CAST Communications

VOL. 24 NO. 2 Winter 2001

CAST (Computers and Systems Technology) is a division of the AIChE (American Institute of Chemical Engineers)

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Important Notice

This issue is the first "on-line-only" copy of *CAST Communications*. We will use the next two issues as a test bed for on-line delivery, with a postcard Table of Contents sent out as a reminder that a new issue has come out. The full issue will be in the same pdf format and in the same location at www.castdiv.org as previous issues. For the issue after that, we may move the newsletter to a password-protected website or to a website announced only to CAST membership.

Please let Peter Rony or Karl Schnelle know what you think about these changes and if we should make them permanent.

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EDITORIAL NOTES

About This Issue

By Peter R. Rony (rony@vt.edu) and
Karl D. Schnelle (kschnelle@dowagro.com)

Once again we honor our CAST Division award recipients, Professor Christos Georgakis (Computing in Chemical Engineering Award), Dr. Chau-Chyun Chen (Computing Practice Award), and Dr. Ashish Gupta (Ted Peterson Student Paper Award). The basis for selecting each winner is described in the article, "2001 CAST Award Winners", by Mark Stadtherr and Karl Schnelle.

We thank Fluent Incorporated authors Engelman, Choudhury, and Marshall for our feature article, "CFD Technology: What Does the Future Hold?" Because this article is available on-line in PDF format, the reader has the added benefit of viewing all the figures in color.

This is the third issue of *CAST Communications* that does not contain the "Meetings, Conferences, . . ." section, which is available only at the CAST division web site, www.castdiv.org/MeetingsandConferences.htm.

E-ADVISORY COMMITTEE

The AIChE has recently created an E-Advisory Committee, of which your editor is a member. Other members include:

- Prof. Tom Edgar, Chair of E-Advisory Committee and former AIChE president;
- Steven R. Smith, Senior Director of AIChE Publications & Information Technology;
- Al Wechsler, AIChE Strategic Planning Facilitation Team Member;
- Eileen Webb, the Chemical Engineering Technology Operating Council;
- Chris Sowa, the Career and Education Operating Council (and AspenTech);
- John Saylor, engineering librarian at Cornell;
- Marty Greubel of Seabury & Smith;
- Hendakar Dandekar, Eastman Chemical;
- Prof. Brice Carnahan, University of Mich.

The issue statement for the committee is as follows:

"AIChE's members and customers are generally computer and web literate. The launch of the Institute's web site has been successful, with use regularly increasing. Member surveys show that they want more products and services available electronically. Our chemical engineering competition is developing sophisticated web sites for their offerings. Our vision to be the global leader will be advanced by increasing our capability to disseminate knowledge electronically. Electronic interaction is required for our international members and customers. Exploitation of electronic interactions with our members and customers will improve the value of AIChE membership, provide a more user-friendly relationship with customers and improve the image of the Institute as a leading technological organization.

***"Implications for AIChE:** It is necessary to increase electronic availability of Institute offerings to attract new members and retain current members. Similarly, products and services need to be made available online in a user-friendly manner to increase revenues. Failure to keep pace electronically would be detrimental to the image and, perhaps, the viability of the Institute.*

***"Data and Questions Suggested to Understand the Issue:** How does AIChE use the E-World to maximize its effectiveness.*

1. *What products, services, and other offerings have been successfully put online by others, and which have not been successful?*
2. *What are the costs for developing a state-of-the-art e-commerce site? What are the benefits and payback time?*
3. *What technical support and customer service are needed to support e-commerce?*
4. *How will online development expand revenues and membership? What have been the experiences of other organizations?*
5. *What are the policies and practices of other organizations for archiving, privacy and fees?*
6. *What specific functions have other organizations outsourced? What are the pros and cons?"*

We would appreciate your perspectives on the E-Advisory Committee issue statement. Please send your comments by email either to the editor, rony@vt.edu, or else to Stephen R. Smith, Senior Director - Publications & Information Technology, American Institute of Chemical Engineers, Three Park Avenue, New York, NY 10016-5901, telephone 212-591-7335, fax 212-591-8883, e-mail steps@aiche.org. Thank you.

FEATURE ARTICLE

CFD Technology: What Does the Future Hold?

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INTRODUCTION

The field of computational fluid dynamics, or CFD, has grown and changed rapidly during the past twenty years. It is tempting to question whether this growth could have been predicted during the early years, or whether the nature of the changes could have been anticipated. Given the advances in computer technology that we have all witnessed during this time – in both hardware and software – it is perhaps even more tempting to question what changes will take place during the next twenty years. While a twenty year perspective on any current technology would be difficult to perform, certain indicators do exist that allow a forecast of trends in the technology to be made. A number of the components of CFD technology are examined below. In addition to summarizing the current states in each of these areas, the anticipated trends that are likely to occur in future generations of CFD software are also described.

MODEL CREATION/CAD INTEGRATION

At the root of every CFD simulation is a discretized model of the solution domain. This consists of a geometric description of the region being modeled (a mixing vessel, for example) and all of the relevant internals. Fitted to this geometry is a grid, or mesh, consisting of triangles or quadrilateral elements for two-dimensional simulations and four-, five-, or six-sided elements for three-dimensional simulations (hexahedra or pyramids, for example). Conservation equations for all the relevant problem variables are solved in each of these elements during a solution until overall balances are achieved.

In the early years, creation of the geometry and grid for CFD purposes was an arduous task. CAD packages, used by manufacturing companies for component design and stress analysis, could not often meet the grid requirements demanded by the CFD solvers of the day. Advances on the solver side as well as on the CAD side have allowed these two technologies to work more closely together in recent years. It is now commonplace for CFD practitioners to pull CAD geometries from their design department, and use either the CAD package or the CFD package to build a suitable mesh for a CFD simulation. Both packages are likely to have automatic meshing tools that build and refine a mesh automatically with only minimal intervention from the user. The CAD/CFD integration will only strengthen in the future. In some cases, it is possible that two of these packages will merge and use a common interface. Perhaps more likely than simply coupling their interface together is that two such packages will couple their calculations together.

For example, the CAD package will be used to design a prototype geometry and corresponding mesh. The CFD solver will perform an analysis on the mesh, from which stresses on the system can be predicted. These stresses will be fed back to the CAD package, where the geometry will be

(continured on next page)

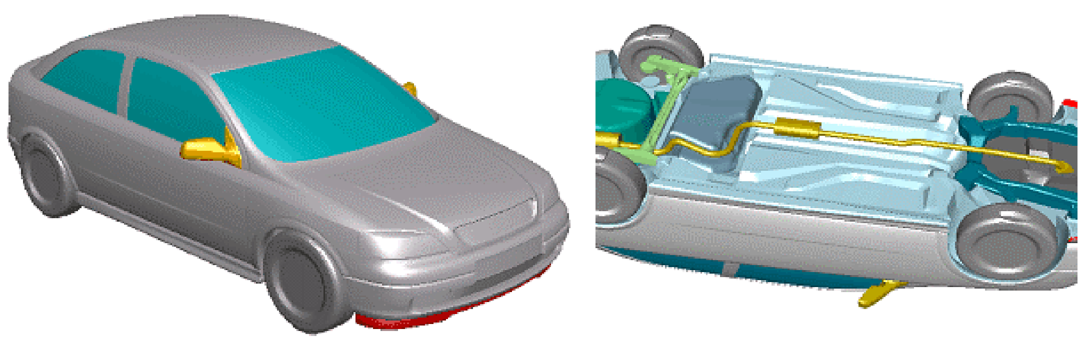

Figure 1: At Opel AG in Germany, engineers use a combination of UNIGRAPHICS for CAD, ANSA for CAD and mesh generation, GAMBIT and TGrid for additional mesh generation, and FLUENT for CFD. Individual vehicle parts and components from a common database at Opel are combined with the body shell data for the ASTRA, shown above, for exterior aerodynamics simulations. Courtesy of Opel AG.

altered in response. The ability to optimize the design of a part or the workings of a process is a common thread that will likely be present in several aspects of CFD modeling in the future.

Along with improved means of building and refining meshes, greater flexibility on the solver side will allow more variety in the mesh itself. In particular, the solvers will have algorithms to make them more tolerant of poor meshes. The algorithms could, for example, reconstruct the mesh in a problem area – during the solution process - so as to improve the mesh quality. This will only be possible with the advent of fully automatic meshing tools that employ all possible grid topologies. An alternative concept that is gaining popularity involves a return to Cartesian meshing algorithms. The so-called adaptive Cartesian meshes employ non-conformal elements, such as those shown in the figure below. Cartesian meshes are popular because they have well-documented advantages for simulations involving complex physics. Hurdles that remain before this technology can be widely used involve boundary fixes, factors that are used in boundary-containing cells that account for effects such as wall shear, boundary layer development, and heat transfer, for example.

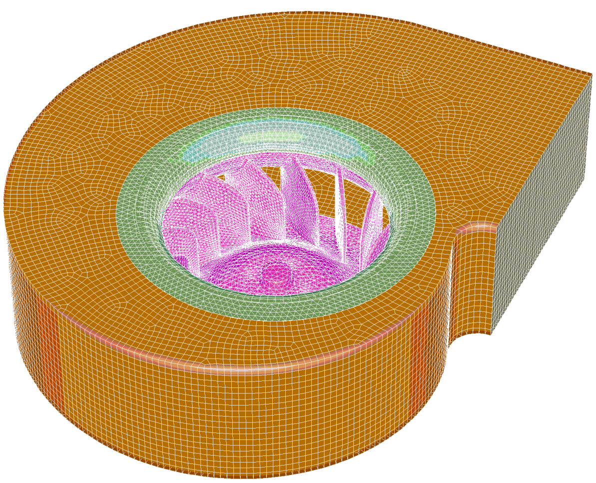

Figure 2: Unstructured hybrid meshes are now popular for CFD applications because they allow many different element types within a single mesh and can handle non-conformal interfaces. These interfaces, which separate the colored regions in the mesh shown, have different mesh topologies on either side.

Numerics and Physical Models

While the computational grid is the foundation of a CFD simulation, the solver numerics and physical models define the structure and, most importantly, the quality of the finished product. Most CFD codes use either the finite volume or finite element method to solve large sets of coupled partial differential equations. Numerous algorithms have been deployed in recent years that serve to minimize the error and time required for this process. These algorithms have been critical to the success of hybrid meshes, containing multiple element topologies in a single simulation. They have also helped push the limits of grid size, making routine work of problems containing several millions of cells. These trends will continue in the future, where increased resolution can be expected from simulations that use even larger cell counts. Advances in numerics will also be able to improve both the spatial and temporal accuracy of the solution. It is expected that control of the solver will become automatic, with adjustment in the solver parameters being performed by the solver itself as it continually monitors the solution progress.

The ability to adapt the mesh to better suit the solution has been available commercially for almost a decade, but the formulations for carrying out this process have been vastly improved over the years. In the future, more improvements are likely to be introduced. For example, the CFD user will not have to intervene to bring about a grid adaption. The solver will assess the solution, detect potential problem spots (say, a steep gradient in one or more flow variables), perform a grid modification automatically, and resume the calculation.

In some cases, two separate regions in a simulation may require different numerical schemes to be treated properly. One example is a glass furnace, where a hot gaseous flame is present in the upper portion of the furnace and a reacting molten glass is present in the lower portion. Today this situation can be handled using two different solvers (one well suited to the flame and one well suited to the glass) that periodically exchange information across their common interface (which then serves as an updated boundary condition). In the future it is expected that independent solvers can be more tightly coupled together to better address problems of this type. Coupled solvers will also be deployed for unusually large simulations where the domain spans several sections. For example, several units in a process loop could be treated together in this manner, with frequent information exchange occurring at the shared boundaries of each.

Many exciting physical models have become available in commercial CFD packages in the past decade, and their success and usability are due in part to the increased capabilities of today's computers. For turbulent flows, the large eddy simulation (LES) model is one example. This transient model, which requires a relatively fine mesh, follows mid- to large-scale turbulent eddies as they grow, change, and decay during multiple cycles. Eddies that are smaller than a typical cell size are assumed to exhibit qualities that are similar from one system to another, so these are described by a simplified model. The cost of performing a transient calculation of this sort on a fine mesh over many eddy lifetimes was considered prohibitive in past years, but it is now within easy reach on most platforms. It has shed new light on phenomena that have been widely observed, from acoustics to instabilities in flames and stirred tanks. Future use of LES will very likely involve reacting flows where turbulent mixing is important. Hybrid solutions can also be expected in which different turbulent models will be used in different regions of a domain, chosen so as to best represent the local conditions.

The modeling of multiple phases is another area that has seen increased sophistication during the past several years. For immiscible fluids, the volume of fluid method has reached maturity in commercial CFD solvers, offering multiple fluids in a simulation and highly accurate interface prediction. The general purpose Eulerian multiphase model is popular for gas-liquid and liquid-liquid mixtures, while its sister, the granular Eulerian multiphase model, has been specifically developed for mixtures containing solids.

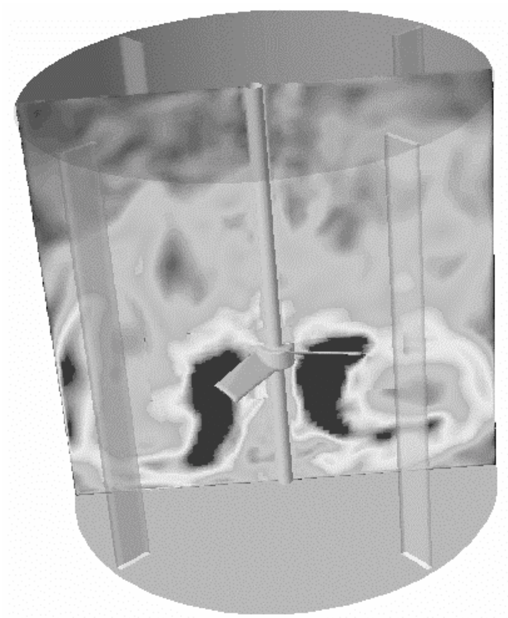

Figure 3: An LES simulation by FLUENT of a Chemineer HE-3 impeller in a stirred tank shows macroscopic fluctuations that have long been observed in the lab but not predicted by simulations until now. (Bakker, et al., 2001)

Multiphase models are now able to describe mixtures of multiple phases of any combination, a capability that has been especially welcomed by analysts of processes such as slurry bubble columns or trickle bed reactors, which involve solids, liquid, and gas. In addition, mass transfer between phases allows for the simulation of evaporation, condensation, and multiphase reacting flows. The future will most likely bring new approaches to multiphase modeling, in addition to more complex physics (for near-wall modeling or interphase turbulence transfer, for example) and improved numerics. The new approaches may be targeted toward specific applications (very-large-particle flows, for example) or applications where certain conditions (regarding the phase volume fractions, for example) prevail, and their strength will lie in their robustness and computational efficiency.

Many models are currently in development, and will be available for general use during the next few years. These include crystallization, with sub-models for the onset of nucleation; plasma models that couple to gaseous flows (used for chemical vapor deposition); electromagnetic models that couple to liquid flows (used for magnetic pumps and ferrofluids); and the ability to model micro- and nano-scale phenomena (such as acoustic vibrations and microelectromechanical systems, or MEMS). The introduction of these models will expand the forefront of CFD modeling into many new application areas during the next decade.

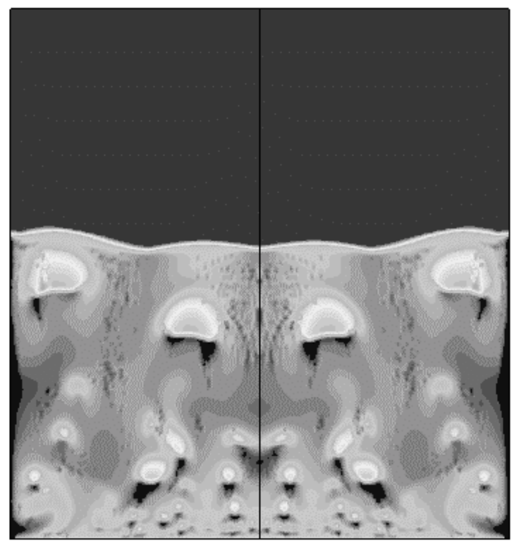

Figure 4: A reacting fluidized bed used for ozone decomposition is simulated in FLUENT using the granular Eulerian multiphase model. Reactions between ozone gas and the particles in the bed convert the ozone to oxygen. Predictions for ozone conversion are in good agreement with published results.

CAE INTEGRATION

While the development of physical models contained in commercial CFD codes will undoubtedly continue, a greater expansion of capabilities will occur through the coupling of CFD software to other computer-aided engineering, or CAE packages. This effort is well underway, as packages for process simulation, stress analysis, and engineering design are now being coupled to CFD software. At the present time, this effort is still in its infancy. Analysts usually need to be trained to use both the CFD and CAE packages that are coupled together. It is often cumbersome for these engineers to maintain a level of proficiency in tools that remain separate entities.

In the future, both CAE and CFD packages will become easier to use, and the process of coupling them together will become more seamless. This will allow design engineers to make use of CFD predictions in their everyday work without necessitating expertise in multiple software products. The ultimate goal will be to make CAE more accessible to a wider audience of engineers within a company, and to make CFD predictions for various designs readily available to these engineers to help guide design changes they wish to make.

OPTIMIZATION

Through CAE integration or within the CFD solver itself, optimization of component design will become more automatic in the near future. Indeed, several organizations are already devising methods to optimize design through the use of repeated CFD simulations. Typically, the results from one simulation are analyzed for stresses, lift and drag coefficients, or other relevant parameters. Adjustments to the geometry are made, based on the preliminary findings, a revised grid is built, and a new solution is run. In-house software is in place in some of these organizations to manage this task, even though manual intervention is still required. This task will soon become automatic, available to all users, and based on built-in conditions that the user supplies to suit the design goals.

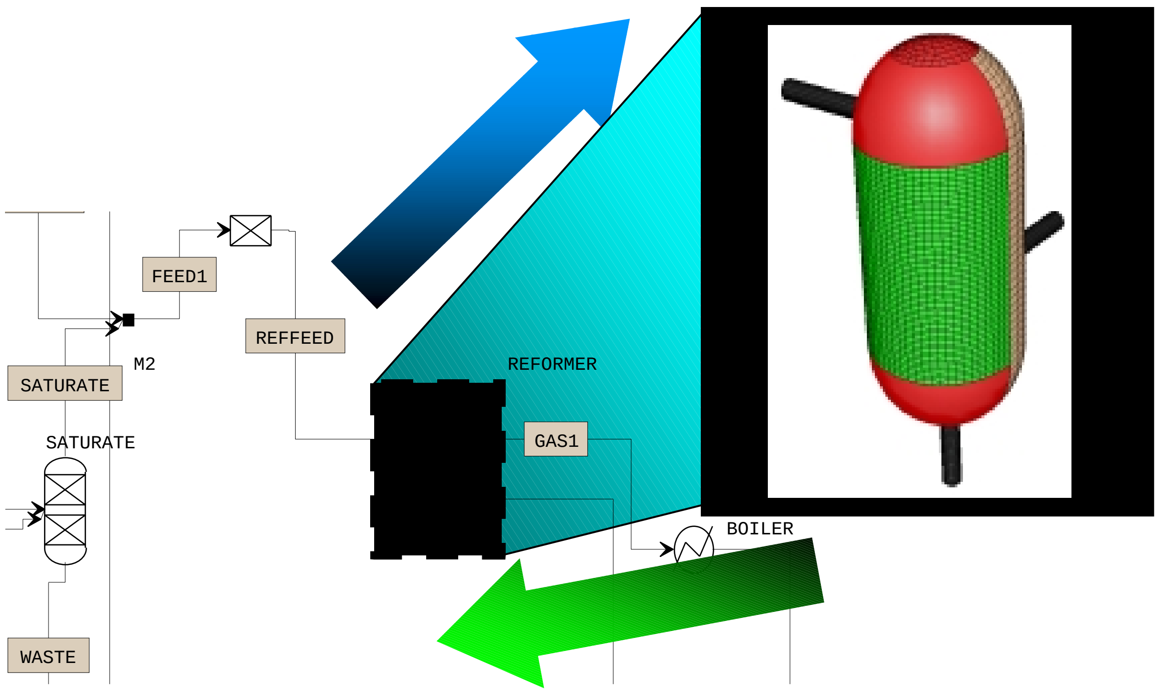

Figure 5: A link between FLUENT CFD software and AspenPlus flowsheet software is one example of CFD/CAE integration. One or more units in the process are modeled using CFD and the results are fed back to the flowsheet for a more accurate portrayal of the operating characteristics of the unit.

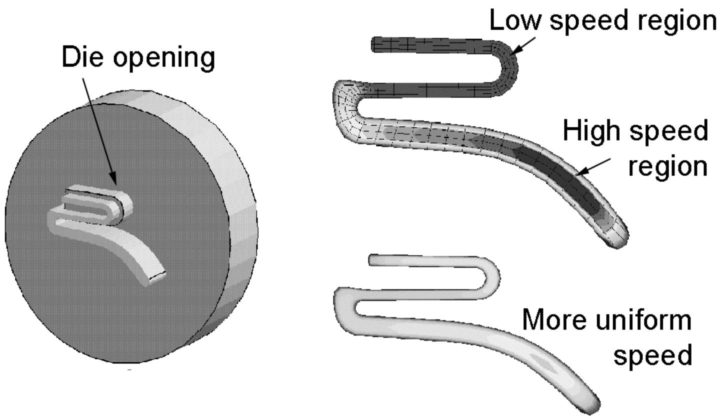

Figure 6: Rubber extruded through a die is shown to have a nonuniform velocity (upper right). The feed opening is enlarged in the die (left) and the result is a more uniform velocity profile in the extruded rubber. This POLYFLOW simulation illustrates how CFD can be used to optimize the design of dies (and other components) for improved product quality. Courtesy of Hutchinson S.A.

VISUALIZATION

One of the most enjoyable aspects of a CFD exercise is the visualization of the results. Velocity vector plots and surface contours of different variables were the hallmarks of early CFD displays. Since then, graphics tools available in both CFD products and third party visualization products have revolutionized graphical output in many ways. A graphical scene is now typically composed of several components, including such things as translucent geometry components, tubes or twisted ribbons to illustrate the flow field, isosurfaces of one variable that can be illuminated or colored by another variable, and "exploded" slices, positioned outside the domain to illustrate the distribution of a variable in one or more regions without cluttering the primary display. In addition to improvements in still images, animation has become an increasingly popular tool, especially because it can convey the results to CFD practitioners and non-practitioners alike. An animation can be used to illustrate transient behavior, such as the emptying of a hopper, or steady-state flow using tracer particles or path lines, moving display planes, and variable points of view. For certain internal flows, the point of view can be attached to an imaginary fluid element, resulting in a so-called "fly-through" of the solution domain. This perspective allows the engineer to gain insight on multiple aspects of the flow fields, including the local speed along the trajectory as well as the helicity, or twist that can result when the fluid passes by protruding geometric features.

Another exciting rend in visualization that will become more developed in the near future is the use of virtual reality. Tools and specialty software products are now available that allow the user to become immersed in a flow field. In some environments, this perspective can offer views on the sides and top as well as in front of the observer. While this "surround" technology is currently only available at a handful of institutions in the US, simplified tools will someday be standard on desktop computers that make use of specialty eyewear. When incorporated with advances in web technology, these visualization options will become available on shared machines, so that engineers in different locations can view and interpret results simultaneously in this format.

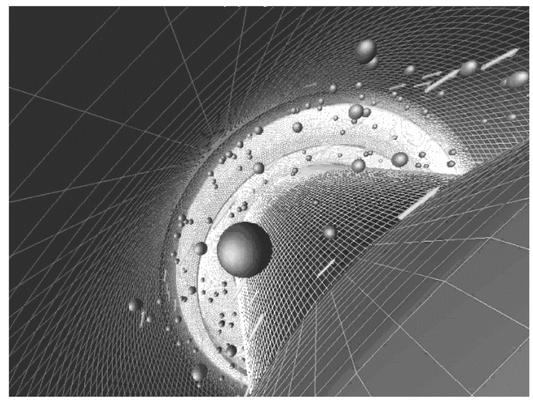

Figure 7: Animation by DX visualization software shows a particle laden flow inside rotating machinery, used to clean debris from the seal chamber of a pump. Courtesy of A. W. Chesterton Company.

USER ENVIRONMENT

Since the early days of commercial CFD codes, the interface has become more user-friendly, evolving from a text-based to a graphical-based format. While text entry is still available for many products, panels offering drop-down menus and point-and-click tools to construct geometry or select modeling options are now experiencing widespread use. Object-oriented programming has allowed for modular code development that will serve to streamline much of the interface functionality as it continues to evolve.

Changes in the interface that can be anticipated during the next several years also involve an increased use of web-based functionality, based on a client / server architecture. In addition to offering general purpose software, corporate intranets will likely provide customized interfaces that allow easy set-up of applications that are particular to the company's business. For example, a chemical process company might have a dozen different cyclone separators in operation at various plants. A web-based custom interface be created that is tailored to cyclone separator modeling. The interface will require input that is relevant only for this type of application. The geometry and grid for each cyclone will

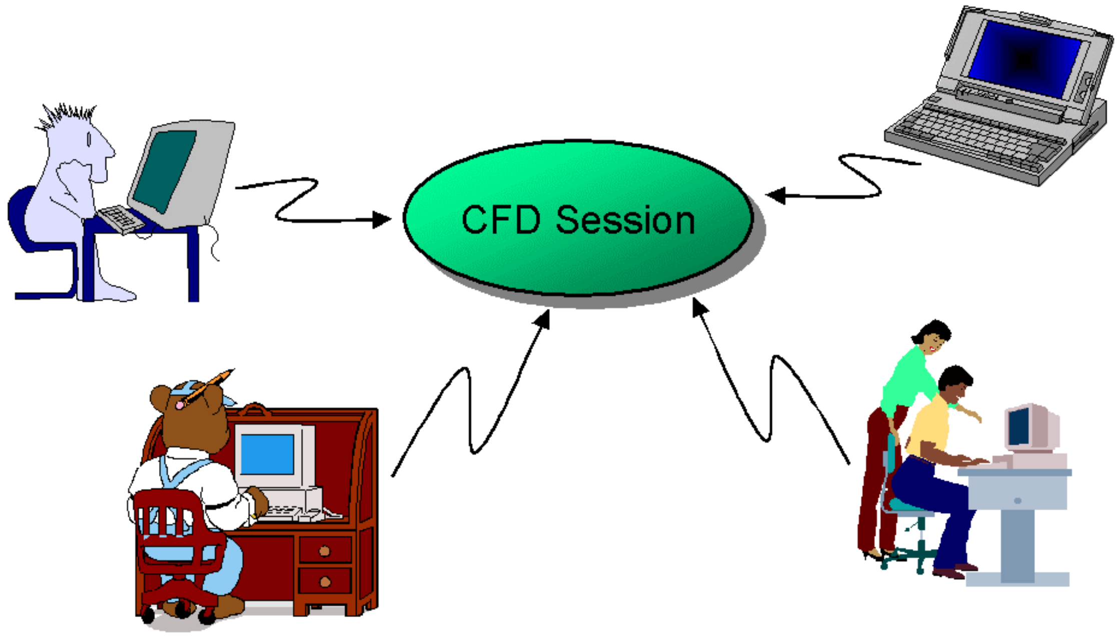

Figure 8: An artist's conception of a web-based CFD session of the future. Multiple clients will be able to connect to a server running the session from a variety of computers, which could include desktop PC's, workstations, laptops, and even hand-held devices. The ability to share results simultaneously will help improve efficiency throughout the organization.

be made available through the corporate intranet in a data repository, and employees can select one (or more) for the purpose of experimenting with modifications to the process parameters.

In addition to web-based setup tools, web-based solver control will become available as well. A company with an extended hardware network will be able to make parallel computing available on a distributed group of machines, controlled by a single desktop, laptop, or hand-held computer. With this structure, a reduced installation of the software will be required on individual personal computers since the bulk of the computational strength will reside on the network. Once the solution is complete, the session can become accessible on the web to multiple clients (engineers) simultaneously for the purpose of viewing the results.

Another benefit of web-based computing will be the easy access between the customer's computer and the software vendor. This access will allow upgrades and bug-fixes to be delivered automatically. It will also allow support engineers to share a session with the client for more efficient responses to questions that arise.

COMPUTING TECHNOLOGY

No discussion about the future of CFD would be complete without mentioning the advances that have been witnessed (and are anticipated) in computational power. It is believed that Moore's Law will continue to prevail for at least another decade, suggesting that by 2011, a computing performance of 10^{11} FLOPS can be expected. Accompanying the speed increases will be further reductions in price for both memory and storage capacity, paving the way for simulations involving ever increasing numbers of cells and more complex physics. As they continue to expand in power and speed, computers will also shrink in size, owing in part to the increased use of chip multiprocessors and more compact storage devices.

To make a corporate network more efficient, tools will become available that do load balancing and resource sharing, keeping track of peak and off-peak demands. Parallel processing will be automatically governed by the needs of a given simulation and the resources available. Automated network management of this type will be largely invisible to the user. It will undoubtedly serve, however, to make the task of performing a CFD simulation considerably easier, thereby making large scale analysis (involving large numbers of cells, for example) open to a wider audience of engineers.

SUMMARY

As these and other changes work their way into CFD codes during the next several years, the result will be software that is more powerful, yet simpler to use. CFD practitioners of the future will not need a long learning curve and extensive training in CFD fundamentals to be successful with their work. Indeed, CFD will become more widely accessible to engineers and technicians alike. Furthermore, the simulations they run will provide a greater depth of understanding about the flow characteristics associated with their process, as a result of increases in accuracy and resolution that can be expected. When CFD is combined with integrated links to other CAE packages, the virtual laboratory of the future will soon become a reality.

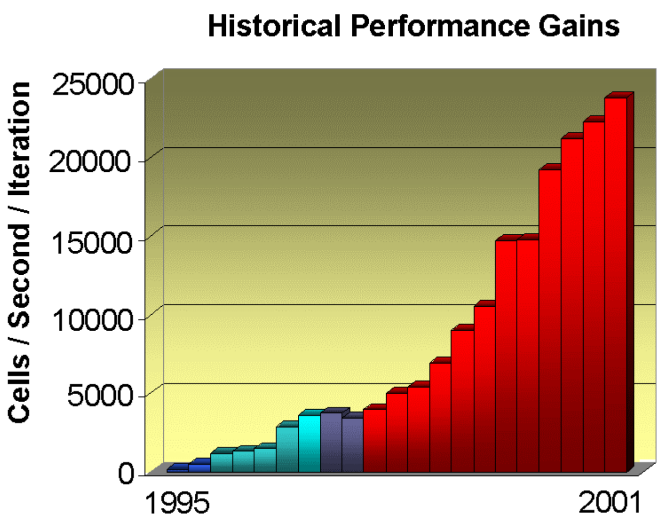

Figure 9: The performance gains for Fluent software products running on a variety of platforms over the years illustrate improvements on both the hardware side as well as on the software side. The latter is a result of advances in solver algorithms.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge contributions from a number of their colleagues at Fluent, including André Bakker, Thierry Marchal, Frank Kelecy, Wei Zhou (now at GE Energy and Environmental Research Corporation), and Lanre Oshinowo (now at Hatch Associates).

REFERENCE

André Bakker, Ahmad Haidari, and Elizabeth Marshall, *Modeling Stirred Vessel Hydrodynamics using Large Eddy Simulation*, presented at the North American Mixing Forum, June, 2001.

QUOTE OF THE DAY

"The greatest problem of the industrial economy is environmental degradation, pollution and the like. The greatest problem of the information economy is privacy. The greatest problem of the bioeconomy of the future will be ethics. When you compare those three, as serious as the privacy issues are, they pale in comparison with the other two. AS TO optimism, I think that the information economy has been incredibly democratizing, much more so than previous economic foundations. The benefits of it have spread to larger numbers of people, despite the digital divide. The major problem of the current information economy, privacy, when seen in an even larger historical perspective is, well, relatively not so bad. The biggest negative is going to be the problem of the bioeconomy. The ethical dilemmas involved are going to be enormous. So I would call it a very cautious optimism."

- Stan Davis in an interview with the online publication Ubiquity (www.acm.org/ubiquity).

2001 CAST AWARD WINNERS

By:
Mark Stadtherr
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&
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We would like to congratulate the three CAST Division award winners for 2001. These announcements include short biographies, followed by selected quotations from supporting letters. The quotations were selected for their particularly strong impact.

Computing Practice Award - Chau-Chyun Chen

For his outstanding leadership and contributions to industrial practice of molecular thermodynamics and fundamental process modeling of complex chemical systems with electrolytes and with polymers. Sponsored by Aspen Technology Inc. and ExxonMobil Corp.

Dr. Chau-Chyun Chen is a founder of AspenTech and the author of the electrolyte and the polymer NRTL models. He is currently responsible for AspenTech's polymers and inorganic process modeling business and technology development. Before joining the company in 1981, he was a research engineer at the Aspen Project at Massachusetts Institute of Technology. He received ScD and MS degrees in chemical engineering from MIT, and a BS degree in chemistry from the National Taiwan University.

"The breadth of processes he has tackled is astounding - ranging from the modeling of the manufacture of industrial polymers to explaining the structure of polypeptides in aqueous solution or representing the behavior of a complex inorganic system."

"Dr. Chen's success is due to his drive, diligence, and sense of devoted service. It is also due to his uncanny (and rare) ability to bridge two cultures: he understands (and contributes to) the fundamental physical chemistry of fluid mixtures as pursued in academic institutions and, simultaneously, he understands exactly what is needed by the practicing chemical design engineer."

"In the application of computers to modern chemical engineering, Chau-Chyun Chen is a giant with few peers."

Computing in Chemical Engineering Award – Christos Georgakis

For his multifaceted and pioneering contributions to process control, through introduction and elaboration of innovative concepts, mentoring of students and leadership in industry-university interactions. Sponsored by Dow Chemical Co. and Mitsubishi Chemical Corp.

Prof. Christos Georgakis is Founding Director of the Process Modeling & Control Research Center at Lehigh University and was a Director of CAST from 1994-7. Some of his research interests include batch process modeling, nonlinear MPC, statistical process monitoring, and the impact of process design on control issues. He received his PhD in Chemical Engineering from the University of Minnesota.

"His research is characterized by a concern to understand and exploit a physical understanding of the problem at hand, and to develop engineering solutions which are fit for purpose, without sacrificing quality and rigor."

"Professor Georgakis was at the forefront of research technology, leveraging the state-of-the-art in computing hardware and software in order to drive toward a solution to the specific issue--but even more, always seeking the larger engineering and scientific principles upon which to provide a general framework for understanding."

"Christos has an infectious enthusiasm for process engineering. His passion for the subject is rivaled only by his quest to develop effective engineering strategies for the operability and control of process systems."

"He has shown a devotion to practically relevant problems but without sacrificing the fundamental nature of the analysis and always staying at the cutting edge of technology."

(continued on next page)

"A computer terminal is not some clunky old television with a typewriter in front of it. It is an interface where the mind and body can connect with the universe and move bits of it about." - Douglas Adams (1952-2001), author of *The Hitchhiker's Guide to the Galaxy*

(continued from page 13)

Ted Peterson Student Paper Award -
Ashish Gupta

For significant developments in process integration, in the AIChE Journal paper "Mass Exchange Networks with Variable Single Component Targets: Minimum Utility Cost Through Linear Programming." Sponsored by Hyprotech, Ltd.

Dr. Ashish Gupta is employed by McKinsey & Company. His expertise is in the areas of process design and large-scale optimization. He received his PhD in Chemical Engineering from UCLA in 1995, and was on the Chemical Engineering faculty at SUNY— Buffalo from 1997-2001.

"The contribution of the paper co-authored by Ashish lies in the fact that [the variable target MEN synthesis problem] was reformulated and solved through linear programming (LP) which was not based on any approximation or problem simplification. Ashish was able to convincingly establish that the solution to the original problem can be derived from the solution to a single LP.... a significant achievement because an LP formulation can be solved even for large, industrial scale problems."

"[This paper] shows that one can solve a related linear programming problem and get to the global optimum of the original problem. This result is far from an obvious one. It has definitely made solving this important problem possible."

"I strongly believe that Ashish's work as a student, later published as a paper in the AIChE Journal, introduced and developed a simple solution method for a very difficult and industrially relevant process integration problem."

Current News - ProcessCity Closes Down

The website, www.processcity.com, previously featured in this newsletter has been shut down. This site now refers the user to AIChE's monthly publication, *Chemical Engineering Progress* at www.cepmagazine.org and to AspenTech at www.aspentech.com.

Current News - Autonomic Computing at IBM

Paul M. Horn, Senior Vice President of IBM Research, says the time is ripe for an assault on the ever-increasing complexity of computing in the Internet era, with its global networks and proliferation of digital devices. At a conference in Scottsdale in October, IBM distributed a paper in which Mr. Horn calls the current version of the complexity problem the industry's "next grand challenge." IBM will also underwrite fifty research projects at universities over the next three to five years — millions of dollars of research grants.

Mr. Horn's paper identifies "autonomic computing" as a means to solve this complexity challenge. This biological metaphor suggests a systemic approach to attaining a higher level of automation in computing. Computer systems could be built that regulate themselves much in the same way as our autonomic nervous system regulates and protects our bodies. Just as a person's nervous system automatically handles all kinds basic functions — heart rate, breathing, digestion, etc. — in response to changing conditions, so, too, should computer systems, according to Mr. Horn.

Similarly, the way to handle the complexity problem is to create computer systems and software that can respond to changes in the digital environment, so the systems can adapt, heal themselves, and protect themselves. Only then, he adds, will the need be reduced for constant human maintenance, fixing and debugging of computer systems.

(Steve Lohr, "Using Humans as a Computer Model", *New York Times*, www.nytimes.com/2001/10/15/technology/ebusiness/15NECO.html, October 15, 2001)

IBM's website calls this concept a radical change in the way businesses, academia, and government design, develop, manage and maintain computer systems. See www.research.ibm.com/autonomic/overview/. A version of Mr. Horn's paper is at www.research.ibm.com/autonomic/manifesto/autonomic_computing.pdf [800 KB].

CHECK OUT

www.castdiv.org

for up-to-date information on CAST

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The Computing and Systems Technology (CAST) Division of AIChE is responsible for the wide range of activities within AIChE that involve the application of computers and mathematics to chemical engineering problems including process design, process control, operations, and applied mathematics. We arrange technical sessions at AIChE Meetings, organize special conferences, and publish this newsletter - *CAST Communications* - twice a year. These activities enable our members to keep abreast of the rapidly changing fields of computing and system technology. The cost is $10 per year, and includes a subscription to this newsletter. Shouldn't you join the CAST Division now? See www.castdiv.org for more details.

Application for Membership

To join the CAST Division, please refer to contact information below. You may also download and print a PDF registration application from AIChE at www.aiche.org/resources/pdflibrary/member.htm. The form is called "Join a Division or Forum -- 2001 Membership Application".

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CAST10 E-Mail List

The following items are used to participate in the list:

1) To post messages to the list, please send mail to:
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3) Archived messages can be found at:
   www.ench.umd.edu/cast10
4) Specific instructions on (un)subscribing and posting messages are located at:
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5) Include keywords as the first line of your message:
   Keywords: software, jobs, education, meetings
   using any or all of the keywords.

The list moderator, adomaiti@Glue.umd.edu , would like to invite comments on the operation of the e-mail list and archive website, especially suggestions for new services.

The Latest Survey Says...

A survey by British PC maker Novatech, intended to take a lighthearted look at techno-glitches, instead revealed the darker side of computing. One out of every four computers has been physically assaulted by its owner, according to the 4,200 respondents. A retired psychology professor from Budapest sums it up: "We treat our machines as if they are persons. We talk to them, we name them, we even sometimes plead with and try to cajole the little god inside each machine. And when the little god turns out to be evil, we beat the machine to purge the demon."
(Wired.com, 5 Jun 2001)

MEETINGS, CONFERENCES, CONGRESSES, AND WORKSHOPS

Location of Meeting Section

To remain as up to date as possible, this meeting section is on-line at www.castdiv.org/MeetingsandConferences.htm. A current screen view is shown below. As announcements are posted on the CAST10 e-mail list, summaries will be added to the website. Other sources of meeting information will be used as well; a direct e-mail to the Editors will ensure that your favorite CAST-related meeting is listed.

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(continued from page 2)

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American Institute of Chemical Engineers

2002 Award Nomination Form*

A. Background Data

1. Name of the Award ____________________________ Today's Date ____________________________

2. Name of Nominee ____________________________ Date of Birth____________________________

3. Present Position (exact title)

____

4. Education

Institution	Degree Received	Year Received	Field

5. Positions Held

Company or Institution	Position or Title	Dates

6. Academic and Professional Honors (include awards, memberships in honorary societies and fraternities, prizes) and date the honor was received. Use separate page.

7. Technical and Professional Society Memberships and Offices. Use separate page.

8. Sponsor's Name and Address

____

____

____

Sponsor's Signature

____

*A person may be nominated for only one award in a given year.

THE DEADLINE FOR AWARD NOMINATIONS IS April 15, 2002.

B. Citation

1. A brief statement, not to exceed 250 words, of why the candidate should receive this award. (Use separate sheet of paper, please.)
2. Proposed citation (not more than 25 carefully edited words that reflect specific accomplishments).

C. Qualifications

Each award has a different set of qualifications. These are described in the awards brochure. After reading them, please fill in the following information about the nominee where appropriate. Use a separate sheet for each item if necessary.

1. Selected Bibliography (include books, patents, and major papers published).
2. Specific identification and evaluation of the accomplishments on which the nomination is based.
3. If the nominee has previously received any award from AIChE or one of its Division, an explicit statement of new accomplishments or work over and above those cited for the earlier award(s).
4. Other pertinent information.

D. Supporting Letters and Documents

List of no more than five individuals whose letters are attached.

	Name	Affiliation
1.		
2.		
3.		
4.		
5.		

Please send the completed form and supplement sheets to the CAST Division 2nd Vice Chair: Babatunde A. Ogunnaike; E.I. DuPont de Nemours and Co.; Experimental Station, E1/104; Wilmington, DE 19880-0101; Phone: (302) 695-2535; Fax: (302) 695-2645; Babatunde.A.Ogunnaike@usa.dupont.com

THE DEADLINE FOR AWARD NOMINATIONS IS April 15, 2002.

CAST Communications

The Semi-Annual Publication of the
Computing and Systems Technology Division of AIChE
Volume 24, No. 2 // Winter 2001
Editor:
Peter R. Rony
Department of Chemical Engineering
Virginia Tech
Blacksburg, VA 24061-0211
Deadlines: December 1, July 1

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