

Grid Application Support Group Case study Schrodinger equations on the Grid

Status report 16. January, 2007.

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GASUC
Grid Application Support Centre

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Introduction

- ABC code
 - Solution of Schrodinger equation for triatomic systems using time independent (ABC) method
 - A single sequential FORTRAN 90 binary
 - Statically compiled with different libraries
 - Task: to execute on the grid with many parameters in a parameter study fashion
 - Provided for GASuc by Department of Chemistry, University of Perugia

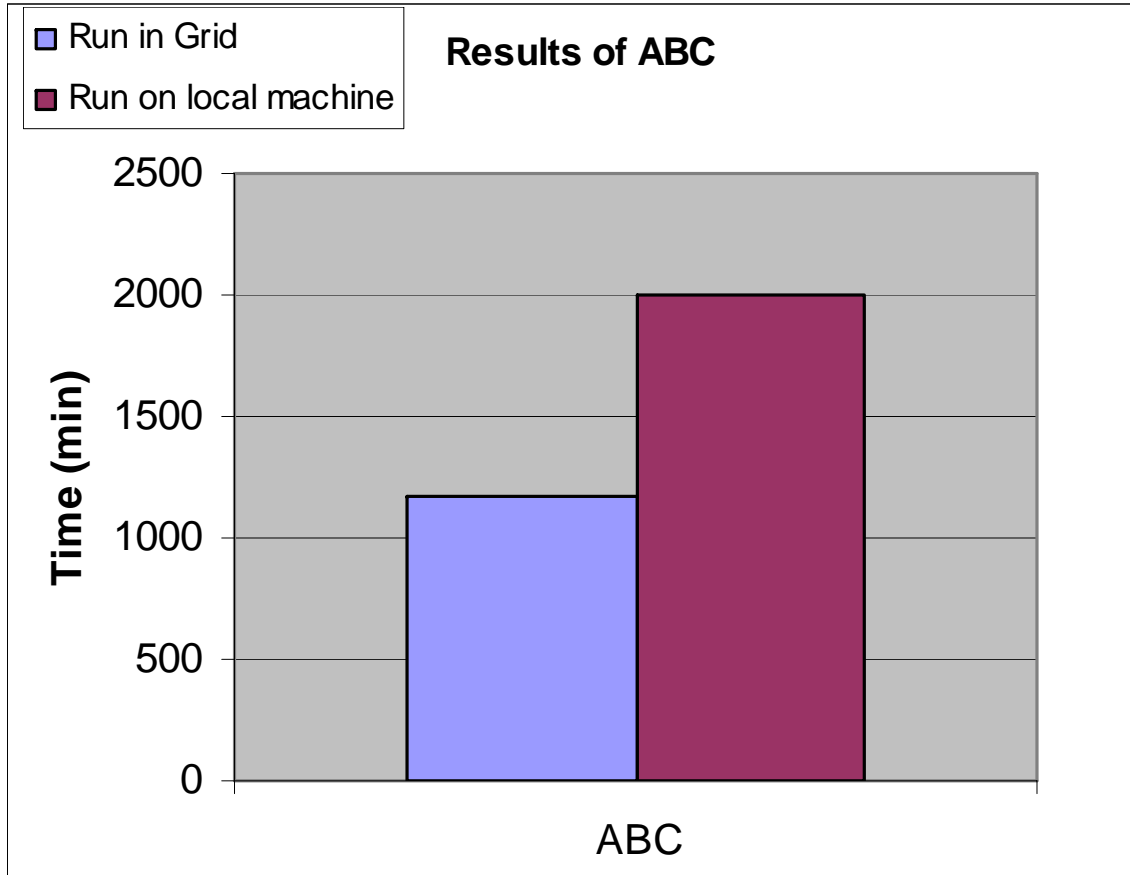
Gridification process

- Chosen infrastructure
 - EGEE
- Chosen tool
 - P-GRADE Portal 2.6
- Chosen grid application structure
 - Workflow with 3 stages:
 - 1st stage: Generator job to generate input parameters for ABC parameter study jobs
 - 2nd stage: ABC simulator jobs (run in SIMD parallelism)
 - 3rd stage: Collector job to pack simulator results into a single archive file (to ease access)

Current status

- ABC workflow is ready and has been executed with 4 parameters on SEE-GRID VO (Southern Eastern European VO)
- Workflow can be managed and monitored through Graphical User Interfaces
- Input parameters can be modified and added through Graphical User Interfaces

Local Vs. Grid execution



- Execution of 4 ABC parameter study jobs
 - on a local machine
 - P4, 3.4GHz, 1GByte
 - on 4 broker selected clusters of SEE VO of EGEE
- Better speed-up can be achieved with more parameter jobs.

Next steps for University of Perugia

1. Try the workflow
 - Browse the results of the finished workflow with 4 parameters
 - Execute another copy of the workflow
 - Configure the workflow
 - Add more input parameters to generate more ABC simulations
2. Feedback to GASuC and decide about possible next steps
 - Migrate workflow to production environment
 - Improve workflow

Workflow information on the next slides

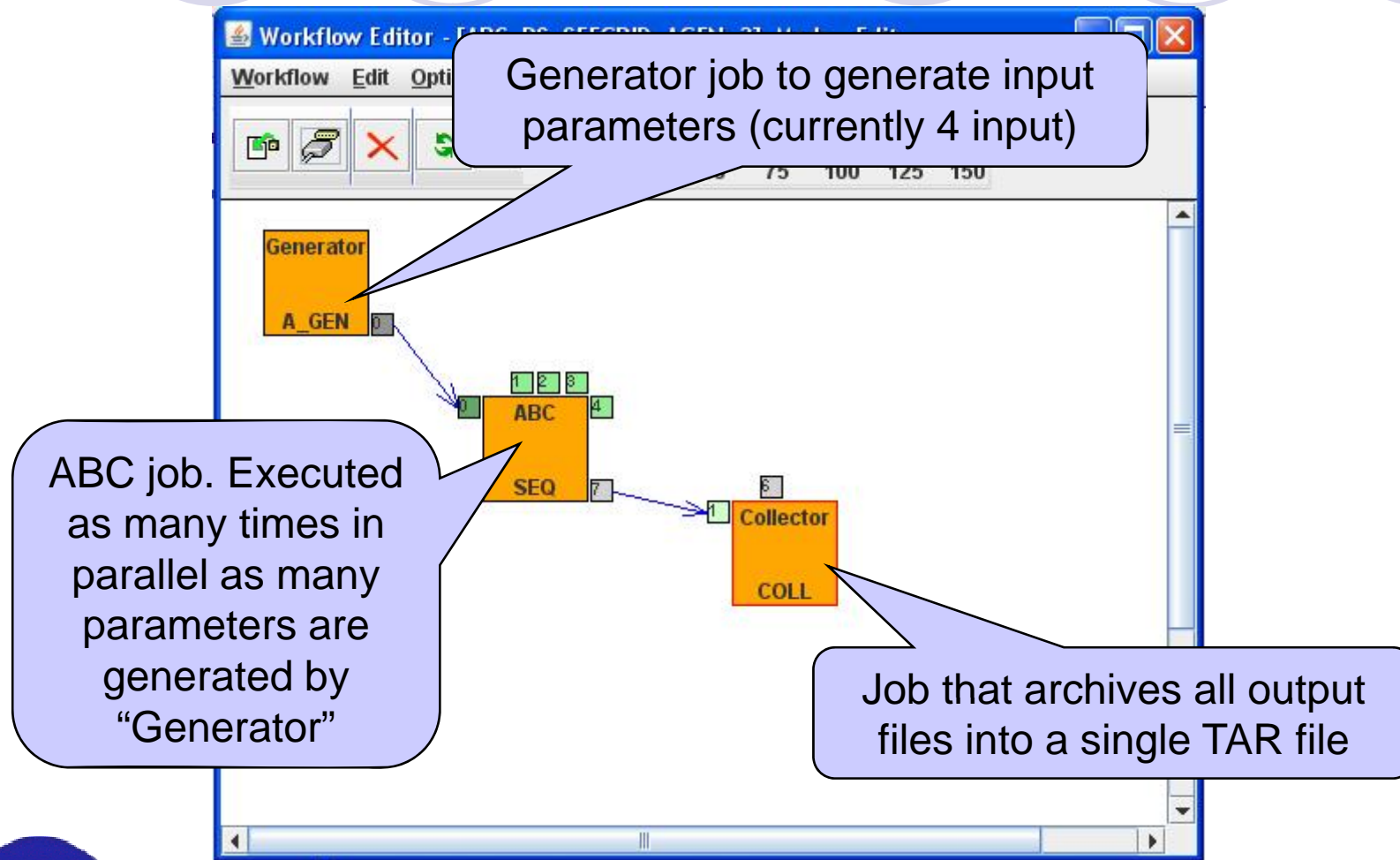


A decorative graphic consisting of seven light purple circles arranged in two rows. The top row has three circles, and the bottom row has four circles. The text is overlaid on these circles.

How to use the ABC workflow

Instruction for users

ABC workflow: explanation of **job flow**



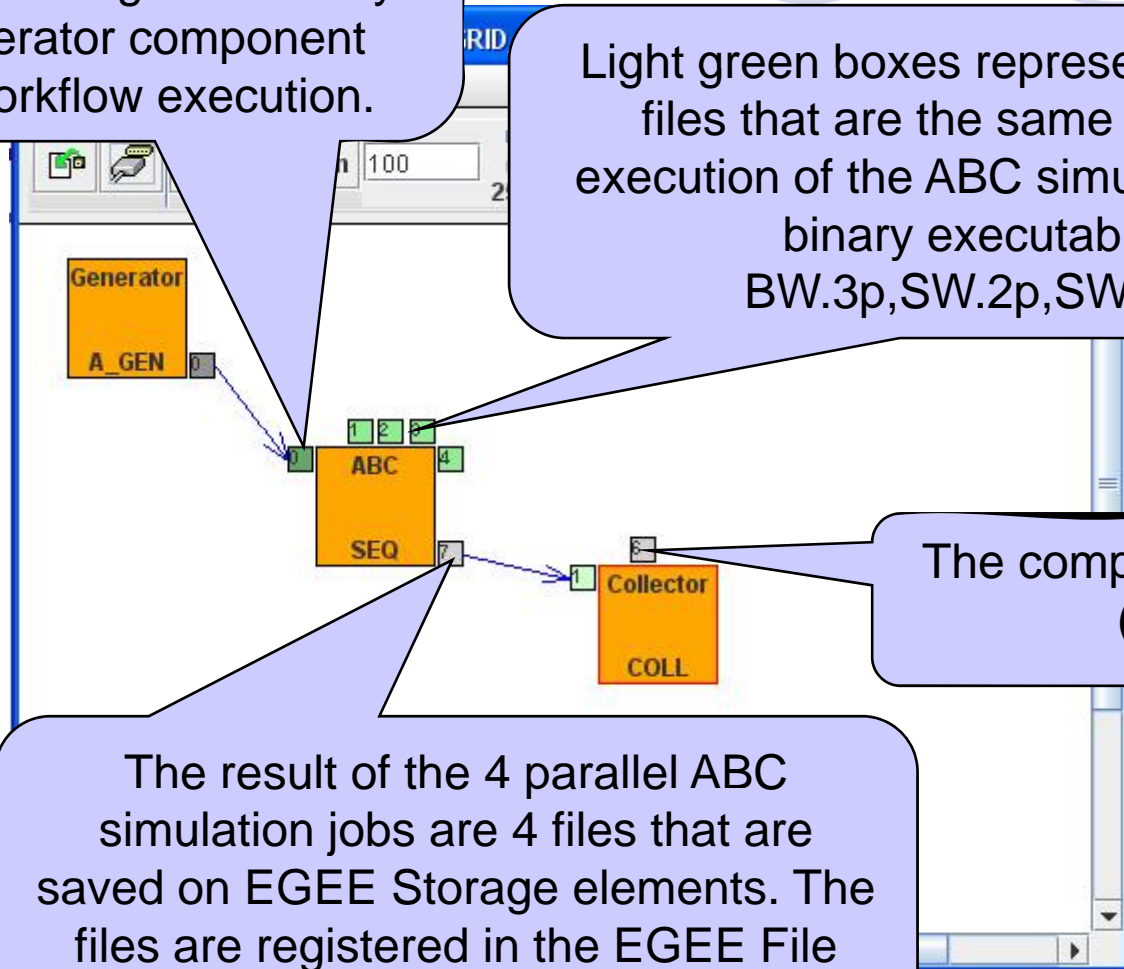
Explanation of **data flow**

Dark green box represents the 4 input files that differ for the 4 ABC simulations. These files are generated by the Generator component during workflow execution.

Light green boxes represent the input files that are the same for every execution of the ABC simulation (ABC binary executable, BW.3p, SW.2p, SW.3p)

The compressed output files (abc.outs)

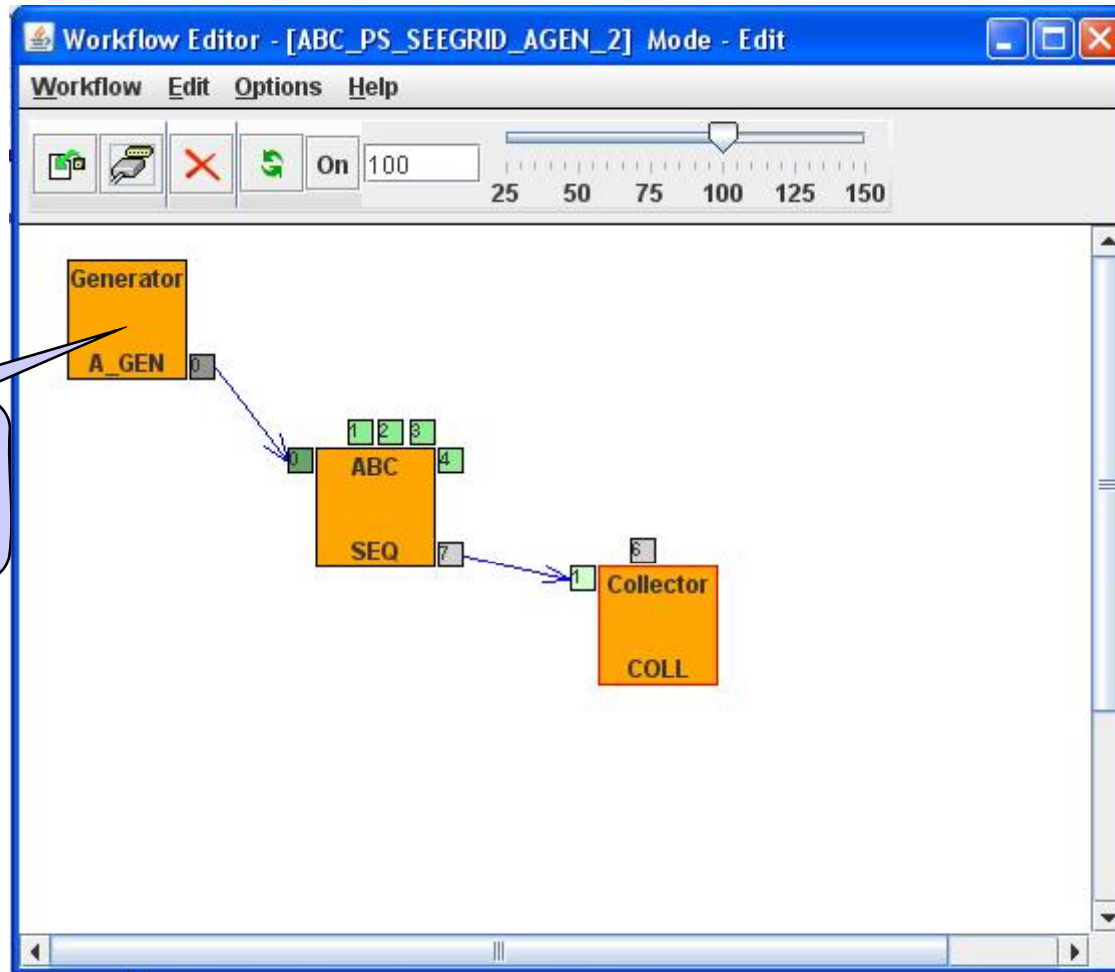
The result of the 4 parallel ABC simulation jobs are 4 files that are saved on EGEE Storage elements. The files are registered in the EGEE File Catalog with Logical File Names.



What should I modify to make a new run?

- Modify input parameters of ABC simulation
- and**
- Modify grid parameters for the workflow

Modify input parameters of ABC simulation



Modify input parameters of ABC simulation

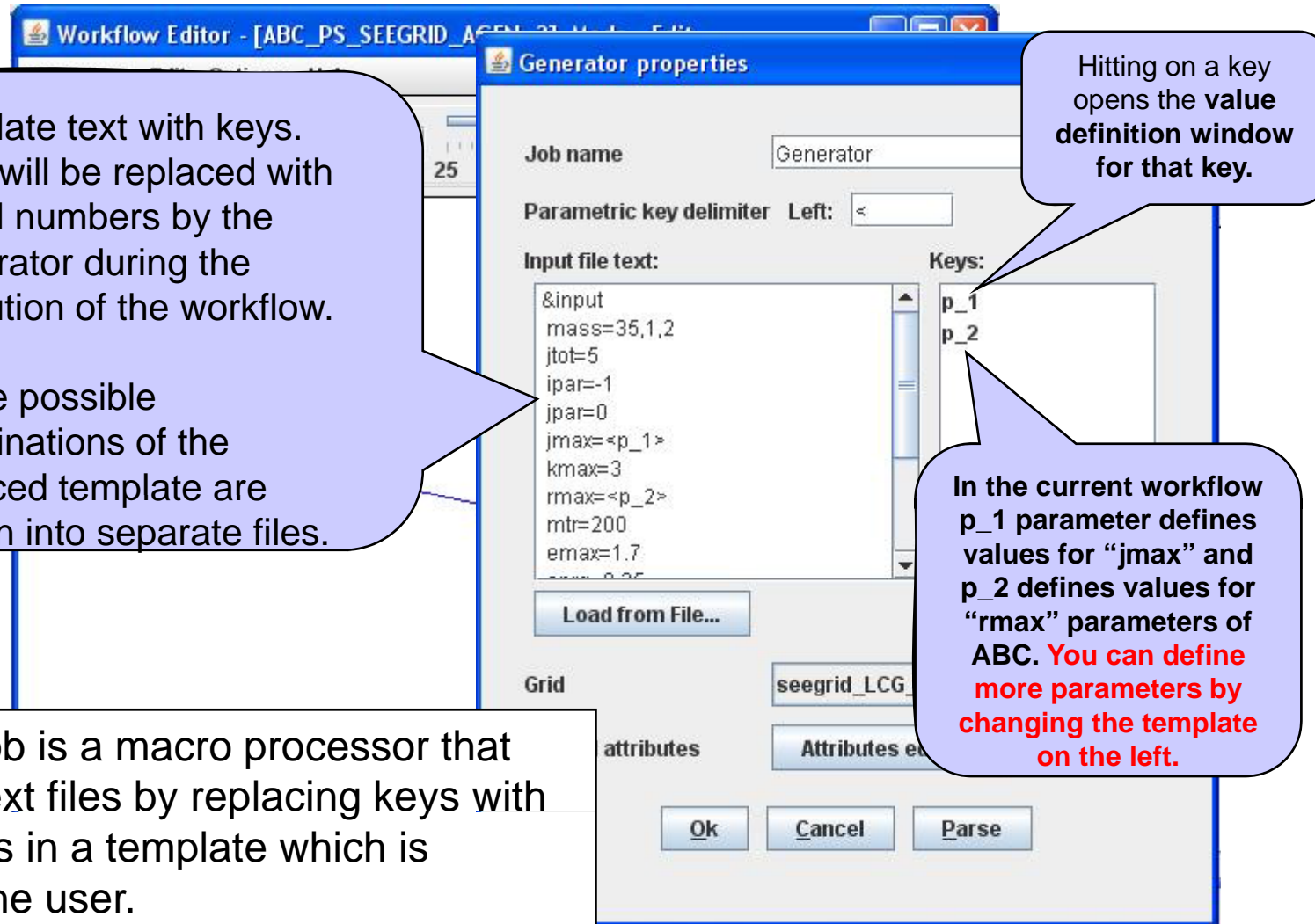
Template text with keys.
Keys will be replaced with actual numbers by the Generator during the execution of the workflow.

All the possible combinations of the replaced template are written into separate files.

Generator job is a macro processor that generates text files by replacing keys with actual values in a template which is defined by the user.

Hitting on a key opens the **value definition window** for that key.

In the current workflow p_1 parameter defines values for "jmax" and p_2 defines values for "rmax" parameters of ABC. **You can define more parameters by changing the template on the left.**



Modify input parameters of ABC simulation

Parameter Key Definition: p_1

Substitution for Parameter key: p_1

Type

- INT
- REAL
- CHAR

Format

Free format

Bound format

Length: Left aligned

REAL

- Exp: -0.M+E M= E=
- Fixed point: W.F W= F=
- Floating point

Generated Items

Total generated items:

Value Definition

- Set:
- Set from local File:
- Range From: To: By:
- Random Seed: Cases: From: To:

OK Cancel Generate

In this form you can define actual values for the selected parameter.

In the workflow the generated values are 17.0 and 21.0 for p_1 and 18.0 and 24.0 for p_2. **You can modify this range in order to define larger parameter sets.**

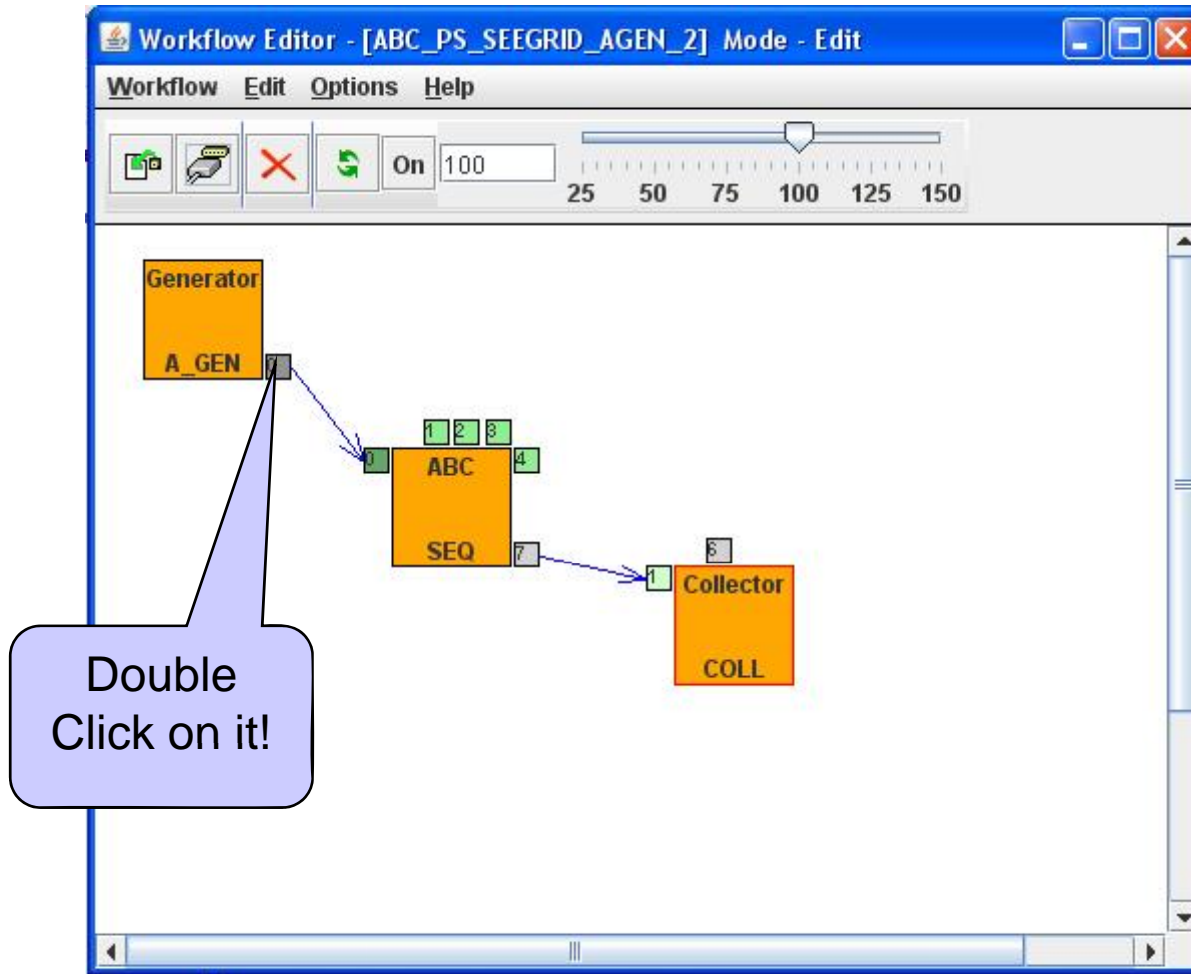
Modify grid parameters for the workflow

- This is necessary because
 - the result files of the Generator job are saved on Storage Elements and are registered in the Grid File Catalog
 - the result files of the ABC jobs are saved on Storage Elements and are registered in the Grid File Catalog
 - File Catalog entries must be different for each workflow execution → Directory names for these files must be changed
- To modify grid directory names
 - Properties of remote files must be modified.

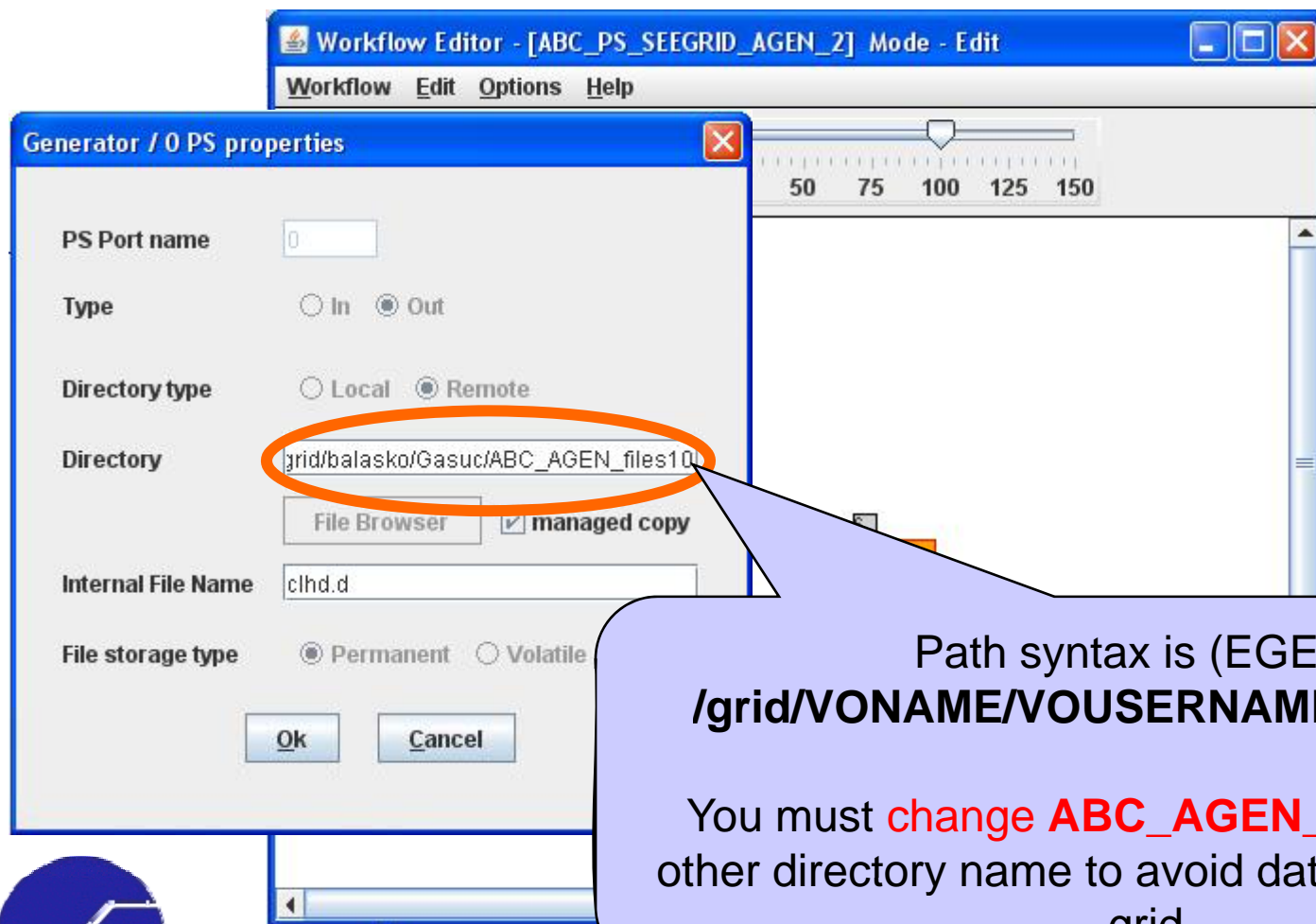
The following slides show how to do it.



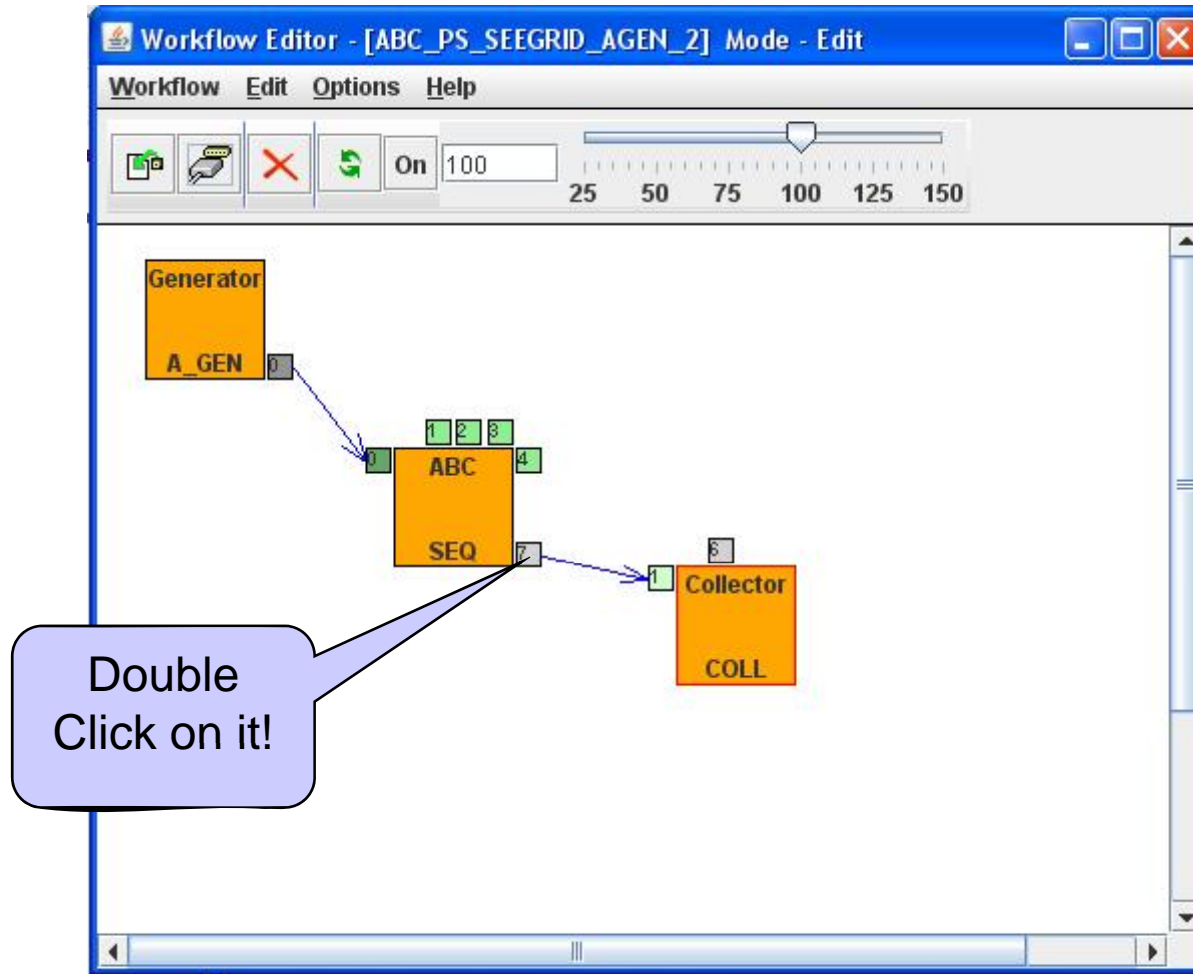
Modify grid parameters for the workflow



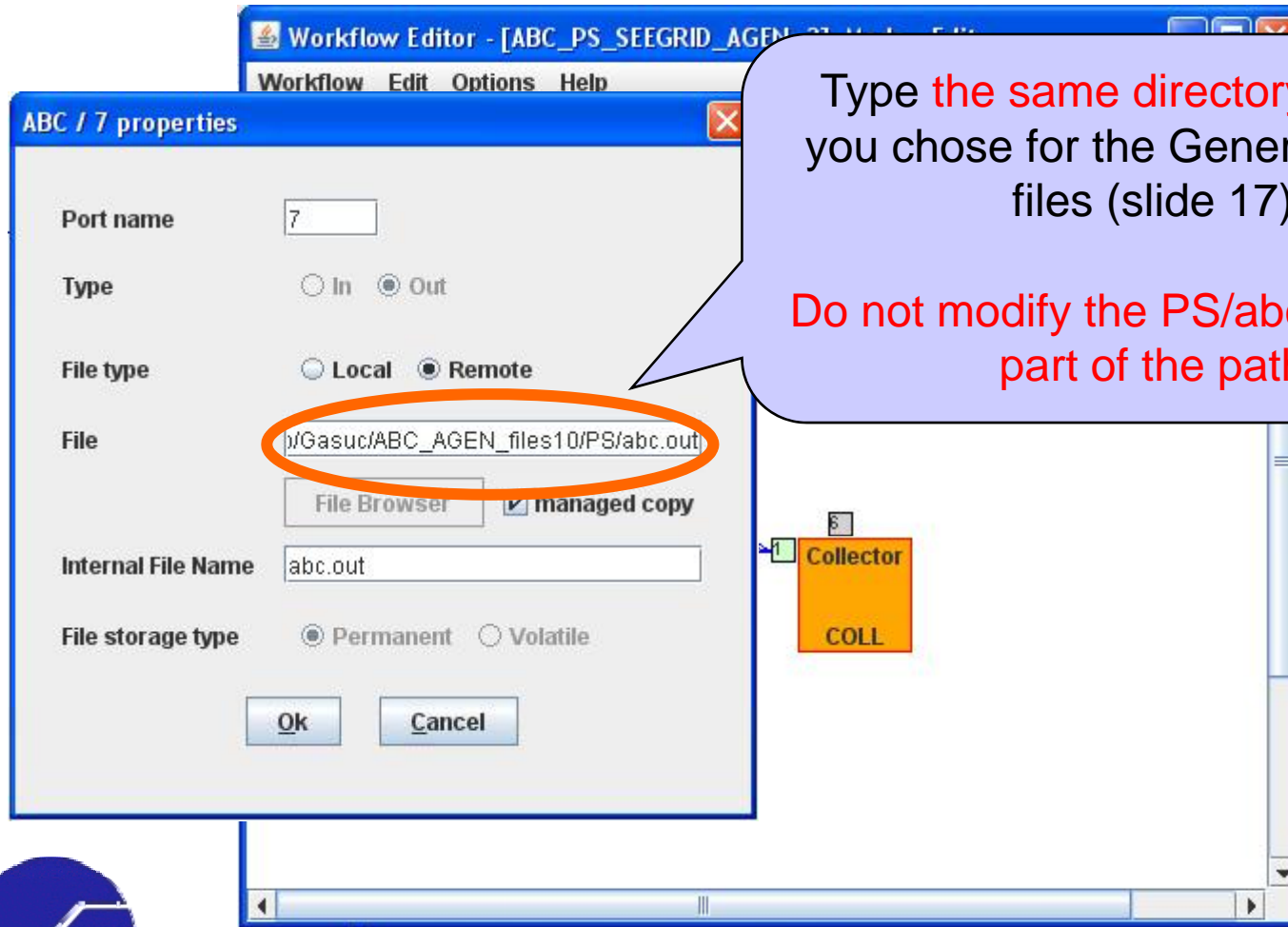
Modify grid parameters for the workflow



Modify grid parameters for the workflow



Modify grid parameters for the workflow



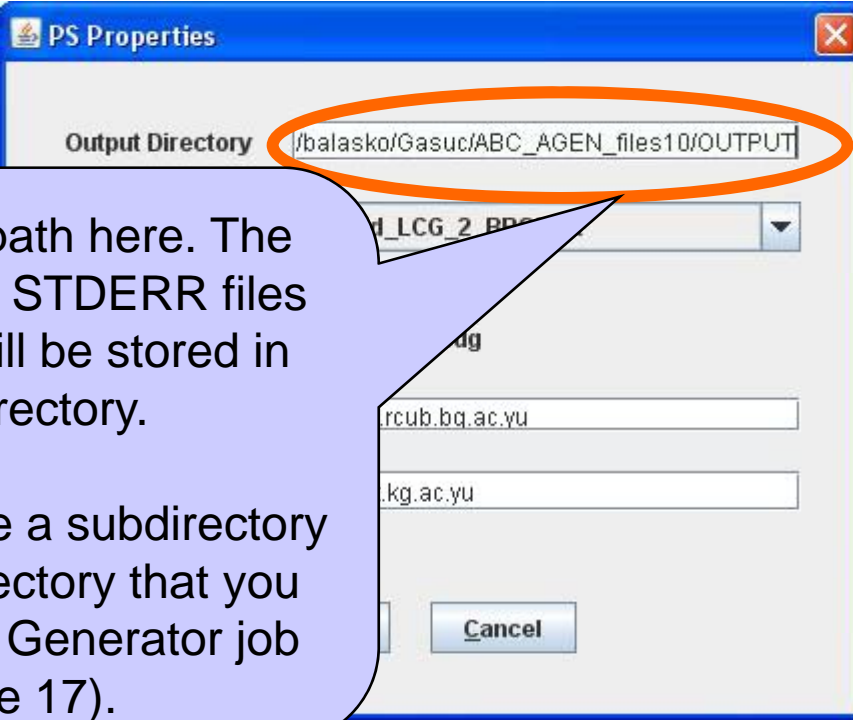
Type **the same directory path** that you chose for the Generator output files (slide 17).

Do not modify the PS/abc.out postfix part of the path!

Modify grid parameters for the workflow

The screenshot shows the 'Workflow Editor' window with the title bar '[ABC_PS_SEEGRID_AGEN_2] Mode - Edit'. The menu bar includes 'Workflow', 'Edit', 'Options', and 'Help'. The 'Edit' menu is open, listing various actions such as 'New', 'New job', 'New port', 'Open', 'Save', 'Save as', 'Import workflow', 'Upload Files...', 'Save resources', 'Refresh', 'Workflow properties', 'PS properties', and 'Exit'. The 'PS properties' option is highlighted. A callout bubble with the text 'Double Click on it!' points to the 'PS properties' menu item. In the background, a workflow diagram is partially visible, showing a 'Collector' node and other components.

Modify grid parameters for the workflow



Type a new path here. The STDOUT and STDERR files of the jobs will be stored in this directory.

Advice: Define a subdirectory within the directory that you chose for the Generator job (Slide 17).

Save and execute the workflow

- Click on “Workflow” then “Save as” and define a new name
- Go back to the Web interface and click on “Refresh” on the Portal interface (*not the browser refresh button*) → The new workflow appears in the list
- Click on “Submit” of the new workflow
- You need proxy certificate to execute the workflow on SEE-GRID resources. We provide you with a proxy for 100 hours. If that proxy expires please contact Akos Balasko to get a new one (balasko@sztaki.hu).

Possible next actions

- **If you are satisfied with the workflow**
 - Setup a P-GRADE Portal for the Compchem VO (SZTAKI)
 - Migrate the application to that VO (SZTAKI)
 - Define more parameters for the application and execute it at a production level (University of Perugia)
 - Train the users (SZTAKI and University of Perugia)
- **If you are not satisfied with the workflow**
 - Discuss potential improvements with GASuC
 - Improve the workflow yourself based on P-GRADE Portal user manual (online at www.portal.p-grade.hu)

The slide features a decorative arrangement of six circles. Two circles are filled with a light purple color, while the other four are hollow with a thin purple outline. The circles are arranged in two rows: the top row has three circles and the bottom row has three circles. The text 'Thank you!' is centered over the top-right circles, and the URL 'www.lpds.sztaki.hu/gasuc' is centered over the bottom-middle circles.

Thank you!

www.lpds.sztaki.hu/gasuc