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Approximate Lattice Matching in Three Dimensions

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Abstract

Given two unit cells, the problem of determining the best match of the lattice of one to the lattice of the other can require large numbers of trial transformations. We present a solution that requires only a limited number of trials.

1. Introduction

A relatively common crystallographic problem is to compare two unit cells and determine whether their lattices are the same or close to each other. Flor *et al.* (2016) have described a solution (COMPSTRU) for more symmetric crystal families. However, for the general case of monoclinic or triclinic lattices a different method is required.

Andrews *et al.* (2023) described a general solution, using the space \mathbf{S}^6 . While effective, this solution in a space based on projections fails to produce the 3D transformations needed for reindexing reflection data and for examining the relationships of structures.

To fill the need to the working crystallographer for transformations to reindex existing data or transform structural data to a new coordinate system, the need is for the 3-space transformations.

Mighell & Karen (1996) give a flow chart that partly encompasses the method here described, but no details are given there. Whereas their method relies completely on Niggli reduction, our method does not, only including Niggli reduction as part of the process. In addition, their description of the generation of alternative unit cells is quite brief, focusing on subcell and supercell transformations.

Attempts to solve the problem by trying a large number of trial transformations can require an unknown and unknowable number of trials of transformations. For closely similar lattices, the Niggli reduced cells are, in general, related by a small number of low-order lattice transformations. Here we describe a straight-forward approach that uses a fixed, modest number of trials and that gives multiple possible matches if they are near or identical to the best match.

2. Notation

\mathbf{P}^3 : Polar coordinate space. It is a compact and smooth alternative to lengths and angles. \mathbf{P}^3 is useful for comparing unit cells. \mathbf{P}^3 is defined as:

$$\mathbf{P}^3: (|\vec{a}|, \alpha), (|\vec{b}|, \beta), (|\vec{c}|, \gamma)$$

\Rightarrow

$$(|\vec{a}| \cos \alpha, |\vec{a}| \sin \alpha)$$

$$(|\vec{b}| \cos \beta, |\vec{b}| \sin \beta)$$

$$(|\vec{c}| \cos \gamma, |\vec{c}| \sin \gamma)$$

also known as (p_1, p_2, p_3)

3. Lattice matching

The general solution approach to matching two lattices has been to test the comparison using a large number of likely transformations. Two problems arise: how many trials to make and how to effectively measure the difference between two lattices.

To avoid the need to examine an unknown number of possible transformations, we propose an algorithm with the following stages. One of the input cells will be designated “reference” and the other (to which the transformations in stage three will be applied) will be designated “mobile”.

1. Convert from both (possibly) centered lattices to primitive. (Apply matrix M_{CR} for reference and M_{CM} for mobile.) (Aroyo, 2016)
2. Niggli reduce both lattices. (Apply matrix M_{NR} for reference and M_{NM} for mobile.)
3. Apply a limited set of transformations to mobile, measuring an agreement factor for each trial, keeping those that meet an acceptable agreement value. This stage creates matrix M_{MR} that transforms the modified mobile to the modified reference. (Niggli, 1928)
4. Compare the results of each transformation using the \mathbf{P}^3 Euclidean distance between the reference and the mobile cell. (Andrews & Bernstein, 2025)

3.1. Finishing

When all of the transformations in stage three have been examined, the group of accepted results needs to be processed. The group might be empty or might contain several possible valid results. We call this the “accepted group”.

In each stage, when a transformation is used, the corresponding matrix is saved for later use. The final transformation chain to convert mobile (in its original lattice

centering) to reference (in its original centering) is

$$M_{CM} * M_{NM} * M_{MR} * M_{NR}^{-1} * M_{CR}^{-1}.$$

This matrix chain needs to be computed for each member of the accepted group.

Of course, for a given reference/mobile pair, only M_{MR} is different for accepted trials.

The immediate question is “how many transformations will need to be tested in stage three”. We have chosen to use all the unimodular matrices (*i.e.* with determinant = 1.0), with elements -1, 0, +1. (Direct computation shows that there are 3480 such matrices.) Each transformation is tested and acceptable results are accumulated to be “finished”.

There is an infinite number of unimodular matrices, corresponding to the fact that for a given lattice, there is an infinite number of possible choices of unit cell. However, the mathematical group that describes the unimodular matrices has a small basis set that by iteration can create the complete, infinite set. In principle, that small set (6: identity, x,y,z unit translations, and 2 axis exchanges) would need to be used iteratively to unknown depth to solve the current problem. We have chosen a modest set that is large enough to create a strong algorithm. It includes all of the simple unit translations and lattice vector exchanges; see Figure 1.

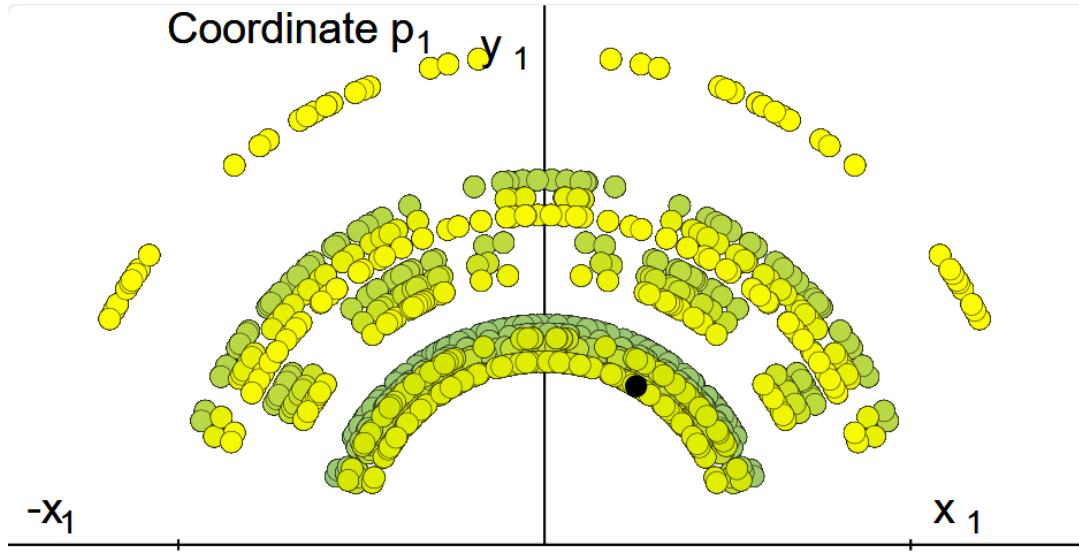


Fig. 1. Graph of (a, α) as coordinate p_1 of P^3 representation (Andrews & Bernstein, 2025) with the initial point shown in black. The initial point has been transformed by the 3480 unimodular matrices described in the text. Many of the generated points are hidden by the symmetry of generation.

4. Examples

4.1. example 1

More than one acceptable match was found

Test input

p 5.17 3.18 7.74 90. 104.5 90. (reference)

p 30.9616 3.1800 8.1608 90.00 171.18 90.00 (mobile)

```

Result of matching
--- Match 1 ---
Quality: EXCELLENT P3 Distance 0.000)

Transformation Matrix:
[ 1.0000,  0.0000,  4.0000]
[ 0.0000,  1.0000,  0.0000]
[ -1.0000,  0.0000, -3.0000]
Matrix determinant: 1.0000
Reference cell: P      5.170      3.180      7.740     90.000    104.500    90.000
Transformed cell: P      5.170      3.180      7.740     90.000    104.500    90.000

```

```
*** SUCCESS: Excellent match within P3-relative threshold ***

--- Match 2 ---
Quality: EXCELLENT (P3 Distance 0.000)

Transformation Matrix:
[ -1.0000,   0.0000,  -4.0000]
[  0.0000,   1.0000,   0.0000]
[  1.0000,   0.0000,   3.0000]
Matrix determinant: 1.0000
Reference cell: P      5.170     3.180     7.740    90.000   104.500   90.000
Transformed cell: P      5.170     3.180     7.740    90.000   104.500   90.000
*** SUCCESS: Excellent match within P3-relative threshold ***
```

4.2. example 2

Test input:

C 12.770 21.235 14.411 136.017 84.071 111.795 (reference)

F 33.151 18.241 20.218 83.054 144.781 120.639 (mobile)

```
==== LATTICE MATCHING RESULTS === =====
Found 1 excellent match
Success threshold: 1.43e-01 (Fixed strict)

--- Match 1 ---
Quality: EXCELLENT (0.000 )
P3 Distance: 0.000
S6 Angle: 0.00
Transformation Matrix:
[  0.0000,  -0.5000,   0.5000]
[  1.0000,   0.5000,   0.5000]
[  0.0000,   0.5000,   0.5000]
Matrix determinant: 0.5000
Reference cell: C      12.770     21.235     14.411    136.017    84.071    111.795
Transformed cell: C      12.770     21.235     14.411    136.017    84.071    111.795
*** SUCCESS: Excellent match within P3-relative threshold ***
```

4.3. example 3

A case where more than one accepted match was found. (Personal communication: Simmons (2025).)

Input:

p 10.25 10.74 21.08 87.72 75.97 61.53 (reference)

p 10.25 10.74 21.08 78.96 75.97 61.49 (mobile)

```

--- Match 1 ---
Quality: EXCELLENT (0.010 )
P3 Distance: 0.010
S6 Angle: 0.01
Transformation Matrix:
[ -1.0000,  0.0000,  0.0000]
[ -1.0000,  1.0000,  0.0000]
[  0.0000,  0.0000, -1.0000]
Matrix determinant: 1.0000
    Reference cell      p    10.25     10.74     21.08     87.72     75.97     61.53 (reference)
    Transformed cell: P    10.250    10.739    21.080    87.714    75.970    61.502
*** SUCCESS: Excellent match within P3-relative threshold ***

--- Match 2 ---
Quality: EXCELLENT (0.023 )
P3 Distance: 0.023
S6 Angle: 0.03
Transformation Matrix:
[ -1.0000,  0.0000,  0.0000]
[  0.0000, -1.0000,  0.0000]
[ -1.0000,  0.0000,  1.0000]
Matrix determinant: 1.0000
    Reference cell      p    10.25     10.74     21.08     87.72     75.97     61.53 (reference)
    Transformed cell: P    10.250    10.740    21.087    87.674    75.893    61.490
*** SUCCESS: Excellent match within P3-relative threshold ***

```

4.4. example 4

Twenty slight variations of a primitive cubic unit cell ($a = 10.0$), expressed in \mathbf{S}^6 , were generated by adding random orthogonal perturbation vectors to the original \mathbf{S}^6 representation. Each perturbation had a length of 0.001 times the \mathbf{S}^6 norm of the cubic cell and was added to the vector $[0, 0, 0, -100, -100, -100]$. The resulting \mathbf{S}^6 vectors were then converted back to unit cell parameters. The modified vectors were lattice-matched to the reference, which is the first entry.

Input:

P	10.000	10.000	10.000	90.000	90.000	90.000	Reference
P	9.994	9.992	9.988	89.958	89.937	89.957	
P	10.002	10.003	9.996	89.957	90.036	90.011	
P	9.996	9.992	9.993	89.994	89.950	89.946	

P	9.990	9.999	10.005	90.058	89.971	89.938
P	9.997	9.999	9.998	90.051	89.949	89.967
P	9.996	9.998	9.990	89.966	89.916	90.033
P	10.002	9.993	9.996	89.980	90.028	89.940
P	10.002	9.992	9.988	89.931	89.977	89.993
P	9.991	9.992	9.991	89.934	89.936	89.982
P	10.002	9.998	10.012	90.030	90.042	89.996
P	10.003	9.990	10.002	89.972	90.061	89.941
P	9.993	10.006	9.992	90.023	89.935	89.995
P	10.002	10.002	10.002	89.968	90.004	90.067
P	10.003	10.010	9.996	90.010	89.956	90.087
P	9.992	10.003	9.994	89.979	89.974	89.983
P	9.999	9.995	9.988	89.934	89.937	90.025
P	10.003	9.990	10.000	89.942	90.012	90.007
P	10.012	9.998	10.002	90.002	90.049	90.023
P	10.008	10.002	10.002	90.012	90.068	89.989
P	9.989	9.996	9.998	89.970	89.993	89.943

and here are the matching results:

Most common transformation matrices:

```
[[-1,0,0,0,-1,0,0,0,1] : 3 mobiles (EXCELLENT, 0.019)
[1,0,0,0,-1,0,0,0,-1] : 2 mobiles (EXCELLENT, 0.013)
[0,0,-1,0,-1,0,-1,0,0]: 2 mobiles (EXCELLENT, 0.022)
[0,-1,0,-1,0,0,0,0,-1]: 2 mobiles (EXCELLENT, 0.020)
[-1,0,0,0,1,0,0,0,-1] : 2 mobiles (EXCELLENT, 0.014)
[-1,0,0,0,0,-1,0,-1,0]: 2 mobiles (EXCELLENT, 0.022)
[1,0,0,0,1,0,0,0,1]   : 1 mobiles (EXCELLENT, 0.016)
[0,1,0,1,0,0,0,0,-1]   : 1 mobiles (EXCELLENT, 0.015)
[0,1,0,0,0,1,1,0,0]   : 1 mobiles (EXCELLENT, 0.017)
[0,1,0,-1,0,0,0,0,1]   : 1 mobiles (EXCELLENT, 0.016)
```

==== BEST MATCH DETAILS ===

Mobile 2: 1.13e-02 (EXCELLENT)

Matrix: [0 0 -1 1 0 0 0 -1 0]

Transformed: 9.996 10.002 10.003 89.989 89.957 89.964

Mobile 15: 1.23e-02 (EXCELLENT)

Matrix: [-1 0 0 0 0 -1 0 -1 0]

Transformed: 9.992 9.994 10.003 89.979 89.983 89.974

Mobile 13: 1.34e-02 (EXCELLENT)

Matrix: [1 0 0 0 -1 0 0 0 -1]

Transformed: 10.002 10.002 10.002 89.968 89.996 89.933

4.5. Example 5

Two reported polymorphic forms of triphenylphosphine oxide hemihydrate, C₁₈H₁₅

PO·0.5H₂O. (Mighell, 2011)

F 19.794 32.54 9.459 90 90 90

```

C 9.4313 32.193 10.8435 90 115.742 90
end

==== PROCESSING INPUT LIST ====
Total results before processing: 500
NC Distance: 6.44756
Range: 4.34e-01 to 6.61e+01
Reference P3 norm: 39.244
Method: Fixed strict
Thresholds:
EXCELLENT <= 1.96e-01 (0.5% of P3)
GOOD      <= 7.85e-01 (2.0% of P3)
POOR      <= 3.14e+00 (8.0% of P3)

==== LATTICE MATCHING RESULTS === =====
Found 2 good matches
Success threshold: 1.96e-01 (Fixed strict)

--- Match 1 ---
Quality: GOOD (0.434 )
P3 Distance: 0.434
S6 Angle: 0.12 degrees
Transformation Matrix:
[ -1.0000,  0.0000, -2.0000]
[ 0.0000, -1.0000,  0.0000]
[ -1.0000,  0.0000,  0.0000]
Matrix determinant: 2.0000
Transformed cell: F    19.535    32.193    9.431    90.000    89.964    90.000
*** SUCCESS: Good match within P3-relative threshold ***

--- Match 2 ---
Quality: GOOD (0.434 )
P3 Distance: 0.434
S6 Angle: 0.12 degrees
Transformation Matrix:
[ 1.0000,  0.0000,  2.0000]
[ 0.0000, -1.0000,  0.0000]
[ 1.0000,  0.0000,  0.0000]
Matrix determinant: 2.0000
Transformed cell: F    19.535    32.193    9.431    90.000    89.964    90.000
*** SUCCESS: Good match within P3-relative threshold ***

```

5. Limitations

The group of all unimodular matrices is an infinite group. Clearly, by limiting this algorithm to matrices with elements -1/0/+1, a complete search cannot be done. However as the examples show, in common cases, the algorithm is effective. One limitation is obvious: if one axial length of the reduced cell is longer than the sum

of the other two axial lengths, then $-1/0/+1$ cannot explore some regions that are available for shorter axial lengths. For instance, if one axis is much longer than the others, then in a matrix for that long axis, the column elements for that axis cannot have more than one element $-1/+1$. Similar arguments apply to the case of a very short axis. In order to treat these more extreme cases using this algorithm, a larger range of element values would need to be examined. The consequence is that the number of matrices and thus the number of trials grows rapidly.

6. Summary

Lattice matching based on unit cell parameters and 3-dimensional transformation matrices is described, including the production of the matrices for transforming unit cell base vectors from a probe's to those of a reference cell.

The described algorithm (CmdLMP3) on a modest laptop computer matched 100 cases in 5 seconds.

7. Availability of code

The code for Lattice Matching (CmdLMP3) and related software tools is available in [github.com](https://github.com/duck10/LatticeRepLib.git), in <https://github.com/duck10/LatticeRepLib.git>. The program CmdLMP3 uses the required files.

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8. Synopsis

A solution is proposed for the problem of best matching the lattices of unit cells that are described in different presentations along with the 3D matrix that defines the relationship between matched lattices.

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