March 2002

CAPE-OPEN Update

an information service provided by the CO-LaN

Issue n°02

CAPE-OPEN 1.0 is Available for Download

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www.colan.org

CAPE-OPEN Update is a publication of the **GCO-Support** project in collaboration with the **CO-LaN**, a non-profit consortium for the development of the **CAPE-OPEN** standard.

Global CAPE-OPEN and **GCO-Support** are funded by the European Community under the «Industrial and Materials Technologies» and «Competitive and Sustainable Growth» Programmes. In addition, **Global CAPE-OPEN** follows the Intelligent Manufacturing Systems initiative promoting collaboration between six international regions.

EDITORIAL:

CAPE-OPEN: Release 1.0 is Ready for Prime Time

SUMMARY

With 5 years' hard work behind us, the involvement of a global Who's Who of universities, software vendors, and industrial companies, and the diligent leadership of a core of visionary CAPE aficionados, Version 1.0 of the CO standard is in place. None of this would have been possible without a collective vision of success, excellent leadership, and might I say dogged determination of a large cast of players to see the effort through. There certainly have been times when many doubted this could happen!

The Global CAPE-OPEN project is now complete, and its goal has been accomplished. Visit the CO-LaN web site (www.colan.org) and see the results. A large number of interface specifications are published and posted on the web site, covering the range of CAPE applications. Plus, the CO standard has been commercially implemented in a number of vendors' PMCs and PMEs (Process Modelling Components and Process Modelling Environments). Later in this newsletter, there is an excellent summary article describing all the elements of the interface standard specifications and their status, plus a list of commercial software that has implemented them.

GOALS & VISION IMPLEMENTED

Release 1.0 has accomplished the CAPE-OPEN goal of providing CAPE practitioners with «plug and play» process modelling software components. A wide range of demonstrations at the GCO final meeting in Cambridge, UK (December, 2001) have proven both the power and success of implementation. A key observation about those demonstrations is that people were able to take the CO standard interface specifications as written, and deliver running models. Minimal support was needed from the GCO experts to make this happen. True plug and play has been delivered. Now it is up to the user community to capture the value inherent in applying best in class solutions to CAPE problems. The simple existence of the possibility for the use of CAPE software components from multiple suppliers is not enough: users must apply their skills and produce process models that solve problems for their companies.

THE WORK REMAINING

* **Interface Specification Refinement.** While there are now a large number of specifications available, there are still a number of specifications that have not been completely tested for interoperability. Beyond this, there are documents that have not been reviewed and therefore are not approved specifications. Though these documents are largely complete specifications, they need to be reviewed to confirm the required quality in order to be deemed CO interface specifications. Details on the status of each specification are covered in the summary article later in the newsletter.
* **New Interface Specifications.** Pending defined needs from the CAPE community, new CO interface specifications will be developed to meet value creation needs. The CO-LaN will serve as the organisation to identify these needs and to organise efforts to address them.
* **Interoperability Testing.** Compliance with the CO standard must be confirmed through testing in the real world. The ITF (Interoperability Task Force) efforts of the GCO project will be taken up by the CO-LaN to assure interoperability of CO compliant PMCs and PMEs.
* **Facilitate the CAPE-OPEN Market.** The CO-LaN industrial users group will work to maintain focus for CAPE users and suppliers, insuring that user needs are addressed in a dynamic market.

CO LaN REORIENTATION

The CAPE-OPEN Laboratories Network (CO-LaN) has been reoriented as an industrial users group. Industrial users pay dues and have the leading role. Software vendors, universities, research institutes, individuals, and other interested parties can join the CO-LaN as associate members: participating in projects, providing insight, and learning. With this new structure and orientation, the CO-LaN is positioned to lead CAPE-OPEN activities into the future. The CO-LaN will foster Special Interest Groups (SIGs) for standards maintenance (expansion and improvement) and development of new standards, both driven by the demand of the CO-LaN members. New members continue to join the CO-LaN to participate in this unique opportunity.

Kerry Irons, Editor

Latest News

The CO-LaN web site has a listing of current events - http://www.colan.org/archive/news.phtml. Please visit to see what's up. Release 1.0 of the CO standard is detailed, and a number of demonstration examples are posted as well. This includes listings of commercial releases of CO compliant software components, the demonstrations from the December, 2001 Cambridge UK final GCO meeting, presentations summarising all aspects of the GCO project, and a host of additional information.

A number of CO Tour events have been held both in public forums and at company sites. This has been a tremendous opportunity to influence CO implementation at the user level. More events are in the planning stages. If your organisation would like to conduct such an event, please contact Bertrand Braunswhweig (Bertrand.Braunschweig@colan.org).

Current Issues

As noted above, the CO-LaN has been redefined as an industrial users group, with participation from the software vendors, universities, research institutes, etc. For the past five years, the CAPE-OPEN and Global CAPE-OPEN projects drove the creation and revision of standards, CO dissemination, training, interoperability testing, etc. This work was done under the signed consortium agreements and, for European organisations, was at least partially funded through EU support to the CO and GCO projects.

As of now, there is no funding available for any of these activities outside of dissemination, and industrial users are paying dues to support the CO-LaN. The work of the CO-LaN will be largely done by the Special Interest Groups (SIGs), and the time that people spend on this will need to have clear value for all the SIG members. While this is a challenge, it also will insure that the CO-LaN is very focused on high value activities.

Global CAPE-OPEN project final summary report

Global CAPE-OPEN raises the CAPE-OPEN standard to a new level

The Global CAPE-OPEN project had its final meeting in Cambridge on 5th/6th December in an event hosted by AspenTech UK Ltd. This marked the end of five years of international EU-supported collaborative work on the establishment of open standards for flowsheet simulation, at first in the CAPE-OPEN project and then in the joint EU/IMS Global CAPE-OPEN project involving partners in three continents. The results, shown in the meeting, exceeded all expectations.

The aim of the projects was to define standard plugs and sockets so that external software components can be used in LegoTM brick plug and play fashion in the main commercial simulators, such as AspenTech's Aspen Plus and Hyprotech's HYSYS. Although the original project scope did not commit to the delivery of commercial implementations of the standards, this is in fact what has happened in the areas of unit operations and thermodynamics. Developers at AspenTech and Hyprotech, who have been central to the implementation and refinement of the standards, have incorporated them into the latest versions of their simulators. Specialist suppliers PSE and Infochem have also produced compatible versions of their respective gPROMS process modelling environment and Multiflash thermodynamics packages, which will be issued shortly. All of these were demonstrated working together reliably and intuitively, by industrial end users. Other suppliers, such as ProSim, Belsim, RSI, and Dechema, are expected to provide the same level of interoperability in their products shortly. Open simulation is now a commercial reality.

As well as these commercial implementations, many other facilities were shown in an advanced state of development. For example, there are wizards to enable existing code to be wrapped into CAPE-OPEN-compliant components for both unit operations and thermodynamics and testers to check components for CAPE-OPEN compliance. There are also specifications for numerical methods, petroleum materials, electrolytes, reactions, on-line and hybrid applications, as well as work aimed at real-time operations, scheduling and planning, and plant lifecycle issues.

Besides these technical developments, the projects have changed the relationships between the participants. All have found that strong collaboration and mutual understanding are essential to deliver the standards and prototypes, while continuing to compete vigorously in all other areas. There was wholehearted agreement with Dr Bertrand Braunschweig from IFP, the project manager of both projects, when he said, "The challenge for the future is to realise the commercial benefits of the hard work and investment of the last five years, but now is the time to celebrate!"

Full details of the standards, the current state of implementation and the project organisation can be found at www.colan.org, which is the web site of the CAPE-OPEN Laboratories Network. This is a not for profit organisation, which has been formed to maintain and develop the standards into the future.

About Global CAPE-OPEN

CAPE-OPEN and Global CAPE-OPEN are funded by the European Community under the Industrial and Materials Technologies Programme (Brite-EuRam III), under contracts BRPR-CT96-0293 and BPR-CT98-9005. In addition, Global CAPE-OPEN follows the Intelligent Manufacturing Systems initiative promoting collaboration between Europe, USA, Japan and other regions.

Members Profiles:

ProSim

ProSim is an independent privately held French company active in Computer Aided Process Engineering (CAPE) since 1989. Compared with the major North-American CAPE software providers, ProSim focuses on providing innovative, high quality software in specific fields, but also makes the difference with services provided. From optimal design to operations improvement, ProSim serves its worldwide demanding clients with state-of-the-art proven technologies. In some niche-markets such as batch processes simulation, nitric acid plants or plate fin heat exchangers, ProSim has gained a leading position with unequaled software solutions. ProSim's addresses the chemical industry including specialty chemicals, petrochemicals, refining, gas processing, food and pharmaceuticals.

ProSim's services include technical assistance or training in process simulation and modeling, as well as project services (modeling services, dedicated models or custom software development, etc.). Thanks to a long term partnership with prestigious university research centers (such as INPT-ENSIACET) and continuous investment in R&D, ProSim has gained a leading position in the field of rigorous batch chemical reactor and distillation column simulation. ProSim has been able to develop original process simulation solutions, to become an active player in CAPE and to successfully address process design and engineering or operation optimization markets.

Early on, ProSim saw the advantage of object oriented software development in the field of CAPE and put several years' investment in the development of OO process simulation framework. A seamless integration of best in class software components delivered by ProSim (specific unit operations, thermodynamic properties servers, solvers, kinetic reactions, …) is an opportunity to strengthen its position on the market. ProSim has already developed a fully CAPE-OPEN compliant thermodynamic properties server making it possible to use this thermo server within other CAPE-OPEN compliant simulation environments. This interoperability has been successfully demonstrated within HYSYS (a video is available on ProSim website: www.prosim.net). A new fully CO compliant software architecture is under development and will be available in a few months.

ProSim is today one of the very few companies able to supply CO compliant software components, but also experienced in making existing legacy codes CO compliant. As there are a number of legacy codes within operating companies (including company-specific thermodynamic or unit operations models) that will have to be wrapped in order to follow their life within a commercial simulation environment, ProSim decided to integrate this new line of services to its portfolio. This new service answers a challenge faced by most of the Chemical Process Industries (either operating companies or engineering firms). If you are thinking of migrating internal codes to CAPE-OPEN, do not hesitate in contacting ProSim. The company operates from offices in Toulouse with highly qualified and experienced technical staff enabling a deep understanding of clients' needs and requirements in order to instantly take into account, analyze and solve even the more complex process industries problems. ProSim's skills include modeling, thermodynamics, numerical algorithms or optimization techniques. ProSim also relies on a network of partners to increase its access to the market or to perform joint developments when appropriate.

To find out more about ProSim, visit its website at: http://www.prosim.net/

For more information please contact us at +33 5 62 88 24 30 or mailto:info-sup@prosim.net

Process System Enterprise

Process Systems Enterprise Ltd (PSE) is a provider of advanced model-based technology and services to the process industries. These technologies address pressing needs in fast-growing engineering and automation market segments of the chemicals, petrochemicals, oil & gas, pulp & paper, power, fine chemicals, food, pharmaceuticals and biotech industries.

PSE was formed in 1997 as a spin-off from London's prestigious Imperial College of Science, Technology and Medicine, to commercialise software originating from Imperial's Centre for Process Systems Engineering. PSE's mission is to become the world's leader in model-based technology for the process industries. Its products support and manage innovation at multiple levels, from the design of products offering new or improved functionality, to the design, operation and control of the processes making those products, all the way to the design and operation of enterprise-wide supply chains.

PSE's gPROMS software family is arguably the world's most advanced process modelling tool available today, supporting the development, maintenance and deployment of models with unprecedented predictive power. gPROMS is used extensively to build models of a wide range of products - from high-performance polymers to fuel cells - and processes - from advanced reactors in the petrochemical industry to crystallisation techniques for large biological molecules. gPROMS underpins the product and process lifecycle with a common modelling framework that can be used for a variety of activities, from the design of experiments for the validation of the process chemistry and the associated estimation of kinetic parameters, to the optimisation of steady-state and dynamic process performance, and on-line model-predictive control.

PSE's second software product is ModelEnterprise, a brand-new tool for modelling enterprise supply chains. ModelEnterprise incorporates hundreds of person-years of research in supply chain optimisation from Imperial College and elsewhere, as well as extensive experience on model-based software design learned from the development of gPROMS. It provides an integrated framework for supporting strategic, tactical and operational decisions, all based on a common enterprise model and a set of powerful techniques for automatically deriving from it models of a level of detail that is appropriate for the particular type of decision under consideration. The first Enterprise Management Application made available within ModelEnterprise is the Optimal Single Site (OSS) scheduling and planning tool, the first of its kind to provide a «profitable-to-promise» functionality. Further tools for multi-site production/distribution planning, and for plant design are currently under development.

PSE believes strongly in working in partnership with its operating company customers and their suppliers, to provide comprehensive solutions. Besides software, PSE offers the ModelCare product, incorporating a range of services aimed at helping customers to get the most out of their investment in tomorrow's technology – today.

PSE is committed to open systems and is strongly supportive of the CAPE-OPEN initiative. Both the gPROMS and the ModelEnterprise product families are based on open architectures that allow third-party software to be incorporated within them, and themselves to be embedded within other software. gPROMS already provides a «socket» that allows CAPE-OPEN compliant physical properties packages to be used within gPROMS models. The gPROMS engine also forms the basis of the gO:CAPE-OPEN software product that allows models developed in gPROMS to be deployed within CAPE-OPEN compliant flowsheeting tools such as Aspen Technology's ASPEN PLUSTM and AEA Hyprotech's HYSYSTM tools. Other products based on gPROMS' open architecture include the gO:CFD tool that allows gPROMS to be used for modelling complex homogeneous and heterogeneous reactions within computational fluid dynamics software such as Fluent Inc.'s Fluent® and CD adapco's STAR-CD®; and gO:Simulink that makes gPROMS modelling and numerical solution technology available within MathWorks Inc.'s MATLAB/Simuling® tool.

PSE is committed to excellence and has strong views on how a technology company should operate in today's business and economic climate. See the PSE web site (http://www.psenterprise.com) for more details.

BELSIM

Belsim is an independent Belgian Company active in the field of Computer Aided Process Engineering (CAPE) which specialises in delivering software, providing solutions and consulting for production accounting, process performance follow-up and optimisation in the refining and chemical industry as well as in the energy sector.

The core business of Belsim is the innovating field of data validation where we are the leaders with the software VALI. This software gives to the plant managers a better insight of the actual plant performance and balances (mass, thermal and thermodynamic balances). Thanks to advanced data reconciliation methods, VALI extracts reliable and accurate information from plant and lab measurements.

The main activities of Belsim can be defined as:

- developing and marketing generic software for process performance analysis and optimisation,
- developing dedicated software solutions,
- marketing and providing engineering services for process studies and for applications based on generic software.

Compliance

Belsim VALI complies with the German VDI 2048 standard.

Belsim VALI has a thermodynamic socket compliant with CAPE-OPEN 0.93.

Belsim company complies with ISO 9001 : 2000 standard.

Some references

Mainly present on the European market, Belsim counts among its customers TotalFinaElf (France), Air Liquide (France), Butachimie (France), BASF (Germany), Wacker Chemie (Germany), Lonzagroup (Switzerland), AtoFina (Belgium), Usinor (Belgium), nuclear power stations in Switzerland and in Germany, Larsen and Toubro (India),...

To share its knowledge and its experience in the field of process analysis, Belsim follows an active policy of partnership with world wide companies such as ABB and Yokogawa-Marex or with local partners as for example BTB Jansky in Germany or SPIRE Technical Services in India.

To find out more about Belsim, visit its website at: http://www.belsim.com/

For more information please contact us at +32 4 259 88 88 or mailto:info@belsim.net

User tips

UNIT OPERATION WIZARD TIP

AspenTech has developed a CAPE-OPEN Unit Wizard (under the Methods and Tools Group of GCO) to provide materials to support the adoption of the CAPE-OPEN standards.

The objective of the Unit Operation Wizard is to help users, who are probably unfamiliar with the techniques required to implement COM components, to build the skeleton of a COM Unit Operation with the minimum effort. A Wizard-style tool is suitable for this type of task because CAPE-OPEN Unit Operations written in Visual Basic can be structured in a standard way and standard implementations of port and parameter objects can be re-used.

The Unit Operation Wizard is an add-in for Visual Basic (VB) that allows a user to create a CAPE-OPEN Unit Operation by filling in data on a sequence of forms. Once data entry has been completed the Wizard generates a Visual Basic project that builds the resulting Unit Operation. Additionally, the wizard creates an installation kit so that the Unit Operation can easily be used on other machines.

Although a COM Unit Operation generated by the Wizard can be compiled, installed and run in a CAPE-OPEN Process Modelling environment (PME), it is not complete. To complete it, a user has to add User Interface forms, and a calculation routine. These are the two features which implement the core behaviour of a Unit Operation and they are too complicated to be automatically generated by the Wizard. The advantage of the Wizard is that it leaves the user free to concentrate on these aspects of the Unit Operation without having to worry about the details of the implementation of COM interfaces and how to write an installation program.

The Unit Operation Wizard is available from AspenTech's Customer Support Hotline and on the CO-LaN web site (http://www.colan.org) and will be a great assistance to users in implementing CO solutions. Documentation explaining the Wizard is available as well. To install the Wizard, you simply download it from either of these two sources, unzip the installation files and run setup.exe. How much easier can it be?

FINAL TIPS

Remember to visit the CO-LaN web site (http://www.colan.org) to better understand both the method and the opportunity of implementing CO standards. If you are a CAPE software developer, you will find CO testers and the CO standards documentation. If you are a CAPE software user, you will find guidance on the use of CAPE tools in a CO-compliant environment. There is a great deal of information on the web site to guide you and offer insight.

Feel free to contact a CO-LaN member to help you focus your activities. These people can answer questions, discuss the philosophy of CO standards, direct you to CO standards experts, and give you a glimpse of current and future activities.

Feedback

While the first edition of the CO-Update newsletter went to some 1500 CAPE practitioners, we don't have any feedback to share. However, we are always looking for your input and suggestions, so please feel free to let us know what you are thinking, your concerns, successes, and failures. We're happy to share your comments with the CAPE community!

Back Issues of CAPE-OPEN Update

You can view back issues of CAPE-OPEN UPDATE on the CO-LaN web site - please visit http://www.colan.org/public/cape-open-update.phtml

Coming events, CO-LaN press releases and other current news

* Visit http://www.colan.org/archive/news.phtml for the latest information!
* CAPE-OPEN Days are planned for BASF (8 April, 2002) and Bayer (9 April, 2002). CO Days are designed to show an organisation's technical professionals and technical leaders how to implement CO standards for their CAPE.
* Wizards are now developed for Unit Operations and Thermodynamics and are available through AspenTech and Hyprotech respectively, and through the CO-LaN web site, http://www.colan.org.
* The CO COSE (CAPE-OPEN Simulation Executive) tester is now ready and available on the CO-LaN web site.
* CO and the CO-LaN will have a strong presence at the ESCAPE 12 conference (http://www.escape12.tudelft.nl/), showing the results of the GCO project, demonstrating Release 1.0 of the CO standard, and showing how CAPE practitioners can successfully implement CO standards.
* A CAPE-OPEN Day is planned for June 19th, all day long, at the ICI Wilton Research Centre, Wilton Middlesborough, UK. Look for further announcements on the colan website.

CAPE-OPEN Update Subscription

If you want to «subscribe» or «unsubscribe» CAPE-OPEN Update, please send an email to mailto:co-update@colan.org with subscribe or unsubscribe as subject, resp. If you need to contact the CO-LaN about the distribution list (if you have trouble unsubscribing or have questions about the list itself), please visit http://www.colan.org/public/cape-open-update.phtml.

From the technical room

Mixed Integer Linear/Nonlinear Programming Interface Specification

MINLP Overview - An Industrial User's Perspective, by Michel Pons, ATOFINA.

Numerical packages for CAPE have been on the market for a long time, typically provided by specialised organisations. However the use of the optimisation routines (contained in those packages) within process modelling environments has been very restricted by the lack of standardised interfaces.

Through the CAPE-OPEN MINLP interface, it will be possible to access seamlessly, from a process modelling environment, the latest optimisation algorithms available. That will provide more robust and more efficient numerical tools to the end-users. For optimisation algorithm developers, implementing the CAPE-OPEN MINLP interface specification will give them access to a larger market where their tools will be put to use immediately.

Bill Morton, University of Edinburgh, is a recognised leader in the field of optimisation algorithms. He stated in January 2001 «It could well be that some of the solvers created both at Dundee (by Roger Fletcher's group) as well as complementary work here would profit from adaptation to the CAPE-OPEN standard. The Dundee solver, FilterSQP, in particular has been widely tested by a number of external users, as well as by the authors and in our group.» In the US, Carnegie Mellon University's Center for Advanced Process Decision-Making is working with the package rSQP++. This package could readily benefit from adopting the CAPE-OPEN MINLP interface specification.

Applications of optimisation are becoming more common in the process industries, especially with data reconciliation for on line optimisation, but also off-line optimisation such as for utility networks. While there are already a number of monolithic packages available and running, the vision is to go beyond the current objective (generally a few percent of increased productivity) for more processes. This can be done, thanks to more robust optimisation tools, available as software components within a general software architecture implementing the CAPE-OPEN MINLP interface specification.

MINLP Interface specification

by Costas Pantelides, Leo Liberti, Panagiotis Tsiakis and Terrence Crombie

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Introduction

Global CAPE-OPEN (GCO) has developed a standard and unified software interface for numerical solvers for both Mixed Integer Linear Programs (MILPs) and Mixed Integer Nonlinear Programs (MINLPs). This article summarises the scope of the interface standard specification and outlines the concepts of MILP/MINLP and their relevance to CAPE practitioners.

Mixed Integer Linear Programs

Mixed integer linear programming (MILP) problems involve the minimisation or maximisation of a linear objective function subject to linear constraints. The optimisation may involve both continuous and discrete (integer-valued) decision variables.

MILPs arise quite frequently in process engineering applications such as:

- supply chain optimisation
- multipurpose plant scheduling
- refinery scheduling
- synthesis of heat exchanger networks

and many others. MILP problems also occur as sub-problems in the solution of mixed integer nonlinear programming problems.

An MILP can be formulated mathematically as follows:

$$\min_{x,y} ax + by$$
$$l \le Ax + By \le u$$
$$x^L \le x \le x^U$$
$$y^L \le y \le y^U$$

where x is a vector of n continuous variables, y is a vector of n' integer variables, a, x^L, x^U are real n-vectors, y^L, y^U are integer n'-vectors, b is a real n'-vector, A is an m x n real matrix, B is an m x n' real matrix and l, u are real m-vectors.

Two important special cases of MILPs are:

- Linear programming (LP) problems.

  In this case, all optimisation decision variables are continuous, i.e. $n'=0$. Such problems also appear frequently in practice, either on their own or as sub-problems in the solution of MILP problems.
- Purely Integer Programming (IP) problems.

  In this case, all optimisation decision variables are discrete, i.e. $n=0$.

Mixed Integer Nonlinear Programs

Mixed integer nonlinear programming (MINLP) problems involve the minimisation or maximisation a nonlinear objective function subject to nonlinear constraints. The optimisation may involve both continuous and discrete (integer-valued) decision variables.

MINLPs arise in many process engineering applications, including:

- process synthesis
- process design
- product design

and others.

An MINLP can be formulated mathematically as follows:

$$\min_{x,y} f(x,y)$$
$$l \le g(x,y) \le u$$
$$x^L \le x \le x^U$$
$$y^L \le y \le y^U$$

where x is a vector of n continuous variables, y is a vector of n' integer variables, x^L, x^U are real n-vectors, y^L, y^U are integer n'-vectors, f: $\mathbf{R}^n$ x $\mathbf{Z}^{n'} \rightarrow \mathbf{R}$ is a (possibly) nonlinear function, g: $\mathbf{R}^n$ x $\mathbf{Z}^{n'} \rightarrow \mathbf{R}^m$ is a list of m (possibly) nonlinear functions and l, u are real m-vectors.

A very important special case of MINLPs is that of nonlinear programming (NLP) problems. In this case, all optimisation decision variables are continuous, i.e. $n'=0$. Most operational (as opposed to design) optimisation problems in process engineering can be formulated as NLPs. NLPs also occur as sub-problems in the solution of MINLP problems.

Generalized Mixed Integer Nonlinear Programs

MILPs can be viewed just a special case of MINLPs where both the objective function and the constraints are linear. Thus, it would appear to suffice defining a standard software interface for MINLPs.

It is worth noting that numerical solvers for nonlinear problems (including NLPs and MINLPs) are often capable of exploiting partial linearity in the problem being solved. Moreover, although possible in principle, the representation of a linear problem in terms of a more nonlinear formulation may entail some inefficiencies from the computational point of view. This indicates that the linear and nonlinear parts of objective function and constraints should be treated separately.

In view of the above, we employ the following definition of a generalized MINLP:

$$\min_{x,y} \; ax + by + f(x, y)$$
$$l \le Ax + By + g(x, y) \le u \qquad (1)$$
$$x^L \le x \le x^U$$
$$y^L \le y \le y^U$$

where x is a vector of n continuous variables, y is a vector of n' integer variables, a, x^L, x^U are real n-vectors, y^L, y^U are integer n'-vectors, b is a real n'-vector, f: $\mathbf{R}^n$ x $\mathbf{Z}^{n'} \rightarrow \mathbf{R}$ is a nonlinear function, A is an m x n real matrix, B is an m x n' real matrix, g: $\mathbf{R}^n$ x $\mathbf{Z}^{n'} \rightarrow \mathbf{R}^m$ is a list of m nonlinear functions and l, u are real m-vectors.

In fact, for ease of manipulation at both the mathematical and the software levels, it is better to group both continuous and integer variables within a single vector x, rewriting the above as:

$$\min_{x} \; ax + f(x)$$
$$l \le Ax + g(x) \le u \qquad (2)$$
$$x^L \le x \le x^U$$
$$x_i \in \mathbf{Z}, \; \forall \; i \in I$$

where x is a vector of n variables , a, x^L, x^U are real n-vectors, f: $\mathbf{R}^n \rightarrow \mathbf{R}$ is a nonlinear function, A is an m x n real matrix, g: $\mathbf{R}^n \rightarrow \mathbf{R}^m$ is a list of m nonlinear functions and l, u are real m-vectors.

We note that:

- the variables in x are characterised by an index i (=1,..,n) and are bounded between given lower and upper bounds x^L and x^U respectively;
- some of the variables x_i are restricted to take integer values; these integer variables are identified via an index set $I \subseteq \{1,...,n\}$;

« all constraints are expressed as double inequalities in the form *lower bound* ≤ *function* ≤ *upper bound*, and are indexed over the discrete domain 1,..,*m*.

Many different variations of this form exist (e.g. involving *equality* constraints of the form *function* = *constant* rather than inequalities, as shown above). However, they are all completely equivalent mathematically and can be transformed to each other via usually trivial mathematical operations.

Scope and Overview of Interfaces

The CAPE OPEN interface specification is aimed at general numerical solvers for MILPs and MINLPs. It also accommodates special cases of these such as solvers for:

« linear programming problems (LPs)
« integer (linear) programming problems (IPs)
« nonlinear programming problems (NLPs).

All these solvers operate on a formal software description of the problem in terms of an *MINLP object*. The latter corresponds to the generalised MINLP mathematical formulation given by equations (2).

A typical scenario for a client program using the interfaces defined in this document would be as follows:

« The client starts by constructing an MINLP object describing the process engineering problem to be solved.
« Once the client constructs the MINLP object, it can then pass it to a *Solver Manager* corresponding to a particular numerical solver to create an *MINLP system*. The latter represents a combination of the problem to be solved (as embodied in the MINLP object itself) and the numerical solution code (as incorporated within the Solver Manager).
« Once the MINLP system object is constructed, the client may invoke its *Solve* method to effect the solution of the problem of interest.
« The client may then retrieve the final values of the variables by invoking the appropriate method of the MINLP object.

The above scenario is entirely analogous to that adopted by earlier CAPE-OPEN specifications for numerical solvers. In particular:

« no attempt is made to standardise the manner in which the MINLP object is actually constructed[1];
« consequently, the MINLP object interface is focussed on allowing a numerical MILP/MINLP solver to obtain all the information that is necessary to solve the problem;
« the MINLP Solver Manager and MINLP System interfaces inherit from the standard CAPE-OPEN ICapeNumericSolverComponent interface which standardises the handling of algorithmic parameters and numerical performance statistics.

Conclusion

The MINLP CAPE OPEN standard is now complete. CAPE practitioners can implement this standard for their in-house software, and CAPE software vendors can deliver CO compliant software components to the CAPE market place using the standard.

Any Feedback ?

Please submit comments and feedback to Kerry.Irons@colan.org . Only the authors are responsible for statements or opinions contained in articles.

1 For example, the CAPE-OPEN specifications for numerical solvers for nonlinear algebraic equations and differential-algebraic equations rely on the problem being described in terms of an Equation Set Object (ESO). CAPE-OPEN does *not* specify how an ESO is constructed.

The CAPE-OPEN Standard 1.0

by Bertrand Braunschweig, president of the CAPE-OPEN Laboratories Network (CO-LaN).

Acknowledgments

This text summarises many other documents authored by contributors of Global CAPE-OPEN from several organisations. It is better not to give any names, since the list would be too long. Many thanks to all.

In addition, this article was reviewed and commented by Peter Banks, Jean-Pierre Belaud, Kerry Irons, Knut Mathisen, Costas Pantelides, Michel Pons, Luis Puigjaner, and Pascal Roux.

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Introduction

The CAPE-OPEN 1.0 standard, a product of several years of collaborative work between partners and contractors of the CAPE-OPEN and Global CAPE-OPEN projects has been recently released and is available for download from the www.colan.org CO-LaN website.

This article aims at giving an overview of the technical elements of the standard - the set of open standard interface specification documents which describe the main software interfaces that process modelling components and environments must provide in order to be CAPE-OPEN compliant. It must be understood that there is no requirement for a piece of software to implement all interfaces specified by CAPE-OPEN. On the contrary, the interface specifications are organised in such a way that each process modelling component (PMC) or process modelling environment (PME) only needs to implement a limited and focused set of interfaces to allow it to interoperate with other software. As an example, a Unit Operation software component (e.g. a model of a distillation column, of a reactor, of a heat exchanger, or a pump etc.) is only required to implement Unit Operation «plug» interfaces, plus a small number of Common Services interfaces, in order to be used with a CAPE-OPEN compliant PME. Should the Unit Operation require direct use of a Physical Properties or of a Chemical Reactions component for internal calculation, then it would have to implement physical properties or chemical reactions «sockets» interfaces in order to gain access to these services.

Note that we have been using the terms socket and plug to refer to the calling and called components respectively: where a software component **A** requires service **S** from component **B** through a published CAPE-OPEN interface specification of service **S**, **A** is said to implement an **S** socket, and **B** is said to implement an S plug.

In the following, we will look at the architecture of CAPE-OPEN 1.0 interfaces, we will briefly address performance issues, and we will give a list of currently available implementations of CAPE-OPEN interfaces in both commercial and research PMCs and PMEs. Some of the text is borrowed from J.-P. Belaud and M. Pons, « *Open Software Architecture For Process Simulation: The Current Status of CAPE-OPEN Standard* », to be presented at ESCAPE-12 conference, The Hague, May 2002, with permission from the authors.

Technical elements of CO 1.0

The CAPE-OPEN interfaces are split in three groups corresponding to three blocks of functionality: business interfaces (also called PMC interfaces), COSE interfaces (also called PME interfaces), and common services. They were introduced by J.-P. Belaud in Vol.1 of this newsletter:

- « *Business interfaces* or *PMC Interfaces* are domain-specific interfaces for the CAPE application domain. They define services provided by CAPE-OPEN compliant process modelling components involved in a CO modelling application. Examples are Unit Operations, Thermodynamic and Physical Properties, Solvers, Physical Properties Data Bases, etc.
- « *COSE (CAPE-OPEN Simulator Executive) Interfaces* or *PME Interfaces* are horizontal interface specifications. They define services provided by CAPE-OPEN compliant PMEs. Services of general use are defined, such as *diagnostics* and *material template* system in order to be called by any CO PMC using a callback pattern.
- « *Common Services Interfaces* define services that may be required by any *Business* and *COSE interfaces*. They support basic functions, such as identification, error handling, collections of objects, parameters, etc.

Business interfaces or PMC Interfaces

The first set, *business/PMC interfaces*, is a comprehensive set of functionalities of process modelling application elements. Let's look at it in detail.

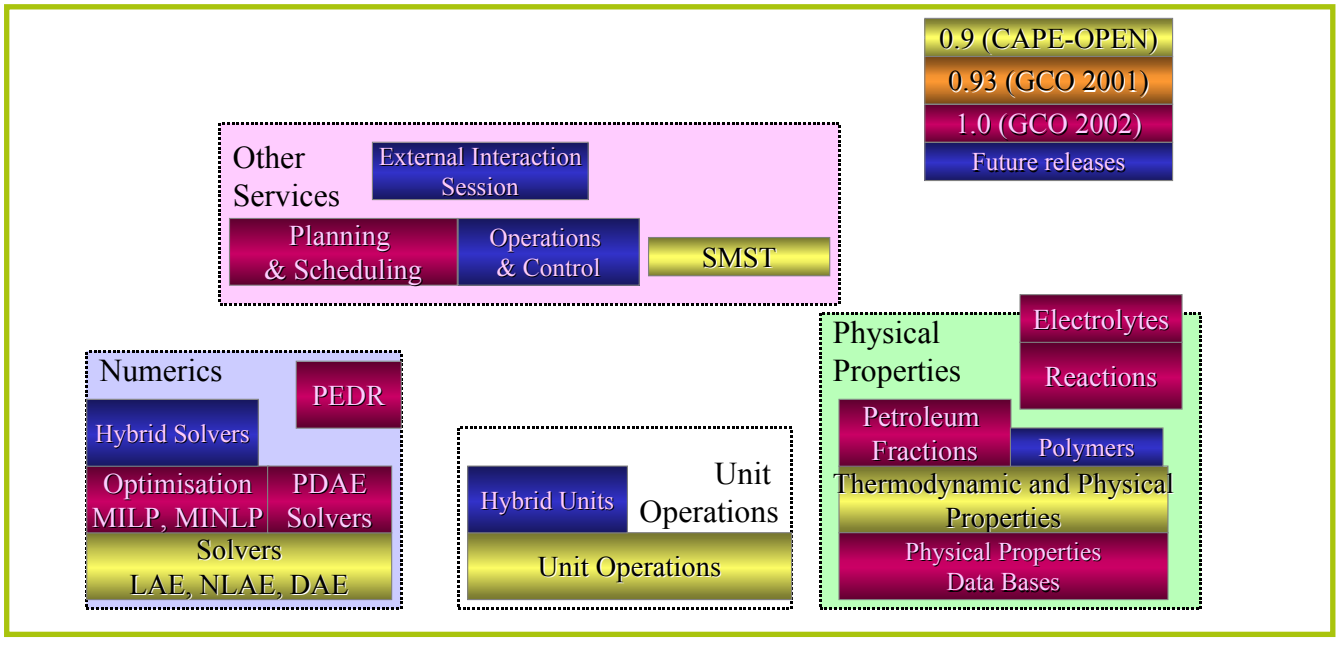

Figure 1. CAPE-OPEN Interfaces for Process Modelling Components

Business interfaces can be roughly grouped in four categories, as shown above: numerics, unit operations, thermodynamic and physical properties, and others. Although it can be debated if chemical reactions/electrolytes interfaces should be kept together with physical properties, we will keep them as such, since is it merely a question of presentation - there are no technical implications.

Version 1.0 updates previously published interfaces (known as «CAPE-OPEN 0.93») and delivers brand new interfaces. These new interfaces have not been as extensively tested as the ones previously published, therefore will be subject to updates after subsequent implementation in operational software. They are identified by the «**New!**» sign.

Several interfaces have been extensively tested and debugged by the Interoperability Task Force of Global CAPE-OPEN, a group of specialists led by Peter Banks and Malcolm Woodman of BP. They are identified by the «**ITF-ed!**» sign.

The ***Numerics*** class groups services related to numeric processing of process models.

- « The base interface in this class is *Solvers*: it focuses on the solution algorithms that are necessary for carrying out steady state and dynamic simulation of lumped systems. In particular, this includes algorithms for the solution of large, sparse systems of non-linear algebraic equations (NLAEs) and mixed (ordinary) differential and algebraic equations (DAEs). Algorithms for the solution of the large sparse systems of linear algebraic equations (LAEs) that often arise as sub-problems in the solution of NLAEs and DAEs are also considered. The CO standard introduces new concepts, such as models and the equation set object (ESO), which is a software abstraction of a set of non-linear algebraic or mixed (ordinary) differential and algebraic equations.
- « **New!** The *PDAE (Partial Diffential Algebraic Equations)* interface defines, on top of the Solvers specification, numerical services for systems with some variables distributed along one or several dimensions. In PDAEs the dependent model variables depend on one or more independent variables. Independent variables are for instance spatial co-ordinates, particulate co-ordinates (in case of population balance models) or time (in case of dynamic models). Thus, models of computational fluid dynamics are also included in this class of problems.
- « **New!** The *Optimisation* interfaces define access to Mathematical Programming optimisation services. They are also based on the *Solvers* architecture. Mathematical programming (IP / LP / NLP / MILP / MINLP) problems involve the minimisation or maximisation a linear / nonlinear objective function subject to linear / nonlinear constraints. The optimisation may involve both continuous and discrete (integer-valued) decision variables. Mathematical programming optimisation problems arise in many process engineering applications, including process synthesis, process design, product design and others. You'll find a technical presentation of these interfaces starting on page 10.
- « The *Hybrid Solvers* interface is not part of CAPE-OPEN 1.0 release and is not addressed here.
- « **New!** The *Parameter Estimation* and *Data Reconciliation* interface (PEDR), at its name clearly states, defines interface to (i) parameter estimation algorithms where the value of a model parameter must be adjusted in order to meet constraints such as experimental data; and (ii) data reconciliation packages which eliminate noisy factors from raw measurements of process variables; The DR and PE are very similar problems in the sense that both are constrained optimization problems. Since a PEDR module may require using external optimisation services, the PEDR module may call an optimisation solver module through a CO-compliant interface.

The ***Unit Operation*** class groups two services related to unit operations.

- « **ITF-ed!** Base *Unit Operation* component: CAPE-OPEN defines a comprehensive set of standard interfaces for unit operation modules being used within modular and steady-state PMEs. A unit operation module may have several ports that allow it to be connected to other modules and to exchange material, energy or information with them. In the material case (which is also the most common), the port is associated with a Material Object. Ports are given directions (input, output, or input-output). Unit operation modules also have sets of parameters. These represent information that is not associated with the ports, but that the

modules wish to expose to their clients. Typical examples include equipment design parameters (e.g. the geometry of a reactor) and important quantities computed by the module (e.g. the capital and operating cost of a reactor).

« *Hybrid Unit Operations* extend the base UO interface towards the processing of batch and hybrid UO's. This interface is not part of CAPE-OPEN 1.0 release and is not addressed here.

The ***Physical Properties*** class groups services related to obtaining or calculating thermodynamic and physical properties of matter, and to handling chemical reactions.

« **ITF-ed!** *Thermodynamic and Physical Properties* base interface: CAPE-OPEN focuses on uniform fluids that are mixtures of pure components or pseudo-components, and whose quality can be described in terms of molar composition. The physical properties operations that have been provided with standardised interfaces are those required for the calculation of vapour-liquid or liquid-solid equilibria or subsets thereof, as well as other commonly used thermodynamic and transport properties. A key concept is that of a Material Object. Typically, each distinct material appearing in a process (in streams flowing between unit operations, as well as within individual unit operations) is characterised by one such object. To support the implementation of the above framework, the CO standard defines interfaces for Material Objects, as well as for thermodynamic property packages, calculation routines and equilibrium servers.

« **New!** *Physical Properties Data Bases* (PPDB) interfaces define a CAPE-OPEN compliant standard interface for connecting a data base with recorded physical property values and model parameters to flowsheeting and other engineering programs. This interface deals with measured, correlated or estimated values of physical property data at discrete values of the variables of state (temperature, pressure, composition).

« **New!** *Petroleum Fractions* (PetroFrac) interfaces extend the standard Material Object for use in the modelling of hydrocarbon fluids processed in refining, petrochemicals and offshore production facilities. They supply additional access to petroleum-specific properties (e.g. RON, MON, cetane index, TBP curves, etc.), and allow characterising parameters of the mixtures. They also introduce a small change in the Unit Operation interfaces in order to distinguish Unit Operations handling petroleum fractions from others.

« *Polymers* interfaces extend the base Thermo interface towards the processing of polymers. This interface is not part of CAPE-OPEN 1.0 release and is not addressed here.

« **New!** *Chemical Reactions/Electrolytes* interfaces support the management and processing of kinetic, equilibrium and electrolytes reaction systems in process models. These interfaces support any reaction model, they are clients to formulate reaction equations, and they support reaction model parameter estimation. Initially planned as two different specifications, Chemical Reactions and Electrolytes were finally merged into one consistent set[1].

The ***Other Services*** class groups various services which do not belong to the three main classes. Only two interfaces are part of CAPE-OPEN 1.0, the others (*Operation and Control* and *External Interaction Session*) are published as drafts, but not officially released. They are not presented here.

« **New!** *Sequential Modular Specific Tools* (SMST) interface. A key part of the operation of sequential modular simulation systems is the analysis of the process flowsheet in order to determine a suitable sequence of calculation of the unit operation modules. This task is typically carried out using a set of tools that operate on the directed graph representation of the flowsheet. The SMST specification defines standard interfaces for the construction of these directed graphs, and for carrying out partitioning, ordering, tearing and sequencing operations on them.

« **New!** *Planning and Scheduling* interface defines interfaces to components delivering procedures and processes for allocating equipment over time to execute the chemical and physical-processing tasks required for manufacturing chemical products, generally in batches. These interfaces deal with managing requirements, production resources, recipes, planning and scheduling problems and their solutions.

[1] At the same time, we publish future draft releases (1.1) of Thermodynamic and Physical Properties, and of Reactions; anyone intending to implement these versions should contact CO-LaN.

COSE (CAPE-OPEN Simulator Executive) Interfaces or PME Interfaces

COSE/PME interfaces define general services that can be requested from CAPE-OPEN compliant process modelling environments such as Hyprotech's HYSYS, AspenTech's AspenPlus, PSE's gPROMS, or RSI's INDISS. All these specifications are **New!** in CO 1.0. The COSE/PME interface is a small and simple interface with only half a dozen methods. It might be extended in the future.

« *Simulation Context* interface specification is the base specification for COSE services. It gathers three functionalities, Diagnostic, Material Template System and Utilities. That results in three interfaces, one for conveying verbose information to the PME, one for allowing the unit to choose between all the Thermo Material factories supported by the COSE, and one for requesting diverse values from the PME.

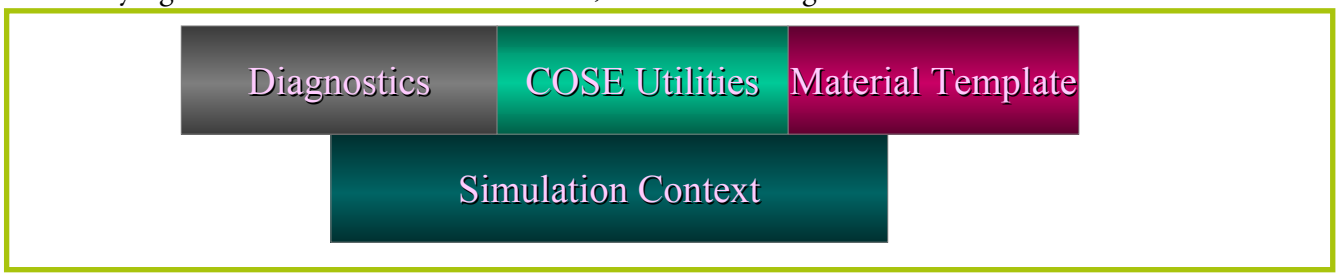

Figure 2. CAPE-OPEN Interfaces for Simulation Executives (or Process Modelling Environments)

« *Diagnostic* interface allows communication of verbose information from the PMC to the PME (and hence to the user). PMCs should be able to log or display information to the user while executing a flowsheet.

« *Material Template* interface provides the mechanisms for accessing CAPE-OPEN Property Packages managed by the COSE, in order to allow PMCs to directly choose and configure material objects as needed.

« *COSE Utilities* provide a small list of other useful functions, in particular the FORTRAN Channel selection which prevents FORTRAN-based PMCs from sending output to channels already used by the COSE.

Common Services interfaces

Common Services interfaces define base services that CAPE-OPEN components can either use or provide, independently of the nature of the component. Some of these specifications were published in release 0.93 last year, some are new. They are gathered in one of the two «Methods and Tools» documents which were developed by the Methods and Tools group of Global CAPE-OPEN: the Common Interfaces Reference Manual.

« **ITF-ed!** *Types and undefined values* are the most basic elements of the CAPE-OPEN 1.0 specification. They define the standard types of all elements passed through CO interfaces: integer values, real values, arrays, character strings, etc. as well as «undefined» values. All CO interfaces rely on the standard types.

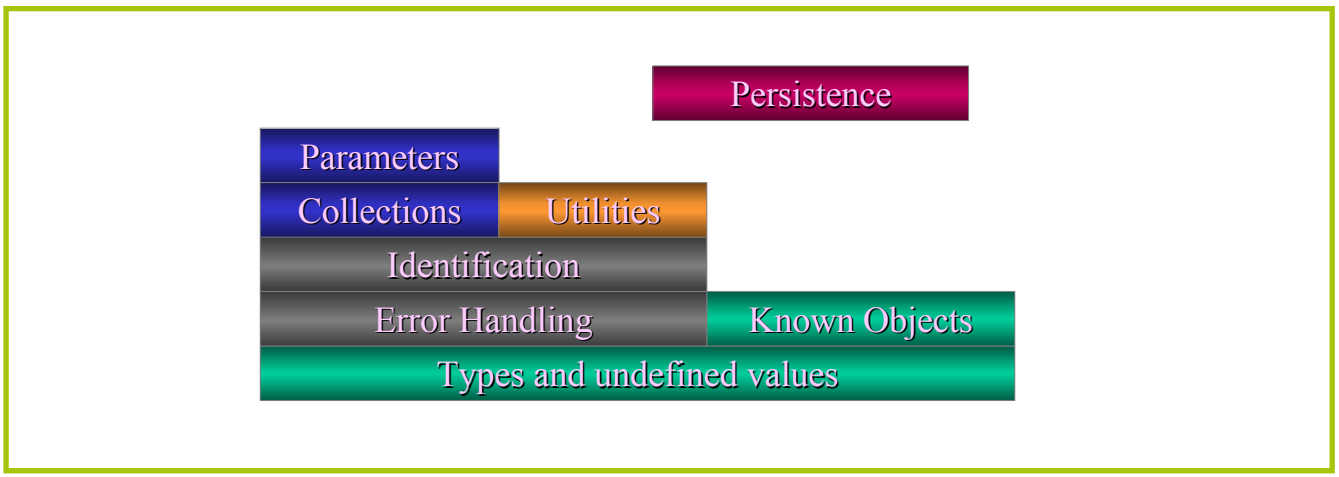

Figure 3. CAPE-OPEN Common Services Interfaces

- **New!** *Known objects* gather a large number of standard identifiers used in interfaces, such as Thermo, PPDB, and petroleum fractions. These are lists of properties names, names of methods; identification of phases, etc., which form a consistent set of names used throughout these interfaces.
- **ITF-ed!** *Error Handling* defines how to manage execution errors (abnormal terminations). When a request is made, if this request is successful it raises no error, otherwise it raises an error. When an error occurs, the execution is immediately aborted. This Error Handling interface gives a classification and a hierarchy of potential errors occurring in CO compliant components. All CO components must implement it.
- **ITF-ed!** *Identification* interface provides the means for all CO components to be identified by name and textual description. All CO components must implement it.
- **New!** *Collections* interface defines a standard way of managing collections of things. The aim of the Collection interface is to give a CO component the possibility to expose a list of objects to any client of the component. The client will not be able to modify the collection, i.e. removing, replacing or adding elements. However, since the client will have access to any CO interface exposed by the items of the collection, it will be able to modify the state of any element.
- **ITF-ed!** *Parameters* interface defines a standard access to component parameters. This specification will be used by CO components wishing to expose some of their internal data to their clients. The interface is made up of two different parts, each corresponding to a different client need: the first part is a fixed, static aspect that describes the Parameter, such as a type, name, description, dimensionality etc. The second part deals with value of the parameter itself. It is expected that the parameter values will change quite frequently both within and outside of the component that needs it.
- **ITF-ed! New!** *Utilities* interface gathers a number of useful functionalities that can be requested from process modelling components. In version 1.0, this interface provides the means to set the simulation context, to collect component parameters, to manage lifecycle of components (creation and termination) and to edit, that is, to open an edit GUI for the component.
- **ITF-ed! New!** *Persistence* interface defines how models and model elements are stored and retrieved. Most simulation environments allow the possibility to store at any moment the state of a simulation case, in order to be able to restore it at any time in the future. In the CAPE-OPEN distributed environment, where different pieces of the simulation may be implemented by different vendors, the Persistence interface proposes a standard mechanism to provide this feature. This interface is different from all others, as it does not define any new method. Instead, it explains how to use standard persistence mechanisms provided by middleware (COM and CORBA) for this purpose

Performance Issues

The Interoperability Task Force of Global CAPE-OPEN spent considerable effort on performance issues in the last months of 2001. The ITF was charged with facilitating the delivery of practical, plug and play interoperability within commercial flowsheet simulators, via industrially-relevant test scenarios and the critical review of the CAPE-OPEN interface specifications for ambiguities and omissions. This capability within mainstream commercial flowsheet simulators is a prerequisite for acceptance of open simulation in the work place.

Good performance is critical especially for thermodynamic and physical properties calculations which are called thousands of times during a process simulation, so that the overhead due to standard interfaces should be minimal. This issue is also of importance for other components but the focus has been on physical properties and thermodynamics since the initial performance degradation was huge in some implementations.

The result of the ITF work is that there is almost no degradation of performance if the interfaces are correctly and efficiently implemented. Revisions of internal implementation of physical properties components by vendors and others (without any revision of the interface specifications) led to orders of magnitudes of improvement, with

Supplier	Software	Interfaces	Technology
AspenTech www.aspentech.com	Aspen Plus 11.1	Thermodynamic and physical properties socket Unit operations socket	COM
	Aspen Properties 11.1	Thermodynamic and physical properties plug	COM
Hyprotech www.hyprotech.com	HYSYS.Plant 2.4	Thermodynamic and physical properties socket Unit operations socket	COM
	Distil	Thermodynamic and physical properties socket	COM
	COMThermo 1.1	Thermodynamic and physical properties plug	COM
Process Systems Enterprise (PSE) www.psenterprise.com	gPROMS	Thermodynamic and physical properties socket Equation Set Object plug Numerical Solvers sockets (linear, nonlinear and differential algebraics)	COM CORBA CORBA
	gO:CAPE-OPEN	Unit operations plug	COM
Belsim www.belsim.com	VALI III	Thermodynamic and physical properties socket	COM
Prosim S.A. www.prosim.net	ATOM Odysseo	Thermodynamic and physical properties plug Dynamic flash unit plug	COM COM
Infochem www.infochemuk.com	Multiflash 3.1	Thermodynamic and physical properties plug	COM
RSI www.rsi-France.com	INDISS	Thermodynamic and physical properties plug and socket Unit Operation plug and socket	COM COM
IFP www.ifp.fr	SPIP FIBER	Thermodynamic and physical properties plug Unit Operation plug	
INP Toulouse - LGC - CNRS www.inp-toulouse.fr/lgc	Numerical Services Provider Continuous Model Builder M&S Flowsheet Server	Numerical Solvers plug Numerical Solvers socket Unit Operation plug Sequential Modular Specific Tools plug	CORBA CORBA COM CORBA
DECHEMA www.dechema.de	DETHERM	Physical Properties Data Bank Plug	COM
RWTH.LPT www.lfpt.rwth-aachen.de		Numerical Solvers plug	CORBA
RWTH.I5 www-i5.informatik.rwth-aachen.de	COM-CORBA Bridge Java Unit Skeleton Java Material Object Skeleton	Bridge Unit Operation plug Material Object and Material Template	COM, CORBA CORBA CORBA
CO-LaN www.colan.org	Tester Suite (1)	Thermodynamic and physical properties plug and socket Unit Operation plug and socket MINLP socket Physical Properties Data Bank socket Sequential Modular Specific Tools socket	COM, CORBA through bridging COM COM COM
NORSK HYDRO www.hydro.com		Heating Tank Unit Operation Fluent Wrap Unit Operation CASE test socket	CORBA
UPC www.upc.es/eq/	MOPEDR MOPP	PEDR Prototype Planning and Scheduling package	CORBA CORBA

(1) The CO-LaN tester suite is a comprehensive set of public-domain tools aiming at helping organisations develop CAPE-OPEN components through detailed compliance checking mechanisms. This is one of the methods that CO-LaN uses to facilitate the migration to CAPE-OPEN, together with additional how-to documents (the *migration cookbook*) and *software wizards*. The Unit Operation wizard is presented in this volume. The tester suite will be presented in Vol. 3. of the CO-Update newsletter.

final values of around 15-20% overhead in calculation time due to CAPE-OPEN interfaces being possible. Such an overhead is not significant and is very quickly compensated by the consequences of Moore's Law, which makes computing speed higher and higher and computing power cheaper and cheaper.

In conclusion, you should not worry about performance of CAPE-OPEN interfaces in general. You should only worry about efficient implementation of CAPE-OPEN compliant physical properties and thermodynamic services: the development of physical and thermodynamic properties plugs or sockets must take serious care of performance, whether the CAPE-OPEN or any other standard is used.

CO-compliant Process Modelling Components and Process Modelling Environments

The table above lists a number of commercial or research PMCs and PMEs providing CAPE-OPEN interfaces. This table cannot be exhaustive since we cannot be aware of all the current developments and migration of existing software packages to CO compliance. If you are interested in specific software package shown in this list, please contact its supplier. If you are interested in any software package **not shown** in the list, please contact its supplier and ask for CO compliance!

A catalogue of CO-compliant PMCs and PMEs will be published and regularly updated on http://www.colan.org.

Conclusions

CAPE-OPEN interfaces match the interoperability needs of the process modelling community; they are debugged; they are efficient; they are publicly available on the web site for anyone to use; they have been implemented in many software packages; in short, they work!

Open process simulation is not a futuristic thing. It is here and now. If you are a supplier, migrate your software to CO compliance; if you are a user, ask for CO compliance from your suppliers.

References

The CAPE-OPEN 1.0 standard is downloadable from http://www.colan.org.

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Any Feedback ?

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