

## **Poster Title:**

More than 20 years of electronic structure computation: Hard- and software evolution (and sometimes revolution) from the early nineties to today.

## **Abstract**

We take a closer look at the evolution of the computational facilities of the Andersen group from the early nineties when the group started the migration from the Cray-XMP at the RZG to the first local IBM RS/6000 520 workstations (20 MHz Clock, 64 MB main memory). These workstations then were connected by shared 10 MBit/s Thinwire Ethernet.

More and more workstations were added and their connection became faster, the institute's first FDDI-Ring and the first switched 10Base-T-Ethernet network were introduced in 1995.

The clustered workstations were augmented in 1996 by the tightly coupled IBM SP/2 parallel computer (8 Nodes, 256MB each) aquired and administered jointly with the Parrinello group. The SP2 was later extended by 10 more SP2 and 8 more SP3 nodes.

In 1997 the Andersen and Parrinello groups proposed a joint backup and archive system which evolved into todays institute wide TSM backup and archive system.

The institute's network backbone was rebuild from scratch based on a fiber to the office approach in 1998 and 1999. The theory groups were among the first to adopt the new concept. The fiber network started with 10MBit/s to the office, today 1 Gbit/s is the standard and up to 10 Gbit/s are possible using the fibers installed back in 1998.

The acquisition of the Regatta SMP parallel computer with 32 IBM Power 4 Cores marked the last AIX based compute server, the Linux revolution started to bring down the cost of software and hardware with the migration from the POWER to PowerPC (Godot) and finally to the Intel architecture (Bohr) using Linux as cluster operating system. All applications were migrated from IBMs XL Fortran compilers to Portland Fortran and finally to the Intel Fortran/C++ compilers and the Intel Math Kernel Library.

In 2013 the group utilizes 832 computing cores in 88 cluster nodes with in total slightly below 3 TB main memory.