An Affordable Concurrent Approach to Positron Polarization Potentials

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

This work supported by the **Robert A. Welch Foundation**.

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Abstract for DAMOP 2000

An Affordable Concurrent Approach to Positron Polarization Potentials[1] PATRICK J. NICHOLS and THOMAS L. GIBSON, Texas Tech University — In order to extend our work on low-energy positron-matter collisions to larger target molecules, we are in the process of purchasing and installing a high-performance, parallel computer for less than $15,000. The system will be constructed from commodity PC-class components, such as Intel Celeron Processors with standard memory, hard drives, and fast ethernet cards. The operating system software, compilers, and standard message-passing routines for this system are available for free from the Beowulf Project. Our modified quantum chemistry codes for generating positron-molecule interaction potentials within the Distributed Positron Model are being converted to parallel form and will be made available for download over the internet. We will present details of our work along with some comparative results.

[1] This work supported by the Robert A. Welch Foundation.

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Motivation

- **Bigger Systems $\Longrightarrow$ More CPU Time**
  - Time to compute V_{pol} for Ar: 12 minutes (serial code)
  - Time to compute V_{pol} for SF_6: 125 days (estimated)
- **Bigger Systems $\Longrightarrow$ More Memory**
- **Bigger Systems $\Longrightarrow$ More I/O**

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Solution

- **Beowulf Cluster**
  - Performance: 100's to 1000's of Megaflops
  - Memory: Gigabytes
  - I/O: Distributed Across Multiple Nodes
  - **Very** Affordable Hardware
  - Standard Software Available for Free
  - Local Control
    - Configuration Optimized for Problem
    - No Sharing Required

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Beowulf Clusters

What is a Beowulf Cluster?

> Beowulf is a project to produce the software for off-the-shelf clustered workstations based on commodity PC-class hardware, a high-bandwidth internal network, and the Linux operating system.
>
> —*Donald Becker*

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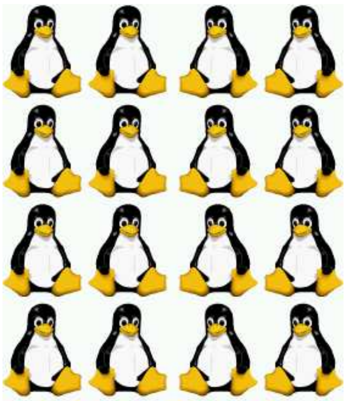
Our Beowulf Cluster—Gamera



$$\Rightarrow$$

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Gamera Hardware

- 16 *e*machines
- 4 Gigabytes aggregate ram
- 64 Gigabytes aggregate disk
- 1 100 base-T 24-port switch

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Gamera Node Hardware

- 500 Megahertz Intel Celeron
- 256 Megabyte ram
- 4.3 Megabyte disk
- Netgear FA310 TX 100 base-T NIC

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Gamera Software

- Linux Mandrake 7.0
- LAM MPI 6.3
- PVM 3.0
- GCC 2.95
- ASCI-Red Optimized BLAS
- ATLAS Optimized BLAS
- PATMOL
- PETLIB

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Gamera Costs

- **Hardware**

– 16 *e*machines:	\$8,160
– 4 Gigabytes ram:	\$3,280
– Network cards, switch, & cables:	\$1,129
– Shelving rack:	\$80

- **Software**

– All software:	\$0

- **Total** \$13,189

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Gamera Performance

# Processors	Execution Time (seconds)	
	Gamera	SGI Origin 2000
1	77.3	70.6
2	41.0	35.7
3	30.7	25.7
4	25.0	19.0
6	18.0	13.7
8	13.8	10.8
12	10.5	8.2
16	8.2	???

Calculations of the ground state energy of CO_2 using a 10s6p2d/5s3p2d basis.

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Gamera Performance

# Processors	Execution Time (minutes)
	Gamera
1	222 (Serial)
16	10 (MPI)

Calculations of the SF_6 ground state energy and two points of the polarization potential for e^+–SF_6.

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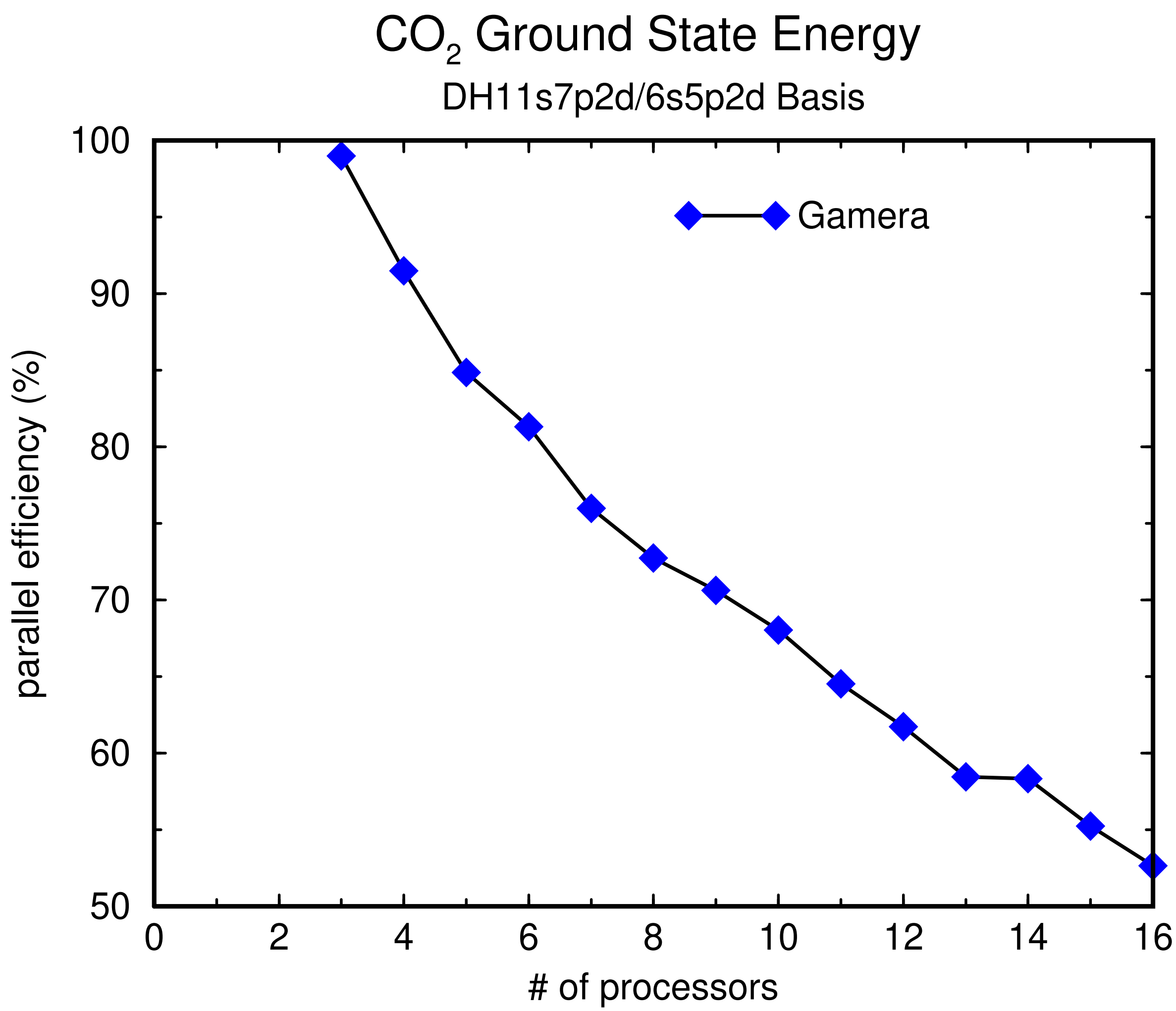
Gamera Results



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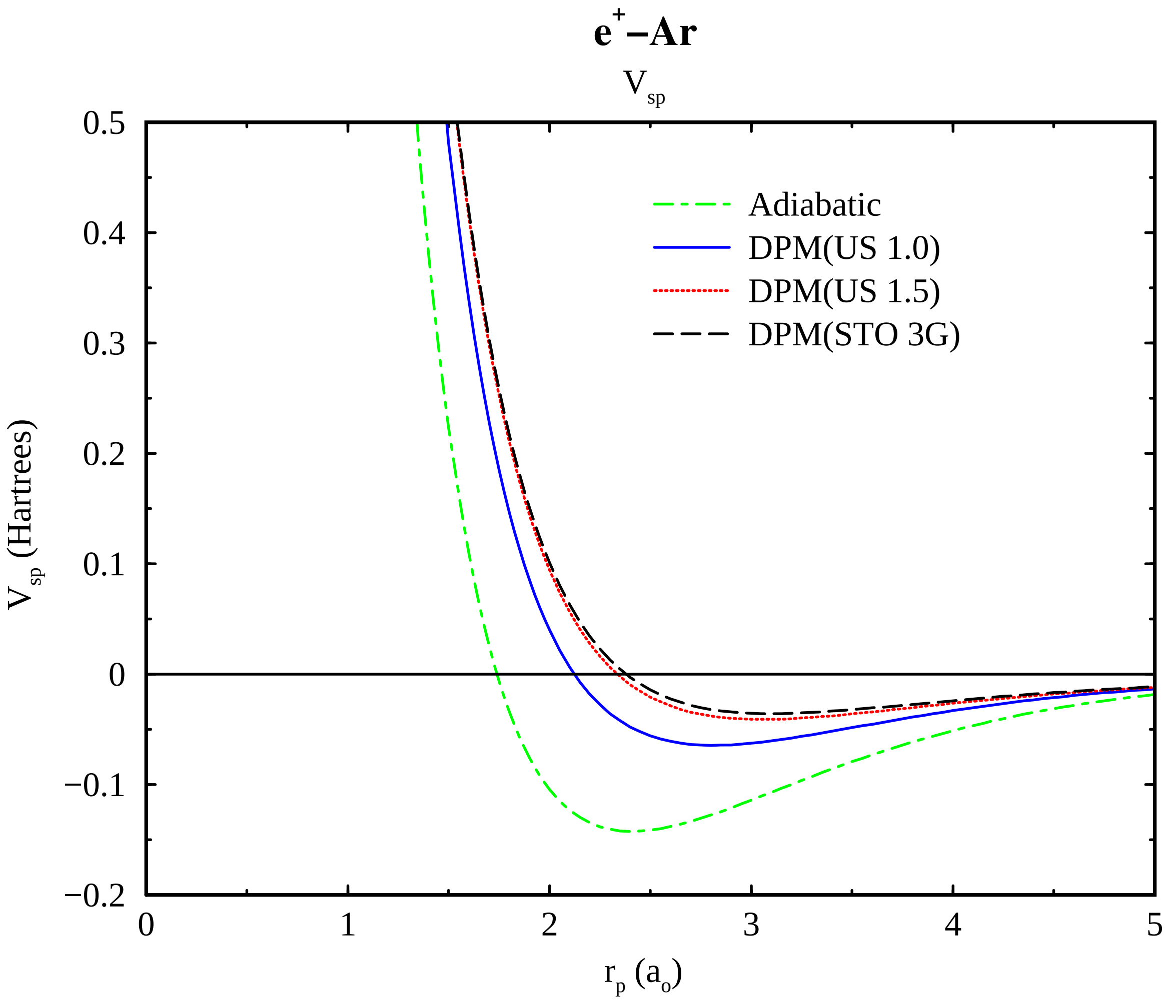
Gamera Results



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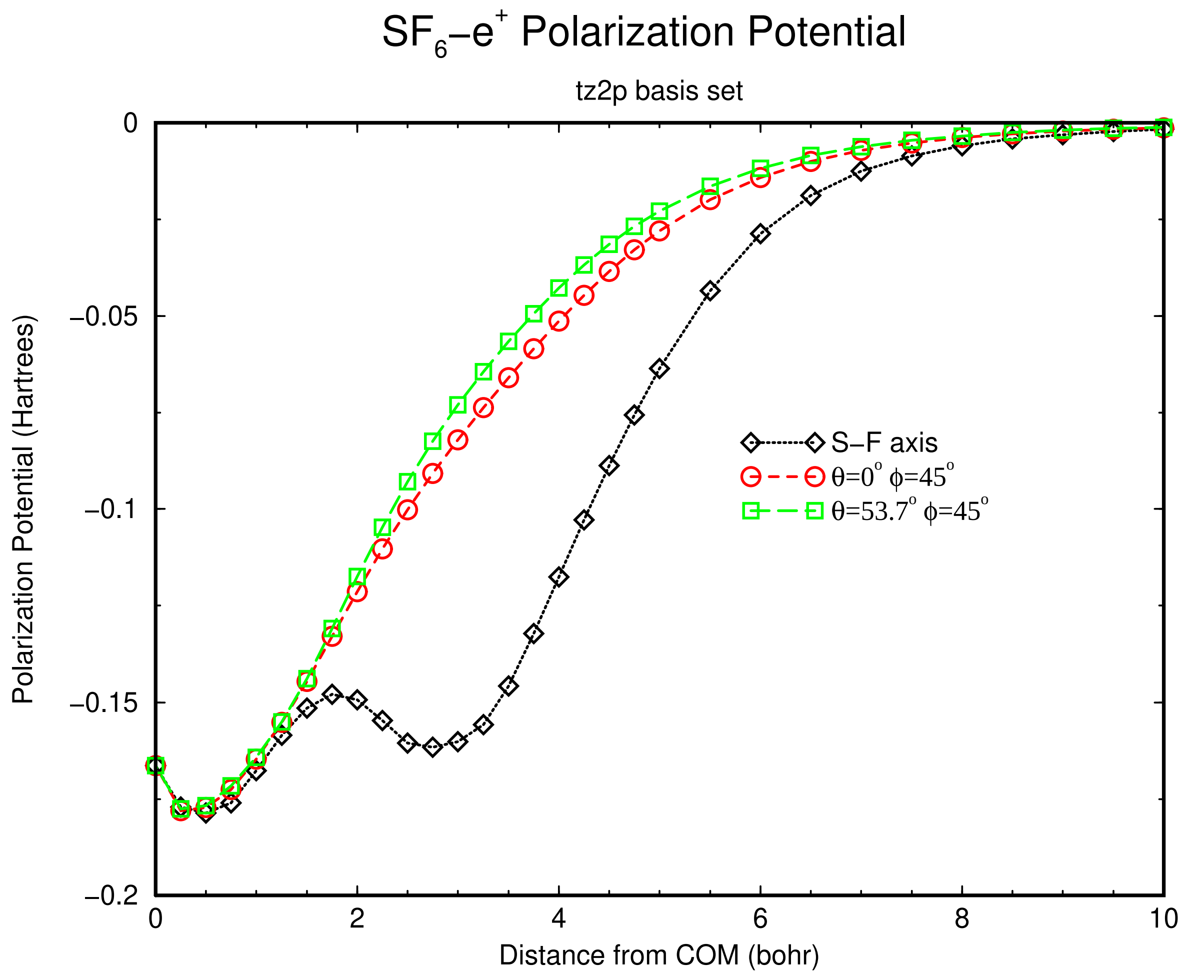
Gamera Results



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Conclusions

- High-Performance Computing $\equiv$ Concurrent Computing
- Affordable Parallel Systems Are Available Now
- Open Source Software and Scientific Applications Are Compatible

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