

Method Development and Deployment

- Scientific Vector Language (SVL)
- Cluster Computing
- Platform Independent
- Interface to Relational Databases and Internet
- MOE/web

MOE™ is a comprehensive system that integrates visualization, molecular modeling, protein modeling, cheminformatics and bioinformatics in one package. In addition to the suite of graphical applications, MOE contains a toolbox for adapting existing applications or creating new applications for Life Sciences. With MOE, expert modelers, application developers and occasional users can benefit from sharing the same software system. Methodology written by application developers can be validated by expert modelers and then deployed to occasional users using either the MOE graphical interface or a Web interface.

Scientific Vector Language (SVL) is the built-in command language, scripting language and application development language of MOE. SVL is a “chemistry aware” computer programming language with over 1,000 specific functions for analyzing and manipulating chemical structures and related molecular objects. SVL is a concise, high-level language and SVL programs are typically 10 times smaller than equivalent programs written in C or Fortran. SVL source code is compiled to a “byte code” representation, which is then interpreted by the base run-time environment making SVL programs inherently portable across different computer hardware and operating systems.

Background Computing. MOE/batch is an adaptation of the MOE run-time environment intended for batch or background calculations that do not require a graphical interface. All non-graphical MOE functionality is accessible. MOE/web technology distributed with MOE is used to create Web Browser interfaces to MOE applications.

Cluster Computing. A standard part of MOE is the MOE/smp distributed computing technology. With MOE/smp, multiple cooperating computers can be used to perform large-scale calculations. A heterogeneous collection of computers including laptops, workstations and multi-processor clusters, all running different operating systems, can be easily harnessed together in a single MOE session. The MOE/smp programming model in SVL makes it easy to parallelize SVL applications.

Computer Platforms. The MOE run-time environment has been ported to a wide variety of computer platforms including Intel computers running Microsoft Windows™, MacOSX or Linux as well as Apple Macintosh, Hewlett-Packard, Sun Microsystems and Silicon Graphics computers running Unix. SVL programs (including MOE's applications) are automatically ported to all platforms upon which MOE runs.

Interface to Relational Databases and Internet. MOE incorporates a tightly integrated and extensible interface to the Java Virtual Machine. SVL programs can take advantage of Java's IT strengths and access data from the internet via FTP, download files from web servers via HTTP and directly access third party database servers such as Oracle and DB2 via JDBC. MOE contains built-in applications to download new entries from the RCSB Protein Data Bank and a relational database browser. It is also possible to write SVL programs that interface with existing applications and libraries.

MOE

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