ADVANCED PROCESS MODELLING FORUM
LONDON
20–21 APRIL 2016

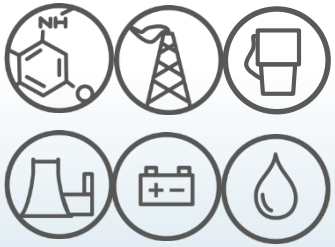
The gPROMS Platform v4.3

Costas Pantelides – Managing Director

gPROMS

gPROMS product family

"Fluids processing world"



g|PROCESS
gPROMS ProcessBuilder
Process MLs

g|WATER — Water MLs

g|UTILITIES — Utilities MLs

g|CCS — CCS MLs

g|POWER — Power MLs

g|OILFIELD — Oilfield MLs

"Formulated products world"

g|FORMULATE
gPROMS FormulatedProducts

Crystallisation MLs — **g|CRYSTAL**

Solids MLs — **g|SOLIDS**

Oral absorption MLs — **g|COAS**

g|FLARE * — Flare & depressurisation MLs

g|FUELCELL — Fuel cell MLs

General mathematical modelling

g|MODEL

gPROMS ModelBuilder provides essentially the full platform functionality

gPROMS

The gPROMS platform

Equation-oriented modelling & solution engine

gSAFT

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* Primarily used internally by PSE for delivery of services

gPROMS Platform

Recent release timeline

- v4.0.0 – April 2014
- v4.1.0 – June 2015
- v4.2.0 – December 2015
- **v4.3.0 – September 2016**
- **v4.4.0 – Q1/2017**

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gPROMS platform v4.3

Highlights – process modelling

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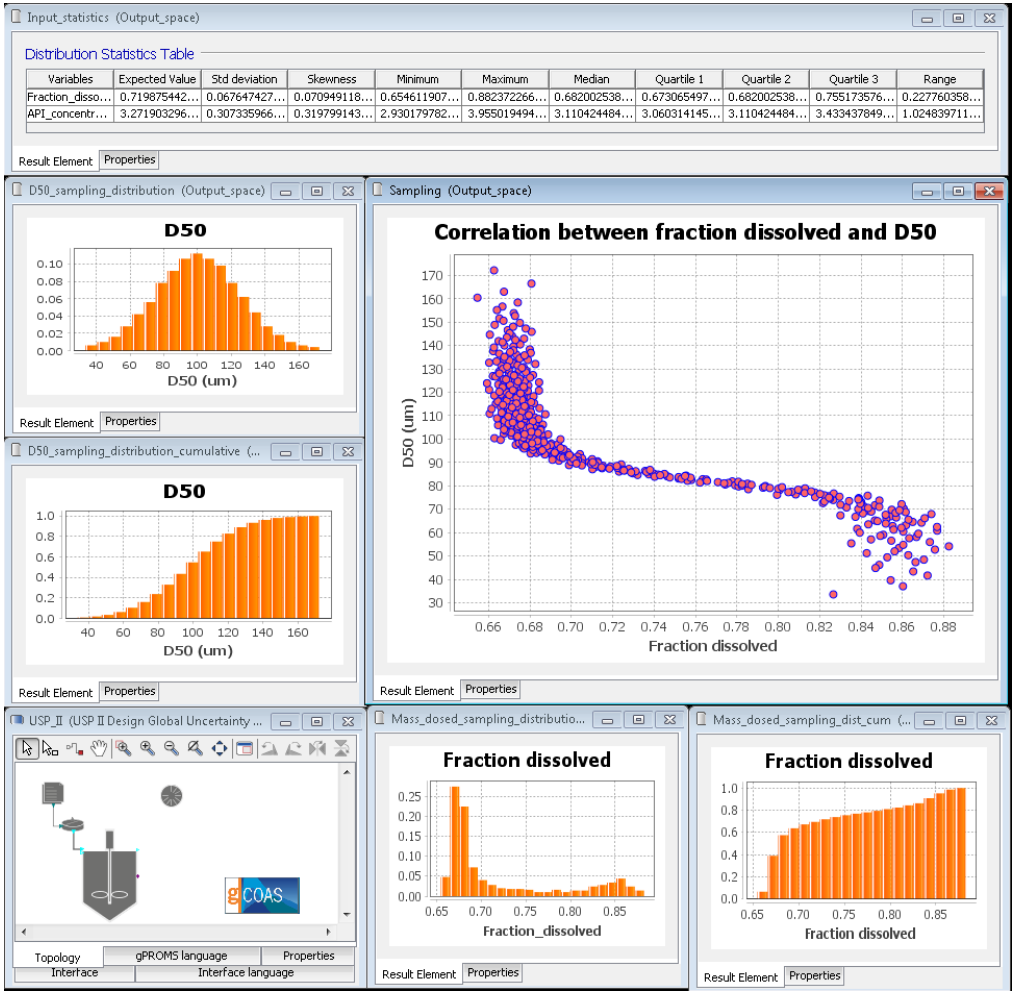
Core capabilities

- Global System Analysis
  - new type of gPROMS activity
- A major new capability
  - applicable immediately to all gPROMS models
- New directions in
  - gPROMS computations
  - interactive results management

Presentation this morning



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Solution power

- New **DAEBDF integrator** now usable for all activities
  - Used for Simulation since v4.2.0
    - ➔ significant improvements in speed & robustness
  - Now available for Parameter Estimation & Optimisation
    - Efficient computation of 1st-order sensitivities

- New **parallelized Parameter Estimation** solver
  - Parallel evaluation of multiple experiments
  - Suitable for execution on multicore machines
    - 4-core machine ➔ 2.7× acceleration
    - 12-core machine ➔ 7× acceleration
  - Straightforward use with existing parameter estimation problems

```
SOLUTION_PARAMETERS
 PESolver := "MAXLKHD" […. "ParallelProcessing" := TRUE,….];
```

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User Interface

- **Units of Measurement** support in all activities
  - Simulation, parameter estimation, optimisation
  - Activity editors & result reports

- More extensive support for “friendly names” for parameters & variables visible to end-users across GUI
  - instead of long pathnames…

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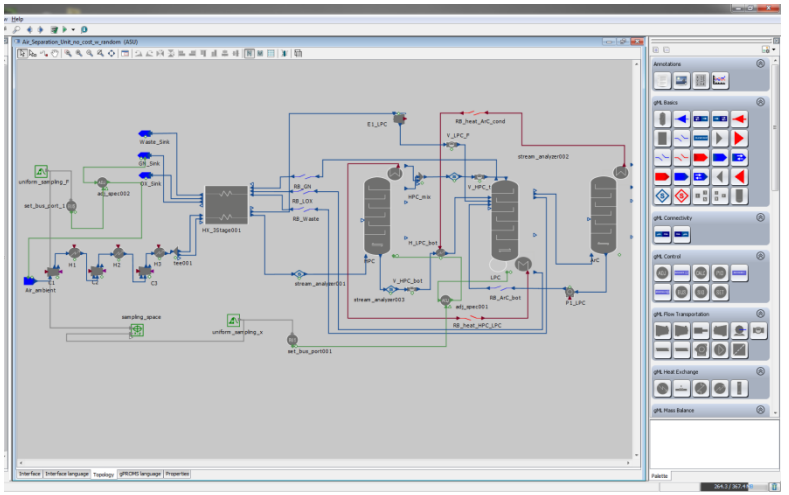
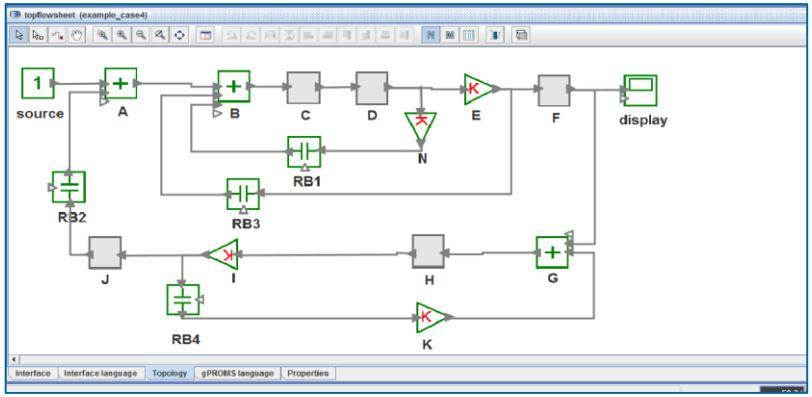
Model Initialisation Procedures (MIPs)

- **Model pruning during MIP execution**
  - Automatically identify & remove all equations/variables not needed during MIP
    - To be post-solved after converged solution is obtained
  - Model Pruning concept & implementation already tested extensively in the context of gPROMS dynamic simulations
    - ➔ Significant enhancement in robustness
      & speed of solution



- **Automatic sequencing algorithm for multiple recycle closure**
  - No need for user to specify order in which recycles need to be handled
  - Can handle flowsheets of arbitrary complexity



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gPROMS platform v4.3

Highlights – materials modelling

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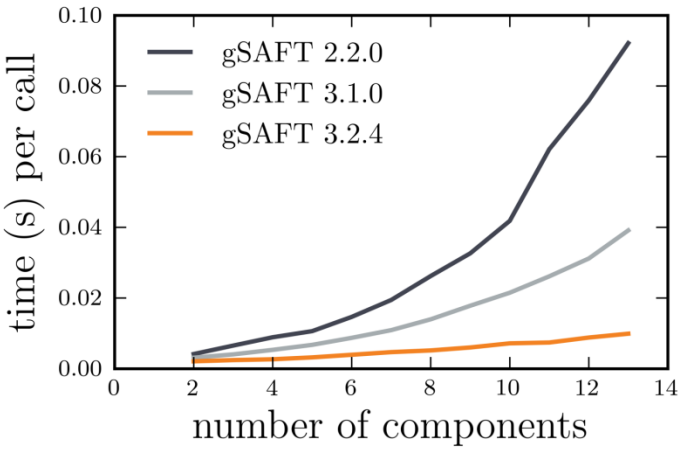
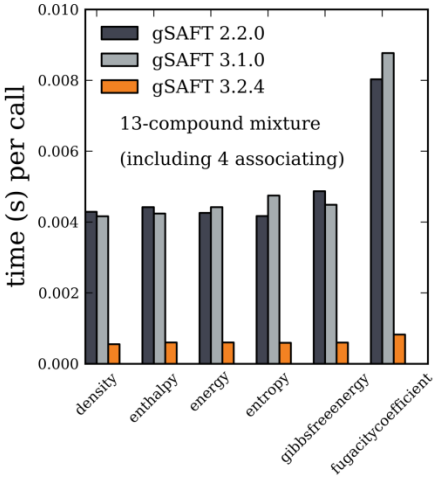
gPROMS v4.3 highlights

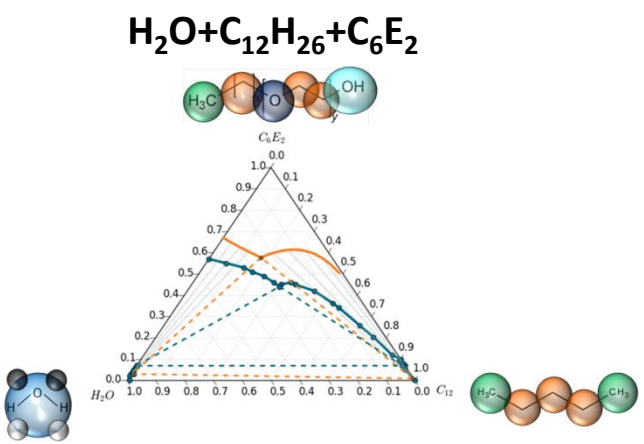
gSAFT advanced materials modelling

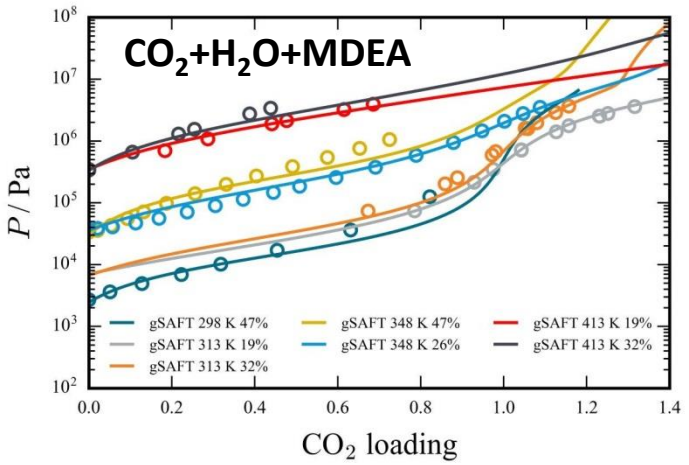
Presentation this morning



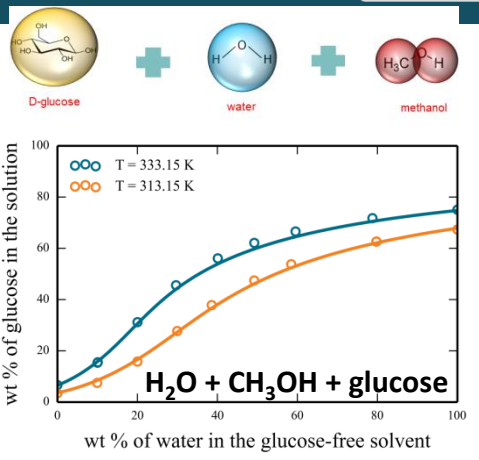
1. Order-of-magnitude performance improvements



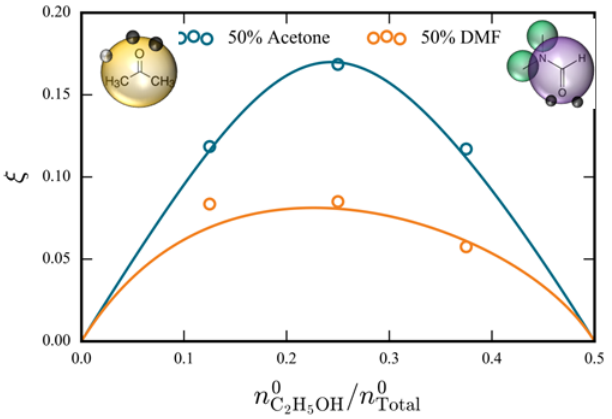




2. Accurate/predictive modelling of increasingly complex systems



3. Predictive modelling of systems with solid phases



4. Predictive modelling of reactive systems

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gPROMS platform v4.3

Supporting online model-based applications

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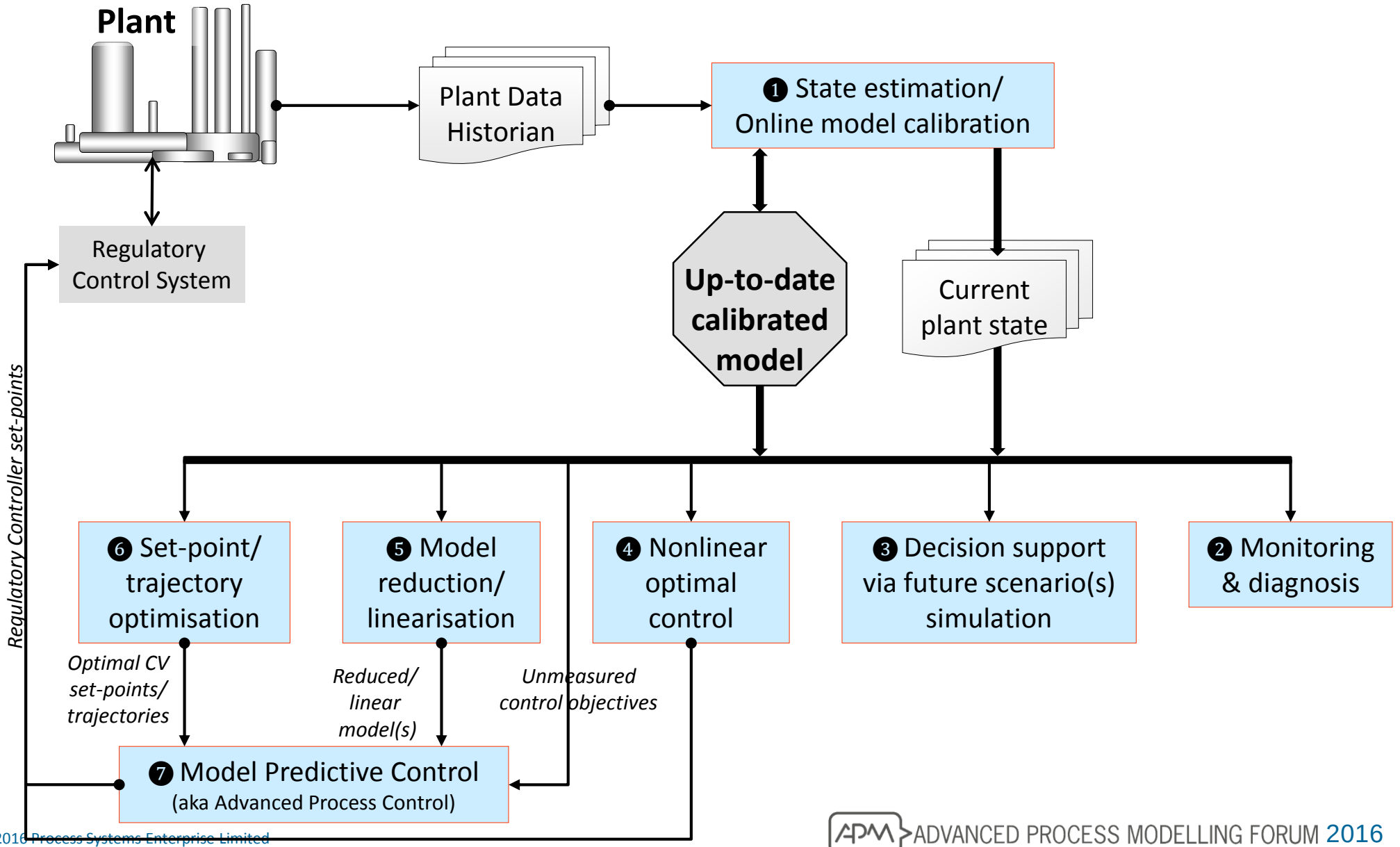
Online Model-Based Applications (OMBAs)

Integrated framework



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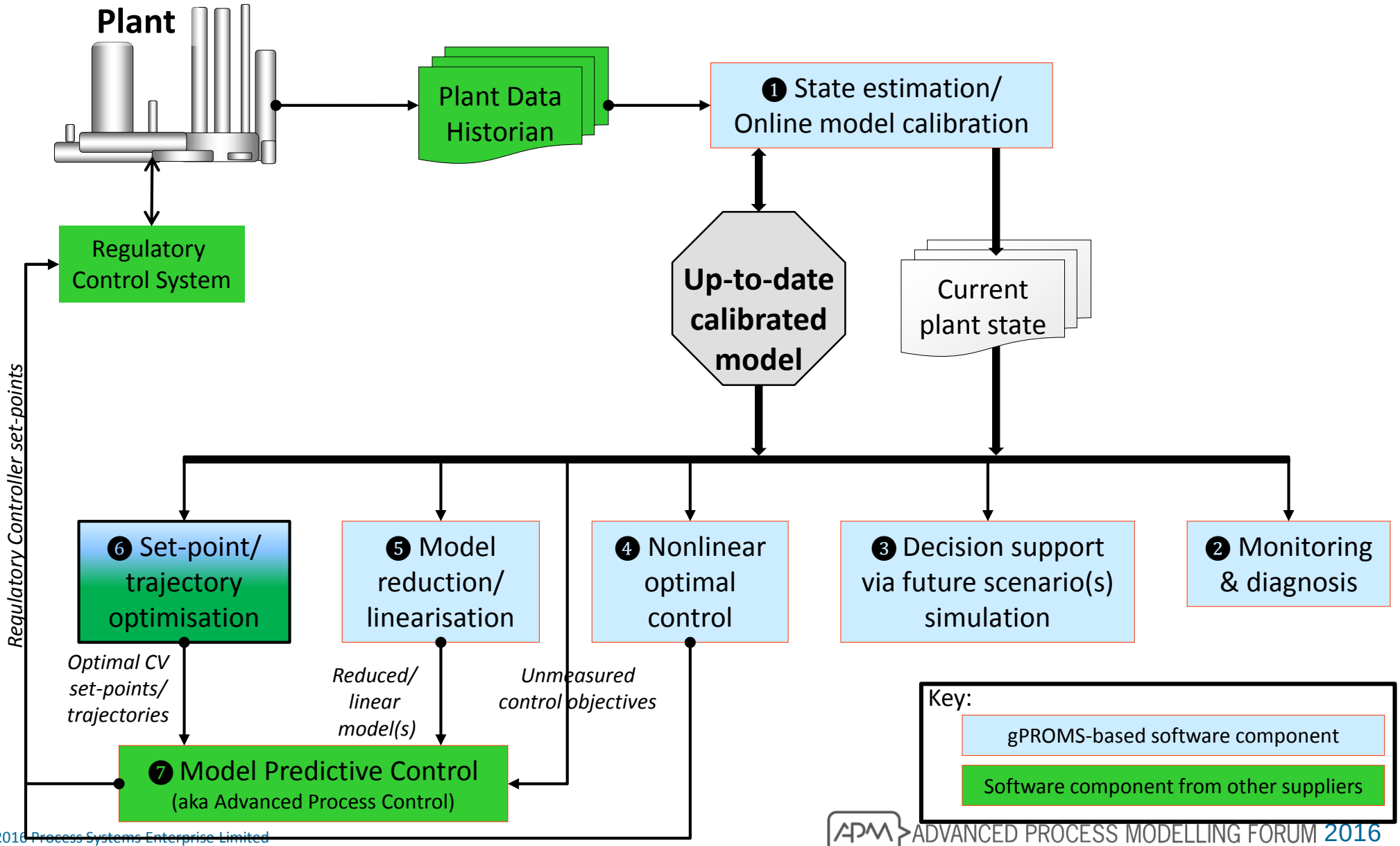
Online Model-Based Applications (OMBAs)

Integrated framework



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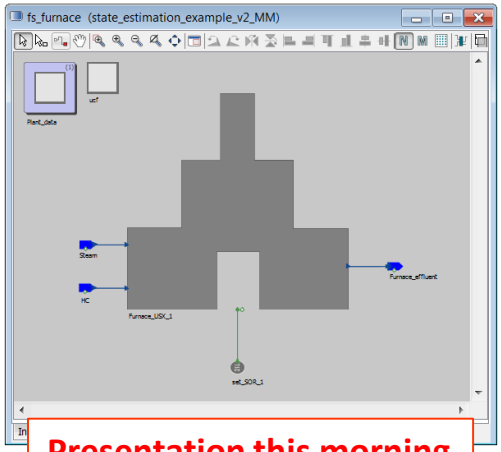
Online Model-Based Applications (OMBAs)

Examples

gCRACKER Online

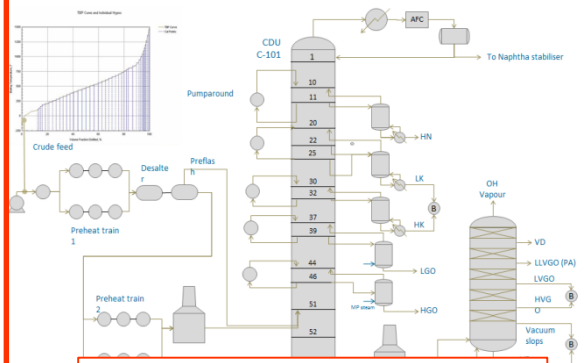
Olefin cracking furnace monitoring



Presentation this morning

ARRMO

Advanced Real-time Refinery Monitoring & Optimisation



Presentation this afternoon

3 other OMBAs under development

- Each OMBA involves one or more gPROMS-based computations…
  - makes use of gPROMS model constructed, validated & tested offline
  - communicates with the gPROMS solution engine to perform calculations
- Each OMBA has a different software architecture…
  - …but makes use of common software elements

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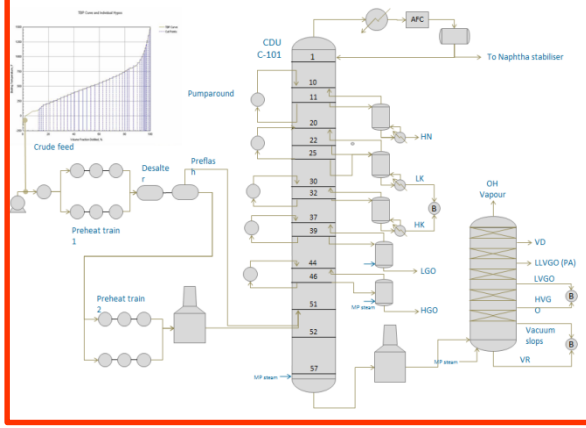
Online Model-Based Applications (OMBAs)

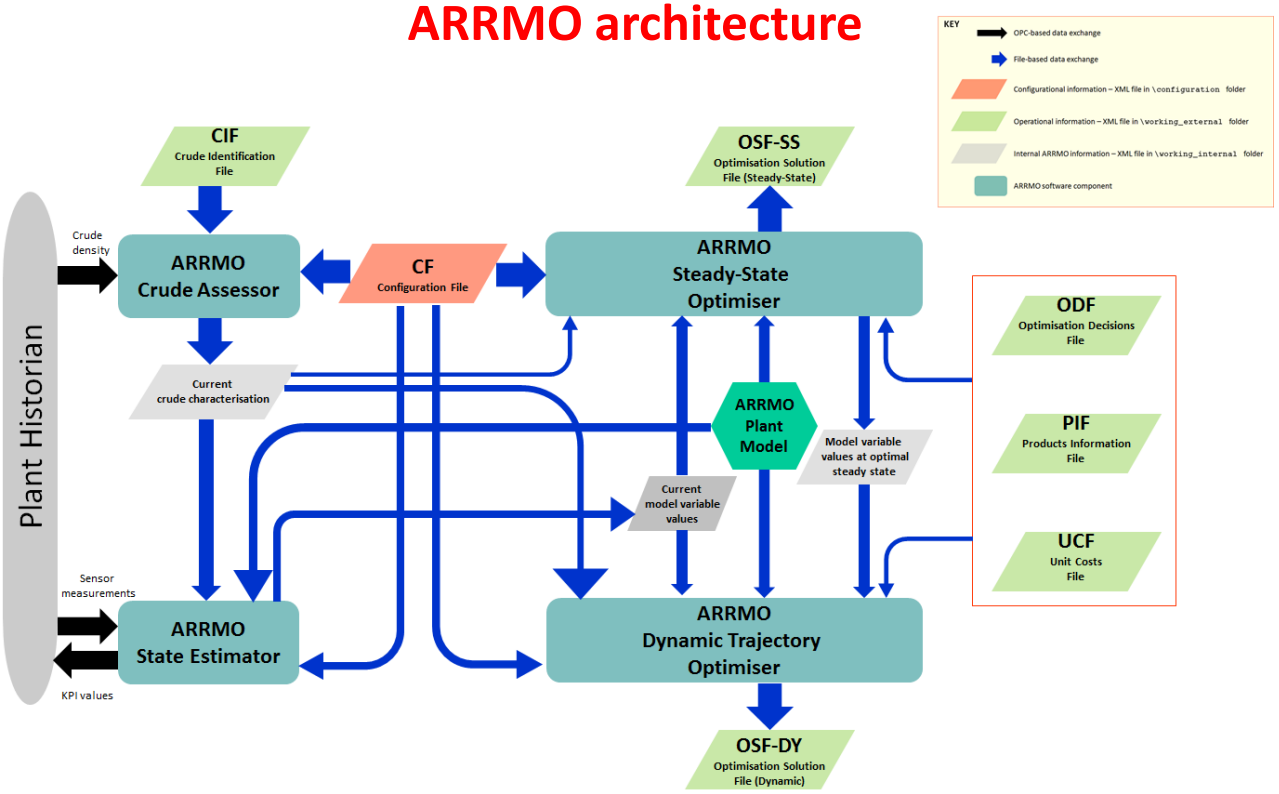
Examples

ARRMO

Advanced Real-time Refinery Management & Optimisation



ARRMO architecture



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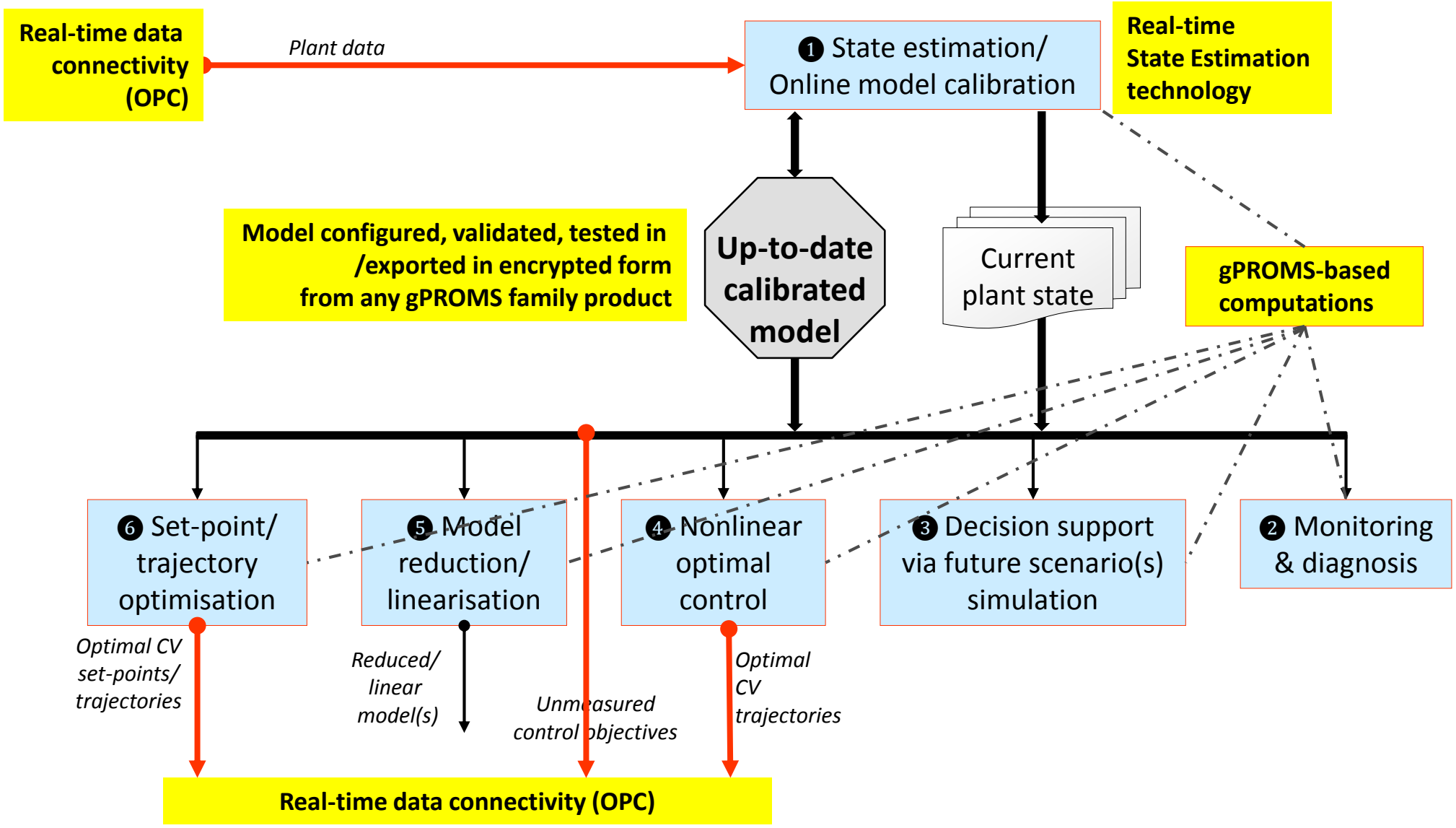
Online Model-Based Applications (OMBAs)

gPROMS technology elements



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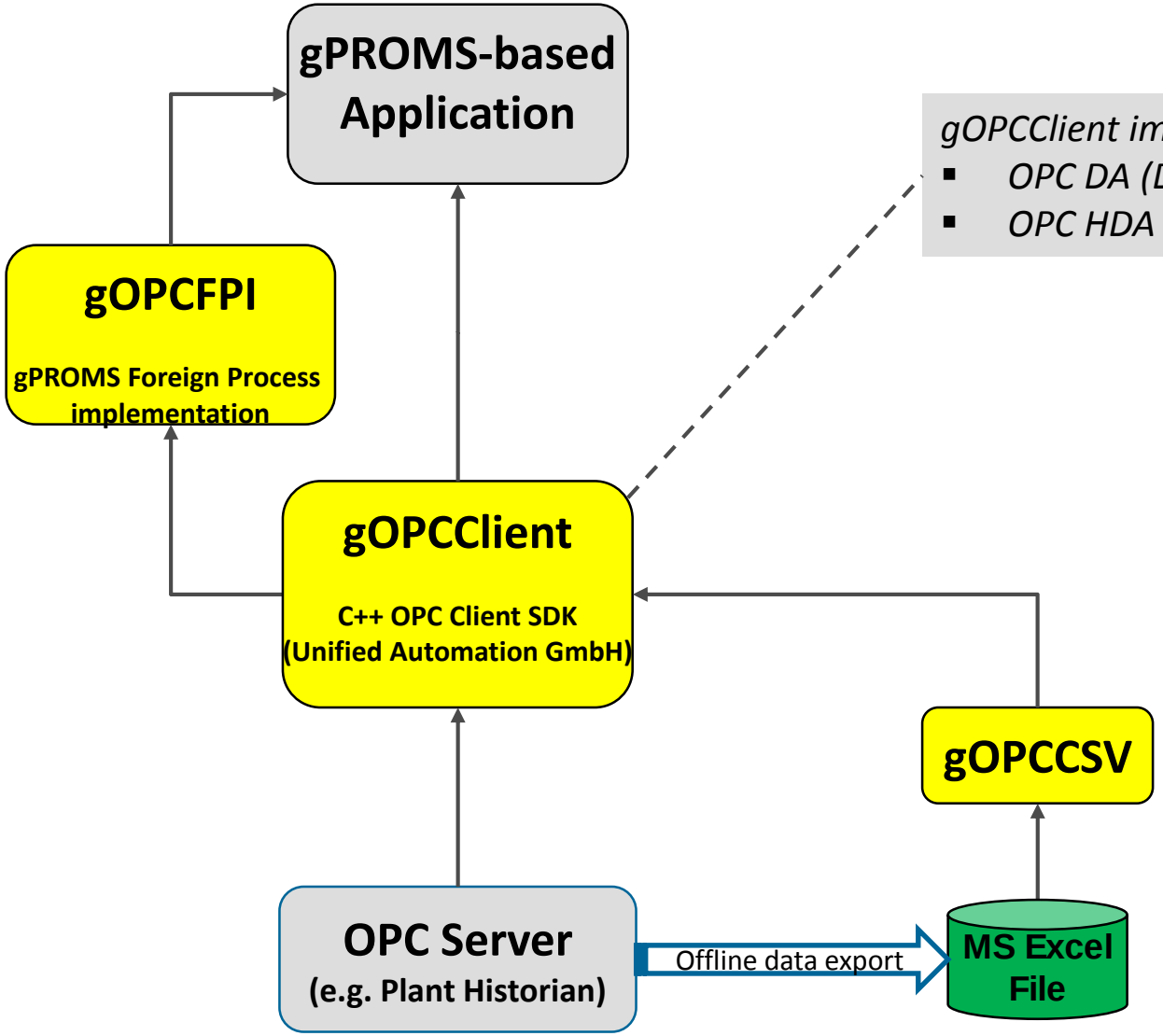
gOPC

gPROMS OPC toolkit in gPROMS v4.3



gOPCClient implements & supports:

- *OPC DA (Data Access): current real-time data*
- *OPC HDA (Historical Data Access): historical data*

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gOPCFPI

OPC Client accessed via gPROMS Foreign Process Interface (FPI)

gPROMS simulation

```
PROCESS StartUpSimulation
UNIT R AS Reactor
. . . . . ..
SOLUTIONPARAMETERS
   FPI := "gOPCFPI::opcconfig.json" ;

SCHEDULE
   SEQUENCE
      PAUSE SIGNALID "operator:start"

      WHILE TRUE DO
          GET
             R.Fin := "FeedFlowrate" ;
             R.Tin := "FeedTemperature" ;
          END

          CONTINUE FOR 10

          SEND
             "Conversion"       := R.Conv ;
             "ExitTemperature" := R.Tout;
          END
      END
   END
```

gOPC configuration file

```
"opcServer":
  {
     "serverName"  :"Matrikon.OPC.Simulation.1",
     "modelTimeUoM":"s",
     "realTimeSpeedUp":"3.0"
  },
 "opcItems":
  [
     {
        "serverTag"     :"R023.FX1432"
        "clientTag"     :"FeedFlowrate",
        "description"   :"Main feed stream flowrate"
      },
     {
         "serverTag"     :"R023.TX0124"
         "clientTag"     :"FeedTemperature",
         "description"   :"Main feed temperature"
      },
      . . . . . .
```

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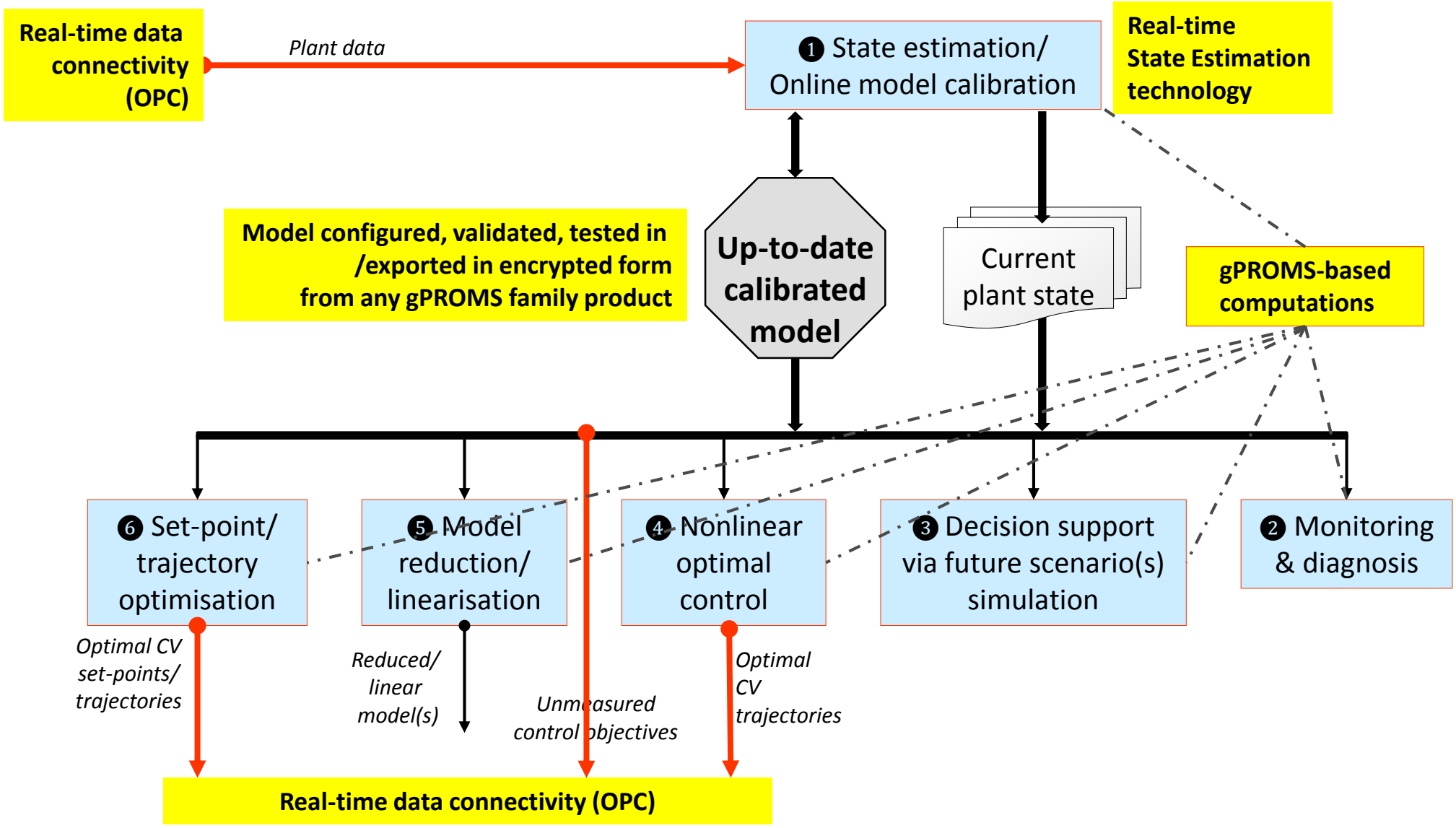
Online Model-Based Applications (OMBAs)

gPROMS technology elements



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Online Model-Based Applications (OMBAs)

gPROMS technology elements

Real-time data connectivity (OPC) ☑

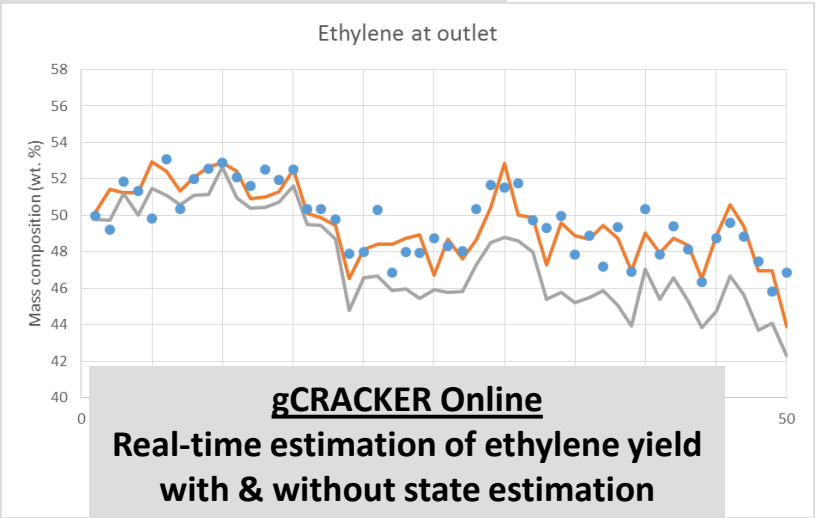
Real-time State Estimation technology

☑ **Model configured, validated, tested in /exported in encrypted form from any gPROMS family product**

gPROMS-based computations ☑

Current focus: full productisation of State Estimation technology

- Packaged as stand-alone gPROMS-based Application (gBA)
- Direct data I/O via OPC interface
- v1.0: Extended Kalman Filter (EKF) algorit
  - Make use of new DAEBDF integrator



gCRACKER Online
Real-time estimation of ethylene yield with & without state estimation

Real-time data connectivity (OPC) ☑

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gPROMS platform beyond v4.3

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gPROMS platform beyond v4.3

Key development directions

1. **Streamlined workflows**
   - Flowsheeting
   - Relating models to experimental R&D
   - Facilitating model deployment within the organisation

2. **High-Performance Computing platforms**
   - Increased range of gPROMS algorithms taking advantage of HPC

3. **Materials modelling**
   - Solids
   - Electrolytes
   - Reactive systems

4. **Online Model-Based Applications**
   - Bringing the benefits of Advanced Process Modelling to process operations

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Thank you