CARAT Manual

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I Introduction to CARAT

Please note that CARAT was developed for crystallographic groups in dimensions up to 6. Most algorithms also work in higher dimensions. However, integer overflow is not trapped in general.

II The structure of relevant files

There are two file types related to CARAT, matrix_TYP and bravais_TYP. Both of them consist of a set of matrices, combined in different ways. Firstly we describe the format of matrices which CARAT is able to read.

II.1 Format of a single matrix in CARAT

A matrix in a CARAT file is represented by a headline which gives information about the dimension of the matrix and the body, which carries the entries of the matrix in question.

The headline has the format

```
NxM   % comment
```

for a matrix which has N rows and N columns. All characters in this line behind % are ignored. There are some abbreviations allowed, and these are N for NxN, Nd0 for an $N \times N$ scalar matrix, Nd1 for an $N \times N$ diagonal matrix, and Nx0 for an $N \times N$ symmetric matrix.

The body consists of the entries of the matrix. Two numbers are separated by any combination of spaces, newlines or tabulators.

For simplicity of the description a couple of examples are given, the left side of these discribing the input, and the right hand side stating it's meaning.

```
3x2  % this will be ignored
1 2
3 4
5 6
```

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix}$$

```
3
1 2 3
4 5 6
7 8 9
```

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

```
3d1 % and also this
1 -1 2
```

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

```
2d0
4
```

$$\begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}$$

All files which are read by CARAT programs consist of a sequence of one or more of these matrices, sometimes with a header line describing to meaning of all these matrices (see below).

II.2 matrix_TYP

Some programs in CARAT will read/output more than one matrix. Therefore we created a file type which is called matrix_TYP and describes a sequence of matrices.

Files of this type will simply begin with $\sharp N$, where N is the number of matrices in the file. If CARAT reads such a file, it will read exactly N matrices and will ignore the rest of the file.

Now we give an example of a file consisting of 3 matrices of dimension 4 which generate a bravais group of Order 384 (which is isomorphic to $C_2 \wr S_4$).

```
#3
4 % generator
 -1 0 0 0
  0 1 0 0
  0 0 1 0
  0 0 0 1
4 % generator
 0 1 0 0
 1 0 0 0
 0 0 1 0
 0 0 0 1
4 % generator
 1 0 0 0
 0 0 0 1
 0 1 0 0
 0 0 1 0
```

II.3 bravais_TYP

Sometimes it is convenient not only to give matrices which generate a group, but feed programs more information, ie. the order of the group, it's normalizer in $GL_n(\mathbb{Z})$.

Therefore the header line of a file of bravais_TYP takes the following form:

```
\sharp gN\ fM\ zO\ nP\ cQ
```

This will cause programs to read $N + M + O + P + Q$ matrices, and interpret the first N matrices as those generating the group, the next M to be a $\mathbb{Z}$-basis of the form space, O matrices representing "centerings", P matrices which form a generating set for the normalizer (in $GL_n(\mathbb{Z})$) modulo the group, and finally Q matrices which generated it's centralizer (again in $GL_n(\mathbb{Z})$).

It is possible to omit one or more of these letter, which will cause programs to think that the described components are not know.

Here are some legal header lines given

```
#g2 f2 n3
```

```
#g2 n4
```

```
#g2 n4
```

Note: Although it is possible to omit components, it is NOT possible to switch them.

The end of a bravais_TYP file states the order of the group. This component is also optional, and takes the following form:

$$p_1^{n_1} \ * \ p_2^n 2 \ \ldots \ * p_m^{n_m} = N\%$$

where $\prod_i p_i^{m_i} = N$ is the order of the described group.

II.4 A format for finitely presented Groups

Some programs we need or generate a presentation for a finite group. CARAT reads them in form of a matrix, which will be interpreted in the following way:

- The biggest entry in modulus is the number of generators of the free group.
- Each ROW of the matrix represents a relation, ie. a word in the generators of the free group. A word $w = x_{i_1}^{\epsilon_1} \cdot x_{i_2}^{\epsilon_2} \cdots x_{i_n}^{\epsilon_n}$ with $\epsilon_j \in \{-1, 1\}$ translate into a row of the matrix by $\epsilon_1 i_1 \ espilon_2 i_2 \ \ldots \ \epsilon_n i_n$.

Again we just give two examples for CARAT presentations (which both are presentations for the A_5).

```
3x10
1 1 0 0 0 0 0 0 0 0
2 2 2 0 0 0 0 0 0 0
1 2 1 2 1 2 1 2 1 2
```

Meaning:

$$\langle x_1, x_2 | x_1 \cdot x_1 = 1, \ x_2 \cdot x_2 \cdot x_2 = 1, \ x_1 \cdot x_2 \cdots x_1 \cdot x_2 = (x_1 \cdot x_2)^5 = 1 \rangle$$

```
3x10
```

III CARAT programmers guide

IV Standalones

IV.1 Bravais_inclusions