Mechanisms for exploiting heterogeneous computing:
Harnessing hundreds of GPUs and CPUs

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Collaborators

- Richard B. Sessions, Amaurys Avila Ibarra
  - University of Bristol, Biochemistry
  - Developers of the docking algorithm and original serial code
- James Price (port to OpenCL)
  - University of Bristol, Computer Science
- Tsuyoshi Hamada, Felipe Cruz (GPUs)
  - University of Nagasaki, Japan

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The Microelectronics Group at the University of Bristol

http://www.cs.bris.ac.uk/Research/Micro/

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The team

Prof David May

Dr Jose Nunez-Yanez

Prof Dhiraj Pradhan

Simon McIntosh-Smith
Head of Group

Dr Kerstin Eder

Dr Dinesh Pamunuwa

Dr Simon Hollis

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7 tenured staff, 6 research assistants, 16 PhD students

Research Group expertise

Energy Aware COmputing (EACO):

- Multi-core and many-core computer architectures
- Algorithms for heterogeneous architectures (GPUs, OpenCL)
- Electronic and Optical Network on Chip (NoC)
- Reconfigurable architectures (FPGA)
- Design verification (formal and simulation-based), formal specification and analysis
- Silicon process variation
- Fault tolerant design (hardware and software)
- Design methodologies, modelling & simulation of MNT based structures and systems

Industrial Collaboration

- The Bristol Microelectronics Group partners with most of Europe's chip industry:
  - ARM
  - Imagination Technology
  - NVIDIA (Icera)
  - Broadcom
  - STMicro, ST-Ericsson
  - Toshiba
  - Infineon
  - Gnodal
  - Picochip
  - And many more…
- XMOS is a successful CPU spin-out from the group
- Global partners include AMD, Intel, IBM, …

Molecular docking

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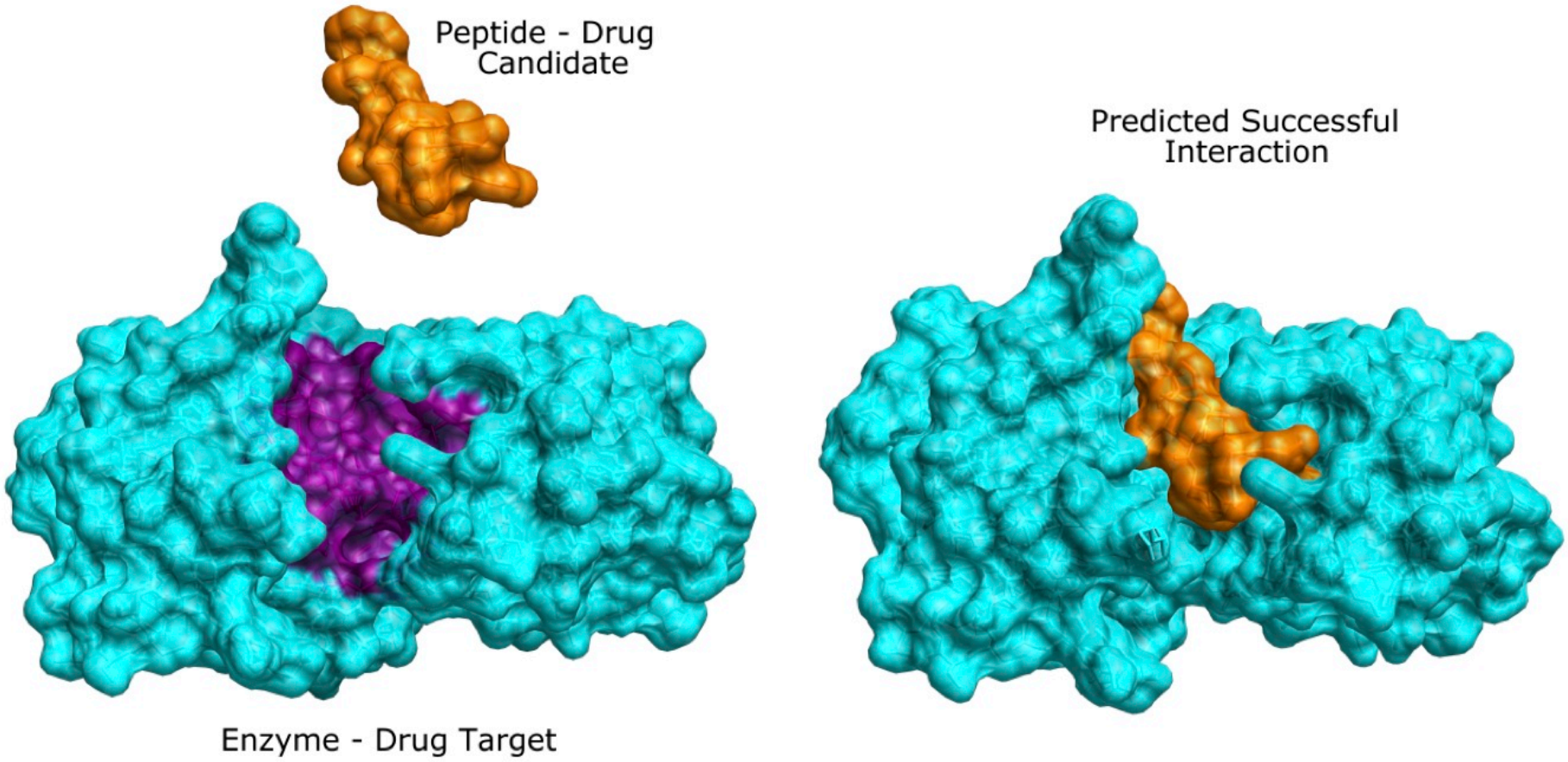
Molecular docking



Proteins typically O(1000) atoms
Ligands typically O(100) atoms

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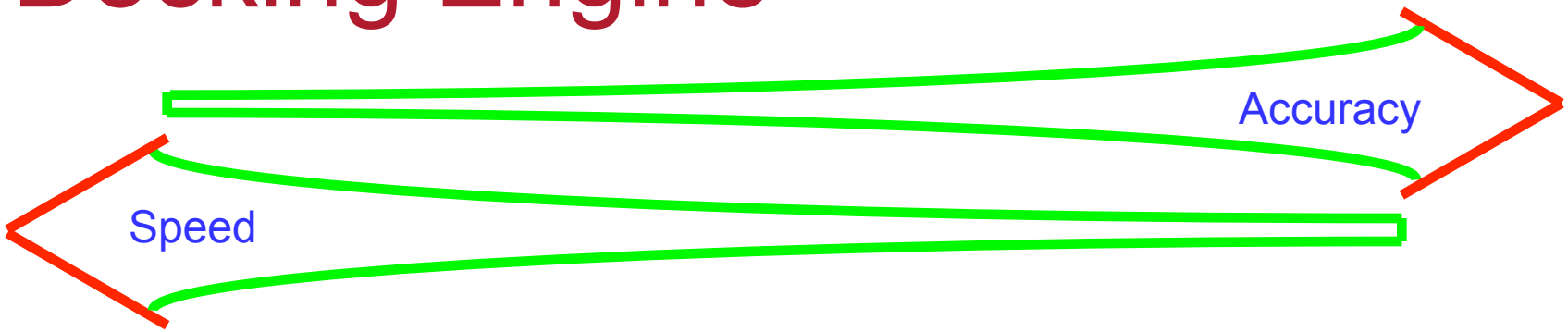
BUDE: Bristol University Docking Engine



Typical docking scoring functions	Empirical Free Energy Forcefield **BUDE**	Free Energy calculations MM[1,2] QM/MM[3]
Entropy:		
solvation	**No**	**Yes**	**Yes**
configurational	**Approx**	**Approx**	**Yes**
Electrostatics	**?**	**Approx**	**Yes**
All atom	**No**	**Yes**	**Yes**
Explicit solvent	**No**	**No**	**Yes**

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1. MD Tyka, AR Clarke, RB Sessions, J. Phys. Chem. B 110 17212-20 (2006)
2. MD Tyka, RB Sessions, AR Clarke, J. Phys. Chem. B 111 9571-80 (2007)
3. CJ Woods, FR Manby, AJ Mulholland, J. Chem. Phys. 128 014109 (2008)

Empirical Free Energy Function (atom-atom)

$$\Delta G_{\text{ligand binding}} = \sum_{i=1}^{N_{\text{protein}}} \sum_{j=1}^{N_{\text{ligand}}} f(x_i, x_j)$$

Parameterised using experimental data†

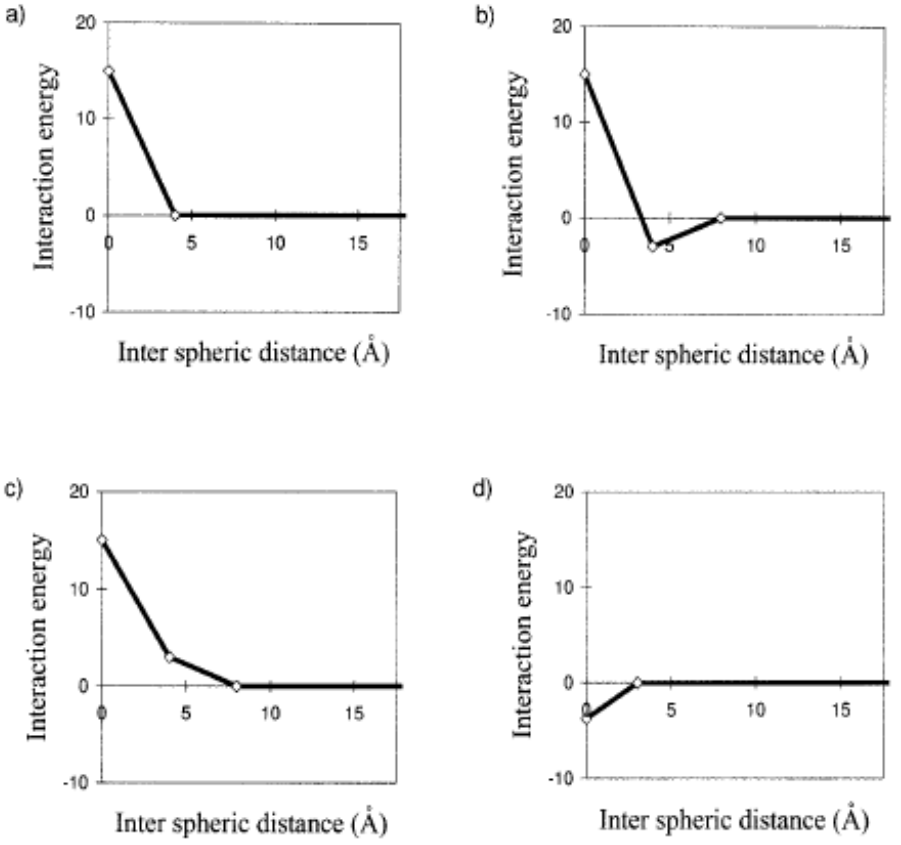

Fig. 1. Inter-residue sphere-sphere interaction energy functions of the force field. a: Between two polar spheres, or between a backbone sphere and any other non hydrogen-bonding sphere. b: Between two non-polar spheres. c: Between a non-polar sphere and a polar sphere. d: Between a hydrogen bond donor sphere and a hydrogen bond acceptor sphere.

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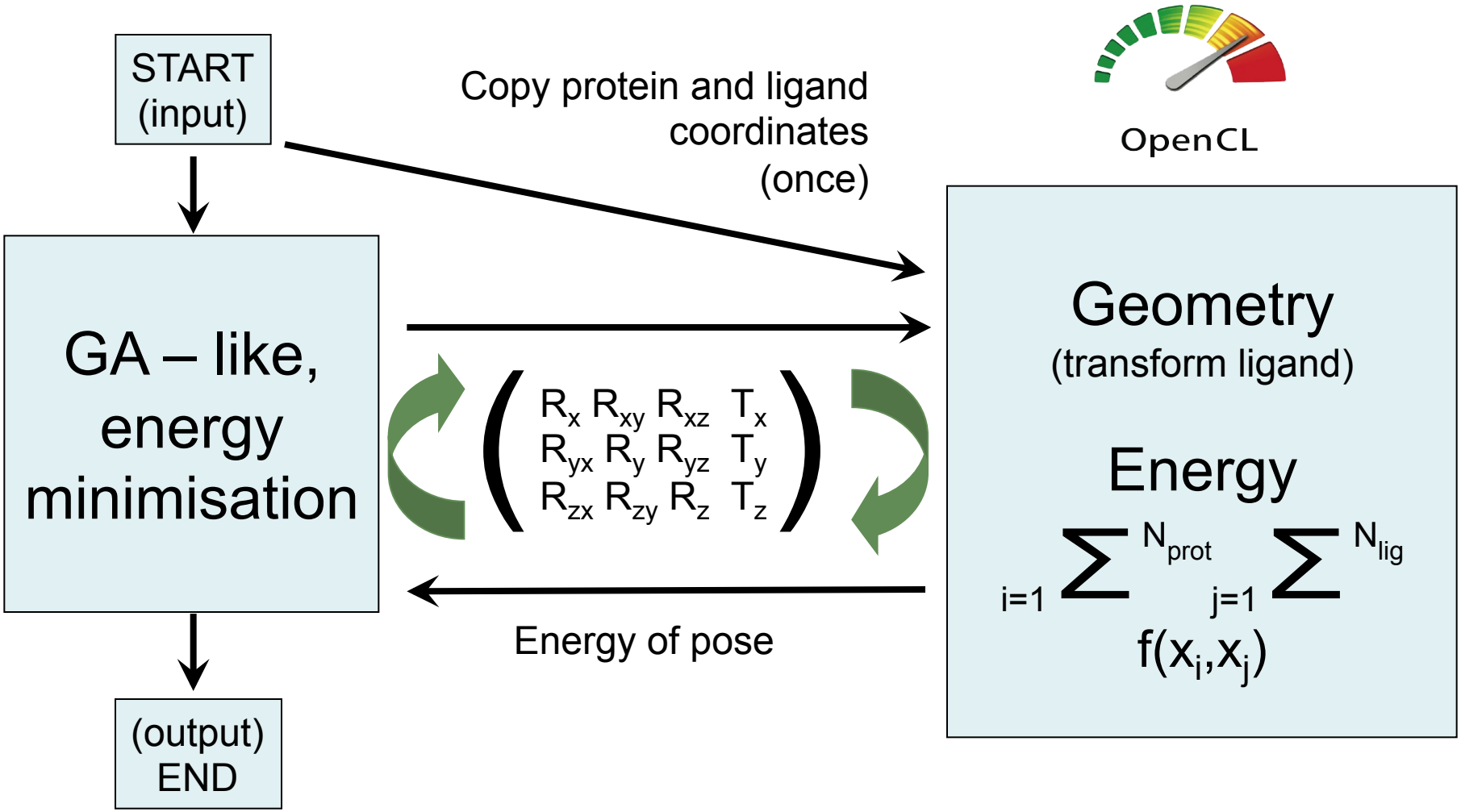
† N. Gibbs, A.R. Clarke & R.B. Sessions, "Ab-initio Protein Folding using Physicochemical Potentials and a Simplified Off-Lattice Model", Proteins 43:186-202,2001

BUDE Acceleration with OpenCL



"Benchmarking energy efficiency, power costs and carbon emissions on heterogeneous systems", Simon McIntosh-Smith, Terry Wilson, Amaurys Avila Ibarra, Jon Crisp and Richard B.Sessions, The Computer Journal, September 12th 2011. DOI: 10.1093/comjnl/bxr091

Multiple levels of parallelism

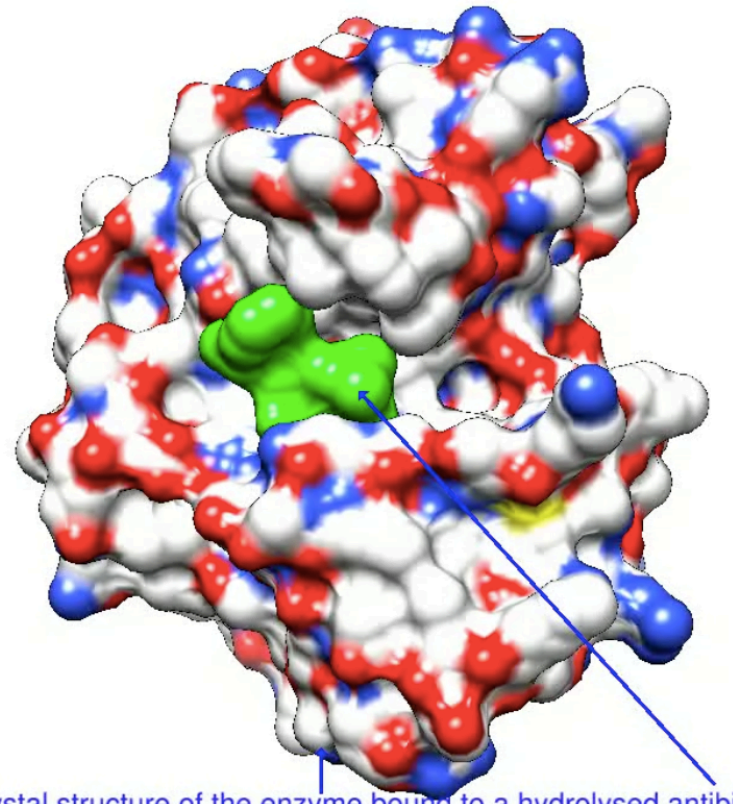
- $O(10^8)$ conformers from $O(10^7)$ ligands
- $O(10^5)$ poses per conformer (ligand)
- $O(10^3)$ atoms per protein
- $O(10^2)$ atoms per ligand (drug molecule)

- Conformers all independent
- Poses can all be independent, but there are benefits in grouping all poses of one conformer to one OpenCL device

- Parallelism strategy:
  - Distribute ligands across nodes – 10^7-way parallelism
  - All the poses of one conformer distributed across all the OpenCL devices in a node – 10^3-way parallelism
  - Each Work-Item (thread) performs an entire conformer-protein docking – 10^5 atom-atom force calculations per Work-Item

How BUDE's EMC works

NDM-1 resistance factor: An enzyme that hydrolyses antibiotics



A crystal structure of the enzyme bound to a hydrolysed antibiotic
Showing the surface (cleaved antibiotic in green)

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Experimental results

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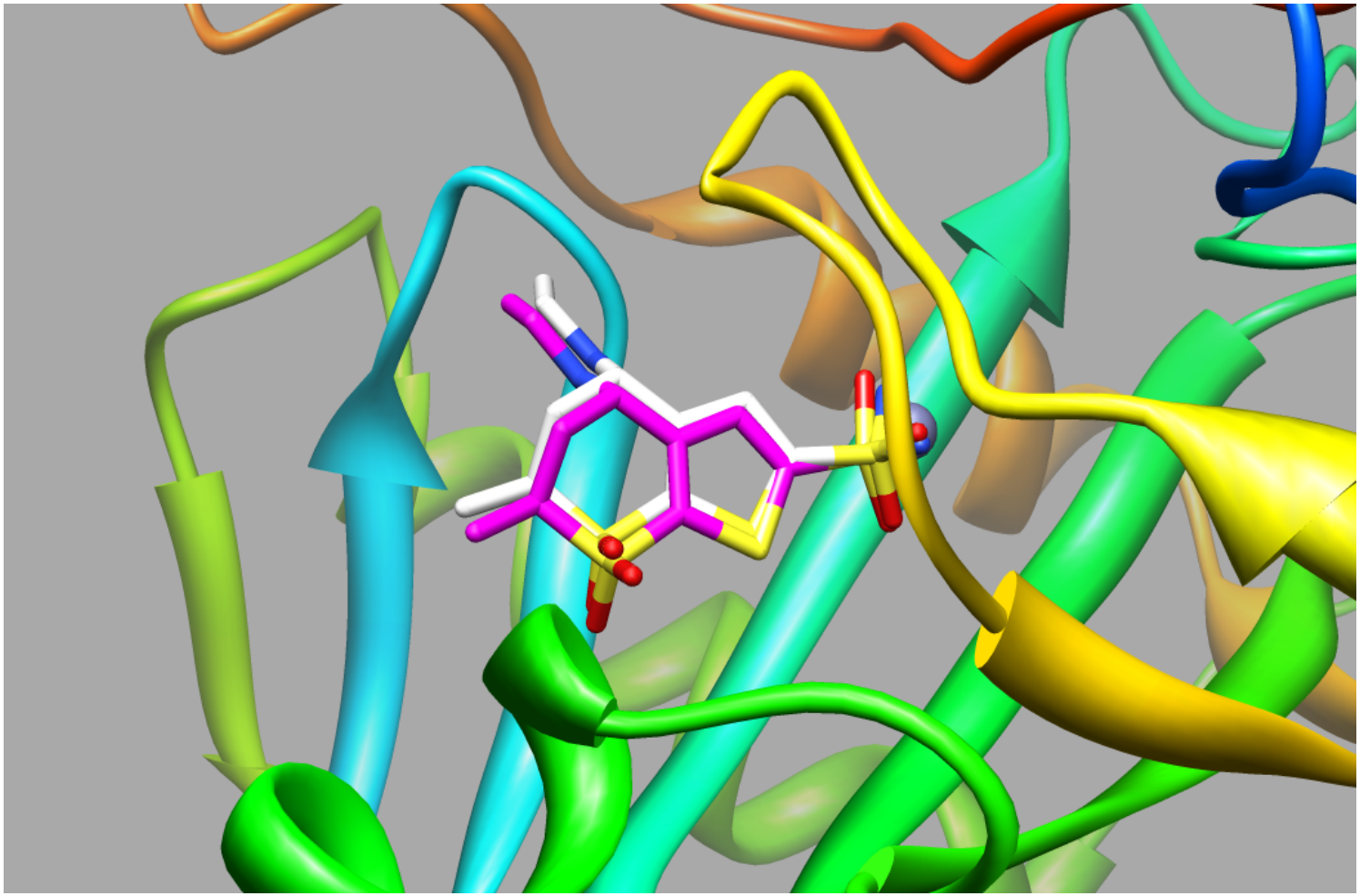
Redocking into Xray Structure



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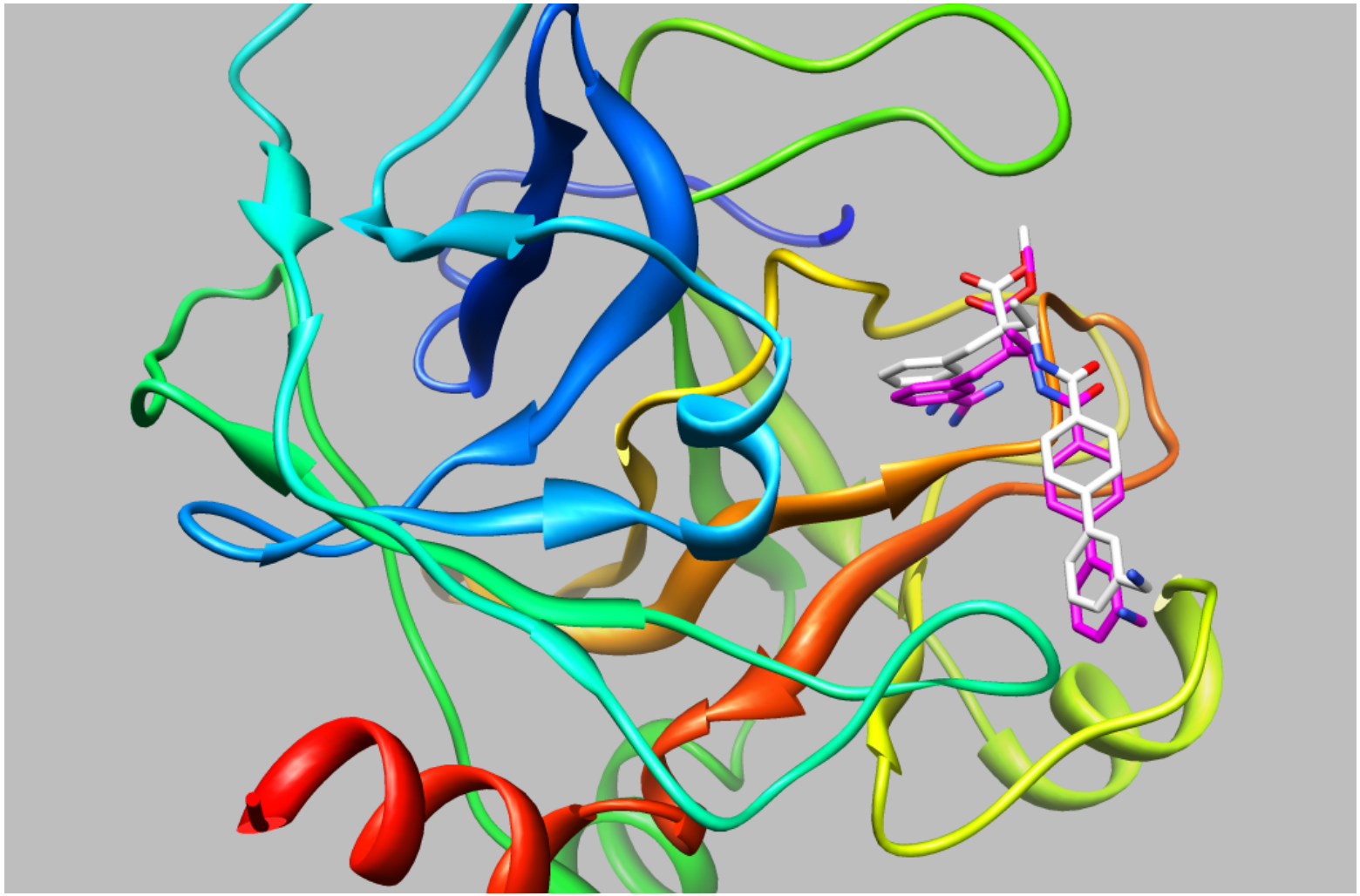
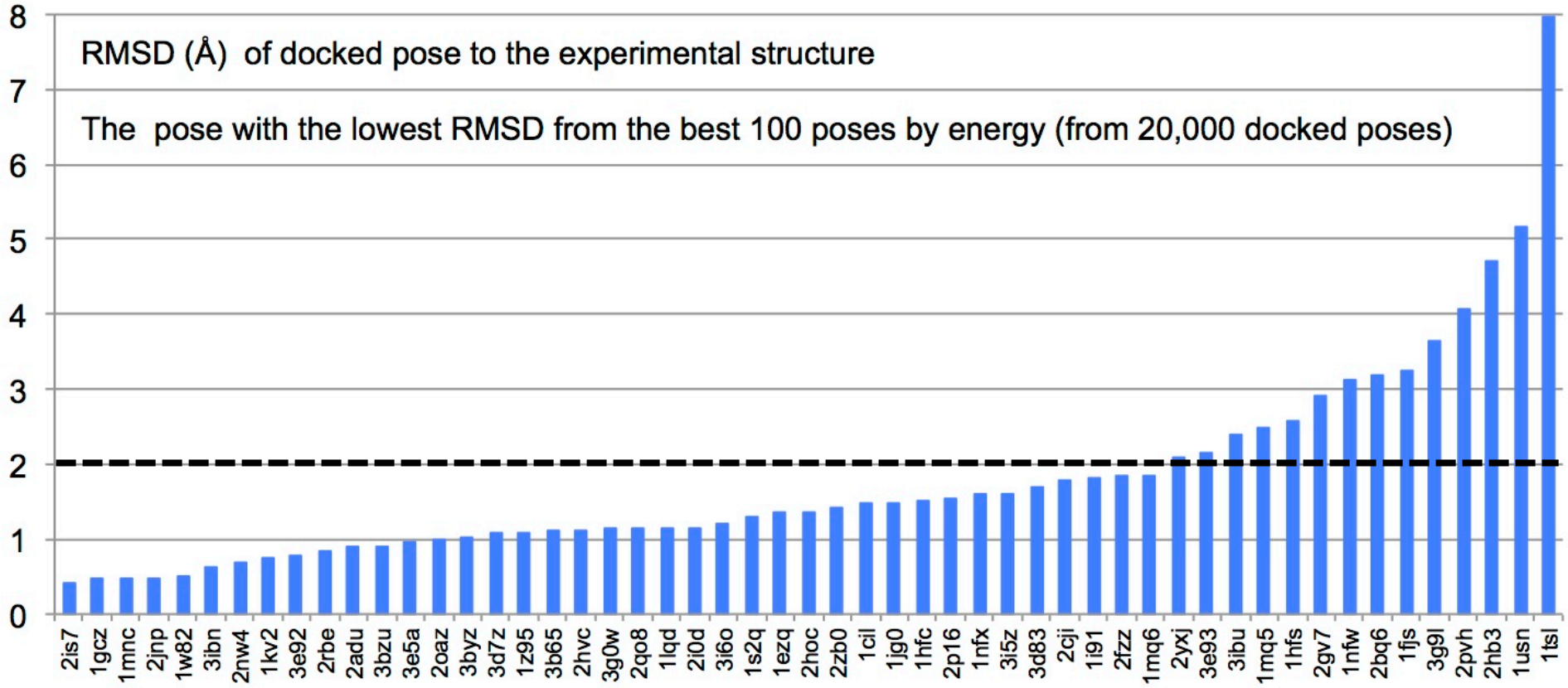
1CIL (Human carbonic anhydrase II)

Another example



1EZQ (Human Factor XA)

The science is working well



53 Experimental results from the Ligand Binding Database

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Heterogeneous Systems

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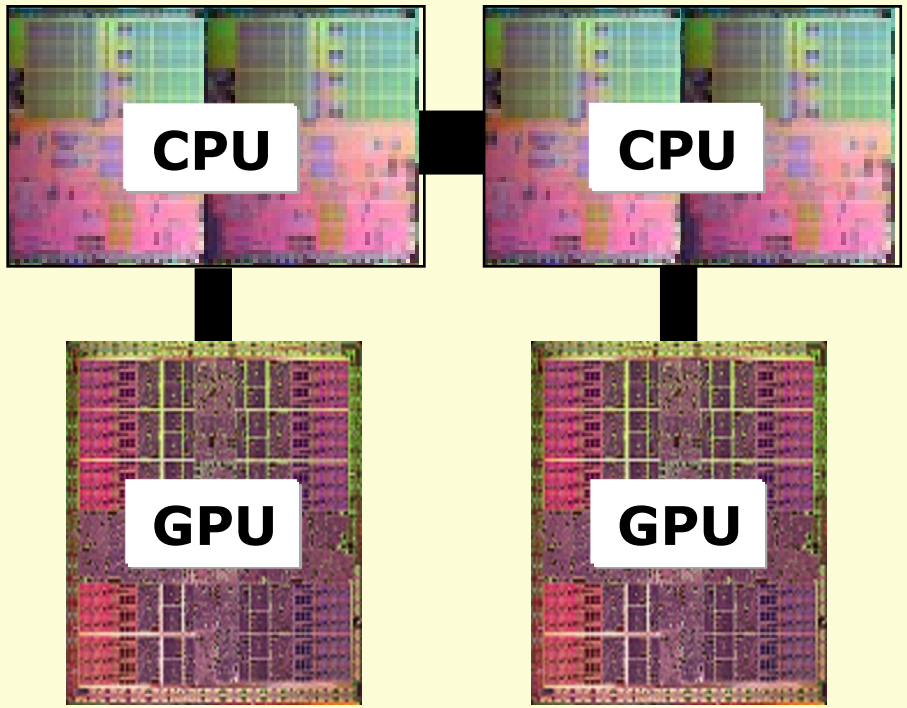
OpenCL for heterogeneous computing

A modern computer includes:

- One or more CPUs
- One or more GPUs



OpenCL (Open Compute Language) lets programmers write a single portable program that uses ALL resources in the heterogeneous platform

Kinds of Heterogeneous Systems

SuperMicro 4 GPU workstation

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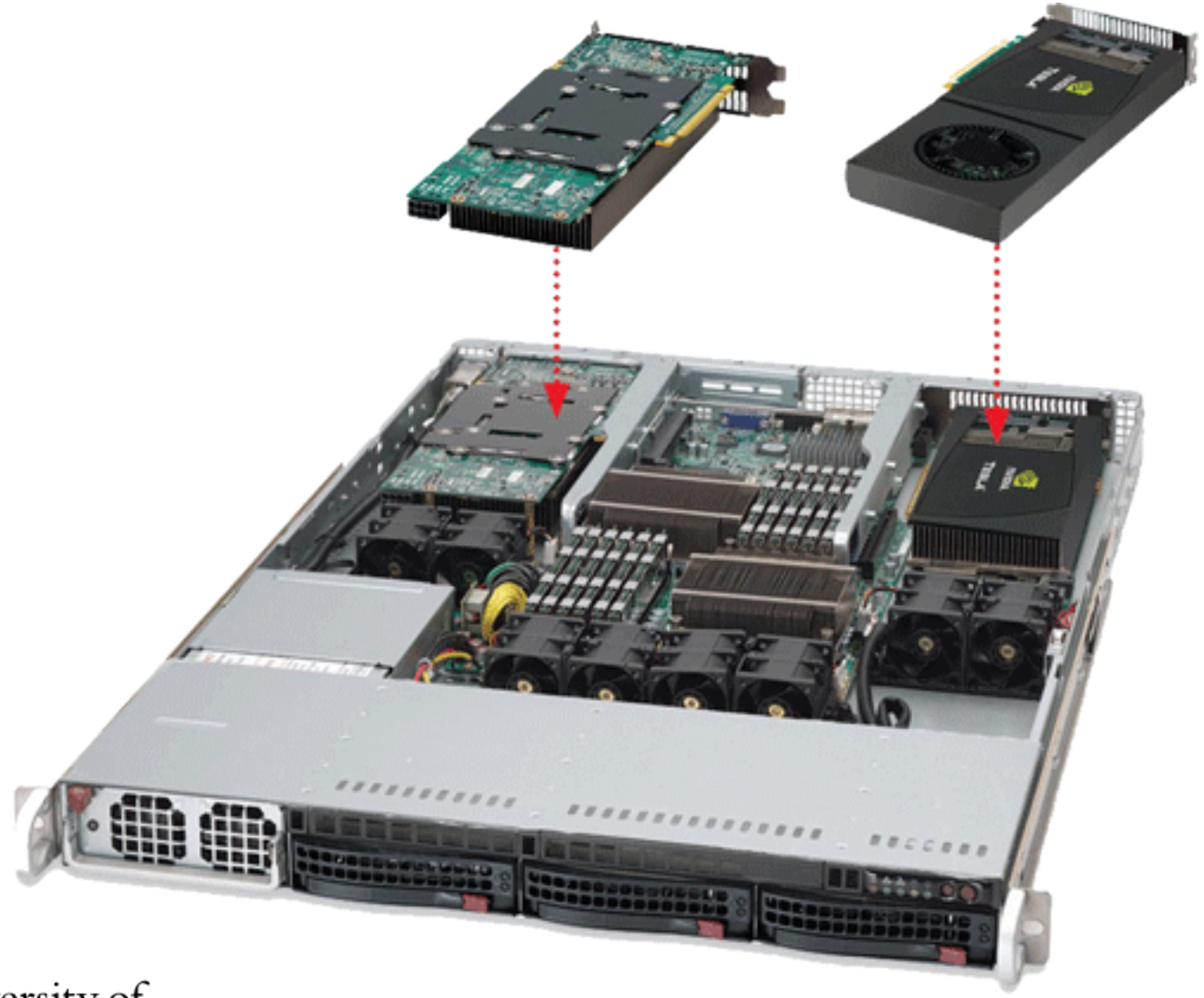
Kinds of Heterogeneous Systems



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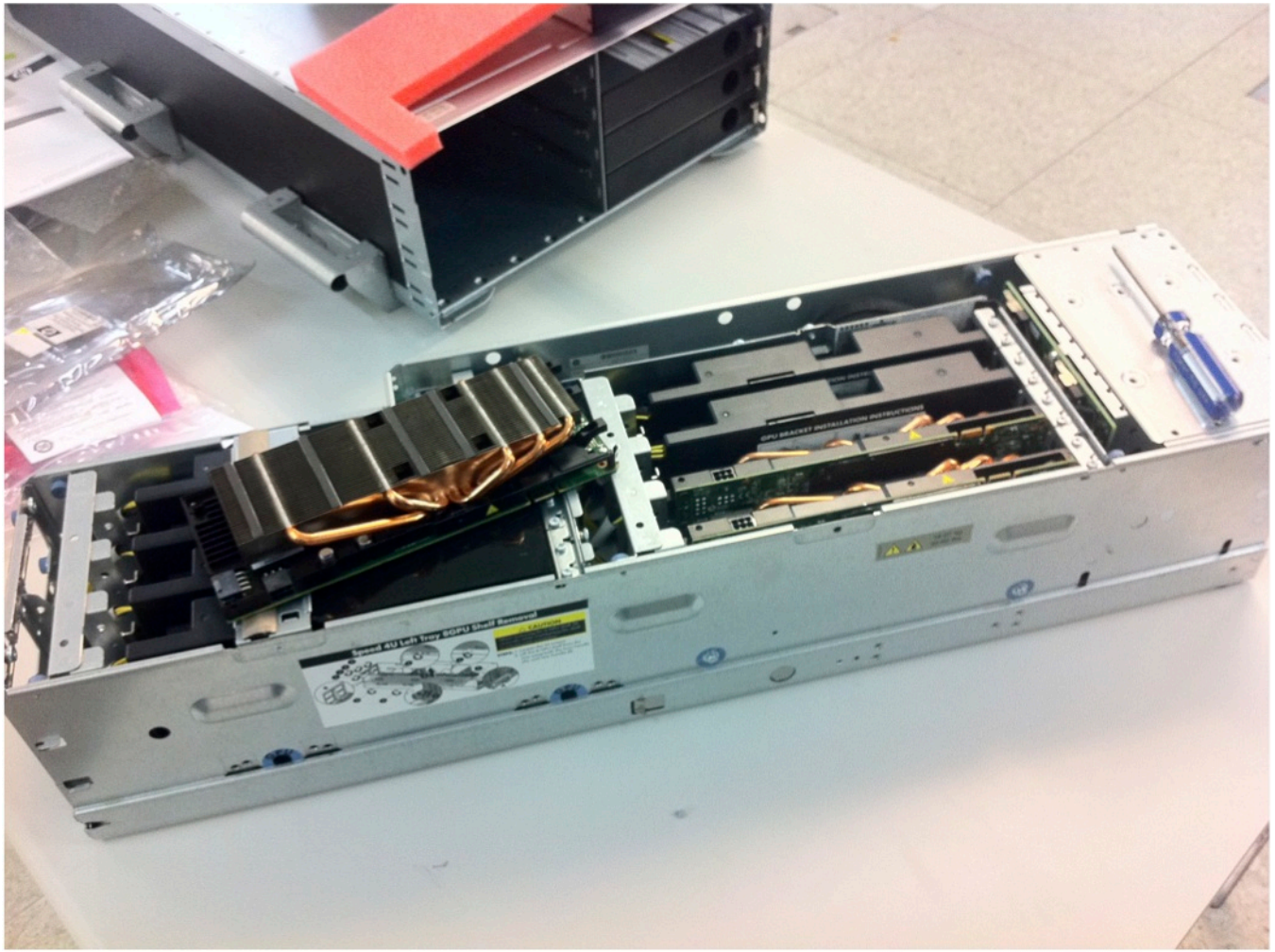
SuperMicro GPU servers – 2 GPUs in 1U

Kinds of Heterogeneous Systems



HP SL390 – 2 CPUs, 8 GPUs in half width 4U

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Kinds of Heterogeneous Systems

Dell PowerEdge C410x – 16 GPUs in 4U

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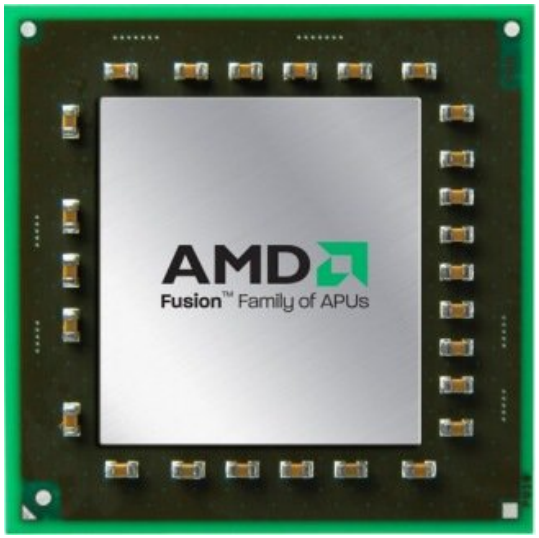
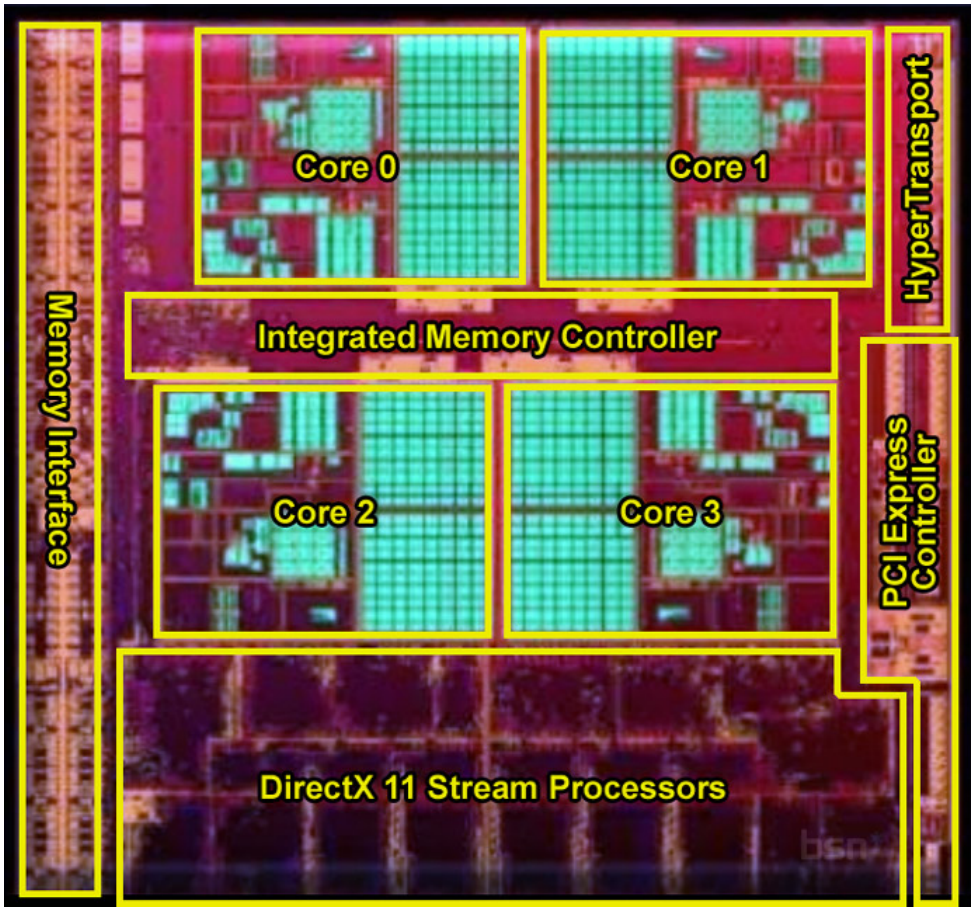
Kinds of Heterogeneous Systems





AMD Llano Fusion APUs

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Kinds of Heterogeneous Systems

Intel Core2 Duo CPU P8600 @ 2.40GHz,
NVIDIA GeForce 9400M integrated GPU, NVIDIA GeForce 9600M GT discrete GPU

Benchmark results

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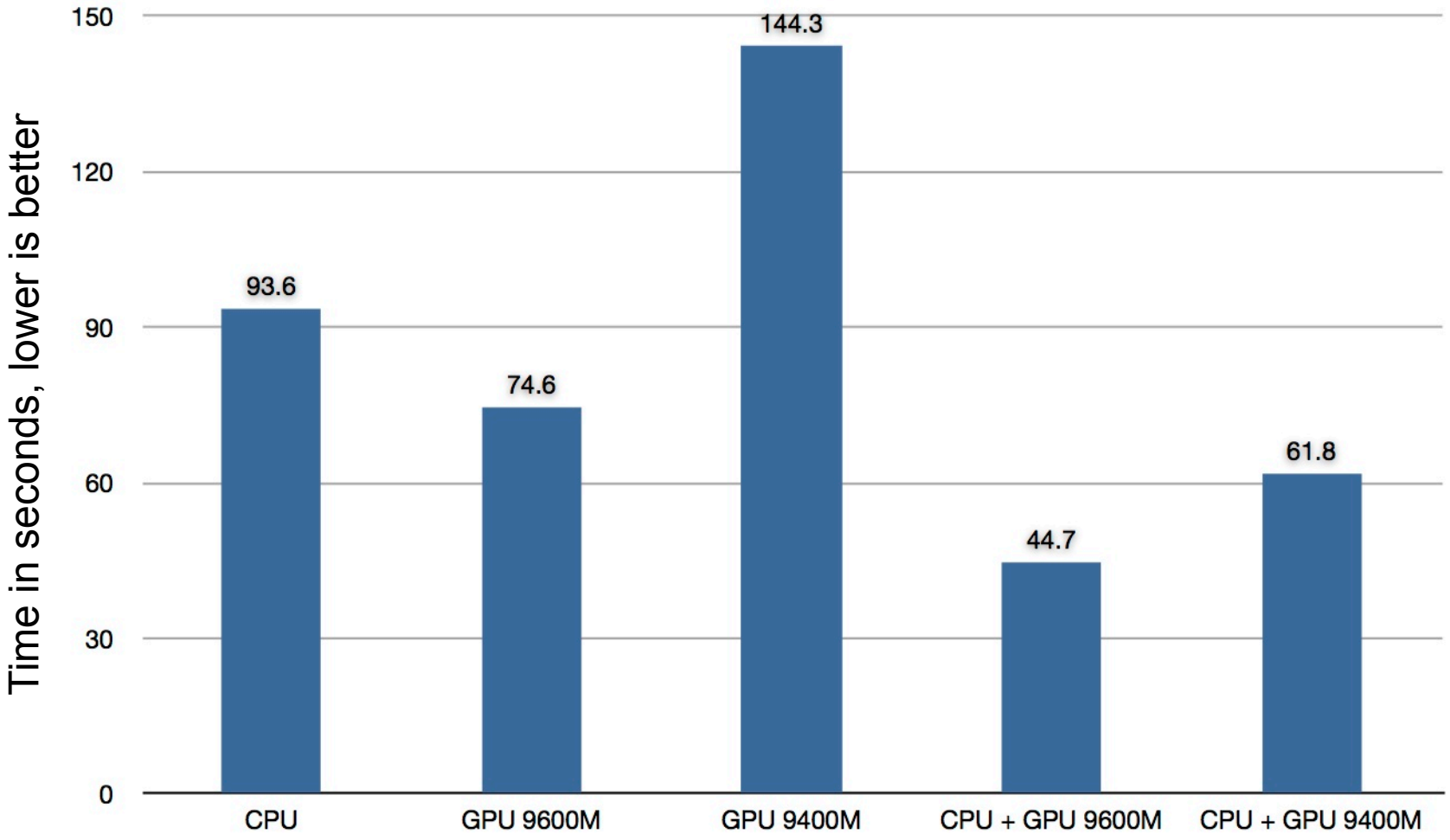
BUDE's heterogeneous approach

1. Discover all OpenCL platforms/devices, including CPUs *and* GPUs
2. Run a *micro benchmark* on each device, ideally a short piece of real work
3. Load balance using micro benchmark results
4. Re-run micro benchmark at regular intervals in case load changes

Benchmarking methodology

- Use the same power measurement equipment for all the systems under test
- Watts Up? Pro meter
- Measures complete system power ‘at the wall’
- Run as fast as possible on all available resources (i.e. all cores or all GPUs simultaneously)

MacBook Pro 2009 results



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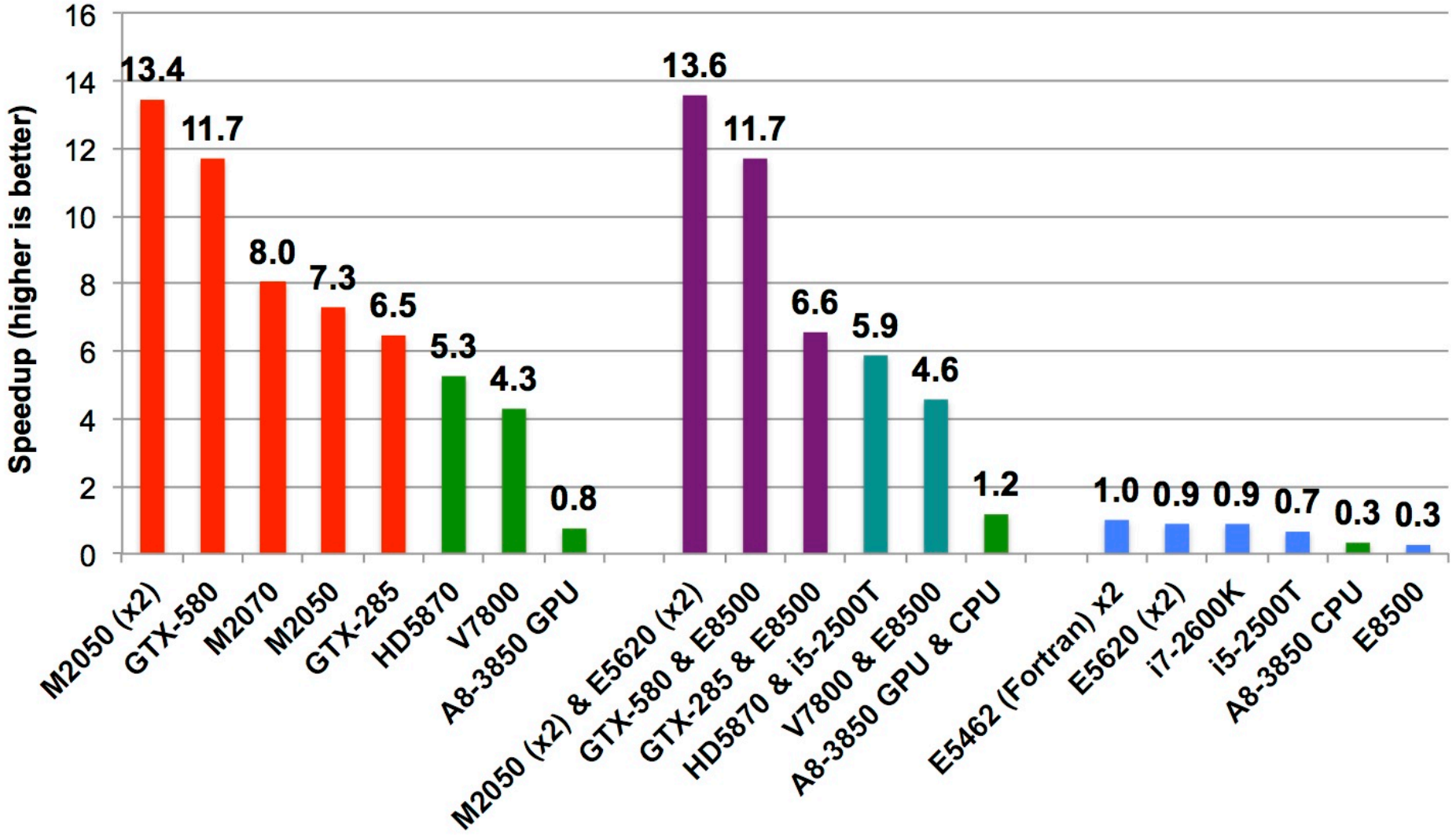
Benchmark results



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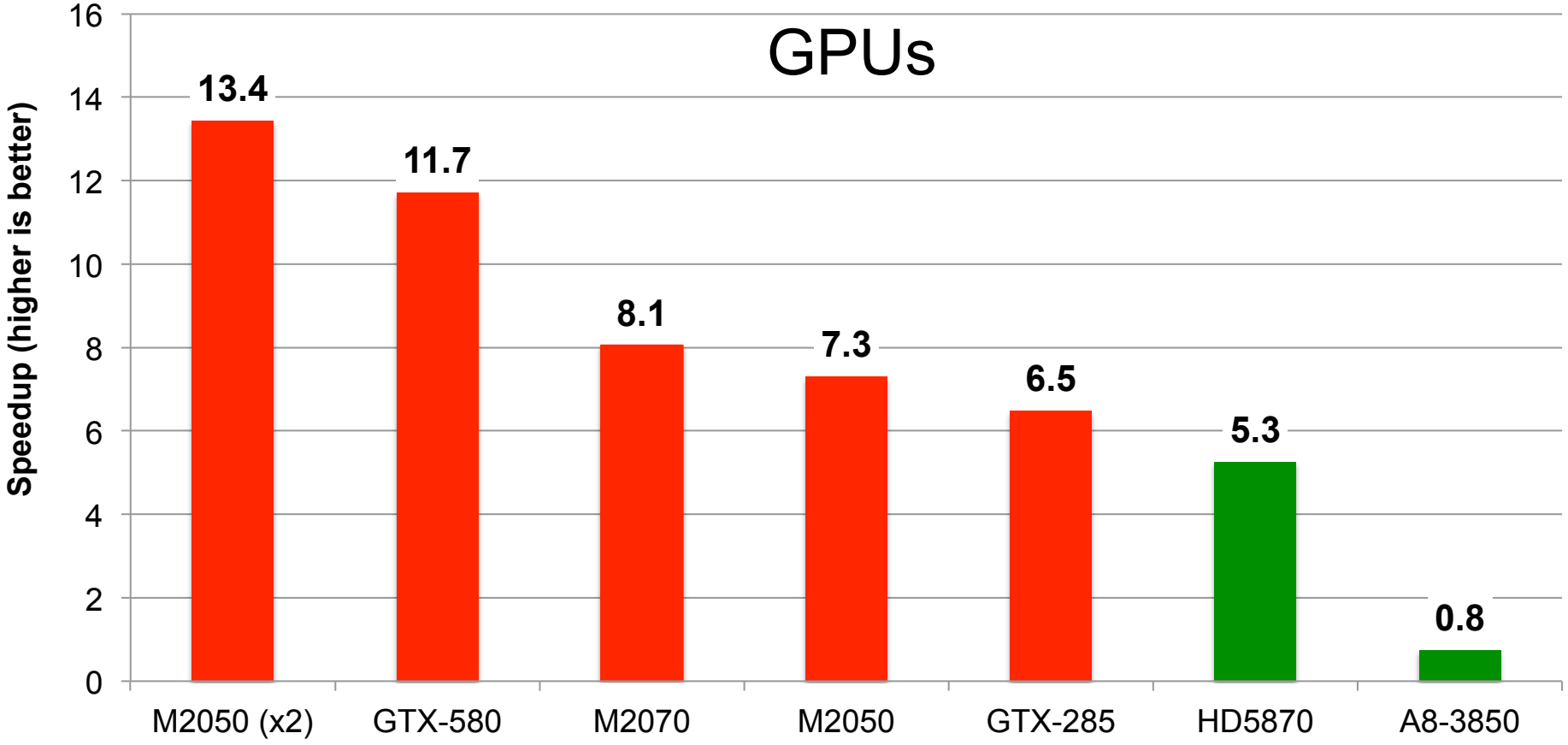
Performance results



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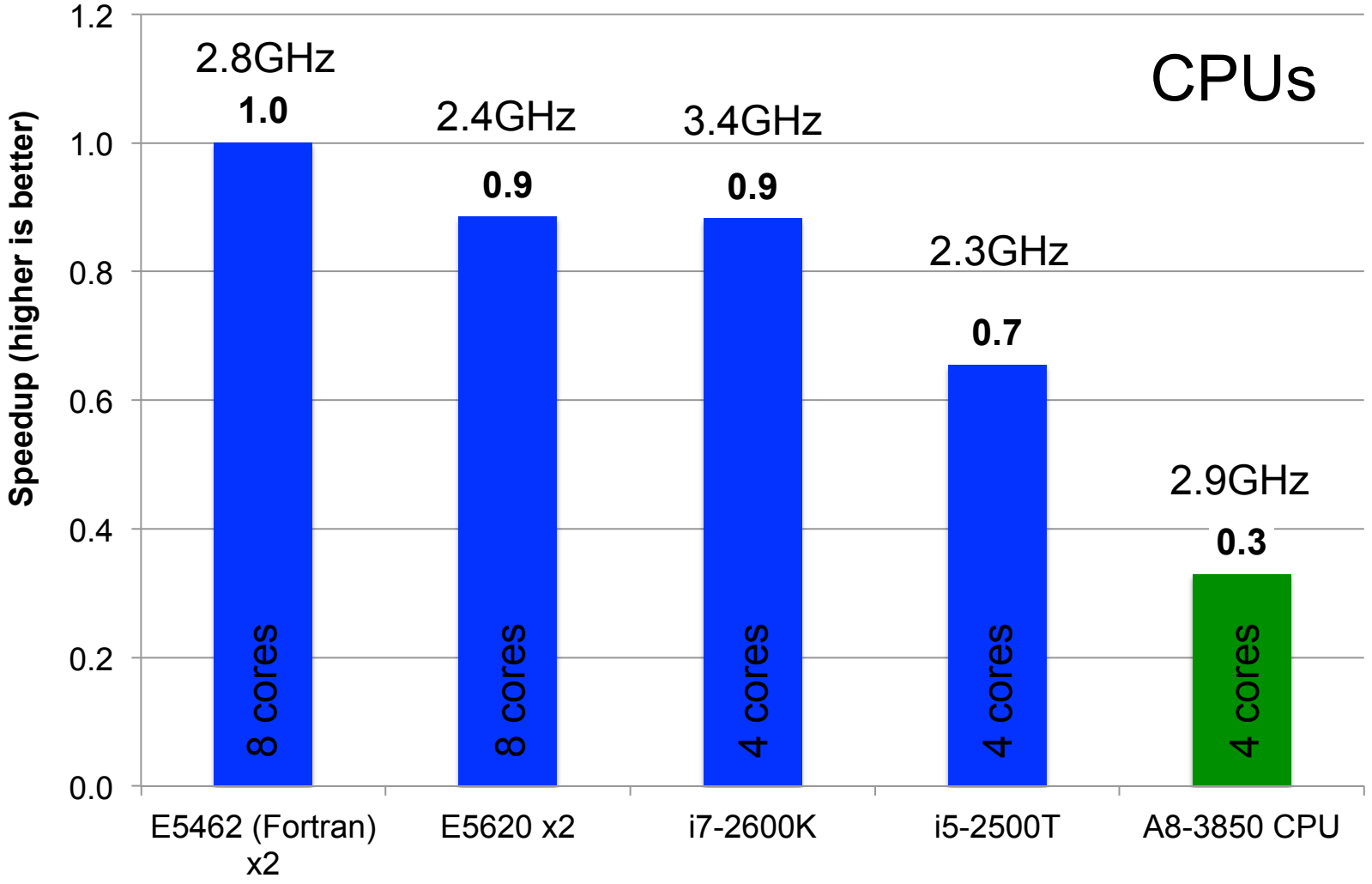
Performance results



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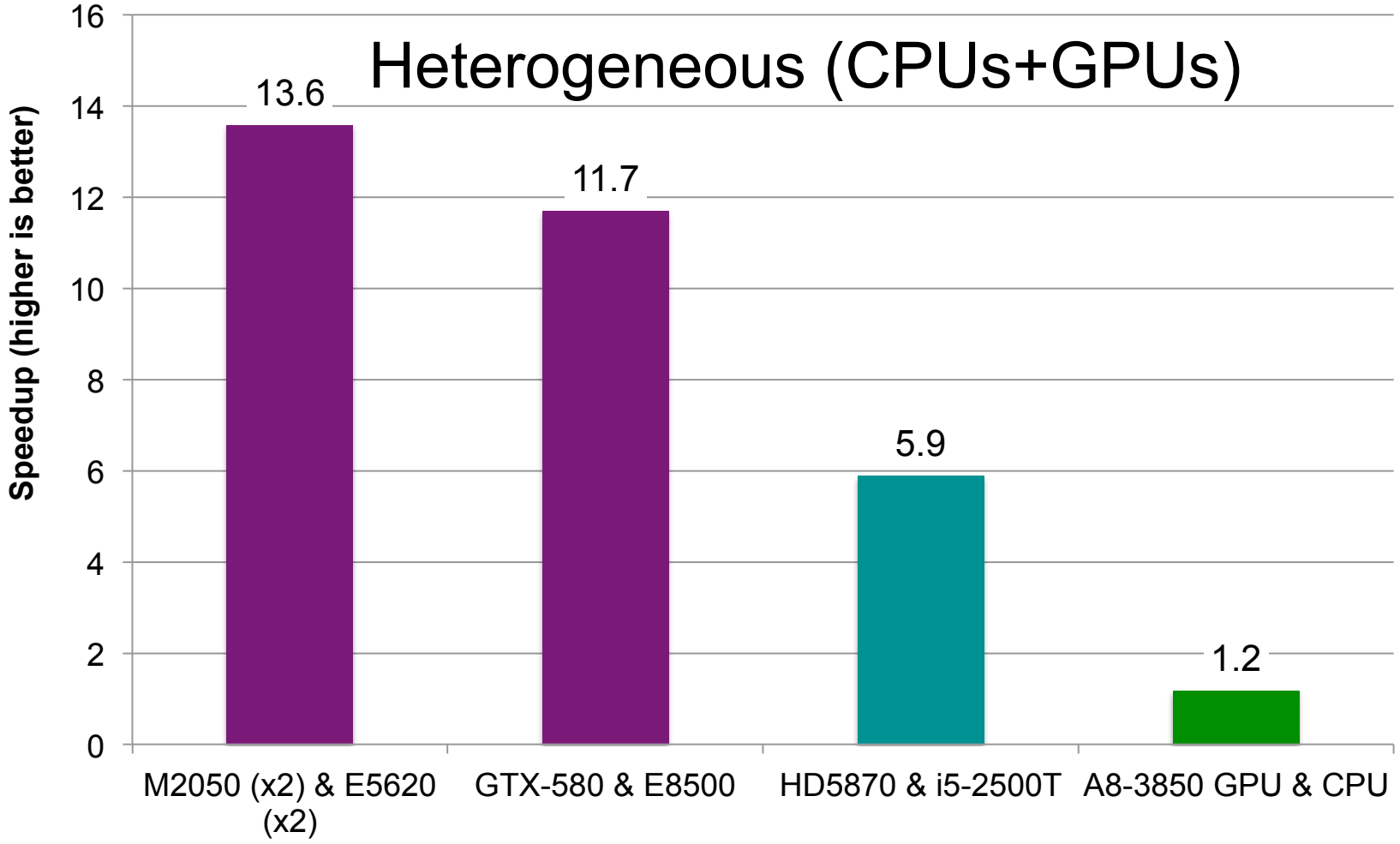
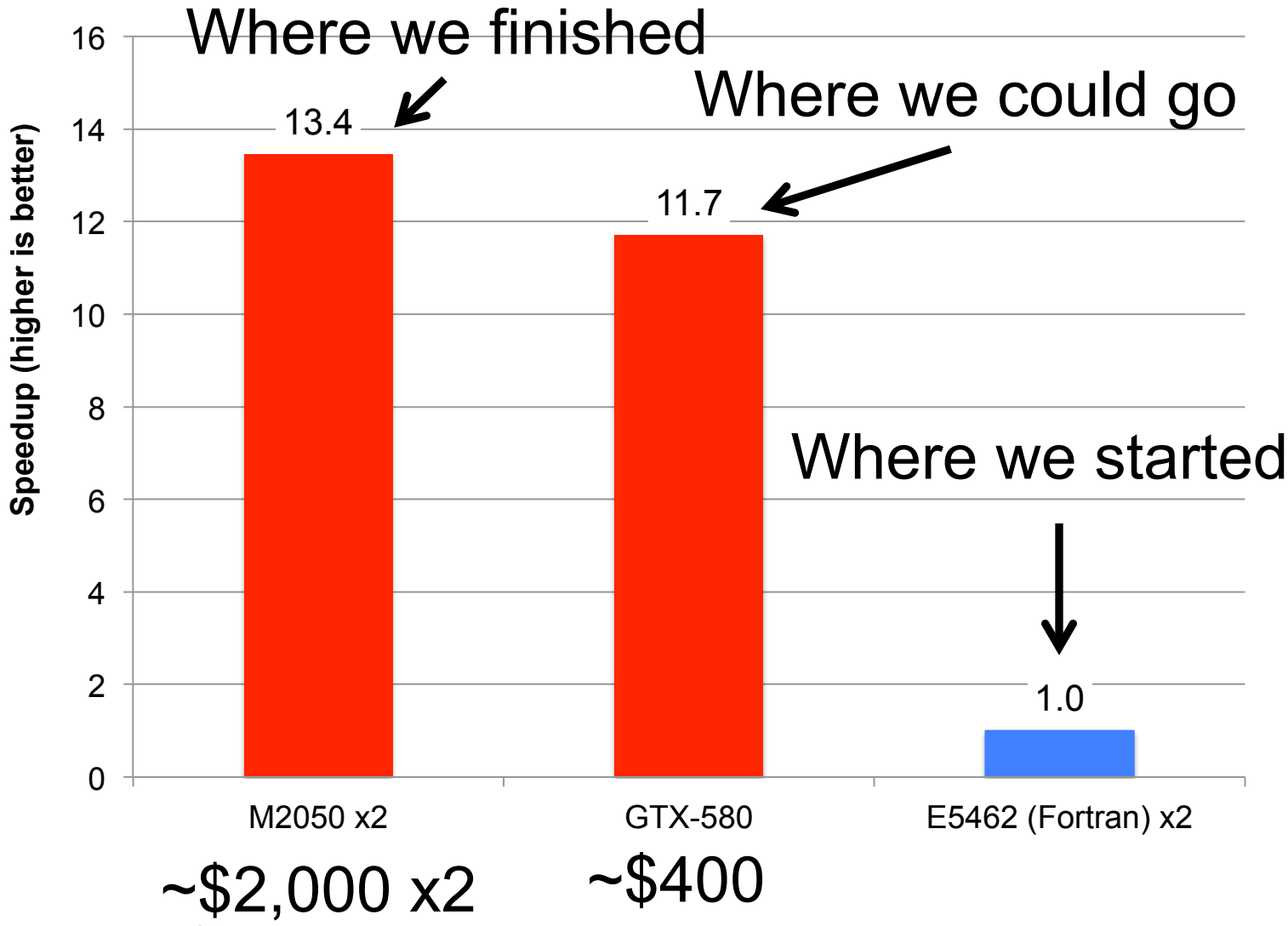
Performance results



Performance results



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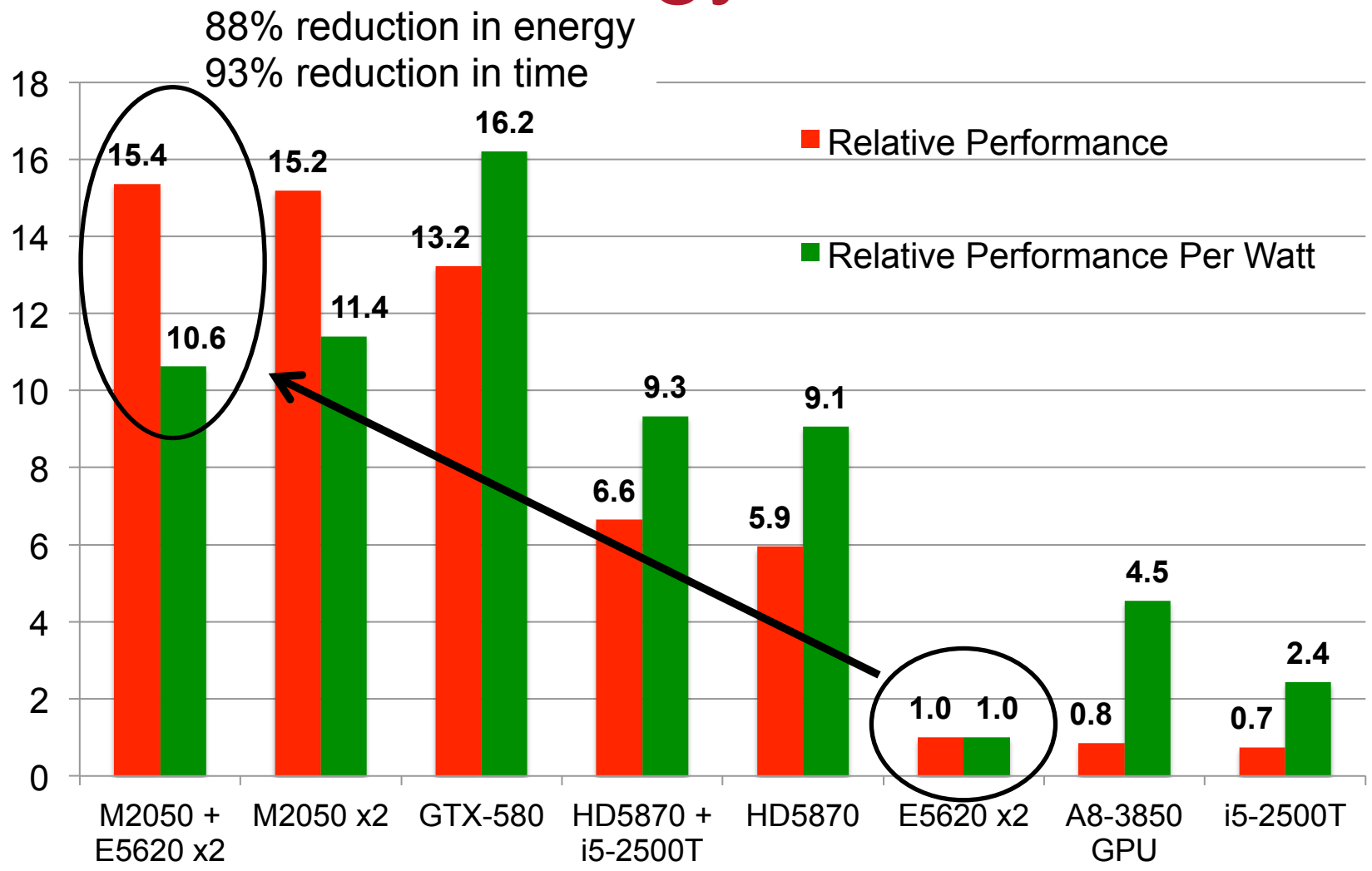
Relative energy and run-time



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Measurements are for a constant amount of work. Energy measurements are "at the wall" and include any idle components.

What does this let us do?

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Potentially save lives

New Delhi Metallo-beta-lactamase-1 (NDM-1) is an enzyme that makes bacteria resistant to antibiotics, giving rise to “superbugs”

http://news.discovery.com/human/superbug-found-in-japan.html

Discovery News > Human News > Japan Detects Antibiotic-Resistant Superbug

JAPAN DETECTS ANTIBIOTIC-RESISTANT SUPERBUG

The first case of an antibiotic-resistant "superbug" in South Asia has triggered a global health alert.

Tue Sep 7, 2010 01:03 PM ET
Content provided by AFP
(1) Comments | Leave a Comment

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Like 168 people like this. Be the first of your friends. Share 83 Tweet 51

The New Delhi metallo-lactamase-1 (NDM-1) gene has created a drug-resistant superbug. Click to enlarge this image.
iStockphoto

THE GIST

- A hospital north of Tokyo detected a drug-resistant "superbug."
- The bacterium has been identified as carrying the New Delhi metallo-lactamase-1 (NDM-1) gene.
- In August a Belgian man became the first such known fatality.

Japan on Monday said it has detected its first case of an antibiotic-resistant "superbug" that surfaced in South Asia and has triggered a global health alert.

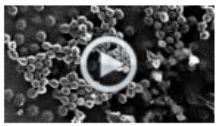
A hospital linked to the Dokkyo Medical University in Tochigi prefecture north of Tokyo detected a drug-resistant "superbug," a bacterium carrying the New Delhi metallo-lactamase-1 (NDM-1) gene, in a patient last year, a hospital official told AFP.

The case follows a warning from the World Health Organization (WHO) last month calling on global health authorities to monitor the drug-resistant superbug that is believed to have spread from India.

"A patient who came home from India, in his 50s, had fever symptoms while he was hospitalized in May last year, and after a blood test the hospital detected an antibiotics-resistant bacterium," the official said, adding that the patient fully recovered.

After examination doctors found that the bacterium contained the NDM-1 gene,

RELATED CONTENT



Take a look at how the swine flu originated and what happens once it

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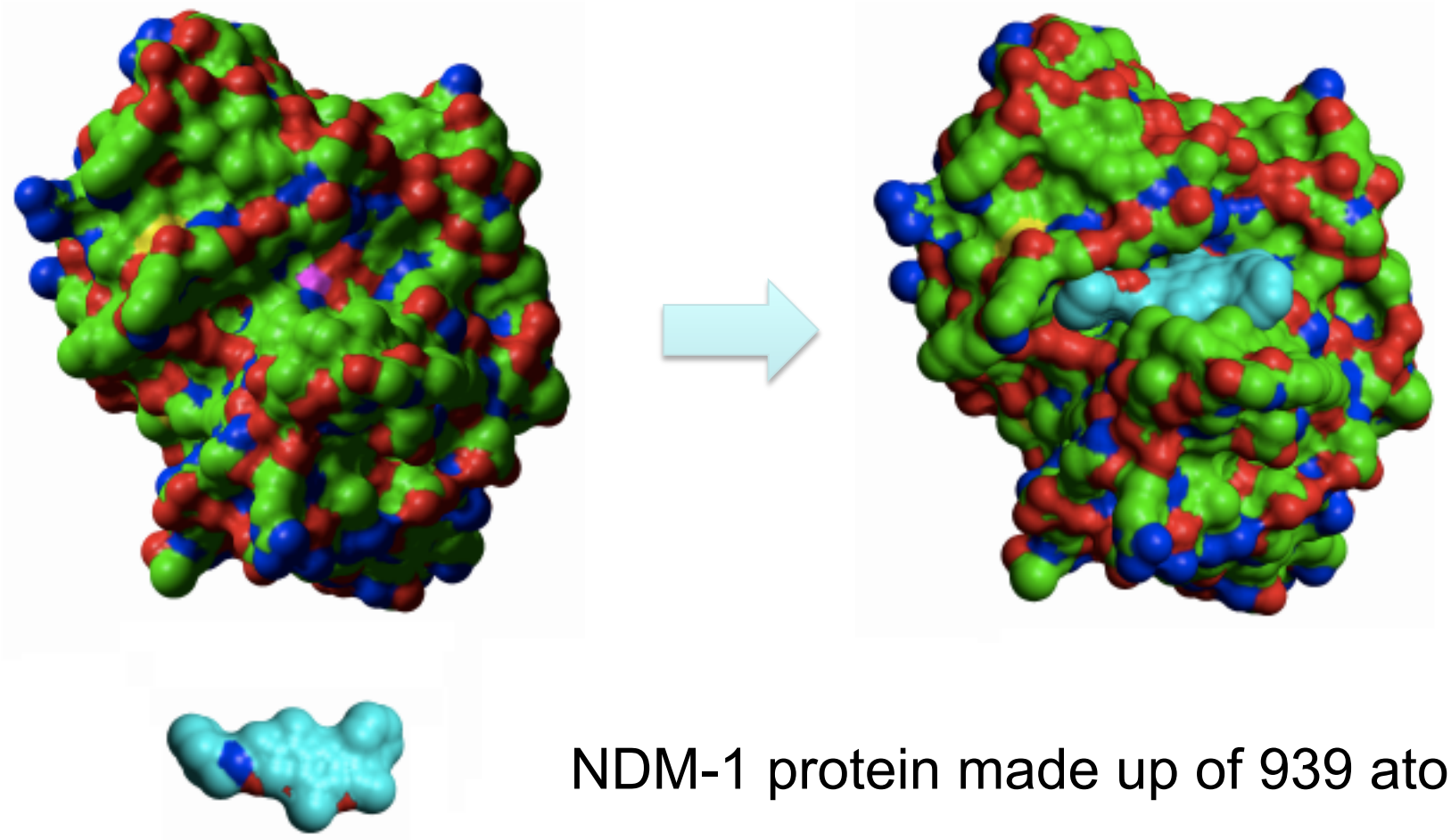
NDM-1 as a docking target



NDM-1 protein made up of 939 atoms

GPU-system DEGIMA

- Used 222 GPUs in parallel for drug docking simulations
  - ATI Radeon HD5870 (2.72 TFLOPS) & Intel i5-2500T
- ~600 TFLOPS single precision
- Courtesy of Tsuyoshi Hamada and Felipe Cruz, Nagasaki

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NDM-1 experiment

- 7.65 million candidate drug molecules, 21.8 conformers each → 166.7×10^6 dockings
- 4.168×10^{12} poses calculated
- ~98 hours actual wall-time
- Top 300 “hits” being analysed, down selecting to 10 compounds for wetlab trials

Future heterogeneous systems

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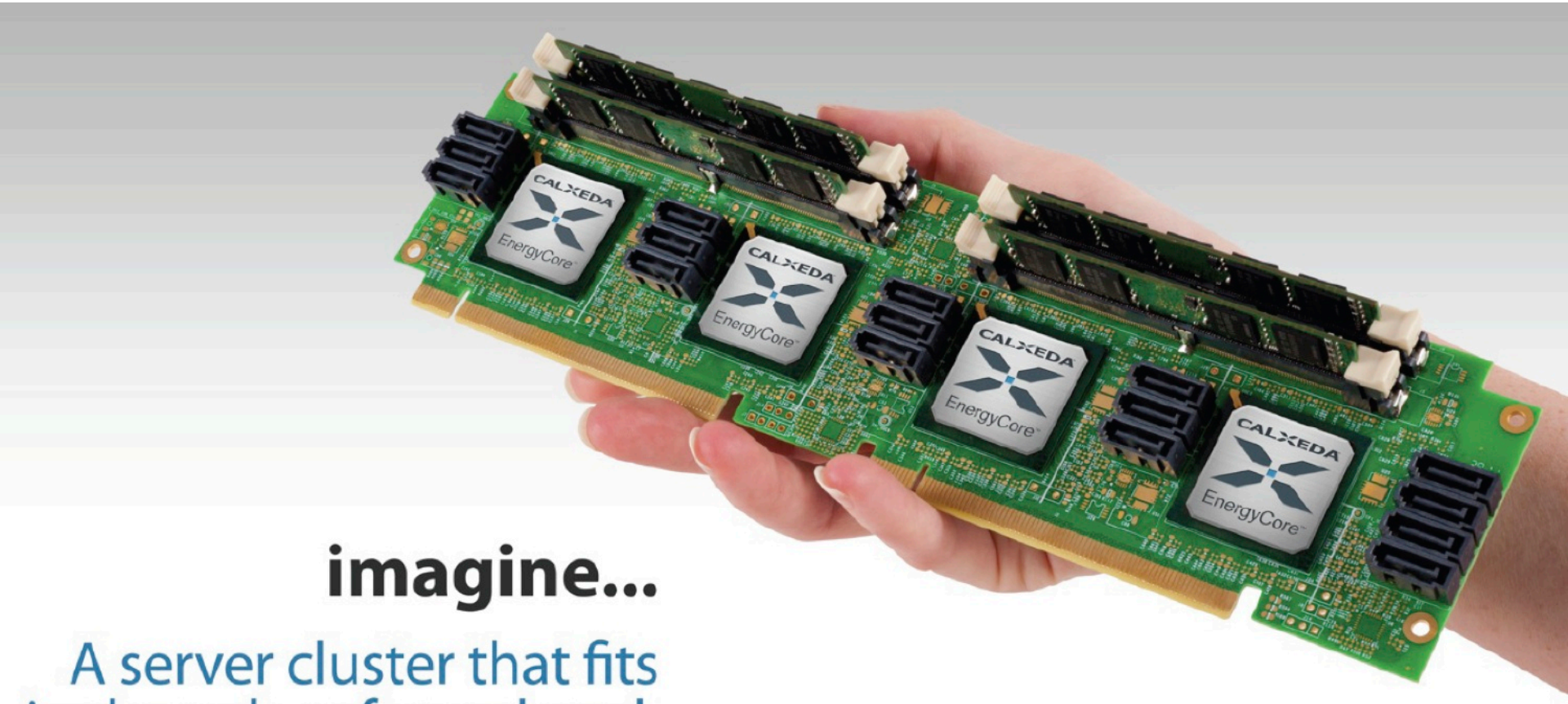
Future heterogeneous systems



imagine...

A server cluster that fits in the palm of your hand.

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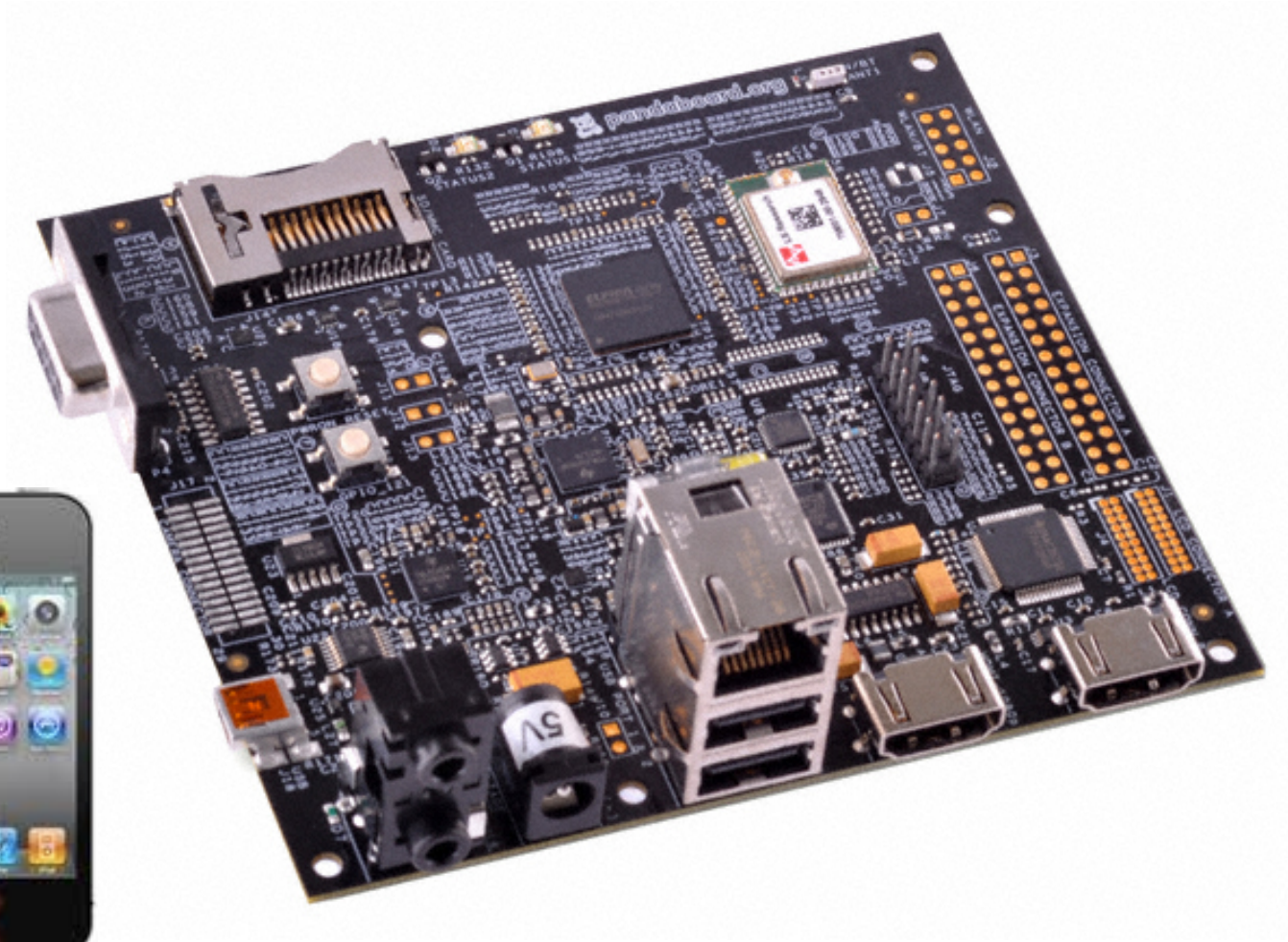
ARM Cortex Quad-core CPU @1.4GHz, 10GbE, 4GB DDR3 DRAM

Future heterogeneous systems



PandaBoard – TI OMAP4, dual core ARM, PowerVR GPU

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Future heterogeneous systems

Sony PSVita – quad core ARM, PowerVR GPU

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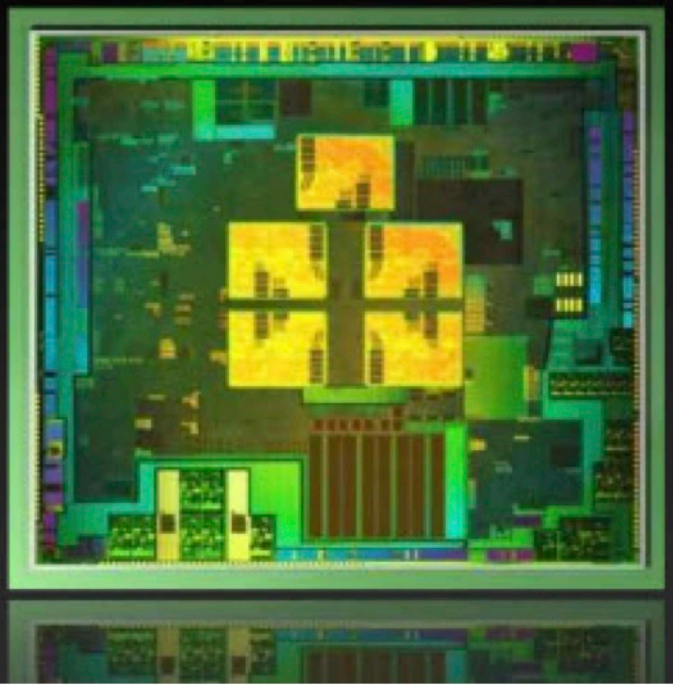
Future heterogeneous systems

Tegra 3

The World's First Mobile Quad Core, with 5th Companion Core for Low Power

CPU	Quad Core, with 5th Companion Core — *Up to 1.4GHz Single Core, 1.3GHz Quad Core*
GPU	Up to 3x Higher GPU Performance — *12 Core GeForce GPU*
VIDEO	Blu-Ray Quality Video — *1080p High Profile @ 40Mbps*
POWER	Lower Power than Tegra 2 — *Variable Symmetric Multiprocessing (vSMP)*
MEMORY	Up to 3x Higher Memory Bandwidth — *DDR3L-1500, LPDDR2-1066*
IMAGING	Up to 2x Faster ISP (Image Signal Processor)
AUDIO	HD Audio, 7.1 channel surround
STORAGE	2-6x Faster — *e.MMC 4.41, SD3.0, SATA-II*



Asus quad-core tablet announced at CES 2012

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Future heterogeneous systems

Conclusions

- OpenCL enables truly heterogeneous computing, harnessing all hardware resources in a system
- GPUs can yield significant savings in energy costs (and equipment costs)
- OpenCL can work just as well for multi-core CPUs as it does for GPUs

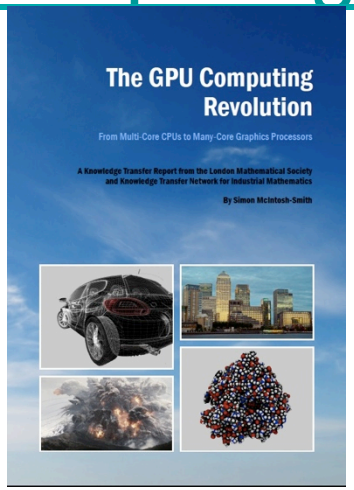
It's possible to screen libraries of millions of molecules against complex targets using highly accurate, computationally-expensive methods in one weekend using equipment costing O(£100K)

For an introduction to GPUs

"**The GPU Computing Revolution**"

A Knowledge Transfer Report from the London Mathematical Society and the KTN for Industrial Mathematics

- https://ktn.innovateuk.org/web/mathsktn/articles/-/blogs/the-gpu-computing-revolution



References

- S. McIntosh-Smith, T. Wilson, A.A. Ibarra, J. Crisp and R.B. Sessions, "Benchmarking energy efficiency, power costs and carbon emissions on heterogeneous systems", The Computer Journal, September 12th 2011. DOI: 10.1093/comjnl/bxr091

- N. Gibbs, A.R. Clarke & R.B. Sessions, "Ab-initio Protein Folding using Physicochemical Potentials and a Simplified Off-Lattice Model", Proteins 43:186-202,200