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BilKristal 2.0: A tool for pattern information extraction from crystal structures

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ABSTRACT

We present a revised version of the *BilKristal* tool of Okuyan et al. (2007). We converted the development environment into Microsoft Visual Studio 2005 in order to resolve compatibility issues. We added multi-core CPU support and improvements are made to graphics functions in order to improve performance. Discovered bugs are fixed and exporting functionality to a material visualization tool is added.

New version program summary

Program title: BilKristal 2.0.
Catalogue identifier: ADYU_v2_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADYU_v2_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 364263
No. of bytes in distributed program, including test data, etc.: 9135815
Distribution format: tar.gz
Programming language: C, C++, Microsoft.NET Framework 2.0 and OpenGL Libraries.
Computer: Personal computer with Windows operating system.
Operating system: Windows XP or higher.
Has the code been vectorized or parallelized?: Multi-core CPU support included.
RAM: 20–60 Megabytes.
Catalogue identifier of previous version: ADYU_v1_0
Journal reference of previous version: Comput. Phys. Comm. 176 (2007) 486
Classification: 8.
External routines: Microsoft.NET Framework 2.0. For the visualization tool, the graphics card driver should also support OpenGL.
Does the new version supercede the previous version?: Yes
Nature of problem:
    Determining the crystal structure parameters of a material is a very important issue in crystallography. Knowing the crystal structure parameters helps the understanding of the physical behavior of a material. For complex structures, particularly for materials which also contain local symmetry as well as global symmetry, obtaining crystal parameters can be very hard.
Solution method:
    The tool extracts crystal parameters such as primitive vectors and basis vectors and identifies the space group from the atomic coordinates of crystal structures.
Reasons for new version:
    Additional features, resolved compatibility issues with the new development environments, performance optimizations, minor bug corrections.
Summary of revisions:

- Capability to export to MaterialVis tool [1] is added. The tool can export the unit cell information extracted from the crystal structure, the raw atomic coordinates and atomic radii into a data file (.dat) that the MaterialVis tool can process.

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- Compatibility issues with Microsoft Visual Studio 2005 up to 2010 are resolved. The original code was developed using Microsoft Visual Studio 2003. However, newer Visual Studio versions were not able to convert and compile the code. Due to the changes in the .NET framework, the converted project produced many errors. In this work, the project is converted into a Visual Studio 2005 project and compilation errors are resolved. We also tested the code with Visual Studio 2010 and the project was successfully converted and compiled.
- Multi-Core CPU support is added. In recent years, multi-core CPUs have become very common. We added the multi-core CPU support in order to utilize the computational capabilities of additional CPU cores. This significantly improves the performance.
- The visualization interface is improved. In particular, the sphere drawing functionality is replaced with an efficient and high quality version that utilizes GPU acceleration.
- For some cases, the fractional coordinates of some of the calculated basis vectors were not all in the $[0, 1)$ range, but at coordinate 1.0 for some axes. These cases were corrected by translating these basis vectors into the $[0, 1)$ range.

Restrictions:

Assumptions are explained in [2]. However, none of them can be considered as a restriction on the complexity of the problem.

Running time:

The tool was able to process input files with more than a million atoms in less than 20 s on a PC with an Athlon quad-core CPU at 3.2 GHz using the default parameter values.

References:

[1] Erhan Okuyan, Ugur Güdükbay, MaterialVis: Crystal and Amorphous Material Visualization Tool Using Direct Volume and Surface Rendering Techniques (Program Summary), Computer Physics Communications, Submitted.

[2] Erhan Okuyan, Ugur Güdükbay, and Oguz Gülseren, Pattern Information Extraction from Crystal Structures, Computer Physics Communications, 176 (2007) 486.