Workshop on CAPE-OPEN 2.0

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Previous episodes

- **CAPE-OPEN 2019 Annual Meeting**
  - **Mark STIJNMAN: thermo (life-cycle, multi-threading), unit operations (equation-oriented, custom GUI), cloud (plug-ins)**

Thermo: proposed solution (Mark STINJMAN)

- Property packages become stateless
  - Model a Property Package as a stateless, pure function object
    - It calculates phase properties as a function of T, P and phase composition
    - It calculates phase equilibrium as a function of input conditions
  - Simplify life cycle
    - Once created, never changes
    - Is either created successfully, or not at all
      - No invalid property packages possible
  - Move complexity to the Package Manager
    - Editing
    - Saving/Loading
    - Preset management

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- **CAPE-OPEN 2020 Annual Meeting**
  - **CTO's views: what is in the pipe from the above**

What could be CAPE-OPEN 2.0 in 2025?

- Thermodynamics (already under development)
  - Close integration between chemical reactions and thermodynamics
  - Manager interface offering enhanced functionality
    - Compared to Property Package Managers
- Unit Operations (preliminary design but need of business cases)
  - Black-box modeling support
- Equation-oriented and dynamic simulation
  - Strong basis exists that could be ported to CAPE-OPEN 2.0
  - Needs a Numerical SIG to make it happen
- Opening to digital twin aspects
- Software engineering aspects
  - Multi-threading / cloud: technical scope of COBIA Phase 3

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- **Management Board meeting on May 17, 2022**
  - **Decided this workshop at CAPE-OPEN 2022 Annual Meeting**
    - **A strategic discussion on the future. Which topics are relevant for process modelling in the future?**
      - **Relation to other standardization bodies to be improved**
      - **COBIA must communicate between Windows and Linux**
      - **Doing cross machine communication in a secure way**
- **Prior to CAPE-OPEN 2022 Annual Meeting**
  - **Market oriented needs listed by Full Members**

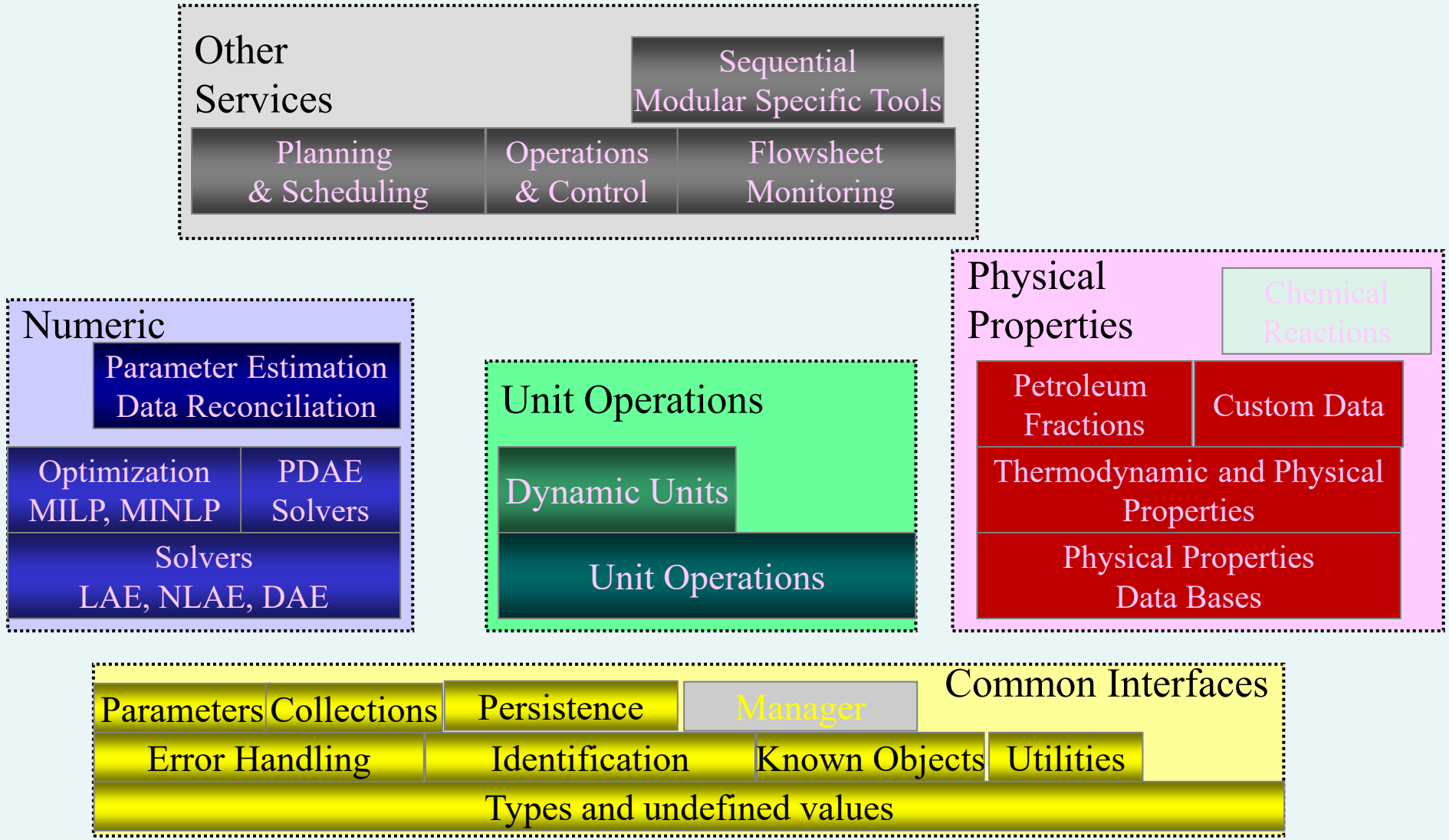
Ideas expressed by CO-LaN Full Members

- **Interface to include surrogate or grey-box models**
  - Common trend to replace or amend rigorous models with data driven models like for example artificial neural networks or gaussian process models or simple parametric models (e.g., linear or quadratic polynomial models).
  - To address these models on the Machine Learning server using for example gRPC could be an issue to be supported by CAPE-OPEN 2.0.
- **Interface to Optimization solvers with reverse communication**
  - Most optimization possibilities within PMEs rely on one solver mostly based on a sequential quadratic programming (SQP). But there are several others and sometimes it makes sense to use alternatives if the selected one fails.
  - The implementation of different optimization solvers into PMEs is not easy since often the objective and constraints are not easily provided via the required interfaces. The easiest way to implement such solvers is the use of reverse communication.
- **SFILES 2.0: An extended text-based flowsheet representation**
  - To encourage researchers and engineers to publish their flowsheet topologies as SFILES 2.0 strings.

CAPE-OPEN 2.0

- « Major » version number increment
  - Indicates a breaking change
- Example:
  - *Change to the CAPE-OPEN Specification that fundamentally alters the interactions between CAPE-OPEN applications*
    - Removal or replacement of an interface from a CAPE-OPEN Specification
    - Originally provided functionality no longer available / need to be accessed through an entirely different means
- Compares to « Patch » version number:
  - Incremented when a feature addition (extension) of the CAPE-OPEN Specification requires modification of the distributed CAPE-OPEN Type Definitions

CAPE-OPEN standard 1.1



Feature additions to CAPE-OPEN 1.1

- Custom Data (published)
  - enables any subclass of Process Modelling Components implementing *ICapeThermoMaterialContext*, to store and retrieve custom data from a Material Object.
- Flowsheet Monitoring (published)
  - provides ability to access all elements in a flowsheet without interfering with the flowsheet.
- Manager (under development)
  - creates and manages a set of Primary PMC objects belonging all to the same category of Primary PMCs.

Additions to CAPE-OPEN 1.1

- Chemical Reactions (under development)
  - replaces version 1.0 of the CAPE-OPEN Chemical Reactions interface specification,
  - allows thermodynamics and reactions to be served from the same source.
- Petroleum Fractions (comments to be replied to)
  - replaces version 1.0 of the CAPE-OPEN Petroleum Fractions interface specification,
  - allows unit operations to read and modify properties specific to the petroleum and gas industry (e.g., cloud point, pour point, Reid vapour pressure),
  - allows run-time re-characterization of the properties of a petroleum fraction.

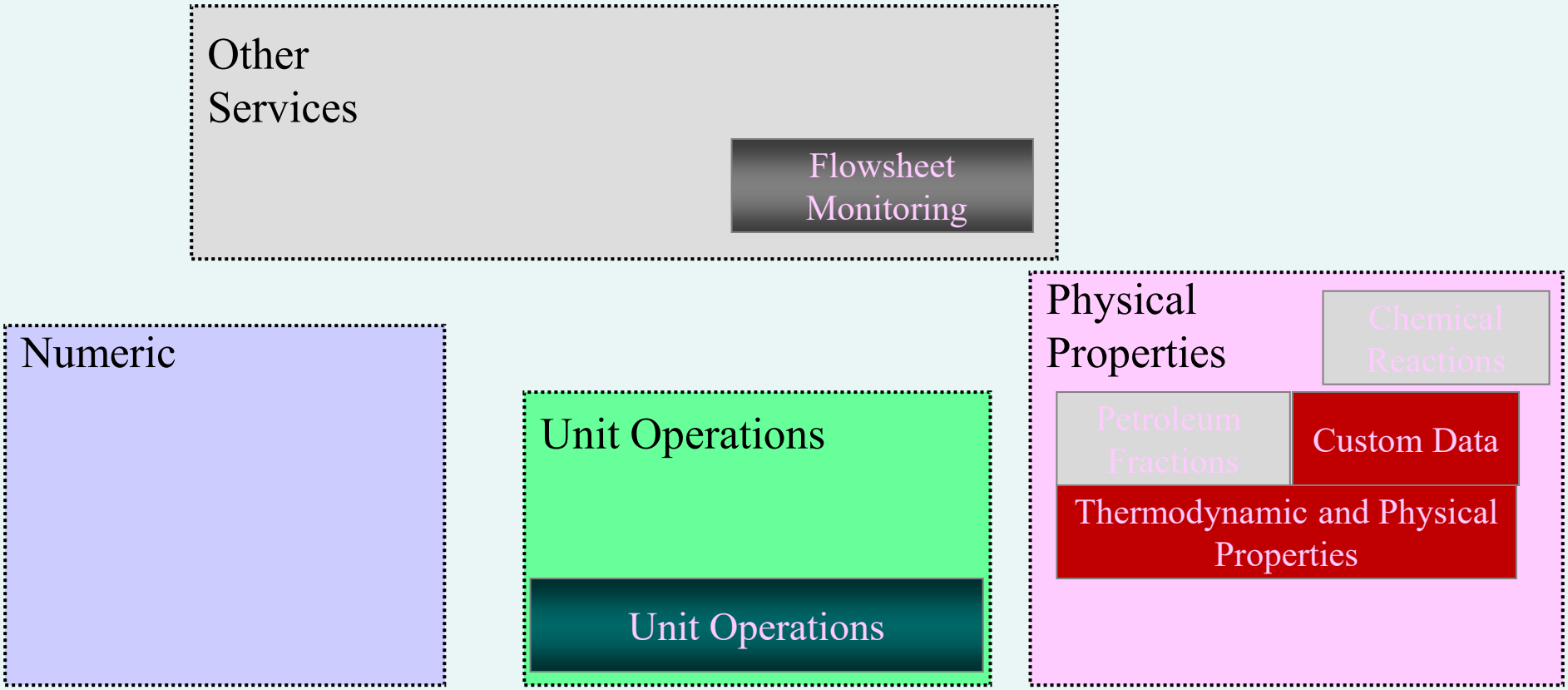
Business specifications with wide adoption

- Thermodynamic and Physical Properties
  - 1.0: early adoption (2000s) by many PMEs and PMCs
    - Aspen Plus, HYSYS, PRO/II, ProSimPlus, Simulis, MultiFlash, ChemCad, COFE, TEA, gPROMS, XChanger Suite, ChemSep, VALI...
  - 1.1: progressive adoption
    - Aspen Plus, HYSYS, PRO/II, COFE, TEA, ProSimPlus, Simulis, PetroSim, ProMax, XChanger Suite, OGT|Suite, MOSAICModelling, COMSOL, ChemSep, MATLAB Thermo …
- Unit Operation
  - 1.0/1.1: early adoption by many PMEs and PMCs
    - Aspen Plus, HYSYS, PRO/II, ProSimPlus, ChemCad, go:CAPE-OPEN, Xchanger Suite, MATLAB Unit Operation, Scilab Unit Operation, …

Business specifications with low adoption

- Numerical solvers
  - Early adoption by EMSO, Diana
  - No adoption by any major commercial software vendor
- Optimization
  - IPOPT
  - No adoption by any major commercial software vendor
- Dynamic Unit Operations
  - Implemented in IndissPlus and in IFPEN Unit Operation(s)
- Petroleum Fractions (revised version)
  - Implemented in PRO/II and in Shell Unit Operation(s)
- Custom Data (published)
  - Implemented in COFE and used by ProTreat PP

CAPE-OPEN standard 1.2



Future of CAPE-OPEN

- Technology wise: COBIA (language bindings/marshalling/…)

- Functionality wise
  - What is missing in CAPE-OPEN 1.X?
  - What are you looking for?

- Implementation wise
  - What should be changed to have more functionality implemented?
  - Boost adoption by software vendors and end-users

Your input please!