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Bioinformatics workflows in the cloud with Unipro UGENE

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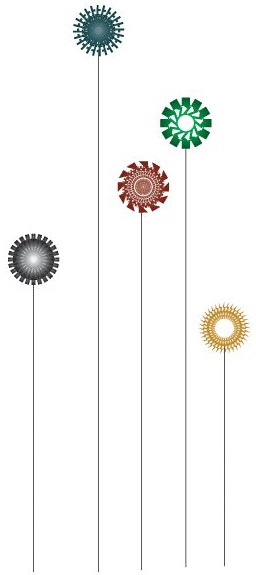
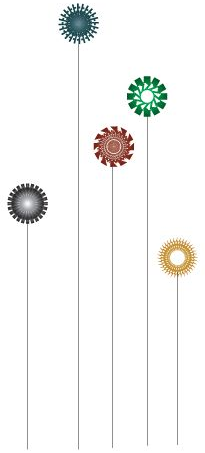


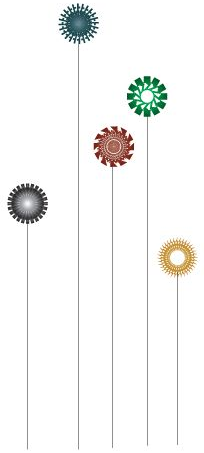
About this tutorial

- Intended audience
  - You are
    - Molecular biologist who uses bioinformatics tools in research
    - System administrator who looks for new software options for an organization
    - Martian secret service agent



Agenda

- Bioinformatics today
- Task complexity factors
- Computational workflows - overview
- Unipro UGENE project: features and capabilities
- UGENE Workflow Designer
- Cloud computing basics
- Running workflows in the cloud
- Free discussion



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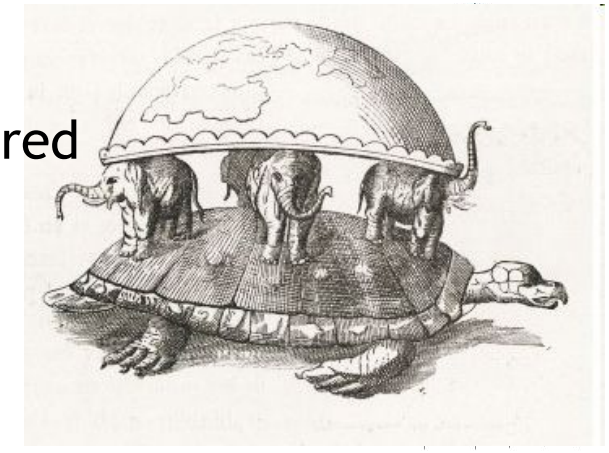
Bioinformatics today

- **Bioinformatics 15 years ago**
  - Pharmaceutical companies were not interested;
  - Life scientists believed that it was an outlet for failed biologists that want to play around with computers;
  - Computer scientists did not even consider it important, they confused it with bio-inspired “computer sciences”.



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Bioinformatics today

- Bioinformatics in 2002

  - Pharmaceutical companies believe that it is the most efficient way to streamline the process of drug discovery;

  - Some life scientists believe it is the solution to all problems in life sciences and that it will allow them to avoid doing some experiments;

  - Computer scientists are very interested. The scope and complexity of the domain makes it the ideal field of application of new software techniques and specialized hardware developments.

Bioinformatics today

- Bioinformatics in 2010
  - Pharmaceutical companies use it routinely, but have realized that it complements rather than replaces experimental work;
  - Computer scientists may have jumped on another fancy subject.
  - The United Nations has designated 2010 the International Year of Biodiversity
  - ….
  - Life scientists use it every day and try to learn on how to deal with >9000 tools and methods available

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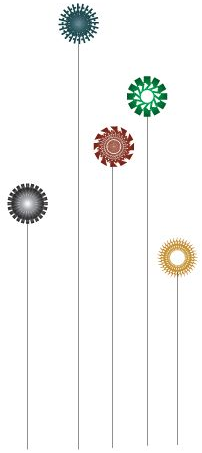
Bioinformatics today

Biological problems that computers can help with:

- I cloned a gene –is it a known gene?
- Does the sequence match? Is the sequence any good?
- Is the sequence similar to other known sequences?
- Which gene family does it belong to?
- The gene I´m interested in was found in another organism, but not in mine. How can I look for it?
- How is the gene expressed in different types of tissues?
- What is the biological function of the protein encoded by the gene?
- Is the gene associated with any disease?

What computer science is to molecular biology is like what mathematics has been to physics

Larry Hunter, ISMB'94



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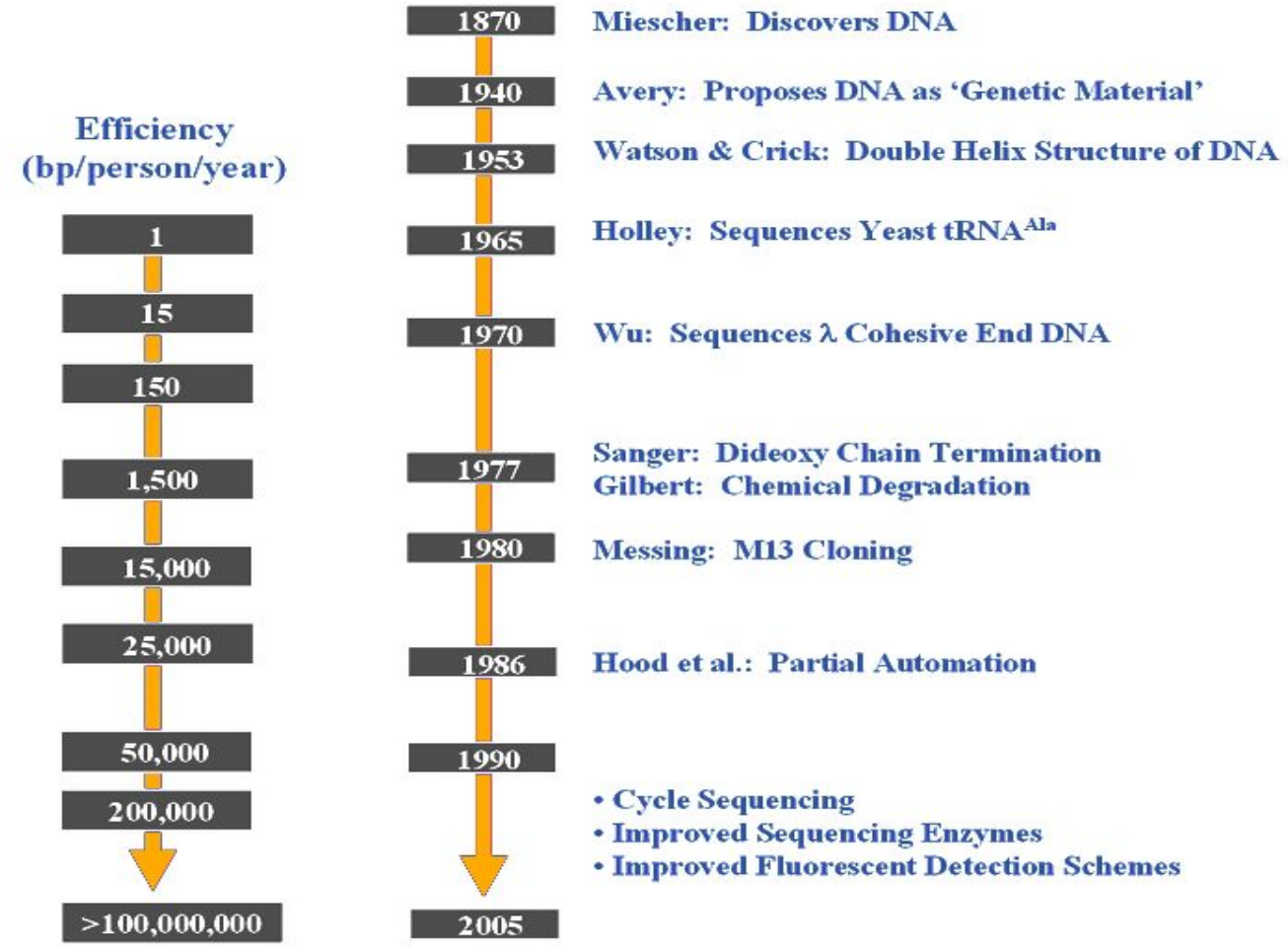
Task complexity factors
Data Volumes



Adapted from Messing & Llaca, PNAS (1998)

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Task complexity factors
Number of databases and protocols

Some words about DNA databases:

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Task complexity factors
Number of available methods, tools, data formats

BLAST,FASTA,SSEARCH,CLUSTAL,MUSCLE,MAFFT,KALIGN,UCLUST,HMMER2,
HMMER3,GARLIC,CONSED,CGVIEW,ERGO,EBBIE,MAUVE,MATTREE,COVE,
PSIBLAST,GOR,PSIPRED,EXPASY,EMBOSS,PHYLIPP,SAM,CASP,BLOCKS,PRIMER3,CSBLAST,HHPRED,BIOCONDUCTOR,M
UMMER,FEAST,BOWTIE,MAQ,SOAP,BIOPERL,POA, PRANK, FOLDALIGN,RMAP,SITECON,SHRIMP,BATWING,ASAP,
BEAST,MEGA,MESQUITE,SEMPHY,TNT,BIOEDIT,BIOPYTHON,GALAXY, TAVERNA, GENEMARK,
AMAP,MEME,PPSEARCH,ELPH,GENESCAN,ARTEMIS,CLANN,GENLUX,CRNPRED,BRAGI,DIP4FISH
ANGIS,AFFYMETRIX,GENECHIP,ARLEQUIN,BIOPHP,BIORUBY,BIOEXTRACT,BIOSLAX,BISKIT,CYTOSCAPE,DAVID,DIALIGN
-T,DIALIGN-TX,DNASTAR,ETBLAST FOLDX,FORMATDB,GENSCAN,GENTLE,GESS,GENMAPP,GENE,ACE, UGENE,ARGO,
DESIGNER,GENEDATA,ENEPATTERN,GENEVESTIGATOR,JALIGNER,MEGAN,ARKA
MODELLER,OLIGO,JPRED,STRIDE,TESS,GLIMMER,BIOECLIPSE,ENSEMBL,ASTERIAS,DPVIEW,
PAUP,PSORT,PHYLOSCAN,PUPASUITE,PYMOL,RAPTOR,RASMOL,STING,SIMBIOSYS,SNAGGER,SOAPLAB,SPLITSTREE,ST
EMLOC,T-COFFEE,PILER,USEARCH,DELTASTAT,DCSE,ASID,ARB,ANGLER,
TREEFINDER,UCSF CHIMERA,UTOPIA,VECTOR NTI,YASS,MUSCA,JASPAR

……

+ 9000 more (from Wikipedia)

- **Facts:**
  - A part of these tools use incompatible data formats
  - A part of these tools are not available for your computer platform
  - A part of these tools are too slow to be used effectively
  - A part of these tools cost money and have not free license
  - A part of these tools has critical bugs that can affect your results
  - A part of these tools lacks documentation
  - A part of these tools are not supported nor developed anymore
  - ...
  - You have no idea what most of these tools about or how to use them …

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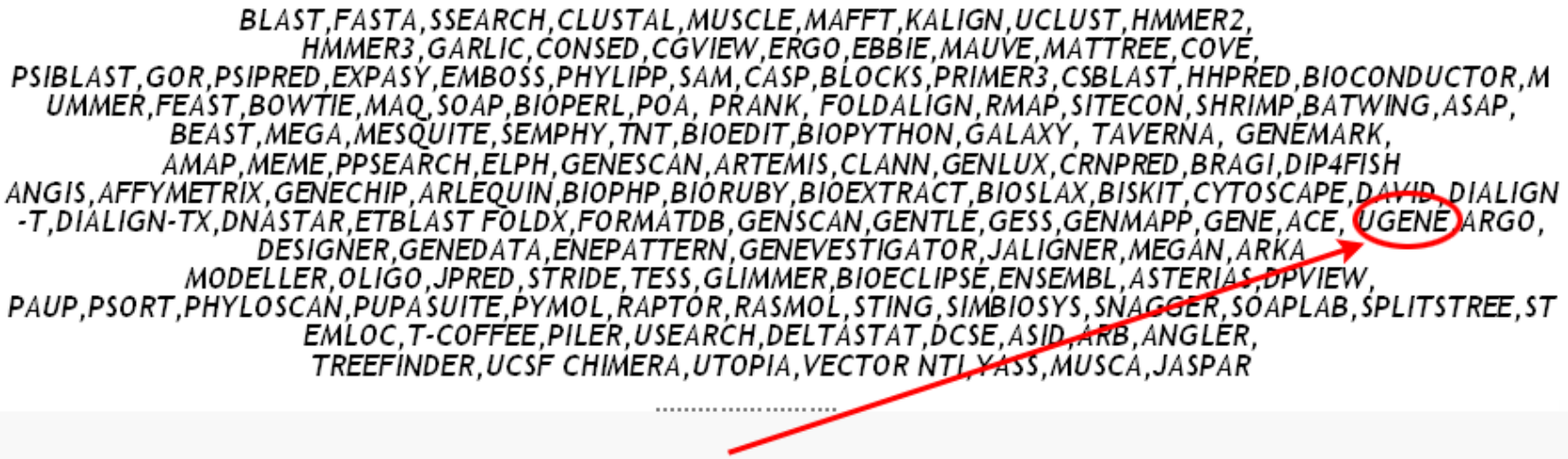
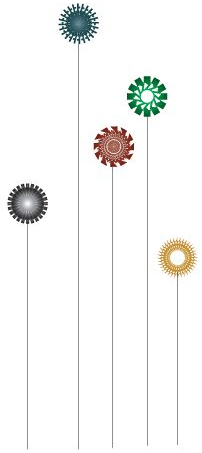
Unipro UGENE project about



- UGENE is one of a number of bioinformatics projects
- The goal of UGENE project is to integrate all other popular bioinformatics tools within a
  - Single application
  - Unified data model
  - Powerful user interface
    - » Do all above in open source



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UGENE capabilities (v1.7.2)

Algorithms:

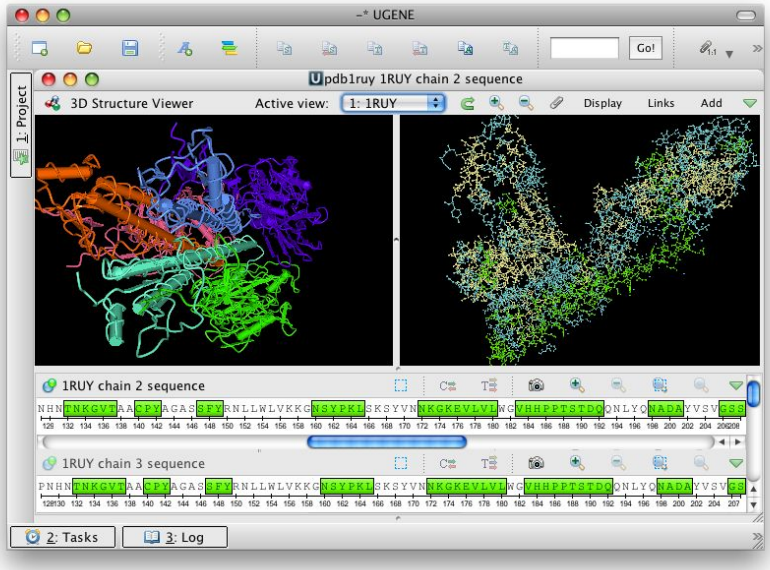
- Multiple sequence alignment using MUSCLE 3,4, KAlign, ClustalW, MAFFT;
- HMM profiles search, based on the source of HMMER2 and HMMER3 tools;
- PCR Primers design using Primer3;
- Protein secondary structure prediction using GORIV and PSIPRED;
- Phylogenetic analysis with Phylip;
- Search for restriction enzymes and integration with REBASE;
- Extremely fast repeat finder;
- DNA to reference assembly using Bowtie and own algorithms;
- Search for transcription factor binding sites using collection of weight and frequency matrix based algorithms (SITECON, JASPAR, UniProbe);
- Various statistical reports: GC content/deviation, I.Entropy, Karlin …
- Classic algorithms: ORFs, Smith-Waterman, protein back-translation;
- Comparing whole genomes using dotplot viewer;

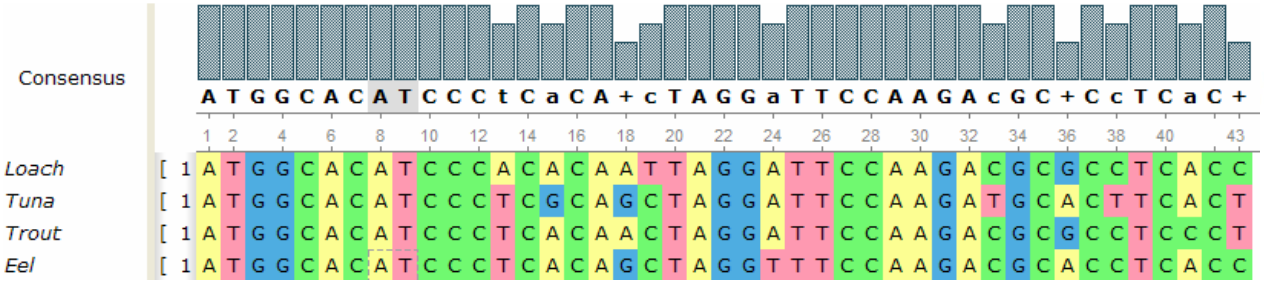
» *more*

UGENE capabilities (v1.7.2)

Visualization:

- DNA/Protein sequence & annotations
- Multiple sequence alignments
- 3D structures and surfaces
- Graphs and statistics
- Phylogenetic trees
- Chromatograms
- Plasmid maps
- Dot-plots





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UGENE capabilities (v1.7.2)

Data formats

- Genbank
- EMBL
- CLUSTAL
- MSF
- STOCKHOLM
- FASTA
- FASTQ
- NEWICK
- NEXUS
- ABI
- SCF
- HMMER2/3
- MMDB
- PDB
- GFF
- SAM
- CSV
- Plain text

- UGENE supports import and export data between all these formats
- All of these formats are auto-detected automatically
- User can work with files stored in gzipped (compressed) form
- Data files can be located on remote servers
- User is provided with powerful scripting language to extend the supported formats list

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UGENE capabilities (v1.7.2)

High performance computing

- UGENE is created to utilize effectively computational power as well as small workstations (P1 MMX, 64Mb RAM) as large data centers

- For the algorithms included UGENE has special optimizations for:
  - Multi-core CPUs
  - SIMD instruction sets (SSE,SSE2,AltiVEC)
  - CELL CPU architecture
  - NVIDIA GPUs with CUDA library
  - ATI GPUs with ATISTREAM library
  - Direct x86/x86_64 assembler snippets
  - Distributed computations

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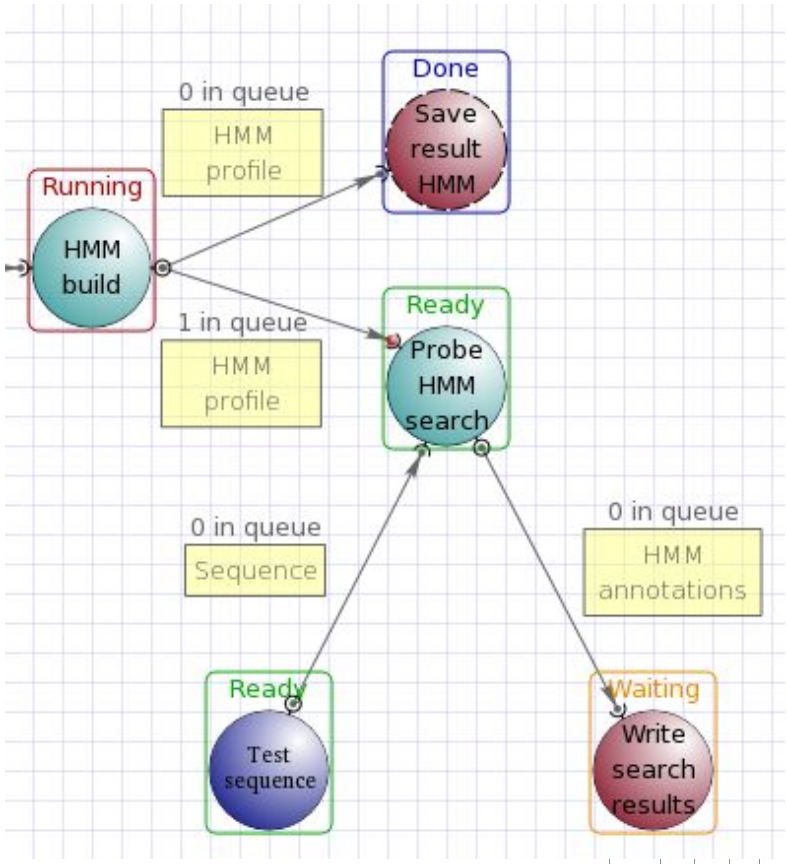
UGENE capabilities (v1.7.2)

Joining all together

- Task complexity
- Rich algorithm libraries
- Unified data formats
- High performance
- Powerful user interface

Workflow Designer



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UGENE Workflow Designer

- Goal
  - to make complex things simple
- Key feature
  - Simplicity
- How?
  - See next slide

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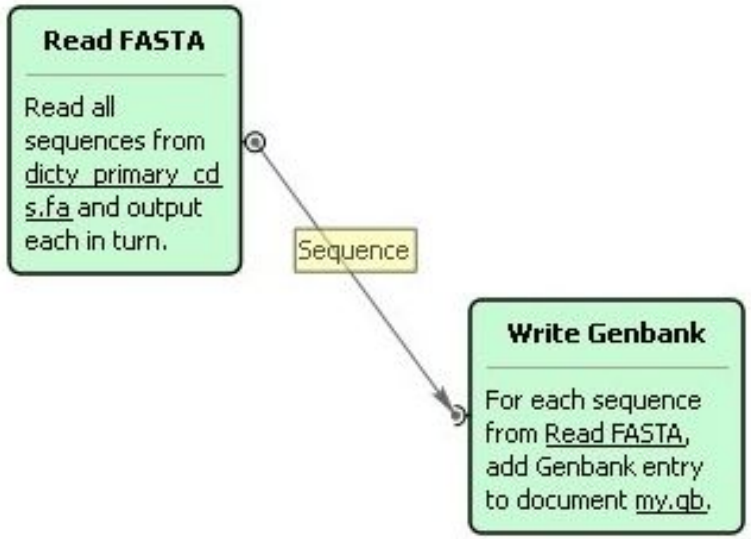
UGENE Workflow Designer

- A complete workflow sample
  (*a screenshot of User Interface)*



- Q: What will this workflow do?

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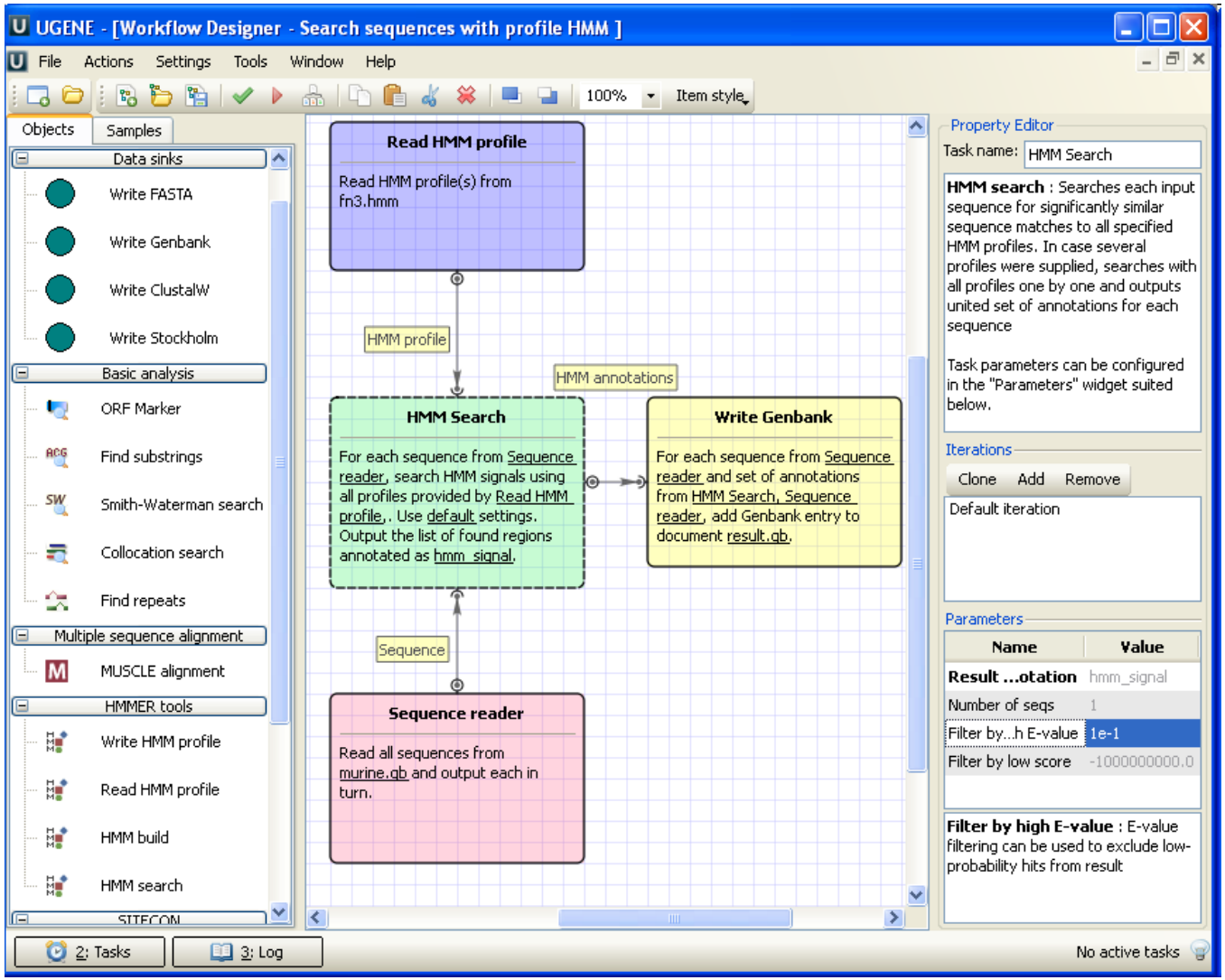
UGENE Workflow Designer layout



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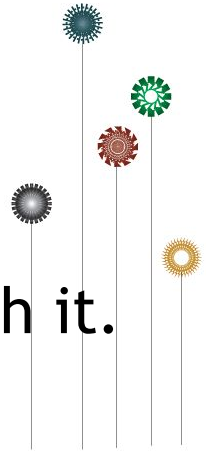
UGENE Workflow Designer basics

- Using drag&drop interface construct computational diagram from a set of algorithmic blocks or processes.
- Processes can be connected with each other using data-flow channels if they have input and output ports of the same data types.
- Each process in a diagram has a set of configurable parameters, specific to the logic of the algorithm it represents.
- Validate the workflow, correct any errors and launch it.



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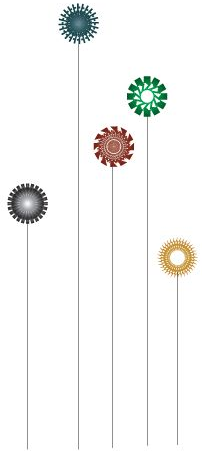
UGENE Workflow Designer practice

- Lesson 1 – Data format conversion
  - Goal: extract sequences from PDB files



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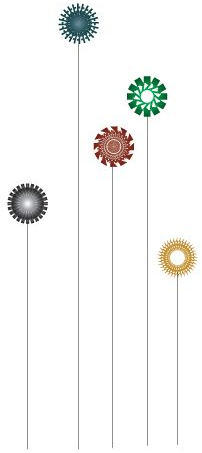
UGENE Workflow Designer practice

- Lesson 2 – Multiple sequence alignment
  - Align multiple files and save the result into desired file format



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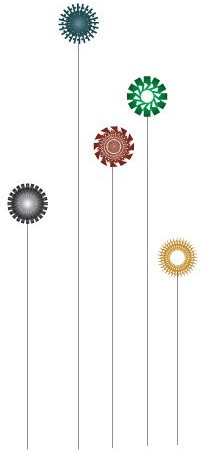
UGENE Workflow Designer practice

- Lesson 3 – Assemble a sequence
  - Run DNA assembly with Bowtie



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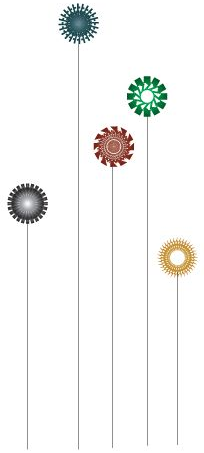
UGENE Workflow Designer reuse

- Run workflow multiple times
  - Run the same workflow multiple times for different data sets



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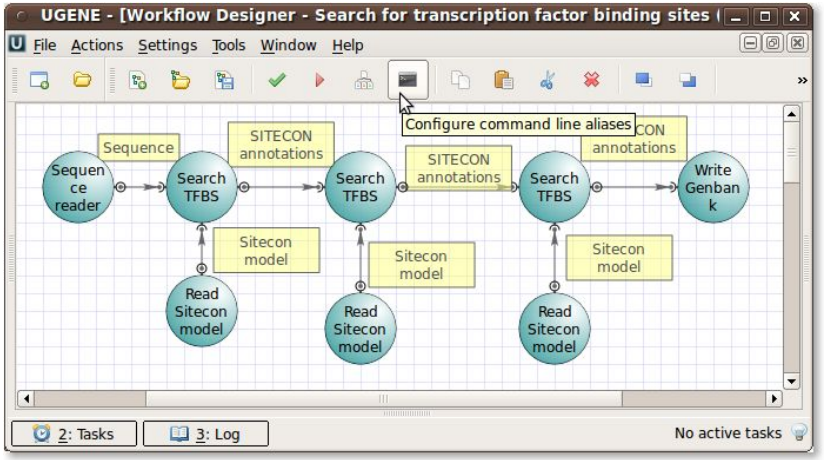
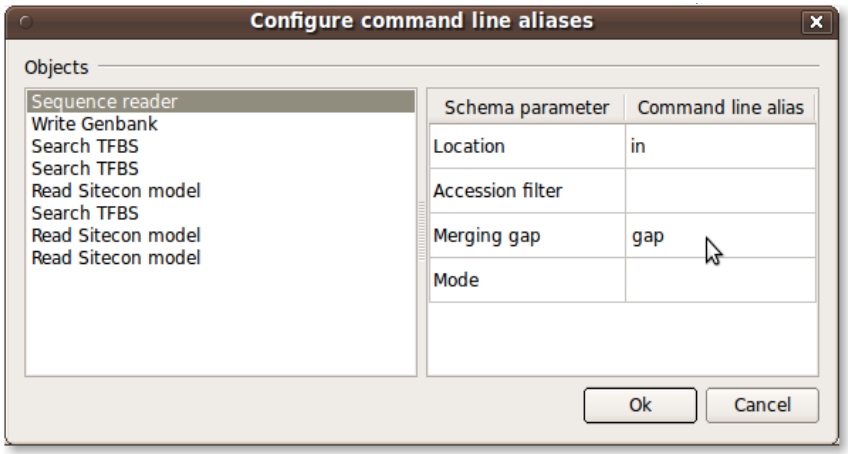
UGENE Workflow Designer reuse

- Create new shell command from workflow
  - Use your own workflow as a stand alone command line tool
  - Example:

```
ugene align --in=file1.aln --out=file2.ali
```

  - Where
    - ‘align’ is the name of the workflow
    - ‘--in’ and ‘--out’ are cmd-line aliases for workflow parameters





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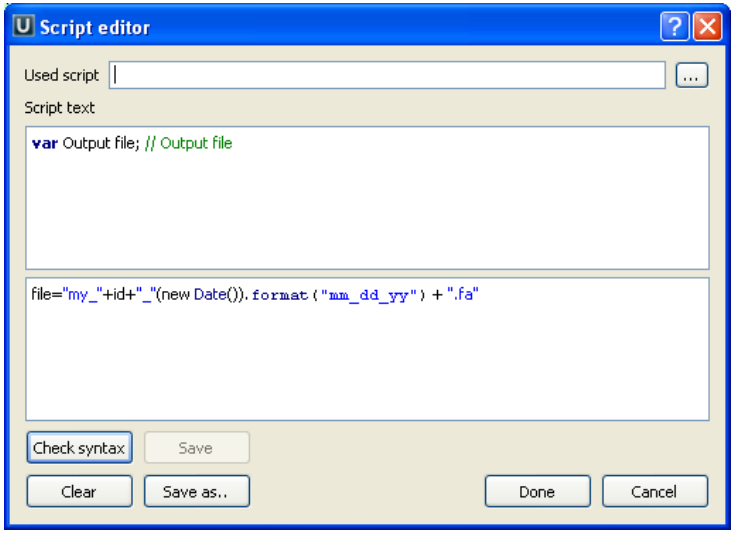
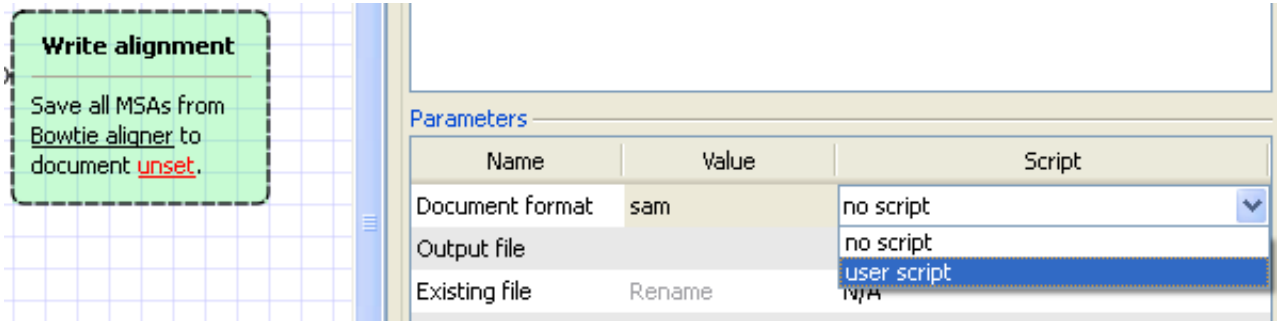
UGENE Workflow Designer reuse

- Script new features
  - use embedded scripting language to design new workflow building blocks





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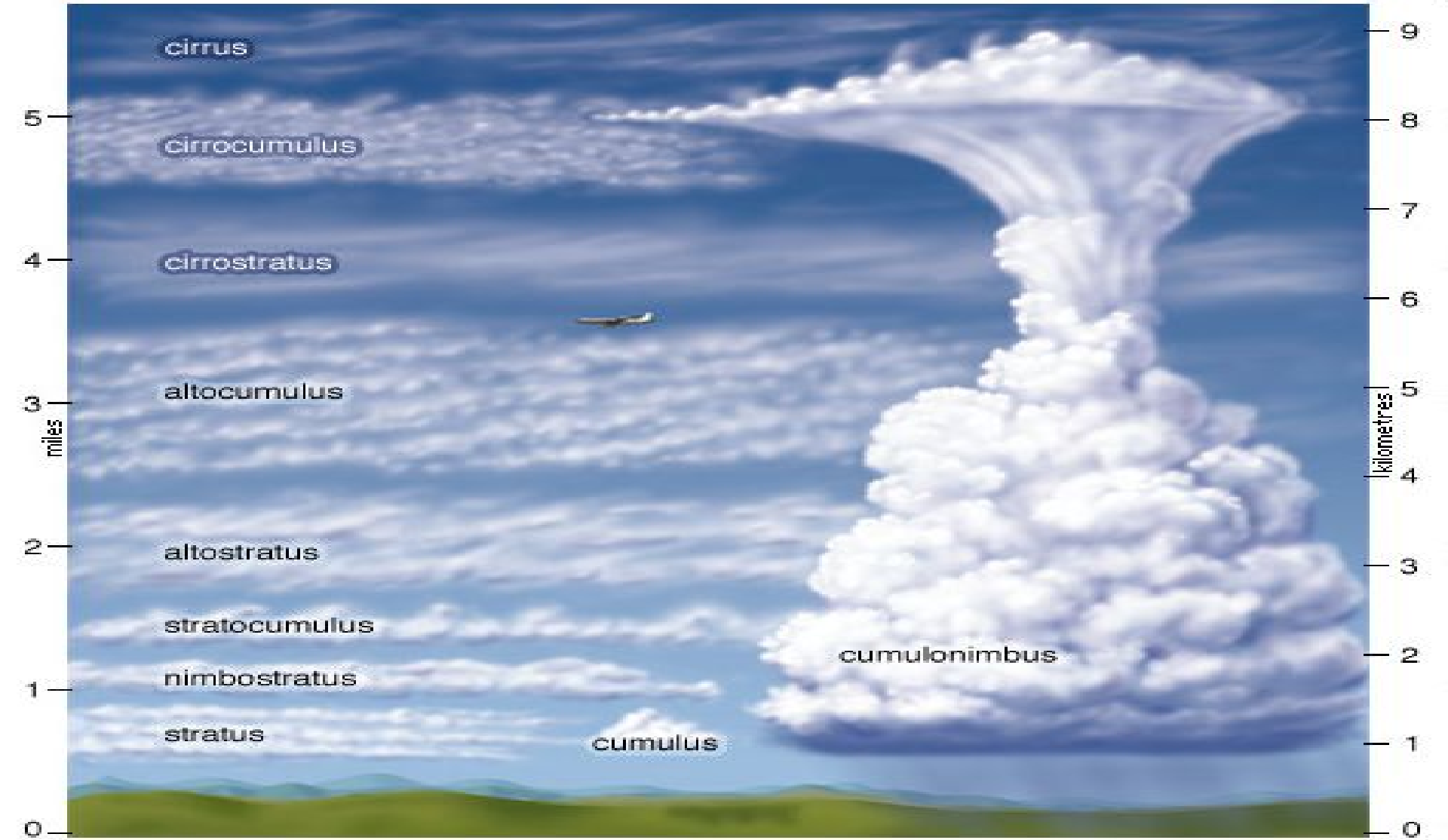
Part 2.
Cloud Computing

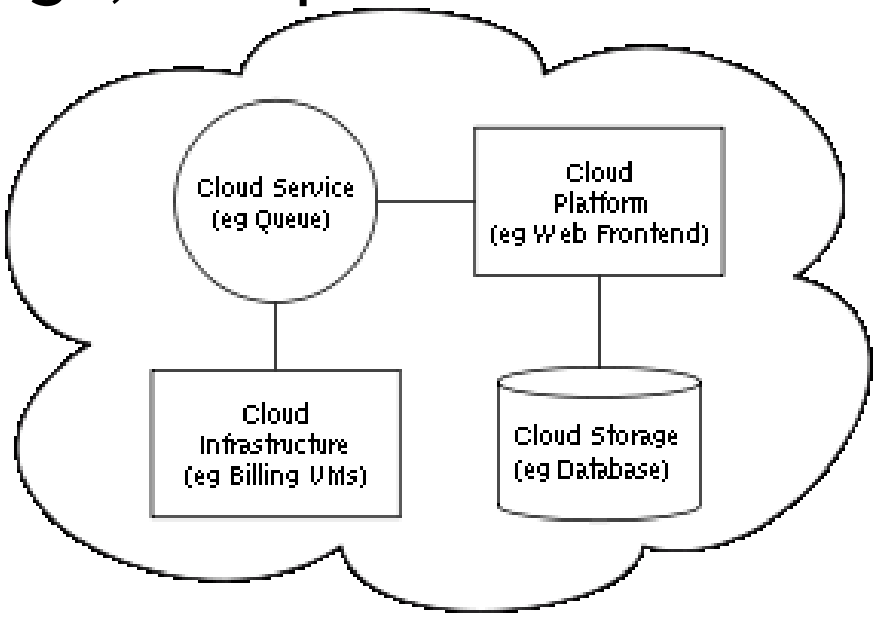


Cloud Computing basics

- Basically: the virtual servers available over the Internet.

- One can use those servers to execute specific functions: storage, computation etc.

The functions provided as ***services***.



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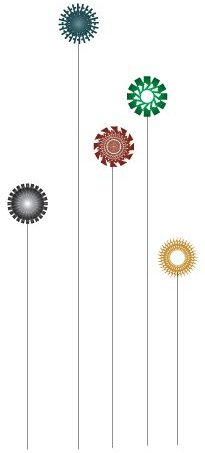
Cloud Computing basics

- Customers **do not own** the physical infrastructure.
  - They consume resources as a service and pay only for resources that they use.
- Cloud providers:
  - Google App server, Amazon EC2, Microsoft Azure, etc…



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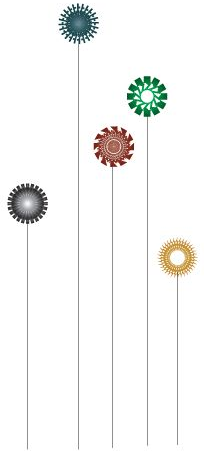
Cloud Computing basics

- The difference between cloud-providers is the type of resources/services their sell
- Example of cloud resources
  - Storage (Box.net, DropBox, Oosah …)
    - Easy and chip to rent a huge amount of storage for your documents
    - Available in different geographical locations 24/7
    - Backup services
    - Can be used for any purpose or limited (only photos, videos…)
    - Have special tools to upload data
      - *Pay per GB, plus web traffic*
  - Hardware and application infrastructure (Amazon, GoogleApp, Azure…)
    - Run your own programs (sometimes limited to certain architecture)
    - Rent storage/CPU/memory resources
    - Use various additional services: load balancing, billing, database accounts
      - Pay per storage, traffic, CPU and memory resources, additional services



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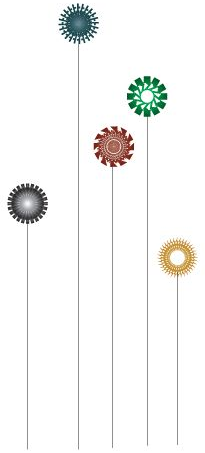
Cloud Computing
basics

- Example of cloud resources (continued…)
  - Software applications
    - Access to preinstalled software application
    - Database
    - Office-like document processing suites
  - Web services
    - A protocols to run complex computations remotely



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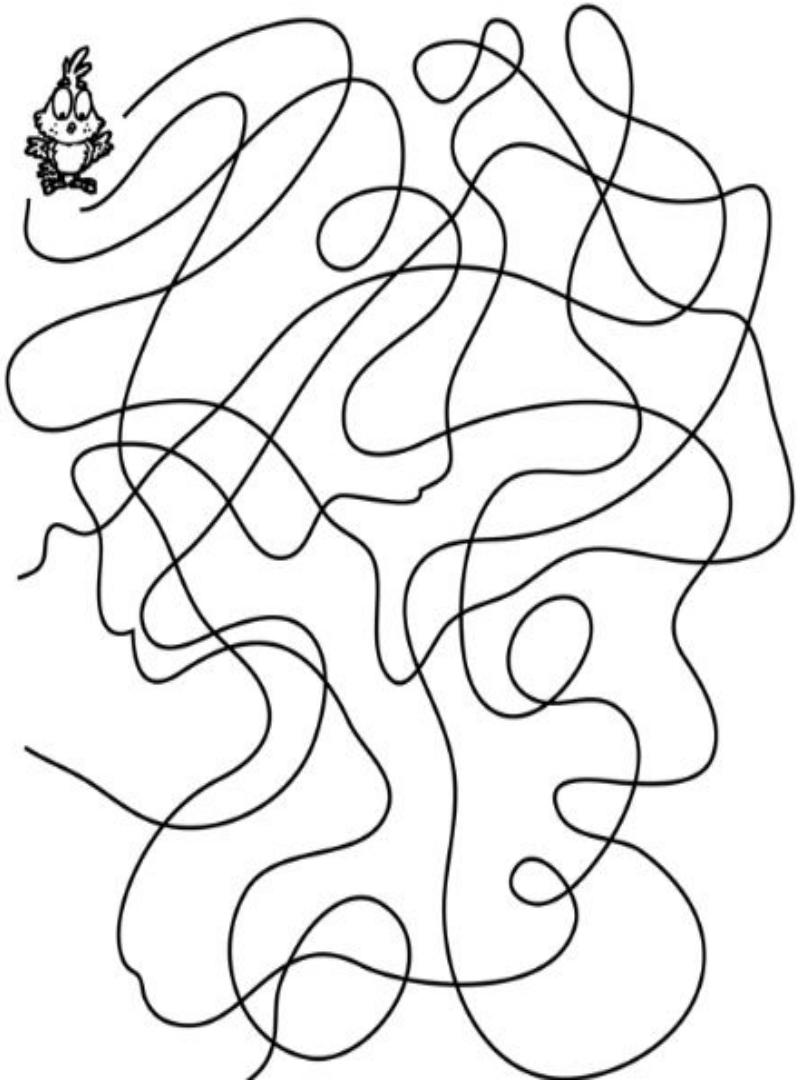
Cloud Computing
UGENE

- UGENE cloud model
  - Server part of UGENE can be installed and utilize resources of infrastructure-level cloud providers (like Amazon EC2)
  - UGENE users will see the UGENE server as remote service and utilize it as a service-level cloud provider



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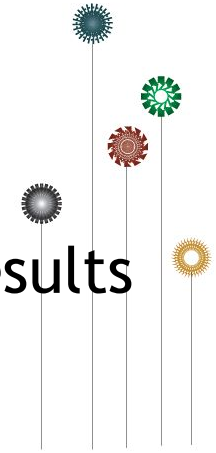
UGENE Workflows in the cloud

- As simple as local workflow:
  - Add remote machine on the cloud
  - Launch the workflow
    - All your local data will be sent to remote computer
    - Check the task progress in “Tasks” area
    - After task is finished, UGENE will fetch the results



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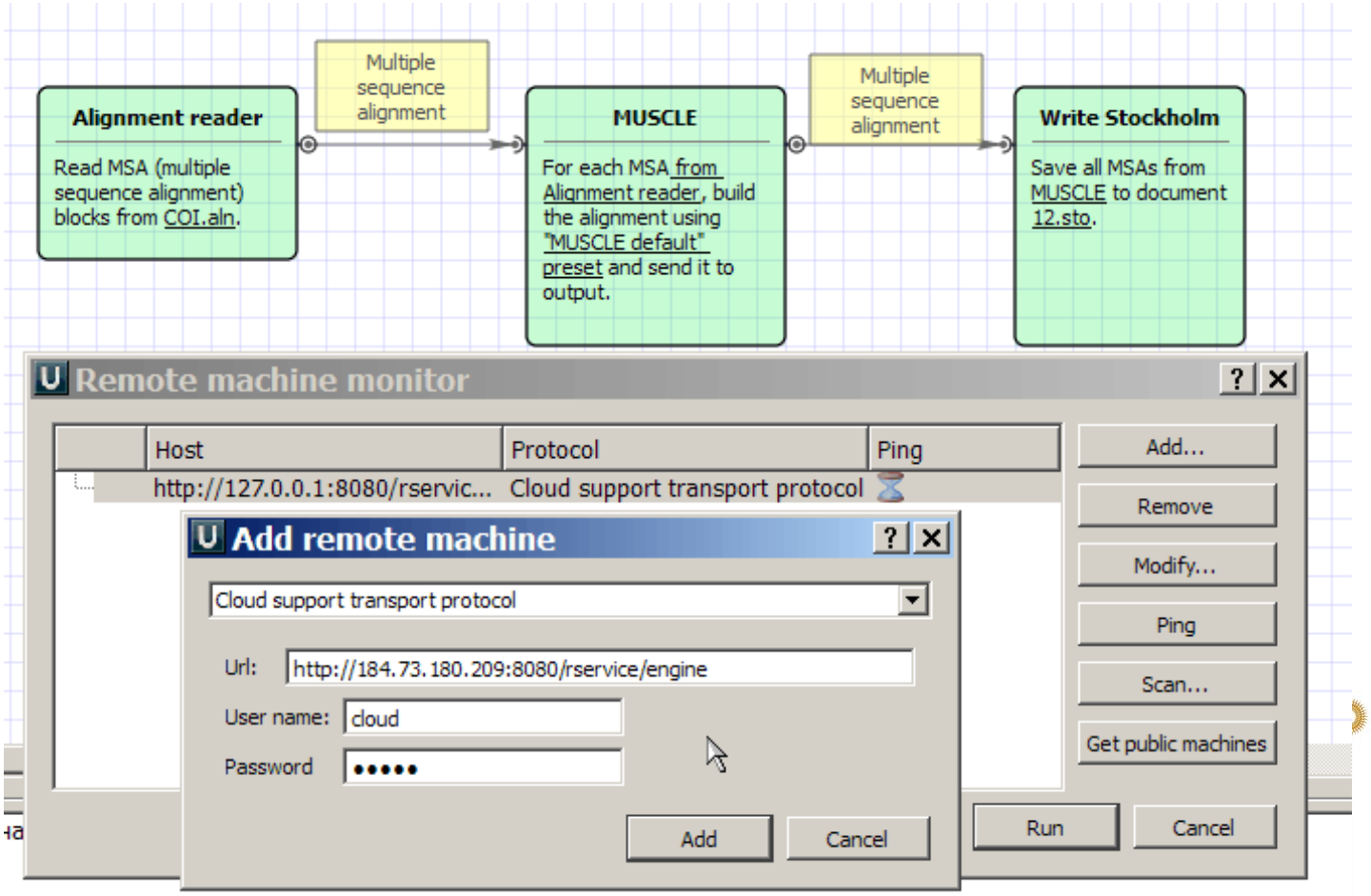
UGENE Workflows in the cloud

Using open Amazon EC2 installation of UGENE:



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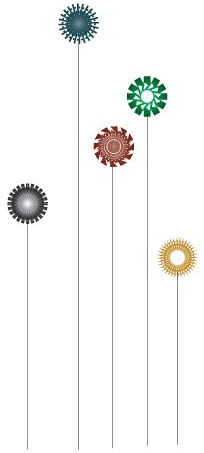
UGENE Workflows in the cloud

- UGENE team provides you with a free account to access to UGENE server instance (see screenshot on the previous page)
  - This account is limited by hardware resources (Amazon is not free for us, unfortunately)
  - You can install the same UGENE service for you organization
    - Using popular cloud provider (example: Amazon)
    - Inside of the private network of your organization!



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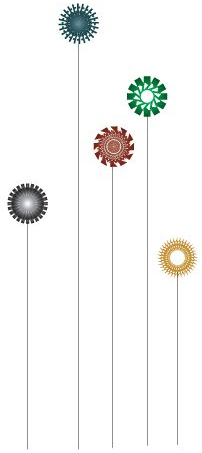
UGENE as a Service for your organization

- Why UGENE as a Service in your private network/organization is a good solution

?



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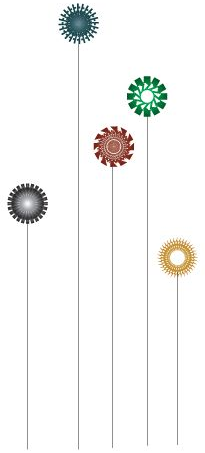
UGENE as a Service for your organization

Show these facts to your network administrators and managers:

- No need to install a lot of software: UGENE package integrates dozens of tools and will get more in the future
- Users can create new algorithms in Workflow Designer that are
  - Safe for execution and secure
  - Effectively utilize distributed environment
- No need to pay license fee or ask additional funds for software
- *Ask us for support if needed!*



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Open Discussion

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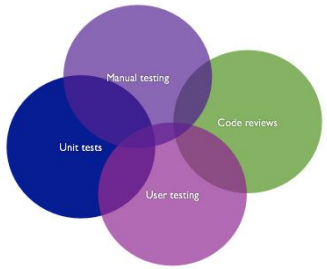
Appendix
Some technical details

- UGENE is written in C++, using QT4 library
- Code license: GPLv2
- Distribution bundle size: 12Mb
- Platform supported:
  Windows, Linux, MacOS
- System requirements:
  Pentium 166MMX, 64Mb RAM
- Test base contains ~5000 tests
- Web-site with additional info
  http://ugene.unipro.ru



UGENE Test Report - precommit testing
generated by UGENE
ПН янв 25 2010 22:10:20

Total Runtime: 207 s	Number of tests	Pass	Fail	Excluded	Success Rate
Total:	1947	1947	0	26	100%
Annotator plugin tests	30	30	0	0	100%
Document format tests	266	266	0	0	100%
Enzymes plugin tests	16	16	0	0	100%
ORFMarker plugin tests	25	25	0	0	100%
Repeat finder tests	177	177	0	0	100%
SequenceWalker tests	10	10	0	0	100%
Smith Waterman Tests classic 2	35	35	0	0	100%
Task tests	10	10	0	0	100%

"ugene" package in Ubuntu
Ubuntu » "ugene" package

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