

Curriculum Vitae - Po-Jen Hsu / 許伯任

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[\(Chinese version\)](#)

Ph.D, IAMS, TIGP, Academia Sinica (2008 - Now)

Research Assistant in Physics, National Central University (2005 - 2008)

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M.S. in Physics, National Central University (2000 - 2003)

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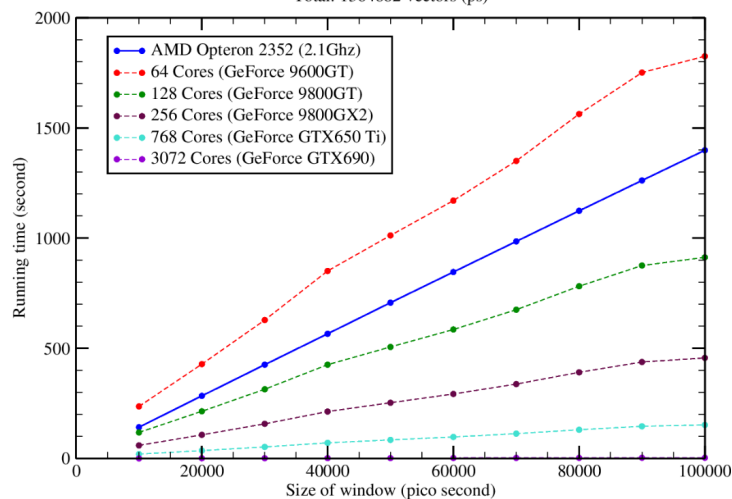
PROJECTS

The following softwares were developed by me and can be modified and distributed under GNU License (GPL). (Click on each subtitle to the corresponding GitHub repository)

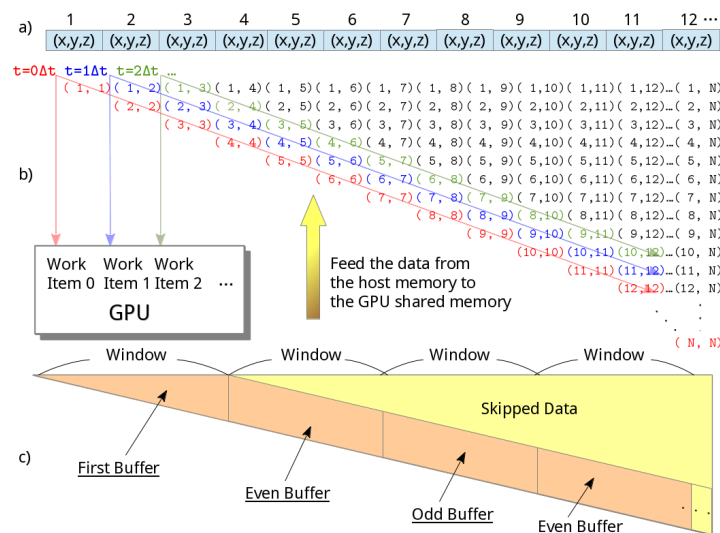
CL-VAF

Vector Autocorrelation Function with GPGPU (OpenCL/C/C++)

Benchmark of GPU versus CPU (VAF Calculation)
Total: 1364882 vectors (ps)



Performance of CL-VAF. (click on image to enlarge)



Three steps of the vector autocorrelation calculation using GPGPU. For a time series of vectors (a), load data to odd or even buffer sequentially (c). Then, assign the vector autocorrelation function to each work item in GPU (b).

The CL-VAF [1, 4, 5, 7, 8] uses the power of GPGPU to calculate the autocorrelation function of multi-dimensional vectors. The code was modified from my another project [TCOM](#) with carefully designed GPGPU parallelism. Instead of using CUDA, I chose OpenCL because of the cross-platform compatibility. OpenCL is supported by vast manufactures including Nvidia, AMD, Intel, ARM (Mobile devices), Apple, and so on whereas CUDA is only applicable on an Nvidia device. The benchmark is based on the consumer-level GPU. For more advanced models such as Nvidia Tesla, the performance should be further improved.

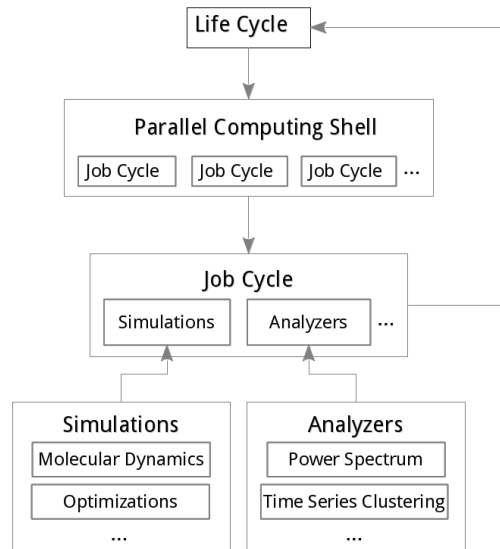
MPI-Tools

MPICH Tools (Shell Script)

The MPI-Tools has vast functionalities which allow users to construct and deploy the parallel computing in a minute. It's written in shell script to achieve the highest cross-platform transferability.

PTMD

Parallel Tempering Molecular Dynamics Simulation Plus Self Analyzers (MPICH/Fortran)

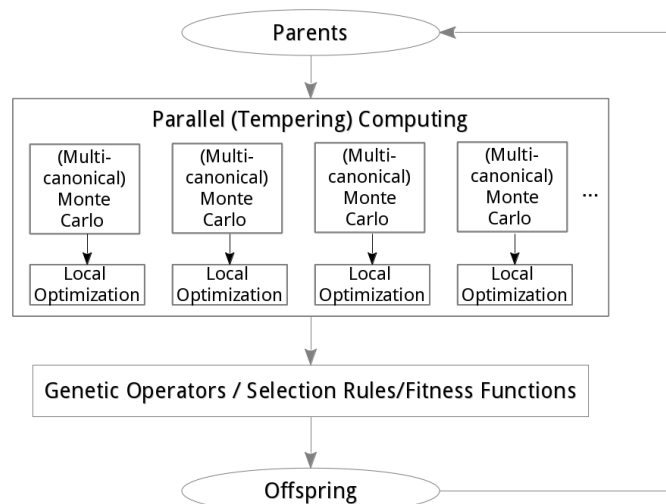


Framework of PTMD.

The PTMD [3-5] is an implementation of the software engineering. It is designed for big data analysis in bioinformatic system and is possible to run numerical simulations and analyze their results in an iterative way. The parallel computing shell allows most kinds of computation to be set and ran in parallel easily. Up to now, most analyzers were designed for time series clustering, time series statistics, and moment analysis.

PTMBHGA

Parallel Tempering Multicanonical Basin-hopping Plus Genetic Algorithm (MPICH/Fortran)



Framework of PTMBHGA.

The PTMBHGA [3-5,9-11] is a combination of several state-of-art optimization techniques, including genetic algorithm, parallel tempering Monte Carlo, simulated annealing, basing-hopping, and multicanonical Monte Carlo. The program was designed to be flexible for either a single run or integration of any optimization technique. I gained most knowledge of optimization from this project.

D-Tools

Tools for Diffusion Theory (C/C++)

The D-tools [1] helps reducing the tedious preparation of the diffusion theory calculation. This is one topic of my Ph.D thesis collaborated with Dr. [Arnaldo Rapallo](#).

TCOM

Vector Autocorrelation Function with MPICH (MPICH/Fortran)

The TCOM [1, 4, 5, 7, 8] is an MPICH version of vector autocorrelation calculation. Later, I wrote CL-VAF with GPGPU implemented.

OTHER INFORMATION

- Constructor and maintainer of PC clusters (Linux/Unix) and mail/version control (SVN/Git) system in [Prof. San-Kiong Lai's Lab](#).
 - [Best Team Presentation Award, 4th Hope Meeting, 2012, Japan](#).
 - Main speaker of open sources in physics in [ICOS2009](#). ([slides](#))
 - Chinese translations of PhET education project in physics.
 1. [Davisson-Germer Experiment](#)
 2. [Stern-Gerlach Experiment](#)
 3. [Quantum Wave Interference](#)
 4. [Quantum Tunneling](#)
 5. [Quantum Bound States](#)
 6. [Covalent Bonds](#)
 7. [Band Structure](#)
 - Applied statistics [3] and numerical simulation teaching.
 - Time series analysis [2], parallel computing, GPGPU computing, and computation algorithm.
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(Click on the title to download the paper)

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2. Weak correlation effect on the folding of transthyretin fragment studied by the shape similarity technique and time series methods, P. J. Hsu, S. A. Cheong, and S. K. Lai, Europhys Lett. (accepted).
3. A new perspective of shape recognition to discover the phase transition of finite-size clusters, P. J. Hsu, J. Comput. Chem. (accepted).
4. [Melting behavior of Ag₁₄ cluster: An order parameter by instantaneous normal modes](#), P. H. Tang, T. M. Wu, P. J. Hsu, and S. K. Lai, J. Chem. Phys. 137, 244304 (2012).

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6. Dynamical study of metallic clusters using the statistical method of time series clustering, S. K. Lai, Y. T. Lin, P. J. Hsu, and S. A. Cheong, Compt. Phys. Commun. 182, 1013 (2011).
7. Melting behavior of noble-metal-based bimetallic clusters, T. W. Yen, P. J. Hsu, and S. K. Lai, e-J. Surf. Sci. Nanotech. 7, 149-156 (2009).
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10. Multi-canonical basin-hopping: a new global optimization method for complex systems, L. Zhan, B. Piwowar, W. K. Liu, P. J. Hsu, S. K. Lai, and Jeff Z. Y. Chen, J. Chem. Phys. 120, 5536 (2004).
11. Structures of metallic clusters: mono- and polyvalent metals, S. K. Lai, P. J. Hsu, K. L. Wu, W. K. Liu, and M. Iwamatsu, J. Chem. Phys. 117, 10715 (2002).