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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  
extension 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; P2₁/c, V = 1421 Å³, 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 x 10⁷, 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.

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Germany.
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.

We are grateful to Elna Pidcock and Wei Dong of the CCDC, and to Alastair Florence and Norman Shankland of the University of Strathclyde, for their help in testing and validating GDASH.

Table 1

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<th>Single PC</th>
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<td>DASH 3.1 mode</td>
<td>GUI</td>
<td>MDASH</td>
<td>MDASH</td>
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<tr>
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<td>16</td>
<td>16</td>
</tr>
<tr>
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<td>2</td>
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References