Astrophysical Algorithms on Novel HPC Systems

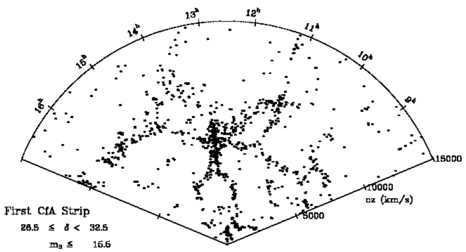
Robert J. Brunner, Volodymyr V. Kindratenko
University of Illinois at Urbana-Champaign
rb@astro.uiuc.edu, kindr@ncsa.uiuc.edu

Objectives

- **Demonstrate the practical use of novel computing technologies, such as those based on Field-Programmable Gate Arrays (FPGAs) and Graphics Processing Units (GPUs), for advanced astrophysical algorithms and applications involving very large data sets**
- **Make the developed data analysis tools available to NASA research community**

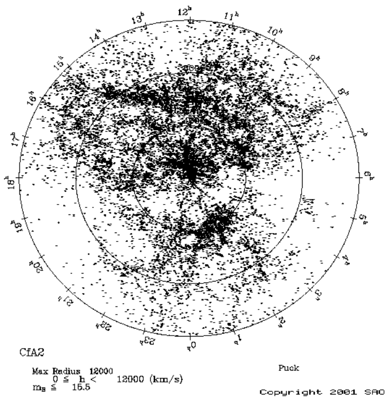
Digit{ized|al} Sky Surveys

From Data Drought to Data Flood



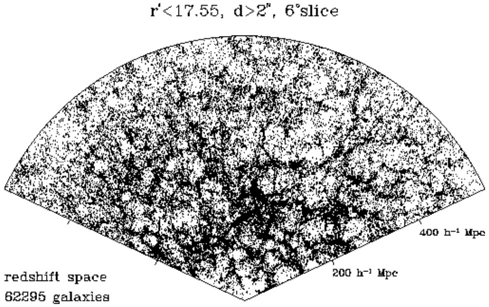
1977-1982
First CfA Redshift Survey

spectroscopic observations of 1,100 galaxies



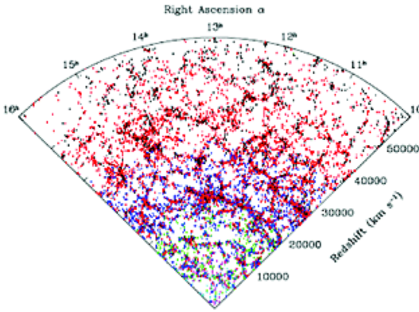
1985-1995
Second CfA Redshift Survey

spectroscopic observations of 18,000 galaxies



2000-2005
Sloan Digital Sky Survey I

spectroscopic observations of 675,000 galaxies



2005-2008
Sloan Digital Sky Survey II

spectroscopic observations of 869,000 galaxies

Sources: http://www.cfa.harvard.edu/~huchra/zcat/
http://zebu.uoregon.edu/~imamura/123/images/
http://www.sdss.org/

Example Analysis: Angular Correlation

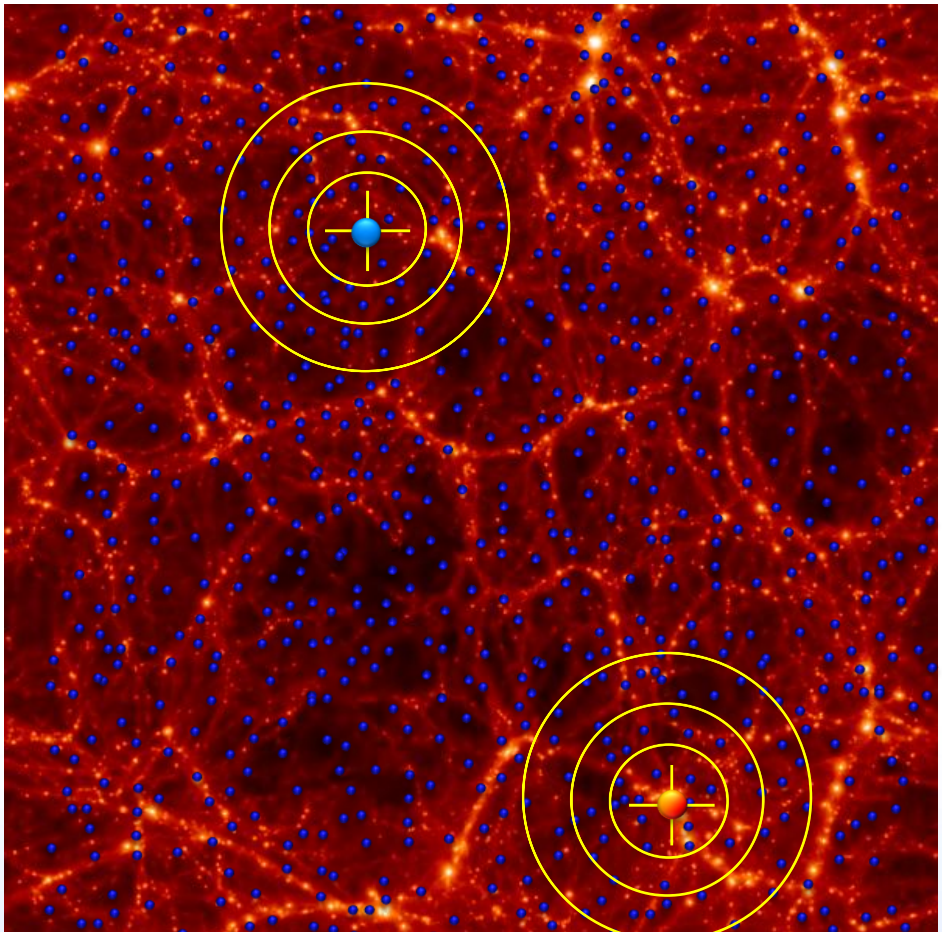


Image source: http://astro.berkeley.edu/~mwhite/

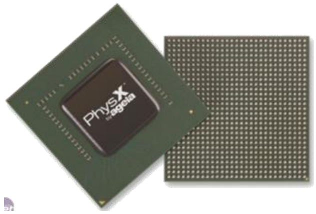
- **TPACF (ω(θ)) is the frequency distribution of angular separations θ between celestial objects in the interval (θ, θ + δθ)**
  - θ is the angular distance between two points
- **Blue points (random data) are, on average, randomly distributed, red points (observed data) are clustered**
  - Random (blue) points: ω(θ)=0
  - Observed (red) points: ω(θ)>0
- **Can vary as a function of angular distance, θ (yellow circles)**
  - Blue: ω(θ)=0 on all scales
  - Red: ω(θ) is larger on smaller scales
- **Computed as**

$$\omega(\theta) = \frac{\frac{1}{n_D^2} \cdot DD(\theta) - \frac{2}{n_D n_R} \sum DR_i(\theta)}{\frac{1}{n_R^2} \sum RR_i(\theta)} + 1$$

Special-Purpose Processors

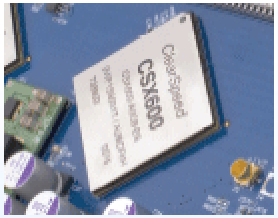
- **Field-Programmable Gate Arrays (FPGAs)**
  - Digital signal processing, embedded computing

- **Graphics Processing Units (GPUs)**
  - Desktop graphics accelerators

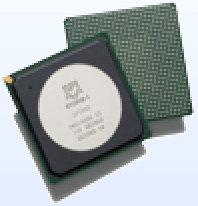


- **Physics Processing Units (PPUs)**
  - Desktop games accelerators

- **Sony/Toshiba/IBM Cell Broadband Engine**
  - Game console and digital content delivery systems



- **ClearSpeed accelerator**
  - Floating-point accelerator board for compute-intensive applications



- **Stream Processor**
  - Digital signal processing

Why not HPC Systems?

- **The gap between the application performance and the peak system performance increases**
  - Few applications can utilize high percentage of microprocessor peak performance, but even fewer applications can utilize high percentage of the peak performance of a multiprocessor system
- **Computational complexity of scientific applications increases faster than the hardware capabilities used to run the applications**
  - Science and engineering teams are requesting more cycles than HPC centers can provide
- **I/O bandwidth and clock wall put limits on computing speed**
  - Computational speed increasing faster than memory or network latency is decreasing
  - Computational speed is increasing faster than memory bandwidth
  - The processor speed is limited due to leakage current
  - Storage capacities increasing faster than I/O bandwidths
- **Building and using larger machines becomes more and more challenging**
  - Increased space, power, and cooling requirements
    - ~$1M+ per year in cooling and power costs for moderate sized systems
  - Application fault-tolerance becomes a major concern

Summary of Year 1 Progress

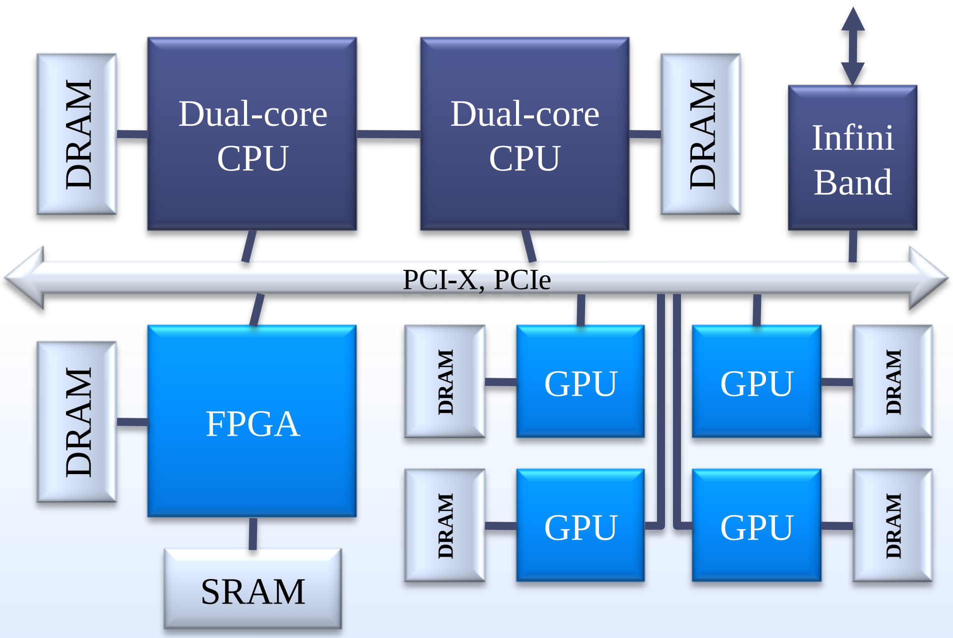
- **Two-point angular correlation algorithm implemented on SRC-6 reconfigurable computer**
  - 2 GFLOPS on an FPGA vs. 80 MFLOPS on a CPU
  - 24x speedup over a 2.8 GHz Intel Xeon
  - 3.2% of power of the CPU-only based system
  - V. Kindratenko, R. Brunner, A. Myers, *Dynamic load-balancing on multi-FPGA systems: a case study*, In Proc. 3rd Annual Reconfigurable Systems Summer Institute - RSSI'07, 2007
- **Two-point angular correlation algorithm implemented on SGI RASC RC100 reconfigurable module**
  - V. Kindratenko, R. Brunner, A. Myers, *Mitrion-C Application Development on SGI Altix 350/RC100*, In Proc. IEEE Symposium on Field-Programmable Custom Computing Machines - FCCM'07, 2007
- **Instance based classification algorithm**
  - Reference implementation of the n-nearest neighbor kd-tree based classification algorithm

Conclusions from Year 1

- **Novel ways of computing, such as reconfigurable computing, offer a possibility to accelerate astrophysical algorithms beyond of what is possible on today's mainstream systems, but**
  - Such systems are expensive and
  - Are not easy to program
- **We should look at architectures based on commodity accelerators, e.g., GPUs**

NCSA's Heterogeneous Cluster

- **16 compute nodes**
  - 2 dual-core 2.4 GHz AMD Opterons, 8 GB of memory
  - 4 NVIDIA Quadro 5600 GPUs, each with 1.5 GB of memory
  - Nallatech H101-PCIX FPGA accelerator, 16 MB SRAM, 512 MB SDRAM



Summary of Year 2 Progress

- **Extended two-point angular correlation function implementation from previous year to work on a cluster consisting of multi-core SMP nodes using Message Passing Interface**
- **Implemented compute kernel of the cluster application on a Nallatech H101 FPGA application accelerator board using DIME-C language and DIMEtalk API and expanded the application to utilize FPGA accelerators available in all cluster nodes**
- **Experimented with the two-point angular correlation compute kernel on the NVIDIA GPU G80 platform using CUDA development tools**
- **Extended our reference *n*-nearest neighbor *kd*-tree based implementation of the instance based classification code to work on a multi-core SMP system via pthreads and tested it with multi-million point datasets**

GPU Results

- **Single Node Performance**
  - Dataset
    - 32K observed points
    - 100 x 32K random points
  - Analysis parameters
    - no jackknifes re-sampling
    - Min angular distance: 1º
    - Max angular distance: 100º
    - Bins per decade of scale: 5
  - GPU vs. CPU speedup
    - 25x for 32K dataset
    - 22x for 8K dataset
    - 60x for optimized kernel that works only with small datasets

- **Observations**
  - Single-precision floating-point
    - Cannot perform calculations for angular separations below 1 degree
  - 32-bit integers
    - Overflow in bin counts
    - Requires additional storage and code to deal with overflow
  - Read-after-write hazard is very costly to work around

FPGA Results

- **Single Node**
  - Dataset
    - 97K observed points
    - 100 x 97K random points
  - Analysis parameters
    - 10 jackknifes re-sampling
    - Min angular distance: 0.01 arcmin
    - Max angular distance: 10000 arcmin
    - Bins per decade of scale: 5
  - One CPU core
    - 44,259 seconds
  - Four CPU cores per node
    - 11,159 seconds (3.9x speedup)
  - One FPGA
    - 7,166 seconds (6.2x, 1.6x)
- **8-node Cluster**
  - Dataset
    - 97K observed points
    - 100 x 97K random points
  - Analysis parameters
    - 10 jackknifes re-sampling
    - Min angular distance: 0.01 arcmin
    - Max angular distance: 10000 arcmin
    - Bins per decade of scale: 5
  - One CPU core per node
    - 5,428 seconds
  - Four CPU cores per node
    - 1,449 seconds (3.8x speedup)
  - One FPGA per node
    - 881 seconds (6.2x, 1.6x)

Conclusions from Year 2

- **As architectures based on commodity accelerators are becoming readily available, they too offer a possibility to accelerate astrophysical algorithms beyond of what is possible on today's mainstream systems**
  - At a substantially smaller cost as compared to highly tuned and specialized systems such as SRC-6
  - Still suffer from some of the hardware limitations and difficulties with programming

Year 2 Outreach Highlights

- **NSF STCI grant: *Investigating Application Analysis and Design Methodologies for Computational Accelerators***
- **V. Kindratenko, C. Steffen, R. Brunner, *Accelerating scientific applications with reconfigurable computing*, IEEE/AIF Computing in Science and Engineering, vol. 9, no. 5, pp. 70-77, 2007**
- **T. El-Ghazawi, D. Buell, K. Gaj, V. Kindratenko, *Reconfigurable Supercomputing tutorial*, IEEE/ACM Supercomputing, November 12, 2007, Reno NV.**
- **Reconfigurable Systems Summer Institute (RSSI), July 2007, NCSA, Urbana, IL**

Future Work

- **With the introduction of double-precision floating-point GPU chips later this year, we will research and implement the two-point angular correlation kernel on double-precision GPUs**
- **Extend our existing cluster application to simultaneously take advantage of the multi-core chips as well as the Nallatech H101 FPGA accelerators and NVIDIA GPUs**
- **Investigate the use of FPGAs and GPUs to accelerate the *kd*-tree based range search algorithm used in the *n*-nearest neighbor classifier**

Reconfigurable Systems Summer Institute (RSSI) 2008

- **July 7-10, 2008**
- **National Center for Supercomputing Applications (NCSA), Urbana, Illinois**
- **Organized by**

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