



Davinci

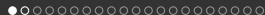
Version 1.0.7 (19 Aug 2018)

A Scientific Software for the Visualization and
Processing of Single-Crystal Diffraction Data
Measured with a Point Detector

Andrew Sazonov

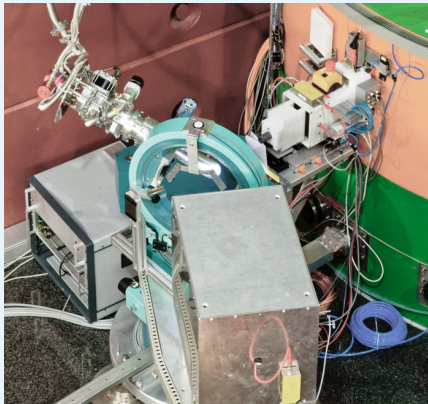
Point detectors in neutron diffraction

Motivation

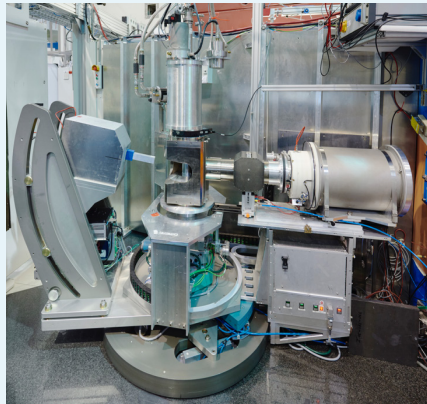


- High accuracy of the measured intensities, especially at short wavelengths.
- HEiDi, POLI (MLZ), 5T2, 6T2 (LLB), D3, D10, D23 (ILL), Zebra/TriCS (SINQ), ...

HEiDi: 4-circle SG diffractometer



POLI: polarised SG diffractometer



License	Open source, GNU GPL v3.0
Programming language	C++11
Dependencies	Qt5 (GUI, etc.), QCutomPlot (plotting), Minuit2 (fitting)
Unit testing	Qt Test framework
Desktop installer	Qt Installer framework, JavaScript (macOS, Linux, Win)
Version control	Git via GitHub
Cont. integration	AppVeyor and Travis (clang, gcc, msvc, mingw)
qmake Project Files	Python scripts
Code styling	Artistic Style
Code documentation	QDoc
User manual	pdfLaTeX (PDF) and Python scripts (HTML)

Input data

- **Raw measured data:** POLI, HEiDi and MIRA at MLZ, 5C2 and 6T2 at LLB

Calculate/extract for each Bragg peak

- **Experimental parameters:** angles, orientation matrix, temperature, field, etc.
- **Miller indices** based on orientation matrix and angles
- **Structure factor** based on peak intensity
- **Full width at half maximum** based on peak intensity and scan data
- **Direction cosines** based on orientation matrix and angles
- **Flipping ratios** (polarised neutrons) based on spin up and down peak intensities

Export data

- **Peak plots as graphics:** vector: PDF, raster: JPEG
- **Output table as text:** general: CSV, specific: ShelX, TBAR/D9, UMWEG, CCSL

Peak location and integration

- The peak and background points can be selected manually or detected automatically using the Lehmann-Larsen method

Acta Cryst. (1974). A30, 580

A Method for Location of the Peaks in Step-Scan-Measured Bragg Reflexions

BY M. S. LEHMANN

Institut Laue-Langevin, B.P. N° 156, 38042 Grenoble Cédex, France

AND F. K. LARSEN

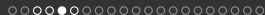
Department of Inorganic Chemistry, University of Århus, DK 8000 Århus C, Denmark

(Received 18 December 1973; accepted 3 March 1974)

A method for location of the peak in a step-scan-measured Bragg reflexion profile is described. It leads to a ratio between the standard deviation of the intensity and the intensity, $\sigma(I)/I$, which is near minimum. The method is based on the observation that if $\sigma(I)/I$ is calculated for all possible peak widths for a given profile then $\sigma(I)/I$ is minimum near the true value of the peak width, and **minimal $\sigma(I)/I$ can thus be used as a criterion for correct location of the peak.** The intensity determined this way is however in general slightly underestimated, and the bias as well as possible corrections are discussed. In addition a simple function resembling $\sigma(I)/I$, which has proved to be useful for practical applications, is given.

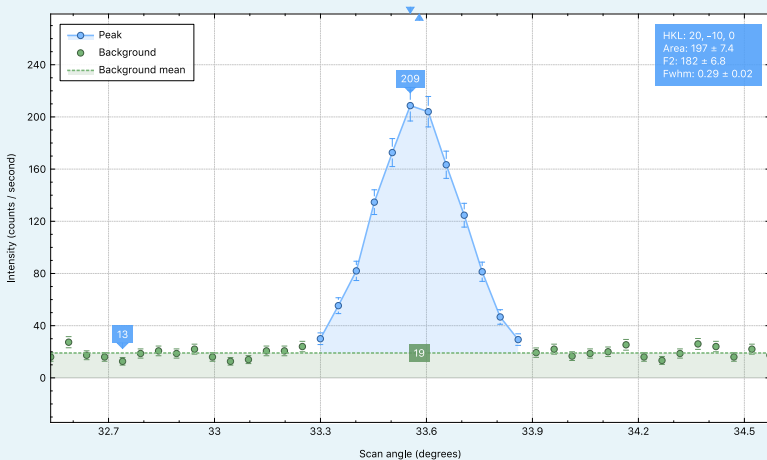
Peak intensity calculation

Davinci features



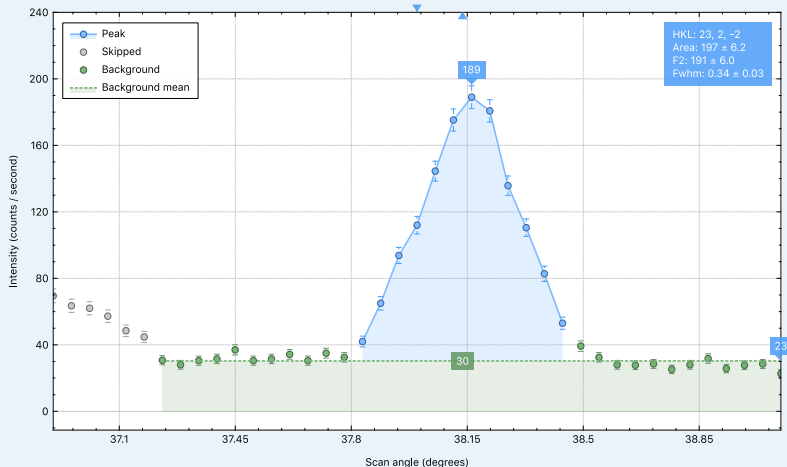
Peak location and integration

- The peak and background points can be selected manually or detected automatically using the Lehmann-Larsen method



Remove neighbours

- The tails from neighbouring reflections can be removed manually or automatically





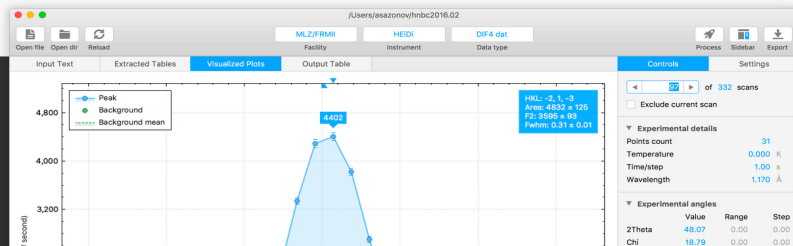
Version 1.0.7 (19 Aug 2018)

A Scientific Software for the Visualization and Processing of Single-Crystal Diffraction Data Measured with a Point Detector

 **Download for macOS**
macOS 10.11 and above, 64-bit

 **Download for Windows**
Windows 7 and above, 32-bit

 **Download for Linux**
Ubuntu 14.04 and above, 64-bit



Davinci Version History

Here you can find the changelog for the Davinci releases.

Version 1.0.7 (19 Aug 2018)

- Adds progress bar to give an indication of how long the data processing is going to take
- Adds more multi-threading features in order to speed up the data processing
- Fixes an issue with ShelX output format in the console version of the program
- Fixes multiple other issues

Version 1.0.6 (09 Jul 2018)

- Adds reading of Psi angle from the NICOS instrument data collection files (Issue #5)
- Adds UMWEG output for the calculation of multiple-diffraction patterns
- Adds some multi-threading features in order to speed up the data treatment

Version 1.0.5 (30 May 2018)

- Adds calculation of the direction cosines (Issue #3)
- Adds reading of Psi angle from the HEiDi instrument data collection files
- Adds natural sort order and sort by date and time to the table widgets
- Adds ShelX output with real (non-integer) Miller indices hkl
- Fixes calculation of the Phi angle in the 4-circle geometry

Davinci User Manual

This page contains the table of contents for the Davinci user manual

1. Introduction

- [1.1. What is Davinci for?](#)
- [1.2. Davinci features](#)

2. Getting Started

- [2.1. Installing Davinci](#)
- [2.2. Launching Davinci](#)
- [2.3. Launching console version of Davinci](#)
- [2.4. Updating Davinci](#)
- [2.5. Uninstalling Davinci](#)

3. How to Use

- [3.1. Davinci user interface](#)
 - [3.1.1. Main window](#)
 - [3.1.2. Sidebar](#)

3.1.1. Main window

The Main Window of the program is located below the Toolbar and it consists of up to 4 tabs, as shown in the figure below. When new files are opened the only first tab is visible. Every next tab appear when the main action on the previous tab is done. You can switch between the available tabs at any time by clicking on their names.



Bug report page: github.com/AndrewSazonov/Davinci/issues

Davinci web



Features Business Explore Marketplace Pricing

Search



Sign in or Sign up

AndrewSazonov / Davinci

Watch 1

Star 0

Fork 0

Code

Issues 1

Pull requests 0

Insights

is:issue is:open

Labels

Milestones

New issue

1 Open 4 Closed

Author

Labels

Milestones

Assignee

Sort

Please provide an AppImage for Linux for download **enhancement**

2

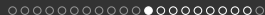
#1 opened on Dec 21, 2017 by probonopd

ProTip! Exclude everything labeled bug with `-label:bug`.



Installer

Davinci workflow



Davinci Installer Setup

Setup - Davinci

Welcome to the Davinci Setup Wizard.

Davinci: A Scientific Software for the Visualization and Processing of Single-Crystal Diffraction Data Measured with a Point Detector.

For more details, visit davinci.sazonov.org

Davinci Installer Setup

Installation Folder

Please specify the directory where Davinci will be installed.

Davinci Installer Setup

Settings

Network **Repositories**

Add Username and Password for authentication if needed.

Use User: Pass: Repository

▼ **Default repositories**

- <http://davinci.sazonov.org/repositories/mc>

Temporary repositories

User defined repositories

Use temporary repositories only

Davinci Installer Setup

Creating Maintenance Tool

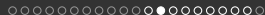
Installation finished!

`/Users/asazonov/Applications/Davinci/Examples/POLLNICOE
/Users/asazonov/Applications/Davinci/Examples/POLLNICOE
/Users/asazonov/Applications/Davinci/Examples/POLLNICOE
/Users/asazonov/Applications/Davinci/Examples/POLLNICOE
/Users/asazonov/Applications/Davinci/Examples/POLLNICOE
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/Users/asazonov/Applications/Davinci/Examples/POLLNICOE
/Users/asazonov/Applications/Davinci/Examples/POLLNICOE
/Users/asazonov/Applications/Davinci/Examples/HEIDI_LOG/
Writing maintenance tool.`

[Installation finished!](#)

Automatic update

Davinci workflow




Open file Open dir Reload

Undefined Facility Undefined Instrument Undefined Data type

Process Sidebar Export

Update



A new version of Davinci is available!

Davinci 1.0.7 is now available.
You are currently using version 1.0.6.

For details, see davinci.sazonov.org

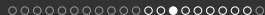
Do you want to restart and install update?

Remind Me Later Install Update Now

Open in the file menu

Open experimental files

Davinci workflow



Open file Open dir Disabled Open existing directory.

Undefined Facility Undefined Instrument Undefined Data type

Process Sidebar Export

+

Drag and drop files/folders here
or
Click the toolbar buttons to browse
or
Open in the file menu

Text view tab

Davinci workflow



Mac OS window titled "/Users/asazonov/Applications/Davinci/Examples/POLI_NICOS/p12062_00074975.dat". The window contains a text editor with a configuration file and a sidebar with search and navigation controls.

File Bar: Open file, Open dir, Reload, MLZ/FRMII (Facility), POLI (Instrument), NICOS dat (Data type), Process, Sidebar, Export.

Input Text:

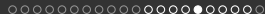
```
172 #      omega_value : -169.39 deg
173 #      variox1_p_i : 10.0
174 #      variox1_piso_value : 6.2e-06 mbar
175 #      variox1_p_heateroutput : 35.9784192523
176 #      variox1_ln2_fill_value : 79.8 %
177 #      variox1_p_window : 60.0 s
178 #      gamma_value : 79.23 deg
179 #      sih_value : 8.18 kstep
180 #      T_setpoint : 1.5
181 #      ytrans_value : -4.00 mm
182 #      T_variox1_window : 60.0 s
183 #      chi1_value : 0.00 deg
184 #      T_d : 0.0
185 #      xtrans_value : 0.51 mm
186 #      T_variox1_i : 0.4
187 #      siv_value : 3.80 kstep
188 #      bmv_value : 180.04 mm
189 #      T_variox1_sample_value : 310.400 K
190 #      bmh_value : 39.98 mm
191 #      theta_m_value : 268.50 kstep
192 #      T_p : 30.0
193 #      liftingctr_value : -2.16 deg
194 #      chi_m_value : 6.30 kstep
195 #      variox1_p_p : 25.0
196 #      variox1_psample_value : 0.6 mbar
197 #      T_i : 0.4
198 #      T_variox1_p : 30.0
199 #      T_variox1_heateroutput : 1.7
200 #      POLI_value : [1.9763, 1.9756, -8.1062] rlu rlu rlu
201 #      variox1_nv_value : 37.0 %
202 #      x_m_value : 45.00 kstep
203 #      bp_value : 10.00 10.00 9.00 20.00 mm
204 ### Scan data
205 # omega Ts ; timer mon1 mon2 ctrl
206 # deg K K ; s cts cts cts
207 -169.42 312.400 1.499 ; 1.01 19768 0 59
208 -169.37 316.300 1.498 ; 1.00 19634 0 68
209 -169.32 318.700 1.498 ; 1.00 19595 0 66
210 -169.27 319.600 1.498 ; 1.00 19587 0 67
```

Controls Panel:

- Go to:** 1 of 4 files, 172 of 240 lines
- Find:** Ignore case, Search for "omega" (9 matches)
- Extract data:** [Button]

Table view tab

Davinci workflow



/Users/asazonov/Applications/Davinci/Examples/POLI_NICOS/p12062_00074975.dat

Open file Open dir Reload

MLZ/FRMII POLI NICOS dat

Facility Instrument Data type

Process Sidebar Export

Input Text	Extracted Tables										Controls	Settings
	Chi1	Chi2	Gamma	Nu	Omega	Detector	Monitor	Monitor1	Monitor2	Absolute		
1	0.00	0.00	79.23	-2.16	-169.42	59	19768	19768		0		
2	0.00	0.00	79.23	-2.16	-169.37	68	19634	19634		0		
3	0.00	0.00	79.23	-2.16	-169.32	66	19595	19595		0		
4	0.00	0.00	79.23	-2.16	-169.27	67	19587	19587		0		
5	0.00	0.00	79.23	-2.16	-169.22	93	19620	19620		0		
6	0.00	0.00	79.23	-2.16	-169.17	83	19614	19614		0		
7	0.00	0.00	79.23	-2.16	-169.13	118	19721	19721		0		
8	0.00	0.00	79.23	-2.16	-169.08	262	19690	19690		0		
9	0.00	0.00	79.23	-2.16	-169.03	734	19936	19936		0		
10	0.00	0.00	79.23	-2.16	-168.98	2006	19392	19392		0		
11	0.00	0.00	79.23	-2.16	-168.93	4476	19750	19750		0		
12	0.00	0.00	79.23	-2.16	-168.88	7173	19812	19812		0		
13	0.00	0.00	79.23	-2.16	-168.83	9623	19813	19813		0		
14	0.00	0.00	79.23	-2.16	-168.79	10256	19958	19958		0		
15	0.00	0.00	79.23	-2.16	-168.74	9776	20083	20083		0		
16	0.00	0.00	79.23	-2.16	-168.69	7425	19738	19738		0		
17	0.00	0.00	79.23	-2.16	-168.64	5244	19820	19820		0		
18	0.00	0.00	79.23	-2.16	-168.59	3301	19785	19785		0		
19	0.00	0.00	79.23	-2.16	-168.54	1760	19762	19762		0		
20	0.00	0.00	79.23	-2.16	-168.49	870	19906	19906		0		
21	0.00	0.00	79.23	-2.16	-168.44	414	19829	19829		0		
22	0.00	0.00	79.23	-2.16	-168.40	278	19919	19919		0		
23	0.00	0.00	79.23	-2.16	-168.35	167	19630	19630		0		
24	0.00	0.00	79.23	-2.16	-168.30	104	19635	19635		0		
25	0.00	0.00	79.23	-2.16	-168.25	81	19479	19479		0		
26	0.00	0.00	79.23	-2.16	-168.20	78	19760	19760		0		

1 of 4 scans

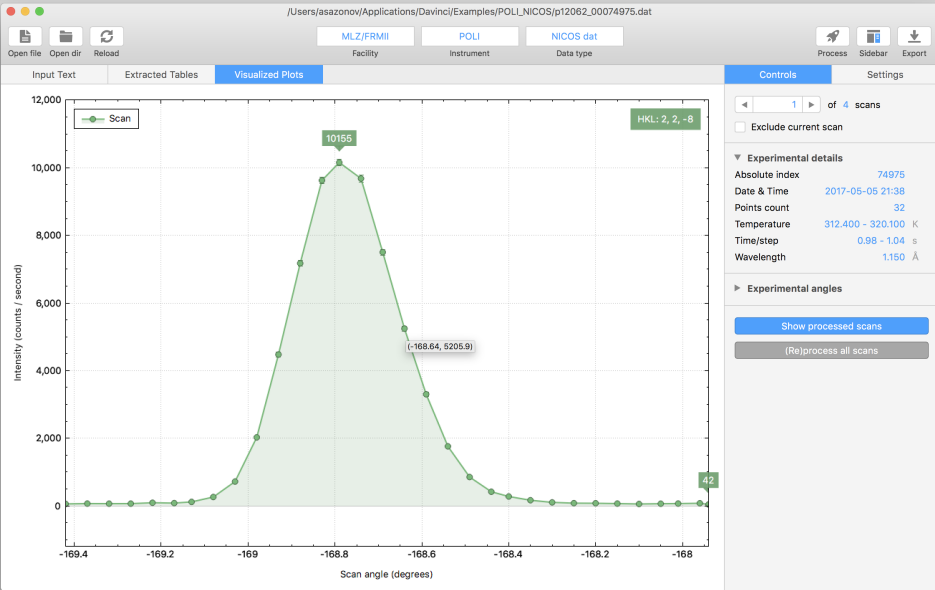
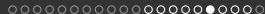
Exclude current scan

Visualize extracted data

Click to visualize the data and switch to the plot view tab.

Plot view tab

Davinci workflow



Plot view tab

Davinci workflow



/Users/asazonov/Applications/Davinci/Examples/POLLI_NICOS/p12062_00074975.dat

MLZ/FRMII POLI NICOS dat
Facility Instrument Data type

Open file Open dir Reload

Input Text Extracted Tables **Visualized Plots**

Controls Settings

◀ 1 ▶ of 4 scans
 Exclude current scan

▶ Experimental details

▼ Experimental angles

	Value	Range	Step
Chi1	0.00	0.00	0.00
Chi2	0.00	0.00	0.00
Gamma	79.23	0.00	0.00
Nu	-2.16	0.00	0.00
Omega	-168.66	1.48	0.05

▶ Scan treatment

▶ Scan correction

▼ Peak integration

Conventional peak integration ▾
Automatically detect background ▾

◀ 6 ▶ 18 ◀ 8 ▶
left background peak right background

Show processed scans
(Re)process all scans

Intensity (counts / second)

Scan angle (degrees)

Legend: Peak (blue line with circles), Background (green line with circles), Background mean (dashed green line).

Peak parameters: HKL: 2, 2, -8; Area: 1518 ± 6.2; F2: 1490 ± 6.1; Fwhm: 0.28 ± 0.01

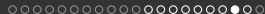
Peak position: 10165

Background position: 69

Scan number: 42

Output table tab

Davinci workflow



/Users/asazonov/Applications/Davinci/Examples/POLI_NICOS/p10394_00134303.dat

MLZ/FRMII POLI NICOS dat
Facility Instrument Data type

Open file Open dir Reload Process Sidebar Export

Input Text	Extracted Tables		Visualized Plots			Output Table				Controls	Settings
Batch	Excluded	Scan	H	K	L	Area	AreaErr	AreaNorm	AreaNorm	1 of 6 scans	Exclude current scan
1	1	0	1	-1.000	0.000	1.000	5346.50	24.73	2877.63		<input type="checkbox"/>
2	1	0	2	-1.000	0.000	-0.001	3339.78	16.94	1793.64		<input type="checkbox"/>
3	1	0	3	2.001	2.001	-7.996	2988.97	12.20	1518.16		<input type="checkbox"/>
4	1								46.20		<input type="checkbox"/>
5	1								07.82		<input type="checkbox"/>
6	1								22.30		<input type="checkbox"/>

Save Output

Save As: p10394_00134303-p12062_00074978.c

Tags:

Output

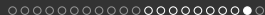
- 5C2
- 6T2_XML
- HEIDI_DIF4
- HEIDI_LOG
- Output
- POLI_NICOS

General comma-separated, real (*.csv)
ShelX with direction cosines, integer (*.hkl)
ShelX with direction cosines, real (*.hkl)
TBAR/D9, integer (*.tb)
UMWEG, integer (*.obs)
CCSL flipping ratios, integer (*.fli)

New Folder Cancel Save

Console version

Davinci workflow



```
AsMBP:Davinci asazonov$
AsMBP:Davinci asazonov$ ./DavinciConsole --help
Usage: ./DavinciConsole [options]
Davinci v1.0.7 (19 Aug 2018)
http://davinci.sazonov.org
A Scientific Software for the Visualization and Processing of Single-Crystal Diffraction Data Measured
with a Point Detector
Copyright (C) 2018 Andrew Sazonov.

Options:
  -h, --help           Displays this help.
  -p, --path <file/dir> File/dir to open.
  -o, --output <file>  File to save output data.
  -f, --format <type>  Output file format <type>: general, shelx, tbar,
                        umweg, ccsl.

AsMBP:Davinci asazonov$
AsMBP:Davinci asazonov$
AsMBP:Davinci asazonov$
AsMBP:Davinci asazonov$
AsMBP:Davinci asazonov$
AsMBP:Davinci asazonov$ ./DavinciConsole --path Examples/HEiDi_DIF4/hnbc2016.02
Davinci v1.0.7 (19 Aug 2018)
http://davinci.sazonov.org
A Scientific Software for the Visualization and Processing of Single-Crystal Diffraction Data Measured
with a Point Detector
Copyright (C) 2018 Andrew Sazonov.

Number of treated files: 1
Number of treated reflections: 332
Output file: /Users/asazonov/Applications/Davinci/Examples/HEiDi_DIF4/hnbc2016.csv

The program is finished successfully.
AsMBP:Davinci asazonov$
```

Peak fitting

- Gaussian, Lorentzian, Pseudo-Voigt peak shape functions and their asymmetric versions

Other instruments

- Single-crystal diffractometers Zebra (TriCS) at SINQ and D3, D10, D23 at ILL

Resolution function table

- Determine the widths table from the good peaks and use it to locate the weak peaks

Save state

- Save the current data processing progress in file (xml, yaml, json?) for later use

Thank you for your attention!