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Report on Subcontract CFS-160043-WTEC2 between Chenega Federal Systems, LLC and WTEC2

Phase I: Identification of Successful International Models for Scalable Engineering Codes

Background

The purpose of this task is to identify successful international models for scalable engineering codes. This task responds to a DoD need for engineering codes that can efficiently run large and complex simulations. DoD areas of interest include computational biology, chemistry and materials science; computational structural mechanics; climate/weather/ocean modeling and simulation; computational fluid dynamics; and computational electromagnetics and acoustics.

Task methodology included analysis of information contained in published literature and on the Web, individual discussions, and written queries. Several techniques were used to identify the most widely used engineering codes and those with interesting scaling properties. A database, presented in Appendix B, was prepared that included one hundred of the most commonly used engineering codes. From this database foreign codes that appeared to be widely used and to scale well were extracted, along with a few similar domestic codes. After further analysis a set of about fifty codes in the DoD areas of interest was assembled, as presented in Appendix A. Characteristics of these codes and comments on the business models for their development are presented in subsequent sections.

Parallel Computation and Scaling

The Scaling Barrier

Most engineering software suffers from a scaling barrier that seriously limits the user's ability to model complex engineered systems. To understand this barrier and its pernicious effect it is helpful to review a few concepts. Today most computers include multiple processors, arranged to share the workload in parallel. Even PCs often contain four or more processors on one chip; the largest HPC systems include more than one hundred thousand processors on more than ten thousand chips. Parallel computers were first introduced in the 1990s to overcome the inherent speed and power limits of a single processor. Unfortunately, advances in software, including algorithms and programming techniques, to use parallel computers have come much slower than the hardware advances.

Reasons for This Barrier

Many contemporary engineering codes were first created in the 1990s before the advent of parallel processing. Converting, or "parallelizing," these serial codes to use parallel computers effectively is usually expensive and time-consuming; in some cases even the basic approach and algorithms to solve the problem must be re-invented.

For several reasons much of the development of codes with good scaling properties requires grueling labor, with few aids from compilers or other tools. This contrasts with scalar codes, for which many good optimizing compilers exist. As a result, there are few scientists or engineers who know how to produce good scalable codes or who are willing to invest the time to learn.

A recent study conducted by the Council on Competitiveness under government sponsorship documented the scaling barrier and showed that most commercial engineering codes do not scale to use more than about one hundred processors, and in some important cases do not use parallel processing at all.[1,2,3] The study included surveys of ISVs (independent software vendors) and users of ISV-supplied engineering codes, as well as a workshop that evaluated the survey data and formulated findings and recommendations. The surveys did not include foreign ISVs or foreign users.

Findings by the study lead to several plausible reasons for this scaling barrier, including lack of R&D funds for ISVs to improve their codes, lack of trained personnel, licensing and business models that discourage use of highly scaled codes, and lack of access to highly parallel systems.

The study pointed out that research codes developed at universities and national laboratories in several disciplines of science and engineering have achieved much greater scale-up by employing novel scientific algorithms and improved computer science. However, for a variety of economic, technical and organizational reasons very few of these codes have become commercialized or seen wide use. Their existence shows that it is possible to break the scaling barrier, but their lack of use shows that, practically speaking, the scaling barrier remains. The study concluded that federal funding patterns have changed in recent years to discourage the types of long-term effort required to commercialize research codes. This conclusion is supported by a National Academies study of HPC that concluded "…from the committee's visits to DOE sites, members got the clear impression that there are no incentives for the transfer of codes developed at those sites to industrial use and no significant funding to facilitate the transfer."[4]

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[1] *Accelerating Innovation for Competitive Advantage: The Need for HPC Application Software Solutions*, July, 2005, Council on Competitiveness, http://www.compete.org/publications/detail/383/accelerating-innovation-for-competitive-advantage-the-need-for-better-hpc-application-software-solutions/

[2] *HPC Software Study Part A: Current Market Dynamics*, Council on Competitiveness, July 2005, http://www.compete.org/publications/detail/392/hpc-software-study-part-a-current-market-dynamics/

[3] *HPC Software Study Part B: End-User Perspectives*, July 2005 Council on Competitiveness, http://www.compete.org/publications/detail/393/hpc-software-study-part-b-end-user-perspectives/

[4] *Getting Up to Speed: The Future of Supercomputing*, The National Academies Press, 2004, http://www.nap.edu/openbook.php?record_id=11148&page=191

Successes and Approaches Outside of the United States

A very recent study by the World Technology Evaluation Center[5] updated these conclusions in an international context. It concluded that the European Union has for some time led the United States in theoretical algorithm development for important areas of science and engineering and that community code developments are much stronger within the European Union than in the United States, with national strategies and long-term support. It identified several European engineering codes that are in widespread use and have achieved good scaling.

In contrast engineering codes in the United States tend to be commercial and/or closely restricted in their usage. Often they are supplied only in object (binary) code format, affording users no opportunity to examine the underlying algorithms or search for areas whose improvement would improve scaling.

Search for Factors Leading to Successful Scaling

Development and sustainment of engineering codes that are user friendly, powerful, and easily scaled requires successful management of several factors. A study of large codes in the Department of Energy nuclear weapons laboratories indicates that control of technical factors is necessary but not sufficient for scalable software development.[6] Among the factors that appear important are the following:

1) Technical advances required to achieve good code scalability. These could include better physical models, better algorithms, better computer science, and better access to suitably large computer systems.
2) Business model used in developing the code. This includes:
    a) Funding Model (private funding, government funding, contributions, volunteer effort)
    b) Organizational Model (private company, university, government center, volunteer community, individual)
    c) Leadership Model (charismatic leader, appointed leader, steering committee, volunteer leaders)
    d) Intellectual Property Model (proprietary, open source, public domain, informal)
    e) Sustainment Model (license fees, contributions, sustained government funding, sustained private funding, embedding in an ongoing research group)
    f) User Input Model (excluded, help desk, developer outreach, Wiki, open source community)

In our analysis of scalable codes we have looked at these factors and intend to examine them closely in Phase II of the study, especially during the workshop planned for this phase, to see which ones correlate with successful scalability.

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[5] *International Assessment of Research and Development in Simulation-Based Engineering and Science*, World Technology Evaluation Center, 2009, http://www.wtec.org/sbes/SBES-GlobalFinalReport.pdf

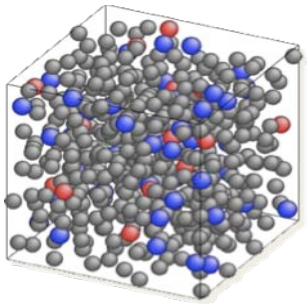
[6] *Computational Science Demands a New Paradigm*, D. E. Post, L. G. Votta, Physics Today, 2005, 58(1): p. 35-41.

Computational Technology Areas

The research community in the Department of Defense High Performance Computing Modernization Program focuses on hundreds of projects throughout the country. These projects are categorized into ten areas called Computational Technology Areas (CTAs). This study addresses five of these areas. For each area, we use an S-box [S] to indicate that a code is potentially a scalable foreign code, and we use an R-box [R] to indicate that a code is potentially a scalable domestic (or reference) code. This notation is used here and in Appendix A.

Computational Biology, Chemistry, and Materials Science

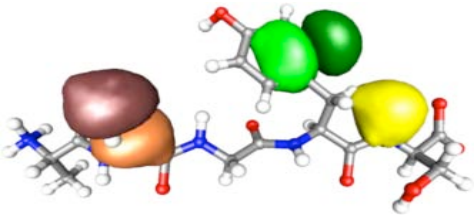
This computational technology area covers computational tools used to predict basic properties of chemicals and materials, including nano- and biomaterials. Properties such as molecular geometries and energies, spectroscopic parameters, intermolecular forces, reaction potential energy surfaces, and mechanical properties are of interest. Within the DoD, quantum chemistry, molecular dynamics, statistical mechanics, and multiscale methods are used to design new chemical, polymer, nano- and bio- molecular systems, for fuel, lubrication, laser protection, explosives, rocket propulsion, catalysis, structural applications, fuel cells, and chemical defense. Solid-state modeling techniques are employed in the development of new high-performance materials for electronics, optical computing, advanced sensors, aircraft engines and structures, semiconductor lasers, advanced rocket engines components, and biomedical applications. Also of interest are methodologies that cover bioinformatics tools, computational biology, and related areas, such as cellular modeling.



The methods employed in this area include both static and dynamic approaches. In all cases, the computer time and memory required increase rapidly with the size of the system. Computational chemistry methods are either empirical or *ab initio* methods. Empirical or semi-empirical methods use experimental results while *ab initio* methods are based entirely on theory.

Density Functional Theory (DFT) methods are often considered *ab initio* methods for determining the molecular electronic structure even though some functionals use parameters derived from empirical data. Car and Parrinello proposed a strategy based on DFT, pseudopotentials, and plane waves for computational condensed matter. Although very powerful, the Car-Parrinello approach requires N^3 computer operations where N is the number of atoms in the system. These are referred to as $O(N^3)$ methods. Even on the fastest computers, such complexity becomes prohibitive for calculations involving 10^6 atoms or more. Fortunately, the principle of nearsightedness (things often depend on near items, not on things far away) made it possible to determine the electronic ground state of a system with a number of operations that increases linearly with N. These are referred to as O(N) methods. With such linear scaling, it is possible to handle problems that are twice as large by using only twice as many processors.

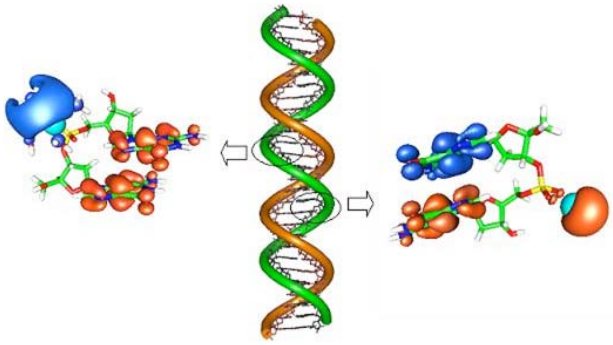
s *ONETEP*



ONETEP (Order-N Electronic Total Energy Package) is a quantum-mechanical materials simulation using DFT, under development by Mike Payne and his associates at Cambridge University in the United Kingdom. The code is in beta release and uses an approach that exhibits O(N) scaling as number of atoms increases. Previous codes were $O(N^3)$ or worse. The overall linear scaling and controlled accuracy have been achieved in testing by the developers.

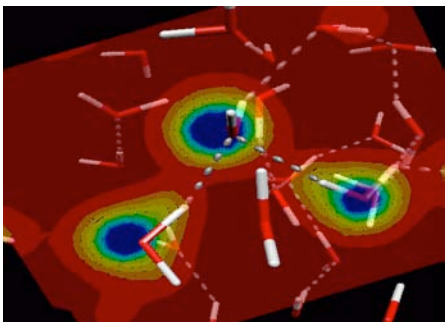
s *OpenMX*

OpenMX (Open Source Package for Material Explorer) is a program package for nanoscale material simulations based on DFT, norm-conserving pseudopotentials, and pseudo-atomic localized basis functions. It is an open source code originally developed by Taisuke Ozaki, Japan Advanced Institute of Science and Technology.



In the current version of OpenMX, three O(N) methods are available: a divide-conquer method, a generalized divide-conquer method, and a Krylov subspace method. For all the calculations of O(N), cluster, and band calculations, the number of processors that one can use for the parallel calculations is limited up to the number of atoms in the system.

s *SIESTA*



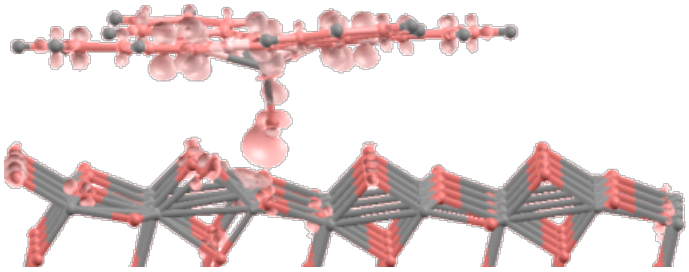
SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is a computer program to perform electronic structure calculations and *ab initio* molecular dynamics simulations of molecules and solids. The code is free to academics, and nonacademic distribution is handled by Nanotec Electronica. Mainly developed in Spain, contributors to the code live around the world.

Because O(N) linear scaling was carefully implemented, the code is very efficient for large systems and moderate precisions. The need for higher precisions and the addition of many new functionalities imposed compromises on the O(N) philosophy. However, efficiency is still one of SIESTA's strongest points. Moreover, SIESTA is an integral part

of the Barcelona Supercomputer Center (BSC) software stack and users may apply for BSC projects to run SIESTA.

s *Quantum ESPRESSO*

Quantum ESPRESSO is an open source framework for plane wave DFT calculations. It is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft). Quantum ESPRESSO uses MPI parallelization. Data structures are distributed across processors organized in a hierarchy of groups, which are identified by different MPI communicator levels. The CP (Car-Parrinello) version was demonstrated to run on up to 4000 processors.



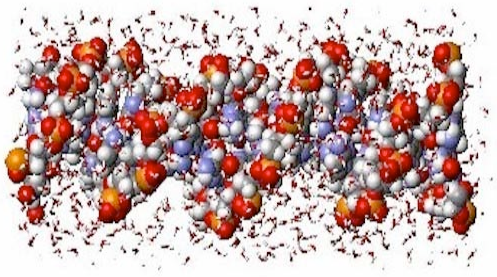
An initiative of the DEMOCRITOS National Simulation Center(Udine - Trieste) and of its partners, Quantum ESPRESSO was developed in collaboration with the CINECA National Supercomputing Center in Bologna, the Ecole Polytechnique Federale de Lausanne, Princeton University, and the Massachusetts Institute of Technology.

s *DL_POLY*

DL_POLY is a general purpose serial and parallel molecular dynamics simulation package developed at Daresbury Laboratory by W. Smith, T.R. Forester and I.T. Todorov. Long-term funding is provided by the British Government. The code is supplied free-of-cost to academic scientists and is suitable for simulations up to order 1 million atoms on 8-1024 processors. The code exhibits weak scalability.[7]

s *GROMACS*

GROMACS is primarily designed for biochemical molecules such as proteins and lipids that have numerous complicated bonded interactions, but since GROMACS is extremely fast at calculating the nonbonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems, e.g. polymers.

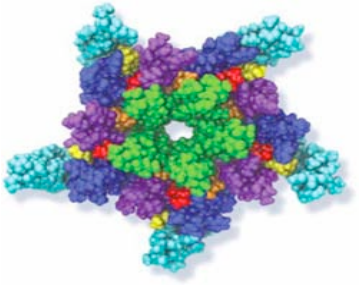


[7] http://www.cse.scitech.ac.uk/arc/dlpoly_scale.shtml

GROMACS is an open source code and was first developed in Herman Berendsen's group, department of Biophysical Chemistry of Groningen University, The Netherlands. It is a team effort, with contributions from several current and former developers all over the world. GROMACS can be run in parallel, using standard MPI communication. It simulates the Newtonian equations of motion for systems with hundreds to millions of particles. It is considered to be the world's fastest molecular dynamics (MD) and trajectory analysis software.

R *NAMD*

NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. The software is developed and distributed by the Theoretical and Computational Biophysics Group at the Beckman Institute of the University of Illinois (Urbana-Champaign).



NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters using gigabit ethernet. Major components of NAMD are written in Charm++, a locally developed language that simplifies parallel programming. NAMD exhibits strong scalability.

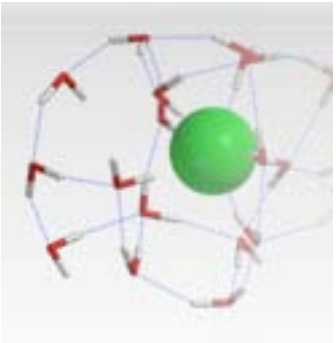
R *NWChem*

NWChem provides many methods to compute the properties of molecular and periodic systems using standard quantum mechanical descriptions of the electronic wavefunction or density. In addition, NWChem has the capability to perform classical molecular dynamics and free energy simulations. These approaches may be combined to perform mixed quantum-mechanics and molecular-mechanics simulations. NWChem development has been devoted to providing maximum efficiency on massively parallel processors.

NWChem has been developed by the Molecular Sciences Software group of the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL). Most of the implementation has been funded by the EMSL Construction Project. NWChem is available free of charge, subject to the terms and conditions of the EMSL Software User Agreement.

NWChem is a computational chemistry package that is designed to run on high-performance parallel supercomputers as well as conventional workstation clusters. It aims to be scalable both in its ability to treat large problems efficiently, and in its usage of available parallel computing resources.

R *Q-Chem/Spartan*

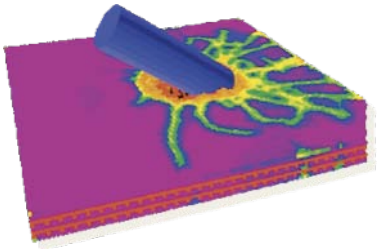


Q-Chem is a commercial *ab initio* quantum chemistry package. Its capabilities range from the highest performance DFT/HF calculations to high level post-HF correlation methods. Q-Chem tackles a wide range of problems in commercial, academic, and government laboratories. Spartan is front-end graphic software. The code is available for clusters and parallel environments.

Computational Structural Mechanics (Finite Element Analysis)

Computational structural mechanics is almost always carried out by finite element analysis (FEA) and is the principal application of FEA. However, FEA can be used for many other problems involving two and three-dimensional structures, such as thermal analysis, electromagnetics, acoustics, and fluid flow.

FEA is used for both static analysis and dynamic analysis. Static analysis investigates properties of structures at rest, including determination of stresses, vibration modes, standing waves, and similar properties.



Dynamic analysis is used to determine the time evolution of a system undergoing change, using appropriate non-linear equations of motion. Generally these equations may be solved using either straightforward time stepping (called explicit methods), or iteratively in time (called implicit methods.) Implicit methods tend to allow longer time steps while preserving accuracy than do explicit methods; therefore implicit methods are more efficient for studying the long-time evolution of a system. However, implicit methods require exchange of information about the system at greater distances than do explicit methods, thus are usually much harder to scale than are explicit methods.

Because explicit methods FEA codes and implicit methods FEA codes are quite different in their scaling properties, we have grouped them into two different subcategories.

Explicit Methods FEA Codes

S *PAM-CRASH*

PAM-CRASH is a commercial French code supported by the ESI Group (esi-group.com) that is widely used in the European automotive and aircraft industries. It reportedly scales better than most FEA codes and is reported to run a two-million-element problem well on 1024 CPUs. PAM-CRASH may be derived in part from DYNA3D, developed at Lawrence Livermore Laboratory.

LS-DYNA

LS-DYNA is a commercial American code derived from DYNA3D. It is supported by the Livermore Software Technology Corporation, whose president, John Hallquist, was the original developer of DYNA3D.

Implicit Methods FEA Codes

s *Code_Aster*

Code_Aster is an open source code supported by Électricité de France (EDF) and widely used in the French nuclear industry. It is capable of calculating structural mechanics, 3D thermal analyses, mechanical analyses, linear and nonlinear statics and dynamics. The code has been developed over eighteen years, primarily by EDF and the French Commissariat a l'Energie Atomique (CEA.) The latest version 10.0 was released May 5, 2009. A parallel version of the code exists, but it scales to only a few tens of processors.

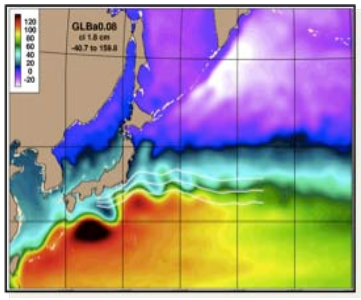
s *Elmer*

Elmer is an open source code supported by the CSC – IT Center for Science, Finland. The CSC actively solicits community help and trains users. Although implicit, the code appears to scale linearly to a few hundred processors using the Message-Passing Interface (MPI) standard. Development started in 1995. The code is stable and supported. Code capabilities include structural mechanics, fluid dynamics, electromagnetics, and heat transport. The code includes a preprocessor, FEA engine and postprocessor. It interfaces with several mesh generation tools.

U.S. commercial codes include ABAQUS, ANSYS, MSC/NASTRAN, and NX NASTRAN (spun off from MSC/NASTRAN.)

Climate/Weather/Ocean Modeling and Simulation

This area includes modeling and simulation codes that attempt to understand and predict regional and global climate changes. Recently, this area has received significant attention due to the global warming controversy.



Historically, weather prediction was a reason for developing the earliest parallel computers because parallel computing was perceived to be necessary for success. Even today, parallel processing is essential for obtaining realistic results.

In this group, special attention is given to ECHAM-MAECHAM (Germany), IFS (supported by ECMWF, an international consortium of 31 countries), and LES (United States: National Center for Atmospheric Research - NCAR).

CM2

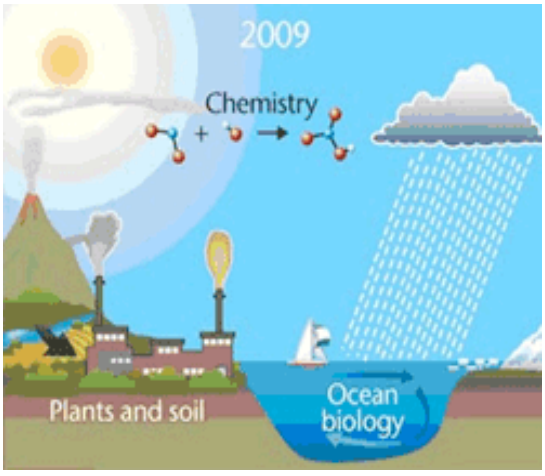
The U.S. Geophysical Fluid Dynamic Laboratory (GFDL) CM2.1 coupled model is representative of the state of the art in global climate modeling. The CM2 models became GFDL's workhorse models for computer modeling studies of decadal to century time scale climate variability and change in 2004, and their results figure prominently in the Intergovernmental Panel on Climate Change Fourth Assessment Report (IPCC AR4) and the U.S. Climate Change Science Program (CCSP) reports. The CM2 global climate models consist of atmospheric, land, ocean and sea ice components that interact with each other. The GFDL CM2.0 and CM2.1 models have been shown to be credible at reproducing the decade to decade variations in global mean surface air temperature observed during the 20th century. Both models have been used to conduct a suite of climate change simulations for the 2007 IPCC assessment report and are able to simulate the main features of the observed warming of the twentieth century.

s *ECHAM-MAECHAM*

Notably, ECHAM was used in the Fourth Intergovernmental Panel on Climate Change (IPCC) assessment report. ECHAM and MEACHAM are both comprehensive general circulation models of the atmosphere. The codes run on the NEC SX6, a vector parallel computer. In a vector CPU, the basic machine instruction operates on multiple units of data at a time. It may take a while for a pipeline to fill up and start producing results, but it is very efficient once it does.

HadCM3

HadCM3 (Hadley Centre Coupled Model, version 3) is a coupled atmosphere-ocean general circulation model (AOGCM) developed at the Hadley Centre in the United Kingdom. It was one of the major models used in the IPCC Third Assessment Report in 2001. HadCM3 is composed of two components: the atmospheric model HadAM3 and the ocean model (which includes a sea ice model). The Stern Review on the Economics of Climate Change, issued in 2006, was based on Met Office Hadley Centre scientific research.



S *IFS*

IFS (Integrated Forecast System) aims to provide a single software system for delivering a state-of-the-art forecast model. Scalability is achieved through CPU optimization, OpenMP, and Message-Passing Interface (MPI) parallelization. Nowadays, a forecast for five days ahead is of the same quality as a forecast for two days ahead in August 1979.

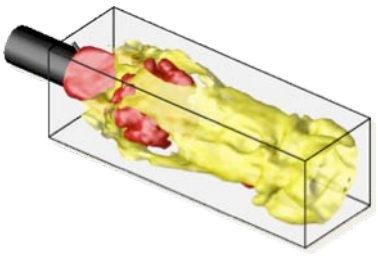
R *LES*

LES (Large Eddy Simulation) seeks to predict the motion of the largest and most important eddies (coherent patches of swirling fluid) uncoupled from the small eddies. This uncoupling is important because the large eddies are resolvable on a computational mesh (a collection of chunks of the physical problem) which can be handled by a supercomputer. LES is written to run on massively parallel computer architectures using the MPI and OpenMP programming models.

This computational technology area also includes the following codes:

CCSM (Community Climate Systems Model): General circulation model
HYCOM (Hybrid Coordinate Ocean Model): Ocean modeling
NEMO (Nucleus for European Modeling of the Ocean): Ocean and climate modeling
PSTSWM (Parallel Spectral Transform Shallow Water Model): Global atmospheric circulation modeling
SEA (Southampton - East Anglia Parallel Ocean Circulation Model)**:** Ocean modeling
WRF (Weather Research and Forecasting Model): Weather forecasting

Computational Fluid Dynamics



Computational fluid dynamics (CFD) codes are widely used to study fluid and gas flows within and around bodies, including steady flows, turbulent flows, reactive flows, and pulsed flows as in shock dynamics. Although FEA can be used to model fluid flow, usually CFD codes use a finite-difference approach to advancing the nonlinear fluid equations. Some codes allow alternate approximations to actual fluid/gas behavior, such as compressible vs. incompressible, viscous vs. inviscid, thermally conductive or not, etc. Solution grids are often regular and fixed in time, although some codes allow for adaptive (Lagrangian) grids whose points follow the fluid in time. Especially with fixed grids CFD codes typically scale well.

S *OpenFOAM*

OpenFOAM (Open Field Operation and Manipulation) is an open source British CFD code with extended capabilities including chemical reactions, solid dynamics, and electromagnetics. The development model appears not to be funded by large external source, rather by a champion at a small company, who has mobilized an open source community to produce one of the better CFD codes with reasonable scalability. Code development is managed by OpenCFD Ltd., in England, that makes money supporting and applying the code. The code uses modern program techniques, written in C++ using an object oriented model. OpenFOAM has been available since 2004 with continuous development. The latest release is version 1.6 released July 28, 2009.

FLUENT

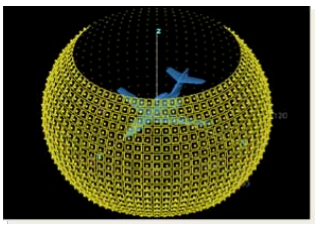
FLUENT is the most commonly used U.S. commercial CFD code. It contains the broad physical modeling capabilities needed to model flow, turbulence, heat transfer, and reactions for industrial applications ranging from air flow over an aircraft wing to combustion in a furnace, from bubble columns to oil platforms, from blood flow to semiconductor manufacturing, and from clean room design to wastewater treatment plants. FLUENT is supported by ANSYS, Inc. and licensed on commercial terms. Advanced parallel processing numerics can efficiently utilize multiple, multi-core processors in a single machine and in multiple machines on a network. Dynamic load balancing automatically detects and analyzes parallel performance and adjusts the distribution of computational cells among the processors so that a balanced load is shared by the CPUs even when complex physical models are in use.

STAR-CD

STAR-CD is an international CFD code with capability in fluid dynamics, thermal and stress analysis, and continuum mechanics. It is capable of simulating engineering problems that involve turbulence, combustion, heat transfer, reacting flows and multiphase physics. STAR-CD is a commercial code supported by CD-adapco.

Computational Electromagnetics and Acoustics

Several FEA and CFD codes have electromagnetic capability, including OpenFoam and Elmer. These codes are typically restricted to low-frequency static fields. They are not well suited for high-frequency propagation or transient field analysis.



AMS

AMS (Auxiliary Space Maxwell Solver) is a scalable solver for Maxwell's equations under development by Lawrence Livermore National Laboratory high frequency and transient code that solves Maxwell's equations directly for the electromagnetic fields, presumably including displacement currents. It promises extreme scalability.

Integrated Code Suites

SALOME-MECA

SALOME-MECA is an integration platform that includes pre- and post-processing for numerical simulation and integrates with Code_Aster (finite element), Code_Saturne (CFD), SYRTHES (heat transfer), OpenFOAM (CFD), and other solvers. SALOME interfaces with CAD format standards such as STEP. It includes geometry and mesh generation, data preparation, and post-visualization. High level integration and customization routines are written in Python. It uses CORBA for inter-process communication. SALOME-MECA is open source and is supported by Electricite de France and the Commissariat a l'Energie Atomique, both of France. The code has been stable with ongoing development since 2000. The latest release is SALOME v5.1.2, released on July 31, 2009. It runs of parallel computers with different levels of scalability depending on the chosen solvers.

CAELinux

CAELinux is and integrated suite for multiphysics that includes SOLOME-MECA (integrating framework), OpenFOAM (CFD), Code_Aster (FEA), DynELA (nonlinear explicit FEA), Code_Saturne (CFD), Elmer (FEA), gmsh (mesh generation), Impact (nonlinear explicit FEA), and Paraview (visualization). It is distributed as a bootable DVD built on the Ubuntu Linux distribution. The suite is developed and supported by Electricite de France. The most recent release was issued in 2009.

Is the United States Losing Ground?

Our analysis of specific engineering codes – encompassing Computational Structural Mechanics; Computational Biology, Chemistry, and Materials Science; Climate/Weather/Ocean Modeling and Simulation; and Computational Fluid Dynamics – tends to support the conclusion that the U.S. is losing ground selectively, especially in computational biology, chemistry, and materials science codes. This is consistent with the recent WTEC study of Simulation-Based Engineering and Science that reached similar conclusions regarding the use of simulation. Table 1 summarizes that status of leading codes in these areas. Succeeding paragraphs discuss the details and implications of this table.

Table 1. Characteristics of Selected Foreign and U.S. Engineering Codes

Code	Method	Type	Origin	Scalability
Chemistry, Biology, and Materials Science				
CONQUEST	O(N) Quantum	Open Source	UK/Japan	Excellent
ONETEP	O(N) Quantum	Academic/Commercial	UK	Excellent
OpenMX	O(N) Quantum	Open Source	Japan	Excellent
Siesta	O(N) Quantum	Academic/Commercial	Spain	Excellent
Quantum ESPRESSO	Quantum	Open Source	Italy	Good
Q-Chem	Quantum	Commercial	U.S.	Good
NWChem	Quant./Newt.	Free restricted	U.S.	Excellent
DL_POLY	Newtonian	Academic/Commercial	UK	Excellent
GROMACS	Newtonian	Open Source	Netherlands	Excellent
NAMD	Newtonian	Open Source	U.S.	Excellent
Structural Mechanics				
PAM-CRASH	Explicit FEA	Commercial	France	Good
LS-DYNA	Explicit FEA	Commercial	U.S.	Good
Code_Aster	Implicit FEA	Open Source	France	Fair
Elmer	Implicit FEA	Open Source	Finland	Good
Abaqus	Explicit/Implicit	Commercial	U.S.	Fair
Climate/Weather/Ocean Modeling				
ECHAM-MAECHAM	GCM	Open Source	Germany	Good
IFS	Forecast	Restricted	Europe	Good
LES	Ocean	Open Source	U.S.	Good
HadCM3	GCM/Ocean	Not Available	UK	Good
CM2	GCM/Ocean	Open Source	U.S.	Good
Fluid Dynamics				
OpenFOAM		Open Source	UK	Good
Fluent		Commercial	U.S.	Good
Star-CD		Commercial	International	
Overflow		Free/restricted	U.S.	Excellent

Chemistry, Biology, and Materials Science: The U.S. lags Europe and Japan, especially in O(N) quantum codes. An earlier generation of codes (not discussed here) was mostly created in the U.S., but these are no longer competitive for large problems. Substantial U.S. government funding initially produced NWChem, a competitive suite of codes, but the ongoing funding stream has been reduced.

This appears to be an area where strong academic capability, patient government funding, and stable committed teams are producing and sustaining strong codes. Reports that some of these foreign codes are given limited distribution tied to area of application are disturbing.

The quantum code ONETEP illustrates the way these codes are developed. The code was designed and written using government funding, starting in 2000, by academics at three

UK universities to exploit recent theoretical advances allowing O(N) scaling. O(N) means that the computation time scales linearly with N, the number of electrons. This is a tremendous improvement over the best previous codes that scaled as $O(N^3)$, including CASTEP written by some of the same team. Only recently, approximately nine years later, has the patient government investment paid off in this new-generation code. Reflecting the government funding, the cost of the code is free to UK academics, but everyone else pays commercial license fees.

Structural Mechanics: The U.S. seems to be in parity with the rest of the world in commercial codes. However, Code_Aster and Elmer are well-supported open source codes with no U.S. equivalents.

Code_Aster is supported by Électricité de France (EDF) as part of a robust suite of engineering codes under the integration platform SOLOME-MECA. These codes are developed and supported by EDF and the French Commissariat a l'Energie Atomique. Current releases are used for production engineering design, including of nuclear reactors, and are regularly updated to incorporate theoretical advances. The suite provides multi-physics simulation of mechanical, chemical, and electronic systems; the modules are linked together through standard interfaces. Pre- and post-processing modules are included. The code is included in the integrated CAELinux suite that can be freely downloaded.

Elmer has been supported by the Finnish government since 1995 at the Finnish IT Center for Science. In addition to structural mechanics, the code has modules for heat transfer, fluid flow, acoustics, and electromagnetism. The Center offers training and maintains extensive documentation. Frequent updates to the code are produced. Free source code availability allows the user community to submit improvements to the code or to modify it for particular needs.

Climate/Weather/Ocean Modeling and Simulation: The U.S. may be leading in climate and ocean modeling, thanks to strong leadership from the National Center for Atmospheric Research and patient government funding. Europe may be leading in weather forecasting, thanks to strong performance by the European Center for Meso-scale Weather Forecasting (ECMWF) and adequate government funding.

Fluid Dynamics: The U.S. appears to be in parity with the rest of the world. However, we have no open source code equivalent to OpenFOAM, a UK code. Overflow, produced by NASA, is very competitive for external fluid dynamics (flow around free bodies.)

In the past, groups that developed codes in the United States had a large advantage in their computational facilities relative to rivals in either Europe or Asia. This is no longer clearly the case, now that the dominant cost in the United States is labor rather than equipment. Development resources are broadening across the world and leveling out.

Regarding system-level tools and middleware, there has been a trend towards moving these tools into the public domain, driven by the success of the open-source development of the Linux operating system and the closely related GNU software tools. Thus obtaining access to existing system-level software and middleware is now easier and less expensive than it has ever been. This has also contributed to a leveling of the playing field for software development in general.

The planned workshop in Phase II of this project should shed additional light on the U.S. position in scalable software development.

Appendix A: Candidate Scalable Codes

S Scalable Code
R U.S. Reference Code

1. Computational Chemistry, Biology, and Materials Science

New O(N) Codes – Better scaling but less accurate

ADF (Amsterdam Density Functional)
Application area: Quantum chemistry
Lead organization: Scientific Computing and Modeling NV (SCM)
Contributor(s): Dr. Stan van Gisbergen, Prof. Evert Jan Baerends, Prof. Tom Ziegler
Development model: Commercial but developed mainly at Vrije Universiteit, Amsterdam and University of Calgary, Canada
Why this code is interesting: ADF is suitable for calculations on atoms and molecules (in gas phase or solution). It can be used for the study of such diverse fields as molecular spectroscopy, organic and inorganic chemistry, crystallography and pharmacochemistry.
Status of code: Latest version is ADF2008.01
Scalability: Latest version increases the max number of atoms to 30000. Most parts of ADF, including BAND, have been efficiently parallelized for both shared-memory and distributed memory systems, such as multi-core multi-CPU machines or simple Linux clusters. For most standard types of calculation, including NMR, analytical Hessian, and TDDFT calculations, ADF approaches perfect parallel scaling fairly well, even for a significant number of CPU's.
Website(s): http://www.scm.com/,
http://www.scm.com/Products/Overview/parallel.html,
http://www.scm.com/News/Newsletters/NewsletterDec08.html,
http://www.csc.fi/english/research/software/adf
Other information: One of chemistry codes maintained by CSC in Finland. A separate program in the ADF package, BAND, is available for the study of periodic systems: crystals, surfaces, and polymers.

CONQUEST
Application area: O(N) density functional theory code
Organization: University College London, UK
Contributor(s): Mike Gillan (University College London), David R. Bowler (University College London), Tsuyoshi Miyazaki (National Institute for Materials Science (NIMS) Japan), R. Choudhury (University College London)
Development model:
Why this code is interesting: While the success of density functional theory (DFT) has led to its use in a wide variety of fields such as physics, chemistry, materials science and biochemistry, it has long been recognized that conventional methods are very inefficient for large complex systems, because the memory requirements scale as N^2 and the CPU requirements as N^3 (where N is the number of atoms). The principles necessary to develop methods with linear scaling of the CPU and memory requirements with system

size (O(N) methods) have been established for more than ten years, but only recently have practical codes showing this scaling for DFT started to appear. The development of the CONQUEST code, which performs O(N) DFT calculations on parallel computers, has a reported ability to handle systems of over 10000 atoms. The code can be run at different levels of precision, ranging from empirical tight-binding, through *ab initio* tight-binding, to full *ab initio*, and techniques for calculating ionic forces in a consistent way at all levels of precision. Illustrations were reported of practical CONQUEST calculations in the strained Ge/Si(001) system.
Status of code: After successful beta testing, the code will be released without restriction (beyond the GPL license) though significant technical support will not be offered without some form of collaboration.
Scalability: Reported efficient parallelization (up to 512 processors), efficient linear scaling (on systems of up to 23,000 atoms), ground state convergence and atomic relaxation on systems containing up to 23,000 atoms
Website(s): http://hamlin.phys.ucl.ac.uk/NewCQWeb/bin/view, http://www.psi-k.org/workshops/workshops_2007/Files_1335.pdf,
http://www.cecam.fr/dbfiles/latex/tp_proposal_wid158.pdf,
http://www.cecam.org/workshop-158.html
Other information: Psi-k, cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. CONQUEST is listed here, but the link http://www.cmmp.ucl.ac.uk/~conquest/ is broken.

S **DL_POLY**
Application area: Molecular dynamics simulation of materials
Lead organization: Computational Science and Engineering Department, Science & Technology Facilities Council Daresbury Laboratory
Contributor(s): W. Smith, T.R. Forester, I.T. Todorov
Development model: Development centered at Daresbury Laboratory, under Dr. W. Smith. Several university collaborators contribute to code development and provide training in code use. Long-term funding provided by the British Government. Code is supplied free-of-cost to academic scientists.
Why this code is interesting:
Status of code: DL_POLY_3 is the latest version.
Scalability: Suitable for simulations up to order 1 million atoms on 8-1024 processors. Exhibits weak scalability.
Website(s): http://www.cse.scitech.ac.uk/ccg/software/DL_POLY/

R **NWChem**
Application area: Quantum chemistry
Lead organization: NWChem has been developed by the Molecular Sciences Software group of the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL). Most of the implementation has been funded by the EMSL Construction Project.

Contribuor(s): Richland (WA), US: E. J. Bylaska, W. A. de Jong, N. Govind, K. Kowalski, T. P. Straatsma, M. Valiev, D. Wang, E. Apra, etc.
Development model: NWChem is available free of charge, subject to the terms and conditions of the EMSL Software User Agreement.
Why this code is interesting: NWChem provides many methods to compute the properties of molecular and periodic systems using standard quantum mechanical descriptions of the electronic wavefunction or density. In addition, NWChem has the capability to perform classical molecular dynamics and free energy simulations. These approaches may be combined to perform mixed quantum-mechanics and molecular-mechanics simulations. NWChem development has been devoted to providing maximum efficiency on massively parallel processors.
Status of code: The latest version is NWChem version 5.1.1. This release includes a number of new capabilities, new supported platforms, and bug fixes.
Scalability: NWChem is a computational chemistry package that is designed to run on high-performance parallel supercomputers as well as conventional workstation clusters. It aims to be scalable both in its ability to treat large problems efficiently and in its usage of available parallel computing resources. Most of the tool and scalable algorithm development has been funded by the High Performance Computing and Communications Initiative (HPCCI) grand-challenge software program and the DOE-2000 ACTS Tools project.
Website(s): http://www.emsl.pnl.gov/docs/nwchem/nwchem.html
Other information: One of chemistry codes maintained by CSC, Finland

S **ONETEP**
Application area: Quantum-mechanical materials simulation using DFT
Lead organization:
Contributor(s): Dr Peter Haynes, Dr Arash Mostofi, Prof Mike Payne, Dr Chris-Kriton Skylaris, Dr Nicholas Hine
Development model:
Why this code is interesting: Code is one of a new generation that uses algorithms allowing O(N) scaling as number of atoms increases. Previous codes were $O(N^3)$ or worse.
Status of code: In beta release
Scalability: Questions as to whether it scales past a few hundred atoms on a few hundred processors
Website(s): http://www2.tcm.phy.cam.ac.uk/onetep/,
http://www2.tcm.phy.cam.ac.uk/onetep/Main/People,
http://www.soton.ac.uk/~compchem/papers/paper17.pdf

S **OpenMX**
Application area: OpenMX (Open source package for Material eXplorer) is a program package for nanoscale material simulations based on density functional theories (DFT), norm-conserving pseudopotentials, and pseudo-atomic localized basis functions.
Organization: OpenMX, Japan

Contributor(s): T. Ozaki (Japan Advanced Institute of Science and Technology), H. Kino (National Institute of Materials Science, Japan), J. Yu (Seoul National University, Korea)
Development model: Open source. Code originally developed by Taisuke Ozaki. Supported by CREST-JST, NAREGI, ACT-JST, and SYNAF-NEDO.
Why this code is interesting: *Ab initio* density functional theory (DFT) with local density approximation (LDA) or generalized gradient approximation (GGA) has been applied to investigate many physical properties of a wide variety of solids with tremendous success in the past decades. Nevertheless, most electronic structure methods used so far to carry out the DFT calculations have suffered from the fundamental problem of cubic scaling, and hence are not applicable to large complex systems such as nanomaterials and biomolecules. Therefore, there has been considerable effort in recent years to develop alternative O(N) fast linear-scaling electronic structure methods. The OpenMX code is a freely available program package that implements the O(N) methods. ADPACK (Atomic Density functional program PACKage) is also available. ADPACK is a program package for atomic density functional calculations, in which either the Schrödinger or Dirac equation under a spherical atomic potential is numerically solved within a local density approximation or a generalized gradient approximation to the exchange-correlation energy. Professor Taisuke Ozaki from Japan Advanced Institute of Science and Technology (JAIST), is the principal author of OpenMX and ADPACK.
Status of code: Latest code release is OpenMX 3.4 (release date 23 June 2008) with a patch (17 March 2009).
Scalability: The computational effort of the conventional diagonalization scheme scales as the third power of the number of basis orbitals, which means that it could be a bottleneck when large-scale systems are calculated. On the other hand, the O(N) methods can solve the eigenvalue problem in O(N) operation in exchange for accuracy. Thus, O(N) methods could be efficient for large-scale systems, while a careful consideration is always required for the accuracy. In OpenMX Ver. 3.4, three O(N) methods are available: a divide-conquer method, a generalized divide-conquer method, and a Krylov subspace method. For all the calculations of O(N), cluster, and band calculations, the number of processors that you can use for the parallel calculations is limited up to the number of atoms in your system. (See http://www.openmx-square.org/openmx_man/.)
Website(s): http://www.openmx-square.org/. For discussion of technical issues on OpenMX and ADPACK, an online forum was created in 2005.
Other information: Psi-k, cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. However, OpenMX is not listed here.

s **SIESTA**
Application area: Local orbital DFT
Organization: SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is distributed freely for academics (see http://www.icmab.es/siesta/). Nanotec Electronica has an agreement with SIESTA authors for Non Academic distribution (see http://www.nanotec.es/products/siesta.php).

Contributor(s): Jose A. Torres (Universidad Autónoma de Madrid (UAM)), Emilio Artacho (University of Cambridge), Javier Junquera (Universidad de Cantabria, Spain), Alberto Garcıa (ICMAB, Barcelona, Spain), Pablo Ordejon (ICMAB, Barcelona, Spain), Daniel Sanchez-Portal (DIPC, San Sebastian, Spain).
Development model: The core development team consists of number of academics from Spain, but the team includes contributors around the world.
Why this code is interesting: SIESTA is both a method and its computer program implementation, to perform electronic structure calculations and *ab initio* molecular dynamics simulations of molecules and solids.
Status of code: Initially, SIESTA was a purely serial code. This was convenient for many "modest" users, who used single workstations, and this gave it a rapid popularity. Later, parallelism was added "on top," with priority given to not compromising serial execution, and without revising the algorithms for good parallelism. Today, parallel computers and clusters have become ubiquitous, and a new parallelization of SIESTA has become a priority. In this effort, the Barcelona Supercomputing Center (see http://www.bsc.es/) has become a key partner. SIESTA is now an integral part of the BSC software stack and users can apply for BSC projects to run SIESTA.
Scalability: SIESTA was born in 1996 to implement, in self consistent DFT, the O(N) techniques developed for tight-binding in the early 1990s. Because O(N)was carefully imposed in all the code, this was very efficient, specially for large systems and moderate precisions. Later, the need for higher precisions, and the addition of many new functionalities, imposed compromises to the O(N) philosophy, but efficiency kept being one of SIESTA's strongest points.
Website(s): http://www.icmab.es/siesta/,
http://www.nanotec.es/products/siesta.php
Other information: Psi-k, a cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. SIESTA is on the list.

Older $O(N^3)$ Codes

Amber
Application area: Molecular simulation
Lead organization: University of California, San Francisco
Contributor(s): D.A. Case, T.A. Darden, T.E. Cheatham, III, C.L. Simmerling, J. Wang, R.E. Duke, etc.
Development model: Amber is developed in an active collaboration of David Case at Rutgers University, Tom Cheatham at the University of Utah, Tom Darden at NIEHS, Ken Merz at Florida, Carlos Simmerling at SUNY-Stony Brook, Ray Luo at UC Irvine, and Junmei Wang at Encysive Pharmaceuticals. Amber was originally developed under the leadership of Peter Kollman, and Version 9 was dedicated to his memory.
Why this code is interesting: Amber refers to two things: a set of molecular mechanical force fields for the simulation of biomolecules (which are in the public domain, and are used in a variety of simulation programs); and a package of molecular simulation programs.

Status of code: The current version of the code is Amber version 10, which is distributed by University of California, San Francisco subject to a licensing agreement. The Mail Reflector exists to provide a forum for discussions on the use of the Amber software and for release of bug fixes.
Scalability: "The parallel scaling of Amber has improved a lot recently."
Website(s): http://ambermd.org/

CASTEP
Application area: Electronic structure on extended systems using plane wave DFT.
Organization: CASTEP was originally created by Prof. M.C. Payne and subsequently developed by various UK academics, primarily from the TCM group in Cambridge. For various technical reasons, it was felt in 1999 that the original code was in need of a total redesign and rewrite, and so the CASTEP Development Group was created to do just that, using modern coding styles and Fortran90. CASTEP is marketed commercially by Accelrys, along with Materials Studio, their graphical frontend for MS Windows. In the United Kingdom there is an academic distribution, maintained by UKCP.
Contributor(s): Mike Payne, Matthew Segall, Matt Probert, Stewart Clark, etc.
Development model: Commercial (Cambridge, UK), sold by Accelrys as Materials Studio.
Why this code is interesting: CASTEP is a software package which uses density functional theory to provide a good atomic-level description of all manner of materials and molecules. CASTEP can give information about total energies, forces, and stresses on an atomic system, as well as calculating optimum geometries, band structures, optical spectra, phonon spectra and much more. It can also perform molecular dynamics simulations.
Status of code: In April 2002 the first version of new CASTEP debuted in Materials Studio 2.1.5. The code was capable of parallel, ultrasoft calculations for electronic relaxation, using either a self-consistent minimizer or a nonself-consistent density mixing minimizer. Geometry optimizations and molecular dynamics simulations could also be performed, as could calculations of band structures. By this time the development team had grown to eight members, and the code exceeded 170,000 lines. It had taken approximately two and a half years to develop. Since then many new features have been added such as linear response, Ensemble DFT, transition state searches, and a new NMR module. CASTEP continues to be developed actively, and is used by researchers around the world.
Scalability:
Website(s): http://www.castep.org/
Other information: Psi-k, a cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. CASTEP is not on the list.

R **CHARMM**
Application area: Force-field-based molecular dynamics for biological macromolecules
Lead organization: Department of Chemistry and Chemical Biology, Harvard University. For-profit companies should contact Accelrys, Inc. (http://accelrys.com/).

Contributor(s): Cambridge (MA), U.S.: Martin Karplus, Bernard Brooks DHHS/NIH/NHLBI
Development model: The CHARMM Development Project involves a network of developers in the United States and elsewhere working with Professor Karplus and his group at Harvard to develop and maintain the CHARMM program.
Why this code is interesting: CHARMM is a versatile and widely used molecular simulation program with broad application to many-particle systems. It has been developed with a primary focus on the study of molecules of biological interest, including peptides, proteins, prosthetic groups, small molecule ligands, nucleic acids, lipids, and carbohydrates, as they occur in solution, crystals, and membrane environments. A variety of systems, from an individual organic molecule to a large oligomeric protein in its solvent environment, can be simulated.
Status of code: The current version is CHARMM 36. A CHARMM forum exists.
Scalability: CHARMM has been ported to numerous platforms in both serial and parallel architectures.
Website(s): http://www.charmm.org/, http://www.charmm.org/old_site/, http://www.charmm.org/ubbthreads/ubbthreads.php?ubb=cfrm
Other information: One of chemistry codes maintained by CSC, Finland

CPMD
Application area: *Ab initio* molecular dynamics
Lead organization: CPMD is copyrighted jointly by IBM Corp and by Max Planck Institute, Stuttgart, and is distributed free of charge to nonprofit organizations.
Contributor(s): Michele Parrinello, Jurg Hutter, D. Marx, P. Focher, M. Tuckerman, W. Andreoni, etc.
Development model: The CPMD consortium has been established in 2001 in order to coordinate the development and distribution of the CPMD code. It is a virtual organization that comprises all the users and developers of the CPMD code around the world. This organization is coordinated by Prof. Michele Parrinello (Chair of Computational Science, ETH Zurich) and Dr. Wanda Andreoni (Program Manager of Deep Computing Applications at IBM Zurich Research Laboratory). The first version of the code was developed by Jurg Hutter at IBM Zurich Research Laboratory starting from the original Car-Parrinello codes.
Why this code is interesting:
Status of code: The current version is CPMD Version 13.3.2
Scalability: CPMD runs on many different computer architectures and it is well parallelized (MPI and Mixed MPI/SMP).
Website(s): http://www.cpmd.org/

CP2K
Application area: Plane wave DFT, atomistic and molecular simulations
Lead organization: ETH Zurich, Switzerland)
Contributor(s): G. Lippert, J. VandeVondele, J. Hutter, M. Parrinello
Development model: Open source. Over a dozen researchers are listed on the development team (see http://developer.berlios.de/project/memberlist.php?group_id=129)
Why this code is interesting:

Status of code: Code comes with little documentation and without any warranty. No official release has been made.
Scalability:
Website(s): http://cp2k.berlios.de/

CRYSTAL
Application area: Gaussian orbital DFT/Hartree Fock
Lead organization: The CRYSTAL program was jointly developed by the Theoretical Chemistry Group at the University of Torino (http://www.theochem.unito.it/) and the Computational Materials Science group in CLRC (http://www.cse.scitech.ac.uk/cmg/) in Warrington, UK.
Contributor(s): Pisa, Italy: R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C.M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I.J. Bush, Ph. D'Arco, M. Llunell
Development model: License fee of 1000 – 9000 Euros.
Why this code is interesting: The program computes the electronic structure of periodic materials within Hartree-Fock, density functional, or various hybrid approximations. The Bloch functions of the periodic systems are expanded as linear combinations of atom-centred Gaussian functions. Powerful screening techniques are used to exploit real space locality. The code may be used to perform consistent studies of the physical, electronic and magnetic structure of molecules, polymers, surfaces, and crystalline solids.
Status of code: Source code is not provided. Latest version is CRYSTAL06.
Scalability:
Website(s): http://www.crystal.unito.it/, http://www.cse.scitech.ac.uk/cmg/CRYSTAL/
Other information: Psi-k, a cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. CRYSTAL is on the list.

Dalton
Application area: Quantum chemistry
Lead organization: Department of Chemistry, University of Oslo, Norway.
Contributor(s): Oslo, Norway: C. Angeli, K. L. Bak, V. Bakken, O. Christiansen, R. Cimiraglia, etc.
Development model: Open source. As the code is distributed for free, official user support is not provided.
Why this code is interesting: Dalton is a powerful molecular electronic structure program, with an extensive functional for the calculation of molecular properties at the HF, DFT, MCSCF, and CC levels of theory.
Status of code: Dalton 2.0 was released on March 4, 2005. The most important and largest extension to the code is the addition of a complete Density Functional Theory (DFT) module, including up to quadratic response properties as well as an extensive open-shell (spin-restricted) module.
Scalability:
Website(s): http://www.kjemi.uio.no/software/dalton/dalton.html

FLEUR: The Jülich FLAPW code family
Application area: Electronic structure in solid state physics
Lead organization: Institute of Solid State Research, Jülich, Germany
Contributor(s): Stefan Blügel, Gustav Bihlmayer, Daniel Wortmann, Christoph Friedrich
Development model: The code is distributed free of charge but without any warranties. The FLAPW code FLEUR was developed since 1998 predominately by Dr. Gustav Bihlmayer and many collaborators of the group of Prof. Stefan Blügel at the Institute Theory I, Institute für Festkörperforschung, Forschungszentrum Jülich. The code includes previous developments of many researchers including e.g., M. Weinert and R. Podloucky.
Why this code is interesting: FLEUR is a new FLAPW-Code the development of which is partly funded by the European Research Network (Psik). The FLAPW-Method (Full Potential Linearized Augmented Plane Wave Method) is an all-electron method which within density functional theory is universally applicable to all atoms of the periodic table and to systems with compact as well as open structures. It is widely considered to be the most precise electronic structure method in solid state physics.
Status of code: Version 0.25 current as of 05/07/2006. There is no warranty and no support.
Scalability: Massive parallelization: Both the k-point loop and the eigenvalue-problem are parallelized and scale very well on MPI machines.
Website(s): http://www.flapw.de/pm/index.php?n=Main.HomePage

GAMESS
Application area: Quantum chemistry
Lead organization: Mark Gordon's Quantum Theory Group, Ames Laboratory, Iowa State University
Contributor(s): Ames (IA), U.S.: M.S. Gordon, M.W.Schmidt
Development model: A site license for GAMESS is available at no cost to both academic and industrial users.
Why this code is interesting: GAMESS is a program for *ab initio* molecular quantum chemistry. Briefly, GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Correlation corrections to these SCF wavefunctions include configuration interaction, second order perturbation theory, and coupled-cluster approaches, as well as the density functional theory approximation.
Status of code: The latest version is dated January 12, 2009. The version changes periodically when some new scientific capability appears.
Scalability: Most computations can be performed using direct techniques, or in parallel on appropriate hardware.
Website(s): http://www.msg.chem.iastate.edu/gamess/. An independent Google Groups discussion forum exists for GAMESS users. The group's home page is at: http://groups.google.com/group/gamess
Other information: Psi-k, a cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. GAMESS is not on the list.

GAMESS-UK
Application area: Electronic structure
Lead organization: Computing for Science (CFS). CFS was founded in the UK in 1992 by an international consortium of established academic and industrial figures in the area of molecular electronic structure and modeling, Drs. M.F. Guest, J.H. van Lenthe, J. Kendrick, and K. Schoeffel.
Contributor(s): M.F. Guest (Cardiff University, UK), H.J.J. van Dam (Daresbury Laboratory, UK), P. Sherwood (Daresbury Laboratory, UK), J.H. van Lenthe (Utrecht University, The Netherlands), J. Kendrick (Bradford University, UK), K. Schoeffel (Norsk Hydro A/S, Norway)
Development model: A license to run the GAMESS-UK program for non-commercial research can be provided to individual research groups, to research institutions, or to computer centers. In all cases, the license normally specifically excludes any commercial use of the program. In order to support the ongoing process of method and code development, a nominal service charge is typically requested for the supply of the software to academic groups outside of the UK. This charge is used exclusively for the ongoing support and development of the code, and no personal profits are made by any of the authors.
Why this code is interesting: By collaborating with both academia and industry CFS is targeting key areas that emphasize the computational requirements of 'Grand Challenge' projects. In particular, the development of combined QM/MM methodologies and the exploitation of massively parallel architectures will allow GAMESS-UK to simulate chemical systems involving several thousands of atoms, enabling the study of many complex chemical phenomena at a molecular level.
Status of code: The current version is GAMESS-UK Version 7.0
Scalability: GAMESS-UK is currently available in two different versions for parallel machines: (1) a replicated data version that relies on the virtual shared memory model provided by the Global Array toolkit (the "GA version"). This is the default parallel version of the code and the one that should be used by most users of GAMESS-UK and (2) a largely distributed-data version that is parallelised using MPI (the "MPI version") and makes use of MPI-based tools such as BLACS and ScaLAPACK. Within the MPI build it is also possible to configure GAMESS-UK to run in "taskfarming" mode, for batch processing numerous small jobs under the umbrella of a single GAMESS-UK job. The MPI version has limited functionality, but scales well on large parallel machines and, due to it's largely distributed data strategy, is best used for extremely large calculations.
Website(s): http://www.cfs.dl.ac.uk/
Other information: Both GAMESS-UK and the U.S. GAMESS have been extensively modified and enhanced since they branched from the original 1981 GAMESS code.

Gaussian
Application area: Quantum chemistry
Lead organization: Wallingford (CT), US: Gaussian, Inc.
Contributor(s): Mike Frisch, Gary Trucks, Jim Cheeseman
Connecticut, US: John Pople, Walter Kohn
Development model: Commercial

Why this code is interesting: Gaussian is a series of electronic structure programs. Starting from the basic laws of quantum mechanics, Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types. It can be used to study molecules and reactions under a wide range of conditions, including both stable species and compounds which are difficult or impossible to observe experimentally such as short-lived intermediates and transition structures.
Status of code: Current Gaussian 09 Revision: A.02
Scalability:
Website(s): http://www.gaussian.com/

S **GROMACS**
Application area: Molecular dynamics
Lead organization:
Contributor(s): Erik Lindahl (Stockholm Center for Biomembrane Research, Stockholm, Sweden), David van der Spoel (Biomedical Centre, Uppsala, Sweden), Berk Hess (Stockholm University, Stockholm, Sweden)
Development model: Open source. GROMACS was first developed in Herman Berendsens group, department of Biophysical Chemistry of Groningen University, The Netherlands. It is a team effort, with contributions from several current and former developers all over the world.
Why this code is interesting: GROMACS is primarily designed for biochemical molecules like proteins and lipids that have a lot of complicated bonded interactions, but since GROMACS is extremely fast at calculating the nonbonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems, e.g. polymers.
Status of code: GROMACS 4 was released in October 2008.
Scalability: GROMACS can be run in parallel, using standard MPI communication. It simulates the Newtonian equations of motion for systems with hundreds to millions of particles. For parallel performance benchmarks, see http://oldwww.gromacs.org/content/view/26/39/.
Website(s): http://www.gromacs.org/
Other information: GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. Hess, B., Kutzner, C., van der Spoel, D. and Lindahl, E. J. Chem. *Theory Comput.*, 4, 435-447 (2008)

LAMMPS
Application area: Molecular dynamics
Lead organization: LAMMPS is distributed by Sandia National Laboratories, a US Department of Energy laboratory.
Contributor(s): Albuquerque (NM), US: Steve Plimpton, Paul Crozier, Aidan Thompson
Development model: LAMMPS is distributed as an open source code under the terms of the GPL.
Why this code is interesting: LAMMPS is a classical molecular dynamics simulator designed for parallel machines. It can model atomic, polymeric, biological, metallic, or

granular systems using a variety of force fields and boundary conditions and can be easily modified and extended.
Status of code: The current version of LAMMPS is July 7, 2009. The last major release is also available on SourceForge (http://sourceforge.net/projects/lammps/files/).
Scalability: LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality.
Website(s): http://lammps.sandia.gov/

MOLCAS
Application area: Quantum chemistry
Lead organization: It is not primarily a commercial product and it is not sold in order to produce a fortune for its owner (the Lund University).
Contributor(s): Lund, Sweden: R.Lindh
Development model: Licensed commercially
Why this code is interesting: The basic philosophy of MOLCAS is to be able to treat, at the same level of accuracy also, highly degenerate states, such as those occurring in excited states, at the transition state in some chemical reactions, in diradicaloid systems, heavy metal systems, etc. This is a more difficult problem since the single determinant approach will not work well in such cases. The key feature of MOLCAS is the multiconfigurational approach. MOLCAS contains codes for general and effective multiconfigurational SCF calculations at the Complete Active Space (CASSCF) level, but also employing more restricted MCSCF wave functions (RASSCF). It is also possible, at this level of theory, to optimize geometries for equilibrium and transition states using gradient techniques and to compute force fields and vibrational energies.
Status of code: MOLCAS 7.4 has been released
Scalability: The size of the systems that can be treated with MOLCAS have been limited due to limitations in storing two-electron integrals for large basis set. This limit has now been moved substantially to larger systems by the introduction of a Cholesky decomposition of the two-electron integrals. This feature is introduced in MOLCAS-7 and can be used for the SCF, CASSCF, CASPT2, RASSI and MP2 codes. It speeds up all calculations by orders of magnitude and extends the size of the basis sets that can be used.
Website(s): http://www.teokem.lu.se/molcas/

Molpro
Application area: Quantum chemistry
Lead organization:
Contribuotr(s): H.-J. Werner (Universität Stuttgart, Germany) and P. J. Knowles (Cardiff University, UK)
Development model: Commercial license
Why this code is interesting: **Molpro** is a complete system of *ab initio* programs for molecular electronic structure calculations, designed and maintained by H.-J. Werner and P. J. Knowles, and containing contributions from a number of other authors. As distinct from other commonly used quantum chemistry packages, the emphasis is on highly accurate computations, with extensive treatment of the electron correlation problem

through the multiconfiguration-reference CI, coupled cluster and associated methods. Using recently developed integral-direct local electron correlation methods, which significantly reduce the increase of the computational cost with molecular size, accurate *ab initio* calculations can be performed for much larger molecules than with most other programs.
Status of code: Molpro version 2009.1 was released on August 7th 2009.
Scalability: MPI-2 parallel implementation is provided.
Website(s): http://www.molpro.net/
http://www.molpro.net/info/current/doc/molpro.bib

R **NAMD**
Application area: Molecular dynamics
Lead organization: The software is developed and distributed by the Theoretical and Computational Biophysics Group at the Beckman Institute of the University of Illinois (Urbana-Champaign), US.
Contributor(s): Urbana-Champaign (IL), US: Klaus Schulten, Laxmikant V. Kalé, Robert D. Skeel
Development model: Open source.
Why this code is interesting: NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.
Status of code: Current version is NAMD 2.7b1. NAMD uses the popular molecular graphics program VMD for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR.
Scalability: NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters using gigabit ethernet. NAMD exhibits strong scalability.
Website(s): http://www.ks.uiuc.edu/Research/namd/
Other information: Laxmikant Kale, Robert Skeel, Milind Bhandarkar, Robert Brunner, Attila Gursoy, Neal Krawetz, James Phillips, Aritomo Shinozaki, Krishnan Varadarajan, and Klaus Schulten. NAMD2: Greater scalability for parallel molecular dynamics. *Journal of Computational Physics,* 151:283-312, 1999.

S **Quantum ESPRESSO** [Need to check whether this is O(N) or O(N^3)
Application area: Framework for plane wave DFT calculations
Lead organization: Quantum ESPRESSO is an initiative of the DEMOCRITOS National Simulation Center (Udine-Trieste) and of its partners, in collaboration with the CINECA National Supercomputing Center in Bologna, the Ecole Polytechnique Federale de Lausanne, Princeton University, and the Massachusetts Institute of Technology.
Contributor(s): Paolo Giannozzi. Gerardo Ballabio, Carlo Cavazzoni
Development model: Open source, development started in 2002.
Why this code is interesting: Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft).
Status of code: Current stable version (v. 4.1) of the code, released July 20, 2009.

Scalability: Quantum ESPRESSO uses MPI parallelization. Data structures are distributed across processors organized in a hierarchy of groups, which are identified by different MPI communicator levels. CP (Car-Parrinello version) demonstrated to run on up to 4000 processors.
Website(s): http://www.quantum-espresso.org/, http://www.democritos.it/events/espresso-tutorial.php, http://users.aims.ac.za/~paolo/tutorial_overview.pdf
Other information: Psi-k, a cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. ESPRESSO is on the list.

R **Q-Chem/Spartan**
Application area: *Ab initio* quantum chemistry
Lead organization: Pittsburgh (PA), US: Q-Chem, Inc. Q-Chem is a developer and provider of quantum chemistry software for *ab initio* electronic structure calculations.
Contributor(s): Martin Head-Gordon
Development model: Commercial
Why this code is interesting: Q-Chem is a comprehensive ab initio quantum chemistry package. Its capabilities range from the highest performance DFT/HF calculations to high level post-HF correlation methods. Q-Chem tackles a wide range of problems in commercial, academic, and government laboratories. Spartan is front-end graphic software.
Status of code: Q-Chem 3.2 is current version, March 2009.
Scalability: Code is available for clusters and parallel environments.
Website(s): http://www.q-chem.com/, http://www.wavefun.com/, http://www.computational-chemistry.co.uk/qchem.html. Open forum is available at USC: http://iopenshell.usc.edu/forum/.

Quickstep (part of CP2D)
Application area:
Lead organization: ETH Zurich, Switzerland
Contributor(s): J. VandeVondele
Development model: Open source
Why this code is interesting:
Status of code:
Scalability:
Website(s): http://cp2k.berlios.de/quickstep.html, https://www.zora.uzh.ch/3175/, http://gow.epsrc.ac.uk/ViewGrant.aspx?GrantRef=EP/F011652/1

TURBOMOLE
Application area: Quantum chemistry
Lead organization: In 2007, the TURBOMOLE GmbH (Ltd) was founded by the main developers of the program: R. Ahlrichs, F. Furche, C. Hättig, W. Klopper, M. Sierka and F. Weigend. The company took over the responsibility for the coordination of the

scientific development of the program, to which it holds all copy and intellectual property rights. Virtually all revenues of the company are spent exclusively on the further program development.
Contributor(s): Karlsruhe, Germany: Reinhart Ahlrichs, F. Furche, C. Hättig, W. Klopper, M. Sierka, F. Weigend
Development model: TURBOMOLE is a quantum chemical program package, initially developed in the group of Prof. Dr. Reinhart Ahlrichs at the University of Karlsruhe and at the Forschungszentrum Karlsruhe. Until 2007 the main development of the program was conducted by students and postdoctoral researches in the group of Ahlrichs, who usually changed their field of work after leaving the group. Therefore, the code was well localized at and, consequently, owned by the University of Karlsruhe. However, in the last years the situation has changed. Reinhart Ahlrichs is retired now and several people, who started their work with TURBOMOLE in Karlsruhe, still make significant contributions and feel responsible for the program, but do no longer reside in Karlsruhe. It was thus necessary to arrange the development of TURBOMOLE in a different manner, namely as a TURBOMOLE company. TURBOMOLE GmbH has granted exclusive responsibility for the distribution, support as well as the software management of TURBOMOLE to COSMOlogic (http://www.cosmologic.de/index.php?cosName=main_qChemistry).
Why this code is interesting: With almost 20 years of continuous development TURBOMOLE has become a valuable tool used by academic and industrial researchers. It is used in research areas ranging form homogeneous and heterogeneous catalysis, inorganic and organic chemistry to various types of spectroscopy, and biochemistry. The philosophy behind the development of the code was, and still is, its usefulness for applications: *"Applications to molecules with more than 100 atoms -of all kinds- are mainly carried out in connection with experiments to check, correct and to predict properties of molecules and their existence."* (Reinhart Ahlrichs)
Status of code: The latest version is TURBOMOLE 6.0.
Scalability: TURBOMOLE is one of the fastest and most stable codes available for standard quantum chemical applications. Unlike many other programs, the main focus in the development of TURBOMOLE has not been to implement all new methods and functionals, but to provide a fast and stable code which is able to treat molecules of industrial relevance at reasonable time and memory requirements.
Website(s): http://www.turbomole.com/, http://www.cosmologic.de/index.php?cosName=main_qChemistry

VASP/VAMP
Application area: Electronic structure on extended systems using plane wave DFT.
Organization: VASP Group at Universität Wien
Contributor(s): Jürgen Hafner (Universität Wien), Georg Kresse (Universität Wien)
Development model: Commercial (Vienna, Austria). VASP has roots in CASTEP/CETEP (version 1989), and has diverged from it roots significantly.
Why this code is interesting: A scientific visualization package for examining output files generated by VASP is available (General Public License): http://vaspview.sourceforge.net/
Status of code: VASP 5.2.2 is the latest release, which is a “mild” update of VASP 4.6.

Scalability:
Website(s): http://cms.mpi.univie.ac.at/vasp/, http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html
Other information: Psi-k, a cooperative organization and website for *ab initio* (from electronic structure) calculation of complex processes in materials is available at http://www.psi-k.org/. A list of electronic structure and related software is available at http://electronicstructure.org/software.asp. VASP is mentioned in the list.

2. Finite Element Analysis (FEA); including mechanics, electromagnetics, CFD and other physics

FEA: Implicit codes solve millions of coupled simultaneous equations. Explicit codes solve millions of uncoupled simultaneous equations.

Explicit methods FEA – requires more time steps but easier to scale

R **LS-DYNA**
Application area: Explicit method FEA for transient dynamics and nonlinear stress analysis
Lead organization: Livermore Software Technology Corp.
Contributor(s): John Hallquist
Development model: Started at LLNL in 1970s as DYNA3D, spun off to LSTC in 1989 as commercial code.
Why this code is interesting: Widely used for crash-testing of vehicles. Scales well. Significant development underway to run tasks currently requiring implicit methods.
Status of code: Stable and supported
Scalability: easily parallelized since explicit method: runs on 65K processors (BlueGene/L), 256 processors (Cray XD1)
Website(s): http://www.lstc.com/lsdyna.htm, http://blog.d3view.com/wp-content/uploads/2007/06/benson.pdf,

S **PAM-CRASH**
Application area: Explicit method Finite element analysis, structural mechanics
Lead organization: esi-group.com, France
Contributor(s):
Development model: commercial, possibly originally derived from DYNA3D
Why this code is interesting: Widely used in automotive and aircraft industries. Scales better than most FEA codes. Direct competitor to LS-DYNA
Status of code: Supported commercially. Proprietary.
Scalability: http://uk.reuters.com/article/idUK61541+18-Mar-2009+MW20090318 1024 CPUs 2-million elements
Website(s): http://www.esi-group.com/products/crash-impact-safety/pam-crash

Implicit Methods FEA – more versatile but harder to scale

s **Code_Aster**
Application area: Implicit method Finite Element Analysis, structural mechanics, 3D thermal analyses, mechanical analyses, linear and nonlinear statics and dynamics
Lead organization: Électricité de France (EDF)
Contributor(s): EDF-R&D plus user community
Development model: Open source; much of development work done by EDF and CEA. 18 years of development in this code and its predecessors.
Why this code is interesting: Part of integrated SALOME-MECA platform. Many types of material models. Carefully tested by EDF
Status of code: Version 10.0 released May 5, 2009
Scalability: Parallel version exists, scalability only to a few tens of processors http://www.iop.org/EJ/article/1742-6596/125/1/012063/jpconf8_125_012063.pdf?request-id=2ff050e9-d7c7-4c6c-8ad5-41ee7248a2f0
Website(s): http://en.wikipedia.org/wiki/Code_Aster, http://www.code-aster.org/V2/spip.php?rubrique2, http://www.code-aster.org/V2/UPLOAD/DOC/Presentation/plaq_V7_GB.pdf
Other information: Much of the documentation is in French.

s **Elmer**
Application area: Implicit (?) finite element analysis multiphysics.
Lead organization: CSC – IT Center for Science, Finland
Contributor(s): Peter Rabeck, Thomas Zwinger
Development model: Open source with CSC doing most of the work. Actively soliciting help and training users.
Why this code is interesting: Appears to scale using iterative methods. Encompasses several types of physics including structural mechanics, fluid dynamics, electromagnetics, and heat transport. Includes preprocessor, FEA engine and postprocessor. Interfaces with several mesh generation tools.
Status of code: Development started in 1995. Stable and supported
Scalability: Appears to scale linearly to a few hundred processors using MPI.
Website(s): http://www.csc.fi/english/pages/elmer, http://www.csc.fi/english/pages/elmer/presentations
Other information: A list of FEA codes, including Elmer, is maintained at http://en.allexperts.com/e/f/fi/finite_element_analysis.htm

ABAQUS, ANSYS, MSC/NASTRAN, NX NASTRAN
Application area: Implicit method FEA
Lead organization:
Contributor(s):
Development model: Commercial and proprietary
Why this code is interesting: Harder to parallelize implicit codes
Status of code:
Scalability:

Website(s):
Other information: These are widely-used commercial implicit FEA codes. As implicit codes, none of them scales well.

Open CASCADE
Application area: 3D solids modeling and numerical simulation framework for CAD/CAM/CAE.
Lead organization: Open CASCADE S.A..S., France
Development model: Open source
Why this code is interesting: Code is developed by a company and maintained as open source. Integrated with the SALOME-MECA platform.
Status of code: Developed since early 90s, version 6.3 released 2008
Scalability:
Website(s): http://www.opencascade.org/, http://www.opencascade.com/
Other information: EDF website indicates that Open CASCADE is superseded by SALOME-MECA

3. Climate/Weather/Ocean Modeling and Simulation

Note: Many ocean models are listed at http://www.ocean-modeling.org/

CM2
Application area: Climate modeling
Lead Organization: Geophysical Fluid Dynamics Laboratory (GFDL), Princeton, NJ
Contributor(s): Tom Delworth (GFDL)
Development model: Developed through U.S. Government funding in government laboratory
Why this code is interesting: The U.S. Geophysical Fluid Dynamic Laboratory (GFDL) CM2.1 coupled model is representative of the state of the art in global climate modeling. The CM2 models became GFDL's workhorse models for computer modeling studies of decadal to century time scale climate variability and change in 2004, and their results figure prominently in the Intergovernmental Panel on Climate Change Fourth Assessment Report (IPCC AR4) and the U.S. Climate Change Science Program (CCSP) reports. The CM2 global climate models consist of atmospheric, land, ocean and sea ice components that interact with each other. The GFDL CM2.0 and CM2.1 models have been shown to be credible at reproducing the decade to decade variations in global mean surface air temperature observed during the 20th century. The models are able to simulate the main features of the observed warming of the twentieth century.
Status of code: The final configuration of the GFDL CM2.0 model was determined in early 2004. The first IPCC-related experiment to be run using CM2.0 (CM2Q_Control-1860_d2) was launched in late April 2004. Other CM2.0 IPCC-related experiments followed until the simulations were completed during autumn 2004. The second member of the CM2.x family of models, CM2.1, was finalized in the late summer of 2004 and the first CM2.1 IPCC-related experiments were launched in September 2004. Only model output (not the code) is available.
Scalability:
Website(s): http://data1.gfdl.noaa.gov/, http://nomads.gfdl.noaa.gov/CM2.X/

s **ECHAM-MAECHAM**

Application area: Climate general circulation model
Lead organization: Max Planck Institut für Meteorologie, Germany
Contributor(s): Erich Roeckner, Max Planck Institute for Meteorology
Development model: Models are made available to the scientific community under the MPI-M Software License Agreement.
Why this code is interesting: ECHAM is a comprehensive general circulation model of the atmosphere. Depending on the configuration the model resolves the atmosphere up to 10 hPa (ECHAM) or up to 0.01 hPa (MAECHAM). The former model has been used extensively to study the climate of the troposphere, the latter allows to include also the middle atmosphere. ECHAM was used in the Fourth Intergovernmental Panel on Climate Change (IPCC) assessment report.
Status of code: The current versions are ECHAM5-MAECHAM5
Scalability: Uses NEC SX6 vector parallel computer
Website(s): http://www.mpimet.mpg.de/en/wissenschaft/modelle/echam/, http://ipcc-wg1.ucar.edu/wg1/Report/AR4WG1_Print_Ch08.pdf (see Chapter 8 on Atmosphere-Ocean General Circulation Model – AOGCM evaluation). http://www.innovations-report.com/html/reports/earth_sciences/report-51622.html
Other information: About the computer:
http://www.hoise.com/primeur/02/articles/monthly/CL-PR-10-02-1.html

HadCM3

Application area: Climate general circulation model
Lead organization: Hadley Centre, United Kingdom
Contributor(s): Alan Dickinson, Director of Science and Technology Hadley Centre
Development model: Open source. Use of the model within the academic community is supported by the National Centre for Atmospheric Science (http://ncas-climate.nerc.ac.uk/).
Why this code is interesting: HadCM3 (Hadley Centre Coupled Model, version 3) is a coupled atmosphere-ocean general circulation model (AOGCM) developed at the Hadley Centre in the United Kingdom. It was one of the major models used in the IPCC Third Assessment Report in 2001. HadCM3 is composed of two components: the atmospheric model HadAM3 and the ocean model (which includes a sea ice model). Other configurations of the Hadley Centre model include atmosphere-only, ocean-only, or an atmosphere coupled to a single-layer or reduced resolution ocean, as well a substantially lower resolution version called FAMOUS. The Stern Review on the Economics of Climate Change, issued in 2006, was based on Met Office Hadley Centre scientific research.
Status of code: The HadCM3 code (Ported Unified Model) was developed on Cray supercomputers, but much work has also gone into producing a ported version of the UM which will run on other platforms including other supercomputers, Unix workstations, personal computers and Beowulf clusters. HadCM3 is normally run using version 4.5. Version 5.5 is now also available, which includes new dynamics, but its coupled climate version (HadGEM) is currently only available to non-Hadley-Centre users under special agreement, so version 4.5 remains popular. For use on other machines, the code for the

UM can be obtained from the Hadley Centre (http://badc.nerc.ac.uk/data/pum/), but access is currently suspended until further notice.
Scalability: As indicated in the status, the model has been implemented on a wide range of parallel computing environments.
Website(s): http://cfpub.epa.gov/crem/knowledge_base/crem_report.cfm?deid=157605, http://www.noc.soton.ac.uk/coapec/models.php, http://www.meto.gov.uk/

HYCOM (Hybrid Coordinate Ocean Model)
Application area: Ocean modeling
Lead organization: University of Miami, Rosenstiel School of Marine and Atmospheric Science
Contributor(s): Miami (FL), US: Alan Wallcraft, George Halliwell, Rainer Bleck, Eric Chassignet
Development model: Open source
Why this code is interesting: In HYCOM, each coordinate surface is assigned a reference isopycnal. The model continually checks whether or not grid points lie on their reference isopycnals and, if not, tries to move them vertically toward the latter. However, the grid points are not allowed to migrate when this would lead to excessive crowding of coordinate surfaces. Thus, in shallow water, vertical grid points are geometrically constrained to remain at a fixed depth while being allowed to join and follow their reference isopycnals over the adjacent deep ocean.
Status of code: The latest release is 2.1.34.
Scalability: HYCOM is targeted to uniprocessors and multiprocessor computers using MPI and OpenMP parallelization.
Website(s): http://hycom.rsmas.miami.edu/hycom-model/index.html

S **IFS (Integrated Forecast System)**
Application area: Medium-range weather forecasting and modeling
Lead organization: European Centre for Medium-Range Weather Forecasts (ECMWF) (http://www.ecmwf.int/). ECMWF is an international organization supported by 31 Member States (http://www.ecmwf.int/about/overview/). ECMWF provides operational medium- and extended-range forecasts (http://www.ecmwf.int/products/forecasts/d/charts) and a state-of-the-art super-computing (http://www.ecmwf.int/services/computing/overview/ibm_cluster.html) facility for scientific research (http://www.ecmwf.int/research/). WCMWF pursues scientific and technical collaboration (http://www.ecmwf.int/about/cooperation/) with satellite agencies and with the European Commission. ECMWF does not carry out climate simulations. However, through its core activity, ECMWF is contributing significantly to climate change studies. Moreover, the EC-EARTH initiative (http://www.ecmwf.int/about/cooperation/EC-leaflet.pdf) by several Member States aims to develop a climate version of the IFS.
Contributor(s): Erland Källén (Head of Research Department) +44 118 949 9003, Agathe Untch (Numerical Aspects Section Head) +44 118 949 9704, Nils Wedi (http://www.ecmwf.int/staff/nils_wedi/index.html), +44 118 949 9000; ECMWF, Shinfield Park, Reading, RG2 9AX, UK.
Development model: Code is free to member countries

Why this code is interesting: Development of IFS was started in 1987 with the aim of providing a single software system delivering a state-of-the-art forecast model. Since then, the code has been in a state of continuous development, incorporating improvements to scientific formulations, modifications to allow efficient utilization of a range of High Performance Computer (HPC) architectures, and technical changes to the structure and expression of the code to improve both its efficiency and maintainability.
Status of code: Current version is Cy31ri, 12 September 2006
Scalability: Scalability is achieved through CPU optimization, OpenMP, and MPI parallelization. Nowadays, a forecast for five days ahead is of the same quality as a forecast for two days ahead in August 1979. ECMWF now uses an IBM Supercomputer comprising 2 clusters each with 155 pSeries p5-575+ servers, each server having 16 1.9 GHz Power5+ processors. The performance of the system is about 4 TFLOPS (sustained). Systems planned for the future call for a sustained performance of 20 teraflops from early 2009, with a gradual increase to between 150 and 200 teraflops sustained by 2015.
Website(s): http://www.ecmwf.int/research/ifsdocs/CY31r1/index.html

s **LES** (Large Eddy Simulation)
Application area: Atmospheric and oceanic flows
Lead organization: Boulder (CO), US: National Center for Atmospheric Research (NCAR)
Contributor(s): Peter Sullivan, Chin-Hoh Moeng, Edward Patton
Development model: The NCAR LES code is freely available to the outside community. Over the years it has been adopted by outside researchers to study a variety of geophysical flows. Requests for the code can be made to Peter Sullivan (pps@ucar.edu), Chin-Hoh Moeng (moeng@ucar.edu), Edward Patton (patton@ucar.edu). The current NCAR LES code was first built in 1984 by Moeng (1984) to study clear convective planetary boundary layers (PBLs) and since then has continuously evolved to include a variety of physical processes, e.g., clouds, chemistry, shear and stable stratification, vegetative surface canopies, and Langmuir cells and wave breaking in the ocean mixed layer. The basic numerical algorithm is a mixed pseudo-spectral finite difference code with third-order Runge-Kutta time stepping utilizing a staggered vertical grid with options for variable spacing. This base algorithm has been extended to a cell centered co-located grid architecture that allows for the resolution of time varying sinusoidal waveforms.
Why this code is interesting: Understanding turbulent flow is central to many important problems including environmental and energy related applications (global change, mixing of fuel and oxidizer in engines and drag reduction), aerodynamics (maneuvering flight of jet aircraft) and biophysical applications (blood flow in the heart, especially the left ventricle). Turbulent flow is composed of coherent patches of swirling fluid called eddies. These range in size from large storm systems such as hurricanes to the little swirls of air shed from a butterfly's wings. Large Eddy Simulation (LES) seeks to predict the motion of the largest and most important eddies uncoupled from the small eddies. This uncoupling is important because the large eddies are resolvable on a computational mesh (a collection of chunks of the physical problem) which can be handled by a supercomputer.

Status of code: The NCAR LES code will continue to evolve to take advantage of new computer hardware and algorithm developments as well as advances in subgrid-scale parameterizations.
Scalability: The code is written to run on massively parallel computer architectures using the Message-Passing Interface (MPI) and OpenMP programming models. Work in the vertical (z-) direction is partitioned across compute nodes using MPI with horizontal (x-y) work split across multiple OpenMP threads.
Website(s): http://www.mmm.ucar.edu/applications/les/les.php

NEMO (Nucleus for European Modelling of the Ocean), Paris, France
Application area: Ocean and climate modeling
Lead organization: LOCEAN-IPSL, Paris is coordinator of the Systems Team. Evolutions and reliability of NEMO are organised and controlled by a European Consortium between CNRS, Mercator-Ocean, UKMO and NERC.
Contributor(s):
Development model: NEMO is available under CeCILL license (public license).
Why this code is interesting: NEMO is a state-of-the-art modeling framework for oceanographic research, operational oceanography seasonal forecast and climate studies.
Status of code*:* The latest version is NEMO release nemo_v3_1
Scalability:
Website(s): http://www.nemo-ocean.eu/

PSTSWM (Parallel Spectral Transform Shallow Water Model)
Application area: Global atmospheric circulation modeling
Lead organization: Oak Ridge National Laboratory
Contributor(s): PSTSWM was originally developed by P. H. Worley at Oak Ridge National Laboratory and by I. T. Foster at Argonne National Laboratory as part of the Department of Energy CHAMMP research program. Worley has been responsible for most subsequent development.
Development model: Research code
Why this code is interesting: PSTSWM is a message-passing benchmark code and parallel algorithm testbed that solves the nonlinear shallow water equations on a rotating sphere using the spectral transform method. It is a parallel implementation of STSWM, developed by J. J. Hack and R. Jacob at the National Center for Atmospheric Research (NCAR) and used to generate reference solutions for shallow water test cases.
Status of code: Version 6.9 now available
Scalability: PSTSWM was developed to evaluate parallel algorithms for the spectral transform method as it is used in global atmospheric circulation models. Multiple parallel algorithms are embedded in the code and can be selected at run-time, as can the problem size, number of processors, and data decomposition.
Website(s): http://www.csm.ornl.gov/chammp/pstswm/index.html, http://www.csm.ornl.gov/chammp/
Other information: World Wide Web climate groups are listed at http://www.csm.ornl.gov/chammp/Climate/climategrps.html

SEA (The Southampton - East Anglia Parallel Ocean Circulation Model)
Application area: Ocean modeling
Lead organization: University of East Anglia, Norwich, UK
Contributor(s): Dave Stevens, Matt Beare, Andrew Coward, Beverly de Cuevas, John Johnson, Catherine Richmond, David Webb
Development model: Open source
Why this code is interesting: SEA is a three-dimensional finite difference, primitive equation, ocean general circulation model, based around the successful Bryan-Semtner-Cox formulation. As part of an on-going project the aim of SEA is to provide an ocean general circulation model (OGCM) suitable for running in a wide variety of configurations, on a wide range of computer platforms, both parallel and sequential. The technical intricacies of parallelism are, as much as possible, hidden from the user, thus easing the transition from traditional scalar computers, to clusters of workstations and massively parallel processors (MPPs).
Status of code: The latest version is SEA version 3.1 (December 1998).
Scalability: SEA is designed to give good performance on high powered workstations, clusters of workstations and message passing massively parallel processing systems, rather than vector processors.
Website(s): http://www.uea.ac.uk/menu/acad_depts/mth/ocean/SEA/

WRF (Weather Research and Forecasting Model)
Application area: Weather forecasting
Lead organization: National Center for Atmospheric Research (NCAR), Boulder (CO), US
Contributor(s): Jimy Dudhia (NCAR), Bill Skamarock (NCAR), Xiang-Yu Huang (NCAR)
Development model: Open source
Why this code is interesting: The current WRF (Weather Research and Forecasting Model) software framework (WSF) supports two dynamical solvers: the Advanced Research WRF (ARW, Users' page) developed and maintained by the Mesoscale and Microscale Meteorology Division of NCAR, and the nonhydrostatic Mesoscale Model (NMM, Users' page) developed by the National Centers for Environmental Prediction with user support provided by the Developmental Testbed Center.
Status of code: The latest version is WRF Version 3.1
Scalability: The software is designed to be a flexible, state-of-the-art atmospheric simulation system that is portable and efficient on available parallel computing platforms.
Website(s): http://www.wrf-model.org/users/users.php, http://www.mmm.ucar.edu/wrf/users/, http://www.dtcenter.org/wrf-nmm/users/ http://www.ncar.ucar.edu/index.php/ncar/articles/modeling_the_atmosphere_at_video_game_speed

CCSM (Community Climate Systems Model)
Application area: General Circulation Model for predicting climate; includes atmospheric models, ice models, land models, ocean models, and the coupler that links them all together
Lead organization: National Center for Atmospheric Research

Contributor(s):
Development model: open source, large community, modular structure allowing different sub-models to be used
Why this code is interesting: Major climate model, used for IPCC studies
Status of code: Stable, long-term development, version 3.0 released June 2004
Scalability: highly scalable
Website(s): http://www.ccsm.ucar.edu/models/ccsm3.0/

4. Computational Fluid Dynamics (CFD)

FLUENT
Application area: Fluid dynamics
Lead organization: ANSYS, Inc., Canonsburg (PA), US.
Contributor(s):
Development model:
Why this code is interesting: FLUENT software contains the broad physical modeling capabilities needed to model flow, turbulence, heat transfer, and reactions for industrial applications ranging from air flow over an aircraft wing to combustion in a furnace, from bubble columns to oil platforms, from blood flow to semiconductor manufacturing, and from clean room design to wastewater treatment plants.
Status of code: The current version is ANSYS 12.0.
Scalability: Advanced solver technology provides fast, accurate CFD results, flexible moving and deforming meshes, and superior parallel scalability. Scaling of ANSYS FLUENT Advanced parallel processing numerics can efficiently utilize multiple, multi-core processors in a single machine and in multiple machines on a network. Dynamic load balancing automatically detects and analyzes parallel performance and adjusts the distribution of computational cells among the processors so that a balanced load is shared by the CPUs even when complex physical models are in use.
Website(s): http://www.ansys.com/products/fluid-dynamics/fluent/

S **OpenFOAM** (Open Field Operation and Manipulation)
Application area: CFD including chemical reactions, solid dynamics, electromagnetics.
Lead organization: OpenCFD Ltd, UK
Contributor(s): Henry Weller
Development model: Open source. Code development managed by small company that makes money supporting and applying the code. Larger open source community that contributes to development.
Why this code is interesting: Development model appears not to be funded by large external source, rather by a champion who has mobilized an open source community to produce one of the better CFD codes with reasonable scalability. Code uses modern program techniques, written in C++ using object oriented techniques. Code has been available since 2004 with continuous development. Henry Weller, head of OpenCFD and champion of OpenFOAM, was trained at Imperial College, London.
Status of code: Stable with ongoing development – latest code release OpenFOAM version 1.6 released 7/28/2009
Scalability: Reportedly scales well to hundreds of processors, e.g. http://openfoamfoorumi.com/wordpress/?p=24

Website(s): http://opencfd.co.uk/openfoam/index.html, http://foamcfd.org/
Other information: A list of CFD codes, including OpenFOAM, is maintained at http://www.cfd-online.com/Links/soft.html. A review is available at http://www.innovative-cfd.com/free-cfd.html

STAR-CD
Application area: Fluid dynamics, thermal and stress continuum mechanics
Lead organization: CD-adapco (New York, London, Yokohama)
Contributor(s): Steve MacDonald, President of CD-adapco
Development model: Commercial
Why this code is interesting: The latest release, STAR-CD V 4, introduces the capability to perform structural analysis calculations using a methodology based upon its industry-leading CFD solver technology, the first time that a comprehensive solution for flow, thermal, and stress simulation has been available in a single general-purpose commercial finite-volume code. It is capable of simulating engineering problems that involve turbulence, combustion, heat transfer, reacting flows and multiphase physics.
Status of code: The latest version is STAR-CD V 4
Scalability:
Website(s): http://www.cd-adapco.com/products/STAR-CD/index.html

OVERFLOW
Application area: Compressible Navier-Stokes 3D fluid dynamics. Time advancement uses first-order implicit methods
Lead organization: NASA Langley and Ames
Contributor(s): Pieter Buning, Bob Meakin, Dennis Jespersen
Development model: Government-funded
Why this code is interesting: Widely used for aeronautics studies in government and industry
Status of code: In long-term production; open-source distribution limited to permanent U.S. residents
Scalability: Scales efficiently to hundreds of processors or more
Website(s): http://aaac.larc.nasa.gov/~buning/codes.html
Other information: http://www.hq.nasa.gov/hpcc/insights/vol5/overflow.htm, http://halfdome.arc.nasa.gov/cfd/CFD4/New_Page/Overflow-D2.htm, http://www.innovative-cfd.com/computational-fluid-dynamics-software.html

5. Computational Electromagnetics and Acoustics

Several FEA codes have electromagnetic capability. In addition, the following code shows promise for good scaling.

AMS (Auxiliary space Maxwell Solver)
Application area: Scalable solver for Maxwell's equations
Lead organization: Lawrence Livermore National Laboratory
Contributors: Tzanio Kolev and Panayot Vassilevski, LLNL; Jinchao Xu, Penn State University; Ralph Hiptmair, ETH, Zurich; Joseph Pasciak, Texas A&M University
Development model: Government funding of small team

Why this code is interesting: Extreme scalability if the code becomes a production code
Status of code: Experimental
Scalability: AMS exhibits weak scalability: the solution time is constant as the problem size and processor workload simultaneously increase.
Website(s): https://www-eng.llnl.gov/mod_sim/mod_sim_em.html, http://www.scidacreview.org/0901/html/bt.html#electro, https://www-eng.llnl.gov/mod_sim/mod_sim_em.html, http://www.docstoc.com/docs/640864/LLNL-LLNL-Falgout-FY---Fiscal-Year-2006-Accomplishments

6. Integrated Code Suites

CAELinux
Application area: Integrated suite for multiphysics. Pre-assembled codes include SALOME-MECA (integrating framework), OpenFOAM (CFD), Code_Aster (FEA), DynELA (non-linear explicit FEA), Code_Saturne (CFD), Elmer (FEA), gmsh (mesh generation) , Impact (non-linear explicit FEA), Paraview (visualization).
Lead organization: Electricite de France
Contributor(s):
Development model: Open source, free download of .iso file to burn boot DVD with full system including Ubuntu Linux (run from DVD or install)
Why this code is interesting: This Linux distribution packages several codes for CFD, FEA, heat transfer, and electromagnetics, with mesh generation and other preprocessing, postprocessing, and GUI front-ends to simplify problem generation, solution, and analysis.
Status of code: CAELinux 2009 released; several prior releases
Scalability: Some codes scale, others not
Website(s): http://caelinux.com/CMS/index.php?option=com_frontpage&Itemid=1

s **SALOME-MECA**
Application area: Integration platform for pre and post-processing for numerical simulation.
Lead organization: Commissariat a l'Energie Atomique (CEA) and Electricite de France (EDF.)
Contributor(s):
Development model: Integrates large companies, small companies, private laboratories and public laboratories in France to develop unified code.
Why this code is interesting: Framework under which user can run Code Aster (Finite Element), Code_Saturne (CFD), SYRTHES (heat transfer), OpenFOAM (CFD), and other solvers. SALOME interfaces with CAD format standards such as STEP Includes geometry and mesh generation, data preparation, and post-visualization. High level integration and customization in Python. Uses CORBA for inter-process communication.
Status of code: Stable with ongoing development since 2000. Follow-on to Open CASCADE. Latest release is SALOME v5.1.2, 7/31/2009. CAELinux 2009 is an integrated prepackaged Linux distribution based on Ubuntu that includes Solome-Meca and several other integrated codes..
Scalability: Claims to run on parallel computers.

Website(s): http://www.salome-platform.org/home/presentation/overview, http://caelinux.com/CMS/index.php?option=com_frontpage&Itemid=1

Appendix B: Comprehensive List of Engineering Codes

Codes are listed in alphabetical order. In the first column "*com*" means commercial, and "*free*" means without cost but not necessarily open source.

ABAQUS *com*	finite element analysis	http://www.simulia.com/products/abaqus_fea.html Providence (RI), US
ABINIT *free (GPL)*	DFT materials: molecules and periodic solids	http://www.abinit.org/, http://www.abinit.org/developers/abinit-dev-doc/abinit-1/Highlight_90.pdf/, http://www.abinit.org/about/presentation.pdf, Xavier Gonze (Belgium), since 2000
ADF *com*	density functional program for quantum chemistry	http://www.scm.com/ Amsterdam, The Netherlands: S. J. A. van Gisbergen
ALE3D	multi-physics modeling	LLNL. https://wci.llnl.gov/codes/ale3d/ http://endo.sandia.gov/SEACAS/Documentation/SEACAS.html
Alya System	large scale computational mechanics	http://www.bsc.es/plantillaA.php?cat_id=552 Barcelona, Spain: M. Vázquez, G. Houzeaux, J.M. Cela
Amber *com*	molecular dynamics	http://ambermd.org/ San Francisco (CA), US: D.A. Case, T.A. Darden, T.E. Cheatham, III, C.L. Simmerling, J. Wang, R.E. Duke, etc.
AMR *free*	gas dynamics	Includes Hpyerclaw, LBNL, CA, https://ccse.lbl.gov/Publications/car/ParHyper.pdf, https://seesar.lbl.gov/CCSE/Research/Hyperbolic/index.html
ANSYS *com*	multiple engineering packages	http://www.ansys.com/ Canonsburg (PA), US
ANSYS Workbench *com*	multiphysics framework	http://www.ansys.com/assets/brochures/workbench-platform-12.0.pdf
AVUS *free with restrictions*	CFD	Parallel, implicit unstructured grid Navier-Stokes flow solver developed by the Computational Sciences Branch of the Air Force Research Laboratory, WPAFB, Ohio, http://www.afrl.hpc.mil/software/info/avus/
Babel *free*	file format converter for chemistry codes	http://openbabel.sourceforge.net/, Open Babel wiki
Band	a density functional band-structure program (part of ADF)	http://www.scm.com/

CalculiX *free*	structural finite element	http://www.calculix.de/ Germany: Guido Dhondt, Klaus Wittig
Cart3D	analysis package for conceptual and preliminary aerodynamic design	http://people.nas.nasa.gov/~aftosmis/cart3d/
CASTEP *com*	atomic-level materials modeling	http://www.castep.org/ Cambridge, UK: Mike Payne
CCPForge	collaborative software development	http://ccpforge.cse.rl.ac.uk/ Warrington, UK
CDF++		Metacomp. http://www.metacomptech.com/ http://www.afrl.hpc.mil/software/info/cfd++/
CHARMM *com*	force field based molecular modeling program for biological macromolecules	http://www.charmm.org/ Cambridge (MA), US: Martin Karplus
CM2 *model output available*	climate modeling	http://data1.gfdl.noaa.gov/, http://nomads.gfdl.noaa.gov/CM2.X/ Geophysical Fluid Dynamics Laboratory, Princeton, NJ
Cobalt *com*	CFD, especially unsteady flow	Derived from code developed at WPAFB, now known as AVUS, Cobalt Solutions, LLC, http://www.cobaltcfd.com/index.php/site/software/cobalt/
Code_Aster *free*	structural mechanics finite element	http://www.code-aster.org/V2/spip.php?rubrique2 France
Code_Saturne *free*	fluid dynamics	http://research.edf.com/the-edf-offers/research-and-development/softwares/code-saturne-107008.html France
Corina *com*	a program to generate 3D structures	http://www.molecular-networks.com/software/corina/index.html
COMET	finite-volume-based program package for modelling coupled physics problems	CD-adapco http://www2.hlrn.de/doc/comet/index.html#general
CP2K *free*	atomistic and molecular simulations	http://cp2k.berlios.de/ Zurch, Switzerland: G. Lippert, J. Hutter, M. Parrinello

CPMD *free to nonprofits*	Car-Parrinello molecular dynamics	http://www.cpmd.org/ Stuttgart, Germany: Michele Parrinello, Jurg Hutter, D. Marx, P. Focher, M. Tuckerman, W. Andreoni, etc.
CRUNCH	multi-element unstructured grid, all-speed Navier-Stokes code (from incompressible to supersonic flows)	Craft Technologies, http://www.craft-tech.com/html/products.html
CRYSTAL *com*	solid state chemistry and physics	http://www.crystal.unito.it/ Pisa, Italy: R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C.M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I.J. Bush, Ph. D'Arco, M. Llunell
CTH *com*	shock wave physics	Sandia National Labs, http://www.sandia.gov/media/NewsRel/NR2001/cth.htm
Dalton *free*	quantum chemistry	http://www.kjemi.uio.no/software/dalton/dalton.html Oslo, Norway: C. Angeli, K. L. Bak, V. Bakken, O. Christiansen, R. Cimiraglia, etc.
Discover *com*	module for force field based molecular modeling (Discovery Studio).	http://accelrys.com/products/discovery-studio/
Discovery Studio *com*	modeling environment for molecular and drug design studies	http://accelrys.com/products/discovery-studio/
DL-POLY *free to academics*	molecular dynamics	http://www.cse.scitech.ac.uk/ccg/software/DL_POLY/ Warrington, UK: William Smith
DMol3	density functional program for quantum chemistry	Part of Materials Studio http://accelrys.com/products/materials-studio/
DYNA3D *free with restrictions*	explicit FEA	Lawrence Livermore National Laboratory, https://www-eng.llnl.gov/mdg/mdg_codes_dyna3d.html
DynELA	large deformation FEA	http://pantale.free.fr/DynELA/frame.htm, in French

ECCE	computational chemistry visualization and graphics	http://ecce.pnl.gov/
Elmer *free*	FEA multiphysics (fluid dynamics, struct.mech., eletromag, heat)	http://www.csc.fi/english/pages/elmer (Parallel scaling demonstrated, uses iteration; may scale to hundreds of nodes) Thomas Zwinger, Peter Rabeck
EPIC	explicit, dynamic, Lagrangian finite-element code for the simulation of the mechanical and thermal responses of solids	Network Computing Services Inc. http://www.afrl.hpc.mil/software/info/epic/ http://epic.org/privacy/socialnet/default.html
ESPRESSO *free*	materials modeling	http://www.quantum-espresso.org/ Princeton, US
FEAP *com*	general purpose finite element	http://www.ce.berkeley.edu/projects/feap/ Berkeley (CA), US
Fluent	CFD application	Ansys. http://www.afrl.hpc.mil/software/info/fluent/ http://www.fluent.com/
FreeCFD	fluid dynamics	http://www.freecfd.com/about/ Emre Sozer, Ez Hassan
GAMESS *free*	molecular electronic structure	http://www.msg.chem.iastate.edu/gamess/ Ames (IA), US: M.S. Gordon, M.W.Schmidt
GAMESS-UK *free to UK academics*	molecular electronic structure	http://www.cfs.dl.ac.uk/ Warrington, UK: M.F. Guest, I. J. Bush, H.J.J. van Dam, P. Sherwood, J.M.H. Thomas, J.H. van Lenthe, etc.
Gaussian *com*	computational chemistry	http://www.gaussian.com/ Connecticut, US: John Pople, Walter Kohn
GeoFEM *free*	finite element for solid earth	http://geofem.tokyo.rist.or.jp/ Tokyo, Japan: Hiroshi Okuda, Jun Yin, Kengo Nakajima
GMSH *free*	finite element mesh generator	http://geuz.org/gmsh/ Belgium: Christophe Geuzaine, Jean-François Remacle
gOpenMol *free*	molecular visualization and analysis program	http://www.csc.fi/english/pages/g0penMol/index_html

GPAW *free*	DFT in real space and scaling to hundreds of processors	Based on the projector-augmented wave (PAW) method. https://wiki.fysik.dtu.dk/gpaw/
GROMACS *free*	molecular dynamics	http://www.gromacs.org/, most recent release gromacs 4.0.5, 5/19/2009, biological molecules?
HadCM3 *free*	general circulation	http://cfpub.epa.gov/crem/knowledge_base/crem_report.cfm?deid=157605, http://www.noc.soton.ac.uk/coapec/models.php, http://www.meto.gov.uk/ Hadley Centre, United Kingdom
HYCOM *free*	ocean modeling	http://hycom.rsmas.miami.edu/hycom-model/modelcode.html Miami (FL), US: Alan Wallcraft, George Halliwell
ICEPIC *free*	particle-in-cell magnetohy-drodynamics	Peter Mardahl, Air Force Research Lab, NM
Impact *free*	explicit finite element	http://impact.sourceforge.net/, http://impact.sourceforge.net/Impact_and_GiD_integration_paper.pdf Jonas Forssell, Sweden
ISAAC *free*	fluid dynamics	http://isaac-cfd.sourceforge.net/ Hampton (VA), US: Joseph H. Morrison
Jaguar	high-performance *ab initio* package for both gas and solution phase simulations	Schrodinger http://www.schrodinger.com/ProductDescription.php?mID=6&sID=9
KRATOS	FEA multiphysics	http://kratos.cimne.upc.es/kratoswiki/index.php/Main_Page, http://www.cimne.com/kratos/, a framework somewhat like PETsC
LAMMPS *free*	molecular dynamics	http://lammps.sandia.gov/ Albuquerque (NM), US: Steve Plimpton, Paul Crozier, Aidan Thompson
LISA *commercial*	finite element	http://www.lisa-fet.com/, http://www.freebyte.com/cad/fea.htm Canada
LS-DYNA *com*	finite element analysis	http://www.lstc.com/lsdyna.htm Livermore (CA), US: John O. Hallquist
Materials Studio *com*	a modeling environment comprising a number of accelrys modules	http://accelrys.com/products/materials-studio/

MCNPX	code for modeling the interaction of radiation with everything.	http://www.arl.hpc.mil/Applications/description.php?sw=MCNPX https://mcnpx.lanl.gov/
MolCAS *com*	quantum chemistry	http://www.teokem.lu.se/molcas/ Lund, Sweden: R.Lindh
MolPro *com*	system of *ab initio* programs for molecular electronic structure calculations	http://www.molpro.net/ http://www.molpro.net/info/current/doc/molpro.bib Stuttgart, Germany: H.-J. Werner and P. J. Knowles
MOPAC *free to academics*	Molecular Orbital Package: semi-empirical quantum chemistry program based on Dewar and Thiel's NDDO approximation.	http://openmopac.net/
NAMD *free*	scalable molecular dynamics	http://www.ks.uiuc.edu/Research/namd/ Urbana-Champaign (IL), US: Klaus Schulten, Laxmikant V. Kalé, Robert D. Skeel
NASTRAN *com*	finite element analysis	http://www.mscsoftware.com/ Santa Ana (CA), US
NEC	Numerical Electromagnetics Code	Lawrence Livermore National Laboratory. http://www.afrl.hpc.mil/software/info/nec/ http://www.nec2.org/
Nemesis	experimental finite element code	http://www.nemesis-project.org/index.php/Main Page, F.E. Karaoulanis
NWChem *free*	parallel quantum chemistry	http://www.emsl.pnl.gov/docs/nwchem/nwchem.html Richland (WA), US: E. J. Bylaska, W. A. de Jong, N. Govind, K. Kowalski, T. P. Straatsma, M. Valiev, D. Wang, E. Apra, etc.
OCTA *free*	multiscale polymer code	http://octa.jp/ Nagoya, Japan: Masao Doi
ONETEP *com*	quantum-mechanical calculations	http://www2.tcm.phy.cam.ac.uk/onetep/ Cambridge, UK: Mike Payne, Peter Haynes, Chris-Kriton Skylaris, Arash A. Mostofi
OOFEM *free (GPL)*	FEA – explicit and implicit	http://www.oofem.org/en/oofem.html, Borek Patzak, Prague Czech Republic. Reportedly scales well using MPI
OpenFVM *free*	fluid dynamics	http://openfvm.sourceforge.net/, parallel version uses PETSc

OpenFOAM *free*	fluid dynamics	http://www.opencfd.co.uk/openfoam/ Caversham Reading Berkshire, UK
OVERFLOW *free with restrictions*	fluid dynamics	http://www.hq.nasa.gov/hpcc/insights/vol5/overflow.htm, Pieter Buning, NASA Langley
PAM-CRASH *com*	explicit FEA physics-based simulation	http://www.esi-group.com/products/crash-impact-safety Paris, France: Alain de Rouvray
ParMETIS *free download*	parallel mesh partitioning	http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview University of Minnesota, George Karypis, ParMetis 3.1.1 released 11/18/08
PETSc *free*	data structures and routines for parallel solution of PDEs	Argonne National Laboratory, http://www.mcs.anl.gov/petsc/petsc-as/,
Prometheus *free*	scalable unstructured finite element solver	http://www.columbia.edu/~ma2325/prometheus/, solved problems of over 76M degrees of freedom on 1024 processors; built on PETSc
Qbox *free download*	first principles molecular dynamics	http://eslab.ucdavis.edu/software/qbox/index.htm, Francois Gygi, UC Davisdesigned for large parallel computers
Q-Chem Spartan *com*	quantum chemistry	http://www.q-chem.com/ http://www.computational-chemistry.co.uk/qchem.html Pittsburgh (PA), US: Martin Head-Gordon
Quantum ESPRESSO	electronic-structure calculations and materials modeling	DEMOCRITOS National Simulation Center. http://adsabs.harvard.edu/abs/2009arXiv0906.2569G
Quickstep *free*	part of CP2K	https://www.zora.uzh.ch/3175/ http://gow.epsrc.ac.uk/ViewGrant.aspx?GrantRef=EP/F011652/1 Zurich, Switzerland: J. VandeVondele
Salome *free*	multiphysics simulations	http://www.salome-platform.org/home/presentation/overview/ Paris, France
SCTB	evaluates the total energy, atomic forces, and virial, as well as the electronic structure of a collection of atoms	NRL. http://cst-www.nrl.navy.mil/bind/sctb/

SEACAS	Engineering Analysis Code Access System (SEACAS)	Sandia. http://endo.sandia.gov/SEACAS/Documentation/SEACAS.html
SESP standards group	Software Engineering Support Program	http://www.cse.scitech.ac.uk/ccg/reports/SESP_report.shtml Warrington, UK: Graham Fletcher, Jens Thomas, Chris Greenough
SIERRA/ PRESTO	three-dimensional explicit, transient dynamics code for the analysis of solids	SNL. https://cfwebprod.sandia.gov/cfdocs/CCIM/docs/cug09_paper_rajan.pdf
SIESTA *free to academics*	electronic structure	http://www.icmab.es/siesta/ Madrid, Spain: Arturo Baró
Sybyl *com*	discovery software for computational chemistry and molecular modeling	http://www.tripos.com/
STAR-CD *com*	fluid dynamics	CD-adapco, http://www.cd-adapco.com/about/index.html
Tinker 4.2 *free*	molecular mechanics and dynamics	http://dasher.wustl.edu/tinker/
TurboMole *com*	efficient parallel *ab initio* and DFT program	http://www.turbomole.com/ Karlsruhe, Germany: Reinhart Ahlrichs, F. Furche, C. Hättig, W. Klopper, M. Sierka, F. Weigend
VASP/VAMP *com*	materials modeling	http://cms.mpi.univie.ac.at/vasp/ Vienna, Austria: Jurgen Hafner, Georg Kresse
VMD	Graphical tool for MD visualization and analysis	http://www.ks.uiuc.edu/Research/vmd/
WIEN2k *com*	chemical structure of solids	http://www.wien2k.at/ Vienna, Austria: P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz
Wind-US *free with restrictions*	fluid dynamics	NPARC Alliance, http://www.innovative-cfd.com/cfd-analysis-software.html

XPATCH	set of prediction codes and analysis tools that use the shooting-and-bouncing ray (SBR) method	Saic. http://www.saic.com/products/software/xpatch/
Zoltan	efficient mesh generation	http://www.cs.sandia.gov/~kddevin/papers/Zoltan_Tutorial_Slides.pdf, http://www.cs.sandia.gov/Zoltan/, Sandia National Lab, v3.1 released 9/08

Electronic Structure Codes: http://electronicstructure.org/software.asp