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MDASH: a multi-core-enabled program for structure solution from powder diffraction data

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The simulated annealing approach to structure solution from powder diffraction data, as implemented in the *DASH* program, is easily amenable to parallelization at the individual run level. Modest increases in speed of execution can therefore be achieved by executing individual *DASH* runs on the individual cores of CPUs.

1. Introduction

DASH (David *et al.*, 2006), a computer program for structure solution from powder diffraction data, which has recently been adapted to run on distributed computing systems, can also be run efficiently on a single computer having more than one CPU, or (as is increasingly common) a single computer containing a CPU with multiple cores.

2. *MDASH* overview

MDASH is a graphical user interface (GUI) driven program that takes, as input, files generated using *DASH* and controls their execution on a single standalone PC. Full details of this file generation and subsequent execution by *DASH* are given in a paper describing *GDASH* (Griffin *et al.*, 2009), and only program aspects that are specific to *MDASH* are discussed here.

3. Program description

3.1. Running jobs using *MDASH*

On running *MDASH*, a user selects a .grd file generated previously using *DASH*, whereupon *MDASH* displays a summary of the job (Fig. 1). Pressing the 'Start' button will commence the job. *DASH* is invoked by *MDASH* with an execution priority of 'below normal' and all detected CPU cores are used, although these settings can be configured by the user. *MDASH* constantly monitors and displays job progress, and by default, when a job is complete, *MDASH* invokes the normal GUI version of *DASH* to display the results.

4. *DASH* program performance when invoked using *MDASH*

The performance of *MDASH* running on a PC equipped with a 2.4 GHz Core2Quad CPU and a PC equipped with dual quadcore Xeon 2.5 GHz CPUs has been evaluated using the moderately challenging optimization problem of solving the crystal structure of famotidine form B (Shankland *et al.*, 2002; $P2_1/c$, $V = 1421$ Å^3, $Z' = 1$, 13 degrees-of-freedom, 1.64 Å resolution) from synchrotron X-ray powder diffraction data. In order to generate easily measurable execution times, the total number of simulated annealing (SA) moves per run was set to 1×10^7, about a factor of ten higher than is actually necessary to solve the structure. The results are summarized in Table 1 and show essentially linear scaling with the number of available cores.

5. Software and hardware environment

MDASH itself runs under MS Windows XP (SP2) and MS Windows Vista and requires the MS .Net 2.0 Framework (or higher) to be installed; this is present by default in XP SP2 and Vista. No installer is required; one simply places the MDASH.EXE file in a convenient location and creates a shortcut to it if desired. Although *MDASH* itself has very modest memory requirements, given that the program invokes multiple copies of the *DASH* executable, it is desirable to have as much memory as possible installed on the PC on which it is running. The exact amount required depends upon the size of the problem being studied with *DASH*, but as a general rule, we would recommend at least 2 GB RAM for a quadcore PC and at least 4 GB RAM for a dual quadcore setup.

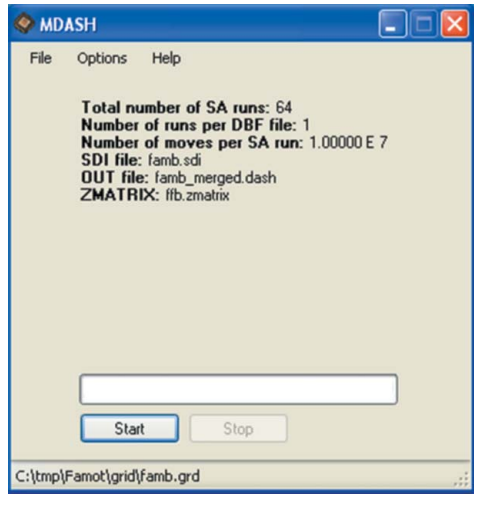

Figure 1
The main *MDASH* window, showing the parameters and files for a *DASH* job.

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5.1. Prerequisites

In order to deploy *MDASH* correctly, *DASH* Version 3.1 or higher must be installed on the PC on which *MDASH* is installed. Note that a site licence is not necessary in order to have more than one copy of the *DASH* executable running on a standalone PC.

6. Documentation and availability

The *MDASH* executable is supplied as an 'unsupported extra' in the *DASH* Version 3.1 software distribution available from the Cambridge Crystallographic Data Centre. Whilst *MDASH* itself does not require a licence, it does require a licenced copy of *DASH* in order to operate.

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Table 1
MDASH performance on a test SA job under different conditions.

	Single PC	Single PC	Single PC
DASH 3.1 mode	GUI	*MDASH*	*MDASH*
Number of SA runs	16	16	16
Number of CPUs	1	1	2
CPU architecture	Core2Quad	Core2Quad	Xeon E5420
Number of cores utilized	1	4	8
CPU speed	2.4 GHz	2.4 GHz	2.5 GHz
Total elapsed time	126 min	28 min	12 min
Relative speed rating	1	4.5	10.5

References

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