Tesla Bio Workbench

Recommended Configurations

Updated 5/24/11

Code	Desktop Workstation Configurations	Data Center Configurations
AMBER	GPUs - 2-4 Tesla C2070 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 12 GB or more	GPUs per node - 2 or more Tesla M2090 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU per server - 12 GB or more per server
CUDA-BLASTP	GPUs - 4 Tesla C2070 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 24 GB or more	Not applicable (CUDA-BLASTP is not MPI enabled)
CUDA-EC	GPUs - 1 Tesla C2070 GPU (CUDA-EC supports a single GPU so far) CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 8 GB or more	Not applicable (CUDA-EC is not yet MPI enabled)
CUDA-MEME	GPU - 1 Tesla C2070 GPU (CUDA-MEME supports single GPU so far) CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 8 GB or more	Not applicable (CUDA-MEME is not yet MPI enabled)
CUDASW++ (Smith-Waterman)	GPUs - 2 Tesla C2070 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 12 GB or more	Not applicable (CUDASW++ is not yet MPI enabled)
GPU-HMMER	GPUs - 4 Tesla C2070 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 24 GB or more	Not applicable (GPU-HMMER is not yet MPI enabled)

GROMACS	GPUs - 1 Tesla C2070 GPU (GROMACS supports single GPU so far) CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 16 GB or more	Not applicable (CUDA version of GROMACS is not yet MPI enabled)
HOOMD	GPUs - 4 Tesla C2070 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 24 GB or more	Not applicable (HOOMD is not yet MPI enabled)
LAMMPS	GPUs - 4 Tesla C2070 GPUs CPU and Main Memory - 2.33 GHz (or faster) Quad-Core x86 CPU - 24 GB or more	GPUs per node - 2 or more Tesla M2090 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU per server - 16 GB or more per server
MUMmerGPU	GPUs - 1 Tesla C2070 GPU (MUMmerGPU supports a single GPU so far) CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 8 GB or more	Not applicable (MUMmerGPU is not yet MPI enabled)
NAMD	GPUs - 4 Tesla C2070 Computing CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 24 GB or more	GPUs per node - 2 or more Tesla M2090 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU per server - 16 GB or more per server
TeraChem	GPUs - 4 Tesla C2070 GPUs CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 24 GB or more	Not applicable (TeraChem is not yet MPI enabled)
VMD	GPUs - 3 Tesla C2070 GPUs + 1 Quadro 5000 GPU for visualization CPU and Main Memory - 2.33 GHz Quad-Core x86 CPU - 24 GB or more	Not applicable (VMD is a desktop visualization application)