



LIBPF: A LIBRARY FOR PROCESS FLOWSHEETING IN C++

Barcelona, October 4th 2006





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Market for Modeling of
Continuous Processes

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LIBPF



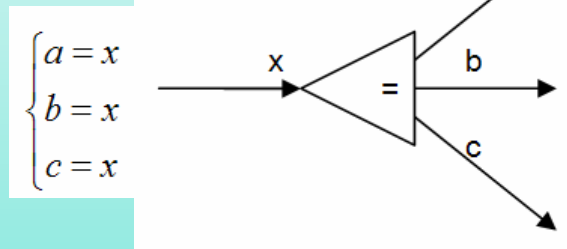
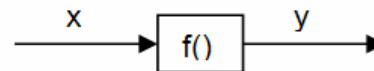
What is Process Flowsheeting ?

- Concentrated parameters, deterministic modelling of a continuous process based on a directed graph
 - ◆ edges are {material, signal, energy} streams
 - ◆ vertexes are transformations on streams
- See Westerberg et al. 1974

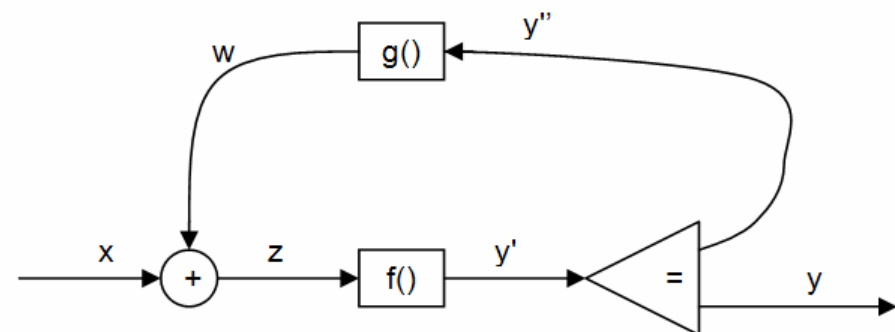


Any equation (set) can be seen as a directed graph

$$y = f(x)$$



$$\begin{cases} z = x + w \\ y' = f(z) \\ y = y' \\ y'' = y' \\ w = g(y'') \end{cases}$$





WHAT ?

MARKET

TOOLS

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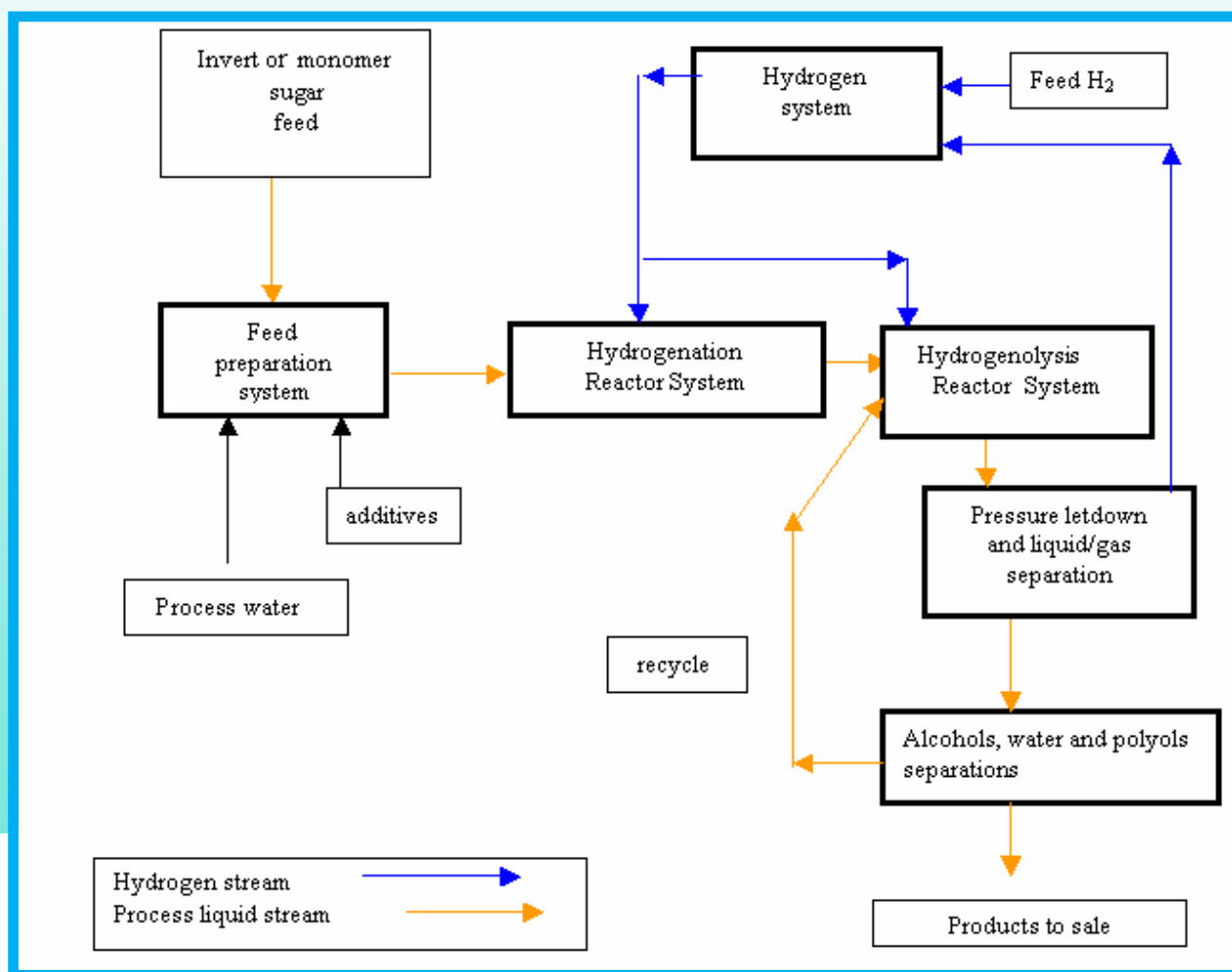
Process flowsheet example

domain:

chemical
engineering

process:

polyols
from biomass



October 4th 2006



Other names for Process Flowsheeting...

- Stock-flow diagrams in econometric models
- “network structure” in LCA (Life Cycle Assessment)
- Heating Ventilation and Air Conditioning (HVAC) modelling



State of Modeling of Continuous Processes in the Industry

■ Required skills:

- ◆ Modeling
- ◆ Software Engineering
- ◆ Process knowledge

Challenges

Large unexploited potential



WHAT ?

MARKET

TOOLS

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Challenges

Single or small-series realizations of processes

Complexity

Safety and reliability

Many different models used by different people in different phases of the project



Many different models 1/2

Feasibility study

Conceptual process design

Basic of pilot plant

Pilot plant data reconciliation processing and interpretation

Basic engineering of production unit

Operations



WHAT ?

MARKET

TOOLS

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Many different models 2/2

CHEMISTRY
EXPERT

PROCESS
ENGINEER

PROCESS
LICENCE SALESGUY

PLANT
OPERATOR

CONTROL
SPECIALIST



WHAT ?

MARKET

TOOLS

LIBPF

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Requirements for industrial modelling solutions

Customization

Integration

Reliability

Maintainability



Req 1: Customization

- Each project will be different
- In terms of solution provider, development tool has to be flexible
- But limit project cost **otherwise it will be impossible to enter the market**



Req 2: Integration

- Need for interfaces: OPC, ODBC
- Need to support different hardware:
 - ◆ Workstation
 - ◆ DCS
 - ◆ Industrial PC
- Need to support different operating systems



Req 3: Reliability

- Provide correct results if solution exists
- Provide and log errors (communication, data consistency, computation)
- Never crash
- No memory leaks (for long execution times)



Req 4: Maintainability

- Short term: low cost to fix bugs
- Long term (25 years): can upgrade, update and recompile
- Own or can freely access source code
- Own or can freely access development tools



Tools & Options

Commercial process simulators: gProms, ACM, HySys, AspenPlus, PROII, ChemCAD ...

Mathematical toolboxes: Matlab, Mathematica...

Spreadsheets (!)

Programming languages: C++, FORTRAN, Java, Phyton, ObjectPascal ...



Commercial process simulators

pros	cons
<ul style="list-style-type: none">■ Short development time■ Libraries of models available■ Can compile	<ul style="list-style-type: none">■ Dependence on tool provider■ Can do no real research■ Small user community = big bugs



Mathematical toolboxes

pros

- Reliable and easy to use
- Libraries of models and control algorithms available
- Can compile via C converters

cons

- Dependence on tool provider
- Interpreted
- Objects and data structures not designed for chemical engineering



Programming languages

pros	cons
<ul style="list-style-type: none">■ Language is vendor-independent, international standard = Portability■ Can be faster	<ul style="list-style-type: none">■ Tough and risky■ Steep learning curve■ Maintainability ?



LIBPF

- Description and Scope
- Capabilities and Applications
- Design
- License



What is LIBPF ?

- **LIBPF** = C++ **LIB**Rary for **P**rocess **F**lowsheeting
- A collection of **objects and methods** to streamline the modelling activity
- Resolution of NLAE (Non-Linear Algebraic Equation) and DAE (Differential Algebraic Equations)
- Version 0.6, 30000 Lines Of Code (LOC)



Scope

- General purpose
- Simple models
- First principle (mass and energy balances, equilibria, rating relations)
- Concentrated parameters
- Modelling of whole processes (flowsheet)



Levels of modelling

- semiempirical, local: rule of thumb, soft sensor

LIBPF

- first principle, system: concentrated parameters, entire process

- first principle, local: CFD, detailed design of single unit



Capabilities 1/3

- Components:

- ◆ fluids

- ◆ biotech (protein, lipid, carbohydrate, ash)

- Properties:

- ◆ ideal vapor-liquid (dilute systems)

- ◆ SRK equation of state



Capabilities 2/3

- Unit operations:
 - ◆ mixer, 2 or more inlets
 - ◆ flow splitter (tee), 2 or more outlets
 - ◆ spawn (duplicates the inlet)
 - ◆ fixed-yield separator, 2 or 3 outlet streams
 - ◆ vapour-liquid flash
 - ◆ isentropic compressor/expander
 - ◆ reactive **multi-stream** heat exchanger
 - ◆ fuel cell
 - ◆ countercurrent non-reactive adiabatic HTU/NTU column
 - ◆ **multistage units obtained combining any of above**



Capabilities 3/3

- Flowsheet resolution:
 - ◆ Supports feedback specifications
 - ◆ Sequential (direct substitution) or
 - ◆ **Simultaneous**



Applications

- Fuel cell system modelling
- Absorption/stripping
- Low pressure gas cleaning / processing
- Biotech processes



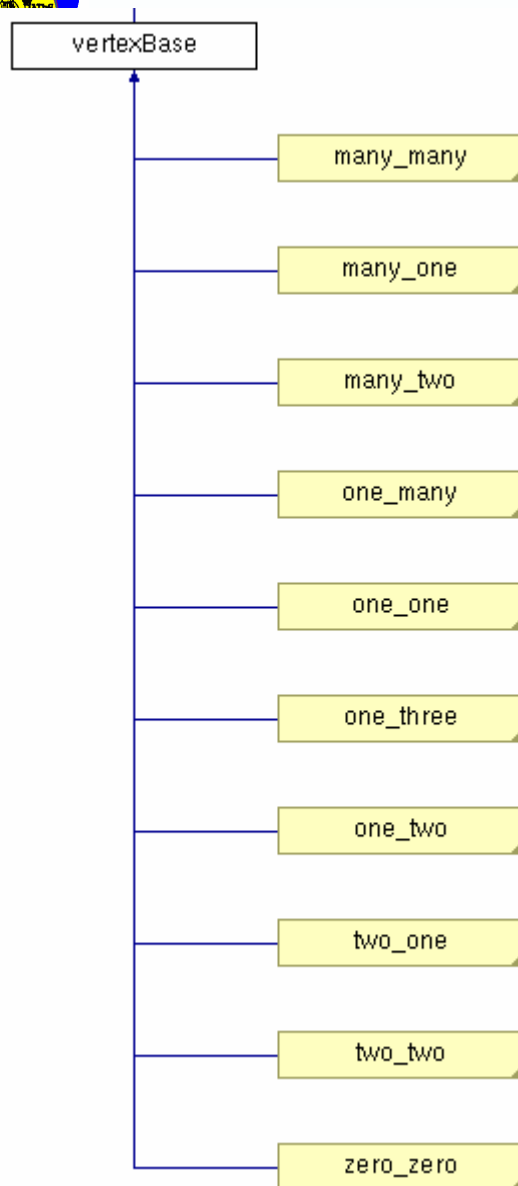
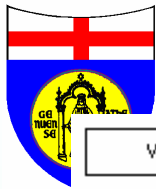
LIBPF design

- Flowsheeting in C++
- Portability
- Persistency to external database
- Small footprint salculation kernel
- Analytical derivatives
- Dimensional check of equations



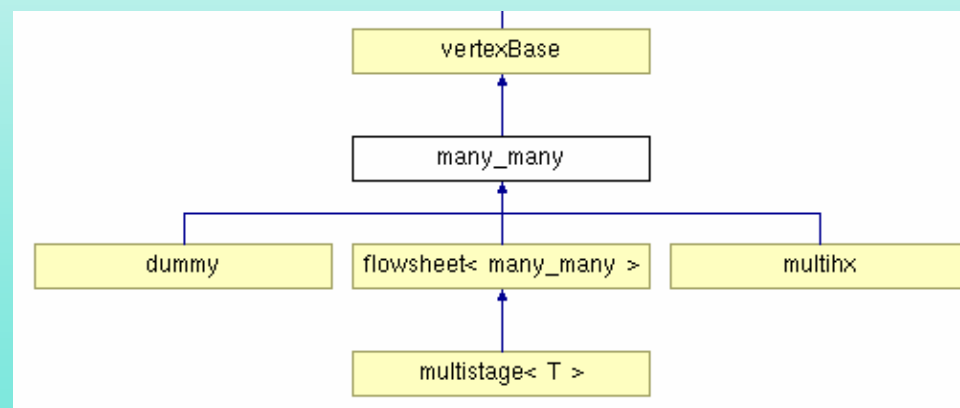
Flowsheeting in C++

- A flowsheet is a parameterized graph
 - ◆ Edges = Streams
 - ◆ Vertexes = Blocks
- Can use graph algorithms to analyze connectivity, find solution path



Vertex taxonomy

- Vertex models inherit from connectivity capability
- flowsheets can be vertexes in turn



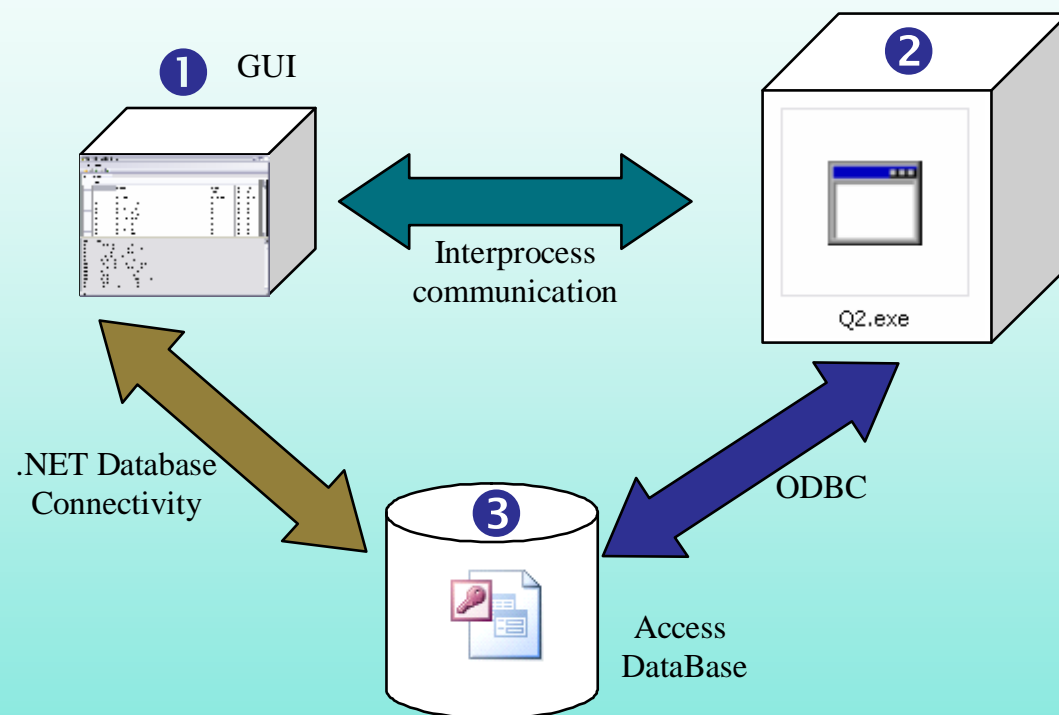


Portability

- International Standard “*Programming Language C++*” ISO/IEC 14882:1998
- **Mac OSX** 10.2.8; GNU gcc 4.0.1
- **Windows** XP Professional SP2; GNU gcc 4.0.1, Microsoft Visual C++ 2005
- Debian **Linux** 3.1; Intel C Compiler 9.1, GNU gcc 4.0.2



Persistency to database



- ① User Interface
- ② Calculation kernel:
console application
from C++ source
- ③ Relational
Database



Calculation kernel

- Small footprint: 1 ~ 4 MB
- Standalone, no weird dependency
- Can be installed on industrial PC, i.e. Windows XP Embedded





Analytical derivatives

- In LIBPF derivatives are not obtained with numerical perturbation (finite differences)
- Derivatives are analytical, obtained without source transformation via operator overloading
- Sparse and dense derivatives supported



Dimensional check of equations

- We want reliable engineering computations
- Options for dimensional consistency check:
 - ◆ compile-time using template metaprogramming, very slow compile
 - ◆ run-time, slows execution but can be turned off for production executable

LIBPF



Dimensional check of equations

```
Qdouble v;                                // the dimension is not known yet

Qdouble P(101325, "Pa");                   // pressure
Qdouble T(298.15, "K");                   // temperature
Qdouble R(8314.4, "J/(kmol*K)");          // gas constant

v = R * T / P;                             // now v becomes a molar volume

diagnostic(0, "Molar volume = " << v);

v = Qdouble(0.0, "kg/m3");                 // error !
```

```
main *** Molar volume = 24.4652 kmol^-1 m^3
UOM error in function: operator=
terminate called after throwing an instance of
'errorUOM'
```



License

Open source approach unsuitable

Free academic license

Flexible commercial licencing options



Open source approach unsuitable

- Open source does not stimulate innovation
- User community is too small
- “Hard” open source is not compatible with industry confidentiality requirements
- Current open source projects struggling (ASCEND, SIM42, OpenSim)



Free academic license

- Researchers can get compiled form (DLL/LIB) of the library complete with headers and examples
- Allowed teaching and research, but commercial uses not allowed
- Objectives:
 - ◆ Increase impact
 - ◆ Test on the field
 - ◆ Create a community



Conclusions

LIBPF can do Process Flowsheeting in C++,
no need for extra tool

LIBPF can help manage the entire life cycle of
a modeling solution

Flexible licencing, inclusive free academic
license



Visit www.libpf.com !

The screenshot shows the LIBPF website homepage. At the top, there is a navigation bar with links: home, products, demos, documentation, news, events, and a log in button. A search bar is also present. The main content area is titled 'Homepage' and includes a welcome message, a description of LIBPF as a tool for prototyping and deploying small applications, and a 'Quick Access' section with links to download brochures, read a case study, and download demos. A 'More information' section provides links to contact, a forum, and documentation. The right sidebar contains 'news' and 'upcoming events' sections. The footer includes a thank you message and a link to the website.

LIBPF

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you are here: home

navigation

- Home
- Products
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- News
- Events
- Contacts

Homepage

Homepage for LIBPF, the LIBrary for Process Flowsheeting in C++

Welcome to the homepage of the LIBPF, the C++ LIBrary for Process Flowsheeting.

LIBPF is a tool to **rapidly** prototype and deploy small applications implementing computations for training, process engineer support, on-line process diagnostic, data reconciliation. It basically is a library of objects and methods and a general purpose programming tool for the resolution of **NLA**E (Non-Linear Algebraic Equation) and **DAE** (Differential Algebraic Equations) sets.

Quick Access

For a **quick introduction** to LIBPF:

- Download product [brochures](#);
- Read the Salt & Pepper case [study](#)
- Download and install [demos](#)

More information

For more information on LIBPF:

- [Contact us](#)
- The [LIBPF forum website](#) hosts a FAQ (Frequently Asked Questions) and an Announcement forum open for **anonymous access**;
- You can [register](#) on the LIBPF forum website to be able to **post in the General/Questions forum** - this also automatically subscribes you to the LIBPF news bulletin;
- Browse the [Documentation/Papers](#) section on this website to find some **scientific** papers with insight into LIBPF technologies.

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news

- LIBPF website up 2006-08-31
- Alfa website 2006-08-22
- More news...

upcoming events

- Launch of LIBPF website
World Wide Web, 2006-09-01
- EMSS2006
Barcelona (Spain), Hospital de Sant Pau, 2006-10-04
- ESCAPE 17
Bucharest (Romania), 2007-05-27
- Previous events...
- Upcoming events...