EASI-STRESS

EUROPEAN ACTIVITY FOR STANDARDIZATION OF INDUSTRIAL RESIDUAL STRESS CHARACTERIZATION

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D4.3 Software for on-line data analysis

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List of Abbreviations

DEC	Diffraction Elastic Constants
FEM	Finite Elements Modelling
FWHM	Full Width at Half Maximum
GUI	Graphical User Interface
GV	Gauge Volume
HDF	Hierarchical Data Format
LRI	Large-scale Research Infrastructure
NeXus	Neutron, X-ray, (muon) Science
OS	Operating System
RS	Residual Stress
WP	Work Package
XRD	X-ray Diffraction

List of Symbols and Units

exx	Elastic strain in x-direction	-
eyy	Elastic strain in y-direction	-
ezz	Elastic strain in z-direction	-
sxx	Normal stress value in x-direction	MPa
syy	Normal stress value in y-direction	MPa
szz	Normal stress value in z-direction	MPa
s_vm	Equivalent Von Mises stress	MPa

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Executive summary

In this document we describe the harmonization of the data produced at different LRIs, which will be the input for the common software, and the common software itself, and it's output files. The NeXus file format was chosen and a new application definition (NXstress) specifically for strain and stress was developed and outlined. We further describe the common software for strain and stress calculations as well as the first working mechanism and structure of the software. The next steps will be to describe in more depth the special measurement cases and compile equations and workflows that should be included in the common software. We have also drafted a first structure of the output files from the common software specifically in the HDF5 format. Since this is not yet a commonly adopted data format by the user community, we have also implemented an ASCII output file based on the information from the deliverable 5.1.

1. Introduction

1.1 EASI-STRESS

Residual stress determination can be accomplished through the measurement of elastic lattice strains at the crystalline level using X-ray or neutron radiation. These measurements can be carried out in polycrystalline materials based on their diffraction signal in laboratories (X-ray), at high-energy synchrotron radiation facilities, or neutron facilities. The latter two are considered as Large-scale Research Infrastructure (LRI); all of the above methods have been used for around three decades for internal stress characterization [1-5]. Standards for strain / stress determination are already available for laboratory X-ray methods as well as for neutron methods [6-10]. Despite previous round-robin exercises to demonstrate the feasibility and precision of respective methods, conducted either as part of or supporting the development of guidelines and standards, knowledge residing at LRIs of these techniques has not yet been widely adopted by industries or is not even known. Additionally, while there is a European standard for laboratory X-ray measurements, there are currently no general stress determination guidelines using synchrotron X-ray radiation, let alone a harmonised guideline which encompasses the different techniques. The project EASI-STRESS aims to address some of these gaps through its work packages (WPs): industrial confidence in the methods is enhanced by validation and benchmarking of neutron, synchrotron X-ray, and laboratory-based techniques with predictive numerical models with benchmark samples in WP2; residual stress determination using different methods at the LRIs are harmonised in terms of measurement protocols and ontologies (WP3), and harmonised metadata and residual stress analysis algorithms in a common software are addressed in WP4. A setup of industrial service functions for residual stress is initiated through a series of round-robin measurements of industrial cases in WP5. Finally, WP6 aims to produce a technical specification for synchrotron X-ray stress measurements to bring the method closer to a standardized technique.

This document describes the heart of the data analysis workflow harmonisation initiative: the common software for residual stress determination and the standardisation of the data input and output format. The subsequent information is the starting point for simple data analysis and further development of the common software for more complex residual stress determination.

1.2 The common software in EASI-STRESS

Different software packages for strain / stress calculation are already available [11-16]. However, there are limitations on the general usability of a software package for different types of measurement or data formats. While certain programs are built only for a specific instrument or instrumental set-up, others, for example, are more general but read only specific data formats. The need for funding to acquire commercial software packages or licenses for executing certain codes poses another problem. This does not only limit the data analysis workflow and the interchangeability of research results, but also efforts in terms of accessibility and reproducibility. Therefore, there is a need for a more "common" software that allows to harness and analyse data from different sources, set-ups, and techniques. This is the purpose of the WP4 common software, which will be called "SOFTware-Analyser for Industrial Stress", *SOFT-AIS,* from now on. It will read data and meta-data from all LRI in the EASI-STRES project and allow strain and stress calculations through a user friendly interface. Furthermore, its output will be aligned with industrial RS simulation software in terms of content and formats.

Interchangeability of data is achieved by adapting the in the scientific environment widely used NeXus data format, based on HDF5, to our needs. However, laboratory X-ray techniques use commercial equipment that is sold together with software packages that process the data more or less

automatically from the measured raw data to the final stress values. This means that the integration of the (raw) data processing from laboratory X-ray instruments into the proposed common NeXus-stress data format (described below) as an input for the common software is too complex at the moment for the partner institutions (DTI, CETIM etc.) and requires the direct engagement of the equipment and software developers. Therefore, SOFT-AIS is currently not foreseen to be used for the analysis of laboratory X-ray data. A way forward in the activities of maximum harmonization could be to make at least output data formats compatible such that RS analysis results from LRIs could be compared with laboratory X-ray measurement results. SOFT-AIS could provide graphical tools for such analysis in the future. With that said, we propose to compare the calculated stress values from laboratory X-ray measurements with synchrotron and neutron output files in a similar format (HDF5 or ASCII). Note that this will only include strain/stress values and positional coordinates of the measurement. In order to interpret a sensible correlation, further information such as gauge volume (GV) description and wavelength calibration will be needed from the laboratory X-ray operator/responsible before conclusions can be drawn. A similar case will be made for the comparison of the industrial finite element modelling (FEM) of RS addressed in WP5 by industrial partners such as NEMAK, EDF, ArcelorMittal, etc.

Therefore, the subsequent focus of data processing and harmonization at this stage is focused on LRIs. The input data for our common software requires LRIs to have already reduced the data into the proposed NeXus-stress format. This means, each participating instrument saves the raw data and metadata, as well as the fitted peak results, in an individual way since the data reduction process, required to produce the diffractograms, is different for each instrument. The aforementioned individual approach is based on the fact that, despite the similarities of the method, hardware and measuring geometry are very instrument specific. That said, the input into SOFT-AIS is the fitted parameters after data reduction of the raw-data and determination of coordinates with measuring points the sample coordinate-system. These are relevant data for strain/stress calculation and mark the interface between the experiment and data analysis. Data reduction is instrument specific and evolves with technical development. This approach also guarantees that any future instrumental updates and modifications are taken into account. Therefore, it remains in the responsibilities of the LRIs and is not part of the common SOFT-AIS program. However, the output data format from the data reduction, which serves as the input data format for our common software, is harmonized. The specifications for this data format were described in D 4.2 but are again outlined below in this deliverable.

2. Input Data Format

Data reduction and data fitting are to be handled by each instrument-specific data reduction software. By doing so, the development of this software can be independent, thus tailored to the requirements and demands of each instrument and setup. The data reduction and fitting process yield fitted data, typically a set of peak fitting parameters reporting peak position (in diffraction angle, neutron energy, X-ray energy, or d-spacing), intensity, FWHM, among others. The fitted data output from different instruments share many common elements. Additionally, the data analysis algorithm required to bring the fitted data to strain and stress values are largely similar for all instruments. Therefore, metadata and fitted data are proposed to be harmonized as an input for the common software, i.e. the data file format and data structure will be standardized in the dedicated NeXus application definition NXstress [17]. The work of translating the instrument's fitted data output into the standardized format will use the resources of each facility; the present section serves as guidance and a responsible/contact will be nominated to support and validate this translation after the EASI-STRESS project. The standardized

fitted data will become the input for the common software for residual stress determination developed within the EASI-STRESS project.

The philosophy of the analysis workflow is that at any step any information from instrument calibration, sample alignment up to stress calculation is retraceable: values required for stress determination and interpretation must be in the data files, additional data must be either included or referenced.

With these considerations in mind, the proposed data output format from the instrument specific software is formulated as follows:

- Data elements should comprise identifiers pointing to the experiment information. This will allow the data to be traced back to the original information from sample positioning, instrument setup, etc.

- Data elements should include information which capture the details of the data reduction and data fitting performed using the raw data. This will ensure the traceability of the data analysis workflow.

- Data structure should be arranged in such a way that it is easily readable by users and can be easily handled by the common software for further strain and stress determination.

- Data format should be easily amendable and expandable for future developments.

For these reasons, the hierarchical data format (HDF5) file format is well suited for our purposes. HDF5 is an open-source data format, and it uses a "file directory"-like structure which allows organizing data within the file in many differently structured ways. Additionally, it supports heterogeneous and complex datasets to be stored, making it suitable for storing information ranging from simple comments as metadata to more complicated arrays which can also include even pictures. A general, standardized HDF5 data format with a convention for neutron, X-ray, and muon scientific communities already exist and is called NeXus [18] which is maintainted by a committee which assures longevity. For these reasons we have developed a data structure NXstress based on the NeXus convention. NeXus is not specific for strain nor stress, but depending on the applications or measurement methods, different subclasses exist (e.g. small-angle scattering data, electron backscatter diffraction (EBSD), and other diffraction data). During the EASI-STRESS project, a specific NeXus structure application definition for stress and strain analysis of crystalline materials (NXstress) has been developed. A first version of its definitions is already publicly available [17]. Within the NXstress structure, certain entries have to be provided and are marked as "required". Lack of providing these entries will not allow the diffraction data to be treated in order to calculate strain and stress values. Additional entries in the NXstress format (marked as "optional") are supplemental information that can be considered as meta data that allow to, for instance, trace the data processing procedures (by specifying e.g. paths or file names to calibration data), determine instrumental set-ups (by defining e.g. detectors), or specify additional information about the sample (by specifying e.g. the phase name or the space group). By choosing this generally used NeXus system, we guarantee sustainability of the format since there is an active international NeXus support group at multiple facilities that provides updates and upgrades on a regular basis in addition to specific software to read and write these files. This ensures quick and easy adaptation upon, for example, instrument or method modifications, different RS software versions, etc.

As described in the paragraph above, the NXstress format provides some freedom in how the data can be structured since not each and every instrument(al set-up) produces data in the same way. For example, while for SALSA each stress component is stored in a separate file, for beamline P61A, all measurement points from all the different directions are stored in the same file. Therefore, while standardizing the input file format for our common software, the structure can still look different and be adapted to how different instruments and beamlines generate their raw data.

3. Software

3.1 Installation

SOFT-AIS is written in C++ and available for Windows, Linux, and Mac OS. The installation files are currently only available in the shared folders on TEAMS which are only available to EASI-STRESS partners. Since we are still in the development phase, there has not been a release made available for the general public. Nevertheless, there is already a GitHub repository that will be used for storing the software as well as for its documentation. Additionally, this repository will also allow to submit information about issues or problems with the software in addition to feature requests.

While the instructions for the installation are listed in the README file (in the downloadable installation folder) and explain the steps needed for installing SOFT-AIS for each OS, they are also outlined here:

Windows:
First the following requirements and dependencies need to be installed which are also distributed with the installation files:

- Microsoft Visual C++ Redistributable
-HDF5 library (≥1.12.1)

After installing all the prerequisites, execute the installer called

SOFT-AIS_x64_Windows_installer.exe

and follow the onscreen instructions.

It is a user friendly GUI based installer like for most other Windows software. After installation admin right should be assigned to the software. To do this find the executable, right click on it, go to Properties, there choose Compatibility tab, on the tab tick Run this program as an administrator checkbox, click Apply and then OK.

Linux:

The following packages needed to be preinstalled before the installation of SOFT-AIS:

-libgl1-mesa-dev
-libglu1-mesa-dev
-mesa-common-dev
-libxcb-xinerama0
-build-essential
-HDF5 library (1.12.1), separate install guide provided for this library in "Install.txt"

All of these packages can be found in the Linux/Prerequirements folder. The installer (only tested on Ubuntu), with which you can install these packages is

> *apt-get install*

After installing all the prerequirements above, execute the installer called

> *./SOFT-AIS_x64_linux_installer*

and follow the onscreen instructions. It is a user friendly GUI based installer. To start the software run the SOFT-AIS.sh command from the install directory (add execution right if necessary)

macOS:

The following packages needed to be preinstalled before software installation:

> *HDF5 library (1.12.1)*

This can be installed through homebrew package manager.

> *brew install hdf5*

Info on how to install homebrew can be found here: https://brew.sh/

After this step, you just have to copy the SOFT-AIS application to the macOS Application folder and that's it. You should be able to run the software from where you have downloaded it.

> *Common_software_x64_installer.exe*

This will open a user friendly graphical user interface (GUI) based installer guiding the user with onscreen instructions.

3.2 Using the Software

3.2.1 Layout of the graphical user interface

After opening the GUI of the software, different areas can be seen (Figure 1). There is the *Plot area*, which will be used to display plots of the input data, the calculated strain and stress values as well as its errors. Below is the *Messages Box* which displays all executed steps from the software plus output text, from an algorithm or script, and error messages. The content of the message box will be automatically saved in a log file in the installation folder in the following format: "Fitted_Data_Reader_YYYYMMDD.log". However, in order for this to happen, the execution of SOFT-AIS must be done in administrator mode on Windows. Lastly, on the right is the *Side Bar* located which contains the following execution buttons:

> 1. "*Load in fitted file(s)*": This button allows to load in one or more reduced NeXus data file(s) (in the NXstress format) generated from the actual sample.

> 2. "*Load in reference file(s)*": This button allows to load in one or more reduced NeXus data file(s) (in the NXstress format) generated from the reference sample.

> 3. "*Calculate*": This button executes the calculation of all the strain and stress values.

> 4. "*Save results*": This button allows to save the calculated strain and stress values to be saved simultaneously as a CSV and an HDF5 file.

5. Drop-Down menu: If the software cannot automatically detect the type of input data or which type of calculations to execute, the drop-down menu can be used to select the calculation type.

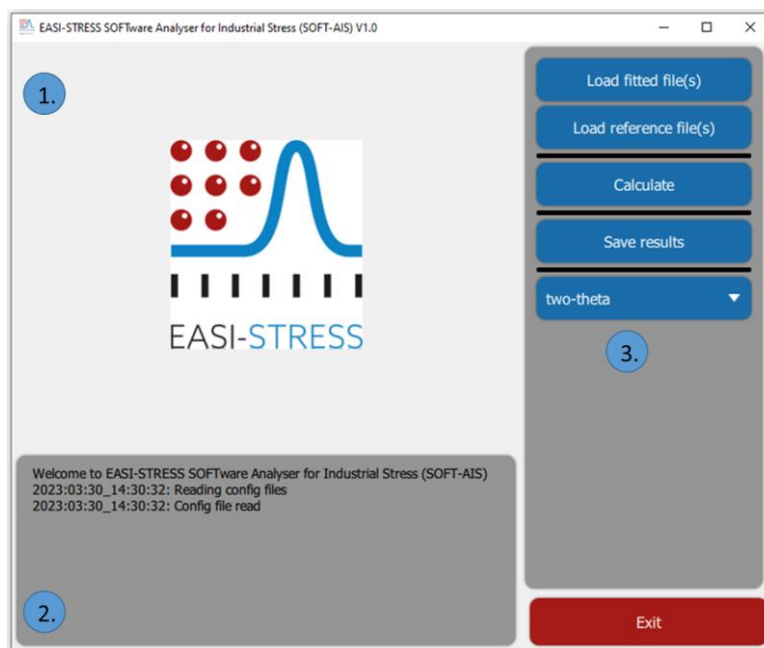6. "*Exit*": This button stop the software and close the graphical user interface.

Figure 1. The GUI of SOFT-AIS with the Plot Area (1), the Message Box (2), and the Side Bar (3).

3.2.2 Executing the software

The steps needed in order to calculate strain and stress are explained in this section. There are two different approaches depending on the nature and amount of reference measurement data. The first step is to load in the measurement data from a NeXus file via the button "*Load in fitted file(s)*". This will be done in one step, depending on the amount of measurement directions, the number of files selected can be more than one. As data gets loaded, the *Message Box* gets updated on the fly and shows the number of measurement points read in. Additionally, also the diffraction type, which determines which set of equations are used for the subsequent calculations, is displayed (Figure 2).

a.) Loading Reference Data

After loading the data, a new window will appear asking for user input on the reference data (Figure 2). If the reference data were collected with reference measurements of a profile, then this step should be aborted by clicking "*Cancel*" and a profile should be loaded via the "Load reference file(s)" button. If the reference data consists of a single value (e.g. in case of a powder), or a single value for multiple directions, these can be entered in the box and confirmed via clicking "*OK*". This will then show the entered value(s) in the *Message Box* and open another window (Figure 3) that requires the user to enter the error associated with this / these value(s). Confirming the input values by clicking "*OK*" will close the window and displays the entered error values in the *Message Box* (Figure 4).
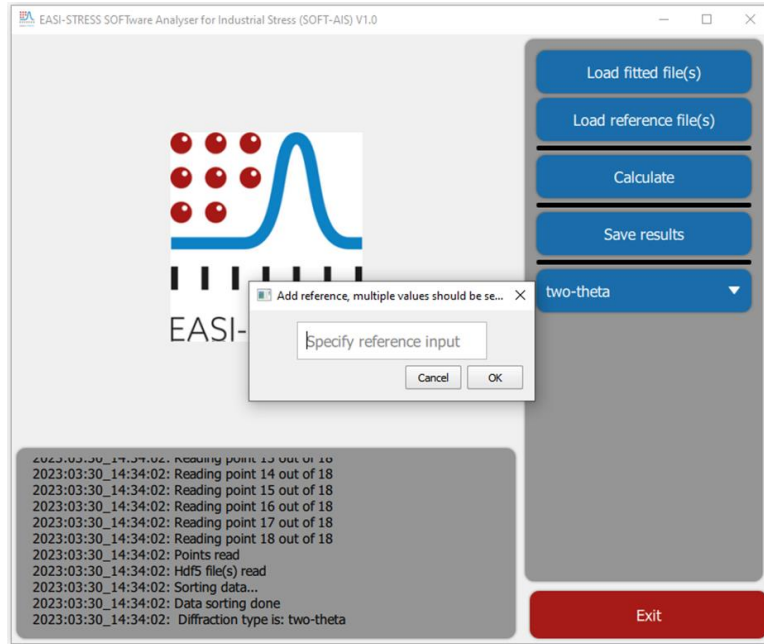
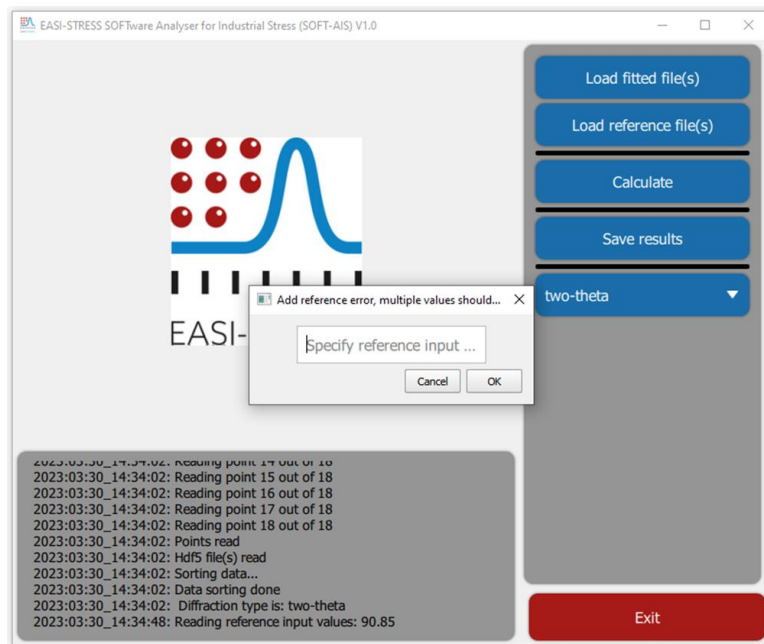*Figure 2. Adding reference information (e.g. d_0 values).*

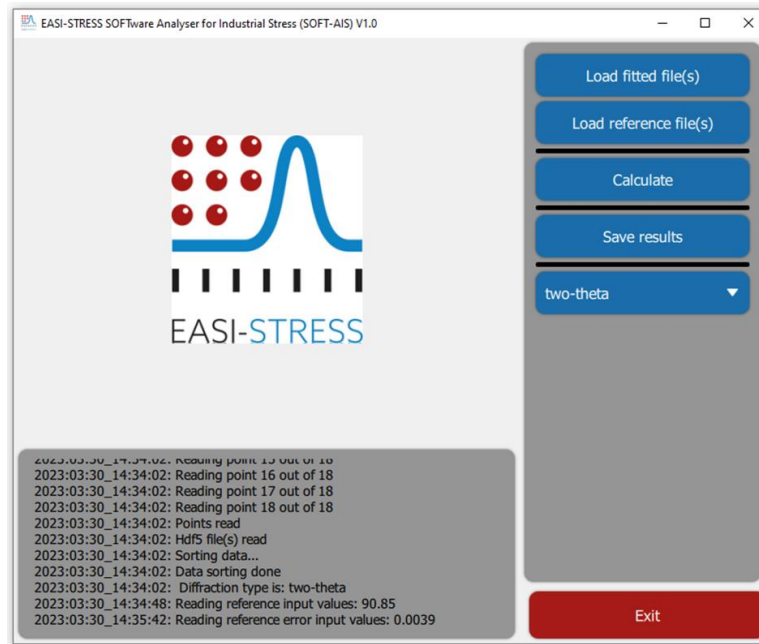*Figure 3. Adding error values for the reference data.*

Figure 4. All the information was read in (see Message Box) and the software is reading for performing calculations.

b.) Calculating Strain / Stress

After all the input data was read in, strain and stress values can be calculated. This can be done by clicking the button "Calculate". This step calculates the strain values and opens up a new window requiring the user to provide first the value(s) for the Young's modulus in GPa (Figure 5) followed by a window asking for the Poisson's ratio (Figure 6). In these windows, either one or multiple values can be entered. In case only one value is provided but multiple measurement directions are used, this value is automatically copied in to the remaining fields for all of the directions. The progress of the calculation can be followed by the output in the *Message Box* which will display after the calculation is finished: "Calculating Stress done" (Figure 7).
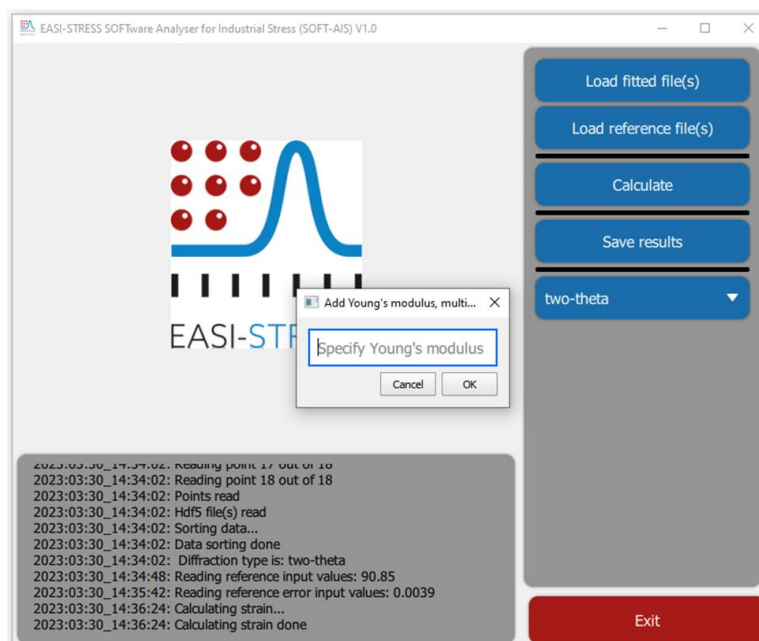
Figure 5. Pop-up window requesting the user to provide the value(s) for the Young's modulus.

![EASI-STRESS logo]
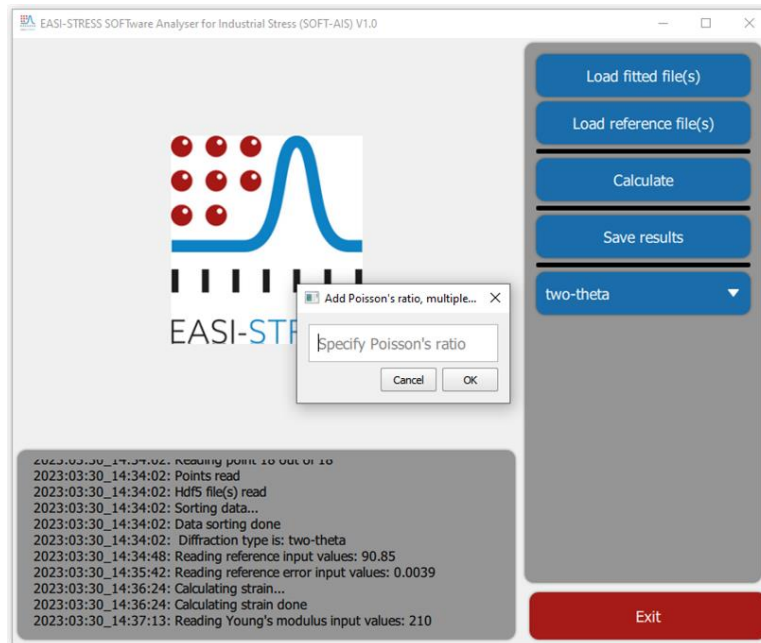
Figure 6. Pop-up window requesting the user to provide the value(s) for the Poisson's ratio.
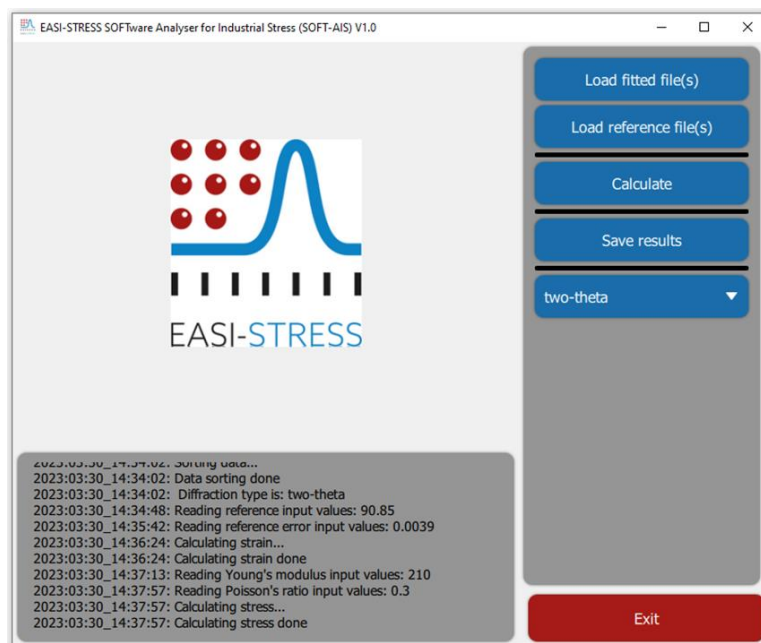
Figure 7. All the calculations are done (see output in the Message Box).

c.) Saving calculated Strain / Stress values

The calculated strain and stress values are currently only stored in memory and cannot be inspected after the calculation unless saved. This must be done explicitly by clicking "*Save results*". This will open up another dialog window which allows to specify the location and name of the to be saved files. This step automatically saves the before calculated data as two files (in a CSV and an HDF5 format) with the same file name.

3.3 Output Data Format

An initial draft of what the output format contain was discussed in depth in D4.2. The output format should be structured in a clear and easily identifiable manner, but also suitable for FE analysis activities as has been defined in the EASI-STRESS WP5. This definition is taken into account in this work.

For the same reasons as used for the fitted data input format, the hierarchical data file format (HDF5) was suggested as the output data format for SOFT-AIS. However, a large part of the user community, whether academic or industrial, still lacks capabilities to process files in this data format. Therefore, another simpler output file format (CSV) is used too.

The residual stress data output in the HDF5 file will comprise three groups, namely "General_info", "Stress_output", and "Strain_output". Similar to the fitted data input file, the "General_info" group of the residual stress data output includes fields describing the instrument used for the experiment, fields about the experiment, and information about the file containing the experimental details, respectively termed "Instrument_identifier", "Experiment_identifier", and "Experiment_info". In the same group, an array, called "Elastic_constant", includes the elastic constant values (Young's modulus and Poisson's ratio) for each strain component.

The "Stress_output" group contains the main information about the residual stress measurement data in "Variable", "Variable_uncertainty", "Variable_name", and "Variable_unit". The variables included in the residual stress output data are measurement point number, measurement point coordinates (in the sample coordinate system), stress values in the different components, the precise dimensions of the gauge volume and its orientation with respect to the sample, and corresponding uncertainties. According to the work of the EASI-STRESS WP5, the inclusion of these variables ensures the compatibility of the residual stress calculation output from the LRIs as a basis for comparison of results from industrial FE modelling activities.

The final group is labelled "Strain_output", which contains n-number of subgroups according to the number of measured strain components for the stress determination (n = 3 for tri-axial stress determination). Each subgroup contains a pointer to the fitted data file, labelled "Data_file". The pointer "Reference_file" refers to a separately fitted data file in case a stress-free reference trend was used to calculate the strains ("None" if the reference is a single value). Meanwhile, the variable "Reference_value" refers to a value that is used as the stress-free reference ("None" if the reference is a profile). The main strain information is stored in "Strain_variable" and "Strain_variable_name". They contain the coordinates of the measurement points (in the sample coordinate system), the strain values, and the strain uncertainties.

While the structure of the CSV output file format is based on what was illustrated in D5.2, this version is still under development. An example of its present version is depicted in Figure 8. The information content will be extended, but this is currently comprised in the content of this file: the name of the input file(s) and the input reference file(s), the elastic diffraction constants, the measurement point coordinates (in the sample coordinate system), the strain values (and its uncertainties), the stress values (and its uncertainties), and the Von Mises stress values (and its uncertainties).

```
Input files:
C:/Users/paecklar/Documents/NEXUS/SALSA/SALSA_NORMAL_multiple_point_test_3.h5
C:/Users/paecklar/Documents/NEXUS/SALSA/SALSA_RADIAL_multiple_point_test_3.h5
C:/Users/paecklar/Documents/NEXUS/SALSA/SALSA_TANGENTIAL_multiple_point_test_3.h5

Input reference files:
C:/Users/paecklar/Documents/NEXUS/SALSA/SALSA_NORMAL_multiple_point_test_3_d0_same_values.h5
C:/Users/paecklar/Documents/NEXUS/SALSA/SALSA_RADIAL_multiple_point_test_3_d0_same_values.h5
C:/Users/paecklar/Documents/NEXUS/SALSA/SALSA_TANGENTIAL_multiple_point_test_3_d0_same_values.h5

Youngs modulus    210      210      210
Poissons ratio:   0.3      0.3      0.3
Strain unit:   microStrain
Stress unit:   MPa
```

X	Y	Z	exx	exxError	eyy	eyyError	ezz	ezzError	sxx	sxxError	syy	syyError	szz	szzError	s_vm	s_vmError
1.5	0	0	74.0042	49.3151	342.614	48.0478	-510.47	52.5109	0.584025	16.3924	43.9749	16.145	-93.831	17.0276	122.04	56.0366
2	0	0	75.1202	44.8752	318.806	43.021	-608.612	44.8156	-13.8752	14.7505	25.4894	14.3856	-124.324	14.7387	134.523	46.0883
2.5	0	0	11.7456	51.2787	389.707	45.7856	-383.909	50.3547	4.02278	16.6771	65.078	15.5994	-59.8907	16.4924	108.236	60.6819
3	0	0	-57.606	52.489	383.474	41.5552	-303.185	43.307	-6.55743	16.5242	64.694	14.3516	-46.2279	14.6856	97.3503	61.088
3.5	0	0	-146.491	48.5266	323.038	46.5586	-276.605	55.3656	-35.7863	16.2788	40.0607	15.8994	-56.8048	17.6451	88.2538	76.6715
4	0	0	-73.9289	48.925	350.374	47.1382	-159.464	46.1058	2.23044	15.972	70.7717	15.6176	-11.5867	15.4152	76.3929	86.6761

Figure 8. The information currently included in the CSV output format.

4. Next steps

An initial survey was sent to all EASI-STRESS partners to get additional input regarding which (additional) features would be useful. The feedback we received can be found in the Appendix. The first round of implementations and upgrades will be primarily based on this information. However, after the first release of SOFT-AIS and some initial trial period, in addition to an EASI-STRESS internal workshop, a second in-depth survey will be distributed to gauge further interest on new features and requests for changes. Additionally, we have also identified a list of features that are foreseen to be implemented of which a few highlights are listed below:

- Data Integration: Sometimes the amount of data points and its locations vary in the measurements for the different strain/stress directions as well as for the reference measurement. Without additional data treatment, this makes it impossible to calculate stress values. Therefore, we are implementing an integration method which will create an equal amount of data points for the different directions. This will be an adequate interpolation routine.
- Drop-Down DEC: Currently, the user has to input the diffraction elastic constants (DEC) for the material of interest when performing the stress calculations. A feature in one of the next releases of the software will be to provide a data base, accessible by a drop-down menu, which will allow to select the diffraction elastic constants for different materials. The information for this menu will be provided to the software by a CSV file which is also stored on the GitHub repository. While we try to provide as much information as possible, we can neither guarantee to know all published values nor to have all of them covered in that file. Therefore, having a generally accessible file will allow not only the developers, but also the entire user community to freely add information to this file whenever new articles are found or published with DEC for another material (or condition). An outline of how this file will look like is shown below (Figure 9).
- *Simulation and laboratory (X-ray) data import:* We aim for allowing the importing and plotting of laboratory X-ray data as well as the results from industrial finite element modelling into the software. This will enable the direct comparison with measured data.
- Online data processing: SOFT-AIS should be able to run a large batch of data so that it allows real time interpretation of measurements at certain large scale facilities, e.g. during *in-situ* or *operando* measurements. This option cannot be used in the same manner at all instruments since this will depend heavily on the online data reduction possibility of the LRIs. However,

where possible, this feature will enable, for instance, the adaptation of experimental parameters or a quicker change of measurement protocols.

Diffraction Elastic Constants												
Entry	Material	Composition	Phase	hkl	Temperature	Youngs modulus	Error	Poissons ratio	Error	Determined	Publication_Name	Publication_Year
1	Al	Al		200		67.2		0.35		simulated	Berechnung der ela	1958
	Al	Al		311		70.2		0.35		simulated	Berechnung der ela	1958
	Al	Al		420		70.3		0.35		simulated	Berechnung der ela	1958
2	Fe	Fe	gamma	200		149		0.34		simulated	Berechnung der ela	1958
3	Inconel 718	Cr19Fe18.5Mo3Nb5.1Al0.5Ti0.9C0.04		111	50	265		0.25		measured	Determination of th	2016
	Inconel 720	Cr19Fe18.5Mo3Nb5.1Al0.5Ti0.9C0.06		311	50	205		0.325		measured	Determination of th	2016

Figure 9. Content of the CSV input file for reading DEC into SOFT-AIS.

5. Summary and Outlook

As mentioned above, the aim of D4.3 is to use the in WP4 establish standard workflows and algorithms for the data analysis of residual stress measurements for the development of the common software. This is being realized with the first version of the common software, called SOFT-AIS, which can process the reduced data from LRIs in a NXstress format to calculate and save strain and stress values. The results of the analysis will also be used for comparisons with laboratory X-ray measurements and FEM. This will be achieved with our common RS software and a compatible data output format for the residual stress results.

We have discussed the standardized input and output format for SOFT-AIS as well as some future features and implementations in the software. While the common data format, the algorithm, and mathematical formulation behind the common software were previously described in D4.2, they have evolved due to the course of the software development. A clear line has been drawn between instrument specific tasks for data reduction and data processing as well as data analysis, which is the objective of our common software SOFT-AIS.

While the official EAI-STRESS project homepage will go offline sometime after the end of the project, the GitHub repository with the software will remain online and accessible indefinitely. However, the question still remains about who or even which institution(s) will be able to maintain and advance the software after the end of the EASI-STRESS project. Extending and implementing the NXstress file format to other LRIs and instruments outside the consortium is also currently under discussion.

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APPENDIX

In this section are the responses from the EASI-STRESS partners during the first survey listed.

	What must be included in the software? In other words, what capabilities, functions, calculations, options, ... are an absolute necessity for your application of the software?
2	Everything after fitting peaks to get changes in 2theta, or strains. This level of abstraction means that there is a need to deliver peaks at specific locations. It should be relatively straightforward after that to apply elastic constants of your choice to end up with stresses.
3	For strain: different d0 reference approaches (constant value, 3D dependent, component dependent, time-temperature dependent). It would be good to be able to plot 2Thetha trend vs strain to see the impact of the particular d0 hypothesis and compare a few cases simultaneously (same input for components and then different d0) For stress: it would be good to update error calculations (see T.Pirling file)
4	It is necessary to have a fast efficient way of calculating part. The input data has to be open source.
5	We should be able to get out the stress values and the different measured positions.
6	Uniform report for customers. Creation of report in common format as excel, pdf, csv...
7	Selection of input files / fixed and variable d0 / possibility to exclude measuring points and ranges / possibility of plotting strain, stress and every parameter which is stored in the file / "Superplot" = combined plots / a click on a data point shows the actual value from a pull-down menue plots of raw-data with fit or fit-parameter values etc can be chosen / a kind of logfile which gives the possibility to automatically parametrise a new session / 3D-plots for maps / interpolation of data points
8	Calculations of stress and strain, line profiles, maps and then visualise them. Ability to rotate coordinates to find stress in secific diections, ability to extract a line scan from a 2D map, Ability to compare multiple types of data or multiple components f stress/strain on a linescan or along a line from a 2D map.
9	-Error bars; -Full width at half maximum (FWHM), to have an indication of "work-hardening" and internal disorder; -Have a preview of the results, to correct whatever is needed, without attending the end of the whole measurement + data analysis time.
10	use my XRD measurements to measure RS from different devices with the same software extract the results in a format that can be opened with excel, python or a notepad visualise the data (curve, tables....)
11	Ability to trace data flow through all of the different stages of capture and processing. Logging the key set up features - component geometry, measurement location and orientation etc
13	Due to my position and point of view from the quality aspects of a company I prefer not to get into the software at all. I focus on the final report of the measuremnt and a complient or non compliant statement in respect to for example overall stress levels, stress level spikes or effective residuel stress reduction visualisation

	Apart from strain / stress calculations, what has the highest priority for you? **In other words, what would be most important for your applications?**
2	1) Ability to load part information/geometries and visualise locations of measurement 2) As above, with gauge volumes 3) As above, with beam path lengths minimized.
3	Temperature & displacement.
4	Some plots that help estimate the accuracy of the measurements. Being able to plot two samples in the same graph to compare stress levels Exporting a plot of the stress and strain. x: position, y: stress (or if 2D map, x,y: position; z: stress) Exporting tabels of the strain and stress levels, peak widths, peak intensity, ... (in ascii or excel format)
5	Visualization of the plots
6	intuitive usage / comfortable plotting functions, 2D and 3D / selection of ranges
7	Ability to alter stress free reference to see its implications, and the ability to use different d zero values at differentpoints -possibly interpolating in cases where the d zero references are widely spaced but the strain measurements are not. Comparions of measured stresses with model or other results. Ability to turn single crystal elastic constants into diffraction elastic constants (say using a korner model).
8	-Error bars; -Full width at half maximum (FWHM), to have an indication of "work-hardening" and internal disorder; -Have a preview of the results, to correct whatever is needed, without attending the end of the whole measurement + data analysis time; -Data superimposition (eg. measuring 2-phases metal).
9	-measure the intensity ratio to estimate the texture -
10	1 calculating uncertainties in measurements. 2 It would be good to also include the option to specify uncertainties in calibration (such as d0 measurements) and in material properties like elastic modulus and then combine these to give and overall value. 3 Stress intensity factor estimations for common geometries (eg plate and cylinder)
11	To identify to which extend residual stresses are still present in the part after the applied stress relief heat treatment cycle.
12	I would like to put a strong interest on the measurment of applied stress as well. This could be due to applied mass or force or others. This in combination with functionality should give an indication of part livetime. Also the development of stress is of importanse in positive sense or negative sense if stress is wanted.

|	What are some features that you would consider a "nice to have" option?
2	Sensitivity analysis on the basis of different elastic constants, that is the ability to either load multiple analyses simultaneously, or to allow error bars to contain some uncertainty on elastic constants.
3	include different failure criteria used in industry and simulations such as von Mises equivalent stress
4	Microstructural link.
5	Comparison to modelling is still very interesting and important, so beeing able to upload modelling output and make plots with the data - subtract them to see differences etc. could be cool (the data would of cource have to be put in the same coordinate system)
6	On 3Dplots extract 2D cuts
8	If our software can analyse diffracton rings then dealling with spotty rings then great and the caking of difraction profiles to form line scan profiles.
9	-Data superimposition (eg. measuring 2-phases metal). -Strained image of the gauge volume.
10	display data from e.g. LXRD, SALSA on the same curve/table,
11	logging additional data about the component, eg materials, weld type and technique, number of passes and possibly also weld parameters like speed, power etc
12	To investigate if the blasting process for surface treatment induces compression stress into the surface of the part.
13	Based on our exerience in stress measurment it is seen mandatory to address industry with an interesting tool is: A questionary what informations are necessary on the part, A list of premeasurments to be executed by the sience partner, standardisation of report, some example of question data and interpretion

	What should the graphical interface contain? **What (type of) plots should be able to be visualized?**
2	Beyond trends in stress along specific measurement points, the ability to 'lock on' a measurement and see FWHM, and integrated intensity. See your 'anatomy of a peak' :)
3	For display: it could be the opportunity to be able to plot automatically 2Thetha-Strain-Stress with respect to location and see it as 3D plots. Sample reference system may be also specified in a sketch together with GV
4	Honestly, I would not spend a single minute developing any GUI. Just open format as .vtk could be postprocess in Paraview.
5	Position vs. stress Position vs. peak width it would of course be cool to be able to show that on top of a sketch or CAD drawing of the component, but that would more be nice to have.
6	In addition to the measured stresses: stress differences, von Mises stresses, and contouring plots (for both strain and stresses when appropriate). Plotting of measured points (when possible)
7	2D and 3D, superplot, select ranges, exclude points
8	Line scans with multiple data and error bars and trend lines 2D maps where we can control the scales to be in sensible gradations (e.g. 0, 100, 200, 300MPa) and to enable like for like plots. We should be able to extract plots to data files. Some way or representing the stress tensor variation across a 2D field (Maybe by arrow sizes and orientations).
9	- scatter data - 2D map - contour map (if not too hard) -Strained image of the gauge volume (if not too hard)
10	Strain in function of sin²psi for LXRD data Stress in function of x or y or z coordinate
11	no preferences
12	The world of industry is the CAD file in step formate and pictures. Thus the report should link the result onto this respectively

	Since this might have changed over time, which common software **output file format(s) would be most useful for you and/or your users/customers/clients?**
2	HDF5 is fine.
3	.csv , .txt. vtk, .xml, hfd5...
4	simple image files for plots and excel or ascii for tabels
5	Excel, pdf, word, csv...
6	Hdf 5 and ASCII in parallel
7	nexus I think.
8	Excel Txt jpeg/tif (if needed to export images)
9	I'm old school, a python or an excel suits me^^
10	non-proprietary database formats since this enables easiest processing in custom software and assessment pipelines
11	no preferences
12	Here is a big difference between system engineering and quality. We intend to have a report with the key findings. System engineering might be interested in the raw data to use them for as input for further analysis in house

Do you currently use or process HDF5 files in your data workflow / simulation workflow?

🔵 Yes	7	
🟠 No	6	

Do you think that your users/customers/clients are capable of processing HDF5 files?

🔵 Yes	4	
🟠 No	7	
🟢 Does not apply to our organiz...	1	
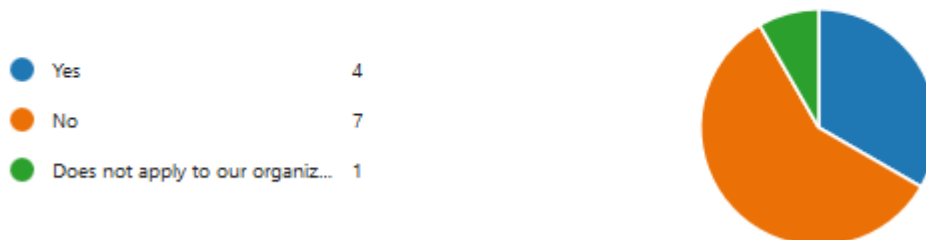
Please add here any other comments you might have regarding the software	
2	I don't think there's an issue with the file format, HDF5 is more than sufficient. I honestly am unaware of another data format that a) performs as well and b) has a significant uptake.
3	we can have the option in the software to SAVE output as hdf5 or excel is the INPUT that must be harmonised NXStress format
4	HDF5 is the future, specially for R&D. However none commercial software has implement it yet.
6	Creating a Windows ".exe" file to run the software