VITESS Tutorial

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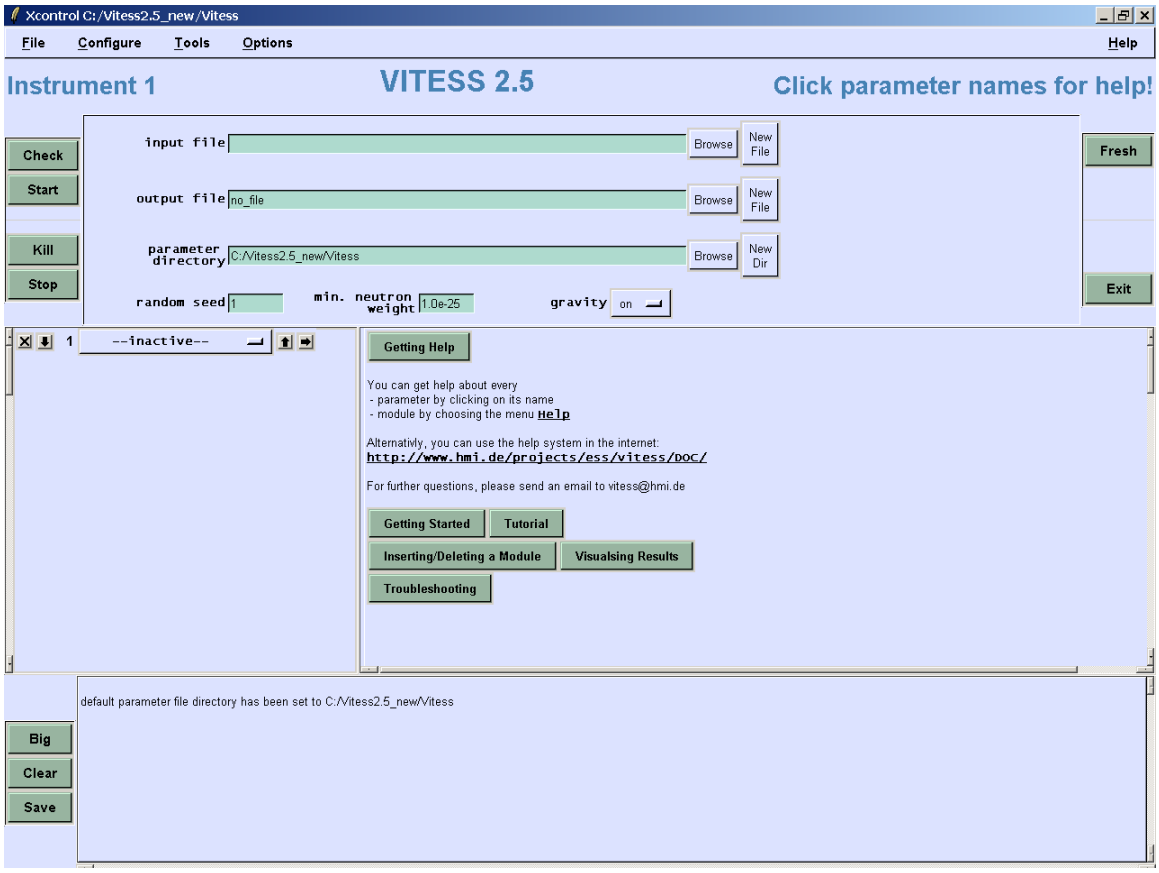
1. *How VITESS works?*

Whilst neutrons can complement other sources of radiation, they excel in a number of domains and are ensured a unique place at the forefront of modern scientific research. Clearly one of the beauties of neutron scattering is that there are so many alternatives on the technique. There is for example, crystallography for the study of molecules in atomic detail, and also reflectometry for looking at the structure of surfaces such as cell membranes. Another aspect of the neutron scattering technique, which involves scattering of neutrons at very small angles (SANS), can be used to resolve larger, intermolecular distances in a complex of several molecules, such as viruses that contain proteins and nucleic acids, or cell membranes made of lipids. Alternatively, quasi-elastic neutron scattering (QENS) is a technique capable of providing a very detailed look at the local dynamics of the molecules on length scales of 1 – 10's of Å and time scales of 10^{-12} sec.

In the last years, Monte Carlo (MC) simulations have proven to be a very essential and frequently implemented tool in the optimization of existing instruments and conception of neutron scattering instrumentation for new facilities. Free open source and user-friendly software packages have become available in recent years, and since then they provide an important aid for the developers of neutron instruments. In this framework the MC simulation software VITESS has been developed at HMI, supported by the HGF-ESS and the SCANS projects.

VITESS is a virtual instrumentation tool for neutron scattering at pulsed and continuous sources developed for the operating systems Unix (SunOS V5.6, OSF1 V4.0), Linux (from version 2.0.3.5) and Windows/DOS. The software package, which has been downloaded by more than 200 users can be obtained from: http://www.hmi.de/projects/ess/vitess/. As shown below, the program is supported by a graphical user interface (GUI), which generates and controls command lines according to a given input.

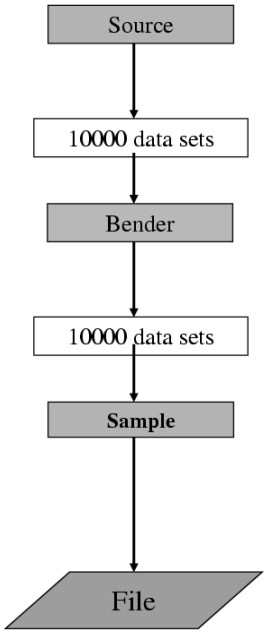


VITESS has an uncomplicated modular structure consisting of independently executable components that describe the instrument components. Each module refers to the coordinate system provided by the preceding module, changing the neutron beam input. On the other hand the output is a function related only to the parameters of the respective module.

The neutron beam input and output represent a number of neutron trajectories. Twelve coordinates describe each trajectory: time, wavelength (λ), probability weight, position (x, y, z,), flight direction ($\cos\alpha$, $\cos\beta$, $\cos\gamma$), spin-state (S_1, S_2, S_3). As the 12 coordinates per neutron trajectory are consecutively written to (or read in) the user can check the changes of the neutron coordinates anywhere in the instrument and generate the statistic of the trajectories.

A simulation comprises one or more modules co-working sequentially that can in principle run simultaneously. The so-called 'pipe' works in the following manner:

a. One trajectory is generated after the other, the parameters are calculated and written to the output
b. After B sets of incoming neutrons (default: B=10000) are collected, the output is transferred to the next module
c. The next module starts after the transfer



2. *Using the modules to create your own instrument*

In VITESS the modules that belong to the hardware have characteristic input parameters allowing an accurate description of the instrument components.

- **Source**: initialises neutrons with randomly distributed parameters (such as, λ, flight direction and spin state) starting over a moderator surface. Source modules for HMI, ISS, ILL, IPNS, SNS and ESS are available in the program but can also be personalized by the use of a binary input file.
- **Monitors:** intermediate information can be obtained, without disturbing the program sequence, by placing the modules monitor and/or write-out anywhere on the sequence.
- **Sample:** VITESS provides 7 different modules to describe various samples: *1) Elastic Isotropic Sample*
  2) Inelastic sample
  3) Powder sample
  4) Reflectometer sample
  5) SANS samples
  6) Single crystal sample
  7) S(Q) sample

Considering that neutron optics is one of the most important techniques to control neutron beam quality and to extract physical quantities, in this project, we also aim to systematically develop modules that lead to the best description of neutron optical devices. The goal is to open new possibilities of neutron scattering experiments. For that reason we have developed the following modules:

- **Guides**
- **Polarization:** a series of modules that allow polarization analysis have been developed, such as: polariser-He3, polariser_SM, super mirror ensemble, resonator Drabkin, gradient flipper, rotating field.

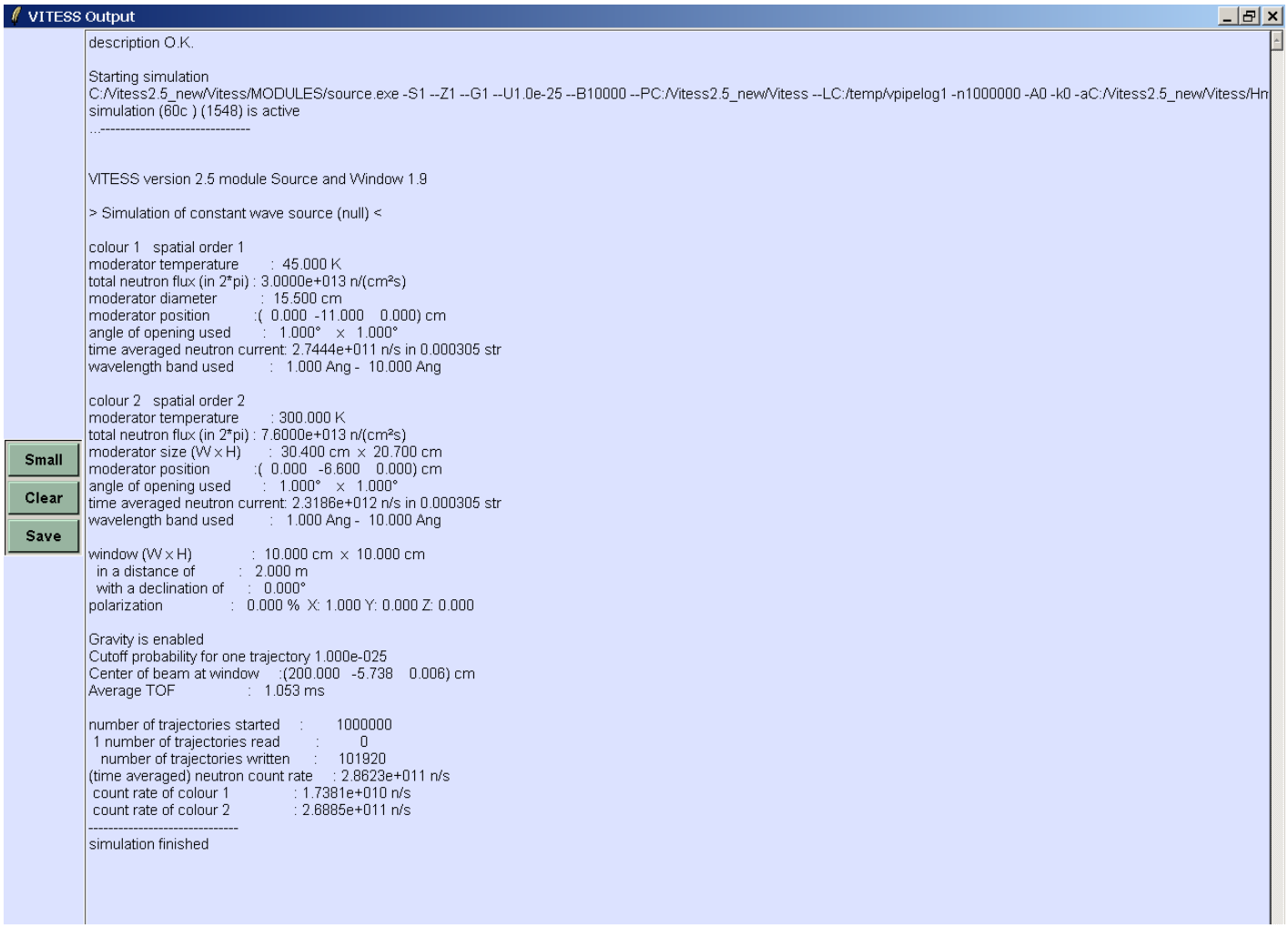
More information on the VITESS modules is available by clicking on "Help" at the menu bar of the VITESS program, or at http://www.hmi.de/projects/ess/vitess/DOC/.

3. *Creating your instrument:*

1. **Start by selecting a source:**
   - i) Click on *"- - inactive- -"*, select *"source"* and choose *"source_HMI"*
   - ii) A new box *"Module 1 source HMI"* will appear on the right side of your screen, under *"moderator description file"* click on *"Browse"*
   - iii) Under *Vitess/Files* select *moderator*
   - iv) Choose HmiMS.mod
   - v) On the *"Module 1 source HMI"* window you can:

     - choose the number of neutron trajectories.
     - choose neutron parameter values: divergency, wavelength, moderator time window, polarization
     - choose values for the propagation window, such as distance between moderator and guide

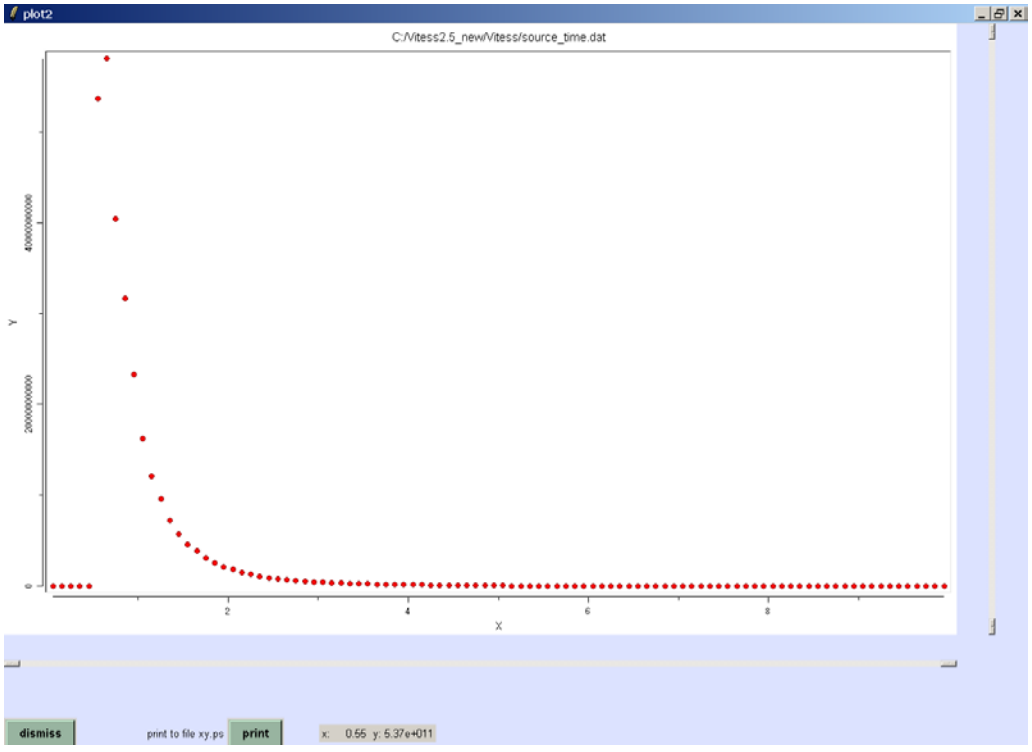
   - vi) Here we will keep the default values for (v) Press start. You should obtain the following output:



2. **Save your instrument:**
   i) under *"file"* select *"SAVE to directory"*
   ii) in later stages you will need to use the command *"SAVE instrument"*

3. **Data visualisation:**
   i) time distribution:

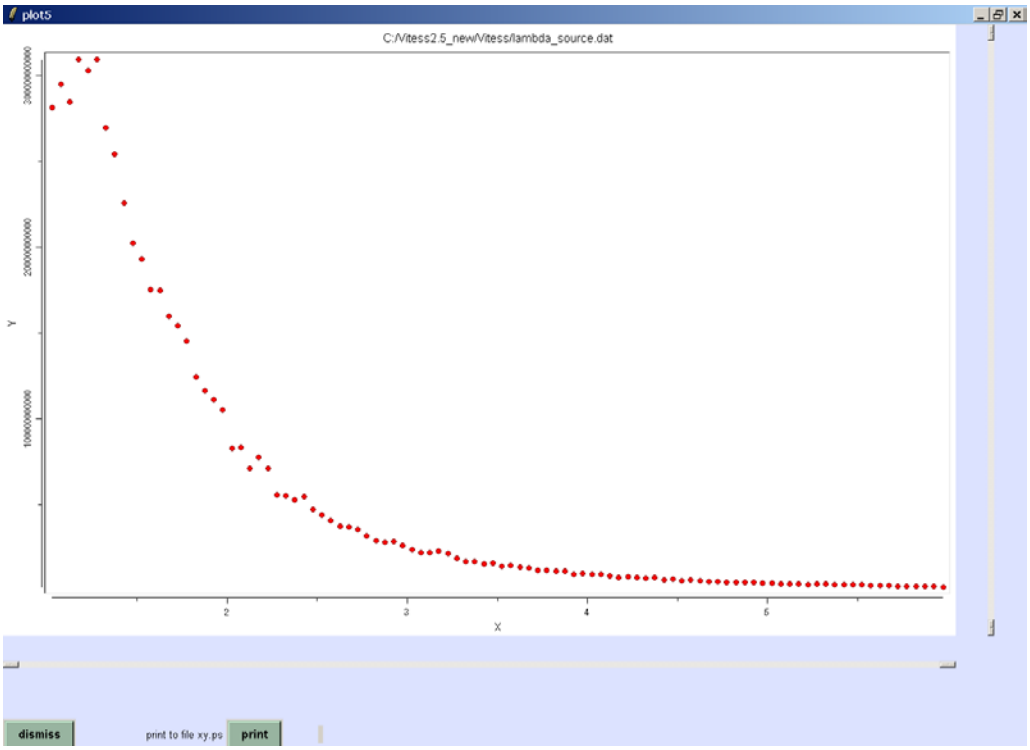
- click on *"- - inactive- -"*, select *"visualise data"* and choose *"mon1_time"*.
- A new box *"Module 2 mon1_time"* will appear on the right side of your screen, give a name to the output monitor file, such as source_time.dat.
- set the number of bins, for example 100, and the time interval, for example 1 to 10 ms.
- If you **do not** wish to have an automatic plot after the simulation, deselect the default choice "*outplot"*.
- Press start. Once the simulation finishes under the window *"Module 2 mon1_time"*, select *"plot"* you should then obtain the following result:



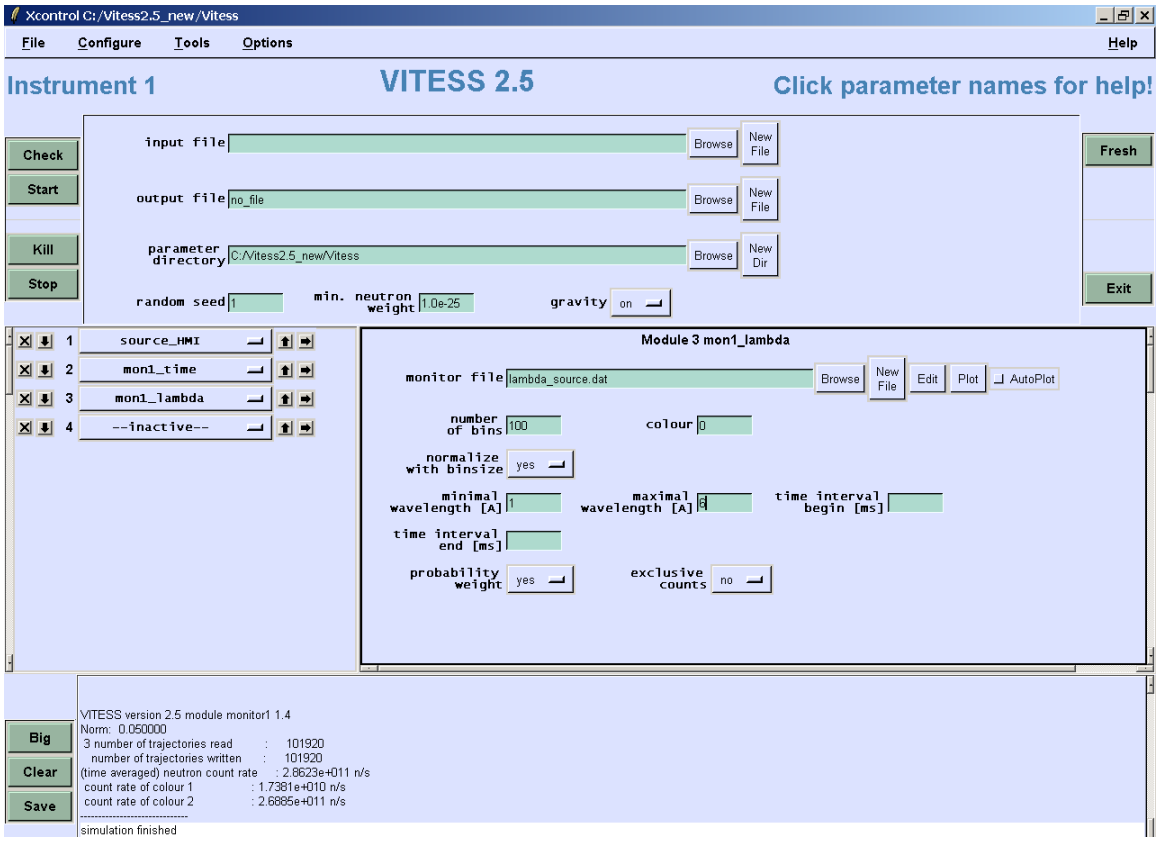
Note: Here the monitor is placed 2 m from the moderator!

ii) Wavelength distribution:

- click on *"- - inactive- -"*, select *"visualize data"* and choose *"mon1_lambda"*.
- A new box *"Module 3 mon1_lambda"* will appear on the right side of your screen, give a name to the output monitor file, such as source_lambda.dat.
- set the number of bins, for example 100, and the wavelength interval, for example 1 to 6 Å.
- If you **do not** wish to have an automatic plot after the simulation, deselect the default choice "*outplot"*.
- Press start. Once the simulation finishes under the window *"Module 3 mon1_lambda"*, select *"plot"* you should then obtain the following result:



At this point your GUI looks like:



4. **Save your new instrument!!!!**

5. **Change your source to HMIcold.mod**. For that you need:
   i) Click on the arrow (➔) that is located beside *source_HMI*, the window *"Module 1 source HMI"* will be displayed, click on *"Browse"*
   ii) Under *Vitess/Files* click on *moderator*
   iii) Choose *Hmicol.mod*

6. Rerun your simulation to check the effect.

7. Narrow down the interval of wavelengths emitted from the source. Rerun your simulation to check the effect.

IMPORTANT NOTES:

i) **Adding a new module**:

- click on *"- - inactive- -"* and select the module

ii) **Adding a new module between existing ones**:

- click on the arrow (🡻) located beside a module, it will create a new *"- - inactive- -"* line above the existing module.

iii) **To find out the module details**:

- click on the arrow (➔) that is located beside the module of interest, a window *"Module # module name"* will be displayed.

iv) **Reloading your instrument**:

- under *"file"* select *"LOAD INSTRUMENT"*

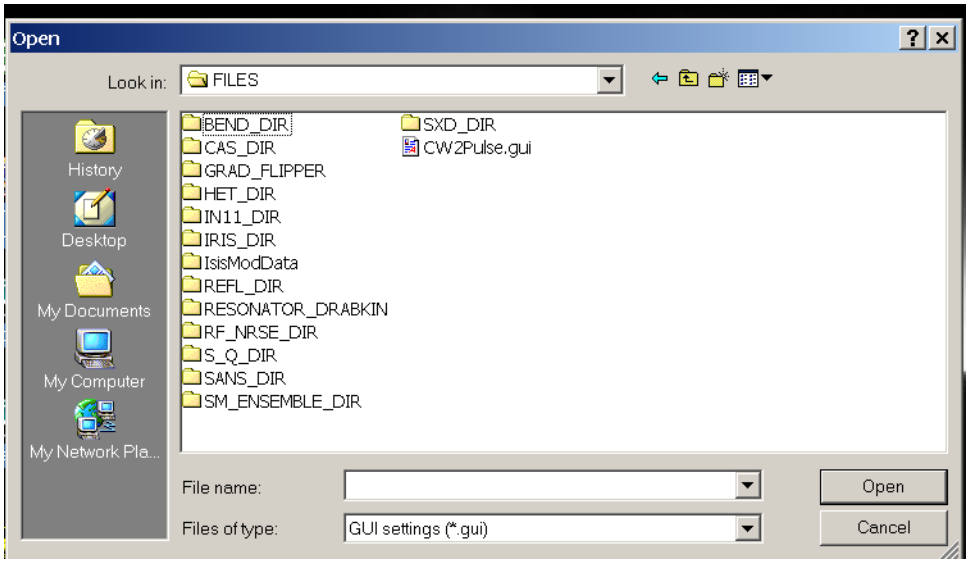
v) **Keeping the results from your previous simulations**:

- under *"options"* choose *"copy results"*, and select *"per simulation"*. If you do **not do** use this option your old simulation data will be over-written!

8. Start building your own machine!

4. *Using the VITESS examples*

1. Under *"File"* select *"LOAD INSTRUMENT"*
2. A window will appear. Click on the folder *FILES*
3. A selection of example files will appear:



4. You can then click in one of the directories and follow up various simulations that were performed using VITESS.

Your comments to this tutorial are welcomed. If you have questions during your simulation do not hesitate e-mailing us: vitess@hmi.de.

References:

- G. Zsigmond and F. Mezei, Simulation of the time-of-flight-backscattering neutron spectrometer IRIS. The Monte Carlo data reduction technique, Physica B 276-278 (2000) 106-107.
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