REVIEW OF CAPE-OPEN NUMERICAL INTERFACES IMPLEMENTATIONS

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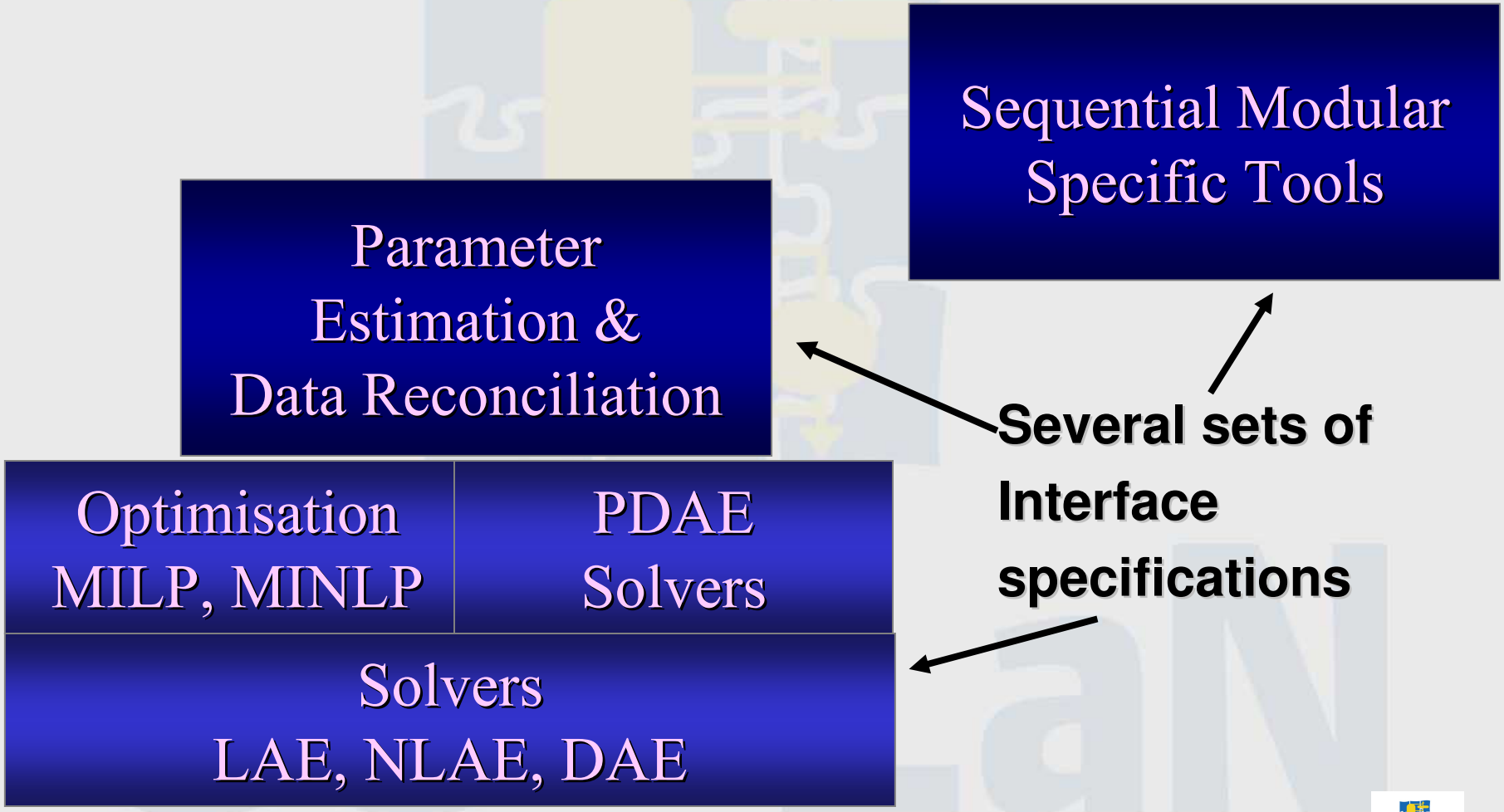
Outline

- What are CAPE-OPEN Numerical interfaces?
- What are the known implementations?
  - Sequential Modular Specific Tools
  - Solvers
- Conclusion & perspectives

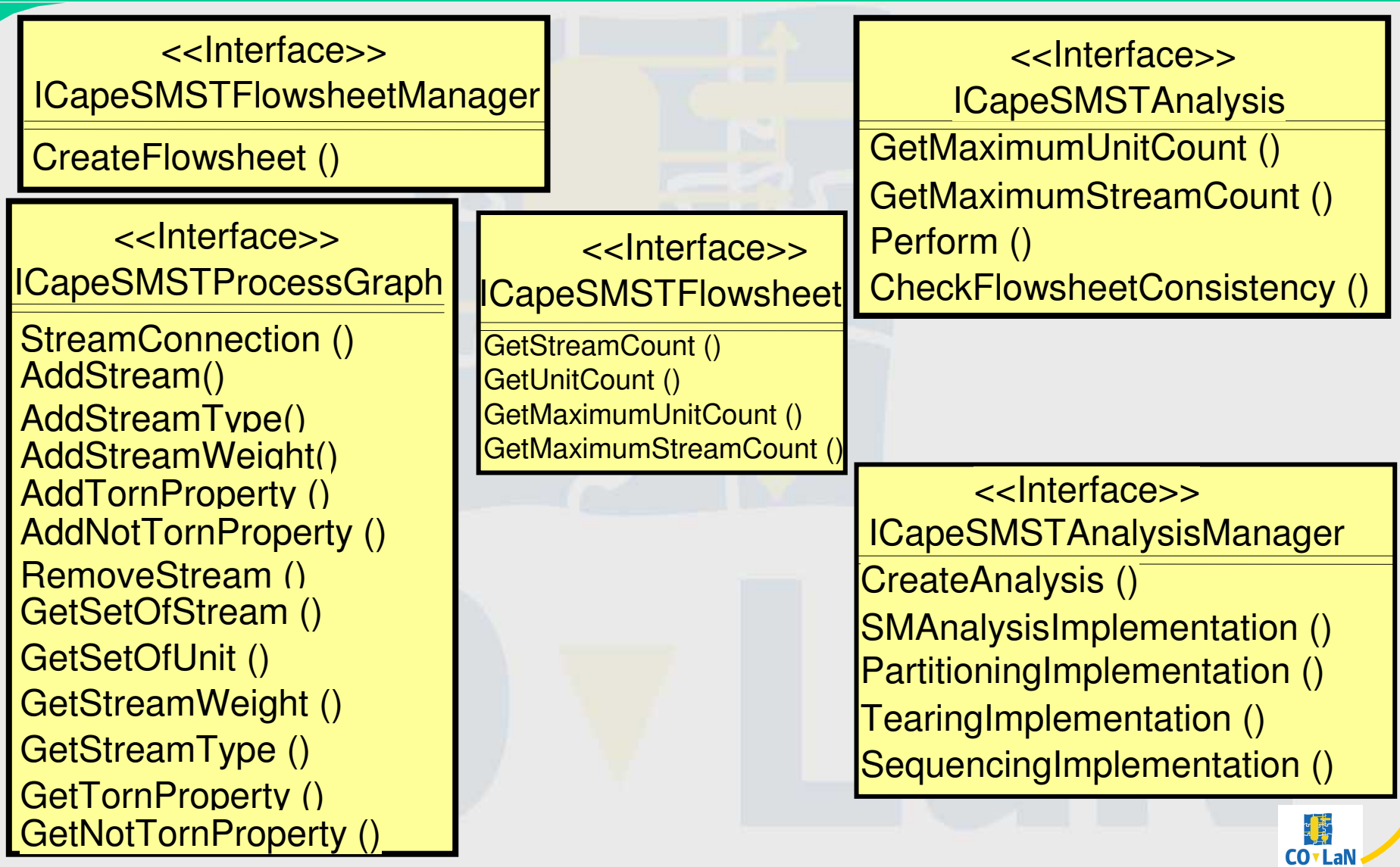
Overview of CO 1.0 interfaces: solvers services and clients



Sequential Modular Specific Tools

- Relates to Graph Analysis Tools
  - Exist at pre-processor level and comprise
    - Partitioning: locate the groups of units (i.e. Partitions) which must be solved together
    - Ordering: to place the Partitions in a proper sequence for computation
    - Tearing: analysis of each Partition to determine tear streams
    - Sequencing: for each Partition where tear streams are determined, search for the computational order of units
- Interface specification developed during CAPE-OPEN project
- As part of the interface specification development, prototypes made by INPT-ENSIACET for plug & socket

SMST interface diagram



Numerical solvers

- Scope is a variety of core model-based activities
  - Steady-state & dynamic simulation
  - Steady-state optimisation
  - Parameter estimation and data reconciliation
- Includes both “modular” and “equation-orientated” systems
- Emphasis on “large-scale” problems

CAPE-OPEN Problem Objects

- **Fundamental principle: complete separation between**
  - **the description of the problem being solved**
  - **the code used for its solution**
- **Describe different types of mathematical problems as different classes with formally defined interfaces**

Mathematical Problem Type	CAPE-OPEN Problem Object
Nonlinear algebraic equations	Equation Set Object (**ESO**)
Differential-algebraic equations	Differential Algebraic ESO (**DAESO**)
Partial differential-algebraic equations	Partial Differential Algebraic ESO(**PDAESO**)
Mixed integer nonlinear programming problems	**minlp** object

CAPE-OPEN Systems

$$\left\{\begin{array}{c}\text{CAPE}-\text{OPEN}\\ \text{System}\end{array}\right\} \equiv \left\{\begin{array}{c}\text{Problem}\\ \text{being solved}\end{array}\right\} + \left\{\begin{array}{c}\text{Numerical code}\\ \text{used for solution}\end{array}\right\}$$

- Each CAPE-OPEN System has method(s) for solving the problem
- Final solution of the problem is placed in the CO Problem Object

CO Numerical Standard

♦ Analysis, Design and Implementation Specifications

➲ the *Solver* package is subdivided into 3 main

Solver involves the CO interfaces :
- Manager
- LA, NLA, DAE, PDAE, MINLP Solver

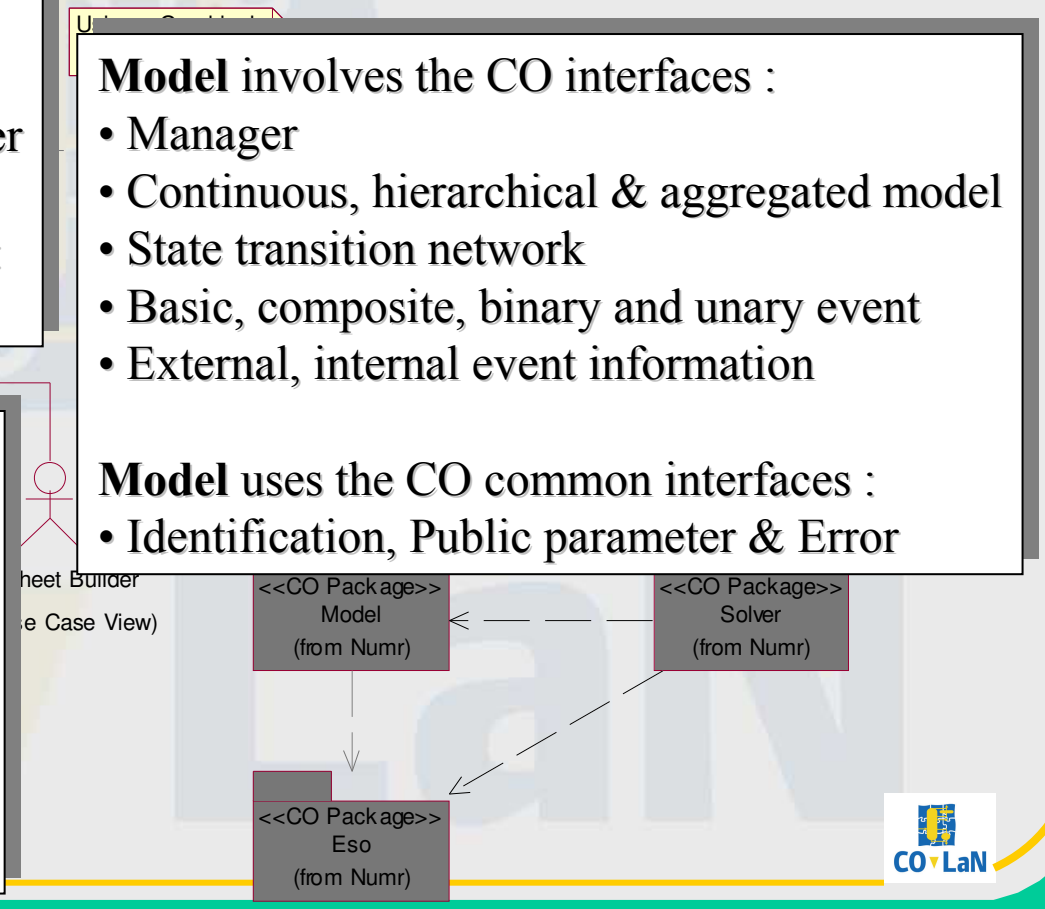
Solver uses the CO common interfaces :
- Identification, Parameter & Error

Model involves the CO interfaces :
- Manager
- Continuous, hierarchical & aggregated model
- State transition network
- Basic, composite, binary and unary event
- External, internal event information

Model uses the CO common interfaces :
- Identification, Public parameter & Error

ESO involves the CO interfaces :
- Manager
- LA, NLA, DA PDA, MINLP ESO
- Global ESO
- Unstructured, full & banded matrix

ESO uses the CO common interfaces :
- Identification, Parameter & error



Solver interface specifications development

- **Specification design**
  - **CAPE-OPEN Project (July 1999): v0.90**
    - **Interface specification for LAE, NLAE, DAE problems**
  - **Global CAPE-OPEN Project (March 2002): v1.0**
    - **Interface specification for MINLP, PDAE, PEDR problems**
- **Prototyping (May 2001)**
  - **Numerical Services Provider and Continuous Model Builder made by INPT-ENSIACET: ESO and DAESO**
    - **See presentation at ESCAPE 11 in Kolding**

Known implementations

SMST implementations

- Tester suite element as a SMST socket
  - Permits test of COM SMST Plug component
- Comment:
  - Simulators having adopted the CAPE-OPEN standards as a basis for their design do not implement SMST interfaces
    - SolidSim
    - CAPE-OPEN to CAPE-OPEN (COCO)
    - Metal Finishing Facility Pollution Prevention Tool (MFFP2T)
  - No value in SMST component?

Solver interface implementations

- **CO-LaN implementations**
  - **Tester suite (June 2002)**
    - **Tester suite element for MINLP components**
  - **Plug component (June 2002)**
    - **LP solver delivered by Universitat of Catalunya under contract from CO-LaN**

Solver interface implementations

- **Commercial implementations**
  - **Aspen Plus (Aspentech): ESO socket**
    - Equation-Oriented Unit Operation Socket, which allows any equation-oriented CAPE-OPEN Unit to run in Aspen Plus EO mode.
    - The Aspen Plus MixNSplit CAPE-OPEN example demonstrates EO support.
  - **gPROMS (Process Systems Enterprise)**
    - gPROMS provides open interfaces for the solution of various types of mathematical problems:
      - Square systems of linear algebraic equations
      - Square systems of non-linear algebraic equations
      - Square systems of mixed ordinary differential and algebraic equations over time and another independent variable
      - Optimization

Solver interface implementations

- **Academic implementations**
  - **DIANA Dynamic simulation and Numerical Analysis tool (Max Planck Institute): solver plugs and socket**
    - **Different nonlinear algebraic and differential-algebraic solvers are implemented, based on existing third party open-source code and can be applied by to the model depending on the special properties of the model.**
    - **The interfaces to models and numerical routines are designed based on the CAPE-OPEN standard.**
  - **EMSO simulator environment (Universidade Federal di Rio Grande do Sul)**
    - **Modifications proposed to set of NUMR interfaces**
      - **Computers and Chemical Engineering 28 (2004), pp 1611-1621**

Solver interface implementations

- **Academic implementations**
  - **ROME (LPT-Aachen): model repository**
    - The repository provides the model through the CAPE-OPEN interface for an equation set object (ESO).
  - **IPOPT (Carnegie Mellon University): NLP plug**
    - A software package for large scale nonlinear optimization of continuous systems
    - IPOPT communicates with CAPE-OPEN compliant MINLP modeling systems through an ICapeMINLP interface.
  - **Universitat Politecnica de Catalunya: PEDR socket**
    - Data Reconciliation as a Framework for Chemical Process Optimization and Control, Chouaib Benqlilou, Antonio Espuna and Luis Puigjaner.
    - Frameworks for sensor placement and data reconciliation

Feedback on MINLP implementation

- **Dr Ying-Sheng Cheng**
  - **« PSE's overall experience with the interface specification has been positive. In particular the amount of effort required to wrap an existing solver with a CAPE-OPEN interface is relatively small. »**
    - **PSE comments on MINLP interface specification, 2002**

- **Yi-dong Lang and Larry Biegler**
  - **« it is relatively easy to make IPOPT CAPE-OPEN compliant »**
    - **The IPOPT Interface to CAPE-OPEN, CO Update 10, 2005**

Conclusions & Perspectives

- Numerical interface specifications have suffered from emphasis on thermodynamic and unit operations in CAPE-OPEN implementations
- Very few implementations of both plug and socket for each set of numerical interfaces
  - Value of standardization grasped by academic researchers mostly
  - No implementation by commercial vendors of numerical code

Conclusions & Perspectives

- Various proposals for improving numerical interface design but no consensus yet
- Need to reactivate Solver Special Interest Group for
  - Maintenance of Numerical interfaces
  - Maintenance of associated Tester elements
  - Developing implementation
- Those interested, please make contact with technologyofficer@colan.org

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