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Condor-COPASI - Integrating COPASI with the Condor high-throughput computing environment

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Overview

Mathematical modelling has become a common tool for improving our understanding of complex biological systems. However, as models become larger and more complex, simulations and analyses require increasing amounts of computational power. Large amounts of power can be delivered by clusters of computers in a high-throughput computing environment. However, exploiting such a system can be difficult for users without the necessary expertise.

We present Condor-COPASI, a server-based software tool that integrates COPASI, a biological pathway simulation tool, with Condor, a high-throughput computing system. Condor-COPASI provides a web-based interface which makes it extremely easy for a user to run a number of model simulation and analysis tasks in parallel. Tasks are transparently split into smaller parts, and submitted for execution on a Condor pool. Result output is presented in a number of formats, including tables and interactive graphical displays.

Background

COPASI

COPASI (COmplex PAthway SImulator) is a software application for simulation and analysis of biochemical networks and their dynamics.

Condor

Condor is a high-throughput computing environment.

- It manages a pool of machines, executing jobs in parallel
- It can run on normal workstations when they are idle, utilizing CPU cycles that would otherwise have gone to waste
- Allows for a powerful computing resource to be obtained for free

In Manchester, the Condor pool provides 2.8 years of computing time every night

COPASI and Condor

We can use COPASI with Condor to speed up certain types of computation

This can only be achieved if we can split our task into multiple jobs to be run in parallel

The submission process for running COPASI tasks on Condor can be difficult for some users:

- Tasks must be manually split into multiple parallel jobs
- The job submission process requires the use of command line tools

Condor-COPASI

To simplify the process of running certain COPASI tasks on Condor, we developed Condor-COPASI - a software tool which automates the process of splitting tasks into parallel and the Condor job submission process.

Condor-COPASI runs on a server, and is accessed though a web-based interface.

The output of completed tasks is automatically collated, and can be displayed in the browser in a variety of formats, including interactive graphical plots

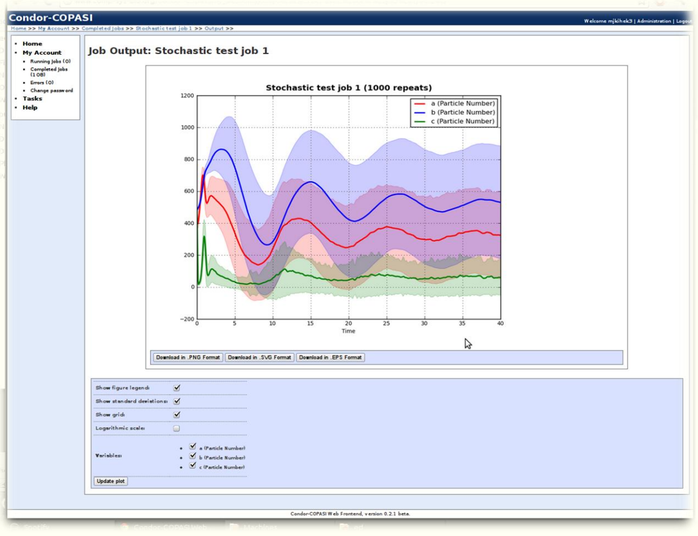

Figure 2: Condor-COPASI screenshot. Plotting the time-course output (particle number means and standard deviations) for 1000 stochastic simulation repeats

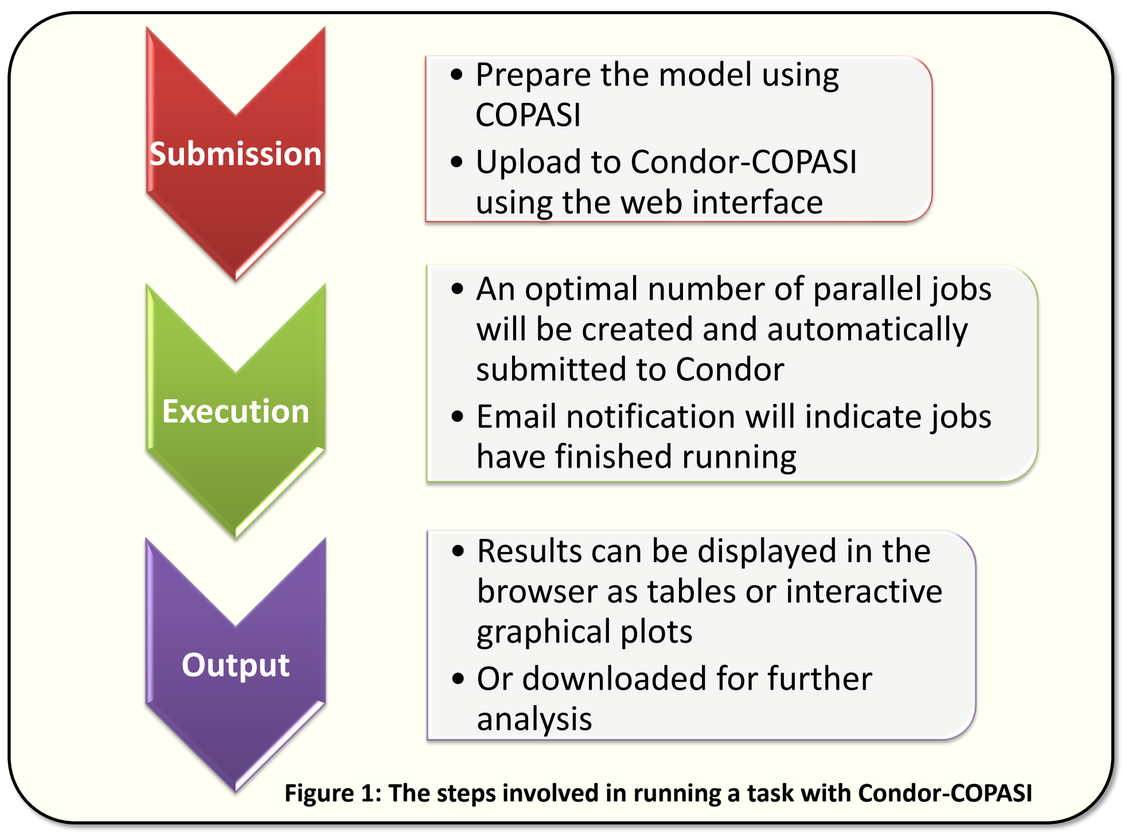

Figure 1: The steps involved in running a task with Condor-COPASI

Task Types

Condor-COPASI can automatically run the following tasks in parallel on Condor:

- **Stochastic simulation repeats**
- **Optimization repeats**
- **Optimization repeats with different algorithms**
- **Parameter estimation repeats**
- **Global sensitivity analysis**
- **Monte Carlo simulation**
- **Parameter scan**

Examples

Vast decreases in run time can be achieved when running tasks with Condor-COPASI. For example:

Task type	Run time with Condor -COPASI	Total CPU time used
Global sensitivity analysis	**5 hours**	**128 hours**
Stochastic simulation repeat	**20 hours**	**2283 hours**
Monte Carlo simulation	**31 hours**	**3961 hours**
Optimization repeat	**25 minutes**	**61 hours**

Project information

Condor-COPASI is free, open source software

It is available for download and, and can be used by anyone with access to a Condor Pool

It only needs to be installed once on a server – it can then be accessed by multiple users

A full user manual and deployment instructions are available on the website

More information: http://code.google.com/p/condor-copasi