



USER MANUAL
AIR POLLUTION APPLICATION

WP1.4.3

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1. INTRODUCTION

STEM-II is an Eulerian air quality model with simulates transport, chemical transformations, emissions and depositions in an integrated framework. It is used to know in advance how the meteorological conditions, obtained from a meteorological model (COAMPS, included in the project), will affect the emissions effects of As Pontes Power Plant (A Coruña, Spain).

The Air Pollution application is based on the MPI parallelization of the STEM-II model with the inclusion of an interactive GUI for representing the output.

The program is designed for the Power Plant technicians. Running this application they can see graphically and in real time, the pollution that a specific combustion generates. Experts can interact with the model choosing different species to be visualized at several high levels. With the help of this tool they can make decisions in order to fulfilling the EU directives about pollution.

The model is computationally intensive, thus, with the help of Grid Computing and the parallelization of the model, the users obtain results in a reasonably time.

Additionally to this document, there are available an installation guide and a developer manual.

1.1. ABBREVIATIONS AND ACRONYMS

STEM-II: Sulphur Transport Eulerian Model version 2

GUI: Graphical User Interface

MPI: Message Passing Interface

MD: Migrating Desktop

COAMPS: Coupled Ocean-Atmosphere Mesoscale Prediction System.

1.2. REFERENCES AND SOURCE CODE

The source code of this application and how to install it is fully described in the Installation Guide of the application.

2. PRODUCT USAGE

The Air Pollution application is available from the Migrating Desktop of the CrossGrid project. There is a specific input in the applications menu.

A specific tab into the Job Wizard allow the user to set the specific input parameters of the model and from the Job Monitoring Dialog the Visualization Plugin can be launched, allowing the user to see graphically the output of the application and interact with the model.

2.1. RUNNING THE PRODUCT

If you run the model into the CrossGrid Testbed there are not specific requirements. But if you install the tool separately, some things must be taken into account.

2.1.1. Operating Requirements

The model is a standalone executable that must be available for the user (see in the installation guide how to obtain it).

If you want to execute the Graphical User Interface of the model, the Migrating Desktop is needed (see the appropriate guide for obtain and install it). But the program can be executed without graphical interactivity, and the binary files with all the pollutants concentrations every hour will be generated. In this case the user only needs the executable and its pool of machines with MPICH (Cluster or Grid).

The user must also provide some input files as the meteorological information, the topology, and the initial concentrations. All that files are in the Storage elements of the CrossGrid project, but must be provided by the user if the application is executed outside the CrossGrid testbed.

2.1.1.1. Local hardware requirements

There are no specific requirements for execute the application. As more power computing nodes we chose, a better performance will be obtained. We recommend not less than Pentium processors with 128Mb of ram memory. The storage requirements are under the couple of GB.

2.1.1.2. Local software requirements

Only the presence of MPICH in the machines where the application is going to be executed is required.

If the user downloads the sources of the application, a Fortran 77 compiler is also needed.

2.1.1.3. Grid infrastructure requirements

There is not necessary any specific Grid infrastructure for running the application, because it can be executed into a cluster. A recommendation is to use network connectivity with a good bandwidth. The communications in the parallel version of the model are the bottle neck of the performance. It is necessary to communicate a big amount of data every iteration.

2.1.2. Step-by-Step User Setup

There is no specific user setup for running this application. If you run the program locally, it is your responsibility, or your system administrator, to have the proper execution permissions.

If you are a CrossGrid user and execute the application from the Migrating Desktop you need a CrossGrid certificate. The proxy is created automatically by the Migrating Desktop. If you run the application in the CrossGrid testbed using only the Resource Broker you must init a proxy before.

2.2. BASIC OPERATION

The Air Pollution mode is available into the CrossGrid Testbed and it can be executed from the Migrating Desktop.

If you want to execute it locally, you can download it from the CVS repository of the CrossGrid project (See the installation guide of the Air Pollution model for details).

2.2.1. Executing from the Migrating Desktop

When the Migrating Desktop has been executed, we can select the Air Pollution application from the applications window.

The input parameters window was included as the first tab of the Job Wizard (Fig. 3-1), allowing the user to set specific parameters of the application. This parameters are the date of the simulation, the start hour and the number of hours of the simulation. Besides this parameters, the user can set another ones not depends on the application, as the number of processors, the target node, the executable path, etc. For interactive purposes of the graphical output, we must add a specific file in the Files tab of the Job Submission Wizard, the ASTEP file, with type out and a refresh of 10 or 20 seconds (it can be shown in the Fig. 3-2). We can select here files for the standard output and the standard error and we can include also a input file for transfer the executable to the execution nodes. When all the parameters have been set, we can submit the Job.

When the program is submitted, we must open the Job Monitoring Dialog into the Migrating Desktop (see Fig. 3-3). In this window, the list of all the jobs the user has submitted is presented. If we select the job that we have just submitted and press the Details button, another window with specific information of our job will be presented (Fig. 3-4).

If the status of the job is running, we can launch the Visualization Plugin by clicking the Visualize button. The representation is a 2-D graph of the concentration of a given pollutant in a level of high will be presented (Fig. 3-5). The concentrations are represented with a background map for a better understanding of the results. The location of the power plant is also indicated. Moreover, a scale with a color code is shown in the right part of the image. This image will be refreshed on real time when new concentration data was available.

This representation is interactive, so the user can vary the pollutant or the level in the visualization plugin, using the drop-down lists in the parameters boxes.

2.2.2. Executing from command line

If the user doesn't want graphical visualization of the results, the program can be submitted as a command line application. The parameters for the application must be provided after the executable name.

If the user submits the job to a Resource Broker, he must set the proper values in the JDL script.

2.3. ADVANCED FEATURES

There is the possibility of submit several jobs simultaneously, with different input parameters, and compare which of them obtain the better results.

2.4. KNOWN PROBLEMS

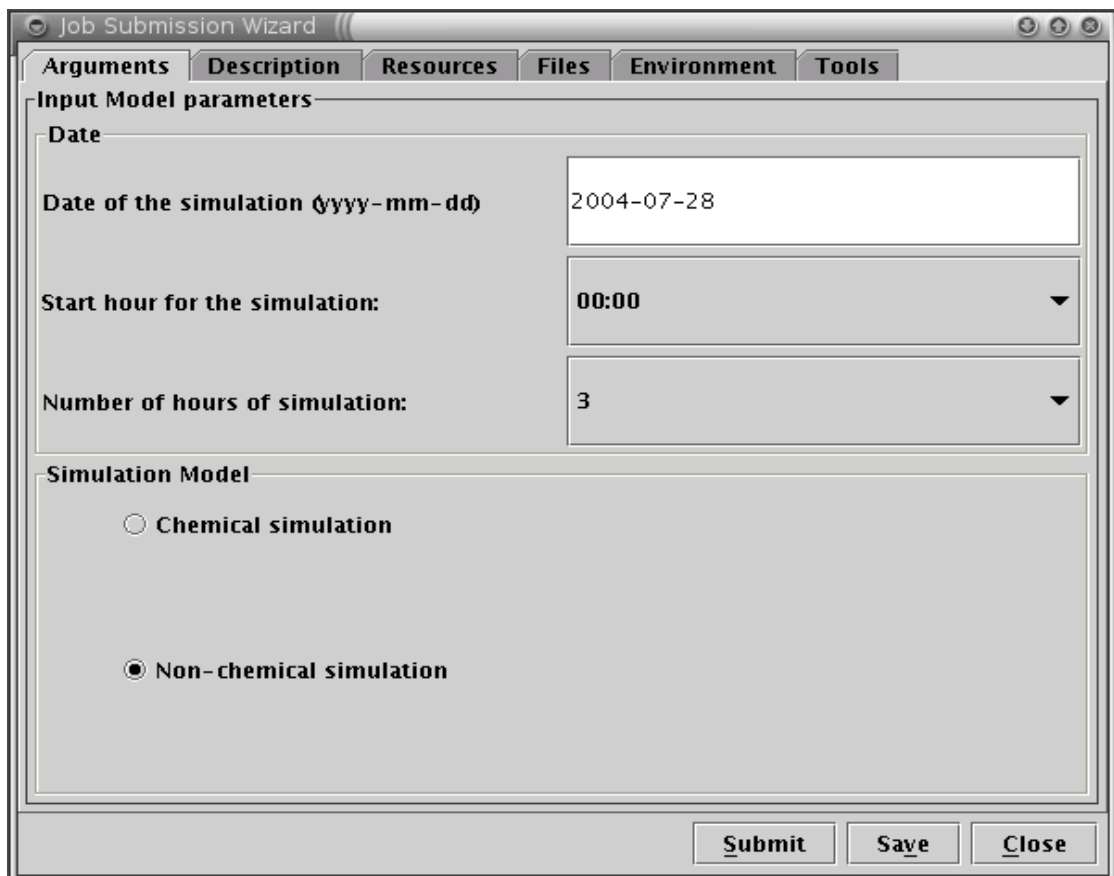
All the known bugs at the moment of write this manual are corrected in the available version.

3. INTERFACE REFERENCE GUIDE

GUI description:

From the Job Parameters Window into the Job Submission Wizard, the input parameters of the application can be set.

- Data of the simulation – It is the date when the simulation starts.
- Start hour of the simulation – When the simulation start.
- Numbers of hours of simulation – How many hours we want to simulate.
- Simulation model – A flag for an only transport simulation or including the chemical reactions



The screenshot shows a window titled "Job Submission Wizard" with several tabs: Arguments, Description, Resources, Files, Environment, and Tools. The "Description" tab is active, showing "Input Model parameters". Under "Date", there are three fields: "Date of the simulation (yyyy-mm-dd)" with the value "2004-07-28", "Start hour for the simulation:" with a dropdown menu showing "00:00", and "Number of hours of simulation:" with a dropdown menu showing "3". Below this is the "Simulation Model" section with two radio buttons: "Chemical simulation" (unselected) and "Non-chemical simulation" (selected). At the bottom right, there are three buttons: "Submit", "Save", and "Close".

Fig. 3-1 Input Parameters Window

In the Files tab of the Job Submission Wizard (Fig. 3-2), the files needed for the application can be specified.

- StdInput, StdOutput and StdError – are generic files for all the submissions. Really are not needed for our application

- ASTEP – Is the file where the output of the program will be stored. This file is read by the output plugin in order to generate the images selected by the user. We add this file pressing the Add button and filling the fields as in the figure. Some of the fields are drop-down lists or open windows for select the information required.
- A new file can be added with the executable name, with the same name of executable that in the Description tab, in the local path where the executable is, of type in and without refresh.

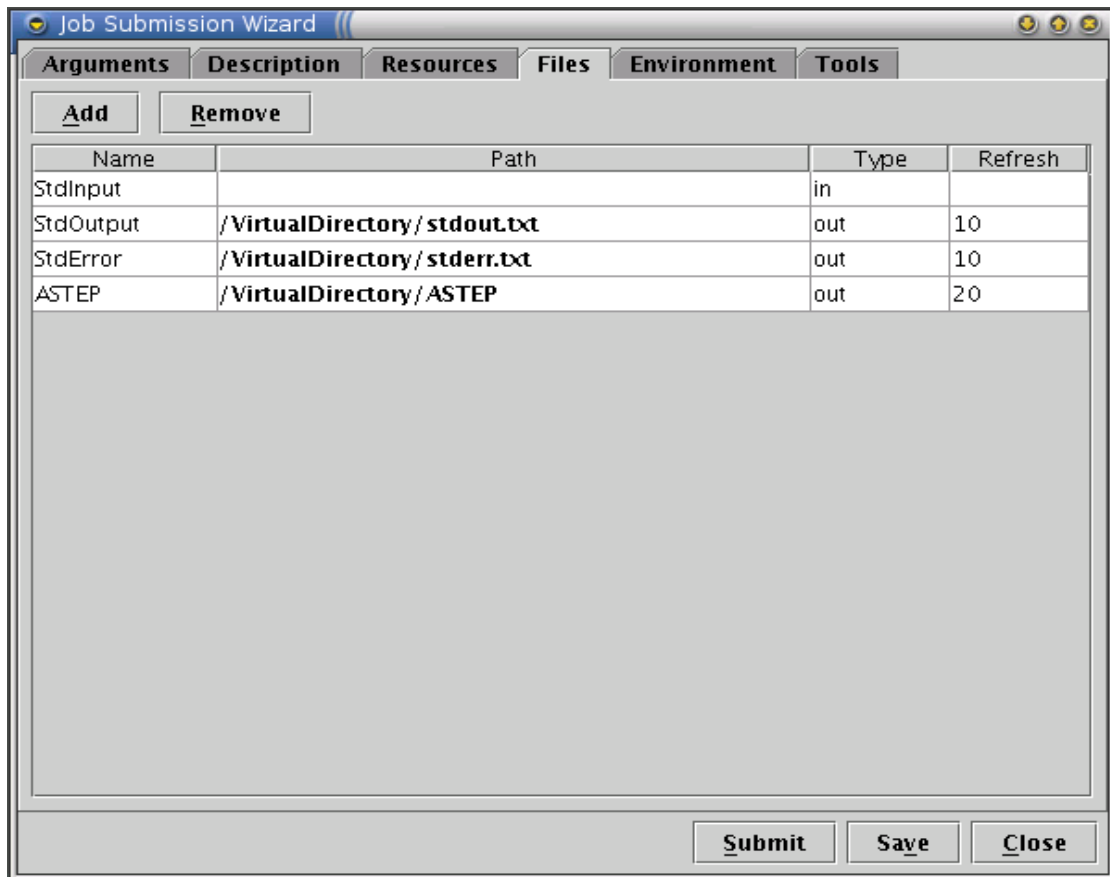


Fig. 3-2 Files Tab

In the Job Monitoring Dialog Window (Fig. 3-3), we can see the list of all the jobs that we have submitted. There are only two buttons with relevance for our application:

- Details – Launch the Job Status Details Window.
- Visualize – Launch the Output Visualization Window for the application.

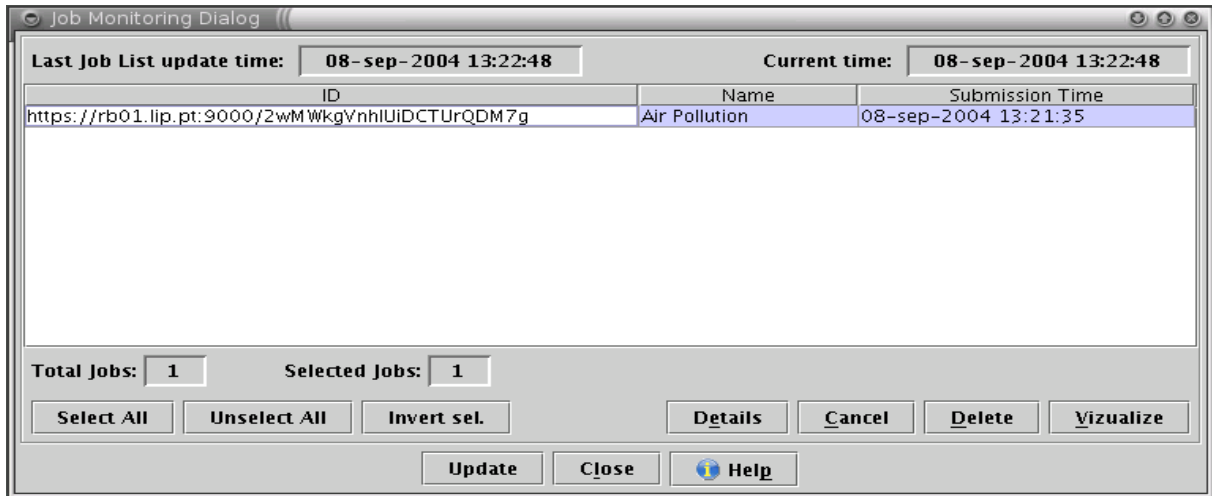


Fig. 3-3 Job Monitoring Dialog

In the Job Status Details Window (Fig. 3-4), the Migrating Desktop shows the details of the job that we have selected. This window it is not auto-refreshable, thus we must refresh it manually.

- Refresh button – Refresh the status of our job.
- Cancel and Delete buttons – Cancel or Delete the Job
- Visualize button – Launch the Output Visualization Window for the Job (if the status is not running, there are no images in this visualization)

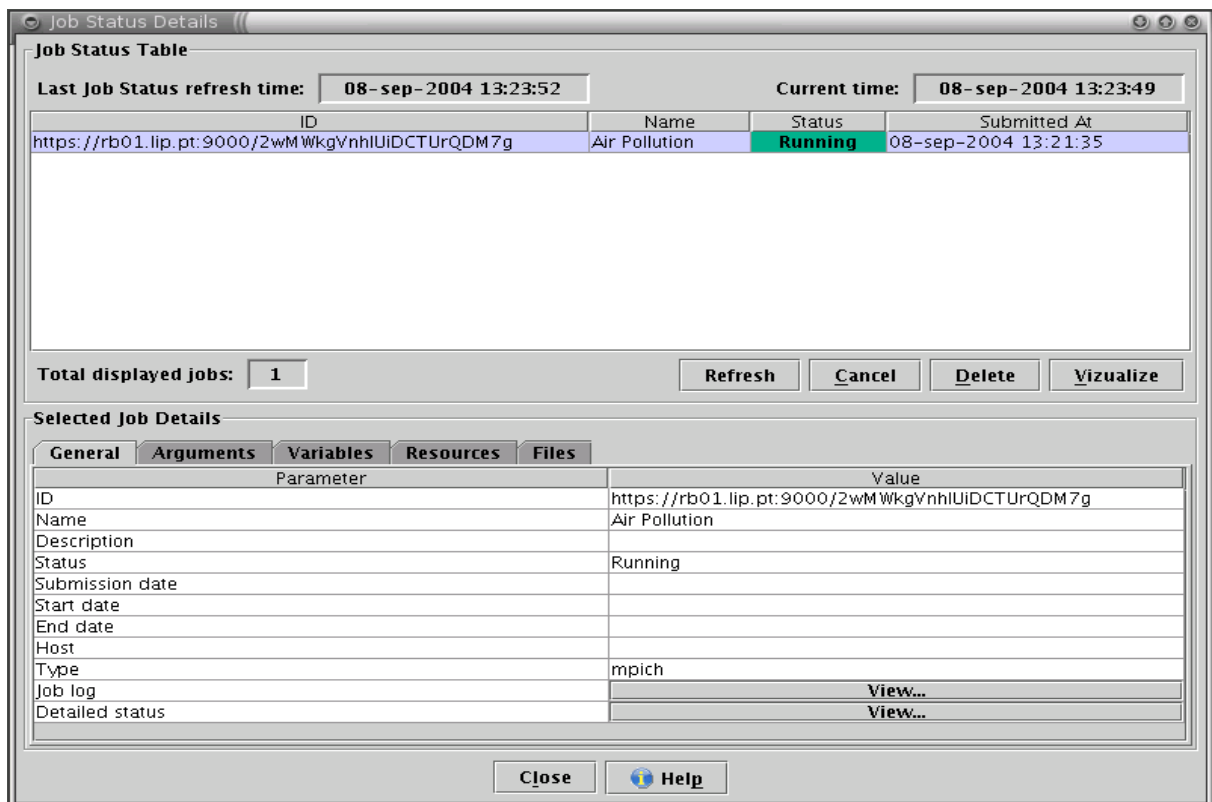


Fig. 3-4 Job Status Details

The Application Viewer or Output Visualization Window. The images in this window are automatically refreshed. The user can vary the desired representation by choosing:

- Type – Pollutant to be represented (drop-down list)
- Level – High level of the 2-D representation (drop-down list)

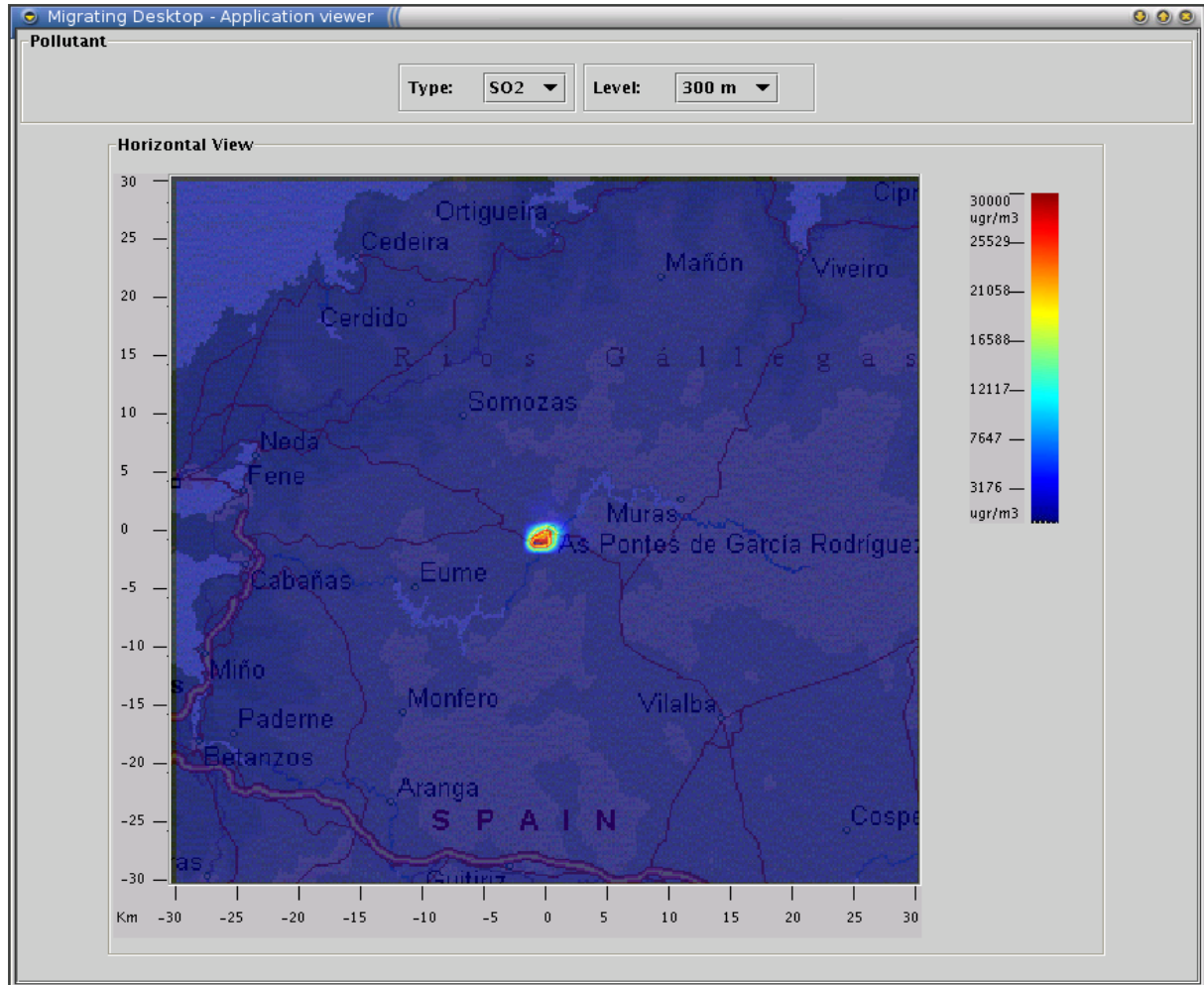


Fig. 3-5 Output Visualization Plugin

Command-line tool sample:

The command line tool *STEMII.exe* uses the following syntax:

```
STEMII.exe date start_hour number_of_hours
```

Where:

- Date** Date of the simulation (YYYYMMDD)
- Start_hour** Start hour of the simulation (0-23)
- Number_of_hours** Number of hours of the simulation (0-23)

4. TROUBLESHOOTING Q&A

Q. The Program execution aborts at the beginning

A. Make sure that you have the input files in the right path (not needed for CrossGrid executions)

Q. There are no images in the Output Visualization Plugin

A. Ensure that the program is already running and that the ASTEP file has been included into the Files tab of the Job Submission Wizard

5. CONTACT INFORMATION AND CREDITS

In case of troubles, please contact the developers at:

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