

Update on CAPE-OPEN standards and CO-LaN activities



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Session on Software architecture, Standards & Interfaces
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Outline

- ◆ **What is CAPE-OPEN?**
- ◆ **CO-LaN**
- ◆ **CAPE-OPEN standards in progress**
- ◆ **Support tools delivered**
- ◆ **Training in CAPE-OPEN**
- ◆ **Conclusions and perspectives**



***Expanding Process Modeling Capability
through Software Interoperability
Standards***

What is CAPE-OPEN?

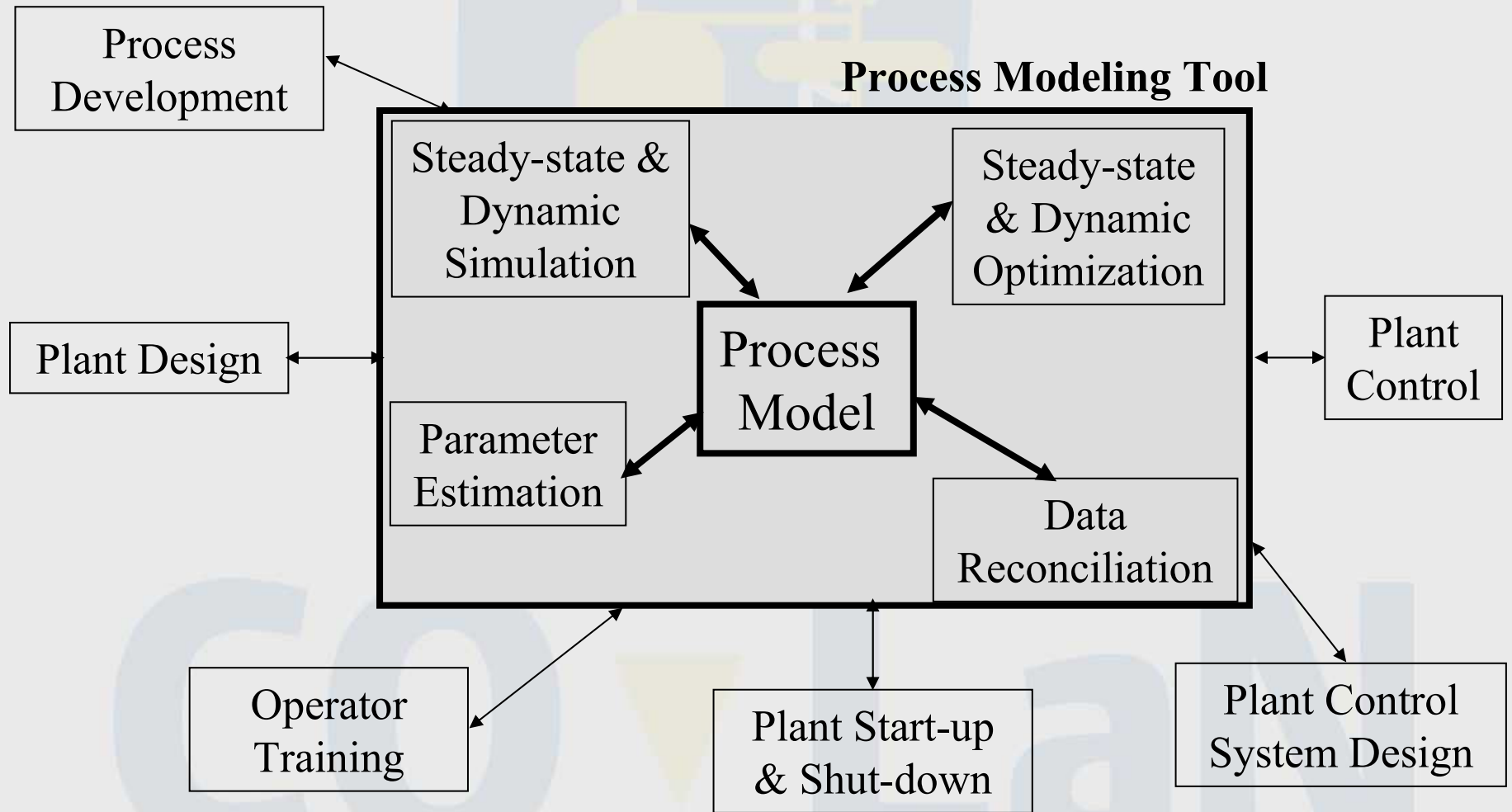
**CAPE-OPEN defines rules and interfaces
that allow CAPE (Computer-Aided Process
Engineering) applications or components
to interoperate**



CAPE-OPEN: a technology for integration

- ◆ A freely available industry standard for interfaces between software components making up process simulation tools
- ◆ The success of a collaboration between software vendors, end-users and academics
- ◆ A proven IT technology implemented in most process simulation tools
- ◆ A growing adhesion by process simulation market leaders and niche software providers

Process modeling and simulation tools



Process modeling: components & environments

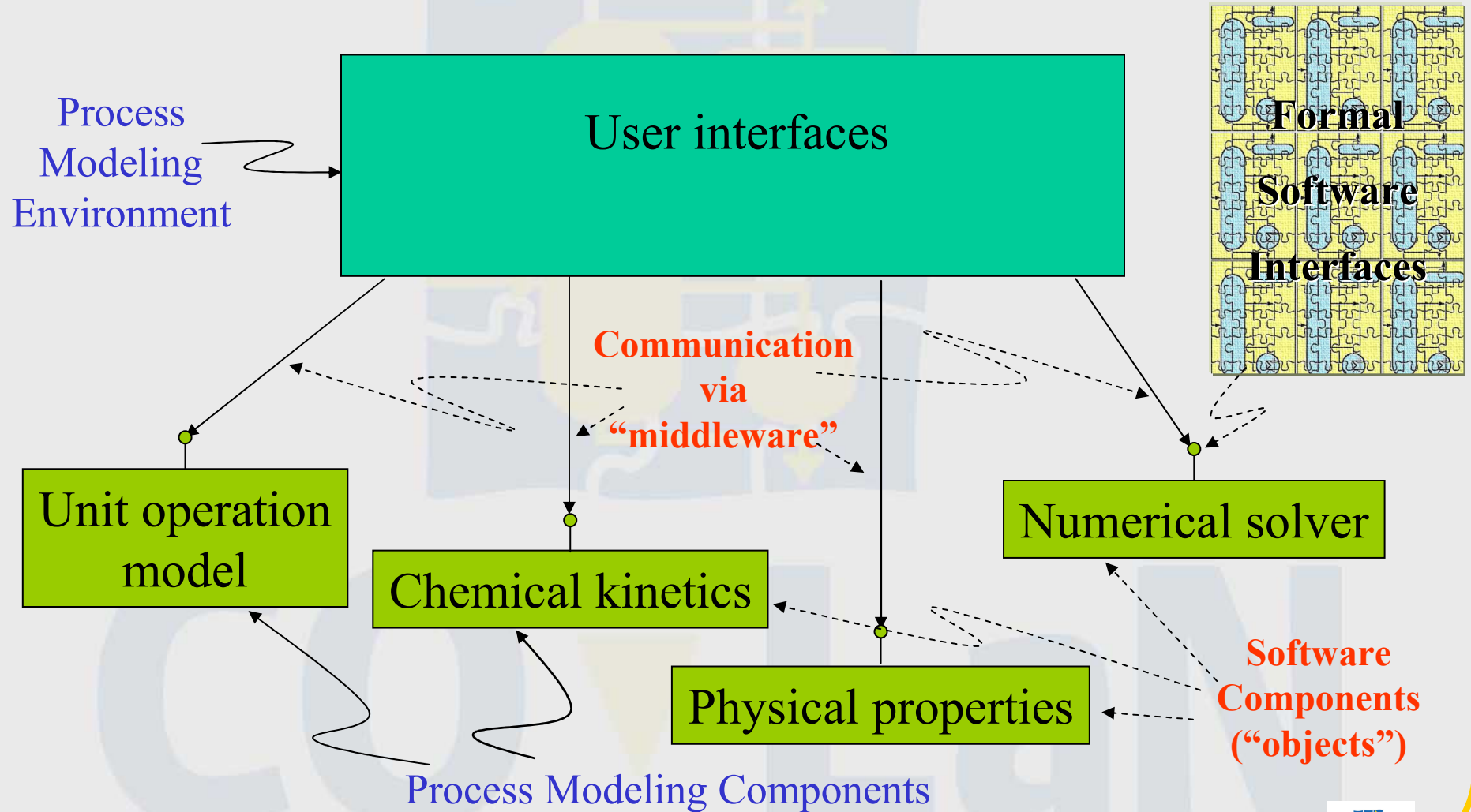
◆ Process Modeling Components (PMCs)

- ⇒ Well-defined pieces of software, relatively narrow function
- ⇒ Wide range of applications
 - Physical properties
 - Unit operation modules
 - Numerical solvers
 -

Process modeling: components & environments

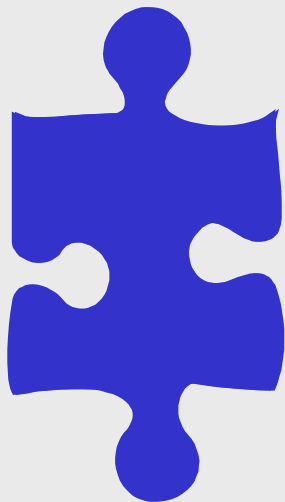
- ◆ **Process Modeling Components (PMCs)**
- ◆ **Process Modeling Environments (PMEs)**
 - ⇒ **Support construction of process model**
 - **From first-principles (modelers) and/or library of unit operation models**
 - ⇒ **Support a number of model-based applications**
 - **Simulation, optimization, parameter estimation...**
 - ⇒ **May make use of one or more PMCs**

CAPE-OPEN in between PME & PMCs

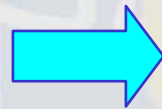


CAPE-OPEN Thermodynamic socket

- ◆ End-user can plug any CO compliant Property Package into a CO compliant Process Modeling Environment.



External CO Property Package:
(Aspen Properties,
PPDS,
UniSim COMThermo,
Aspen Hysys COMThermo,
Simulis Thermodynamics,
MultiFlash,
CO-SPPTS, ...)



CAPE-OPEN PME:
Aspen Plus,
Aspen Hysys,
UniSim Design,
INDISS,
ProSimPlus,
gPROMS,
PRO/II,
COFE,
Xchanger Suite

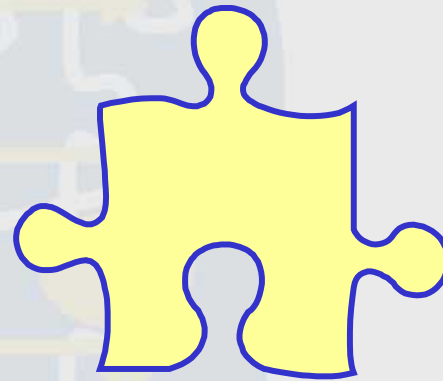
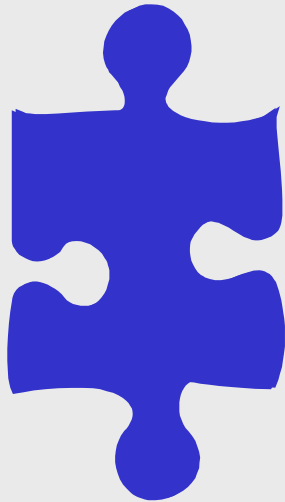


Workflow

- ◆ End-user develops a Property Package in a third-party application (ex. : Aspen Plus, Simulis Thermodynamics, etc...).
- ◆ End-user saves Property Package (PP) configuration to make PP available as a CAPE-OPEN component.
- ◆ End-user opens a PME and selects the external Property Package to be used.
- ◆ The PME asks for physical properties and phase equilibrium calculations to the external Property package through CAPE-OPEN interfaces.

CAPE-OPEN Unit Operation socket

- ◆ End-user can plug any CO compliant Unit Operation into a CO compliant Process Modeling Environment.



CAPE-OPEN PME:
Aspen Plus,
Aspen Hysys,
UniSim Design,
INDISS,
ProSimPlus,
PRO/II,
COFE

External CO Unit Operations:
(XChanger Suite,
Fluent models,
gO:CAPE-OPEN models,
in-house components...)



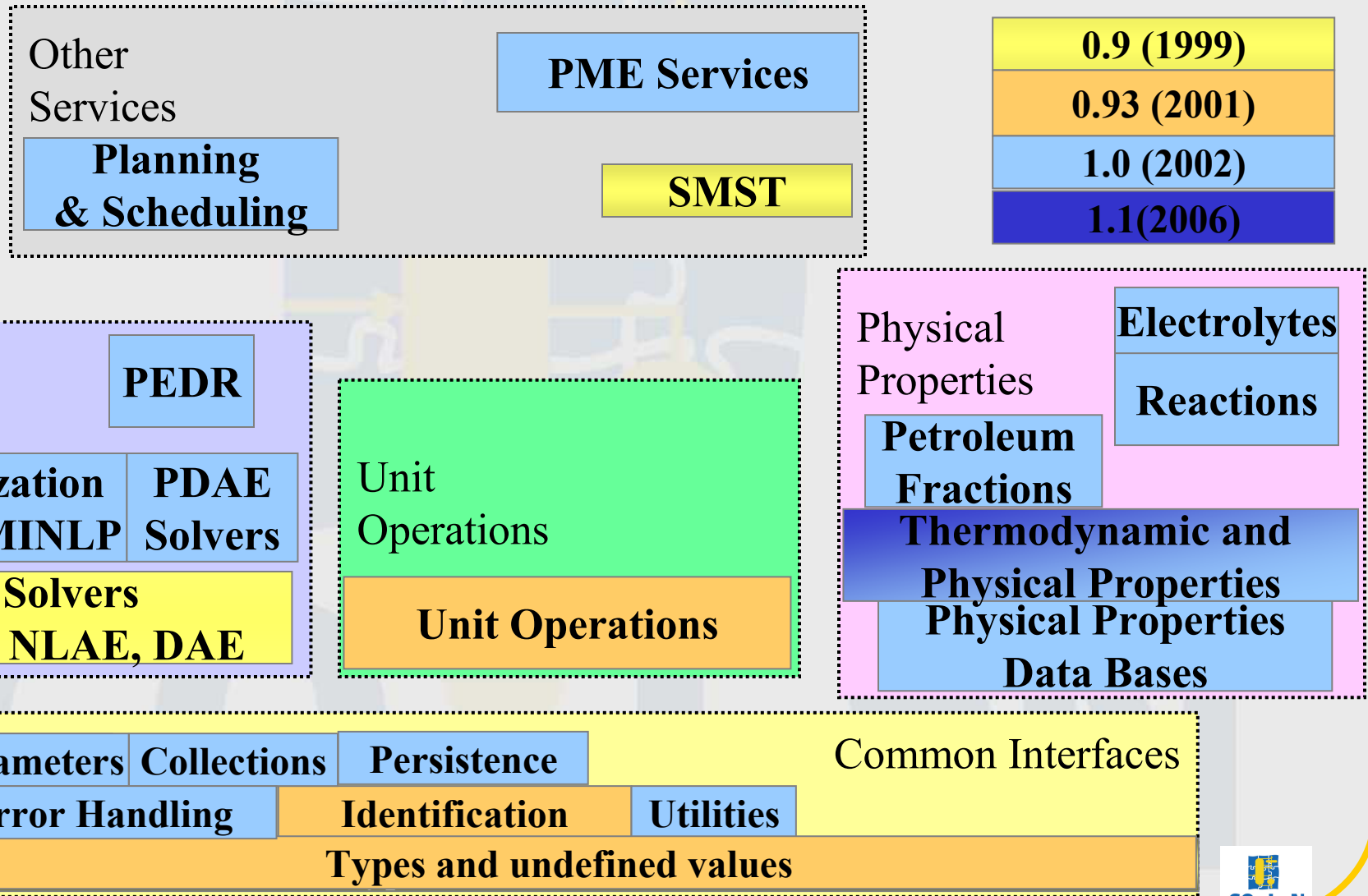
What is CAPE-OPEN?

- ◆ **CAPE-OPEN is not**
 - ⇒ A piece of software
 - ⇒ A data model
- ◆ **CAPE-OPEN is**
 - ⇒ An interface standard
 - ⇒ A documentation set

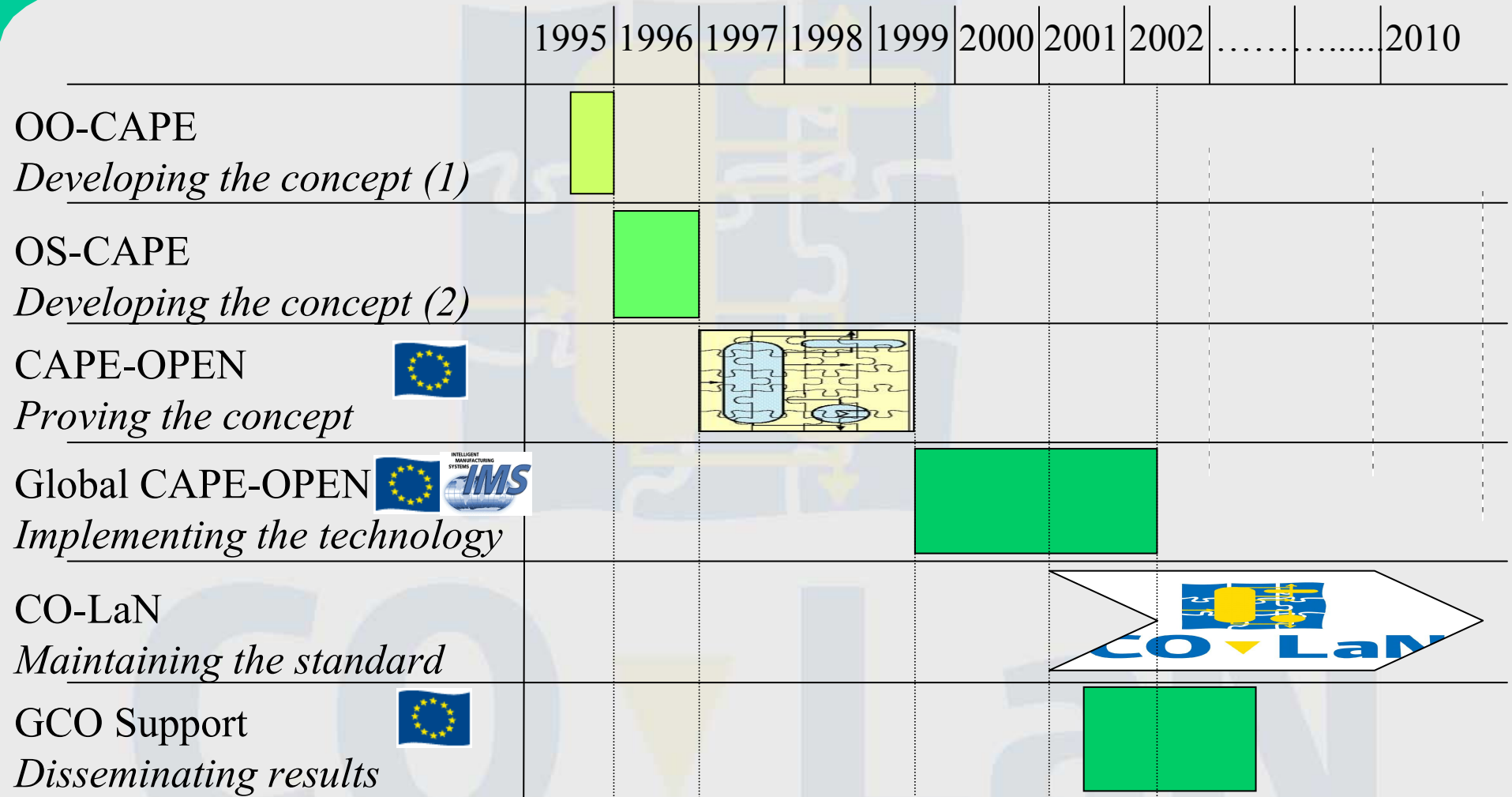
CO  LaN



CO interface specification releases



Making a visionary idea a reality



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**CO-LaN
CAPE-OPEN Laboratories Network**

**A group of end users taking responsibility
for putting resources together to support
ongoing work on the standard**

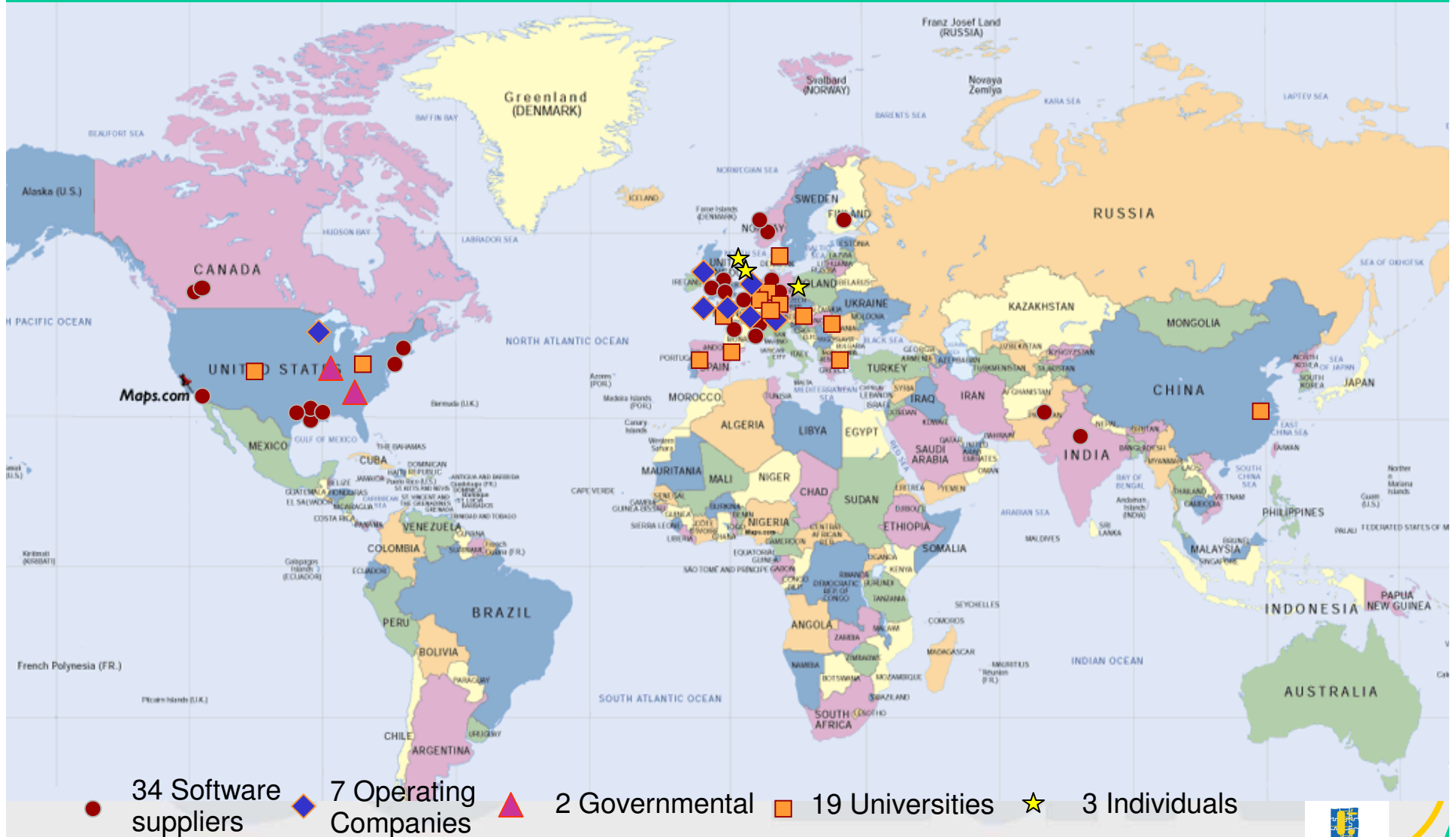


The CAPE community behind CAPE-OPEN



And quite a few more

65 members as of September 2007



Activities

- ◆ **Organize targeted Special Interest Groups on standards**
 - ⇒ Trigger projects open to all members
- ◆ **Develop independent testers and support tools**
 - ⇒ CO-LaN Tester suite, wizards, logger
- ◆ **Disseminate**
 - ⇒ Web site, documents, newsletter
 - ⇒ CAPE-OPEN European and US Conferences
- ◆ **Facilitate interoperability**
 - ⇒ Use software made available in any combination
- ◆ **Deliver training**
 - ⇒ Three training courses organized / sponsored



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CAPE-OPEN standards in progress

Thermodynamic & Physical Properties 1.1

Refinery Reactors



Objectives of Thermo revision 1.1

- ◆ **Improve clarity**
 - ⇒ Remove ambiguities of previous version (1.0)
 - ⇒ Better define purpose and functionality
- ◆ **Simplify implementation**
 - ⇒ Reuse entire sets of methods on different components
- ◆ **Improve reliability**
 - ⇒ Methods to check capabilities before launching calculations

A collaborative development process

- ◆ **Initiated within Global CAPE-OPEN project**
 - ⇒ **Interoperability Task Force headed by BP**
 - **BASF, Aspentech, Hyprotech, TOTAL, Infochem**

- ◆ **Pursued within CO-LaN**
 - ⇒ **Investment in prototyping work**
 - ⇒ **Special Interest Group Thermodynamics**
 - **BASF, Aspentech, Infochem, TOTAL, AmsterCHEM, TUV NEL Ltd, ProSim, TUHH directly involved**
 - **Formally adopted in October 2006 by CO-LaN Management Board after completion of approval process**



Highlights

- ◆ **Workflow**
 - ⇒ **Inquire, Check, Calculate**
- ◆ **Less emphasis on phase equilibrium**
 - ⇒ **Phases as independent entities**
- ◆ **Handling of multiple phases**
 - ⇒ **Phase label and state of aggregation**
- ◆ **Versatile phase equilibrium calculations**
 - ⇒ **Any arrangement of specifications allowed**



Immediate adoption

- ◆ **Process Modeling Environments (PMEs)**
 - **SolidSim (TUHH) since September 2006**
 - **COFE (AmsterCHEM) – since March 2007**
 - **TUWAX (University of Tulsa) – since May 2007**
 - **Aspen Hysys (Aspentech) – November 2007**
- ◆ **Process Modeling Components (PMCs)**
 - **Property Package Managers**
 - **TEA (AmsterCHEM) – since March 2007**
 - **MultiFlash (Infochem) – since April 2007**
 - **Simulis Thermodynamics (ProSim) – November 2007**
 - **COMThermo (Aspentech) – November 2007**
 - **PPDS (TUV NEL Ltd) – December 2007**
 - **Unit Operations**
 - **COUSCOUS (AmsterCHEM) – since March 2007**
 - **PIPE (IFP/TOTAL) – since May 2007**
 - **TUWAX – November 2007**



Special Interest Group Refinery Reactors

◆ Charter:

- ⇒ Revise and develop the necessary CAPE-OPEN interface standards for the use of Refinery Reactor models in Process Modelling Environments

◆ Key Responsibilities:

- ⇒ Develop required extensions to existing interface specifications necessary to implement refinery reactor models as CAPE OPEN units. This may lead to the creation of new interfaces.
- ⇒ Initiate implementation of petroleum fractions in PME and PMC.

◆ Membership

- ⇒ BP, Shell Global Solutions, SimSci-Esscor, Honeywell, Aspentech, IFP



2007 Objectives

From 2007 SIG Charter:

- ◆ Engage Unit and Thermo SIG on modifications required for petroleum fractions.
- ◆ Further refine scenarios to cover functionality required for implementation.
- ◆ Initiate approval process of the revised petroleum fractions interface specification.
- ◆ Finalize two independent prototypes for demonstration at the 2008 CO-LaN Annual General Meeting.



Prototypes

- ◆ **CO “Refinery Reactor”**: UO interacting with compounds defined by modifiable (petroleum) properties
 - ⇒ Sulfur, Viscosity, RON, TBP, metals content
- ◆ **Proto#1: delivered in March 2007**
 - ⇒ Shell, AmsterCHEM, SimSci (PRO/II 8.1 Patch 1)
 - ⇒ Property Calculator - Sulphur
- ◆ **Proto#2:**
 - ⇒ BP, SAIC, Aspentech, Honeywell
 - ⇒ Mixer/blender and RON calculator
 - ⇒ Developed, not yet tested

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Interoperability Support Tools

**Responding to developers' and users'
needs**



Needs for Interoperability Support Tools

- ◆ **Users' need: delivery of reliable, seamless interoperability**
 - ⇒ **Facilitate relationship with support teams if problems arise**
- ◆ **Developers' need: reduce learning curve**
 - ⇒ **Lessen cost of adopting CAPE-OPEN**
- ◆ **CO-LaN's goal: accelerate adoption**
 - ⇒ **Get more components and environments available with CAPE-OPEN interfaces**

Solution proposed by CO-LaN

◆ Simplify processes

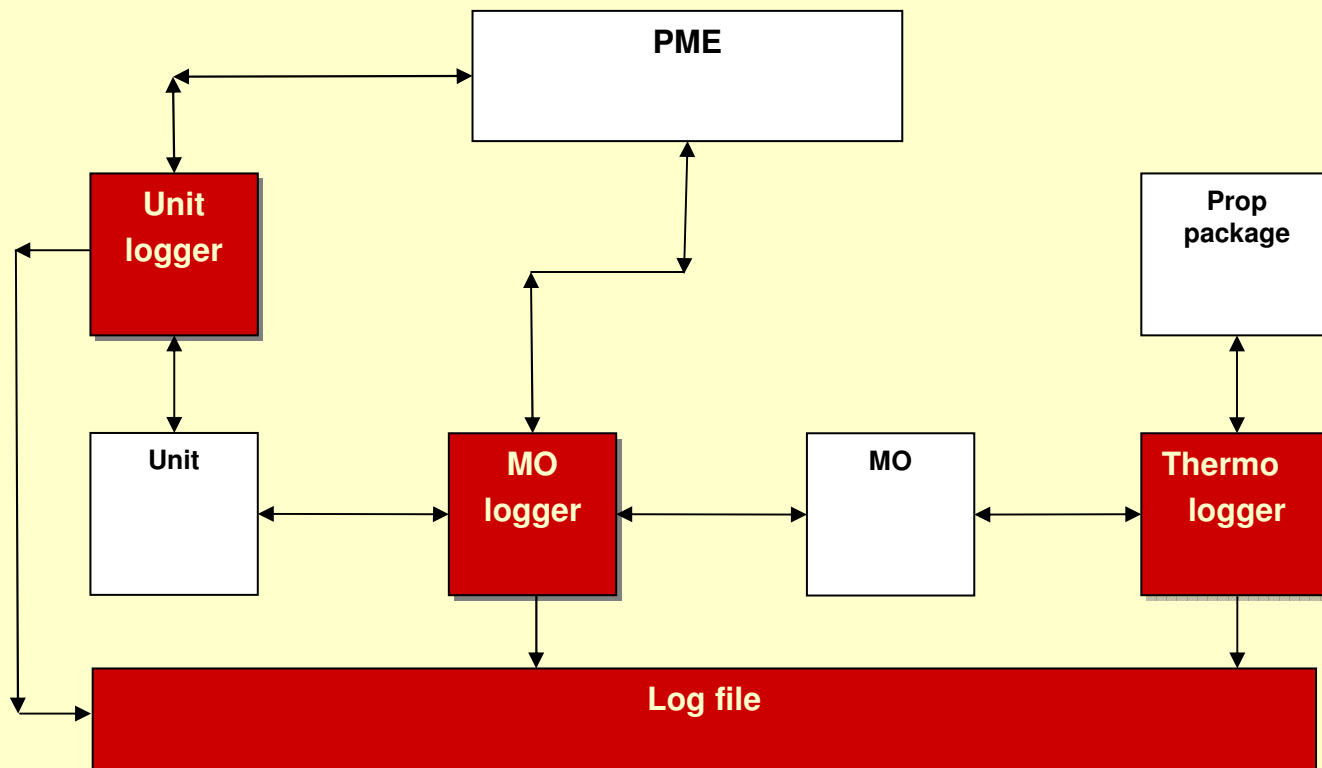
- ⇒ of developing a CAPE-OPEN compliant component
 - Wizards develop most of the code needed around a CAPE-OPEN component automatically
- ⇒ of testing compliance with CO standards
 - A Tester Suite analyzes the CAPE-OPEN interfaces displayed by a component
- ⇒ of analyzing communication between a PMC and a PME
 - A CAPE-OPEN Logging and Testing Tool reports on whatever transactions take place between a PME and a PMC

Interoperability Support Tools: a major commitment from CO-LaN

- ◆ **Unit Wizards: ~25 K\$ development cost for CO-LaN**
 - ⇒ Provides wrappers for Unit Operation components quickly
- ◆ **Tester suite: ~ 90 K\$ development cost for CO-LaN**
 - ⇒ Checks CO compliance of software components
- ◆ **Logging Tool: ~ 45 K\$ development cost for CO-LaN**
 - ⇒ Analyzes communication

CO Logging and Testing Tool (COLTT)

COLTT components inserted in between actual components and PME



Log content

- ◆ COLTT logs all calls made in both directions, via CAPE-OPEN interfaces between a PME and a PMC.
- ◆ Each call to any method from any interface generates a log entry showing:
 - ⇒ Which object made the call
 - ⇒ Which call was made
 - ⇒ Values for the input arguments that were passed
 - ⇒ Return values that were passed back
 - ⇒ Whether the call generated an error and what the error was
 - error codes are explained by a message where possible, or at least translated to a Windows or CAPE-OPEN error name such as E_FAIL or ECapeLimitedImpl.

In-house development support tools

- ◆ **Need for software tools facilitating in-house migration to CAPE-OPEN**
 - ⇒ **Wizards**
 - ⇒ **Libraries**
 - **Simplify function calls by hiding IT technology used**

- ◆ **TOTAL, IFP, SASOL have developed tools for different programming languages:**
 - ⇒ **FORTRAN 90, C++, Pascal**

- ◆ **Donated to CO-LaN or released as open source**



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Training in CAPE-OPEN

Disseminating knowledge



Vendors and CO-LaN offering

- ◆ Initially training in CAPE-OPEN was supposed to be made by software vendors
- ◆ When this did not happen, CO-LaN took actions:
 - ⇒ Push for a Short Course at AIChE Annual Meeting 2006
 - Realized by ProSim SA with CO-LaN support
 - ⇒ Arrange a one-day course on CAPE-OPEN and .NET at the 4th CAPE-OPEN European Conference (2007)
 - ⇒ Arrange for a Short Course at AIChE Annual Meeting 2007
 - Instructors from US EPA and AixCAPE e.V.



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Conclusion and perspectives

CO  LaN



Conclusions and perspectives

- ◆ **CAPE-OPEN projects achieved success**
- ◆ **CO-LaN is on the move for sustained success**
 - ⇒ **Expanding its membership**
 - ⇒ **Enhancing the CAPE-OPEN standards**
 - ⇒ **Delivering tools easing up implementation**
 - ⇒ **Making sure training is delivered**
 - ⇒ **Maintaining CAPE-OPEN awareness high**



Conclusion & perspectives

- ◆ **CAPE-OPEN recognized as THE interface standard in process simulation**
- ◆ **CAPE-OPEN attractive to many process simulation software vendors**
 - ⇒ **Most commercial PMEs now CAPE-OPEN compliant**
- ◆ **Solution adopted by end-users for in-house tools**
 - ⇒ **IFP, SASOL, Air Products,**
- ◆ **Next push from CO-LaN: develop more PMCs**
 - ⇒ **Emphasis**
 - **On tools making implementation easier**
 - **On implementation examples**





Next CAPE-OPEN events later this year:
CAPE-OPEN Short Course, Salt Lake City, Nov 4
4th CAPE-OPEN US Conference, Salt Lake City, Nov 4-9

Thank you
Questions?

