ADVANCED PROCESS MODELLING FORUM 2017
London 25–26 April

The gPROMS Platform

Version 5.0 and beyond

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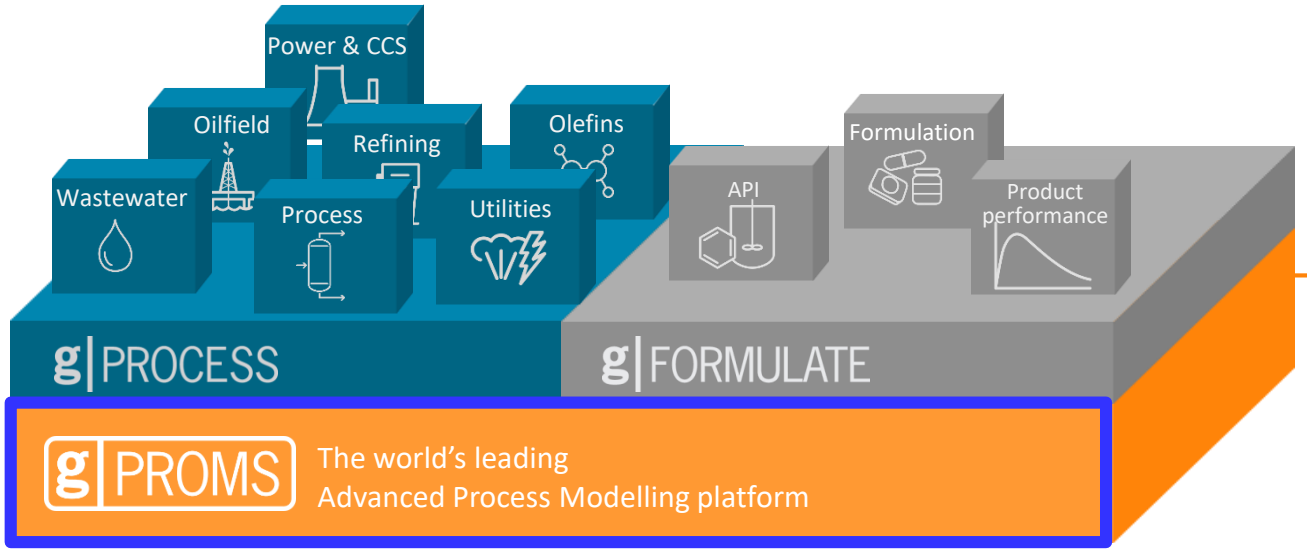
The gPROMS software suite

Offline model development & validation tools

Platform Environments Packaged Libraries



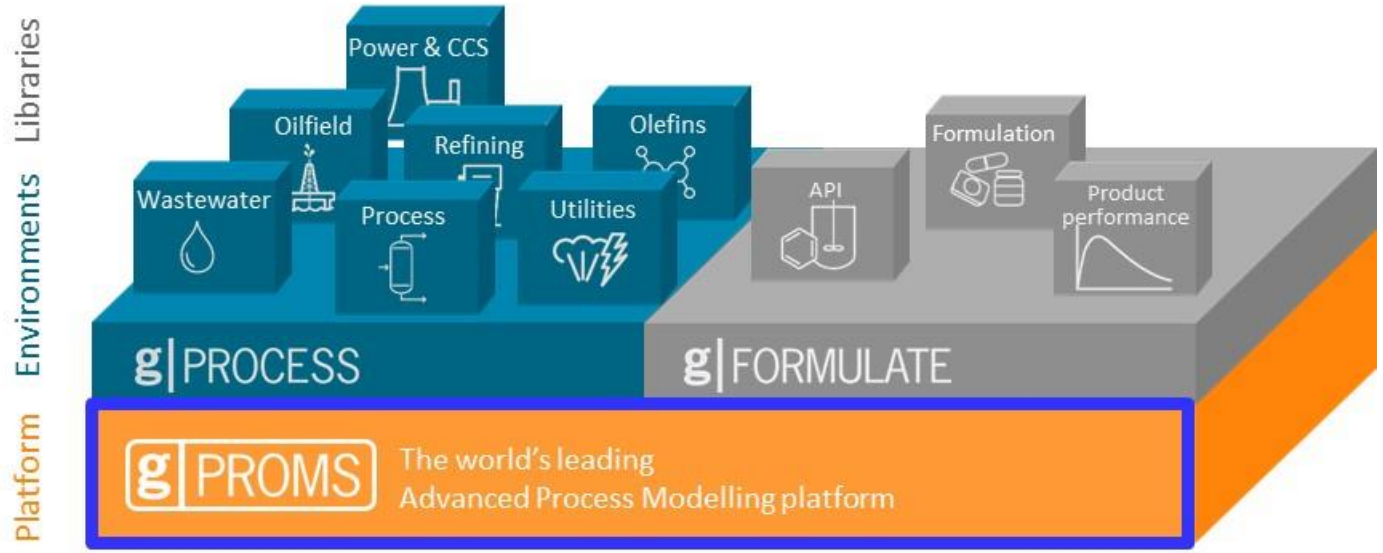
Platform functionality

Process modelling

- Equation-oriented solution power
- Custom model construction
- Steady-state and dynamic simulation and optimisation
- Advanced parameter estimation
- Powerful dynamic and mixed-integer optimisation
- Sophisticated Integrated Modelling Environment
- Global system analysis
- High-performance computing

gPROMS Platform

Recent & forthcoming release timeline for major versions



- v4.0.0 – June 2014
- v4.1.0 – June 2015
- v4.2.0 – December 2015
- **v5.0.0 – May 2017**
- **v5.1.0 – Q2/2018**

gPROMS Platform – 12-month roadmap

Usability

gPROMS v5.0

- Flowsheet-Level Model Initialisation Procedures
  - automated sequencing of recycle breakers
- Units of Measurement
  - now covering all model-based activities
  - both inputs & outputs
- Many more, larger and smaller, enhancements to the GUI

gPROMS v5.1

- Model Initialisation Procedures
  - extended to optimisation & parameter estimation
  - user-specified preferences for order of recycle closing
- Improved management of packaged model libraries
  - new library loading dialog
- Model dialogs with enhanced in-line help

Model-based activities

gPROMS v5.0

- New Global System Analysis
  - Factors
    - deterministic
    - probabilistic
      - univariate
  - Responses
    - time-invariant
  - significantly enhanced GUI
    - input dialogs
    - targeted new result elements
  - already tested extensively in pre-release versions

gPROMS v5.1

- Global System Analysis
  - extended range of probability distributions
    - univariate: lognormal
    - multivariate: discrete probabilistic
  - time-series responses
- Model verification
  - implemented as extension to parameter estimation activity
  - distinguish between
    - experiments for estimation
    - experiments for verification

Mathematical solvers

gPROMS v5.0

- New DAEBDF integrator
  - applied to dynamic simulation, parameter estimation & dynamic optimisation
  - significantly enhanced efficiency
- New LASLU linear algebra solver
  - more efficient alternative to MA48
  - fewer tuning parameters
  - the larger the problem, the larger the improvement
  - immediately usable throughou all gPROMS computations

gPROMS v5.1

- LASLU linear algebra solver
  - improved diagnostics
  - improved robustness for corner cases
- A
  - sc
- New globalised MINLP solver

Large performance gains for steady-state and dynamic simulations, in particular for large problem sizes

Acceleration factors for large models (O(10^5) equations)

Refinery CDU/VDU steady-state optimisation	: ×2.9
Refinery CDU/VDU dynamic simulation	: ×2.0
LDPE reactor dynamic simulation	: ×2.1
Fuel cell system dynamic simulation	: ×3.0

High-performance computing

gPROMS v5.0

- Global System Analysis
  - simultaneous evaluation of multiple samples
- Parameter Estimation
  - simultaneous evaluation of multiple experiments
- Local multiprocessor/ multicore hardware
  - up to 32 cores/workers
- Performance gains already present on standard dual-core laptops (4 logical)

gPROMS v5.1

- Parallelised sensitivity evaluations
  - major impact on efficiency of dynamic optimisation & parameter estimation
- Globalised optimisation solver
- Parallelised linear algebra
- Distributed multiprocessor/ multicore hardware clusters
  - unlimited cores/workers
  - available for GSA initially

Execution transparent to the user

Licensing

gPROMS v5.0

- High-Performance Computing
  - enabling HPC licence
    - allowing computations with up to 32 cores/workers
  - parallelised computations otherwise treated as sequential ones
    - require only single licence for model-based activities, model libraries, physical properties etc.
    - …irrespective of numbers of cores/workers

Mid – late 2017

- Token-based Licensing
  - additional flexibility for complex combinations of products & features
  - co-exists with existing licensing options

Advanced Process Modelling technology

Deployment across the organisation

Advanced Process Modelling technology

Deployment across the organisation

Tier-I

First-principles modellers ("custom modelling")

Primarily R&D
Subject-Matter Experts

Tier-II

Drag-and-drop flowsheeting using model libraries

R&D
Engineering

Tier-III

"Non-modellers" requiring access to model-based calculations

R&D
Engineering
Operations
Commercial

Tier-IV

Model-based applications embedded in operations decision-support systems

Operations

g | PROCESS
g | FORMULATE

g | Web-based Applications

g | Process Operations Solutions

Tier-III gPROMS usage

Putting advanced process modelling in the hands of the masses

Tier III

"Non-modellers" requiring access to model-based calculations

R&D
Engineering
Operations
Commercial

- **Same** types of calculation as those routinely done by Tier-I/II users of PSE's products
- …**but simpler** to use
  - more restricted access to the model
  - customised user interfaces
  - *end-users only require a web browser*
    - *no need for software installation*
    - *no need for powerful hardware*

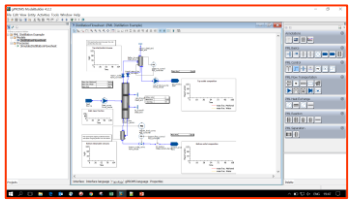
"…just a different way of delivering the benefits of advanced modelling to a wider audience within the organisation"

Tier-III model usage – a 3-step workflow

1. MODEL

Construct & validate model

Tier-I/II model developer



Challenge

achieve good results with limited effort

➔ gPROMS v5.1

2. DEPLOY

Configure appropriate GUI for Tier-III model deployment
Make model accessible to authorised users

Model "configurer"
(often same as model developer)

3. USE

Access & use model in Tier-III mode

Tier-III authorised model user

Advanced Process Modelling technology

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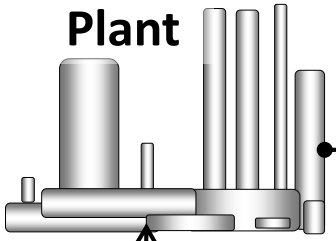
gPROMS Process Operations Solutions

First-principles models in decision support & control for process operation



Plant

Plant Data

Data conditioning

State estimation/ Online model re-calibration

Regulatory Control System

Up-to-date (re-calibrated) model

Current plant state

Regulatory Controller set-points

Set-point/ trajectory optimization

MPC model derivation

Economic MPC

Decision support via future scenario simulation

Monitoring & diagnosis

Optimal CV set-points/ trajectories

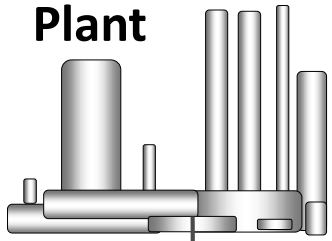
Reduced/ linear model(s)

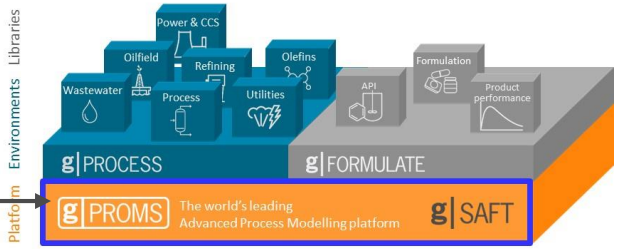
Model Predictive Control
(Linear / Nonlinear)

Unmeasured CVs

Real-time data communication & analysis

All available in gPROMS v5.0





gOPCFPI

DAE EKF Solver
(for use within gPROMS ProcessBuilder/ FormulatedProducts

Plant Data Historian

OPC Server

gOPC Client

gPROMS State Estimation (EKF)
Self-contained gPROMS-based Application

Historical plant data (csv file)

gOPCCSV

gPROMS model (exported, encrypted)

State Estimation configuration file

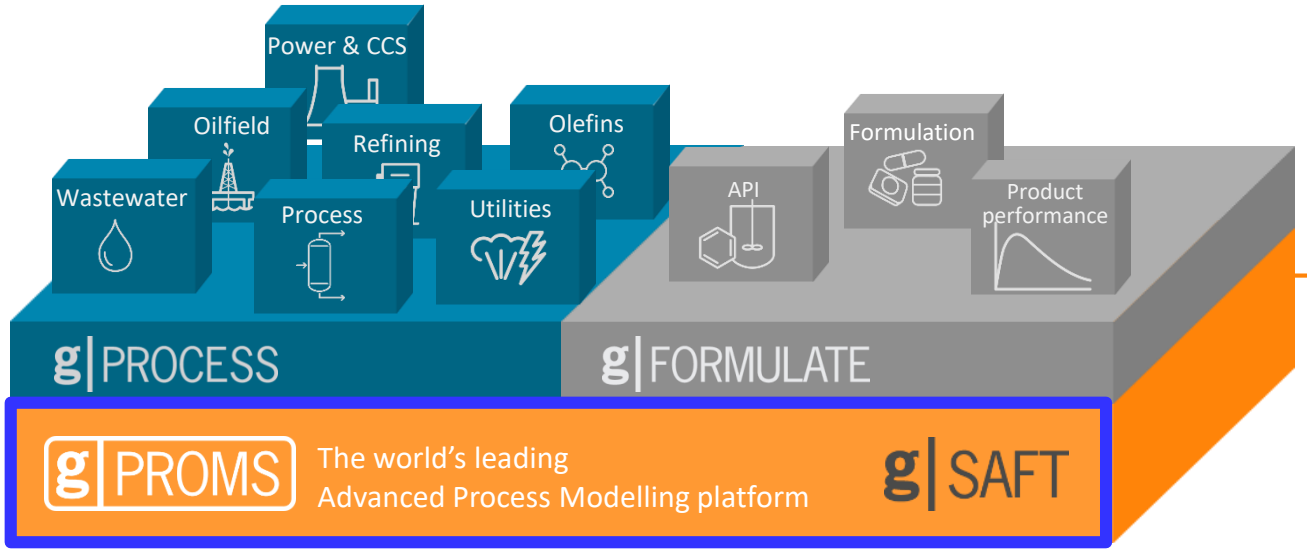
Coming next this morning…

The gPROMS software suite

Offline model development & validation tools

"Simple" products
gPROMS ProcessBuilder

Formulated products
gPROMS FormulatedProducts



Platform Environments Libraries

A single powerful software platform
Effective & efficient
software development & maintenance

Platform functionality

Process modelling

- Equation-oriented solution power
- Custom model construction
- Steady-state and dynamic simulation and optimisation
- Advanced parameter estimation
- Powerful dynamic and mixed-integer optimisation
- Global system analysis
- High-performance computing

Materials modelling

- Molecular & ionic species
- Complex species & mixtures
- Gas, liquid, solid phases
- Phase & reaction equilibrium

Thank you