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Command line programs from LatticeRepLib

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1. Introduction

In the study of various spaces for representing lattices, a number of software tools have been prepared. Some of those are available as simple commandline programs. Most of them have flexible input and output their processed results in a form that another can use that for processing. A few are terminal programs that produce analysis. A small number take no input and generate files for other uses.

2. Data Inputs:

2.1. Table of input types

In general, there are 5 types of input lines, see Table 1. Except for "END", they can be combined in any order.

Table 1. *All these are case-insensitive. If a particular input lattice is invalid, it is rejected with a message.*

Vector Input:	**g** for $\mathbf{G^6}$ vectors
	s for $\mathbf{S^6}$, Delone/Selling scalars
	C3 for $\mathbf{C^3}$ input (without parentheses or commas, "C" would be interpreted as a C-centered unit cell)
	U for DC7 unsorted
RANDOM: Random (valid) unit cell generated	
Crystal lattice input: "A", "B", "C", "P", "R", "H","F", "I" followed by three axis lengths and three angles (in degrees)	
semicolon: lines beginning with a semicolon are treated as comments	
END: ends the data input section	

2.2. Examples of unit cell inputs

P 10 20 30 90 111 90
G 100 400 900 0 -215.02 0
S6 0 -107.51 0 7.51 -400 -792.49
; this is a comment

3. Programs

3.1. Filters - change lattice representation

Table 2. *Programs to convert lattice representations. NOTE: although all can take all of the input types,* $\mathbf{B^4}$. $\mathbf{DC^{13}}$, *Polar write output that cannot be used as input.*

Name	in	out	Output
CmdToB4	y	$\mathbf{B^4}$	For each input, it produces the 4 vectors as a,b,c,d as E3 vectors, and also the lengths of each of those vectors.
CmdToC 3	y	$\mathbf{C^3}$	For each input, produces the $\mathbf{C^3}$ representation in the form (#,#) (#,#) (#,#), which does not conform to the format for input to other programs.
CmdToCell	y	$a, b, c,$ α, β, γ	Converts to the conventional unit cell representation If the input is already unit cell parameters, then the output will be in the same lattice centering as the input.
CmdToDC	y	$\mathbf{DC^{13}}$	Outputs the lengths of the 13 unique vectors describing the Dirichlet cell.
CmdToG6	y	$\mathbf{G^6}$	Converts the input to $\mathbf{G^6}$
CmdToS6	y	$\mathbf{S^6}$	Converts the input to $\mathbf{S^6}$
Radial	y	Polar	CSomputes the polar distances in Angstroms from the first input cell. That is (a,α), (b,β), and (c,γ) as coordinates in complex space.

3.2. Data processing programs

Table 3: Summary of programs manipulating data

Name	in	out	command line params	Output
CmdCmplx	NA	y	_____	Currently, this just outputs some programmed examples.
CmdDelone	y	$\mathbf{S^6}$	_____	Converts input to $\mathbf{S^6}$
CmdDists	y	mod	_____	For on input list of n cells, n-1 distances will be output.
CmdGen	NA	$\mathbf{G^6}$	ngen	- number of examples to generate (optional)
			type	- lattice type to generate (optional); many options c,t,h,o,r,h,m,a, cP, cF,cI, tP, tI, hP, hR, oP, oF, oI, oS, mP, mC, mS, aP, numeric Niggli types - 1-44, Delone types - C1,C3,C5, . . . If no parameters are present, one each of the 44 Niggli types. If only a number is present, that is how many of each of the 44 Niggli types to generate. For usage examples, see Table 4

CmdLM	y	y	————	Lattice Matching. The first input cell is used as the reference. Succeeding cells are matched as well as possible to the reference cell.
CmdNiggli	y	$\mathbf{G^6}$	————	Produces the Niggli reduced cell for each input.
CmdPath	y	$\mathbf{S^6}$	no. of points	If the number of points is not on the command line, the default number to generate is 20. If there is only one point, then the second point is generated as the Niggli reduced cell. If more than two points are input, each successive pair will generate a list of output points; so if 3 cells are input, the output will be 2 times the number of points requested.
CmdPerturb	y	y	n-number of perturbations, parts per thousand to perturb	n cells perturbed normal to the input $\mathbf{S^6}$ vector If a lattice centering (including P) is input, the output is in the same centering. Otherwise, the output is in $\mathbf{S^6}$.
CmdS6Refl	y	$\mathbf{S^6}$	————	For each input, all 24 $\mathbf{S^6}$ reflections are produced.
CmdSella	y	y		SELLA produces 2 output: std::out contains the match of each of the 24 Delone types; SVG for the Grimmer diagram is written to a file with a name such as SEL__2023-01-07.08_56_42.svg with date/time stamp.
CmdSort	y	y	"C3" or "seq'	
CmdVolume	y	mod	————	Outputs the unit cell and the volume of each input cell.
PlotC3	y	mod	————	Plot the three $\mathbf{C^3}$ coordinates. See Figure 1. The gray lines connect successive pairs of points in the input. The output graphics file is an SVG file whose name is in the output in standard output.
SELLA	y	mod	————	Outputs the distances from each of the Bravais lattice types (in s_6).
SVD	y	mod	————	Outputs the singular value decomposition vectors and eigenvalues for the input lattice. This is done in $\mathbf{S^6}$.

- **CmdGen**

3.3. Individual program details

CmdGen is a program for creating examples of various types of lattice types.

There are two optional input parameters. The first is the count of how many samples of each type to generate. The second (if present) is the type of lattices to generate. There is no input data other than the command line parameters. For examples of using CmdGen, see table 4

The is considerable flexibility in the input types. However, they are case-sensitive.
– Niggli types by number 1-44 (see Table 6).

– Delone types by Delone's designation - C1,C3,C5, T1, T2, T5, R1, R3, O1A, O2, O3, O4, O5, O1B, M1A, M2A, M3, M4, M1B, M2B, A1, A2, A3, H4 (see Table 5).
– Crystal system - c,h,t,o,m,a

Table 4. *CmdGen examples*

CmdGen	generates a single example of each of the 44 Niggli types
CmdGen 2	generates two examples of each of the 44 Niggli types
CmdGen 4 aP	generates four examples of each of the two anorthic Niggli types
CmdGen 2 17	generates 2 examples of Niggli 17, which is mC
	Output:
	; Niggli lattice type requested
	; lattice type = 17
	G6 90.428 90.428 142.222 83.992 83.992 22.888 IT# = 17 mC
	G6 79.033 79.033 111.127 -61.421 -73.872 -22.772 IT# = 17 mC
CmdGen 2 C5	generate two examples of Delone type "C5", which is primitive cubic.
	Output:
	; Delone lattice type input
	; lattice type = C5
	G6 181.275 181.275 181.275 0.000 0.000 0.000 IT# = C5 cP
	G6 74.526 74.526 74.526 0.000 0.000 0.000 IT# = C5 cP
CmdGen 1 h	Generate a single example of each of the hexagonal (and rhombohedral) Bravais lattice (per Nigg
	Output:
	; Niggli lattice type input
	; lattice type = 2
	G6 119.828 119.828 119.828 -45.302 -45.302 -45.302 IT# = 2 hR
	;
	; lattice type = 4
	G6 86.837 86.837 86.837 19.813 19.813 19.813 IT# = 4 hR
	;
	; lattice type = 9
	G6 3.688 3.688 145.128 3.688 3.688 3.688 IT# = 9 hR
	;
	; lattice type = 12
	G6 55.273 55.273 136.854 0.000 0.000 -55.273 IT# = 12 hP
	;
	; lattice type = 22
	G6 73.578 73.578 149.339 0.000 0.000 -73.578 IT# = 22 hP
	;
	; lattice type = 24
	G6 101.390 125.771 125.771 -91.974 -67.593 -67.593 IT# = 24 hR
	;

- **SVD**

  On input to a number of lattices, SVD calculates a Singular Value Decomposition. The output consists of the eigenvalues and the six eigenvectors. It is important to check that the form of each cell is the same; for instance, monoclinic cell should have the unique interaxial angle in the same place (*e.g.* β)

  As an example, consider using SVD to compute the information for one of the
  Command line:
  CmdGen 5 33 | CmdSort seq | SVD
  ; SVD
  S6 from input cell 0.000 -31.196 0.000 -71.963 -109.653 -131.880
  S6 from input cell 0.000 -23.060 0.000 -77.367 -110.398 -125.599
  S6 from input cell 0.000 -28.898 0.000 -54.985 -106.336 -82.229
  S6 from input cell 0.000 -56.133 0.000 -103.736 -177.343 -123.204
  S6 from input cell 0.000 -10.111 0.000 -50.618 -91.57100 -98.102

  Output:
  eigenvalue 0; vector 1 0 0 0 0 0
  eigenvalue 413.012; vector 0 -0.1728 00 -0.4007 -0.6616 -0.6097
  eigenvalue 48.3869; vector 0 -0.4009 0 -0.1129 -0.5164 0.7482
  eigenvalue 14.0785; vector 0 -0.7060 0 -0.4581 0.5344 -0.0786
  eigenvalue 8.53435; vector 0 0.5576 0 -0.7853 0.1001 0.2494
  eigenvalue 0; vector 0 0 -1 0 0 0
  The two zero eigenvalues correspond to the invariant interaxial angles (α and γ, in this case).

- **CmdS6Refl**

  CmdS6Refl generates the 24 reflections (see (Andrews *et al.*, 2019)) of each input lattice. Duplicate outputs of each input are not removed.

- **CmdPath**

  CmdPath outputs points along a line between pairs of lattice.
  The number of points per segment is a commandline parameter. If no parameter is input, the default is 20. This is not the number of steps; it is the number of points that will be output for a segment (pair of input lattices).

  1. Only a single lattice is input. A second point will be generated as the Niggli reduced lattice, and series of points will be output between them.
  2. Two lattices are input. Then the points will be created between them.
  3. More than two lattices are input. Then each point and its succeeding point will generate a segment. Each segment will be output as the number of points specified. Note: the final point of one segment and the first point of the next segment will be duplicates.

The line between points is calculated in $\mathbf{S^6}$. The other likely space would be $\mathbf{G^6}$, but the results seem to be the same. As an example, in the case of 3 items input and 5 requested output lattices, the output will consist of 10 lines, 5 for each successive pair of lattices, and the 5th and 6th points will be the same.

Command Line:
CmdPath 5
; Path generator
f 10 10 10 90 90 90 90
end

Output:
; no. of points output is 5
S 0.00000 0.00000 0.00000 -100.00000 -100.00000 -100.00000 1
S 6.25000 6.25000 6.25000 -100.00000 -100.00000 -100.00000 2
S 12.50000 12.50000 12.50000 -100.00000 -100.00000 -100.00000 3
S 18.75000 18.75000 18.75000 -100.00000 -100.00000 -100.00000 4
S 25.00000 25.00000 25.00000 -100.00000 -100.00000 -100.00000 5
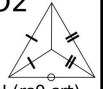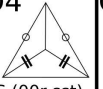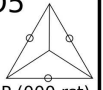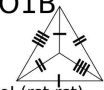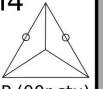
Command Line:
CmdPath 5 | CmdToCell
; To Cell
f 10 10 10 90 90 90
end

Output:
; no. of points output is 5
P 10.00000 10.00000 10.00000 90.00000 90.00000 90.00000
P 9.35414 9.35414 9.35414 85.90396 85.90396 85.90396
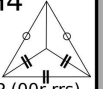P 8.66025 8.66025 8.66025 80.40593 80.40593 80.40593
P 7.90569 7.90569 7.90569 72.54240 72.54240 72.54240
P 7.07107 7.07107 7.07107 60.00000 60.00000 60.00000

Table 5. *The table of Delaunay (1932) describing the 24 Bravais types in* $\mathbf{S}^6$. *It has been redone removing the images of the Dirichlet cells, the not-reduced cells, and adding the "lattice character", which describes the linear manifold of each type. The crystal family types have been renamed to modern usage: Q changed to T for tetrahedral, K changed to C for cubic, and T changed to A for anorthic. Where Delone in some places included two types in one table cell, they have been split into two (for example: "M1" becomes "M1A" and "M1B"). Note that five types (O3, M3, M2B, A2, and A3) are not normal crystallographic types. They are boundary types, and they have fewer free parameters than the generic type requires. For instance, O3 (character: rs0 rs0) has only two free parameters (r and s), whereas an ordinary orthorhombic type requires three variables.*

	1	2	3	4	5
C	C1 cI (rrr rrr)		C3 cF (rr0 rr0)		C5 cP(000 rrr)
T	T1 tI (rrs rrs)	T2 tI (rr0 rrs)			T5 tP(000 rrs)
R	R1 hR (rrr sss)		R3 hR (rr0 sr0)		
O	O1A oF (rrs rrt)	O2 oI (rs0 srt)	O3 ∗ oI (rs0 rs0)	O4 oS (00r sst)	O5 oP (000 rst)
O	O1B oI (rst rst)				
M	M1A mC (rrs ttu)	M2A mC (rs0 stu)	M3 ∗ mC (rs0 ts0)	M4 mP (00r stu)	
M	M1B mC (rst rsu)	M2B ∗ mC (rs0 rst)			
A	A1 aP (rst uvw)	A2 ∗ aP (rs0 tuv)	A3 ∗ aP (rs0 tu0)		
H				H4 hP (00r rrs)	

∗ The right angles have no relationship to symmetry.

Table 6. *Roof/Niggli symbol, International Tables (IT) lattice character, Bravais lattice type, unsorted* $\mathbf{DC^7}$ *subspace, boundary polytope. Note that the variables r, s and t are non-negative, and u, v and w may be positive, negative or zero as constrained below.*

Roof/ Niggli Symbol	IT Lattice Char	Bravais Lattice Type	Unsorted DC^7 Subspace	Boundary Polytope
44A	3	**cP**	$(r, r, r, 2r, 2r, 2r, 3r)$	$12345 = 12\hat{3} = 12\hat{4} = 12\hat{5}$
44C	1	cF	$(r, r, r, r, r, r, 2r)$	12679ACD
44B	5	cI	$(r, r, r, 4r/3, 4r/3, 4r/3, r)$	$12F2'F' = 1\hat{2}\hat{F}$
45A	11	**tP**	$(r, r, t, r + t, r + t, 2r, 2r + t)$	$1345 = 1\hat{3} = 1\hat{4} = 1\hat{5}$
45B	21	**tP**	$(r, s, s, 2s, r + s, r + s, r + 2s$	$2345 = 2\hat{3} = 2\hat{4} = 2\hat{5}$
45D	6	tI	$(r, r, r, r - w/2, r - w/2, 2r + w, r),$ $-r \le w \le 0$	$12FF' = 12\hat{F}$
45D	7	tI	$[r, r, r, 2 * r + u, r - u/2, r - u/2, r],$ $-r \le u \le 0$	$12F2' = 1\hat{2}F$
45C	15	tI	$(r, r, t, t, t, 2r, t)$	158BF
45E	18	tI	$(r, s, s, -r/2 + 2s, s, s, -r/2 + 2s)$	$2ADA' = 2\hat{A}D$
48A	12	**hP**	$(r, r, t, r + t, r + t, r, r + t])$	134E
48B	22	**hP**	$(r, s, s, s, r + s, r + s, r + s)$	2458
49C	2	hR	$(r, r, r, 2r - u, 2r - u, 2r - u, 3r - u),$ $0 < u \le r$	$121'2' = \hat{1}\hat{2}$
49D	4	hR	$(r, r, r, 2r + u, 2r + u, 2r + u, 3r + 3u),$ $-r \le u \le 0$	$121'2' = \hat{1}\hat{2}$
49B	9	hR	$(r, r, t, t, t, r, r + t)$	1679ACD
49E	24	hR	$(r, s, s, s + r/3, s + r/3, s + r/3, s)$	$2F2'F' = \hat{2}\hat{F}$
50C	32	**oP**	$(r, s, t, s + t, r + t, r + s, r + s + t)$	$345 = \hat{3} = \hat{4} = \hat{5}$
50D	13	oC	$(r, r, t, r + t, r + t, 2r + w, 2r + t + w),$ $-r \le w \le 0$	134
50E	23	oC	$(r, s, s, u + 2 * s, s + r, s + r, u + 2 * s + r),$ $-s \le u \le 0$	245
50A	36	oC	$(r, s, t, s + t, t, r + s, s + t)$	35B
50B	38	oC	$(r, s, t, s + t, r + t, s, s + t)$	34E
50F	40	oC	$[r, s, t, t, r + t, r + s, r + t)$	458
51A	16	oF	$(r, r, s, r + s + u, r + s + u, -2u, s),$ $-r \le u \le 0$	$1F1' = \hat{1}F$
51B	26	oF	$(r, s, t, -r/2 + s + t, t, s, -r/2 + s + t)$	$ADA' = \hat{A}D$
52A	8	oI	$(r, r, r, 2r + u, 2r + v, -u - v, r),$ $-r \le u \le 0, -r \le v \le 0$	12F
52B	19	oI	$(r, s, s, 2s - u, s, s, -r + 2s + u),$ $0 < u \le r$	
			$(r, s, s, 2s - u, s, s, r + 2s - u),$ $r < u \le s$	$29C = 2AD$
52C	42	oI	$r, s, t, t, t, r + s, t$	58BF
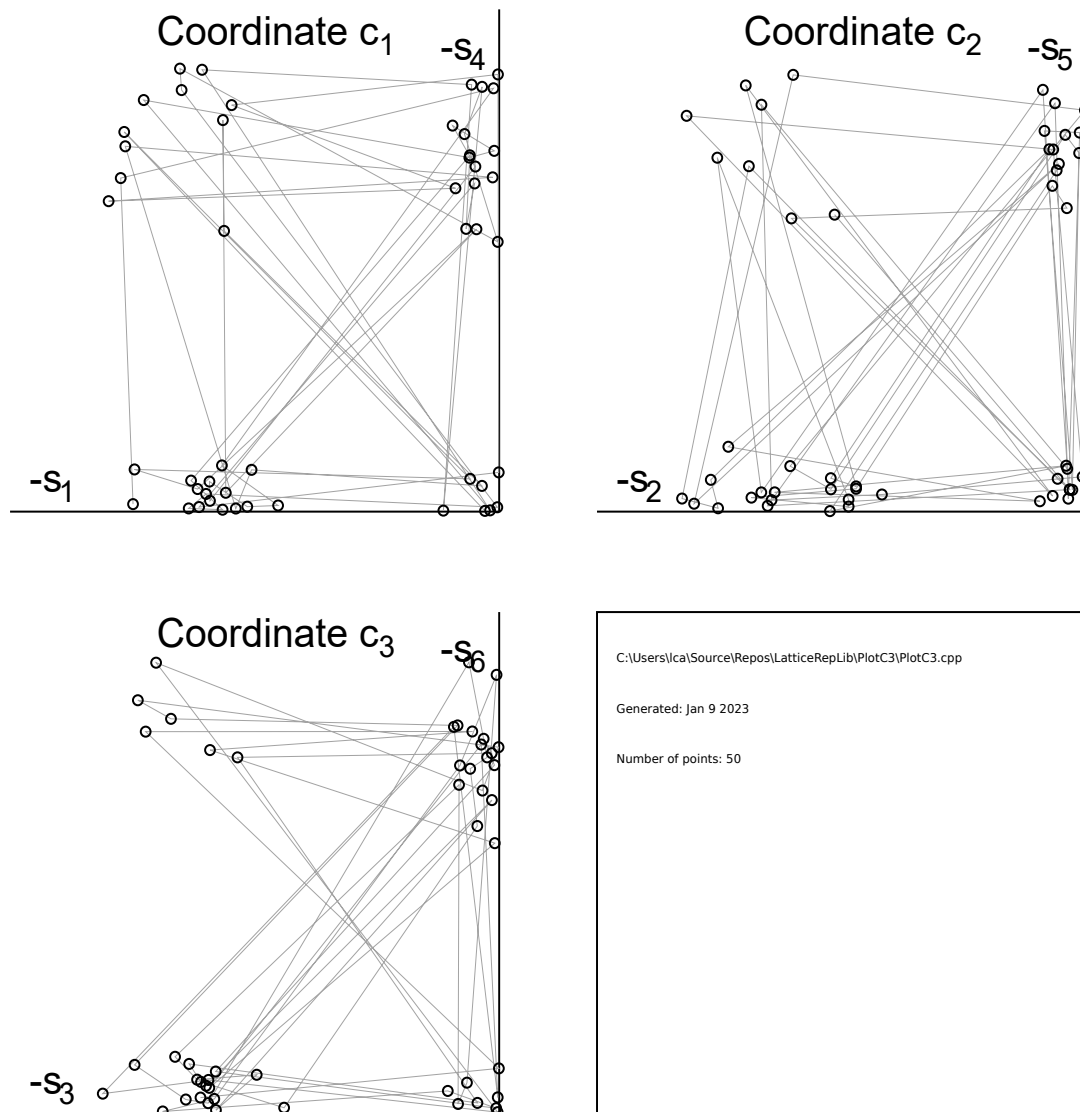
Fig. 1. Output of PlotC3

4. Availability of code

The C^{++} code is available in github.com, in `https://github.com/duck10/LatticeRepLib.git`.

Acknowledgements

Funding information

References

Andrews, L. C., Bernstein, H. J. & Sauter, N. K. (2019). <u>Acta Cryst.</u> A75. Https://doi.org/10.1107/S2053273318015413.

Delaunay, B. N. (1932). <u>Z. Krist.</u> 84, 109 − 149.

Synopsis

Selling reduction and Delone reduction are considered in a space of complex variables.