Petapath

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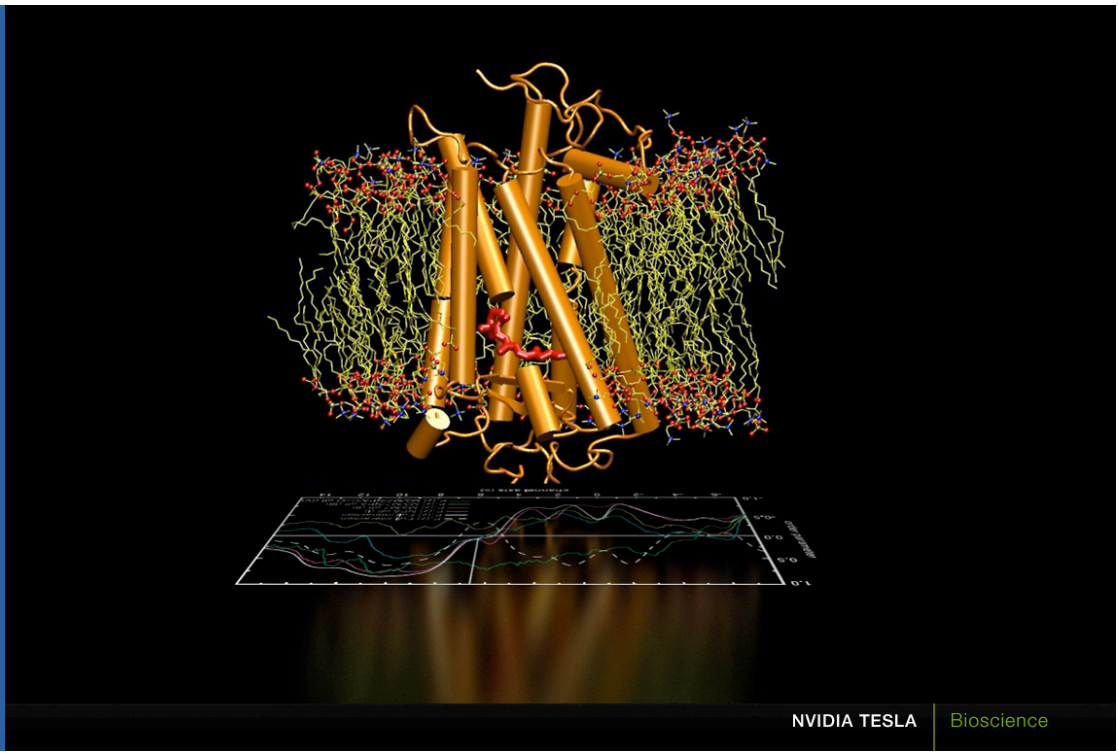

NVIDIA Bio Workbench:
more science more quickly

NVIDIA has always recognised the value of building an open software ecosystem that allows users to make use of GPU accelerated applications with the minimum of effort.

The NVIDIA® Tesla™ Bio Workbench is a new and critically important part of this ecosystem, specifically addressing users in the Life Sciences and Computational Chemistry. The Bio Workbench enables biophysicists and computational chemists to push the boundaries of biochemical research in a practical and cost effective way.

By harnessing the performance of NVIDIA Tesla Computing Solutions, it can turn a standard PC into a "computational laboratory" capable of running complex bioscience, particularly Molecular Dynamics and Quantum Chemistry codes. These include well established codes such as AMBER and other newer codes written from the ground up to support GPUs. All offer substantial improvements in throughput, enabling users to obtain more results more quickly. Bio Workbench codes can also be run on GPU equipped clusters.

The codes can be divided into two groups, and include:

Molecular Dynamics
- ACE MD
- AMBER
- BigDFT (ABINIT)
- GROMACS
- HOOMD
- LAMMPS
- NAMD, TeraChem, VMD

Bio Informatics
- CUDA-BLASTP
- CUDA-EC
- CUDA-MEME
- CUDASW++
- GPU-HMMER
- HEX Protein Docking
- Jacket (MATLAB Plugin)
- MUMmerGPU

Benchmark figures compiled by Ross C. Walker from the San Diego Supercomputer Center show performance improvements, over an x86 reference machine (2.8GHz Intel E5462 dual quad core), ranging from a minimum of 3x faster on a single NVIDIA Tesla C2050 to over 17x depending on the simulation.

Benchmark		8 core (ns/day)	C1060 (ns/day)	C2050 (ns/day)	Speedup
AMBER Implicit Solvent (GB)	TRPCage (304 atoms)	116	254	368.2	**3.17 x**
	Myoglobin (2,492 atoms)	4.4	27.9	49.9	**11.34 x**
	Nucleosome (25,095 atoms)	0.06	0.52	1.04	**17.33 x**
AMBER Explicit Solvent (PME)	DHFR NVE (23,558 atoms)	5.94	11.93	20.7	**3.48 x**
	DHFR NPT (23,558 atoms)	5.33	9.8	18.11	**3.39 x**
	FactorIX NVE (90,906 atoms)	1.67	3.51	5.19	**3.1 x**

Bio Workbench Workshop:

The University of Nottingham

23rd Nov 2010

Room A103
Centre for Astronomy and Particle Physics, Cripps Building

Petapath and NVIDIA would like to invite researchers, students and industrial users to a series of seminars and workshops dedicated to the Bio Workbench, with a particular focus on AMBER 11.

To register visit:
petapath.com/nvidia

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A lot can be achieved in one day

Plan of the day	
10:00 a.m.	Registration opens, morning coffee
11 a.m. - 1 p.m.	BioWorkbench seminar
1 p.m. - 2 p.m.	Lunch and discussions
2 p.m - 5 p.m.	CUDA workshop
5 p.m.	Day end

There will be coffee breaks with light snacks throughout the day

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Our seminars are aimed at users who already have experience with molecular dynamics and bio informatics. While we will start, taking AMBER as an example, by introducing the latest developments in AMBER 11 with particular emphasis on new methods and GPU support, our goal is to give researches an opportunity to trial their preferred codes and data on the GPU enabled cluster.

Taking a selection of these codes we would like to demonstrate and analyse advantage of Fermi compute power and which hardware configurations will work best for the different class of problems. We will then give an overview of the different options available on the GPU and how to improve performance by selecting specific options.

Please help us make the seminars relevant to your compute problems by sending us the input files and benchmarks ahead of the sessions. If you would like to see how your simulations perform on the latest NVIDIA hardware and share this experience with other attendees, then please contact us at least two weeks before the date of the seminar.

The Bio Station

Petapath has worked with Supermicro to architect a deskside supercomputer for Bio Workbench applications. We created the configuration that provides the right balance of bandwidth and compute, and the memory footprint sufficient for large systems.

Bio Station can be configured with up-to 12 CPU cores, four Tesla M2050 Computing Modules or professional Quadro visualization boards.

Supports up-to four double width GPUs

92.31% efficient power supply

- Intel® Xeon® processor 5600/5500 series, with QPI up-to 6.4 GT/s
- Up-to 192GB DDR3 1333/ 1066/ 800MHz ECC Registered DIMM
- 4U tower or rack mount

Registration is open:

www.petapath.com/nvidia