THE_ELEMENTS

/Fire/Air/Water/Earth/

A Distributed Parallel Computer

THE_ELEMENTS is a multiple computer for supporting the project on *Classical and Quantum Mechanical Molecular Dynamics* of TCCC. This distributed parallel system is an effort to create large computational power by accumulating low cost CPUs, memory and data storage using public domain software as far as possible. The current composition of The_Elements is four dual Pentium II systems [FIRE (master)-AIR-WATER-EARTH] with cpus at 350 Mhz, total memory 2GBytes, total hard discs 21 GBytes and all these connected with a fast ethernet switch of 100 Mbits/s.

The system was developed and is currently maintained by Dr. Manolis Founargiotakis (founar@alcyone.cc.uch.gr).

TECHNICAL CHARACTERISTICS

- **CPUs: Eight Pentium II CPUs at 350 Mhz**
- **Motherbords: INTEL BX 100Mhz, Cash Memory 512 KBytes**
- **Memory: 2.048 GBytes (100 Mhz SDRAM)**
- **Discs: 21 GBytes (ULTRA WIDE SCSI)**
- **Network: Bay 350T, 100 Mbits Switch, Backbone 1Gbits, 16 ports**

SOFTWARE

- **Operational System: Linux, Distributor Red Hat 5.1 (Manhattan) (Kernel 2.1.121) (P)**

- **Batch Queuing Program: NQS (Network Queuing System)- Sterling Software Incorporated (P)**
- **Compilers: High Performance Fortran(HPF)/Fortran 90/Fortran 77/C/C++ PortlandGroup (C)**
- **Communication Programs: Message Passing Interface (MPI) Parallel Computing/Local Area Multicomputer (LAM) (P)**
- **Libraries: Numerical Recipes (C) - PETs (P)-**

- **P = Public software**
- **C = Commercial software**
- **L = Local software**

PROJECTS

Non-Linear Classical Mechanical Analysis of Molecular Systems: Periodic Orbit Multiple Shooting Algorithms POMULT (L)
Molecular Quantum Dynamics: Periodic Orbit Assisted Grid Solutions of Time Dependent Schroedinger Equation POATDSE (L)
Molecular Electronic Structure Calculations (Quantum Chemistry) Packages: GAUSSIAN94, GAUSSIAN98 , (C)
MOLPRO98 (C)

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SUPPORT

The project was financed by the Ministry of Education within the program EPEAEK for postgraduate studies in Applied Molecular Spectroscopy.

With the prices of July 1998 the cost of The_Elements in its current composition is: ~7000000 Greek Drachmas (~$25000)

FUTURE DEVELOPMENTS

Scheduled Upgrade in 1999:

16 CPUs, 6 Gbytes memory, 50 Gbytes hard discs.

BENDSMARKS

- **Comparison of memories**
- **Comparison with HP-CONVEX (Exemplar)**
- **Comparison with SUN**
- **Comparison with DIGITAL/Alpha**

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