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# REAL TIME VISUALIZATION OF QUANTUM MOLECULAR DYNAMICS

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# Real Time Visualization of Quantum Molecular Dynamics

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This demonstration displays results of a Quantum Molecular Dynamics (QMD) simulation of the metal cluster $Li_6$ running on the Intel[1] Touchstone Delta at Caltech.

**Usage**

1) To run remotely on the Intel Touchstone Delta at Caltech

cd QMD

go to step 3)

2) To run locally (e.g. if the Delta/network is down)

cd QMD_local

3) Start AVS and enter the QMD application

avs (if you are using a remote X display use the -nohw flag)
click on the 'Applications' button
click on the 'QMD' button

4) Select the desired number of processors by typing with the cursor in the 'No. of processors' value field in the left window. On the Delta this is forced to the range 4-128. On the local IBM RS6000 it can only be one.

5) Click on the 'Start' button to go. A more detailed description of the demo is in the bottom left text window. If all is well, another window will appear; position this by clicking the left mouse button up against the middle of the left-hand border of the screen.

6) If the demo completes successfully, you may keep repeating steps 4) and 5). In case of error you will have to exit from the application after accepting the error condition (click on accept in the dialog box).

7) To exit, click 'exit' at the top of the left-hand window, click 'Return to Main Menu', click 'Exit', click 'Yes'.

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[1] Intel is a registered trademark of the Intel Corporation

## Detailed Description

When the demo (an AVS[2] application) is started, a process is created on the Delta using rsh. This process pipes back five sets of information during each MD step:

1) The electronic density is displayed using an iso-surface.

2) The potential energy is graphed.

3) A simple performance model is used to predict the number of MD steps taken using different numbers of processors.

4) Execution at the module level is traced.

5) Standard output is sent to the terminal window.

## Theory

The simulation uses an all-electron *ab initio* closed-shell spin-restricted Hartree-Fock wavefunction in a 3s1p atomic basis of contracted gaussians. At each time step all unique 2-electron integrals are computed and stored (distributed) in memory for subsequent processing in the Self-Consistent Field calculation. Forces on the nuclei are computed using analytic derivatives. A time step of 0.5 femto-seconds is used to propagate the classical nuclei on the Born-Oppenheimer electronic potential energy surface.

## Parallel Performance

One MD time step takes 1.2 seconds on 128 processors. A performance analysis shows that the execution time beyond 16 processors is dominated by the extensively-tuned matrix transformations (notably diagonalization). On this small system it is not possible to parallelize the diagonalization effectively due to communication latency.

This code is a prototype. The sequential version of this program was developed by the Berlin group, starting from the GAMESS-UK quantum chemistry package. Guest ported the code to the Intel iPSC. Harrison and Fantucci ported the code to the Delta and performed extensive restructuring and optimization. Harrison and Thornton implemented the graphics.

## Acknowledgments

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[2] AVS is a registered trademark of Advanced Visual Systems Inc.

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