Object-oriented modelling applied to hybrid unit operations

Paolo Greppi, Barbara Bosio, Elisabetta Arato

Department of Civil Environmental Architectural Engineering

Università degli Studi di Genova

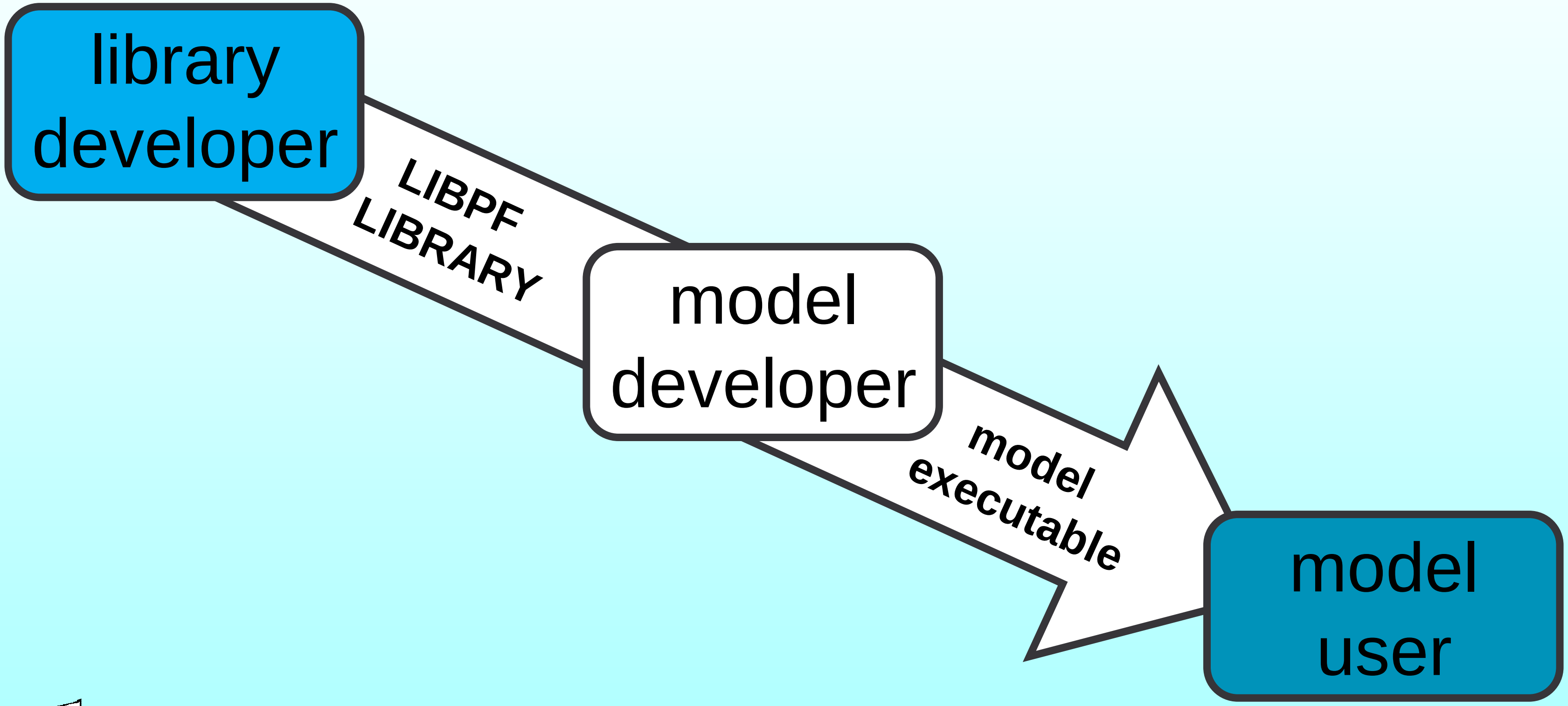
ICheaP-8 - The eight International Conference on Chemical & Process Engineering

ISCHIA Island Gulf of Naples, Italy - June 24-27th 2007

Contents

- Introduction
- Streams, flashes, connectivity, multistage arrangements
- Applications
- Conclusions

Introduction: model workflow



library developer

LIBPF LIBRARY

model developer

model executable

model user

Model development

library developer

- map process simulation entities to
  - **abstract** C++ class types
  - **mixins**: reusable partial classes
  - **concrete** classes

= **LIB**rary for **P**rocess **F**lowsheeting

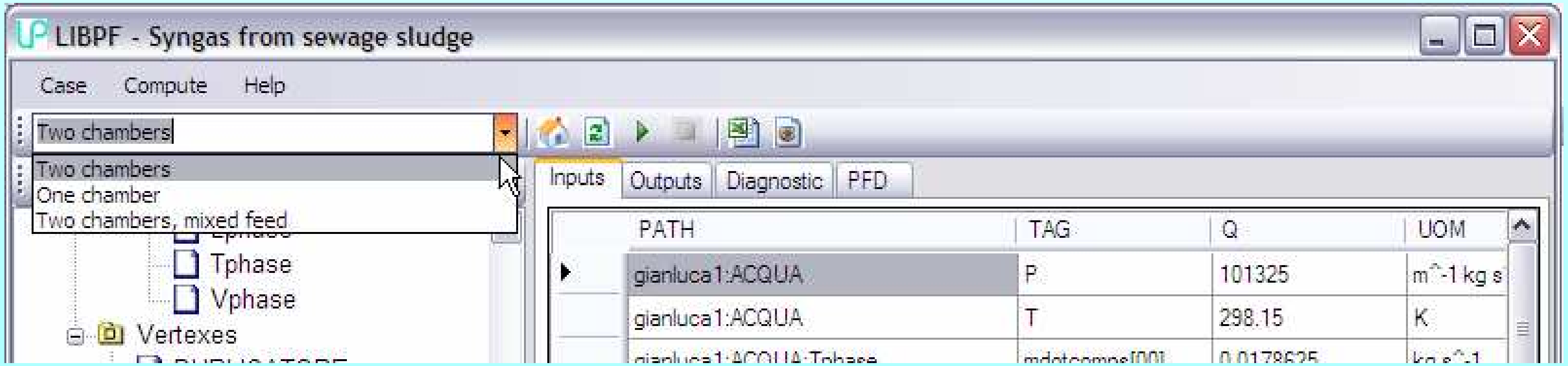
model developer

- pick up concrete classes from **LIBPF**
- write a C++ program representing the system model
- compile it to a standalone executable

Model deployment

model user

- receives system model as an executable
- access via **user interface**
- can change inputs or switch configuration
- each model configuration has a fixed structure


LIBPF - Syngas from sewage sludge

Two chambers

Two chambers
One chamber
Two chambers, mixed feed

PATH	TAG	Q	UOM
gianluca1:ACQUA	P	101325	m^-1 kg s
gianluca1:ACQUA	T	298.15	K
gianluca1:ACQUA:Tphase	mdotcomps[00]	0.0178625	kg s^-1

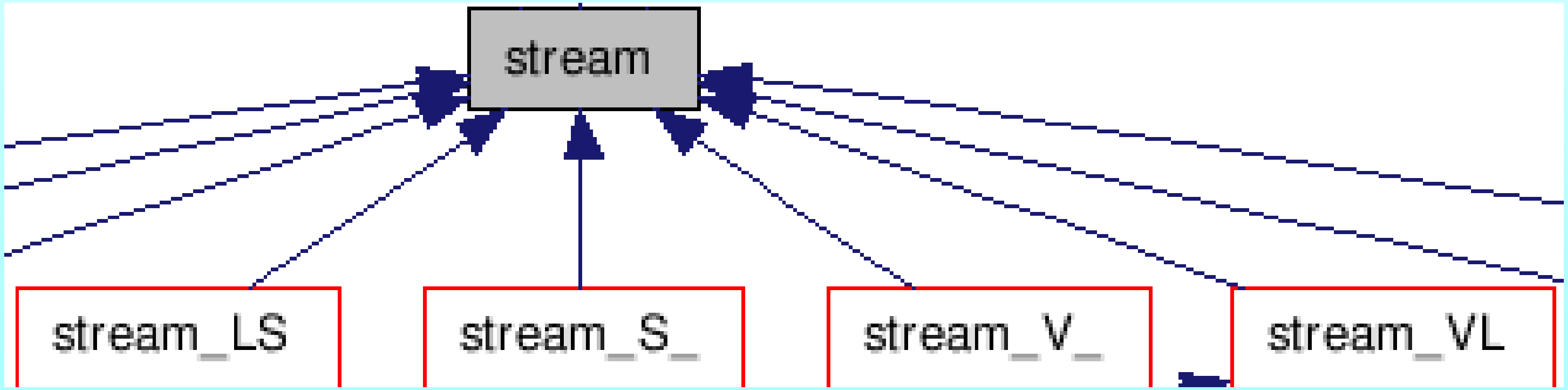
Contents

- Introduction
- Streams, flashes, connectivity, multistage arrangements
- Applications
- Conclusions

The simplest object: **`stream`**

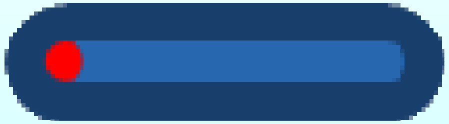
- abstract **`stream`** type

- specialized mixin classes are derived from abstract **`stream`** type

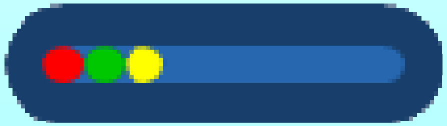


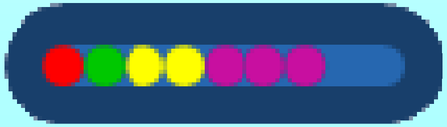
Concrete `stream` types

- every concrete stream type contains at least one **total** phase



- multi-phase streams can have explicit representations of the phases
  - **`stream_VLe...`**
  - **`stream_VLLSSSe...`**

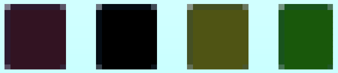




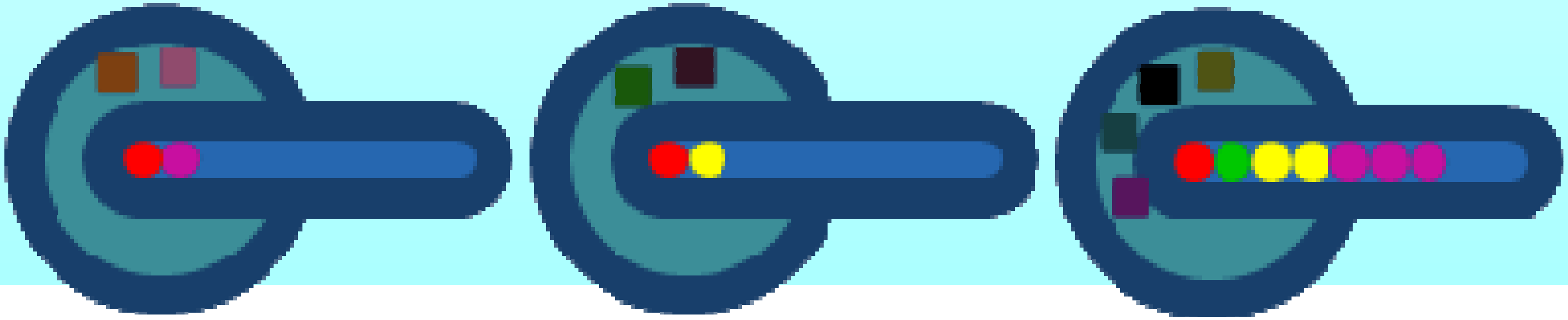
Enter reactions

- Take a generic flash (**`genflash`**) mixin class instance

- add reactions ...

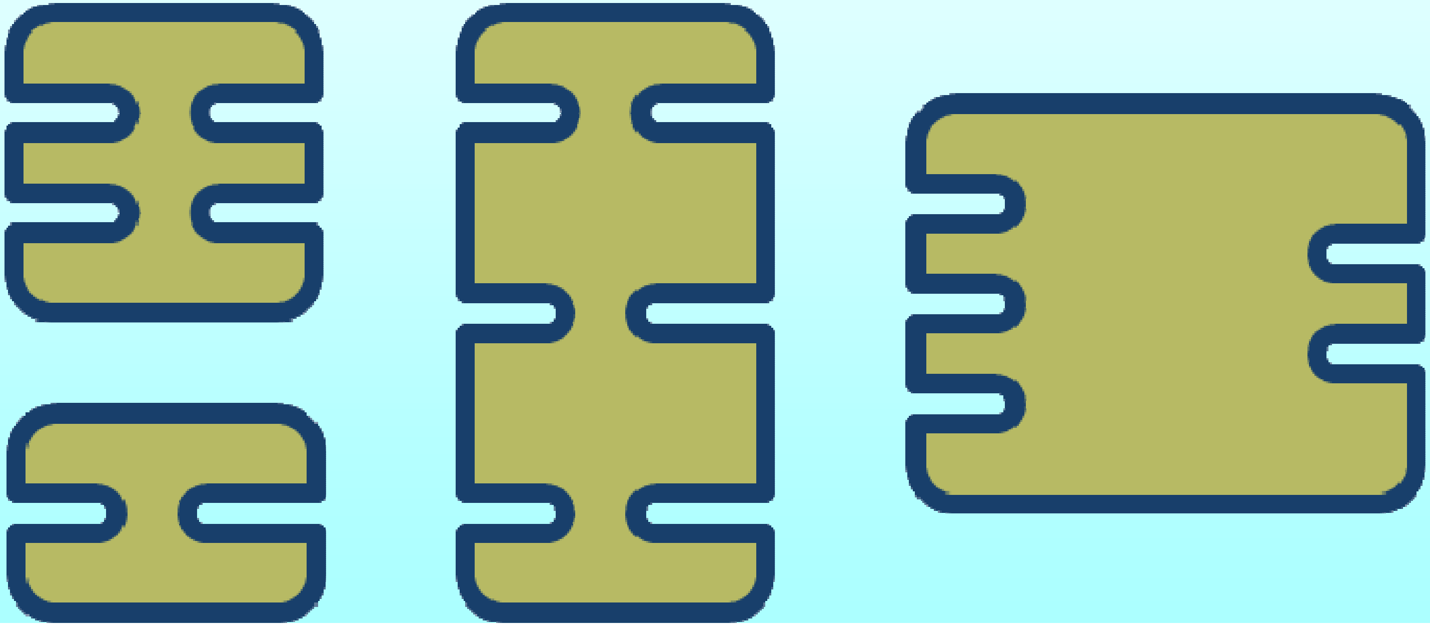


- ... get reactive flashes

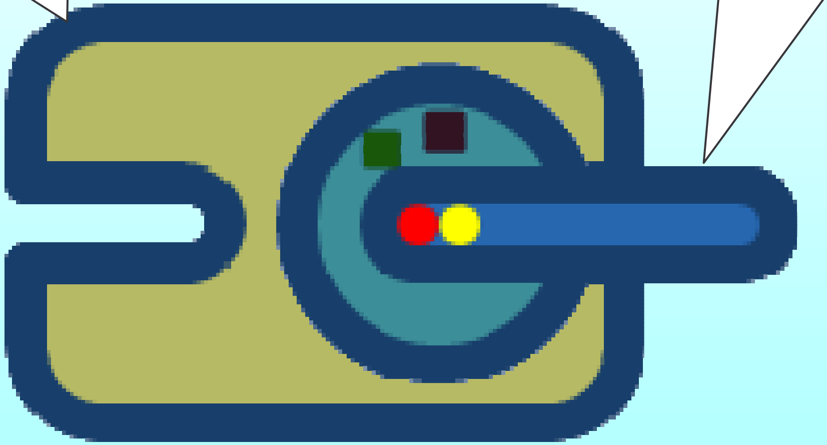


Enter connectivity

Special mixin types represent the capability of units to **connect** to streams



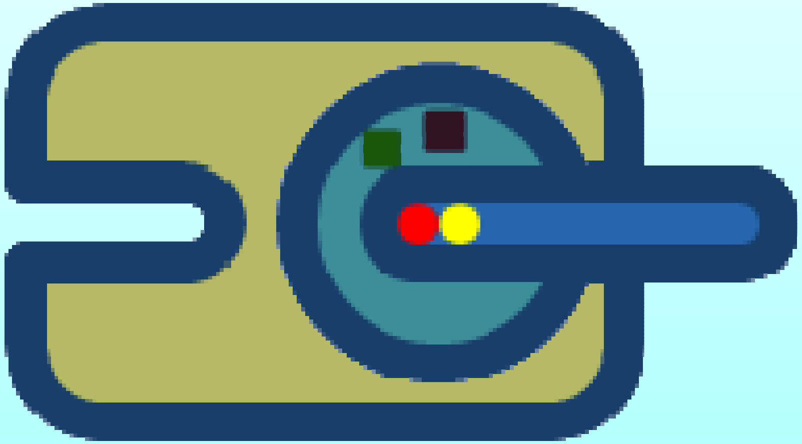
Compose mixins ...



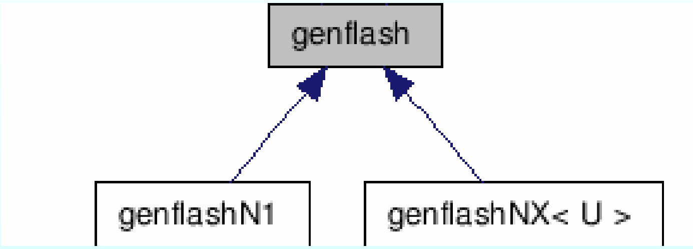
connectivity mixin

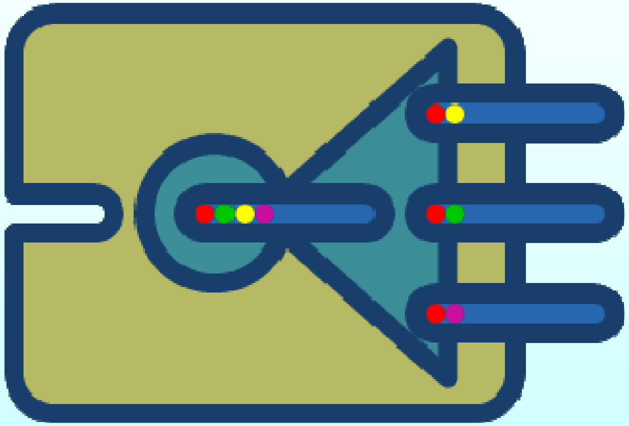
process mixin

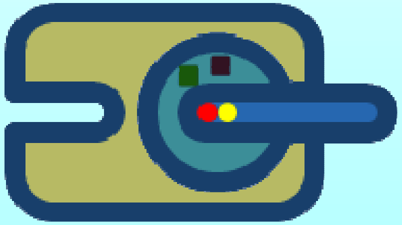
.. get a concrete class

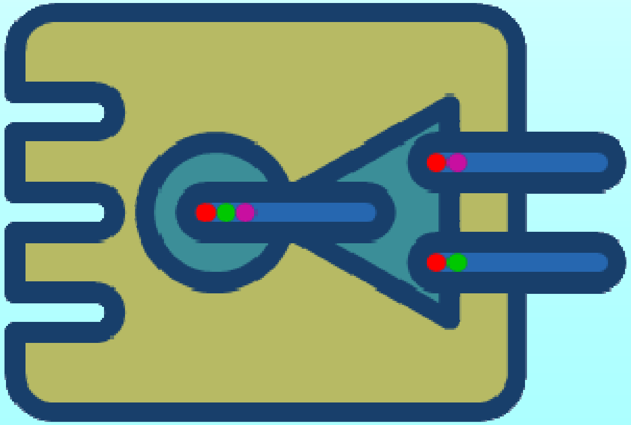


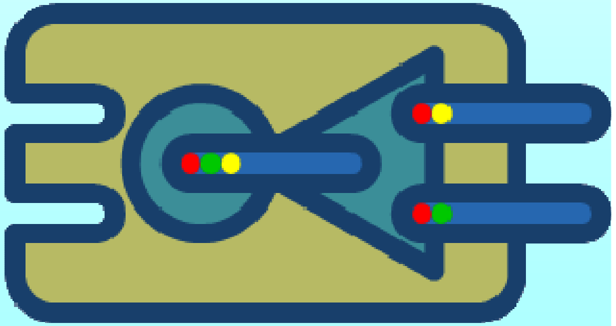
Variations of `genflash` with connectivity





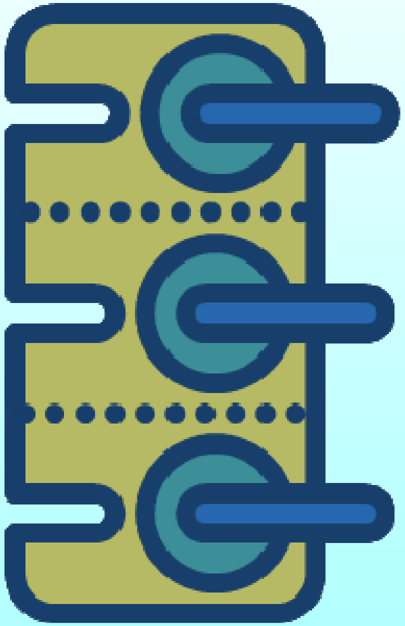






Combinations of generic flashes

- flexible mulstream concentrated parameters model: **`multihx`**
- N reactive streams exchanging heat or mass:
  - (reactive) multi-stream heat exchanger
  - (reactive) membrane unit
  - fuel cell



Multistage arrangements

- Concentrated parameter objects are combined to yield distributed parameter models:
  - 1-D arrangements:
    - columns
    - pipes
  - 2-D arrangements:
    - fuel cells
    - reactive heat exchangers

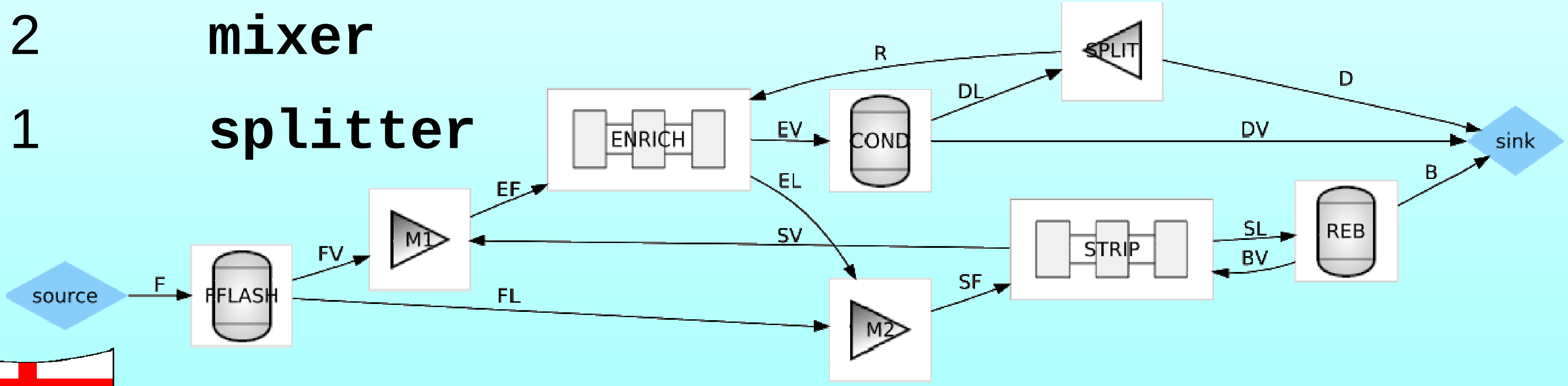
Contents

- Introduction
- Streams, flashes, connectivity, multistage arrangements
- Applications
- Conclusions

Application 1: Simple distillation column

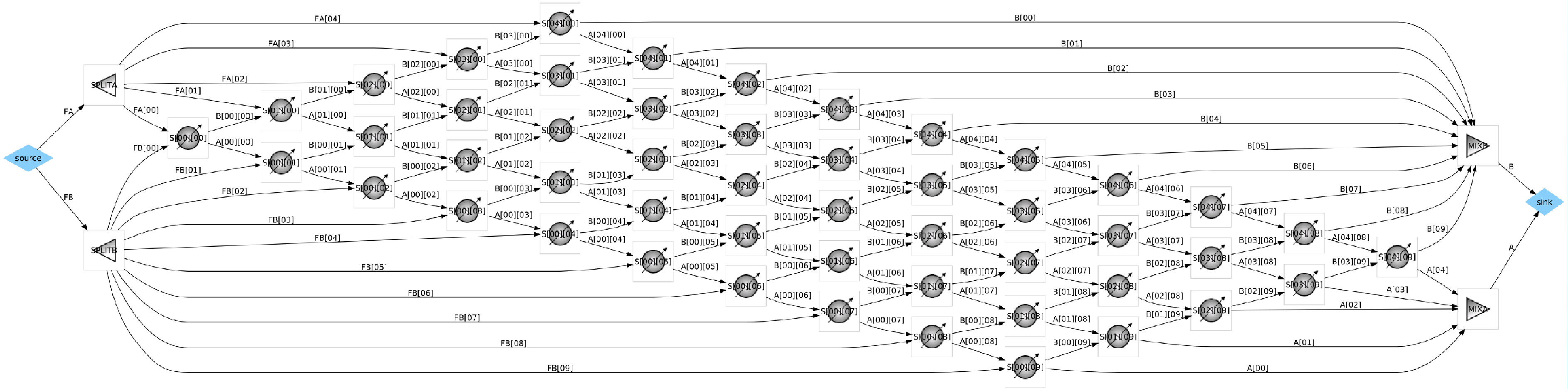
The column was broken down into 8 subunits:

2	**`multistage1D<genflashNX<stream_VL>>`**
3	**`genflashNX<stream_VL>`**
2	**`mixer`**
1	**`splitter`**



Application 2: Distributed parameter planar Fuel Cell

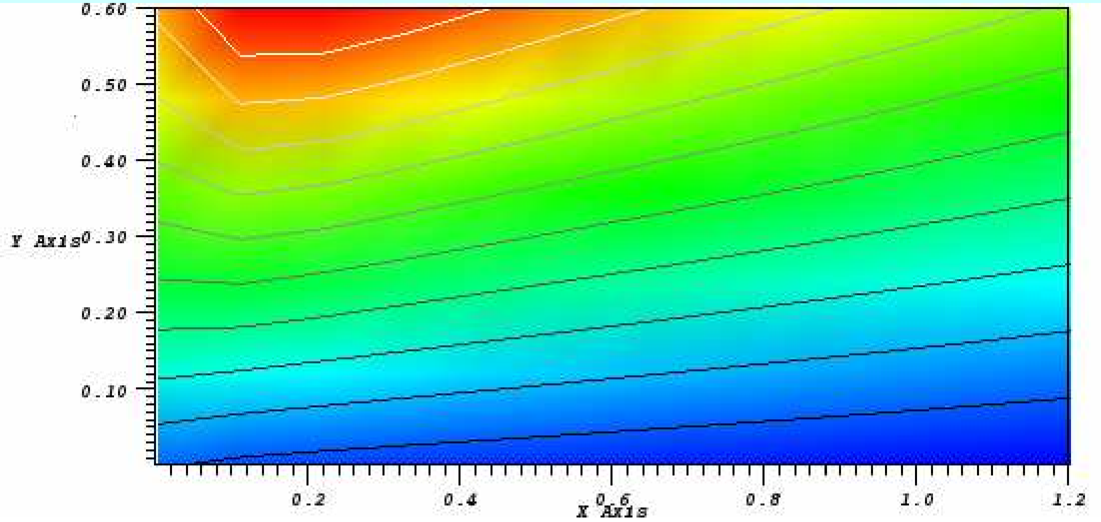
- 5 x 10 **`multihx`** objects



- flowsheet for **cross-flow** arrangement

Application 2: Distributed parameter planar Fuel Cell

- Results match proven tools
- Example: solid temperature plot for MCFC (Molten Carbonate Fuel Cell)



Applications: simulation run duration

LIBPF slower than special-purpose tools

Test case	Reference tool (benchmark)	Benchmark	LIBPF
		Timing, s	Timing, s
Simple distillation column	Commercial process simulator X	1	10
Planar Fuel Cell	Special purpose 2-D finite differences code	2	60

Applications: modelling project duration

modelling of hybrid / complex unit operations

- conventional approach:

  3 man-months

- new approach with model reuse:

  1 man-month

(estimates)

Contents

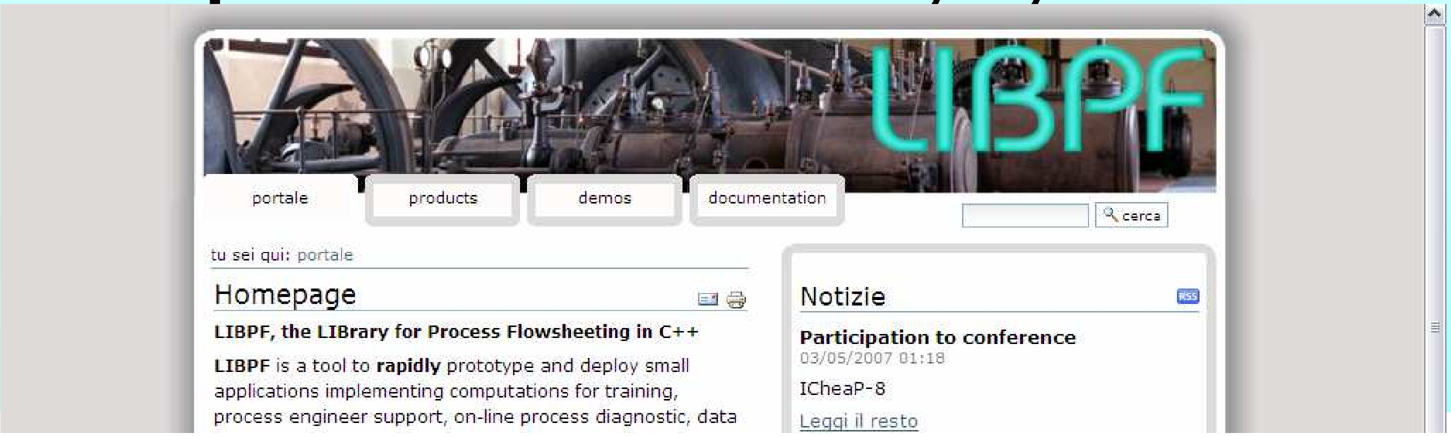
- Introduction
- Streams, flashes, connectivity, multistage arrangements
- Applications
- Conclusions

Conclusions

- **C++** can be used for process simulation using **LIBPF** library
- **Run-time** is slower than with conventional approaches ...
- ... but **project duration** is shorter for hybrid unit operations modelling

Visit libpf.com

- Get C++ header files with the **classes hierarchy**
- Get and run **demos**
- **Request** the LIBPF library by mail



tu sei qui: portale

Homepage

LIBPF, the LIBrary for Process Flowsheeting in C++

LIBPF is a tool to **rapidly** prototype and deploy small applications implementing computations for training, process engineer support, on-line process diagnostic, data

Notizie

Participation to conference
03/05/2007 01:18

ICheaP-8

Leggi il resto