Curriculum Vitae - Po-Jen Hsu / 許伯任

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

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

Military Service (2003 - 2005)

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

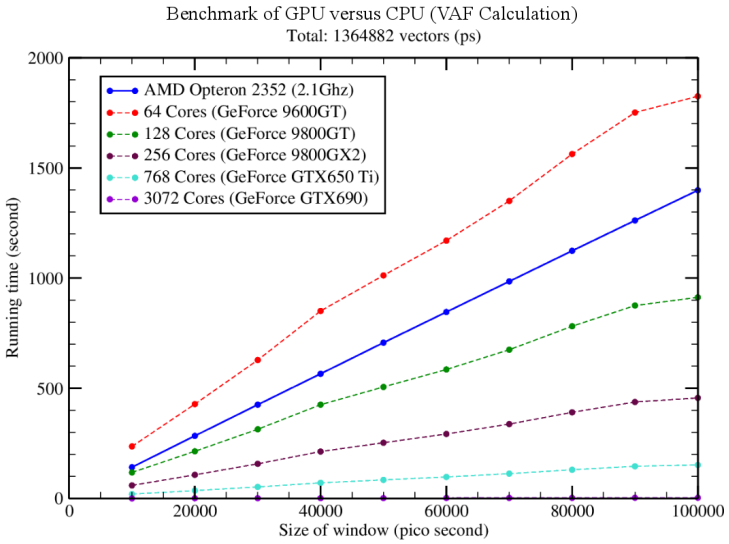
B.S. in Physics, National Central University (1996 - 2000)

PROJECTS

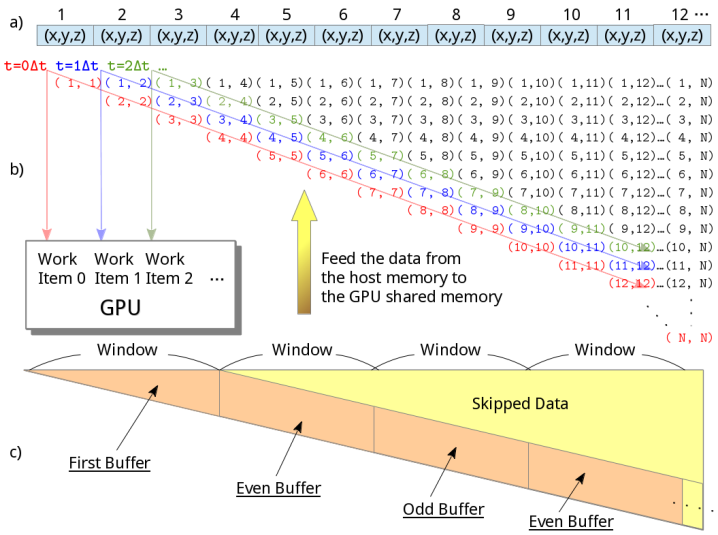
The following softwares were developed by me and can be modified and distributed under GNU License (GPL). (Click on each subtitle to the corresponding GitHub repository)

CL-VAF

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



Performance of CL-VAF.



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 autorrelation function to each work item in GPU (b).

The CL-VAF [1, 2, 4, 5] 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.

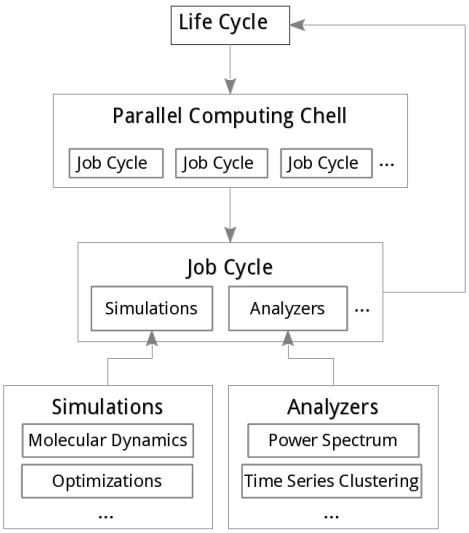
MPI-Tools

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)

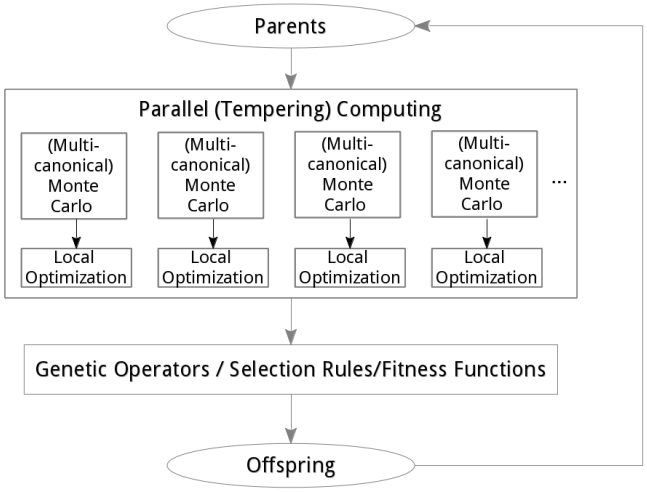


Framework of PTMD.

The PTMD [1 - 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 [6, 7, 8] 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 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, 2, 4, 5] is an MPICH version of vector autocorrelation calculation. Later, I wrote CL-VAF with GPGPU implemented.

I also use matlab and python for light-weight computation and figure organization.

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. Davission-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 and parallel computing lectures.

REFERENCES

(Click on the title to download the paper)

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[2] P.H. Tang, T.M. Wu, T.W. Yen, S.K. Lai, and P.J. Hsu, J. Chem. Phys. 135, 094302 (2011), "Comparative study of clusterAg17Cu2by instantaneous normal mode analysis and by isothermal Brownian-type molecular dynamics simulation"

[3] S.K. Lai, Y.T. Lin, P.J. Hsu, and S.A. Cheong, Compt. Phys. Commun. 182,1013(2011), "Dynamical study of metallic clusters using the statistical method of time series clustering"

[4] T.W. Yen, P.J. Hsu, and S.K. Lai, e-J. Surf. Sci. Nanotech.7, 149-156 (2009), "Melting behavior of noble-metal-based bimetallic clusters"

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[6] P.J. Hsu and S.K. Lai, J. Chem. Phys.124, 044711 (2006), "Structure of bimetallic clusters"

[7] L. Zhan, B. Piwowar, W.K. Liu, P.J. Hsu, S.K. Lai, and Jeff Z. Y. Chen, J. Chem. Phys.120, 5536 (2004), "Multi-canonical basin-hopping: a new global optimization method for complex systems"

[8] S.K. Lai, P.J. Hsu, K.L. Wu, W.K. Liu, and M. Iwamatsu, J. Chem. Phys.117, 10715 (2002), "Structures of metallic clusters: mono- and polyvalent metals"