الجمهورية الجزائرية الديمقراطية الشعبيه

وزارة التعليم العالي والبحث العلمي

People’s Democratic Republic of Algeria

Ministry of Higher Education and Scientific Research

جامعة محمد الصديق بن يحي -جيجل-

Mohamed Seddik Benyahia University – Jijel

Faculty of Natural Sciences

And Life Sciences

Molecular and Cellular Biology

كلية العلوم الطبيعية والحياة

البيولوجيا الجزيئية و الخلوية

Master 01 in Pharmacological Sciences

Logiciel libre and open source

Report

Logiciel libre and open source

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Supervised:

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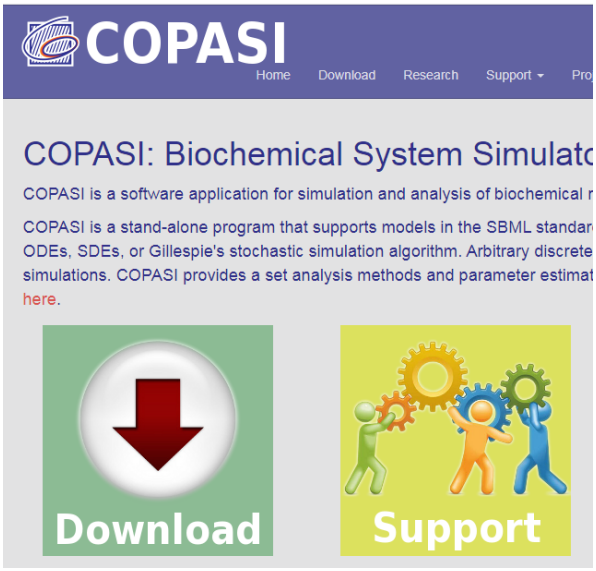
Academic Year: 2025/2026.

PART 1 – Theoretical Study of a Tool (COPASI):



Simulation and modeling is becoming one of the standard approaches to understand complex biochemical processes. Therefore, there is a growing need for software tools that allow access to diverse simulation and modeling methods as well as support for the usage of these methods. In order to meet this need for software in the field, several tools have been developed like EMBOSS, Biopython, COPASI and CellDesigner. Here we present COPASI (Complex Pathway Simulator) which combines all the standards and some unique methods for the simulation and analysis of biochemical reaction networks. (1)

1. General presentation of COPASI:

COPASI is a stand-alone software application designed for the simulation and analysis of biochemical networks and their dynamic behavior. It supports models defined in the SBML standard and allows simulations using ordinary differential equations (ODEs), stochastic differential equations (SDEs), or Gillespie's stochastic simulation algorithm. The software also enables the inclusion of arbitrary discrete events and provides a wide range of analysis tools, including parameter estimation methods. (2)

2. Main functionalities:

- Model creation and editing via graphical interface or SBML import.
- Deterministic and stochastic simulations (ODE-based and Gillespie algorithm).
- Parameter estimation and optimization using experimental data.
- Sensitivity analysis (local and global).
- Metabolic control analysis (MCA).
- Time-course simulations and steady-state analysis.
- Support for SBML (Systems Biology Markup Language).

- Task automation via scripting (Python, COPASI's own API). (2)

3. Technical aspects:

- **License:** GNU General Public License (GPL)
- **Platform :** Windows, macOS, Linux
- **Programming languages:** C++ core, with bindings for Python and Java
- **Model exchange:** Supports SBML Level 2 and 3
- **Dependencies:** Qt for GUI, SUNDIALS for ODE solving
- **Latest stable version:** COPASI 4.40 (as of 2025)**.** (3)

4. Strengths:

- No cost, open-source, and regularly updated.
- User-friendly graphical interface suitable for both beginners and advanced users.
- Comprehensive simulation and analysis tools integrated into one platform.
- Interoperability with other tools via SBML.
- Active development and community support.
- Extensive documentation and tutorials available.
- Widely used and cited in scientific literature. (4)

5. Limitations and weaknesses:

- Steep learning curve for advanced features like parameter estimation.
- Limited native support for spatial modeling.
- GUI can become slow with very large models.
- Less frequent updates compared to some commercial tools.
- Limited built-in visualization customization compared to MATLAB or Python-based tools. (5)

6. Conclusion:

In summary, COPASI is a free open-source tool for modeling and analyzing biochemical networks, offering strong SBML support, deterministic and stochastic

simulations, and advanced analyses such as parameter estimation and metabolic control analysis. While complex models may require complementary tools, COPASI remains a key reference in systems biology research.

PART 2 – Practical Study: Exploration of Zenodo:

1. Presentation of Zenodo:

Zenodo (https://zenodo.org) is an open-access, multidisciplinary repository operated by CERN (European Organization for Nuclear Research), which provides researchers with an easy and stable platform to archive and publish their data and other output. (6)

Platform objectives

- Provide a stable and open-access platform to archive, publish, and preserve research outputs
- Enable easy sharing and citation of data through persistent identifiers (DOIs)
- Support automated archiving workflows via an API for large-scale digitization pipelines
- Ensure that published data comply with FAIR principles (Findable, Accessible, Interoperable, Reusable)
- Facilitate rapid publication of digitized data shortly after creation. (6)

Types of hosted content

- **Research Data:** From small datasets to massive collections (e.g., the 1 TB of herbarium JPEGs mentioned).
- **Publications:** Preprints, reports, conference papers, theses.
- **Software and Code:** Research software tools, scripts, and code packages.
- **Multimedia and Digital Objects:** Images, videos, audio files. The abstract specifically tested digitized specimen images (TIFF, JPEG) and associated label overlays.
- **Rich Metadata:** Supports machine-readable metadata in formats like JSON-LD using standardized terminologies (e.g., Darwin Core for biodiversity data), enhancing interoperability. (6)

Importance of Zenodo for open science and research in NLS:

- Promotes open access to scientific data in Natural and Life Sciences
- Enhances data visibility, reuse, and interoperability through standard metadata and linked data
- Provides long-term preservation of large-scale digitized natural heritage collections
- Assigns DOIs to individual specimens , improving traceability and citation
- Supports collaboration and data sharing across institutions and disciplines

2. The practical steps:

❖ Search for Zenodo in Google (figure 1 and 2).

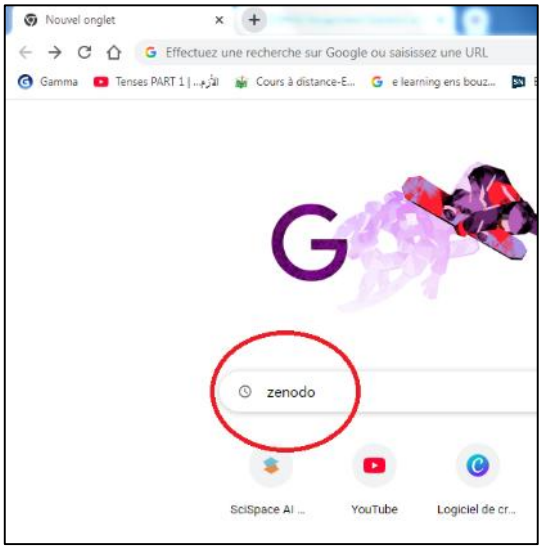


Figure 1: searching for the Zenodo

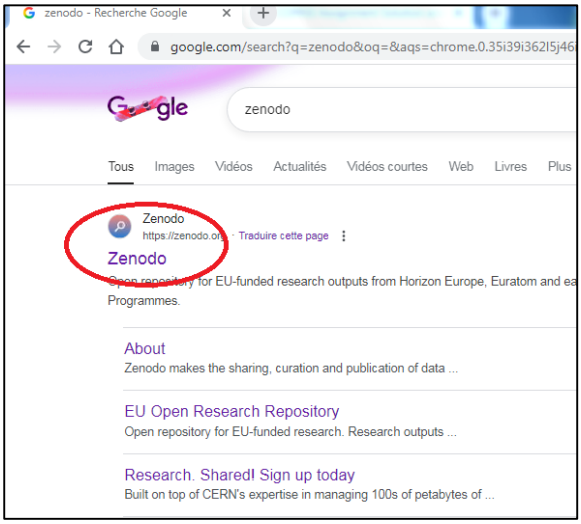


Figure 2: Zenodo Repository Google Search Result

❖ Search for a dataset using genome and select Dataset and CSV as characteristics (figure 3, 4 and 5).

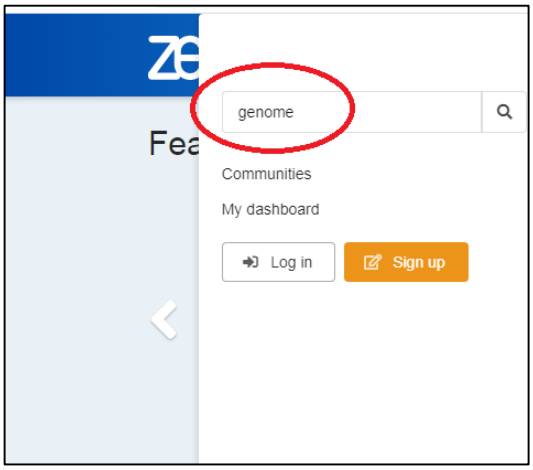


Figure 3: Dataset Search Interface in Zenodo using **genome**

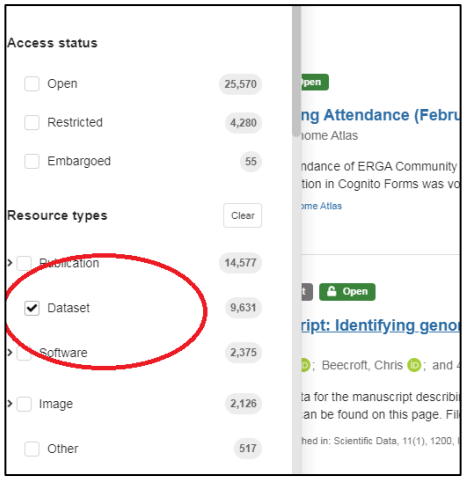


Figure 4: Dataset selecting

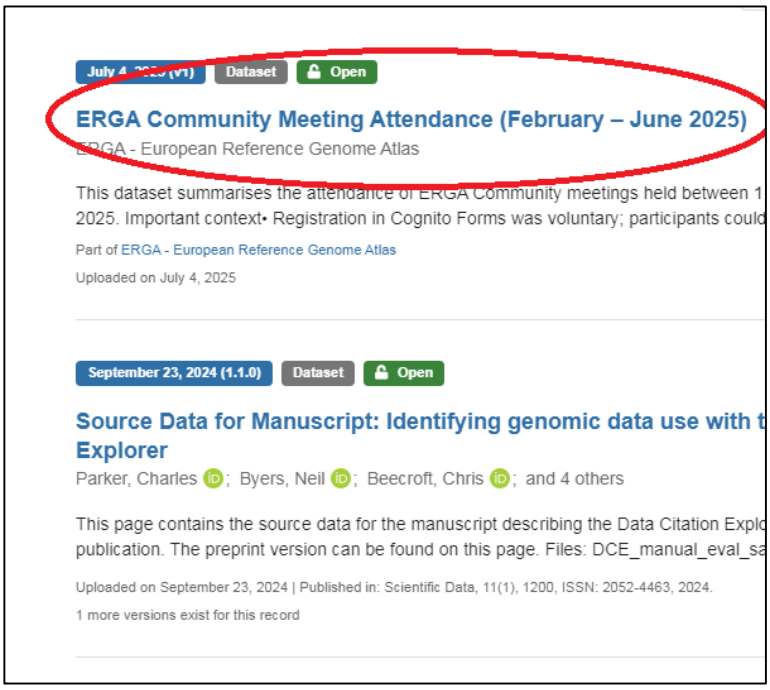


Figure 5: Selected Dataset

❖ Download the selected dataset (figure 6 and 7)

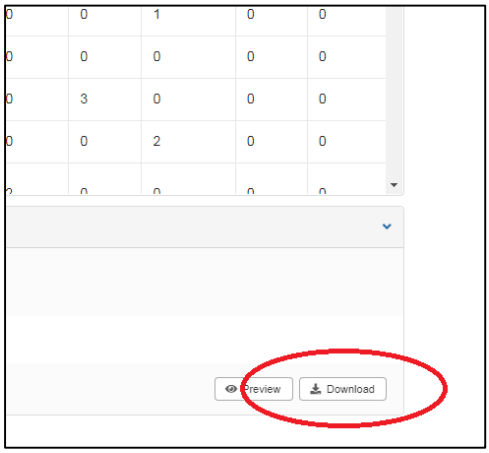


Figure 6: Download Dataset

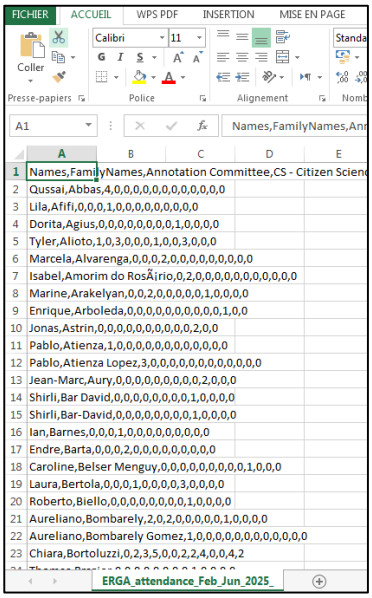


Figure 7: Downloaded Dataset result

❖ Retrieve the dataset metadata using Dublin Core (figure 8 and 9).


```
<?xml version="1.0" encoding="utf-8" ?>
<oai_dc:dc xmlns:dc="http://purl.org/dc/elements/1.1/" xmlns:oai_dc="http://www.openarchives.org/OAI/2.0/oai_dc/" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
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  <dc:creator>ERGA - European Reference Genome Atlas</dc:creator>
  <dc:date>2025-07-04</dc:date>
  <dc:description>&lt;p dir="ltr"&gt;This dataset summarises the attendance of ERGA Community meetings held between 1 February 2025 and 30 June 2025.&lt;/p&gt; &lt;p
    dir="ltr"&gt;&lt;strong&gt;Important context&lt;/strong&gt;&lt;br&gt;&bull; Registration in Cognito Forms was voluntary; participants could join meetings without completing the
    form.&lt;br&gt;&bull; This file is a static snapshot and will not be edited after publication. To ensure future aggregates remain accurate, community members are encouraged to enter
    their given and family names exactly the same way every time they register.&lt;/p&gt; &lt;p dir="ltr"&gt;Each row represents one participant who explicitly consented, via the ERGA
    Cognito Forms survey, to have their name made public. Columns are:&lt;/p&gt; &lt;div dir="ltr"&gt; &lt;table style="width: 78.814628%;"&gt;&lt;colgroup&gt;&lt;col style="width:
    17.92%;"&gt;&lt;col style="width: 81.92%;"&gt;&lt;/colgroup&gt; &lt;tbody&gt; &lt;tr&gt; &lt;td&gt; &lt;p dir="ltr"&gt;&lt;strong&gt;Column&lt;/strong&gt;&lt;/p&gt;
    &lt;/td&gt; &lt;td&gt; &lt;p dir="ltr"&gt;Description&lt;/p&gt; &lt;/td&gt; &lt;/tr&gt; &lt;tr&gt; &lt;td&gt; &lt;p dir="ltr"&gt;&lt;strong&gt;Names&lt;/strong&gt;&lt;/p&gt;
    &lt;/td&gt; &lt;td&gt; &lt;p dir="ltr"&gt;Given (first) name of the participant&lt;/p&gt; &lt;/td&gt; &lt;/tr&gt; &lt;tr&gt; &lt;td&gt; &lt;p
    dir="ltr"&gt;&lt;strong&gt;FamilyNames&lt;/strong&gt;&lt;/p&gt; &lt;/td&gt; &lt;td&gt; &lt;p dir="ltr"&gt;Family (last) name of the participant&lt;/p&gt; &lt;/td&gt; &lt;/tr&gt;
    &lt;tr&gt; &lt;td&gt; &lt;p dir="ltr"&gt;&lt;strong&gt;Committee columns&lt;/strong&gt;&lt;/p&gt; &lt;/td&gt; &lt;td&gt; &lt;p dir="ltr"&gt;One column per ERGA meeting (e.g.
    Plenary, DAC &amp;ndash; Data Analysis Committee, etc.). The cell value is the number of meetings that participants attended for that committee during the reporting period. A value of 0
    indicates no attendance.&lt;/p&gt; &lt;/td&gt; &lt;/tr&gt; &lt;/tbody&gt; &lt;/table&gt; &lt;/div&gt; &lt;p&gt; &lt;/p&gt;</dc:description>
  <dc:description>&lt;p dir="ltr"&gt;&lt;strong&gt;Data provenance&lt;/strong&gt;&lt;br&gt;Participant attendance was collected with Cognito Forms. Only the minimum information
    required for the intended public purpose, names, and attendance counts, has been retained; no e-mail addresses, institutional affiliations, or other personal data are included.&lt;/p&gt;
    &lt;p dir="ltr"&gt;&lt;strong&gt;GDPR &amp;amp; ethics&lt;/strong&gt;&lt;br&gt;All individuals accepted the ERGA privacy notice and provided explicit consent for their names to appear
    in a public archive. The dataset therefore complies with the GDPR principle of lawfulness, fairness, and transparency (Art. 5 (1)(a)) and the data minimisation principle (Art. 5 (1)(c)).
    No special-category data are present.&lt;/p&gt; &lt;p dir="ltr"&gt;&lt;strong&gt;Temporal coverage&lt;/strong&gt;&lt;br&gt;2025-02-01 to 2025-06-30.&lt;/p&gt;
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Figure 9: Dublin core Dataset metadata result

3. The DUBLIN CORE Dataset metadata:

Title	ERGA Community Meeting Attendance (February – June 2025)
Creator	ERGA - European Reference Genome Atlas
Subject	Community meetings, scientific collaboration, research governance, attendance records
Description	The application component monitoring dataset for the Genom application under the MORPHEMIC project.
Publisher	Zenodo
Date	This dataset summarises the attendance of ERGA Community meetings held between 1 February 2025 and 30 June 2025. It includes participant context, registration information collected via Cognito Forms, attendance per meeting, GDPR compliance details, and temporal coverage from 2025-02-01 to 2025-06-30.
format	CSV
type	info:eu-repo/semantics/other
Identifier	doi:10.5281/zenodo.15805327
Source	Online registration and attendance data collected through Cognito Forms for ERGA Community meetings
Relation	Part of the ERGA Community on Zenodo
Coverage	February 2025 – June 2025; Online ERGA Community meetings
Rights	creativecommons.org/licenses/by/4.0/legalcode

PART 3 – BONUS

GitHub created repository website:
https://github.com/allamikram09-sketch/open-source/upload/main

Reference:

(1) Hoops, S., Sahle, S., Gauges, R., Lee, C., Pahle, J., Simus, N., Singhal, M., Xu, L., Mendes, P., & Kummer, U. (2006). COPASI--a COmplex PAthway SImulator. Bioinformatics (Oxford, England), 22(24), 3067–3074. https://doi.org/10.1093/bioinformatics/btl485

(2) COPASI Official Documentation. Retrieved from https://copasi.org

(3) Mendes, P., Hoops, S., Sahle, S., Gauges, R., Dada, J., & Kummer, U. (2009). Computational modeling of biochemical networks using COPASI. Methods in molecular biology (Clifton, N.J.), 500, 17–59. https://doi.org/10.1007/978-1-59745-525-1_2

(4) Bergmann, F. T., & Sauro, H. M. (2006, December). SBW-a modular framework for systems biology. In Proceedings of the 2006 Winter Simulation Conference (pp. 1637-1645). IEEE.

(5) COPASI GitHub Repository. (n.d.). Retrieved from https://github.com/copasi

(6) Dillen, M., Groom, Q., Agosti, D., & Nielsen, L. H. (2019). Zenodo, an Archive and Publishing Repository: A tale of two herbarium specimen pilot projects. Biodiversity Information Science and Standards, (2). https://link.gale.com/apps/doc/A646406315/AONE?u=anon~4a347de5&sid=googleScholar&xid=6324736b