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| **Document Status**   |  |  |  |  | | --- | --- | --- | --- | | **유형** | Draft (초안) | **보안** | Confidential | |

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# Introducing

본 문서는 ‘공개소프트웨어 기반의 개인용 슈퍼 컴퓨팅 플랫폼 구축 및 커뮤니티 운영’ 과제에 대한 개발 분석과 계획에 대하여 서술한 자료임.

# 분석자료

## GPGPU의 기반이 되는 Architecture

* 1. 초기 GPGPU Framework



\* Ref. : 이만희, 박인규, 원석진, 조성대, “GPU를 이용한 DWT 및 JPEG2000의 고속 연산”, 전자공학회 논문지, Vol.44-SP, No.6, pp.9-15, 2007년 11월

* 1. 엔비디아 CUDA 구조
     1. Block Diagram



* + 1. CUDA Software 개발환경

|  |  |
| --- | --- |
| Libraries | Advanced libraries that include BLAS, FFT, and other functions optimized for the CUDA architecture |
| C Runtime | The **C Runtime for CUDA** provides support for executing standard C functions on the GPU and allows native bindings for other high-level languages such as Fortran, Java, and Python |
| Tools | NVIDIA C Compiler (nvcc), CUDA Debugger (cudagdb), CUDA Visual Profiler (cudaprof), and other helpful tools |
| Documentation | Includes the CUDA Programming Guide, API specifications, and other helpful documentation |
| Samples | SDK code samples and documentation that demonstrate best practices for a wide variety GPU Computing algorithms and applications |

* + 1. CUDA 적용 Language

**Fortran:**

o Fortran wrapper for CUDA – <http://www.nvidia.com/object/cuda_programming_tools.html>

o FLAGON Fortran 95 library for GPU Numerics – <http://flagon.wiki.sourceforge.net/>

o PGI Fortran to CUDA compiler – <http://www.pgroup.com/resources/accel.htm>

**Java:**

o JaCuda – <http://jacuda.wiki.sourceforge.net>

o Bindings for CUDA BLAS and FFT libs – <http://javagl.de/index.html>

**Python:**

o PyCUDA Python wrapper – <http://mathema.tician.de/software/pycuda>

**.NET languages:**

o CUDA.NET – <http://www.gass-ltd.co.il/en/products/cuda.net>

**Resources for other languages:**

o SWIG – <http://www.swig.org> (generates interfaces to C/C++ for dozens of languages)

* 1. OpenCL
     1. OpenCL – Open Computing Language



* + 1. OpenCL 적용 이전과 이후



* + 1. OpenCL 조합



* + 1. OpenCL Software



* + 1. OpenCL과 기타 표준과의 관계



* + 1. OpenCL Platform Model



* + 1. OpenCL Memory Model



* + 1. OpenCL Kernel 실행



* + 1. OpenCL SDK 제공

Intel OpenCL SDK : <http://software.intel.com/en-us/articles/opencl-sdk/#resource>   
NVIDIA OpenCL SDK: <http://developer.nvidia.com/opencl>

AMD OpenCL SDK : <http://developer.amd.com/sdks/AMDAPPSDK/Pages/default.aspx>

* + 1. OpenCL Reference.

\* OpenCL The Open Standard for Heterogeneous Parallel Programming, Neil Trevett(Khronos President) , Multicore Expo, March 2009

\* OpenCL Technical Overview, John Roberts(NVidia), Multicore Expo, March 2009

\* OpenCL as an intermediate language for heterogeneous multi-core programming, Alastair F. Donaldson(Codeplay Software Ltd. ), Multicore Expo, March 2009

\* “Apple主導 の OpenCL プロセ サに 自由 をもたらす, Nikkei Electronics, Dec. 08, 2008

\* Khronos Group : <http://www.khronos.org>

\* The OpenCL Specification, version : 1.0, Document Revisions : 43, Khronos OpenCL Working Group

\* Open Standard Industry Update from handhelds to supercomputers, Jon Peddie Research

## GPGPU 적용을 위한 Application 분석.

* 1. AutoDock Vina
     1. 기본 설명

O AutoDock Vina는 신약개발을 위한 Open Source Project

O Molecular docking, virtual screening 기능

O multi-core capability, high performance, 정확도 향상, 사용 용이성 제공

* + 1. 개발자

O Dr. Oleg Trott in the Molecular Graphics Lab at The Scripps Research Institute

* + 1. 결과 형상

flexible docking (green)의 결과가 crystal structures (a) indinavir, (b) atorvastatin, (c) imatinib, and (d) oseltamivir 각각 에 올려있는 모습



* + 1. 참고자료

<http://vina.scripps.edu/>

[O. Trott, A. J. Olson, AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading, *Journal of Computational Chemistry 31 (2010) 455-461*](http://www3.interscience.wiley.com/journal/122439542/abstract)

# 개발계획 (가칭 PSClib : Personal Super Computing Library)

## PSClib

* 1. 필요성

엔지니어, 과학자, 분석가, 기술 전문가들이 GPU를 이용한 데이터 분석 작업에 연산 성능을 최대한으로 이용할 수 있도록 지원. 최근 증대되는 이미지 데이터, 복잡한 분석 알고리즘, 수치해석 모델 등이 기존 CPU의 성능으로는 부족함을 느끼고 있기 때문에 GPU를 추가로 이용하는 것이 필요함.

* 1. 필요 기능

기존 CPU 프로그래밍을 하던 개발자들도 GPU 사용을 쉽게 할 수 있도록 지원해야 하며 이를 위한 해결 방안은 대용량 병렬 알고리즘이나 GPU 메모리 관리의 용이한 개발 환경이 필요함.

가속된 Mathematical, Image Filtering, Simulation Functions

Structural mechanics, fuid dynamics, earth, science, biosciences, medial/diagnostic imaging, financial engineering.

* 1. 참고자료

CUDA Web Site : <http://www.nvidia.com/cuda>

기타 본 문서 ‘관련자료’ 참조

## PSClib Block Diagram



# 관련자료

## GPGPU를 이용한 어플리케이션

|  |  |
| --- | --- |
| **category** | **title** |
| **Government & Defense** | [RealityServer](http://www.nvidia.com/object/realityserver.html) |
| **Government & Defense** | [Ikena: Imagery Analysis and Video Forensics](http://www.motiondsp.com/products/Ikena) |
| **Government & Defense** | [Signal Processing Library: GPU VSIPL](http://gpu-vsipl.gtri.gatech.edu/) |
| **Government & Defense** | [IDL and MATLAB Acceleration: GPULib](http://www.txcorp.com/products/GPULib/) |
| **Government & Defense** | [GIS: Manifold](http://www.manifold.net/index.shtml) |
| **Government & Defense** | [MATLAB GPU Computing: MathWorks](http://www.nvidia.com/object/tesla-matlab-accelerations.html) |
| **Government & Defense** | [MATLAB Plugin: Accelereyes](http://www.accelereyes.com/) |
| **Molecular Dynamics, Computational Chemistry** | [OpenMM library for accelerating molecular dynamics on GPUs](https://simtk.org/project/xml/downloads.xml?group_id=161) |
| **Molecular Dynamics, Computational Chemistry** | [GROMACS using OpenMM](https://simtk.org/project/xml/downloads.xml?group_id=161#package_id600) |
| **Molecular Dynamics, Computational Chemistry** | [NAMD molecular dynamics](http://www.ks.uiuc.edu/Research/gpu/) |
| **Molecular Dynamics, Computational Chemistry** | [VMD visualization of molecular dynamics](http://www.ks.uiuc.edu/Research/gpu/) |
| **Molecular Dynamics, Computational Chemistry** | [HOOMD molecular dynamics](http://www.ameslab.gov/hoomd/) |
| **Molecular Dynamics, Computational Chemistry** | [Acellera: ACEMD bio-molecular dynamics package](http://www.acellera.com/index.php?arg=acemd) |
| **Molecular Dynamics, Computational Chemistry** | [BigDFT: DFT (Density functional theory) electronic structure code](http://inac.cea.fr/L_Sim/BigDFT/index.html) |
| **Molecular Dynamics, Computational Chemistry** | [MDGPU](http://www-old.amolf.nl/~vanmeel/mdgpu/about.html) |
| **Molecular Dynamics, Computational Chemistry** | [GPUGrid.net](http://www.gpugrid.net/) |
| **Molecular Dynamics, Computational Chemistry** | [MATLAB GPU Computing: MathWorks](http://www.nvidia.com/object/tesla-matlab-accelerations.html) |
| **Molecular Dynamics, Computational Chemistry** | [MATLAB plugin: Accelereyes](http://www.accelereyes.com/) |
| **Life Sciences, Bio-informatics** | [GPU HMMER](http://www.mpihmmer.org/) |
| **Life Sciences, Bio-informatics** | [DNA Sequence alignment: MUMmerGPU](http://sourceforge.net/projects/mummergpu/) |
| **Life Sciences, Bio-informatics** | [LISSOM: model of human neocortex using CUDA](http://code.google.com/p/lissom/) |
| **Life Sciences, Bio-informatics** | [Silicon Informatics: AutoDock](http://www.siliconinformatics.com/) |
| **Life Sciences, Bio-informatics** | [MATLAB plugin: Accelereyes](http://www.accelereyes.com/) |
| **Electrodynamics and electromagnetic** | [Acceleware: FDTD Solver](http://www.acceleware.com/fdtd-solvers) |
| **Electrodynamics and electromagnetic** | [Acceleware: EM Solutions](http://www.acceleware.com/electromagnetic-solutions) |
| **Electrodynamics and electromagnetic** | [Remcom XStream FDTD](http://www.remcom.com/xf7-xstream/) |
| **Electrodynamics and electromagnetic** | [SPEAG Semcad X](http://www.semcad.com/simulation/features/hardware.php) |
| **Electrodynamics and electromagnetic** | [CST Microwave Studio](http://www.cst.com/Content/Products/MWS/GPU.aspx) |
| **Electrodynamics and electromagnetic** | [Quantum electrodynamics library](http://code.google.com/p/aeth-drive/) |
| **Electrodynamics and electromagnetic** | [GPMAD : Particle beam dynamics simulator](http://www.hep.manchester.ac.uk/gpmad/) |
| **Medical Imaging, CT, MRI** | [RealityServer](http://www.nvidia.com/object/realityserver.html) |
| **Medical Imaging, CT, MRI** | [GPULib:IDL acceleration](http://www.txcorp.com/products/GPULib/) |
| **Medical Imaging, CT, MRI** | [Acceleware: Imaging Solutions](http://www.acceleware.com/imaging-solutions) |
| **Medical Imaging, CT, MRI** | [Digisens: SnapCT tomographic reconstruction software](http://www.digisens.fr/snapct/) |
| **Medical Imaging, CT, MRI** | [Techniscan: Whole Breast Ultrasound Imaging System](http://www.techniscanmedicalsystems.com/) |
| **Medical Imaging, CT, MRI** | [NVPP: NVIDIA Performance Primitives (early access)](http://www.nvidia.com/nvpp) |
| **Medical Imaging, CT, MRI** | [MATLAB GPU Computing: MathWorks](http://www.nvidia.com/object/tesla-matlab-accelerations.html) |
| **Medical Imaging, CT, MRI** | [MATLAB plugin: Accelereyes](http://www.accelereyes.com/) |
| **Oil & Gas** | [RealityServer](http://www.nvidia.com/object/realityserver.html) |
| **Oil & Gas** | [Acceleware: Kirchoff and Reverse Time Migration](http://www.acceleware.com/default/index.cfm/solutions/seismic-solutions/) |
| **Oil & Gas** | [SeismicCity: 3D seismic imaging for prestack depth migration](http://www.seismiccity.com/) |
| **Oil & Gas** | [OpenGeoSolutions: Spectral decomposition and inversion](http://www.opengeosolutions.com/) |
| **Oil & Gas** | [Mercury Computer systems: 3D data visualization](http://3dviz.mc.com/solutions/oilandgas/ngog/) |
| **Oil & Gas** | [ffA: 3D Seismic processing software](http://www.ffa.co.uk/) |
| **Oil & Gas** | [Headwave: Prestack data processing](http://www.headwave.com/) |
| **Oil & Gas** | [GIS: Manifold](http://www.manifold.net/index.shtml) |
| **Oil & Gas** | [MATLAB GPU Computing: MathWorks](http://www.nvidia.com/object/tesla-matlab-accelerations.html) |
| **Oil & Gas** | [MATLAB plugin: Accelereyes](http://www.accelereyes.com/) |
| **Financial computing and options pricing** | [SciComp: derivatives pricing](http://www.scicomp.com/parallel_computing/GPU_OpenMP) |
| **Financial computing and options pricing** | [Hanweck: options pricing](http://www.hanweckassoc.com/home.html) |
| **Financial computing and options pricing** | [Exegy: Risk Analysis](http://www.exegy.com/PDFs/WHT-0001-A_final.pdf) |
| **Financial computing and options pricing** | [Aqumin: 3D Visualization of market data](http://www.aqumin.com/) |
| **Financial computing and options pricing** | [Level 3 Finance](http://www.level3finance.com/) |
| **Financial computing and options pricing** | [OnEye (Australia): Accelerated Trading Solutions](http://www.oneye.com.au/) |
| **Financial computing and options pricing** | [Arbitragis Trading](http://www.arbitragis-research.com/cuda-in-computational-finance) |
| **Financial computing and options pricing** | [Enabling GPU Computing in the R Statistical Environment](http://brainarray.mbni.med.umich.edu/brainarray/rgpgpu/) |
| **Financial computing and options pricing** | [MATLAB GPU Computing: MathWorks](http://www.nvidia.com/object/tesla-matlab-accelerations.html) |
| **Financial computing and options pricing** | [MATLAB plugin: Accelereyes](http://www.accelereyes.com/) |
| **Math** | [CUDA Acceleration for MATLAB](http://www.nvidia.com/object/tesla-matlab-accelerations.html) |
| **Math** | [Accelereyes: Jacket engine for MATLAB](http://www.accelereyes.com/) |
| **Math** | [GPULib: mathematical functions for IDL and MATLAB](http://www.txcorp.com/products/GPULib/) |
| **Math** | [Integrating Simulink with CUDA using S-functions](http://www.cs.ucf.edu/~janaka/gpu/documentation.htm) |
| **Math** | [Enabling GPU Computing in the R Statistical Environment](http://brainarray.mbni.med.umich.edu/brainarray/rgpgpu/) |
| **Math** | [Mathematica plug-in for CUDA](http://hpc.nomad-labs.com/?p=8) |
| **Math** | [Using NVIDIA GPUs with National Instruments LabView](http://decibel.ni.com/content/docs/DOC-6064) |
| **Electronic Design Automation** | [Agilent EESof: ADS SPICE simulator](http://www.home.agilent.com/agilent/product.jspx?nid=-34346.0.00&cc=US&lc=eng) |
| **Electronic Design Automation** | [Synopsys: Sentaraus TCAD](http://www.synopsys.com/Tools/TCAD/Pages/default.aspx) |
| **Electronic Design Automation** | [Gauda: Optical proximity correction (OPC)](http://www.gauda.com/) |
| **Weather and Ocean Modeling** | [CUDA-accelerated WRF code](http://www.mmm.ucar.edu/wrf/WG2/GPU/) |
| **Video, Imaging, and Vision Applications** | [Axxon Intellect Enterprise Video Surveillance Software](http://www.axxonsoft.com/products/axxon_enterprise/) |
| **Video, Imaging, and Vision Applications** | [Pflow CUDA Plugin for Autodesk 3ds Max](http://www.zhangy.com/main/index.php?module=documents&JAS_DocumentManager_op=viewDocument&JAS_Document_id=26) |
| **Video, Imaging, and Vision Applications** | [RUINS Shatter CUDA Plug-in for Maya](http://www.nshatter.com/index.html) |
| **Video, Imaging, and Vision Applications** | [Bullet 3D Multi-Physics Library with CUDA Support](http://code.google.com/p/bullet/downloads/list) |
| **Video, Imaging, and Vision Applications** | [CUDA Voxel Rendering Engine](http://voxels.blogspot.com/) |
| **Video, Imaging, and Vision Applications** | [NVPP: NVIDIA Performance Primitives (early access) Volume Rendering with CUDA for VTK / Slicer3](http://www.slicer.org/slicerWiki/index.php/Slicer3:Volume_Rendering_With_Cuda) |
| **Video, Imaging, and Vision Applications** | [Furryball: Direct3D GPU Rendering Plugin for Maya](http://furryball.aaa-studio.cz/) |
| **Video, Imaging, and Vision Applications** | [For consumer CUDA applications, visit NZone](http://www.nzone.com/page/nzone_section_andmore.html) |

출처 : CUDA-Accelerated Applications ( <http://www.nvidia.com/object/cuda_app_tesla.html> )

## GPGPU 관련 서적

|  |  |  |  |  |
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| **Front Cover** | **Title** | **Autor / Editor** | **Date** | **Publisher** |
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| GPU Pro 2   |  | | --- | |  | | [GPU Pro 2](http://www.amazon.com/GPU-Pro-2-Wolfgang-Engel/dp/1568817185/ref=pd_sim_b_3) | Wolfgang Engel | 2011-02-14 | A K Peters/CRC Press |
| |  | | --- | |  | | [Gpu Computing Gems Emerald Edition](http://www.amazon.com/GPU-Computing-Gems-Emerald-Applications/dp/0123849888/ref=sr_1_1?ie=%20UTF8&s=books&qid=1298081179&sr=1-1) | Wen-mei W. Hwu | 2011-2-7 | Elsevier Science & Technology |
| |  | | --- | |  | | [Scientific Computing with Multicore and Accelerators (Chapman & Hall/CRC Computational Science)](http://www.amazon.com/Scientific-Computing-Multicore-Accelerators-Computational/dp/143982536X/ref=pd_sim_b_5) | Jakub Kurzak, David A. Bader, Jack Dongarra | 2010-12-07 | CRC Press |
| |  | | --- | |  | | [Cuda By Example: An Introduction to General-Purpose GPU Programming (OpenCL입문 - GPU와 멀티코어 CPU 병렬 프로그래밍)](http://www.amazon.com/CUDA-Example-Introduction-General-Purpose-Programming/dp/0131387685/ref=sr_1_1?ie=UTF8&s=books&qid=1271458526&sr=1-1) | Jason Sanders; Edward Kandrot | 2010-7-29 | Addison-Wesley |
| |  | | --- | |  | | [GPU Pro: Advanced Rendering Techniques](http://www.amazon.com/GPU-Pro-Advanced-Rendering-Techniques/dp/1568814720/ref=pd_sim_b_2) | Wolfgang Engel | 2010-07-01 | A K Peters |
| |  | | --- | |  | | [Opencl入門 - GPU&マルチコアCPU並列プログラミング for MacOS Windows Linux (OpenCL입문 - GPU와 멀티코어 CPU 병렬 프로그래밍)](http://www.amazon.co.jp/OpenCL%E5%85%A5%E9%96%80%E2%80%95GPU-%E3%83%9E%E3%83%AB%E3%83%81%E3%82%B3%E3%82%A2CPU%E4%B8%A6%E5%88%97%E3%83%97%E3%83%AD%E3%82%B0%E3%83%A9%E3%83%9F%E3%83%B3%E3%82%B0-MacOS-Windows-Linux/dp/4798026085/ref=pd_sim_b_2) | 奥薗隆司 | 2010-5-1 | インプレスジャパン |
| OpenCL Programming Book   |  | | --- | |  | | [The OpenCL Programming Book](http://www.fixstars.com/en/company/books/opencl/) | Ryoji Tsuchiyama, Takashi Nakamura, Takuro Iizuka, Akihiro Asahara, Satoshi Miki | 2010-03-31 | Fixstars Corporation |
| |  | | --- | |  | | [Cuda高速gpuプログラミング入門 (CUDA 고속 GPU 프로그래밍 입문)](http://www.amazon.co.jp/CUDA%E9%AB%98%E9%80%9FGPU%E3%83%97%E3%83%AD%E3%82%B0%E3%83%A9%E3%83%9F%E3%83%B3%E3%82%B0%E5%85%A5%E9%96%80-%E5%B2%A1%E7%94%B0-%E8%B3%A2%E6%B2%BB/dp/479802578X) | 岡田賢治 | 2010-3-1 | 秀和システム |
| |  | | --- | |  | | [Programming Massively Parallel Processors](http://www.amazon.com/dp/0123814723?tag=wwwnvidiacomc-20&camp=14573&creative=327641&linkCode=as1&creativeASIN=0123814723&adid=1DT2S034DXS37V3K5FFY) | David Kirk; Wen-mei W. Hwu | 2010-2-5 | Elsevier Science & Technology |
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