Grid Application Support Group Case study
Schrodinger equations on the Grid

Status report 16. January, 2007.

GASuC
Grid Application Support Centre

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Introduction

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- 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

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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

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- 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

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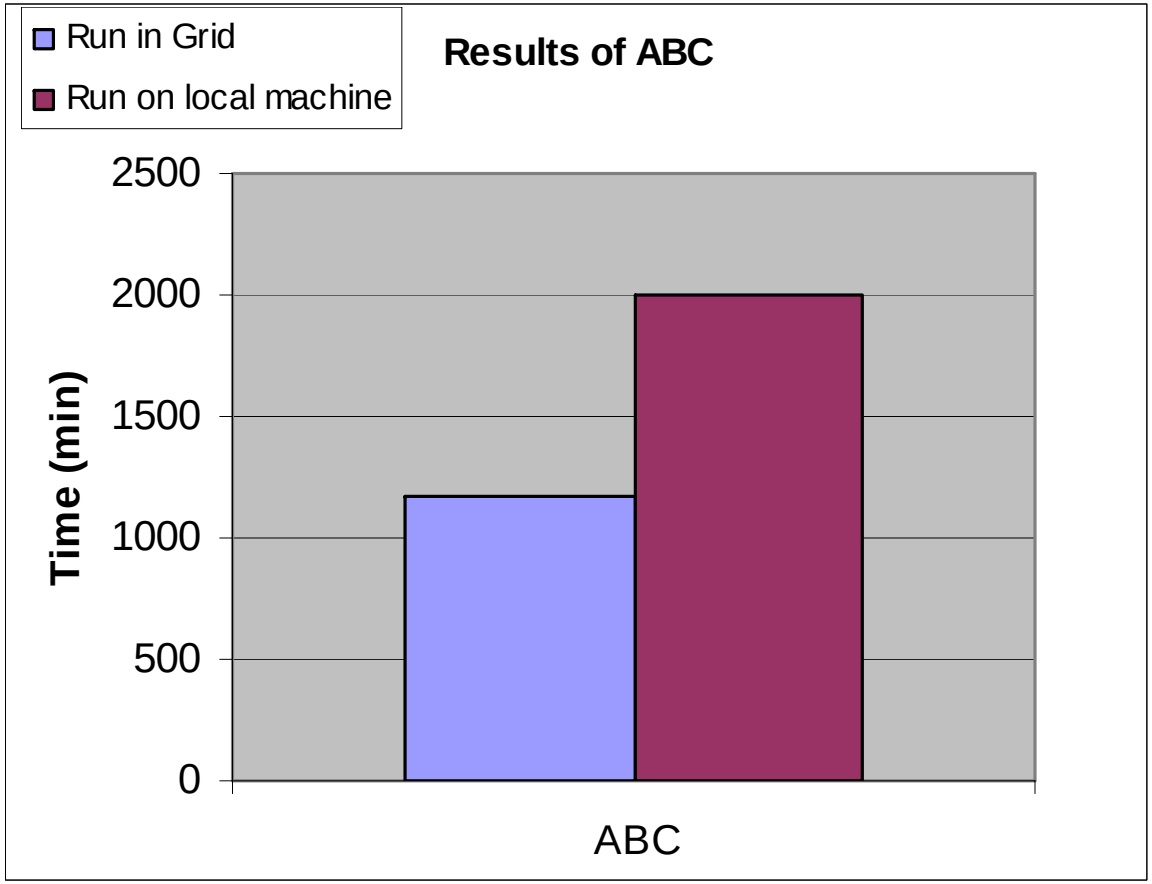
Local Vs. Grid execution



- 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.

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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

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How to use the ABC workflow

Instruction for users

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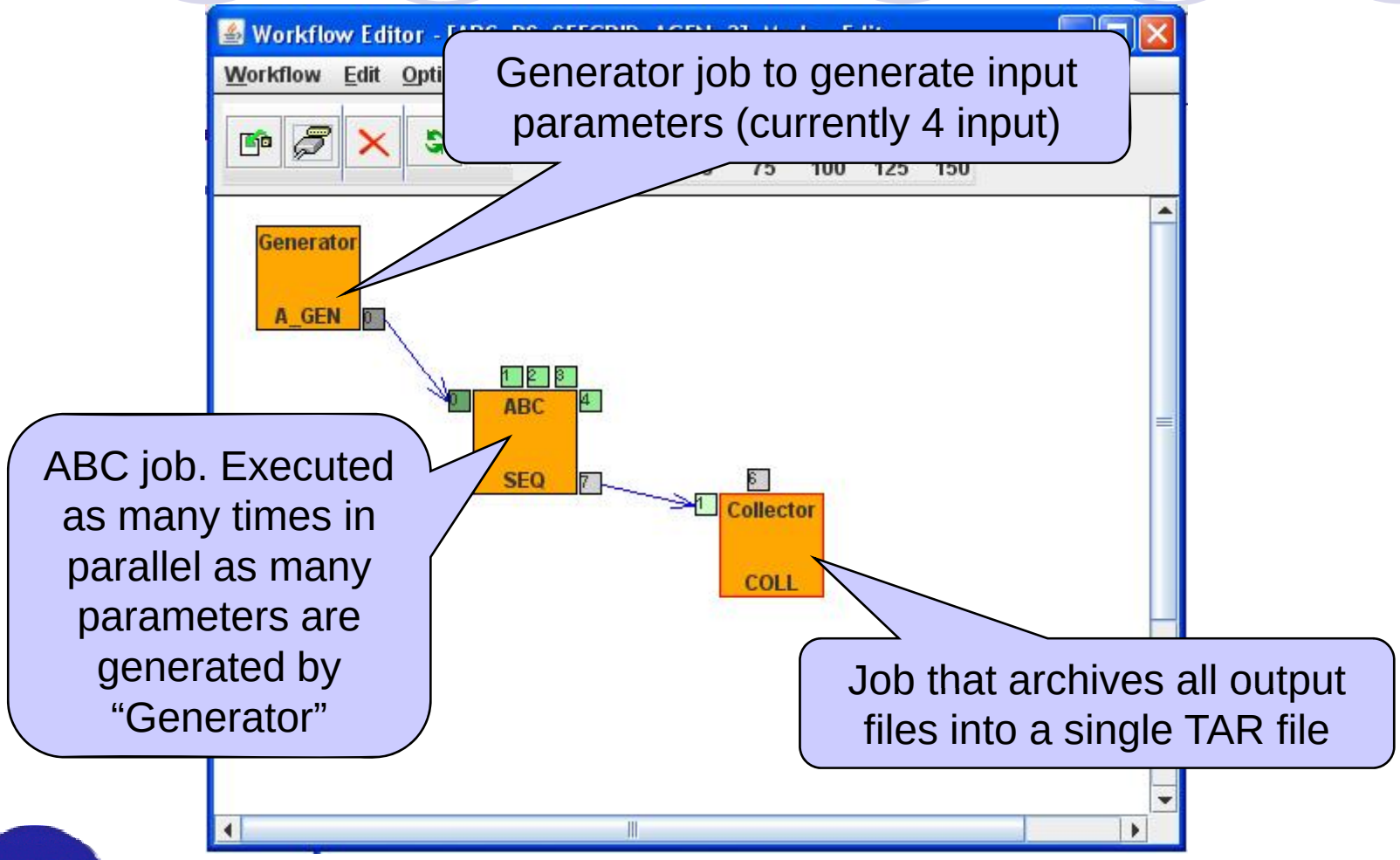
ABC workflow: explanation of **job flow**



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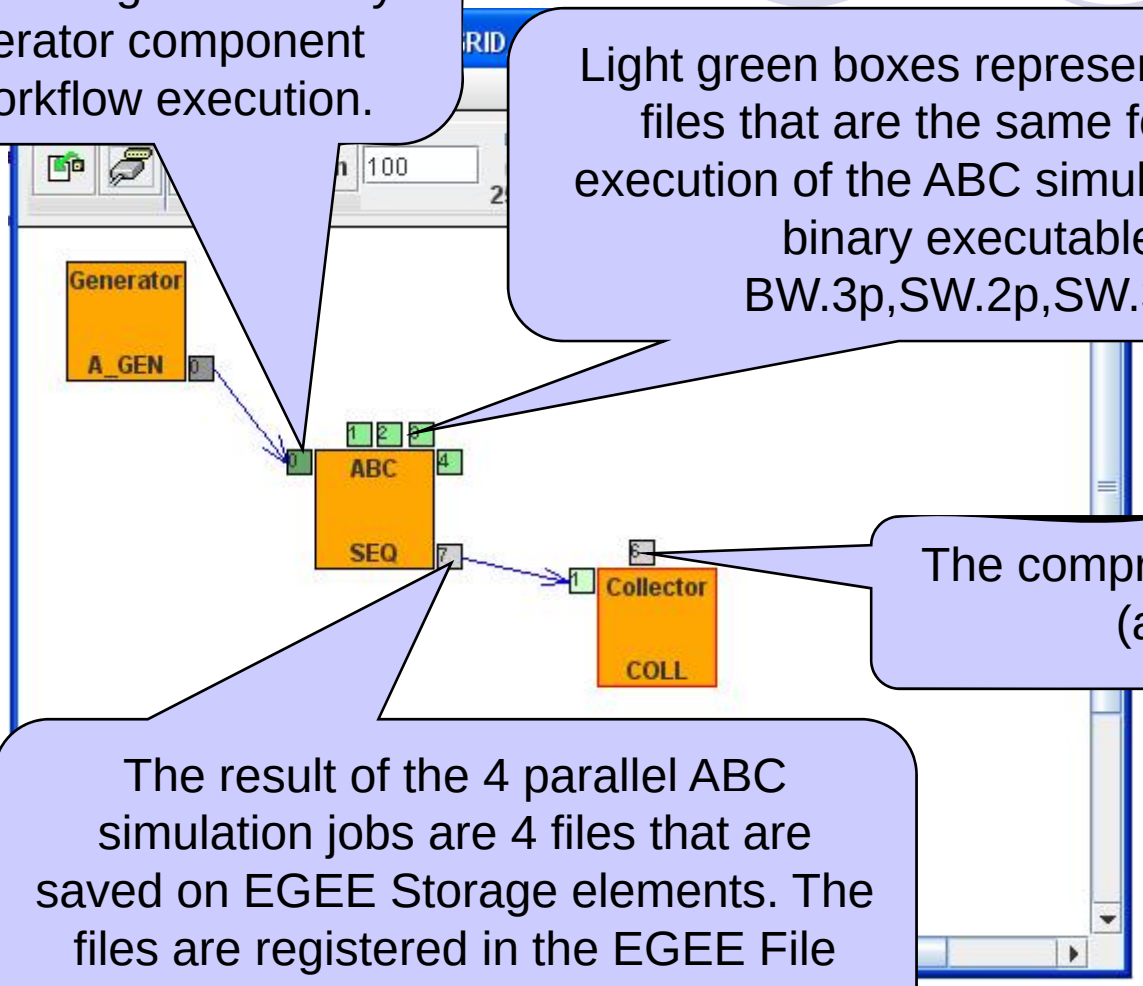
xplanation of **data flow**

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.

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What should I modify to make a new run?

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- Modify input parameters of ABC simulation

and

- Modify grid parameters for the workflow

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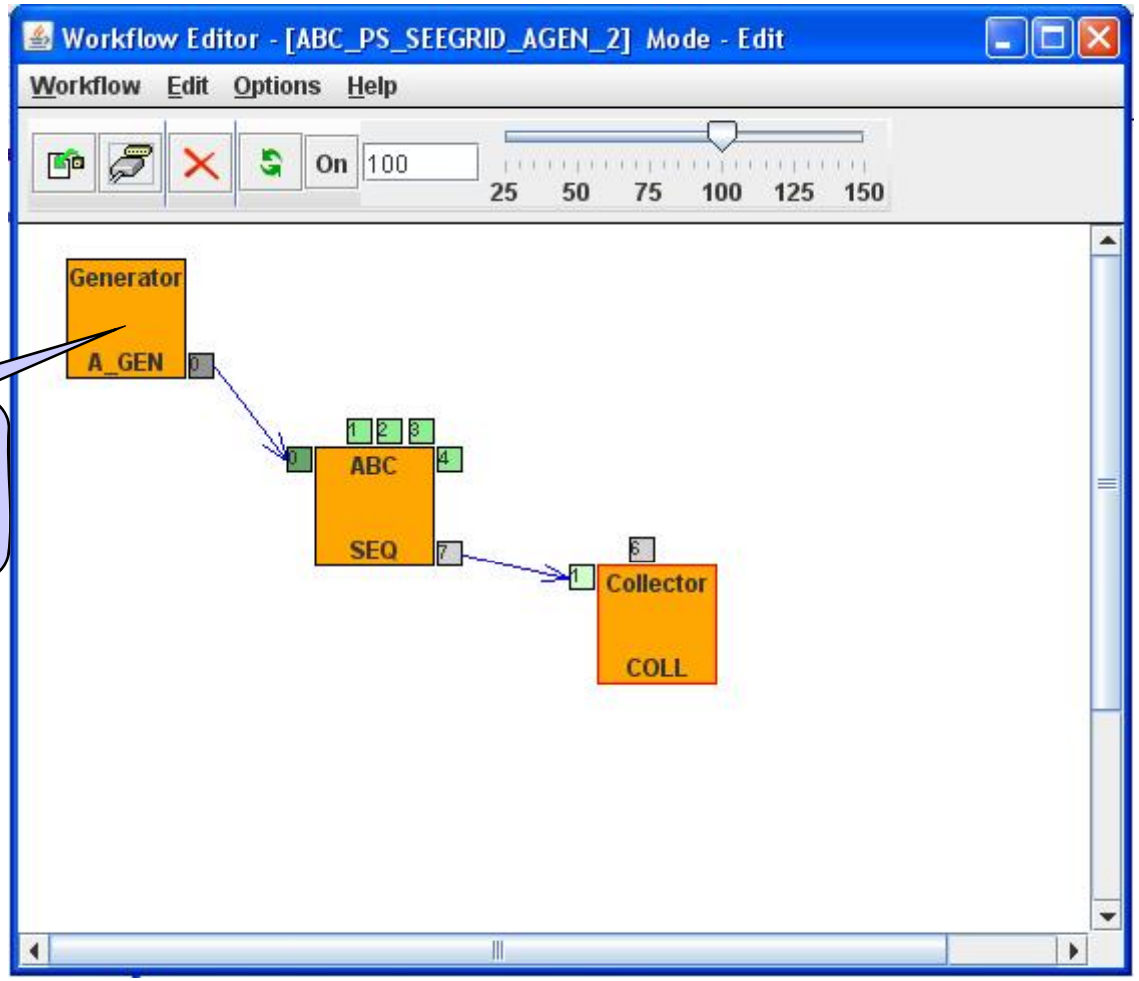
Modify input parameters of ABC simulation



Modify input parameters of ABC simulation

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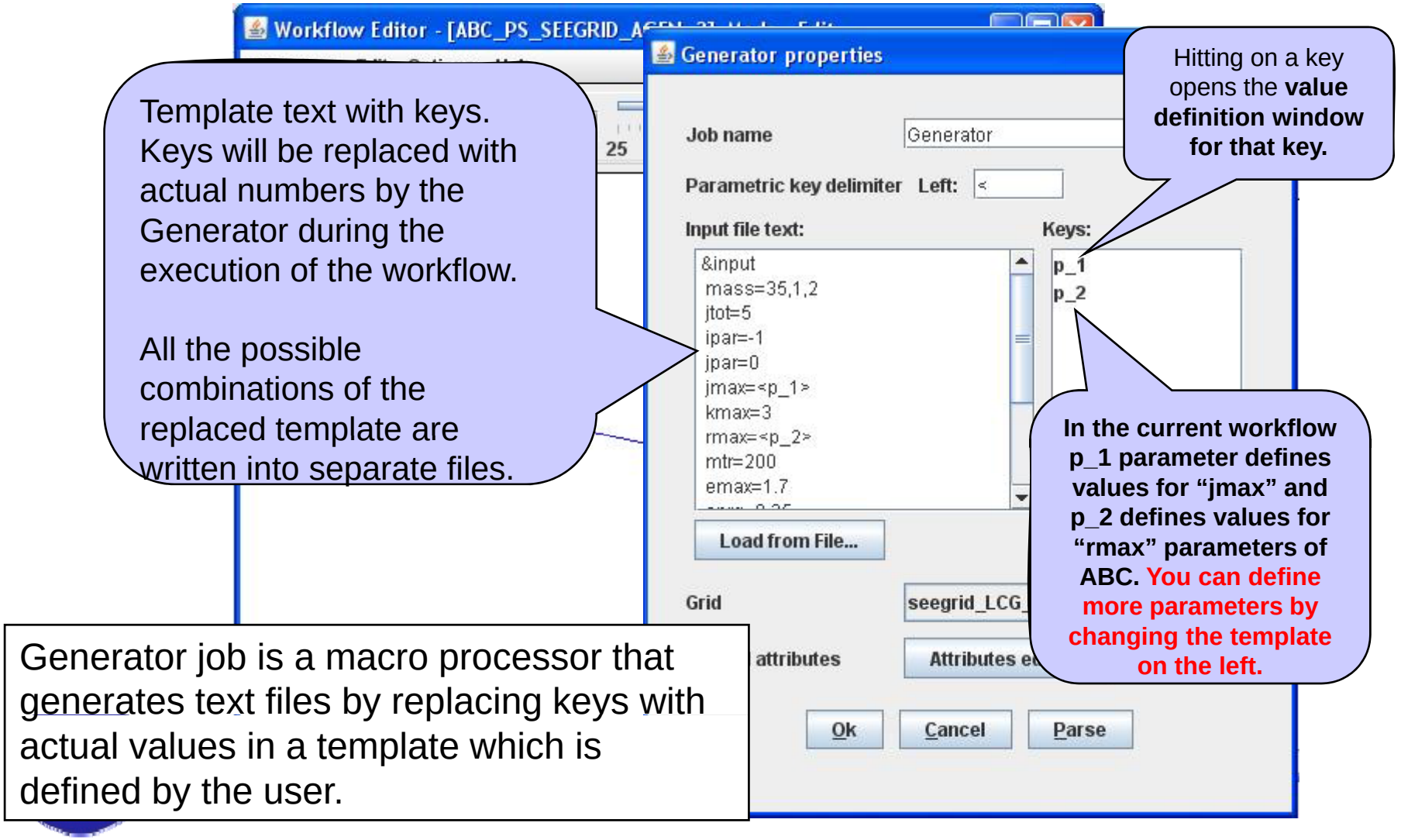

Modify input parameters of ABC simulation

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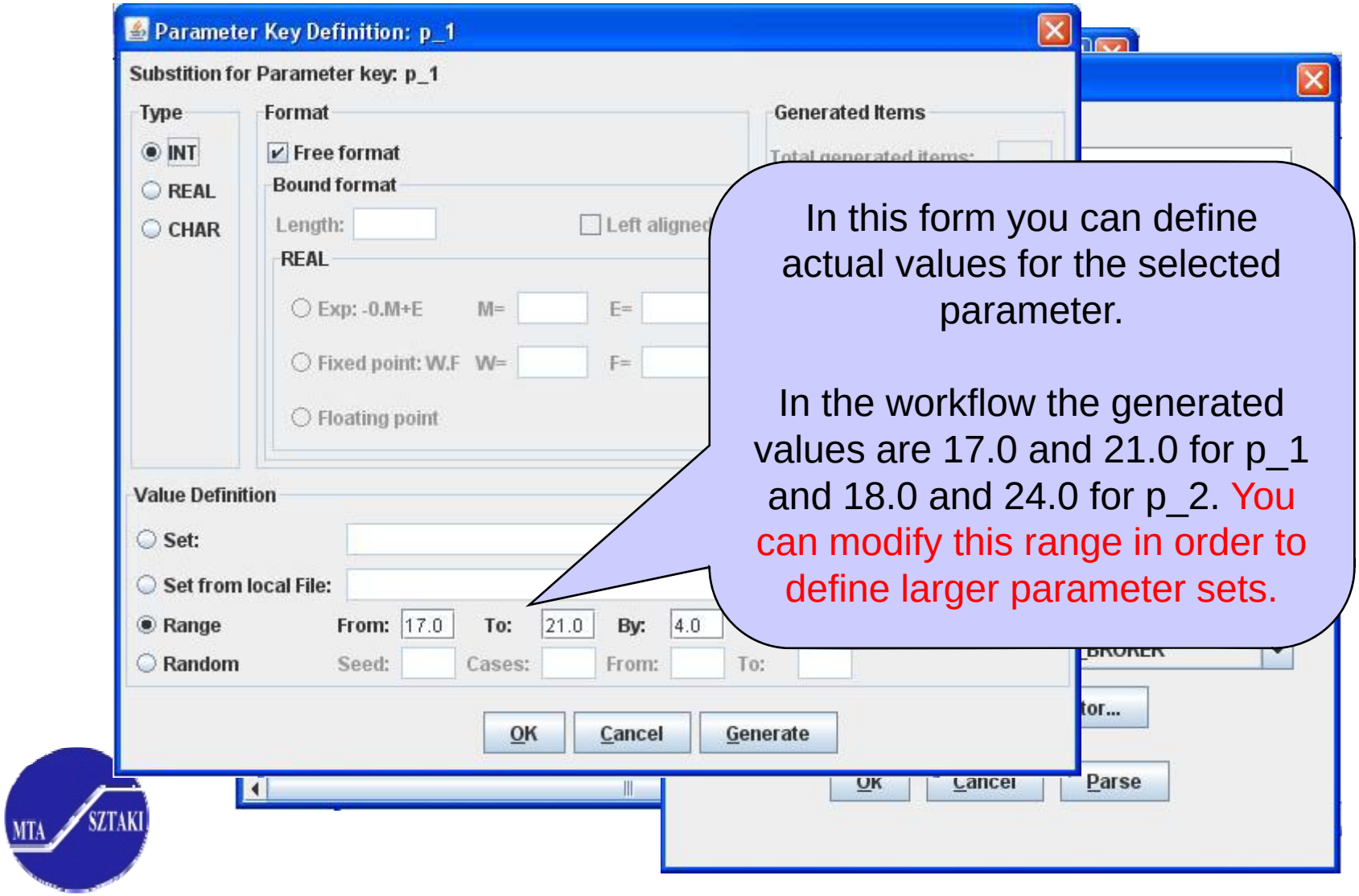

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Modify grid parameters for the workflow

- 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.

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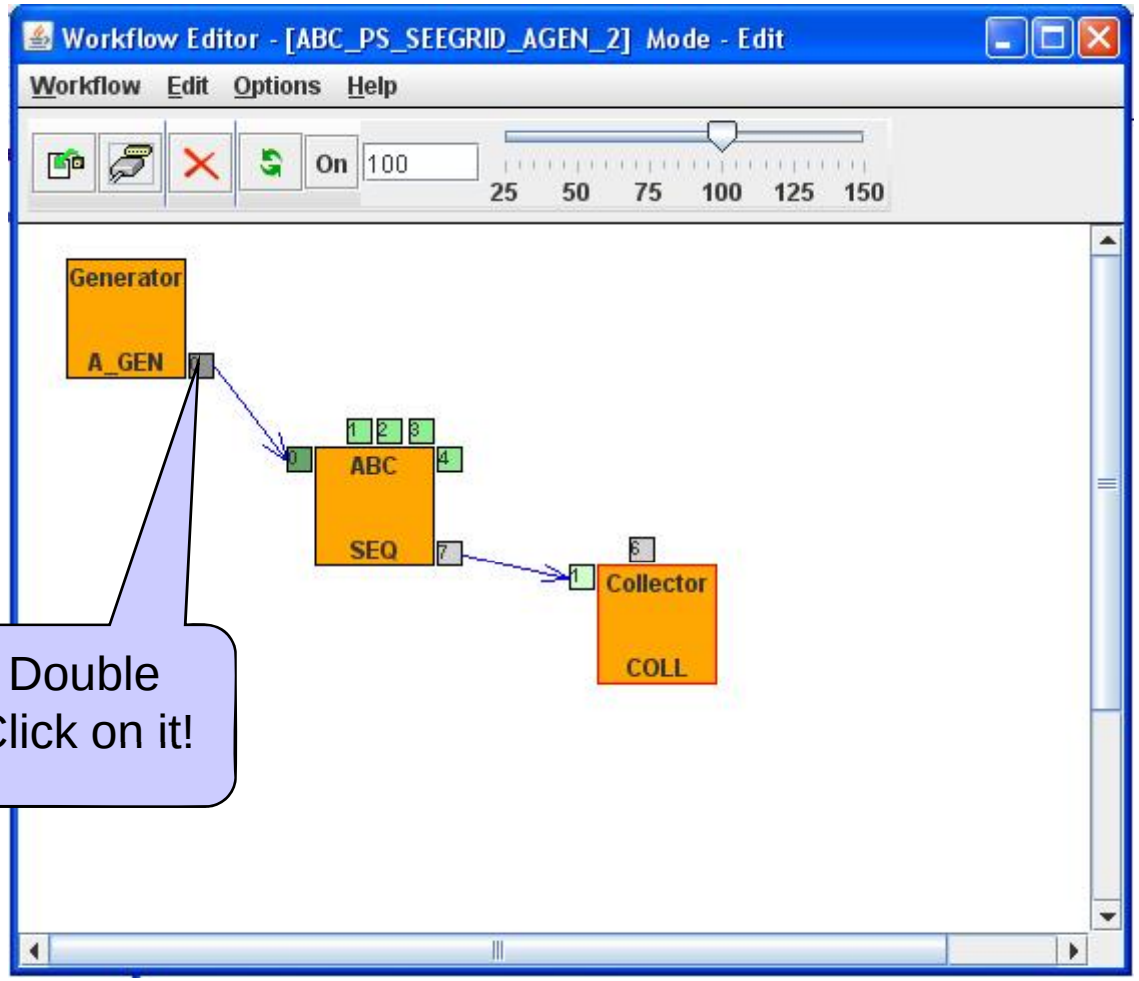
Modify grid parameters for the workflow



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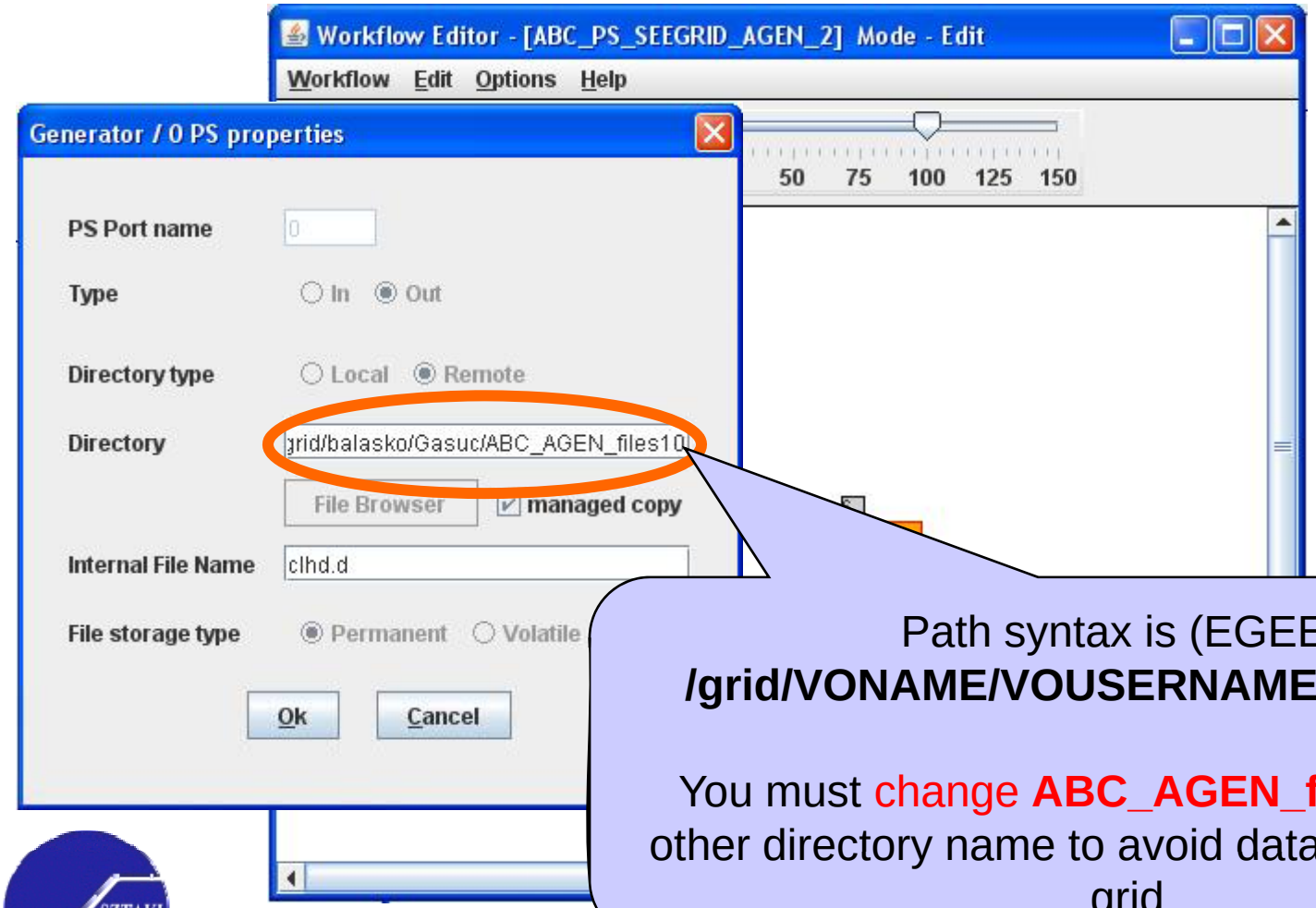
Modify grid parameters for the workflow



Path syntax is (EGEE):
/grid/VONAME/VOUSERNAME/custom_dir

You must change **ABC_AGEN_files10** to any other directory name to avoid data-rewrite on the grid

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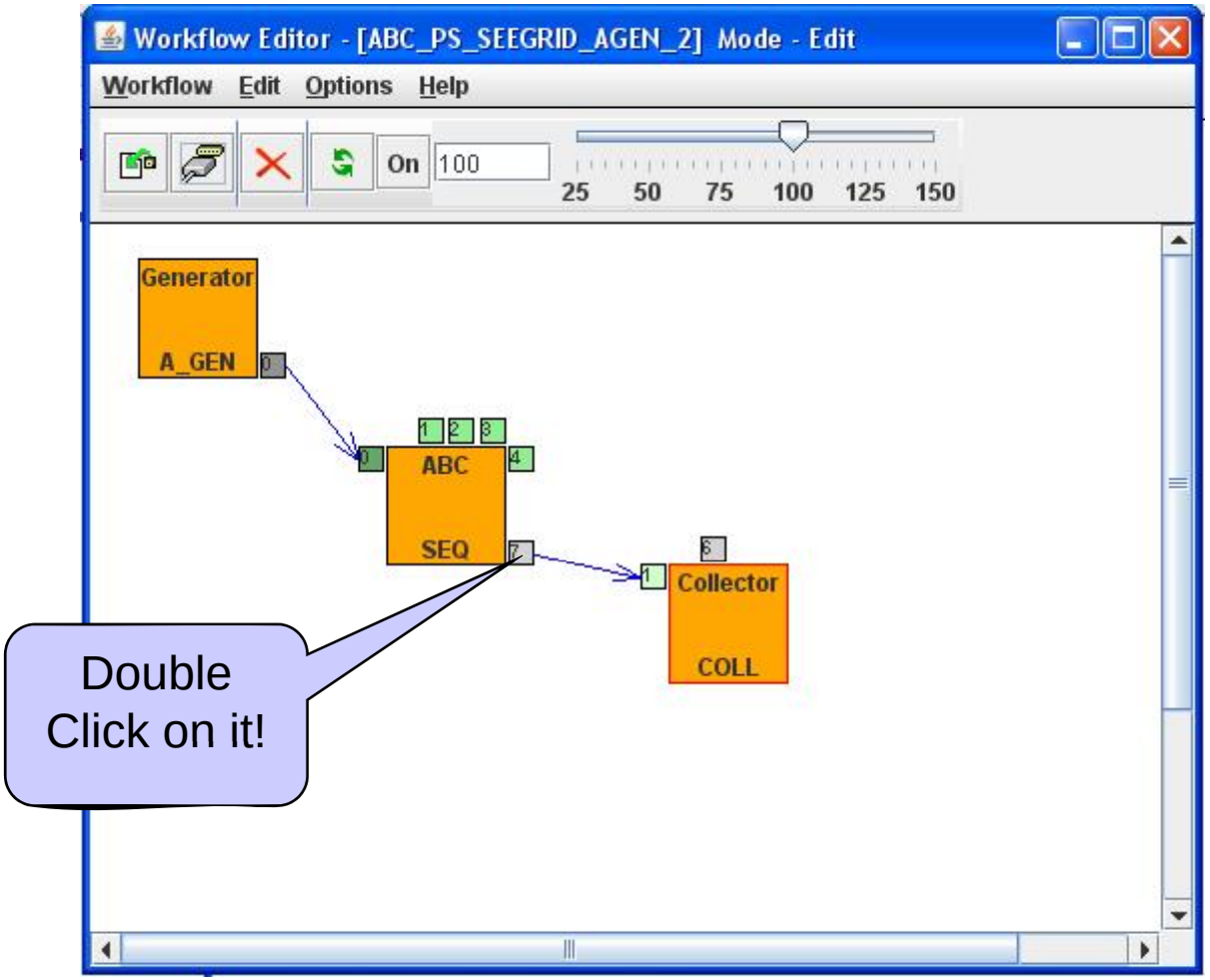
Modify grid parameters for the workflow



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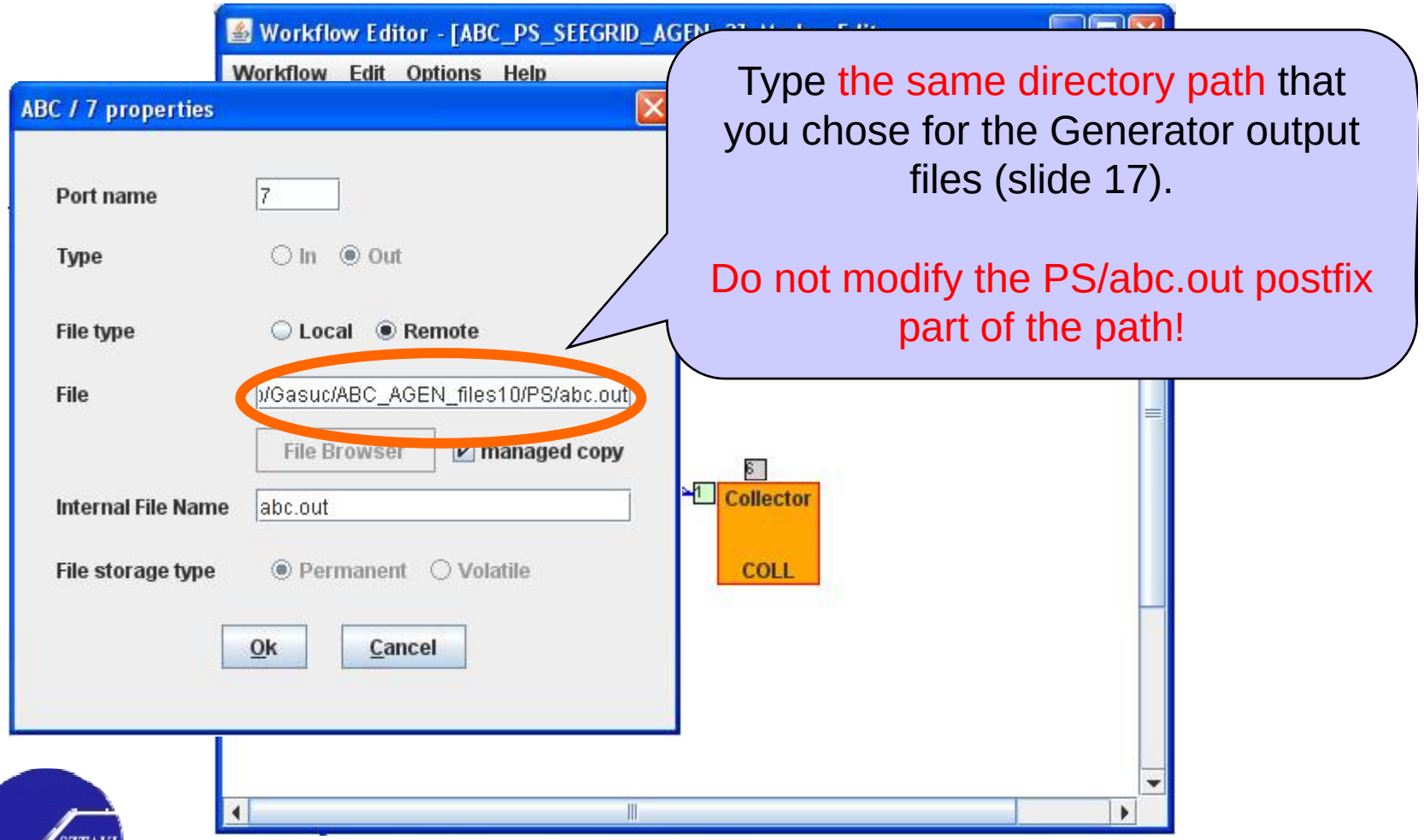
Modify grid parameters for the workflow



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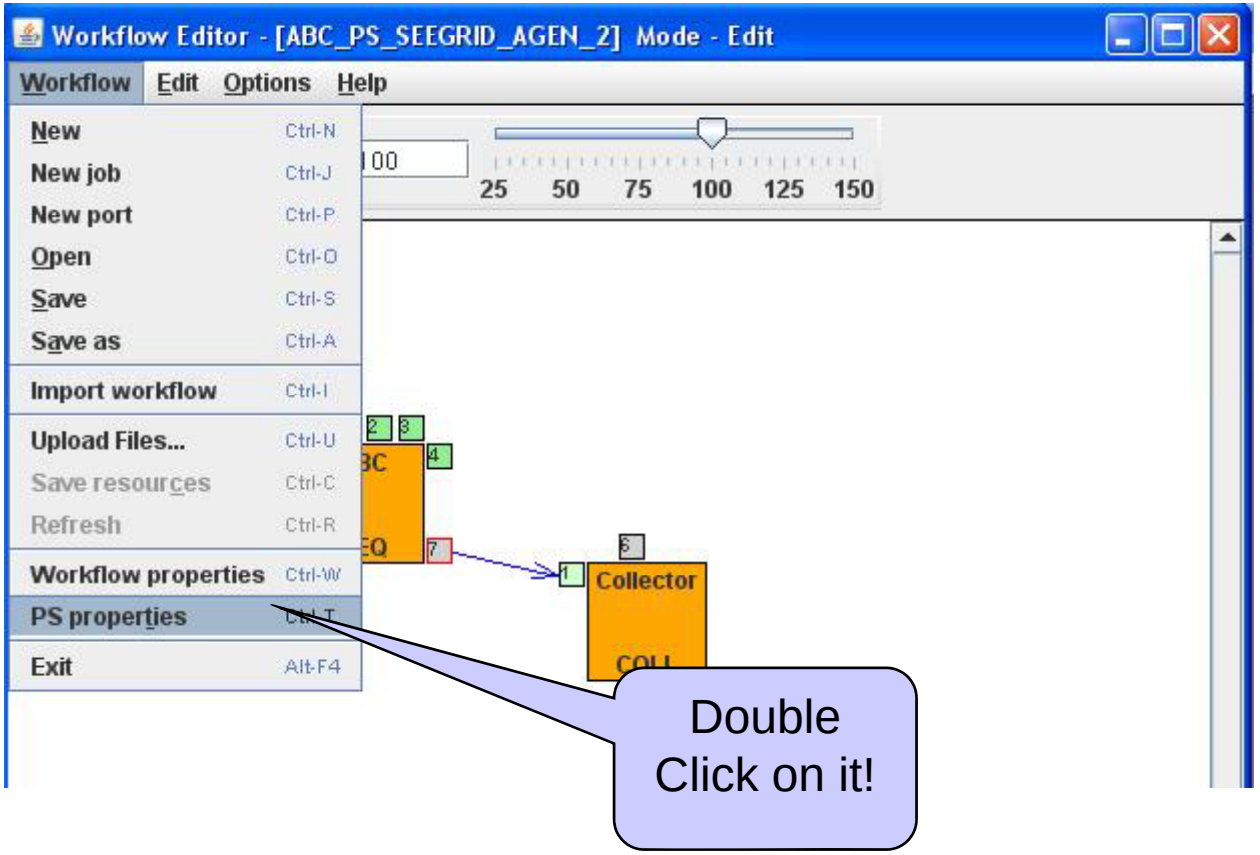
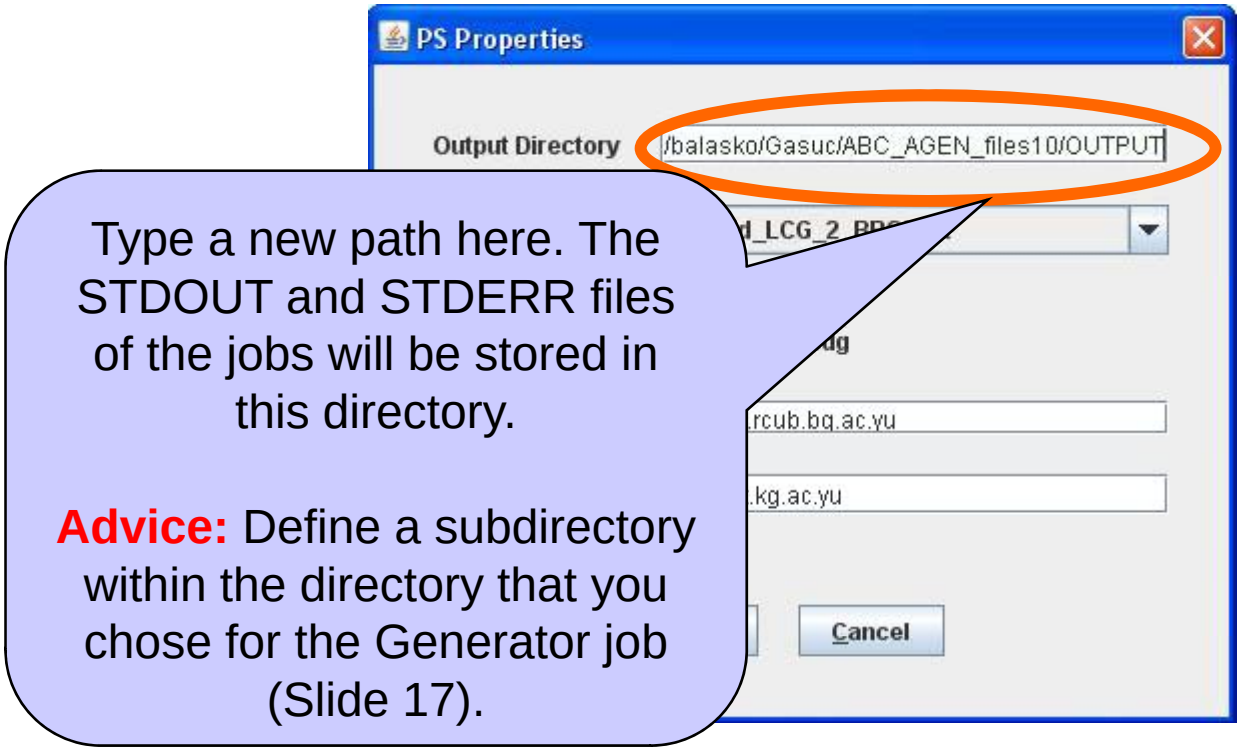
Modify grid parameters for the workflow



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).

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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).

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Possible next actions

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- 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)

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Thank you!

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