Thermo SIG Progress Report 2017

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Thermo SIG Annual Report: Charter

Task:

Develop, maintain and promote Thermodynamic and Physical Properties interface specifications

Key Responsibilities:

- **Maintain and manage existing interface specifications**
- **Assess expansions of interface specifications**
- **Manage the development of expansions**
- **Help organizations to develop implementations**

Thermo SIG Annual Report: Membership

- Bjørn Maribo-Mogensen — Hafnium Labs
- Jasper van Baten — AmsterCHEM (co-leader)
- Mark Stijnman — Shell Global Solutions
- Michel Pons — CO-LaN
- Ryan Liu — Honeywell Process Solutions
- Jian Yong (Jim) Yang — Honeywell Process Solutions
- Richard Szczepanski — KBC Advanced Technologies
- Sergej Blagov — BASF (co-leader)
- Suphat Watanasiri — Aspen Technology, Inc.
- Vicky Athanasiou — Honeywell Process Solutions

Activities 2016-2017

- **Chemical Reactions interface specification v1.1**
  - First ideas first presented at CAPE-OPEN 2012 Annual Meeting in Lyon
  - **Document structure change** done
  - **Design change** done
  - ***RFC by end of January 2018***

- **Recommendation to M&T SIG regarding COBIA**
  - **Advisory: no COBIA support for Thermo 1.0**
  - **Material Template System, in progress...**

Immediate goals 2017: document change

- Formulation of business cases, in progress...
- Restructuration of document done
  - Document treats three concepts
    - A Reaction Server that exposes reactions
    - A Chemical Phase Equilibrium Server
    - Multiple Compound Slates (true and apparent)
  - Initial structure followed CAPE-OPEN template
  - New structure: separate by concepts
    - CAPE-OPEN template applied per concept
      - Textual requirements, Use Cases, Interface descriptions

Document change: Where we stand

- A Reaction Server that exposes reactions
  - Textual requirements done
  - Use Cases done
  - Interface descriptions done
- A Chemical Phase Equilibrium Server
  - Textual requirements done
  - Use Cases done
  - Interface descriptions done
- Multiple Compound Slates (true and apparent)
  - Textual requirements done
  - Use Cases, in progress...
  - Interface descriptions, in progress...

Document change: to complete

- Business cases
- Document heat of reaction consistency issues
- Describe links between various chapters
- Custom Data

Business cases

- Explain expectations of Reaction Package standard:
  - Enumerating example fields of applications:
    - e.g. electrolytes, reuse of reaction definitions between reactors,…
  - Product management issues:
    - e.g. minimum functionality, IPR, package configuration,…
- Justify interface design
    - Reactive Equilibrium distinct from Phase Equilibrium
- Introduce and help navigate through major concepts of the interface:
    - e.g. Reaction server, Chemical Reaction Equilibrium, Multiple Compound Slates

Custom Data

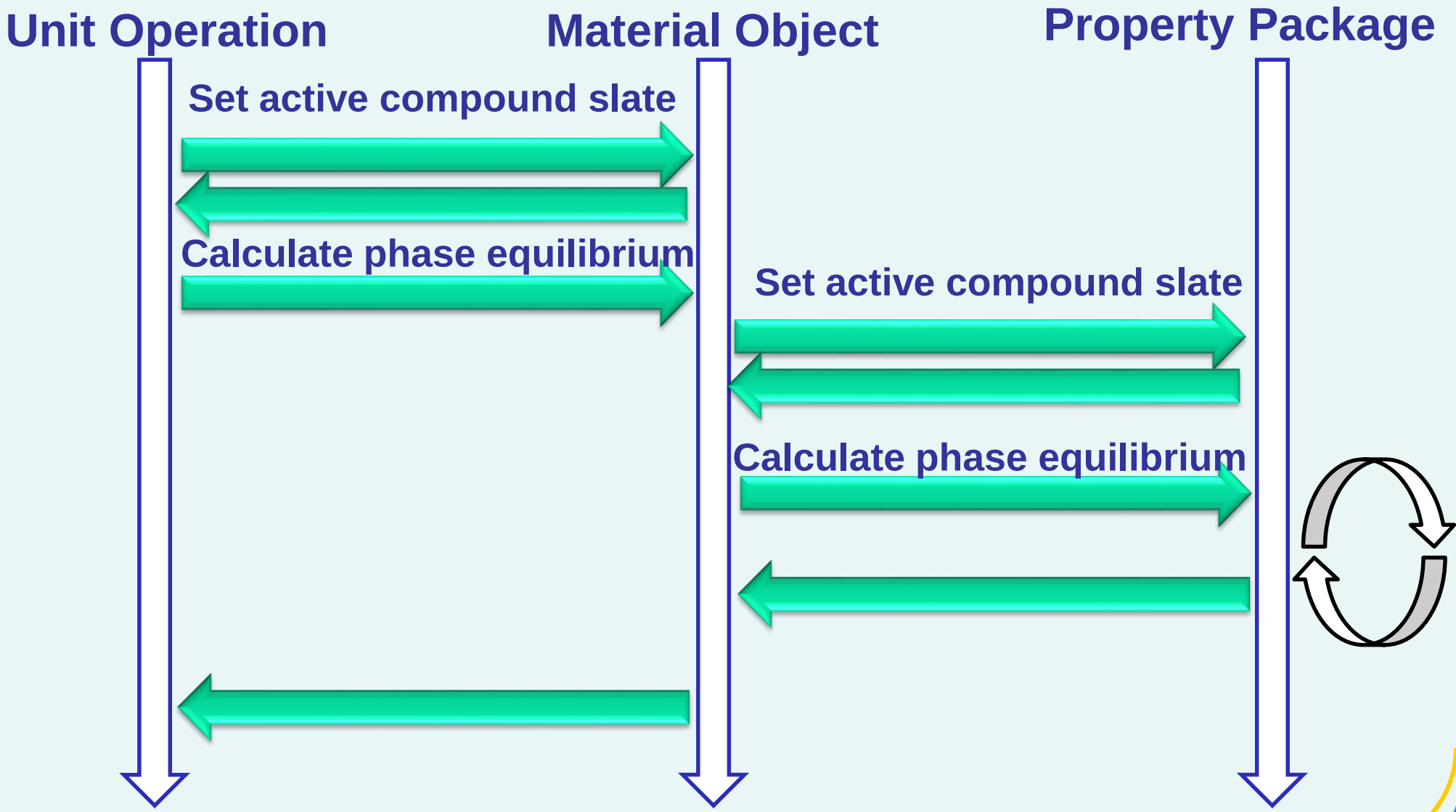
- Custom data lie between PME and PMCs
  - Allows storage of PMC's specific data on Material Object
  - A means to improve performance of chemical equilibrium

- Open questions:
  - Is Custom Data support required or optional?
    - Required:
      - Pro: Easier on PMC, no fallback required
      - Con: *When* required, under which conditions?
  - Persistable and/or clonable?

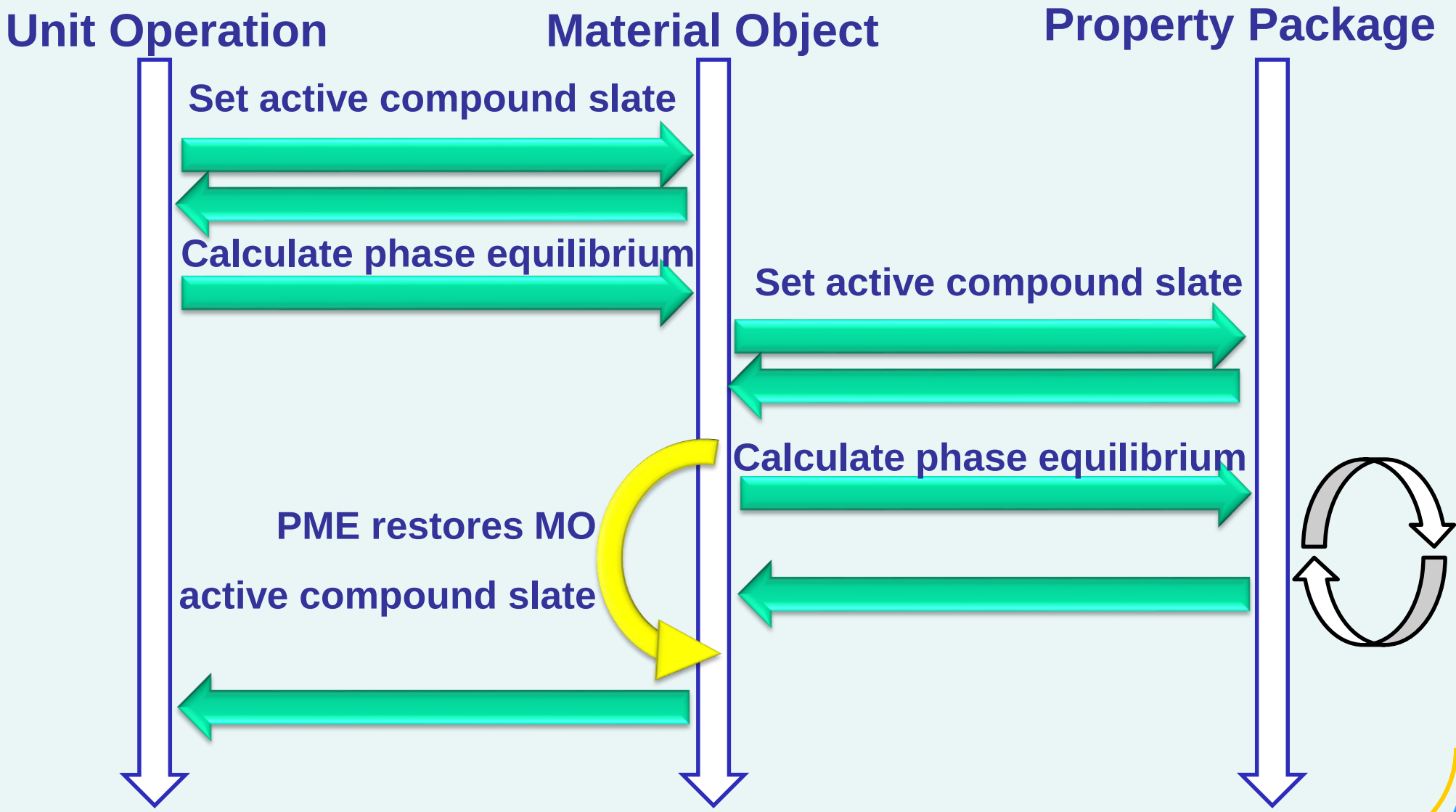
Accomplished 2017: design change

- Reaction Server
  - Drop hierarchy of reactions
  - Clarify differences between Reaction Server and Chemical Phase Equilibrium Server
- Chemical Phase Equilibrium Server
  - (None)
- Multiple Compound Slates
  - Replaced Delegates by active Compound Slate
  - Modified workflow between MOs and PPs/UOs

Active Compound Slate



Active Compound Slate



Advisory on Thermo support in COBIA

- The Methods and Tools Special Interest Group has asked the Thermo Special Interest Group to provide its input on whether Thermo 1.0 should be implemented in COBIA.

- ***The Thermo SIG advises against support for Thermo 1.0 in COBIA:***

  - **Support for 1.0 directly in COBIA: NO** (all new developments use Thermo 1.1 and that includes COBIA)

  - **Translator/adaptor to Thermo 1.0 in COMBIA : NO** (drop backward compatibility with COM-based Thermo 1.0. Market for 1.0 too small. Providing adaptor calls for future support)

Summary and further actions

- Good progress on reactions
  - Taking work offline helped
  - Planning to launch RFC in January 2018

- Interactions with COBIA
  - Advisory on Thermo 1.0
  - Advisory on Material Template System
  - Check COBIA IDL

Questions?

Thank you for your attention!

Go CAPE-OPEN!

CO LaN