com/hprcta2010>

SAAHPC 2011

- **Symposium on Application Accelerators in High Performance Computing 2011**
- Covers all accelerators including GPUs, FPGAs, Cell
- Co-hosted by **NCSA, University of Illinois** and **University of Tennessee, Knoxville**
- 2011 dates and location not announced (June or July)
- Submissions due in April/May 2011

Current news can be found at: saahpc.org