This work supported by the Robert A. Welch Foundation.

Patrick J. Nichols and Thomas L. Gibson
Texas Tech University

An Affordable Concurrent Approach
to Positron Polarization Potentials
I. This work supported by the Robert A. Welch Foundation.

Some comparative results.

made available for download over the Internet. We will present details of our work along with potentials within the Distributed Position Model being converted to parallel form and will be part of Project. Our modified quantum chemistry codes for Generalized Position-Molecule Interaction and standard message-passing routines for this system are available for free from the Downt.

standard memory, hard drives, and fast Ethernet cards. The operating system software, compilers,

will be constructed from commodity PC-class components, such as Intel Celeron Processors with purchasing and installing a high-performance, parallel computer for less than $15,000. The system

low-energy position-matter collisions to larger target molecules, we are in the process of

NICHOLS and THOMAS L. GIBSON, Texas Tech University — In order to extend our work on

An Affordable Concurrent Approach to Position Polarization Potential s PATRICK J.

Abstract for DAMOP 2000
Bigger Systems ↔ More I/O

Bigger Systems ↔ More Memory

(TTU)

- Time to compute \( \Lambda^d \) for SF: 125 days (estimated)
- Time to compute \( \Lambda^d \) for AR: 12 minutes (serial code)

Bigger Systems ↔ More CPU Time

Motivation
TTU

No Sharing Required

Configuration Optimized for Problem

- Local Control
- Standard Software Available for Free
- Very Affordable Hardware
- I/O: Distributed Across Multiple Nodes
- Memory: Gigabytes
- Performance: 100s to 1000s of Megahops

Beverly Cluster

Solution
—Donald Becker

What is a Beowulf Cluster?

Beowulf clusters

system.

a high-bandwidth internet network, and the Linux operating
clustered workstations based on commodity PC-class hardware,
Beowulf is a project to produce the software for off-the-shelf
Our Bow2fly Cluster—Camera
- 1 100 base-T 24-port switch
- 64 GiBabytes aggregate disk
- 4 GiBabytes aggregate ram
- 16 machines

Camera Hardware
Camera Node Hardware

- Netgear PA310 TX 100 Base-T NIC
- 4.3 Megabyte disk
- 256 Megabyte RAM
- 500 Megahertz Intel Celeron
PETLIB
PATMOL
ATLAS Optimized BLAS
ASCI-Red Optimized BLAS
GCC 2.95
PVM 3.0
LAM MPI 6.3
Linux Mandrake 7.0

Camera Software
TTU
<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>\textbullet Total</td>
<td>-</td>
</tr>
<tr>
<td>All software</td>
<td>$0</td>
</tr>
<tr>
<td>\textbullet Software</td>
<td></td>
</tr>
<tr>
<td>Shelving rack</td>
<td>$80</td>
</tr>
<tr>
<td>Network cards, switch, &amp; cables</td>
<td>$1,129</td>
</tr>
<tr>
<td>4 Gigabytes ram</td>
<td>$33280</td>
</tr>
<tr>
<td>16 Emachines</td>
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<tr>
<td>\textbullet Hardware</td>
<td></td>
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<tr>
<td>Camera Costs</td>
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</table>
Calculations of the ground state energy of CO₂ using a 10sp5pd/5sp3pd basis.

<table>
<thead>
<tr>
<th>Energy</th>
<th>SCI Origin 2000</th>
<th>Execution Time (seconds)</th>
<th># Processors</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.2</td>
<td>16</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.2</td>
<td>12</td>
<td></td>
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</tr>
<tr>
<td>10.8</td>
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<td></td>
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</tr>
<tr>
<td>13.8</td>
<td>6</td>
<td></td>
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</tr>
<tr>
<td>18.0</td>
<td>4</td>
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</tr>
<tr>
<td>25.0</td>
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<td>30.7</td>
<td>2</td>
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<tr>
<td>41.0</td>
<td></td>
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</tr>
<tr>
<td>70.6</td>
<td>1</td>
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</tr>
<tr>
<td>77.3</td>
<td></td>
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</tbody>
</table>
Calculations of the Sf6 ground state energy and two points of the polarization potential for $e^{-}\text{Sp}_6$. 

<table>
<thead>
<tr>
<th>Camera</th>
<th>Execution Time (minutes)</th>
<th># Processors</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 (MPI)</td>
<td>16</td>
<td>1</td>
</tr>
<tr>
<td>222 (Serial)</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>
Ground State Energy

CO$_2$ Ground State Energy

Parallel efficiency (%)

# of processors

Results

Gamera

DH11s7p2d/6s5p2d Basis
Polarization Potential (Hartrees)

Distance from COM (bohr)

S-F axis

\( \theta = 0 \), \( \phi = 45^\circ \)

\( \theta = 53.7^\circ \), \( \phi = 45^\circ \)

\( \theta = 53.7^\circ \), \( \phi = 15^\circ \)

Polarization Potential

S-F axis

Results
TTU

We are grateful for support from the Robert A. Welch Foundation.

- Compatible
- Open source software and scientific applications are available now

Conclusions