

UL HPC School 2017

PS6: Bioinformatics Workflows and Applications



UL High Performance Computing (HPC) Team

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Latest versions available on **Github**:



UL HPC tutorials:

<https://github.com/ULHPC/tutorials>

UL HPC School:

<http://hpc.uni.lu/hpc-school/>

PS6 tutorial sources:

<https://github.com/ULHPC/tutorials/tree/devel/advanced/Bioinformatics/>





Summary

- 1 Objectives
- 2 Bioinformatics packages
- 3 Notes
- 4 Practical session
- 5 Conclusion



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Better understand the usage of Bioinformatics packages on the UL HPC Platform.



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- very many associated workflows, thus excellent examples

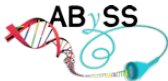


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- several applications in the ABYSS package
- only **ABYSS-P** is parallelized using MPI
 - ↳ started with the **abyss-pe** launcher
- workflow (pipeline) of **abyss-pe** also includes:
 - ↳ OpenMP-parallel applications
 - ↳ serial applications
- Note: compared with other de novo assemblers, the per-node memory requirements are smaller due to ABYSS' task distribution model



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- very large codebase: 1.836.917 SLOC
- many applications in the package, several parallelization modes
- **mdrun**: computational chemistry engine, performing:
 - ↔ molecular dynamics simulations
 - ↔ Brownian Dynamics, Langevin Dynamics
 - ↔ Conjugate Gradient
 - ↔ L-BFGS
 - ↔ Steepest Descents energy minimization
 - ↔ Normal Mode Analysis
- **mdrun** - parallelized using MPI, OpenMP, pthreads and with support for GPU acceleration



Bowtie2/TopHat

Bowtie2: Fast and sensitive read alignment

ultrafast & memory-efficient alignment of sequencing reads to long ref. sequences

TopHat: A fast spliced read mapper for RNA-Seq

alignment of RNA-Seq reads to a genome, to identify exon-exon splice junctions



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- TopHat aligns reads to mammalian-sized genomes using Bowtie
- then analyzes the mapping results to identify splice junctions between exons
- **bowtie2** is OpenMP-parallel
- rest of workflow is sequential



mpiBLAST

mpiBLAST: Open-Source Parallel BLAST

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- two main applications: **mpiblast** **mpiformatdb**
- requires (NCBI) substitution matrices and formatted BLAST databases
- the databases can be segmented
 - ↪ into as many segments as the # of cores that will be used when performing searches
 - ↪ or a multiple, in order to avoid load imbalance
- **mpiblast** requires ≥ 3 processes, 2 used for internal tasks
 - ↪ `mpirun -np 3 mpiblast [...]` only gives you one searcher process!



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.. on real world applications (bioinfo or others):

- make sure you *understand the parallel capabilities* of your software
 - ↔ pthreads/OpenMP vs MPI vs hybrid
 - ↔ use of GPU acceleration



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- make sure you *request the appropriate resources* for the processing needs of your workflow
 - ↪ Does the software always take advantage of more than 1 core or node?
 - ↪ How does it scale? Many obstacles to perfect scalability!



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.. on data management:

- make sure you use *the appropriate storage place*
 - ↪ \$HOME vs \$WORK vs \$SCRATCH
- stage data in/out, archive your (many & unused) 'small' files



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Exercises

- Read and understand the Bioinformatics tutorial

<https://github.com/ULHPC/tutorials/tree/devel/advanced/Bioinformatics/>

- Run the examples

↔ all calculations should be fast

↔ you should attempt the exercises proposed in each section

- Try even more tests, e.g.:

↔ on different node classes

↔ with one core per node on ≥ 2 nodes

↔ vs ≥ 2 cores on single node



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Conclusion

- Bioinformatics applications execution on the **UL HPC Platform**
- Outlined:
 - ↪ different workflows
 - ↪ some of the concepts you should care about when running complex software

Perspectives

- Personalize the UL HPC launchers with the specific commands for ABySS, Gromacs, TopHat, Bowtie, mpiBLAST..



Thank you for your attention...

Questions?

<http://hpc.uni.lu>

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