Editorial

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This issue of the *Journal of Bioinformatics Research and Applications* (IJBRA) showcases selected but considerably revised and extended papers from HiPCoMB-2005, the First IEEE Workshop on High Performance Computing in Medicine and Biology, held in Fukuoka Institute of Technology, Japan, in July 2005. The Workshop brought together about 30 individuals from across the world for participation. Due to the terrific response we have continued the workshop for 2006 and onwards.

This issue of IJBRA has eight high-quality papers that cover a broad range of topics in use of High Performance Computing for Medicine and Biology.

In the first paper titled 'A parallel implementation of 2-D/3-D image registration for computer-assisted surgery', the authors present the design and implementation of a parallel two-dimensional/three-dimensional (2-D/3-D) image registration method for computer-assisted surgery. Their method exploits data parallelism and speculative parallelism, aiming at making computation time short enough to carry out registration tasks during surgery. The experiments show that exploiting both parallelisms reduces computation time on a cluster of 64 PCs from a few tens of minutes to less than a few tens of seconds, a clinically compatible time.

The second paper is titled 'Rotational and translational alignment errors in 3D reconstruction of virus structures at high resolution' and presents the 3D reconstruction of virus structures at high resolution using CryoTEM data that requires a very accurate rotational and translational alignment of individual views obtained experimentally. In this paper they discuss the geometrical foundations and the computational problems raised by rotational and translational alignment and the errors introduced in this process. In the third paper titled 'Concurrent numerical simulation of flow and blood clotting using the lattice Boltzmann technique', the authors describe a novel approach for a concurrent numerical simulation of the unsteady flow within an idealised stenosed artery and a simplified blood clotting process based on a residence time model. The applied numerical scheme is the lattice Boltzmann technique, which proved to be highly efficient particularly for transient flows and complex or varying geometries.

Protein fold recognition aligns a probe amino acid sequence onto a library of representative folds of known structure to identify a structural similarity. In the fourth paper titled 'MESSM: a framework for protein fold recognition using neural networks and support vector machines', the authors present a new framework for protein fold recognition with a Mixed Environment-Specific Substitution Mapping (MESSM). The new framework has three key features. First, an environment-specific amino acid substitution (3D-1D) mapping is generated using artificial neural networks. Second, a mixed substitution mapping is proposed by linearly combining the structurally derived substitution mapping with sequence profile from well-developed amino acid substitution matrices. Third, a support vector machine is employed to measure the significance of the sequence-structure alignment.

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In the fifth paper titled 'High-speed multiple sequence alignment on a reconfigurable platform' the authors present a new approach to multiple sequence alignment MSA on reconfigurable hardware platforms to gain high performance at low cost. To derive an efficient mapping onto this type of architecture, fine-grained parallel Processing Elements (PEs) have been designed. Using this PE design as a building block they have constructed a linear systolic array to perform a pair-wise sequence distance computation using dynamic programming. This results in an implementation with significant runtime savings on a standard off-the-shelf FPGA. In the sixth paper titled 'PRec-I-DCM3: a parallel framework for fast and accurate large scale phylogeny reconstruction', the authors improve the performance of Rec-I-DCM3 via parallelisation. Rec-I-DCM3 is an efficient and accurate meta-method for solving the maximum parsimony problem on large datasets. Experimental results demonstrate that their parallel method, PRec-I-DCM3, achieves significant improvements, both in speed and accuracy, over its sequential counterpart.

In the seventh paper titled 'Numerical solutions of master equation for protein folding kinetics', the authors computationally study the folding rate for a kinetics problem of protein folding by solving a large-scale eigenvalue problem. Three numerical methods, the implicitly restarted Arnoldi, the Jacobi-Davidson, and the QR methods are applied to solve the corresponding large-scale eigenvalue problem of the transition matrix of master equation. Comparison among the implicitly restarted Arnoldi, the Jacobi-Davidson, and the QR methods is performed in terms of the computational efficiency. In the eighth paper titled 'Optimised fine and coarse parallelism for sequence homology', the authors present a technique to effectively combine fine and coarse grain parallelism using general-purpose processors for sequence homology database searches. The results show that the classic Smith-Waterman sequence alignment algorithm achieves super linear performance with proper scheduling and multi-level parallel computing at no additional cost.

We hope the papers in this issue of IJBRA provide a cross-section of the research underway in High Performance Computing in Medicine and Biology.