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Right To Health

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ABSTRACT

"Every citizen of India has a 'Right to health' which has been given by Constitution of India under Article 21 which talks about "Right to life and personal liberty". Although right to health is not specifically mentioned in Article 21 but Supreme Court interpreted as right of life also includes 'right to health'. This right to health also enumerates in Directive Principle of State Policy (DPSP) specifically Article -39(a), 47 and 48A by themselves and collectively cast a duty on 'State' to secure heath of people, improve pubic heath and protect & improve public environment. Although DPSP cannot be enforced by court but it is a guideline for framing of law by government to establish a just society in the country. So, if we say every citizen of India has a Right i.e 'State' shall have obligation to provide such right to every citizen of India. If we examine carefully 'Right to health 'it seems a most violated right which people are hardly aware about it. We should also examine how a State can fulfill his obligation of providing 'Right to health' to every citizen of India. Therefore, the paper tries to critically examine the position of "Right to Health" in India and its implementation in governmental policies.

Definition of health:

Health as defined in the oxford dictionary "the state of being free from illness or injury"(1).

The widely acceptable definition of health is that given by the WHO in the preamble of its constitution, according to World Health Organization, "Health is a state of complete physical, mental and social wellbeing and not merely the absence of disease (2)." In recent years, this statement has been amplified to include the ability to lead a 'socially and economically productive life'. Through this definition, WHO has helped to move health thinking beyond a limited, biomedical and pathology-based perspective to the more positive domain of "wellbeing". Also, by explicitly including the mental and social dimensions of wellbeing, WHO has radically expanded the scope of health and by extension, the role and responsibility of health professionals and their relationship to the larger society (3).

Right to health means that everyone has the right to the highest attainable standard of physical and mental health, which includes access to all medical services, sanitation, adequate food, decent housing, healthy working conditions, and a clean environment (4). Since it is an inclusive right it includes the following (5):

1. Safety food
2. Adequate nutrition and housing
3. Healthy working and environment conditions

4. Health-related education and information
5. Gender equality
6. Safe drinking water and adequate sanitation
7. Maternal, child and reproductive health
8. Equal and timely access to basic health services
9. The provision of health-related education and information
10. Participation of the population in health- related decision making at the national and community levels.

Development of the right to health

Now, we should understand how this right developed in internationally and India.

Internationally, the right to health was first articulated in 1946 constitution of world health organization (WHO), the preamble states that "the enjoyment of highest attainable standard of health is one of the fundamental rights of every human being without distinction of race, religion, political belief, economic or social condition" (6).

The 1948 Universal Declaration of Human Rights also mentioned health as part of the right to an adequate standard of living (article 25) (7).

The right to health was recognized as human right in the 1966 International Covenant on Economic, Social and Cultural right (8).

Every country has ratified at least one international human rights treaty recognizing the right to health. Moreover, States have committed themselves to protecting this right through international declarations, domestic legislation and policies, and at international conferences.

In India

1) Right to health as a fundamental right

Indian constitution has granted certain fundamental rights to its citizen under part III of it, these rights play an important role with reference to health and health care. Article 21 of Constitution of India, "Right to life and personal liberty to all person" through it doesn't provide expressly for healthcare however the liberal interpretation adopted by Indian Supreme Court to word "Life" brought the healthcare it the ambit of word life and declared it as basic right to every citizen of India (9). The concept of personal liberty comprehended many rights, related to indirectly to life or liberty of a person.

2) Right to health under DPSP(Directive Principle of state policy)

Panchayat, Municipality and Health:

Not only the State also Panchayat, Municipalities liable to improve and protect public health. Article 243G says "State that the legislature of a state may endow the panchayats with necessary power and authority in relation to matters listed in the eleventh Schedule". The entries in this schedule having direct relevance to health are as follows

11 -Drinking

23 -Health and sanitation including hospitals, primary health centers and dispensaries.

24 -Family welfare

25 -Women and Child development

26 -Social welfare including welfare of the handicapped and mentally retarded.

Article 243-W finds place in part IXA of the constitution titled "The Municipalities:

5 -Water supply for domestic industrial and commercial purpose.

6 -Public health, sanitation conservancy and solid waste management.

9-Safeguarding the interest of weaker sections of society, including the handicapped and mentally retarded.

16-Vital statistics including registration of births and deaths

17- Regulation of slaughter – houses and tanneries.

Various Indian statute interpreting right to health and their relevant cases

So, if we say that every citizen has a right to health as enumerate under Article 21 and DPSP 39(a), 47& 48A, so on other hand 'State'/ municipality /panchayat shall have obligation/duty to provide such right to every citizen of India.

According to MCkinsey & company, Indian healthcare sector (public & private) faced shortage of workforce and infrastructure. India had 1.7 trained allopathic doctors and nurses per 1,000 population compared to WHO (World Health organization) recommended guideline of 2.5 per population and bed density was .67 per population well below global average of 2.6 and WHO (World Health organization) benchmark of 3.5 per population. It observed by MCkinsey & company that as compared to private sector of Indian healthcare system the public sector of Indian healthcare system is in worse condition.

Therefore, we can say that Indian health care system is in bad condition and the "Right to health" is a fundamental right to every citizen is a most violated right which people are hardly aware about it. The judiciary has not really been active in giving a direction in implementation till the advent Consumer court/ forums, there were hardly any cases of medical negligence. Therefore, we are still far behind in implementing it as fundamental right to its fullest meaning. We can also say that "State" who has obligation to provide right to health to every citizen, it seems to be giving this right to every citizen.

CONCLUSION

India is a developing country. India has second highest world population with funds limited and corruption at root level. So, it will be challenging task for a "State" to provide right to health to all citizen of India but if we see that we have already eradicated "polio "despite of lots of challenges and this proves that if we are committed we can succeed to ensure safety from diseases to every Indian. The government to step in and start working towards developing health care system by doing following acts:

1. There is an urgent need to open more and more medical colleges. Today a lot many people cannot afford to pay heavy bills of private hospitals and since the government hospital are both too crowded and in unhygienic state that people are out of options. Due to this there is shortage of qualified staff in almost all the hospital. Therefore, government should open more medical colleges so that shortage of qualifies staff will be fulfilled in this country
2. Provide more fund for betterment of infrastructure of government hospital
3. Ensuring availability of good and qualified doctors in existing government hospital

4. Private hospitals should be kept in check and should not allow to extorting huge amount of money in name of treatment
5. Strong Legislation required to implement of right to health to the widest interpretation and make it within the reach of all the citizen--- The Right has been inferred to be part of Fundamental rights through various judicial proceeding and strong Legislation required to implement of right to health to the widest interpretation and make it within the reach of all the citizen

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A Review on GPU Accelerated Bioinformatics Tool

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ABSTRACT

Traditional computational methods and software tools developed in the research fields of Bioinformatics, Computational Biology and Systems Biology have a common property which is that they are computationally demanding on Central Processing Units (CPUs), therefore limiting their applicability in many circumstances. To overcome this issue, general-purpose Graphics Processing Units (GPUs) are gaining an increasing attention worldwide, as they can considerably reduce the running time required by standard CPU-based software, and allow more intensive investigations of biological systems. The latest generation of graphics processing units (GPUs) has democratized the use of HPC also as they push desktop computers to cluster level performance. In this review work, we present a collection of GPU enhanced bioinformatics tools developed recently in the past two to three decades to perform computational analysis in various life science disciplines, emphasizing the advantages and the drawbacks in the use of these parallel architectures.

INTRODUCTION:

Bioinformatics has evolved and expanded continuously over the past four decades and has grown into a very important bridging discipline in life science research. The quantities of data obtained by new high-throughput technologies, including micro or Chip-Chip arrays, and large-scale "OMICS"-approaches, such as genomics, proteomics and transcriptomics, are vast and biological data repositories are growing exponentially in size. Furthermore, every minute scientific knowledge increases by thousands pages and to read the new scientific material produced in 24 hours a researcher would take several years. To follow the scientific output produced regarding a single disease, a scientist would have to scan more than a hundred different journals and read a few dozen papers per day **(Pavlopoulos G.A. et. al.; 2008)**.

Typical applications in Bioinformatics, Computational Biology and Systems Biology exploit either physico-chemical or mathematical modeling, characterized by different scales of granularity, abstraction levels and goals, which are chosen according to the nature of the biological system under investigation—from single molecular structures up to genome-wide networks—and to the purpose of the modeling itself. Molecular dynamics, for instance, simulates the physical movements of atoms in biomolecules by calculating the forces acting on each atom, considering bonded or non-bonded interactions **(Rapaport D.C.; 2004) (Haile J.M.; 1997).**

Sequence alignment methods scale the abstraction level from atoms to RNA or DNA molecules, and then up to whole genomes, to the aim of combining or interpreting nucleotide sequences by means of string-based algorithms **(He M. et al.;2011)**.Systems Biology considers instead the emergent properties of complex biological systems—up to whole cells and organs **(Alberghina L. et al.;2005) (Karr J.R. et al.;2012)** focusing either on topological properties or flux distributions of large-scale networks, or on the dynamical behavior of their molecular components (e.g. genes, proteins, metabolites). Although these disciplines are characterized by different goals, deal with systems at different scales of complexity and require completely different computational methodologies, they share an ideal trait d'union: all of them are computationally challenging **(Schulz R. et al.;2009) (Sauro H.M. et al.;2006) (Pop M. et al.;2008).** Computers based on Central Processing Units (CPUs) are constantly improving, offering improved performances thanks to the parallelism granted by multi-threading and the vector instructions provided by e.g. Streaming SIMD Extensions (SSE) **(https://software.intel.com/sites/default/files/m/8/b/8/D9156103.pdf).**Still, computational analyses in life science disciplines often lie on the boundary of feasibility because of the huge computational costs they require on CPUs.

In the latter years, a completely different approach to HPC gained ground: the use of general-purpose multi-core devices like Many Integrated Cores (MIC) co-processors and Graphics Processing Units (GPUs). In particular, GPUs are gaining popularity, as they are pervasive, relatively cheap and extremely efficient parallel multi-core co-processors, giving access to lowcost, energy-efficient means to achieve tera-scale performances on common workstations (and peta-scale performances on GPU-equipped supercomputers) **(Joubert W. et al.;2015)(Bland A.S. et al.;2012).**However, tera-scale performances represent a theoretical peak that can be achieved only by distributing the whole workload across all available cores **(Amdahl G.M.;1967)** and by leveraging the high-performance memories on the GPU, two circumstances that are seldom simultaneously verified. Even in sub-optimal conditions, though, GPUs can achieve the same performances of other HPC infrastructures, albeit with a single machine and, remarkably, without the need for job scheduling or the transfer of confidential information. Being GPU's one of the most efficient and largely exploited parallel technology, in this article we provide a review of recent GPU-based tools for biological applications, discussing both their strengths and limitations.

In this review we describe GPU enhanced tools which nearly nullifies the huge processing time,simplify the analysis and interpretation of biological data by transforming the raw data into logically structured and visually tangible representations. Since the wealth of existing visualization tools makes an exhaustive collection and in-depth discussion of all available software tools impossible, we present a selection of several GPU enhanced bioinformatics tools/softwares, which are broadly applicable. Our survey covers tools invented mainly over the past two or three decades and discusses some of their advantages and shortcomings in order to aid researchers in choosing the most suitable tool for their studies. Finally, we will highlight crucial gaps in the landscape of bioinformatics, discuss how existing tools

could be improved to fill these gaps and lay out the perspectives and goals for the next generation of such GPU enhanced tools.

Literature Survey:

BINDSURF is an efficient and fast blind methodology for the determination of protein binding sites depending on the ligand that uses the massively parallel architecture of GPUs for fast prescreening of large ligand databases. It was developed by a group of scientists from University of Murcia, Spain in 2012 **(Linares I.S. et al; 2012)**. BINDSURF divides the whole protein surface into arbitrary independent regions (also known as spots). With the computational power provided by the efficient exploitation of the parallelism of GPUs, a large ligand database is screened against the target protein over its whole surface simultaneously, and docking simulations for each ligand are performed simultaneously in all the specified protein spots resulting in new spots found after the examination of the distribution of scoring function values over the entire protein surface. Using this approach, it has been found that BINDSURF predicts accurately and at an unprecedented speed the binding sites to which different ligands bind to the same protein in known cases that were problematic to other docking methods.BINDSURF is a stochastic methodology that uses the Monte Carlo energy minimization scheme.

BINDSURF processing times in the computers offered by Ibercivis are equivalent to the lowest-line GPUs which offer great performance at a very low-cost price and, sometimes, even improve the performance results of the high performance line of Nvidia GPUs, code-named Tesla **(Guerrero G.D.et al;2014).**

Deshmukh K.B. et al;2015 describes implementation of Smith-Waterman (SW) algorithm on the Graphics Processing Unit (GPU) with parallel scan approach, aiming to accelerate SW alignment. Also optimization technique are introduces like reduce accessing global memory so that it can helps to reduce a latency time. Proposed system developed using Compute Unified Device Architecture (CUDA), which provides by nvidia GPU. Smith-Waterman algorithm is providing optimal local alignment which has quadratic time and space complexity. In several real time applications huge sequences are aligned to discover structural, functional and evolutionary characteristics of newly generated sequence. To evaluate performance, proposed system uses sequence retrieved from the NCBI site.The proposed algorithm implemented on NVIDIA GTX 680 Graphics card using CUDA.

They have tested the performance of serial implementation of Smith-Waterman algorithm with OpenMP implementation and finally CUDA based implementation of parallel scan approach of SW algorithm. Results shows that CUDA based implementation takes lesser time with an increase in number of input size than that of the serial implementation and OpenMP based implementation of SW algorithm, i.e. the implementation of Smith-waterman algorithm with the parallel scan approach on GPU able to align large biological sequences.There are various algorithm available based on GPU but drawback is that they are able to calculate only score but not alignment for complex biological sequence. Smith waterman algorithm with parallel scan approach provides score as well as alignment for huge biological sequences and increasing efficiency of alignment calculation as compared to serial and OpenMP implementation.

Arioc is a read aligner that uses GPU-based parallel sort and reduction techniques to identify high-priority locations where potential alignments may be found. The Arioc pipeline implementation consists of one-time-only initialization (memory allocation, loading of lookup tables and reference data) followed by iterative batched processing of reads (query sequences). Within each batch, non-gapped alignments are discovered using GPU-based spaced seed alignment. Gapped alignments, using GPU-based seed-and-extend alignment, are computed only for reads for which a satisfactory number of non-gapped alignments are not found. All mappings are finalized (scored and mapped), classified, and reported in multiple concurrent CPU threads. When alignments of DNA sequences are computed to a large genome, a key element in achieving high processing throughput is to prioritize locations in the genome where high-scoring mappings might be expected. Arioc demonstrates significantly greater throughput or accuracy than the other read aligners we evaluated across a wide range of sensitivity settings (**Wilton R. et al., 2015**).

BarraCUDA was developed in 2009 at the Metabolic Research Laboratories, University of Cambridge in collaboration with the Department of Computer Science, University College London. The software development is lead by Dr Brian Lam (Cantab) and Dr Bill Langdon (UCL). BarraCUDA is a sequence mapping software that utilizes the massive parallelism of graphics processing units (GPUs) to accelerate the inexact alignment of short sequence reads to a particular location on a reference genome **(http://seqbarracuda.sourceforge.net/index.html).**

BarraCUDA can align a paired-end library containing 14 million pairs of 76bp reads to the Human genome in about 9 minutes from fastq files to SAM alignment using a NVIDIA Tesla K80. The alignment throughput can be boosted further by using multiple GPUs (up to 8) at the same time **(Klus P. et al; 2012)**.BarraCUDA delivers a high level of alignment fidelity and is comparable to other mainstream alignment programs. It can perform gapped alignment with gap extensions, in order to minimize the number of false variant calls in re-sequencing studies.

BEAGLE is a high-performance library that can perform the core calculations at the heart of most Bayesian and Maximum Likelihood phylogenetics packages. It can make use of highly-parallel processors such as those in graphics cards (GPUs) found in many PCs. The API provides a uniform interface for performing calculations on an expanding variety of computer hardware platforms including GPUs, multicore CPUs, and SSE vectorization. On GPUs, the library provides novel algorithms and methods for evaluating likelihoods under arbitrary molecular evolutionary models, harnessing the large number of processing cores to efficiently parallelize calculations. Current results show speedups of up to 71-fold on a single GPU over CPU-based likelihood calculators. BEAGLE is currently integrated with three state-of-the-art phylogenetic software packages: MrBayes, BEAST, and GARLI, and compatible with many more. Forthcoming extensions include OpenCL support, single-precision SSE vectorization, improved performance for highly partitioned data sets, and additional high-level language wrappers, such as Python **(Ayres D.L. et al; 2012).**

CAMPAIGN is a library of data clustering algorithms and tools, written in ‘C for CUDA’ for Nvidia GPUs. The library provides up to two orders of magnitude

speed-up over respective CPU-based clustering algorithms and is intended as an open-source resource. New modules from the community will be accepted into the library and the layout of it is such that it can easily be extended to promising future platforms such as OpenCL. Its supported features includes K-means (and Kps-means, a K-means variant for GPUs with parallel sorting for improved performance), K-medoids, K-centers (a K-medoids variant in which medoids are placed only once according to a heuristic), Hierarchical clustering and Self-organizing map. The current library is limiting the size of usable datasets to the amount of memory available on the GPU, such as 4GB in case of the Tesla GPU used here for testing, with less memory available on more low-end graphic cards. The first batch of algorithms distributed with the initial release of the library offers one to two orders of magnitude speed-up as compared with CPU reference implementations **(Kohlhoff K.J. et al; 2011)**.

CUDASW++ is publicly available open-source software. It provides a significant performance improvement for Smith-Waterman-based protein sequence database searches by fully exploiting the compute capability of commonly used CUDA-enabled low-cost GPUs.Supported features include Parallel search of Smith-Waterman database with multiple GPU supports.CUDASW++ supports query sequences of length up to 59K and for query sequences ranging in length from 144 to 5,478 in Swiss-Prot release 56.6, the single-GPU version achieves an average performance of 9.509 GCUPS with a lowest performance of 9.039 GCUPS and a highest performance of 9.660 GCUPS, and the dual-GPU version achieves an average performance of 14.484 GCUPS with a lowest performance of 10.660 GCUPS and a highest performance of 16.087 GCUPS **(Liu Y. et al; 2009).**

CUSHAW is a parallelized short read aligner based on the compute unified device architecture (CUDA) parallel programming model. CUDA-compatible graphics hardwares are been exploited as accelerators to achieve fast speed. The algorithm uses a quality-aware bounded search approach based on the Burrows–Wheeler transform (BWT) and the Ferragina–Manzini index to reduce the search space and achieve high alignment quality. The performance evaluation, using simulated as well as real short read datasets, shows that the algorithm running on one or two graphics processing units achieves significant speedups in terms of execution time, while yielding comparable or even better alignment quality for paired end alignments compared with three popular BWT-based aligners: Bowtie, BWA and SOAP2. CUSHAW also delivers competitive performance in terms of single-nucleotide polymorphism calling for an Escherichia coli test dataset. This aligner only provides support for ungapped alignment and has been incorporated to NVIDIA Tesla Bio Workbench **(Liu Y. et al, 2012).**

G-BLASTN is a GPU-accelerated nucleotide alignment tool based on the widely used NCBI-BLAST. G-BLASTN can produce exactly the same results as NCBI-BLAST, and it has very similar user commands. Compared with the sequential NCBI BLAST, G-BLASTN can achieve an overall speedup of 14.80X under ‘mega-blast’ mode. More impressively, it achieves an overall speedup of 7.15X over the multithreaded NCBI-BLAST running on 4 CPU cores. When running under ‘blastn’ mode, the overall speedups are 4.32X (against 1-core) and 1.56X (against 4-core). G-BLASTN also supports a pipeline mode that further improves the overall performance

by up to 44% when handling a batch of queries as a whole. Currently G-BLASTN is best optimized for databases with long sequences **(Zhao K. et al; 2014).**

GPU-BLAST is an accelerated version of the popular NCBI-BLAST using general-purpose graphics processing unit (GPU). The implementation is based on the source code of NCBI-BLAST, thus maintaining the same input and output interface while producing identical results. In comparison to the sequential NCBI-BLAST, the speedups achieved by GPU-BLAST range mostly between 3 and 4.That implies GPU-BLAST can speed up the popular NCBI-BLAST code by nearly four times while producing identical results. Moreover, the implementation is capable of using the GPU along with multiple CPU cores concurrently. The present version of GPU-BLAST only works for BLASTP. The source code of GPU-BLAST is freely available athttp://archimedes.cheme.cmu.edu/biosoftware.html.**(Vouzis P.D. et al; 2010).**

CLUS_GPU-BLASTP is another CUDA implementation of protein BLAST to search multiple query sequences in parallel on GPU-enabled cluster. The head node performs the task of work distribution and result compilation. Subject database is divided into multiple fragments by the head node. Each compute node is allocated a different fragment to be searched against the query sequences. For concurrent processing of query sequences, PBS scheduler is used to schedule the query sequences to different compute nodes. Each participating compute node is GPU enabled. In comparison with the famous GPUBLAST, CLUS_GPU-BLASTP implementation is 2.1 times faster on single compute node. On a cluster of 12 compute nodes, this implementation gives a speedup of 13.2X. In comparison with standard single-threaded NCBI-BLAST, CLUS_GPU-BLASTP achieves a speedup ranging from 7.4X to 8.2X. **(Rani S. et al; 2017).**

GHOSTM is a highly efficient homology search algorithm suitable for graphics processing unit (GPU) calculations that was implemented as a GPU system. The system first searches for candidate alignment positions for a sequence from the database using pre-calculated indexes and then calculates local alignments around the candidate positions before calculating alignment scores. If both of these processes are implemented on GPUs, a system achieves calculation speeds that are 130 and 407 times faster than BLAST with 1 GPU and 4 GPUs, respectively. The system also shows higher search sensitivity and has a calculation speed that is 4 and 15 times faster than BLAST with 1 GPU and 4 GPUs **(Suzuki S. et al; 2012).**

LASSIE is a "black-box" GPU-accelerated deterministic simulator, specifically designed for large-scale models and not requiring any expertise in mathematical modeling, simulation algorithms or GPU programming. Given a reaction-based model of a cellular process, LASSIE automatically generates the corresponding system of Ordinary Differential Equations (ODEs), assuming mass-action kinetics.The computational performance of LASSIE are assessed using a set of randomly generated synthetic reaction-based models of increasing size, ranging from 64 to 8192 reactions and species, and compared to a CPU-implementation of the LSODA numerical integration algorithm.

LASSIE adopts a novel fine-grained parallelization strategy to distribute on the GPU cores all the calculations required to solve the system of ODEs. By virtue of this implementation, LASSIE achieves up to 92× speed-up with respect to LSODA, therefore reducing the running time from approximately 1 month down to 8 hrs to

simulate models consisting in, for instance, four thousands of reactions and species. Notably, due to its smaller memory footprint, LASSIE is able to perform fast simulations of even larger models, whereby the tested CPU-implementation of LSODA failed to reach termination. LASSIE is therefore expected to make an important breakthrough in Systems Biology applications, for the execution of faster and in-depth computational analyses of large-scale models of complex biological systems **(Tangherloni A. et al.; 2017).**

MUMmerGPU is an open-source high-throughput parallel pairwise local sequence alignment program that runs on commodity Graphics Processing Units (GPUs) in common workstations. MUMmerGPU uses the new Compute Unified Device Architecture (CUDA) from nVidia to align multiple query sequences against a single reference sequence stored as a suffix tree. By processing the queries in parallel on the highly parallel graphics card, MUMmerGPU achieves more than a 10-fold speedup over a serial CPU version of the sequence alignment kernel, and outperforms the exact alignment component of MUMmer on a high end CPU by 3.5-fold in total application time when aligning reads from recent sequencing projects using Solexa/Illumina, 454, and Sanger sequencing technologies. MUMmerGPU is low cost, ultra-fast sequence alignment program designed to handle the increasing volume of data produced by new, high-throughput sequencing technologies. MUMmerGPU demonstrates that even memory-intensive applications can run significantly faster on the relatively low-cost GPU than on the CPU **(Schatz M.C. et al.; 2007).**

Parallel-META, a GPU- and multi-core-CPU-based open-source pipeline for metagenomic data analysis, which enabled the efficient and parallel analysis of multiple metagenomic datasets. In Parallel-META, the similarity-based database search was parallelized based on GPU computing and multi-core CPU computing optimization. Experiments have shown that Parallel-META has at least 15 times speed-up compared to traditional metagenomic data analysis method, with the same accuracy of the results **(Su X. et al.; 2011).**

NVBIO is an open source C++ library of reusable components designed to accelerate bioinformatics applications using CUDA. Supported features include data structures, algorithms, and utility routines useful for building complex computational genomics applications on CPU-GPU systems **(http://nvlabs.github.io/nvbio/index.html).**

PEANUT is a read mapper for DNA or RNA sequence reads to a known reference genome.It Achieves supreme sensitivity and speed compared to current state of the art read mappers like BWA MEM, Bowtie2 and RazerS3. PEANUT reports both only the best hits or all hits **(Koster J. et al.; 2014).**

REACTA is a modified version of GCTA with improved computational performance, support for Graphics Processing Units (GPUs), and additional features. The purpose of REACTA is to quantify the contribution of genetic variation to phenotypic variation for complex traits.It's supported features include GRM creation, REML analysis, Regional Heritability (including multi-GPU) **(Cebamanos L. et al. ;2014).**

REACTA is no longer under active development or support. The source code remains freely available. REACTA has been superseded by DISSECT.

DISSECT is a new, easy to use, and freely available software which is able to exploit the parallel computer architectures of supercomputers to perform a wide range of genomic and epidemiologic analyses which

currently can only be carried out on reduced sample sizes or in restricted conditions. In the work of **Xandri O.C. et al.; 2015,**they have showcased this new tool by addressing the challenge of predicting phenotypes from genotype data in human populations using Mixed Linear Model analysis.They have analyzed simulated traits from half a million individuals genotyped for 590,004 SNPs using the combined computational power of 8,400 processor cores. It was found that prediction accuracies in excess of 80% of the theoretical maximum could be achieved with large numbers of training individuals.

SeqNFind is a powerful tool suite that addresses the need for complete and accurate alignments of many small sequences against entire genomes utilizing a unique hardware/software cluster system for facilitating bioinformatics research in Next Generation sequencing and genomic comparisons. Its supported features include Hardware and software for reference assembly, blast, SW, HMM, de novo assembly **(Carr D.A. et al.; 2011).**

MCUDA-MEME is a bioinformatics application based on the MEME algorithm. With properties similar to LAMMPS, MCUDA-MEME is multi-thread and multi process, though in this code each process needs a GPU. In consequence, they must run in different nodes **(Liu Y. et al.; 2011).**

SOAP3 is another GPU-based software for aligning short reads with a reference sequence. It can find all alignments with k mismatches, where k is chosen from 0 to 3. Supported features include short read alignment tool that is not heuristic based; reports all answers **(Liu C.M. et al.; 2011).**

SOAP3-dp is an ultra-fast GPU-based tool for short read alignment via index-assisted dynamic programming.It's supported features includes Borrows-Wheeler Transformation, Dynamic Programming etc.Compared with widely adopted aligners including BWA, Bowtie2, SeqAlto, CUSHAW2, GEM and GPU-based aligners BarraCUDA and CUSHAW, SOAP3-dp was found to be two to tens of times faster, while maintaining the highest sensitivity and lowest false discovery rate (FDR) on Illumina reads with different lengths. Transcending its predecessor SOAP3, which does not allow gapped alignment, SOAP3-dp by default tolerates alignment similarity as low as 60%. Real data evaluation using human genome demonstrates SOAP3-dp's power to enable more authentic variants and longer Indels to be discovered.SOAP3-dp natively supports BAM file format and provides the same scoring scheme as BWA, which enables it to be integrated into existing analysis pipelines **(Luo R et al.;2013).**

UGENE is multi platform open-source software with the main goal of assisting molecular biologists without much expertise in bioinformatics to manage, analyze and visualize their data. UGENE integrates widely used bioinformatics tools within a common user interface. The toolkit supports multiple biological data formats and allows the retrieval of data from remote data sources.It provides visualization modules for biological objects such as annotated genome sequences, Next Generation Sequencing (NGS) assembly data, multiple sequence alignments, phylogenetic trees and 3D structures. Most of the integrated algorithms are tuned for maximum performance by the usage of multithreading and special processor instructions. UGENE includes a visual environment for creating reusable workflows that can be launched on local resources or in a High Performance Computing (HPC) environment. UGENE is written in C++ using the Qt framework. The built-in plugin system and structured UGENE API make it possible

to extend the toolkit with new functionality **(Okonechnikov K. et al.; 2012).**

WideLM fits large numbers of linear models to a fixed design matrix and response. An Nvidia GPU is used to accelerate model fitting, with the CUDA API enabling parallel execution of multiple individual fits. The individual models must have modest size. The package implements a chunking interface to the GPU kernel, allowing the caller to stream model specifications. Hence the number of fits to be performed is essentially unlimited**(https://crantastic.org/packages/WideLM).**

ACEMD is a production-class biomolecular dynamics (MD) engine supporting CHARMM and AMBER force fields. Designed specifically for GPUs it is able to achieve supercomputing scale performance of 40 ns/day for all-atom protein systems with over 23 000 atoms. The ability to model these systems for tens of nanoseconds per day makes it feasible to perform simulations of up to the microsecond scale over the course of a few weeks on a suitable GPU-equipped machine **(Harvey M.J. et al.;2009).**

AMBER is a suite of programs to simulate molecular dynamics on biomolecule. Assisted Model Building with Energy Refinement (AMBER) is a family of force fields for molecular dynamics of biomolecules originally developed by Peter Kollman's group at the University of California, San Francisco. AMBER is also the name for the molecular dynamics software package that simulates these force fields. Specific features include PMEMD Explicit Solvent and GB Implicit Solvent **(Pearlman D.A. et al.; 1995).**

Chemistry at Harvard Macromolecular Mechanics (CHARMM) is the name of a widely used set of force fields for molecular dynamics, and the name for the molecular dynamics simulation and analysis computer software package associated with them.The CHARMM Development Project involves a worldwide network of developers working with Martin Karplus and his group at Harvard to develop and maintain the CHARMM program. It has been developed over the last three decades with a primary focus on molecules of biological interest, including proteins, peptides, lipids, nucleic acids, carbohydrates, and small molecule ligands, as they occur in solution, crystals, and membrane environments. For the study of such systems, the program provides a large suite of computational tools that include numerous conformational and path sampling methods, free energy estimators, molecular minimization, dynamics, and analysis techniques, and model-building capabilities. Calculations with CHARMM can be performed using a number of different energy functions and models, from mixed quantum mechanical-molecular mechanical force fields, to all-atom classical potential energy functions with explicit solvent and various boundary conditions, to implicit solvent and membrane models. Supported features include Implicit (5x), Explicit (2x) Solvent via OpenMM, ported natively to GPUs **(Brooks B.R. et al.; 2009).**

DESMOND is a high-speed molecular dynamics simulations of biological systems. It's code uses novel parallel algorithms and numerical techniques to achieve high performance and accuracy with multi-GPU support. Thecode is written in CUDA C++, that is designed for the execution of molecular dynamics (MD) simulations of biological systems on NVIDIA Graphics Processing Units.The 2016 version of Desmond/GPU used in this report does not support the use of more than one GPU in a

single MD simulation, though replica exchange simulations can use more than one GPU. This change in the software allowed for large improvements in performance and increased simulation system sizes. For a comparison of Desmond performance on CPUs versus GPUs, and for comparative performance of the current version of Desmond/GPU with the previous version, the preceding performance study is to be referred **(Bergdorf M. et al.; 2016).**

ESPResSo is a highly versatile software package for performing and analyzing scientific Molecular Dynamics many-particle simulations of coarse-grained atomistic or bead-spring models as they are used in soft-matter research in physics, chemistry and molecular biology.It's special features include Hydrodynamic / Electrokinetic forces P3M electrostatics.A particular strength of ESPResSo is its efficient treatment of long range interactions for various geometries using sophisticated algorithms like P3M, MMM2D, MMM1D and ELC. It is already equipped with a broad variety of interaction potentials, thermostats, and ensemble integrators; it offers the usage of constraints, masses and rotational degrees of freedom; it allows to move between different ensembles on-the-fly. An efficient MPI parallelization allows the usage of multi-processor architectures. Strict usage of ANSI-C for the core functions and a Tcl-script driven user interface makes ESPResSoplatform independent. This also ensures easily modifiable interfaces to communicate with other MD/MC Packages, real-time visualization and other graphic programs **(Limbach HJ et al.; 2006).**

Folding@home is a distributed computing system first released in 2000 to provide such resources needed to simulate protein folding and other biomolecular phenomena like misfolding, aggregation, and related diseases. Now operating in the range of 5 PetaFLOPS sustained, it provides more computing power than can typically be gathered and operated locally due to cost, physical space, and electrical/cooling load. Its suppoted features include powerful distributed computing molecular dynamics system; implicit solvent and folding **(Beberg AL et al.; 2009).**

GPUgrid.net is a distributed computing project that uses GPUs for molecular simulations.This projrct was initiated from the Universitat Pompeu Fabra in Barcelona,Spain. The main feature of GPUGRID.net is the brute force that it allows in terms of computational power by using accelerator processors, not only as an aggregate, but also as individual volunteered machines.This level of granularity is a fundamental requirement for all-atom molecular simulations as it permits the use of a wide range of protocols on a very volatile grid **(Rinaldi A. et al.;2009).**Specific features include High-performance all-atom biomolecular simulations; explicit solvent and binding.

GROMACS is a parallel message-passing implementation of a molecular dynamics (MD) program that is useful for bio(macro)molecules in aqueous environment is described. The software has been developed for a custom-designed 32-processor ring GROMACS (GROningen MAchine for Chemical Simulation) with communication to and from left and right neighbours, but can run on any parallel system onto which a a ring of processors can be mapped and which supports PVM-like block send and receive calls. The GROMACS software consists of a preprocessor, a parallel MD and energy minimization program that can use an arbitrary number of processors (including one), an optional monitor, and several analysis tools. The programs are written in

ANSI C and available by ftp (information: gromacs@chem.rug.nl). The functionality is based on the GROMOS (GROningen MOlecular Simulation) package **(Berendsen HJ et al;1995)**.Special features include Implicit (5x) and Explicit (2x) Solvent.

HAL's MD package is a high-precision molecular dynamics package for large-scale simulations of the complex dynamics in inhomogeneous liquids. It has been specially designed to support acceleration through CUDA-enabled graphics processors **(http://halmd.org/#)**.It's features include simple fluids and binary mixtures (pair potentials, high-precision NVE and NVT, dynamic correlations), GPU-acceleration of 1 NVIDIA Kepler K20Xm GPU comparable to 100 CPU cores (Benchmarks), high performance and excellent numerical long-time stability (e.g., energy conservation).

HOOMD-blue is a new, open source code for performing molecular dynamics and related many-body dynamics simulations on graphics processing units (GPUs). All calculations are fully implemented on the GPU, enabling large performance speedups over traditional CPUs. On typical benchmarks, HOOMD-blue is about 60 times faster on a current generation GPU compared to running on a single CPU core. Efficient execution is achieved without any lack of generality and thus a wide variety of capabilities are present in the code, including standard bond, pair, angle, dihedral and improper potentials, along with the common NPT, NVE, NVT, and Brownian dynamics integration routines. The code is object-oriented, well documented, and easy to modify **(Anderson J. et al.; 2010).**

LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules,polymers) and coarse-grained or mesoscopic systems. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial decomposition of the simulation domain. Many of its models have versions that provide accelerated performance on CPUs, GPUs, and Intel Xeon Phis. From the implementation perspective, it is a multi-thread and multi-process application which needs at least one GPU to host their processes, but can benefit from the use of multiple GPUs **(http://lammps.sandia.gov/).**

MELD is an OpenMM plugin written for GPUs.It's features include integrative approach to combine physics and information Orders of magnitude faster protein folding than brute force MD. MELD draws Bayesian inferences from semi-reliable data in the context of atomistic REMD computer simulations, to give accurate protein structures.In a way, MELD follows from an old line of thought that if we knew the physical mechanisms for how proteins fold so fast, we could invent fast ways to search their conformational spaces to find native like states **(MacCallum J.L et al.;2015).**

NAMD is a molecular dynamics program designed for high performance simulations of large biomolecular systems on parallel computers. An object-oriented design implemented using C++ facilitates the incorporation of new algorithms into the program. NAMD uses spatial decomposition coupled with a multithreaded, message-driven design, which is shown to scale efficiently to multiple processors. Also, NAMD incorporates the distributed parallel multiple tree algorithm for full electrostatic force evaluation in O(N) time. NAMD can be connected via a communication system to a molecular graphics program in order to provide an interactive modeling tool for viewing

and modifying a running simulation **(Nelson M.T. et al.;1996).**

OpenMM is a library and application for molecular dynamics for HPC with GPUs. OpenMM also includes several methods of time integration and the ability to enforce distance constraints. These features are implemented in three different Platforms: a reference Platform written in C++, a CUDA based Platform for Nvidia GPUs, and an OpenCL based Platform for a variety of GPUs and CPUs.The newest feature of OpenMM is custom forces that let the user specify an arbitrary algebraic expression for the form of their force **(Eastman P. et al.;2015)**. A person with no GPU programming experience can still implement arbitrary functional forms for their nonbonded interactions, and get nearly as good performance as hand tuned GPU code.

SOP-GPU or Self Organized Polymer Model fully implemented on a GPU, is a scientific software package designed to perform Langevin Dynamics Simulations of the mechanical or thermal unfolding, and mechanical indentation of large biomolecular systems in the experimental subsecond (millisecond-to-second) timescale.It features Langevin dynamics simulations using the coarse-grained Self Organized Polymer (SOP) model, Multiple simulation trajectories can be performed simultaneously on a single GPU, Calpha and Calpha-Cbeta models are supported, Simulations of protein forced unfolding, Novel simulations of nanoindentation in silico, Support for hydrodynamic interactions, Up to ~100 ms of simulation time per day, Systems of up to 1,000,000 amino-acids (on GPUs with 6GB or great memory).

Hence, SOP-GPU simulations can be utilized to explore the unfolding micromechanics of protein fibers, and to characterize the visco-elastic properties of viral capsids using the experimental force loads. This makes it possible to interprete the experimental force spectra and force-indentation profiles of biomolecules, obtained in dynamic force spectroscopy assays, and, thus, to bridge the gap between theory and experiments.For the accurate interpretation of the experimental data, dynamic force measurements *in silico* should be performed using the experimentally relevant pulling speeds. This can be achieved in reasonable wall-clock time using the SOP-GPU package **(Zhmurov A. et al.;2010).**

CONCLUSION:

A potential drawback of GPUs is the availability of memory and higher energetic requirements.As a matter of fact, many applications—in particular those processing genome-wide data—require a huge amount of memory, more than the few gigabytes contained on high-end GPUs at the time of writing. However, CUDA allows kernels to directly access CPU's RAM by means of 'pinned memory'. This type of memory is page-locked and can be directly read and written from the GPU, using Direct Memory Access through the PCI-express bus, without any involvement of the CPU.

In general, the most efficient GPU-powered implementations share the following characteristics: they leverage the high performance memories, and try to reduce the accesses to the global memory by exploiting GPU-optimized data structures.

Taking all of these mentioned issues into consideration, it can be anticipated that the increasing availability of GPU-powered tools in various research areas of life sciences—as well as the creation of massive GPU-based infrastructures, providing scientists with hexa-scale performances—will

finally enable the execution of fastest and thorough simulations and analyses of complex molecular structures, or pave the way to ambitious goals like genome-wide analyses and dynamical simulations of detailed mechanistic models of whole cells and organisms.

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