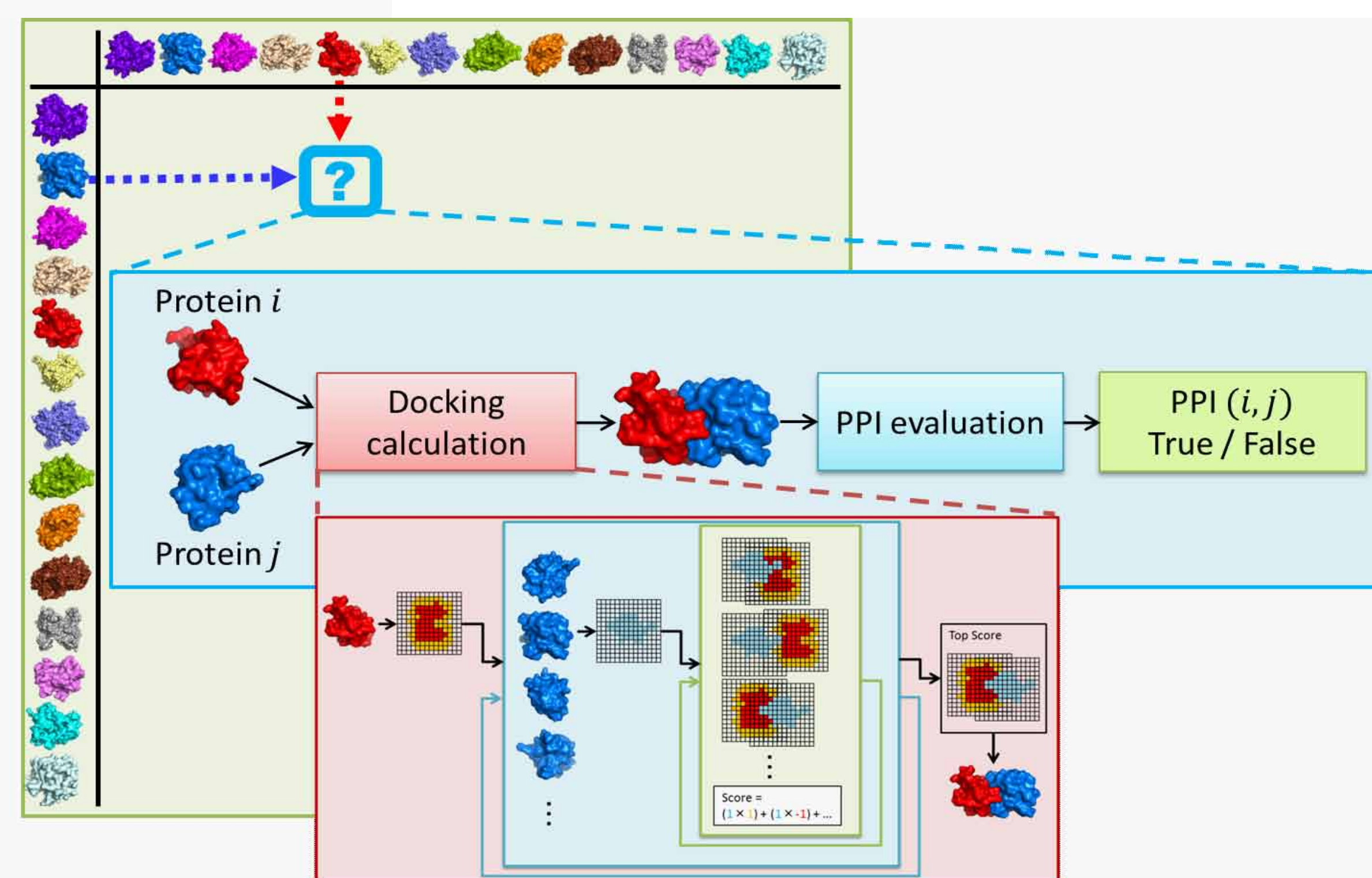


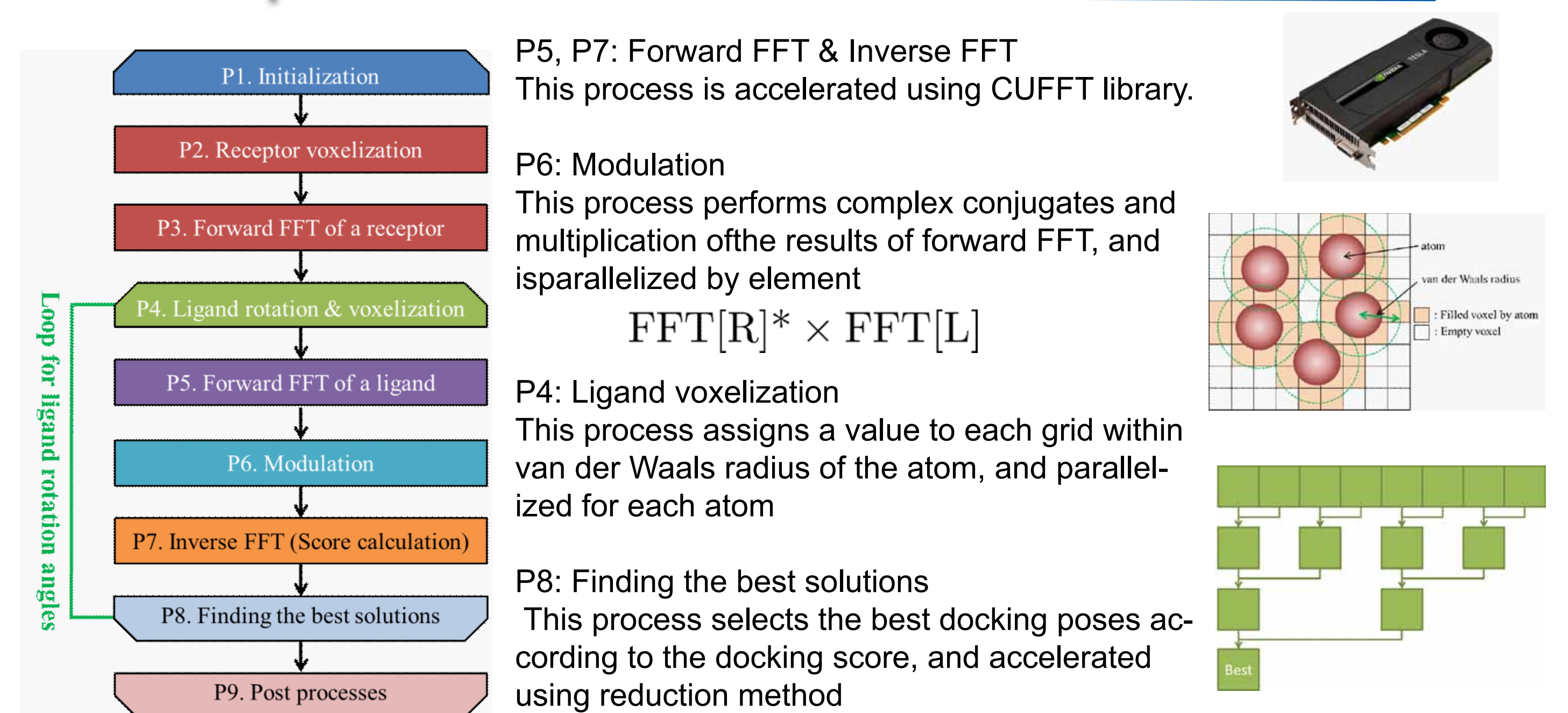


MEGADOCK-GPU: GPU-acceleration of protein-protein docking

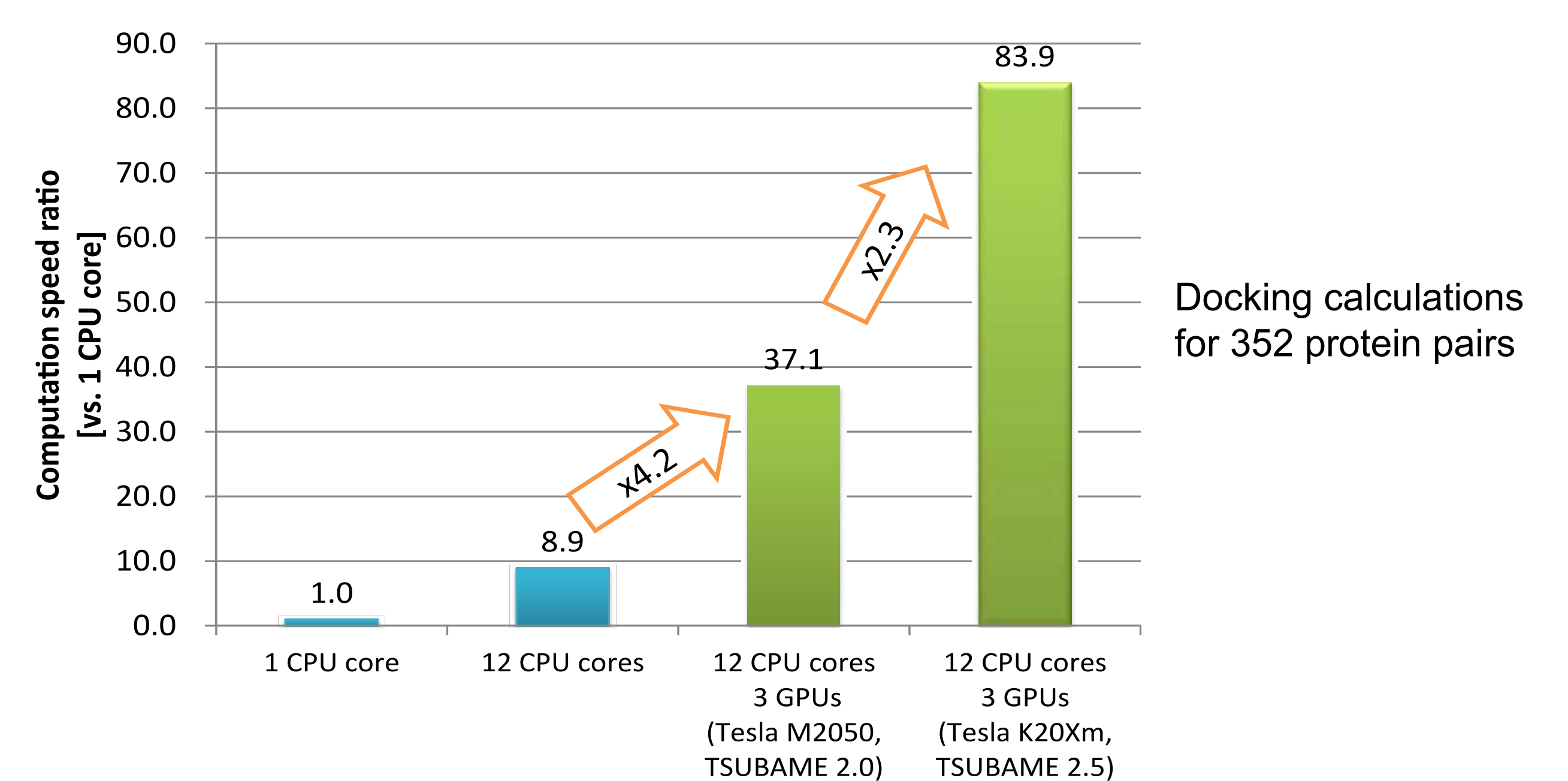
MEGADOCK [M. Ohue, et al., Protein Pept Lett, (2013)]



GPU implementation [T. Shimoda, et al., ParBio2013, (2013)]



Speedup by GPGPU



- Protein docking (rigid-docking based):
 - original rPSC model + electrostatic interaction
 - 3-D convolution by FFT: $O(n^6) \rightarrow O(n^3 \log n)$
- Protein-Protein Interaction (PPI) prediction:
 - post-docking analysis by clustering and threshold logic
 - multi-level MPI parallelization for all-to-all analysis
- PPI network prediction:
 - application to bacterial chemotaxis (about 100x100 pairs)
 - application to lung cancer pathway (about 500x500 pairs)

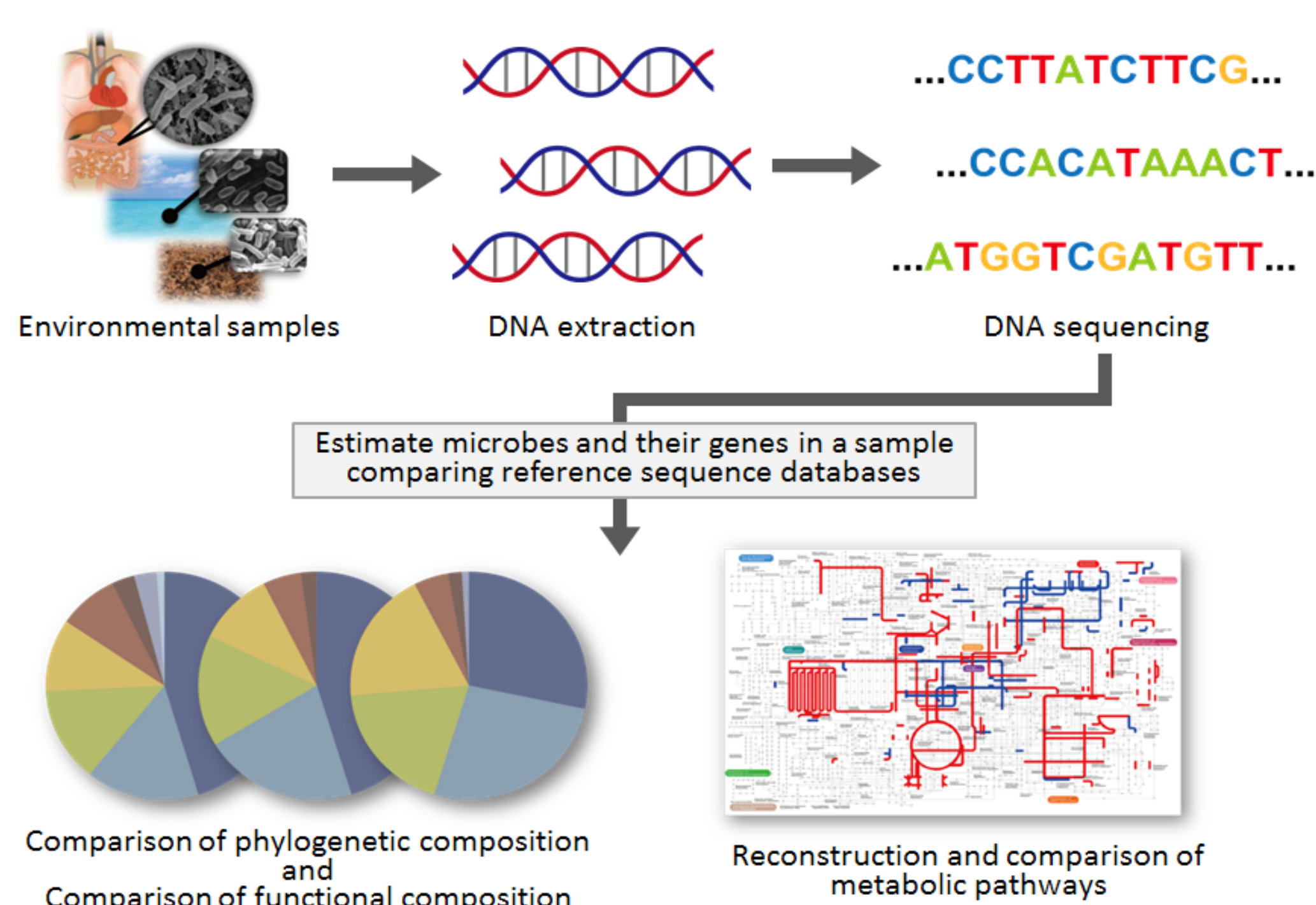
- 83.9-fold speedup with 3 GPUs on TSUBAME 2.5

GHOSTM: GPU-acceleration of sequence homology search

- Fast sequence homology search for metagenomics

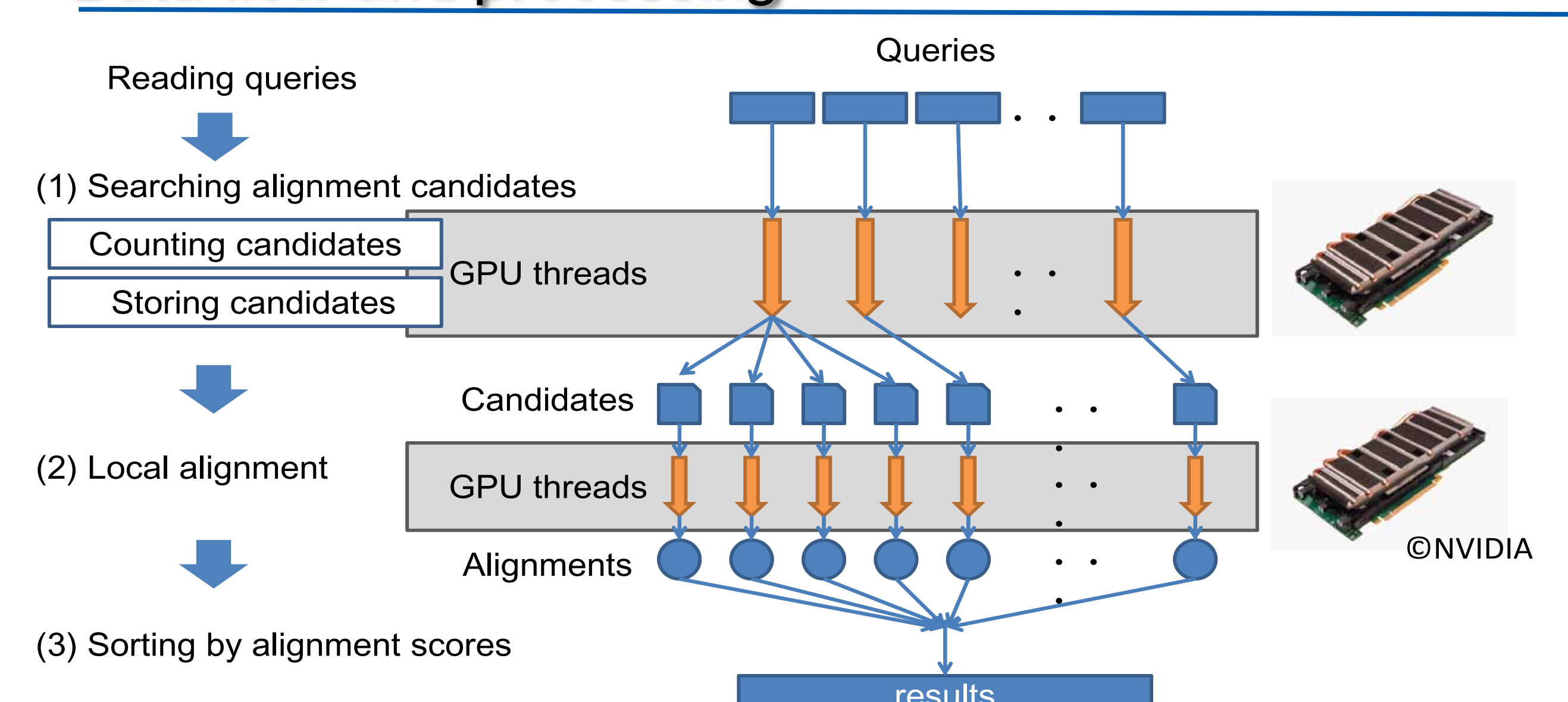
[Suzuki et al., PLoS ONE, (2012)]

- enough sensitive for metagenomic annotation
- similar to BLAST but optimized for GPU-calculation
- implemented on GPUs by NVIDIA CUDA
- approximately **130 times faster** than NCBI BLAST

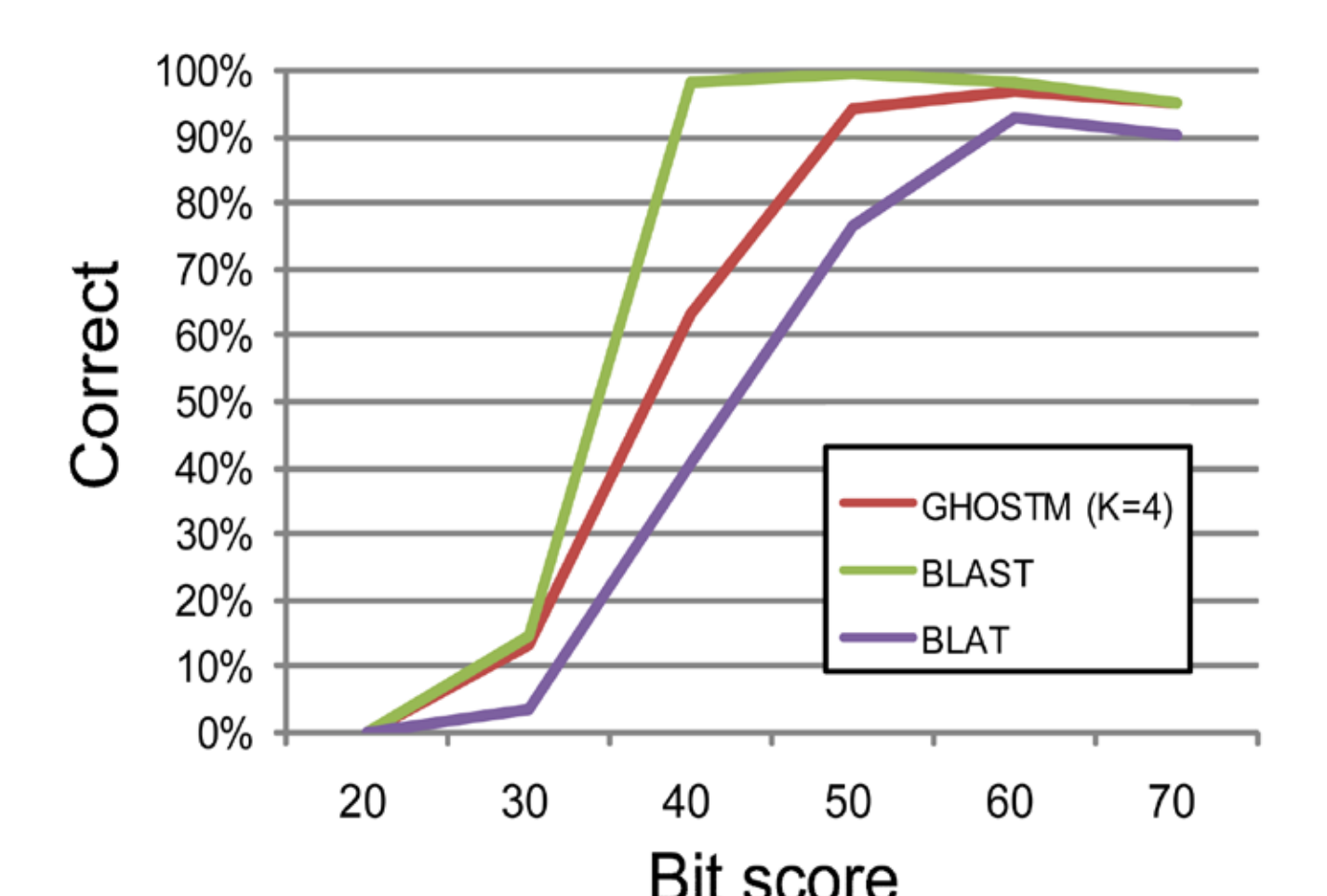
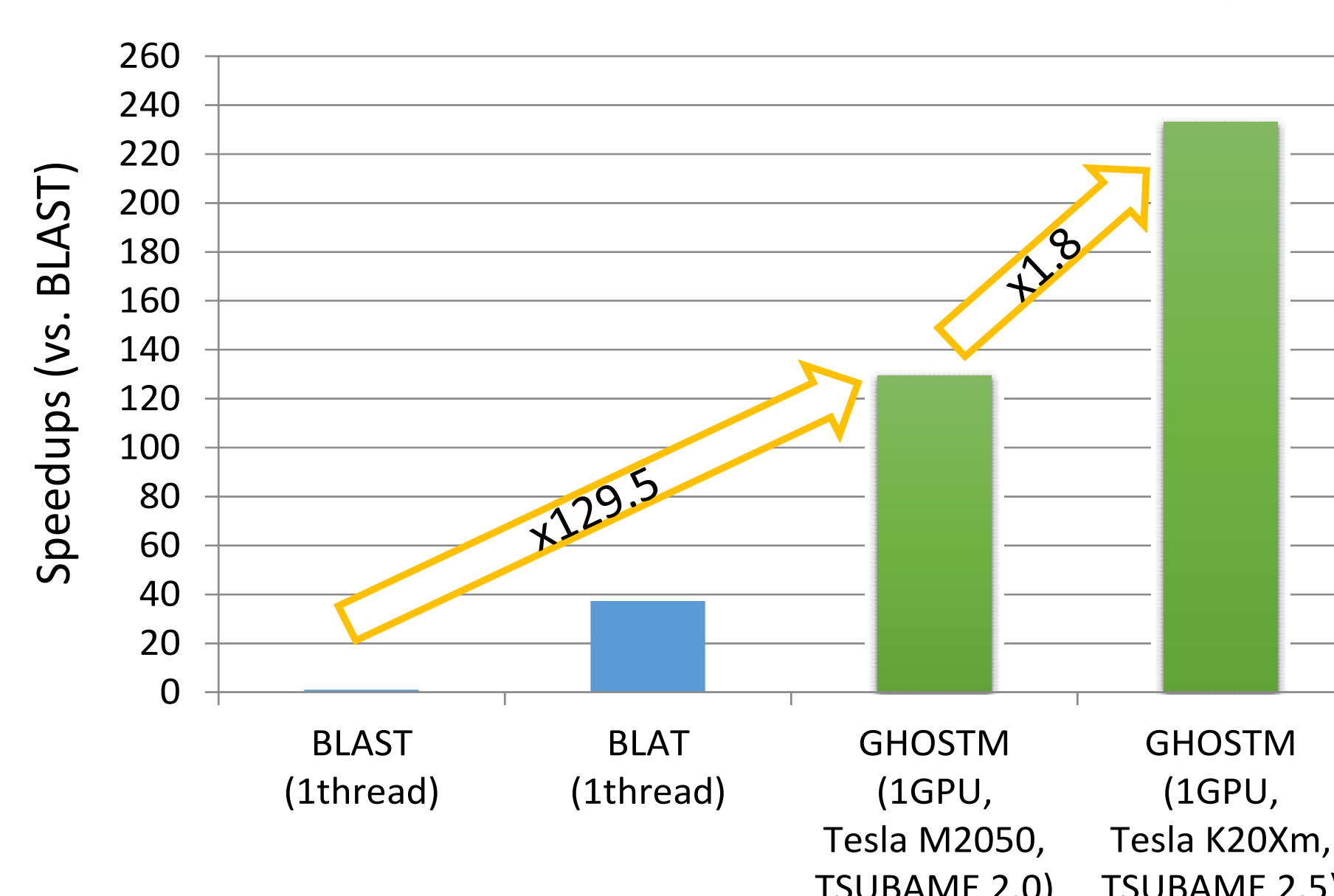


Metagenome analysis: the study of the genomes of uncultured microbes obtained directly from microbial communities in their natural habitats such as soils, seas, and human bodies.

Data flow and processing



Search speed and sensitivity



Correct answer: Smith-waterman local alignment algorithm by using SSEARCH

- 233-fold speedup with 1 GPU on TSUBAME 2.5