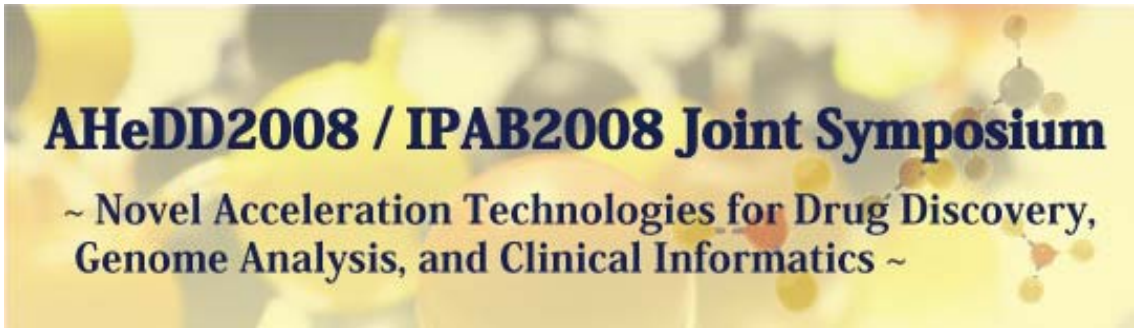

Date: October 16 (Thu) – 17 (Fri), 2008

Place: Yebisu Garden Place, Tokyo, Japan
(SGI Hall, Yebisu Garden Place Tower B1F, 4-20-3 Yebisu, Shibuya-ku)

Participation Fee: Free of charge (Pre-registration required)

URL: http://www.ipab.org/AHeDD2008-IPAB2008-Joint-Symposium

Organizers:

Initiative for Parallel Bioinformatics (IPAB) (President: Prof. Yutaka Akiyama)
AHeDD 2008 Organizing Committee

In cooperation with:

Global COE program "CompView" (Leader: Prof. Osamu Watanabe)
BMDRC, Seoul, Korea (Director: Prof. Kyoung Tai No)
DDDC, Shanghai, China (Director: Prof. Hualiang Jiang)
Japanese Society for Bioinformatics (JSBi)
Chem-Bio Informatics Society (CBI)
Japanese Society for Artificial Intelligence (JSAI)
SIGBIO/SIGMPS/SIGHPC, Information Processing Society of Japan (IPSJ)

Scope:

Accelerator Technology (GPGPU, FPGA, etc.) for bioinformatics and computational life sciences, Computational approaches for Drug Discovery (virtual screening, ADME, etc.), Clinical Informatics, and other topics related to bioinformatics and computational biology research.

Language:

Day 1: Japanese and English
Day2 : English

*Note: Most of talks in Day1 will be given in Japanese, while Day2 presentations are all in English.

Overview

Initiative for Parallel Bioinformatics (IPAB) was founded in 1999 and is a formal non-profit organization. IPAB is a group of individual researchers and private companies aiming at contributing to the research and industrialization of bioinformatics and biomedical computing, by means of state-of-the-art information technologies, like as parallel processing, Grid technology, machine learning, knowledge processing, etc. IPAB2008 is the 9th annual symposium of IPAB and in this year it will be held as a joint event with AHeDD2008.

Asia Hub for e-Drug Discovery (AHeDD) is an international research collaboration group founded in 2004, aiming at exchange of latest ideas and results on computational methods for drug discovery, and also construction of an Asian research community for sharing knowledge, training people, and incubating new business in e-drug discovery. In 2008 IPAB has decided to contribute to AHeDD activity as a Japanese brunch of AHeDD. AHeDD2008 is the fourth international workshop by AHeDD community, which succeeds previous AHeDD2005 (Jeju), AHeDD2006(Seoul), and AHeDD2007(Shanghai). For details, please visit the AHeDD www page at http://www.e-drugdiscovery.org.

AHeDD2008/IPAB2008 Program: (ver.2.5, Sep. 9)

Day 1: Thu., October 16 *"New Direction of IPAB"*

Venue: SGI Hall (Yebisu Garden Place Tower B1F)

10:00-10:05 Opening Address

Prof. Yutaka Akiyama (President of IPAB / Tokyo Tech)

10:05-11:45 Session 1: Accelerator Technology

Coordinator: Prof. Fumikazu Konishi (Tokyo Tech)
(Senior Vice President, Head of Accelerator WG, IPAB)

10:05-10:35 Dr. Toshiyuki Sanuki (DE, IBM Japan, Ltd.)
"Challenges for Petascale Computing"

10:35-11:05 Dr. Yosuke Tamura (CTO, Fixstars, Co.)
"Current state and applied case with software development for Cell/B.E."

11:05-11:35 Dr. Masatsugu Hashimoto (CTO, SGI Japan, Ltd.)
"The Capability of GPU computing"

11:35-11:45 Prof. Fumikazu Konishi (Tokyo Tech)
"Introduction to accelerator WG activity in IPAB"

11:45-13:00 Lunch Break

* Free Lunchon Seminar is planned for audiences.
* Commercial Exhibitions, and Poster Display.

13:00-13:50 Special Talk

Prof. Kenichi Hagihara (Osaka University)
"Medical image processing using GPGPU"

13:50-15:20 Session 2: Clinical Informatics

Coordinator: Prof. Teruyoshi Hishiki (Toho University)
(Vice President, Head of Clinical Informatics WG, IPAB)

13:50-14:20 Prof. Teruyoshi Hishiki (Toho University)
"IPAB's new activity on Clinical Informatics"

14:20-14:50 Prof. Yutaka Suzuki (The University of Tokyo)
"Analysis of full-length cDNAs with next-generation DNA sequencers"

14:50-15:20 Prof. Hiroshi Mizushima (Tokyo Medical and Dental University)
"Integrated database with comprehensive both clinical and molecular information"

15:20-16:00 Cofee Break

*Commercial Exhibitions, and Poster Display

16:00-17:30 Session 3: e-Drug Discovery

Coordinator: Prof. Yutaka Akiyama (Tokyo Tech)
(President, Head of pharmaco-informatics WG, IPAB)

16:00-16:30 Prof. Kyoung Tai No (Yonsei University / BMDRC, Korea)
"Development of e-Organ and It's Application for Drug Repositioning"

16:30-17:00 Prof. Takatsugu Hirokawa (CBRC, AIST, Japan)
"Protein structure-based virtual screening using concavity shape fingerprints"

17:00-17:30 Prof. Weiliang Zhu (DDDC, SIMM, China)
"Exploring Functional Conformations of Target Protein for Drug Discovery by Molecular Dynamics"

17:30 End of Day 1

18:00-20:00 Reception Party

at Beer Station Yebisu (3 min. on foot)
Food and All-you-can-drink Beer at Japanese most famous brewery
Participation Fee: JPY2,000 (planned)

Day 2: Fri., October 17, *"Asia Hub for e-Drug Discovery"*

Venue: SGI Hall (Yebisu Garden Place Tower B1F)

10:30-10:45 Introduction to AHeDD activity

Prof. Kyoung Tai No (Yonsei University / BMDRC, Korea)
Prof. Weiliang Zhu (DDDC, SIMM, China)
Prof. Yutaka Akiyama (Tokyo Tech, Japan)

10:45-12:15 Session 4: Frontiers of Drug Discovery Research

Chair: Prof. Kyong Tai No (Yonsei University / BMDRC, Korea)

10:45-11:15 Dr. Sungchul Chung (STEPI, Korea)
"Opportunities for S&T Cooperation in East Asia"

11:15-11:45 Prof. Yun Tang (East China Univ. of Science and Technology, China)
"New potential inhibitor binding sites identified in HIV-1 integrase"

11:45-12:15 Dr. Tohru Natsume (BIRC, AIST, Japan)
"Systematic Analysis of Protein Interaction Networks"

12:15-13:30 Lunch Break

*Commercial Exhibitions, and Poster Display

13:30-14:20 Special Talk

Prof. Toshihisa Ishikawa (Tokyo Tech, Japan)
"Transporter mechanism-based drug molecular design: High-speed screening, QSAR analysis, and molecular orbital calculation"

14:20-15:50 Session 5: Challenges for Important Targets

Chair: Prof. Weiliang Zhu (DDDC, SIMM, China)

14:20-14:50 Prof. Hong Gil Nam (POSTECH, Korea)
"Molecule-Level Imaging of Pax6 mRNA Distribution in Mouse Embryonic Neocortex by Molecular Interaction Force Microscopy"

14:50-15:20 Prof. Baik Lin Seong (Yonsei University, Korea)
"Common Vaccine Platform for Seasonal and Pandemic Influenza"

15:20-15:50 Dr. Tomoko Niwa (Nippon Shinyaku Co., Ltd., Japan)
"Elucidation of Characteristic Structural Features of Protein Kinases: A Neural Network Approach"

15:50-16:30 Poster Presentation

Explanation by authors. With Coffee service.

16:30-18:00 Session 6: Novel Computing Techniques for Drug Design

Chair: Prof. Hiroshi Chuman (The University of Tokushima, Japan)

16:30-17:00 Prof. Jianfeng Pei (Peking University, China)
"De novo drug design - to be a more practical approach"

17:00-17:30 Dr. Kunqian Yu (DDDC, SIMM, China)
"Drug discovery Grid of China"

17:30-18:00 Dr. Toshio Watanabe (RICS, AIST, Japan)
"Molecular Orbital Calculation for Large Molecule with Sakurai-Sugiura Method on Grid Computing Environment"

18:00 Closing Remark

*Special presentation of Computer demonstration and exhibition (E01-E07)

E01: Fixstars, Co.
E02: Information and Mathematical Science Laboratory Inc.
E03: Tokyo Institute of Technology Global COE program "CompView"
E04: Bestsystems, Inc.
E05: IBM Japan, Ltd.
E06: ClearSpeed Technology, Inc.
E07: (To be announced soon)

*Poster Presentations (P01-P21)

P01: Shen J, Liu GX, Tang Y* (ECUST): "In silico prediction of blood-brain partitioning using a chemometric method called genetic algorithm based variable selection (GAVS)."
P02: Jing Chen, Jianfeng Pei, Dengguo Wei, Qingliang Li, Luhua Lai (Peking Univ.): "Improving virtual screening efficiency by receptor-based pharmacophore model"
P03: Kunqian Yu (DDDC, SIMM): "Drug discovery Grid of China"
P04: Kwang-Hwi Cho, Jeong-Hyun Kim (SoongSil Univ.): "SABA: Secondary structure Assignments program Based on Alpha Carbon"

P05: Ky-Youb Nam, Hanjo Kim (BMDRC): “In silico Integrated Drug Profiling System against Influenza Virus”

P06: Jong Young Joung (Yonsei Univ.): “Property-Weighted Vector driven Docking Algorithm Using Solvation Free Energy Density (SFED) model”

P07: Hwan You (Yonsei Univ.): "Prediction of Binding Free Energy of Protein-Protein complex using Statistical Mechanics Methods"

P08: Hyoungjun Son (Yonsei Univ.): “In silico prediction for phase II enzyme selectivity of UGT and SULT substrates”

P09: Hankil Son (Yonsei Univ.): "Classification of phase II metabolizing enzymes"

P10: Chang Joon Lee (Yonsei Univ.): "RP-Path : A Robust Method for Search Smallest Set of Smallest Rings (SSSR) with Path Included Distance (PID) Matrix"

P11: Young Mook Kang (Yonsei Univ.): "Prediction of Metabolism using MNA Descriptor and Artificial Neural Network"

P12: Su Yeon Kim (Yonsei Univ.): “Development of novel chemicals blocking export of glycogen synthase kinase 3 (GSK3) from nucleus to cytoplasm”

P13: Se Han Lee (Yonsei Univ.): “Solvation Free Energy Calculation Method with the SFED and GSFED Model”

P14: Hiroaki Umeda (RICS, AIST): "Grid-enabled large Fock matrix construction for FMO-MO method"

P15: (RICS, AIST) (Title to be announced)

P16: Fumikazu Konishi, et.al (Tokyo Tech): “he speed-up of Crystallography & NME System (CNS) with hardware SIMD accelerator”

P17: Fumikazu Konishi, et.al (Tokyo Tech): “Development of an instant accelerator environment with Knoppix technology”

P18: Satoshi Matsuoka, Yutaka Akiyama, Akira Nukada, Toshio Endo, Yasuhiko Ogata, Fumikazu Konishi (Tokyo Tech): "HPC-GPGPU: Large-Scale Commodity Accelerated Clusters and its Application to Advanced Structural Proteomics"

P19: Kouta Toshimoto, et.al (Tokyo Tech): “In silico prediction of major drug clearance pathways”

P20: Yutaka Akiyama, et.al (Tokyo Tech): “MEGADOCK- A rapid screening system for all-to-all protein docking analysis”

P21: Yuri Matsuzaki, et.al (Tokyo Tech): “Analysis of protein-protein interactions of signal transduction pathways using a docking prediction program”