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Command line programs from LatticeRepLib

Lawrence C. Andrews[a]* and Herbert J. Bernstein[b]

[a]Ronin Institute, 9515 NE 137th St, Kirkland, WA, 98034-1820 USA, and [b]Ronin Institute, c/o NSLS-II, Brookhaven National Laboratory, Upton, NY, 11973 USA. E-mail: lawrence.andrews@ronininstitute.org

Abstract

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** (or **v** or **g6**) for $\mathbf{G^6}$ vectors
	d (or **d7**) for $\mathbf{D^7}$ vectors
	s (or s6) 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)
RANDOM: Random (valid) unit cell generated	
Crystal lattice input: "**A**", "**B**", "**C**", "**P**", "**R**", "**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*

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	$a, b, c, \alpha, \beta, \gamma$	Converts to the conventional unit cell representation.
CmdToDC	y	$\mathbf{D^{13}}$	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 $\mathbf{S^6}$
CmdGen	NA	$\mathbf{G^6}$	ngen - number of examples to generate (optional)	

			type	- lattice type to generate, many options (optional) 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	?	?	———	Clearly not working the way it should
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.
MultiMetricDists	y	mod	”Y/y”(optional)	Parameter Y/y for maxima style output
PlotC3	y	mod		Plot the three $\mathbf{C^3}$ coordinates
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).

Table 5. *The table of ? 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.

Q U P S T R	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** $\mathbf{DC^7}$ **Subspace**	**Bound- ary 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*	$(r, r, r, 4r/3, 4r/3, 4r/3, r)$	$12\mathrm{F}2'\mathrm{F}' = 1\hat{2}\hat{\mathrm{F}}$
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*	$(r, r, r, r - w/2, r - w/2, 2r + w, r)$, $-r \le w \le 0$	$12\mathrm{FF}' = 12\hat{\mathrm{F}}$
45D	7	*tI*	$[r, r, r, 2 * r + u, r - u/2, r - u/2, r]$, $-r \le u \le 0$	$12\mathrm{F}2' = 1\hat{2}\mathrm{F}$
45C	15	*tI*	$(r, r, t, t, t, 2r, t)$	158BF
45E	18	*tI*	$(r, s, s, -r/2 + 2s, s, s, -r/2 + 2s)$	$2\mathrm{ADA}' = 2\hat{A}\mathrm{D}$
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*	$(r, s, s, s + r/3, s + r/3, s + r/3, s)$	$2F2'\mathrm{F}' = \hat{2}\hat{\mathrm{F}}$
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*	$(r, r, s, r + s + u, r + s + u, -2u, s)$, $-r \le u \le 0$	$1\mathrm{F}1' = \hat{1}\mathrm{F}$
51B	26	*oF*	$(r, s, t, -r/2 + s + t, t, s, -r/2 + s + t)$	$\mathrm{ADA}' = \hat{A}\mathrm{D}$
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*	$(r, s, s, 2s - u, s, s, -r + 2s + u)$, $0 < u \le r$; $(r, s, s, 2s - u, s, s, r + 2s - u)$, $r < u \le s$	$29\mathrm{C} = 2\mathrm{AD}$
52C	42	*oI*	$r, s, t, t, t, r + s, t$	58BF

4. Availability of code

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

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Synopsis

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