



Workflows controlling all essential laboratory activities: analysis planning, data acquisition, automated error recovery, information retrieval, and evaluations - all in one

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Laboratory Automation Conference
Hinxton Hall, Cambridge, UK, Jan., 12, 2010

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- Goal and definitions
- Workflow components for analyses
- Virtual resources
- New workflow components
- Workflow processing architecture
- Conclusions



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- **Goal and definitions**
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Goal

- One workflow for
 - Analysis planning, instrument control, data acquisition, automated error recovery, information retrieval, and evaluations
- Why?
 - Possibility to perform routine analyses **fully automated**



Workflow definition

- A workflow consists of a sequence of connected steps. [...]
- Workflow may be seen as any abstraction of real work, segregated in work share, work split or other types of ordering.
- For control purposes, workflow may be a view on real work under a chosen aspect, thus serving as a virtual representation of actual work.



Workflow definition

The automation of a business process, in whole or part, during which documents, information or tasks are passed from one participant to another for action, according to a set of procedural rules.



Resource

- **Real machine or instrument** on with an activity is processed
- Commands invoke a **process step on a resource**
- **Non-consumable** resource
 - Resource usable repetitively by activities of different samples in a time interval.
 - Examples: **machines, instruments**
- **Consumable** resource
 - Resources usable once in an activity
 - Examples: **reagents, containers**
- Resources linked to specific maintenance workflows

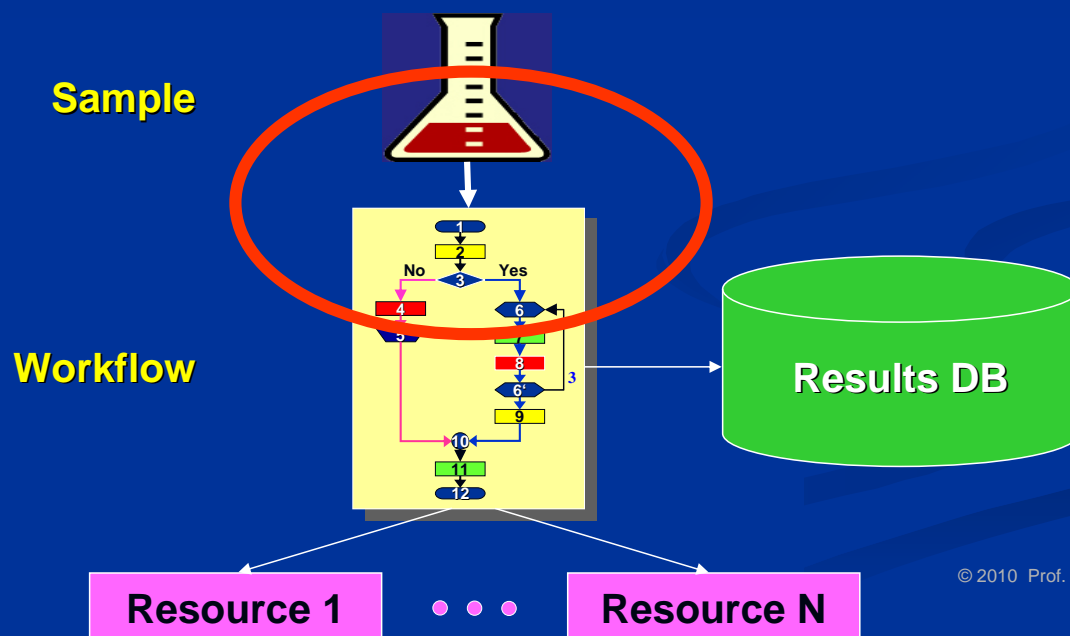


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Job definition

- A **work piece or sample** to be processed on a **set of resources** following a **workflow**.



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General requirements

- Good representation for workflow
- Robust design of activities
- Model to describe variable timing in chemical or biological processes
- Model for control operation processing
- Data model for static and dynamic resource description
- Databases for workflows, resources, results, recovery, ...
- Dynamic scheduler
- Dynamic executor
- Interfaces to the real world – workbench control and data acquisition
- Error detection and recovery system

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Process elements

- Activities („chemical“ or instrument control)
 - A piece of work that forms one logical step within a process – manual or automated.
- Control elements
 - IF, CASE, PARALLEL, LOOP, WHILE, UNTIL, SPLIT, MERGE, CALL, ONERROR
- Parameter operations
 - CREATE, ASSIGN, READ, UPDATE, DROP



Symbol for an activity in a GUI



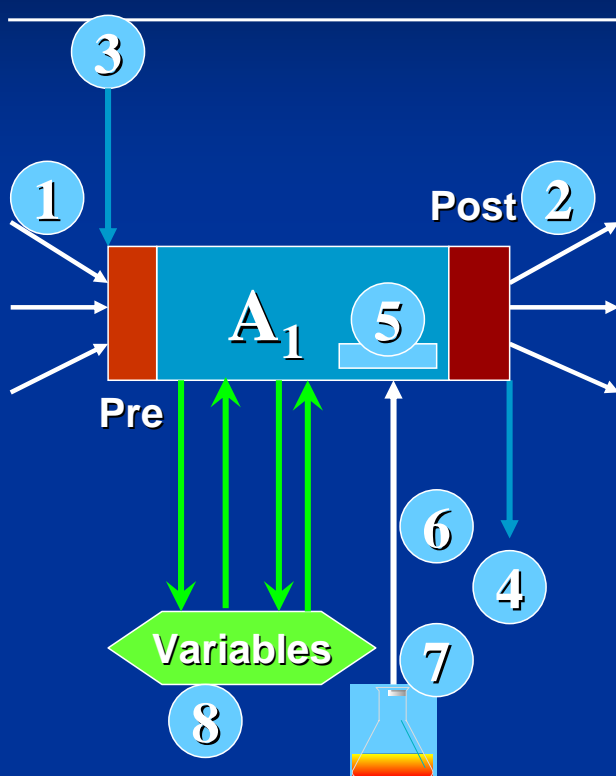
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Design of activities



- 1 Time constraints to the previous activities
- 2 Time constraints to the next activities
- 3 Pre trigger
- 4 Post trigger
- 5 Branching to an error workflow
- 6 Consumables
- 7 Durables
- 8 Variables

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Activity cooperates with resource driver (control, status, results).

Functionality of activities

- Generic software driving instruments
 - Commands, parameters, result structure, error control from System Capability Dataset (OMG LECIS standard)
- Instrument capabilities loaded automatically into workflow editor from SCD
- Runtime system executes capabilities utilizing SCD information



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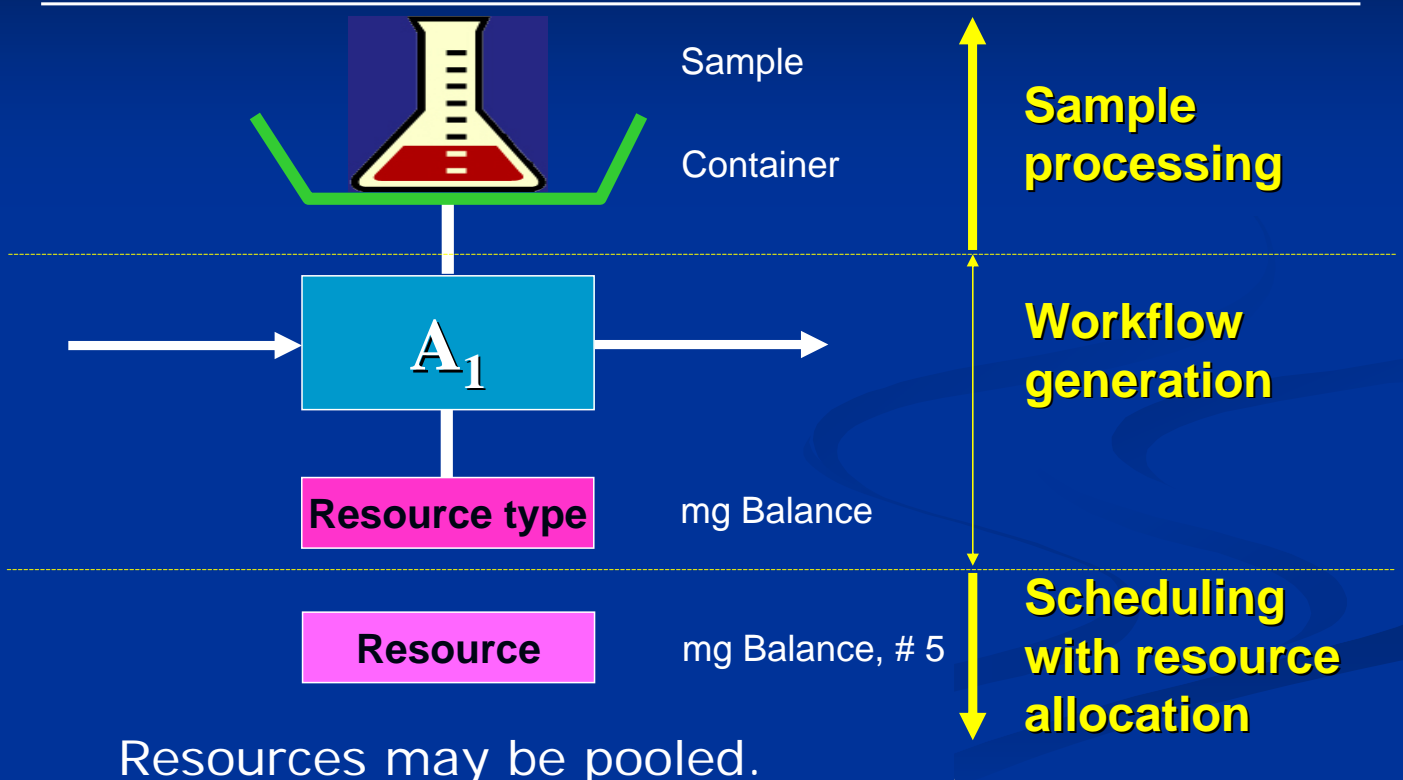
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Ref: <http://www.lecis.org>

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Activity model (1)



Activity model (2)



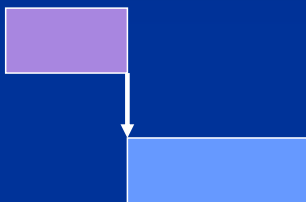
- Interface to resource driver
 - Execute commands
 - Transfer parameters
 - Readout results
 - Check status
 - Detect errors
- Spawn programs
 - ...
- Branch to maintenance workflows



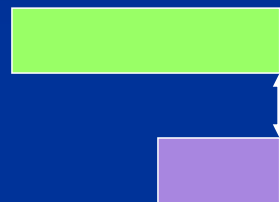
Activity constraints

■ Timing constraints

■ End-to-start



■ end-to-end

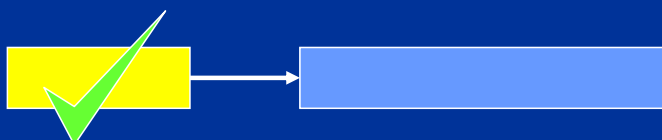


■ start-to-start



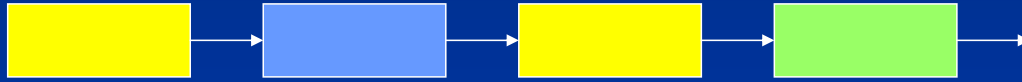
■ Conditional constraints

- Activity can be executed only if one or several conditions are true

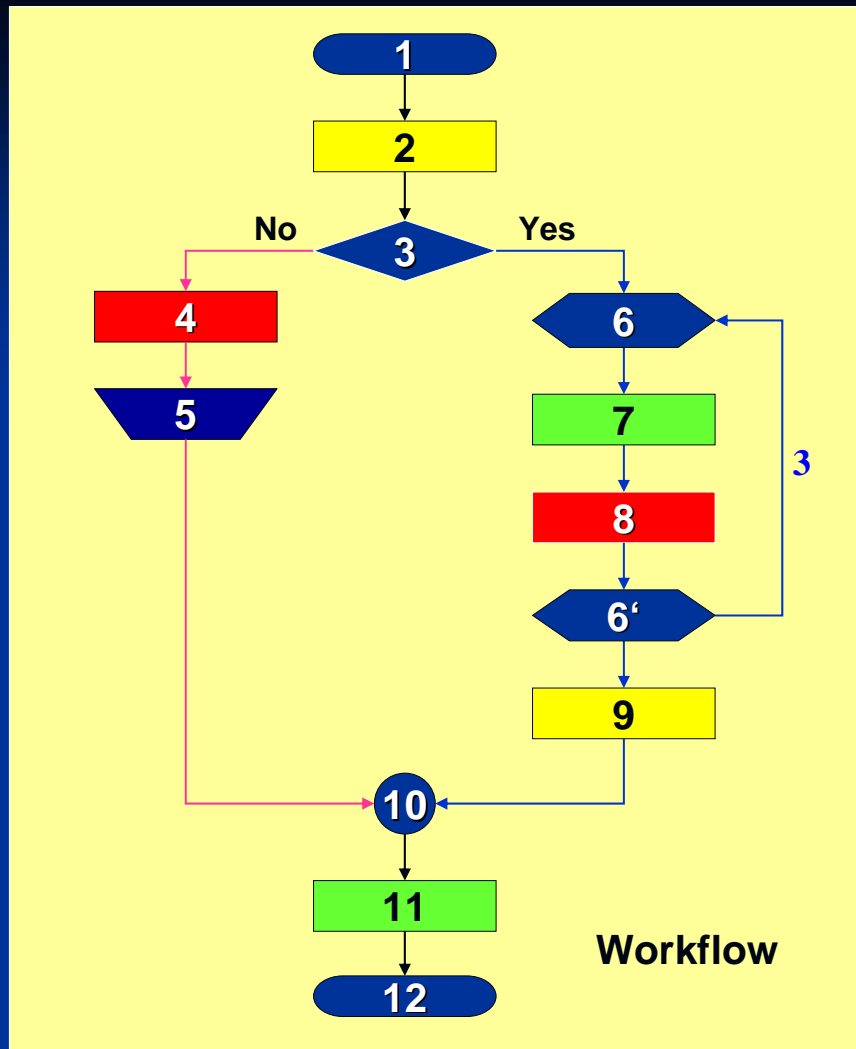
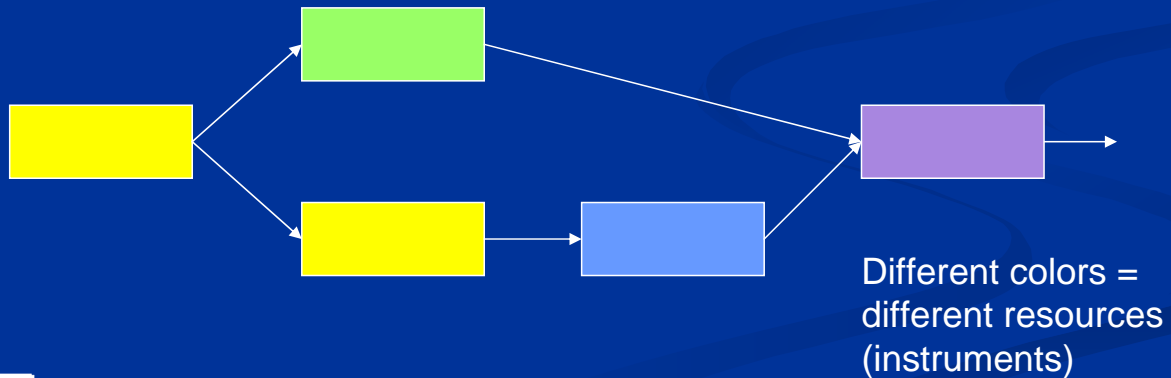


Representation of a workflow

- Activities in a sequence

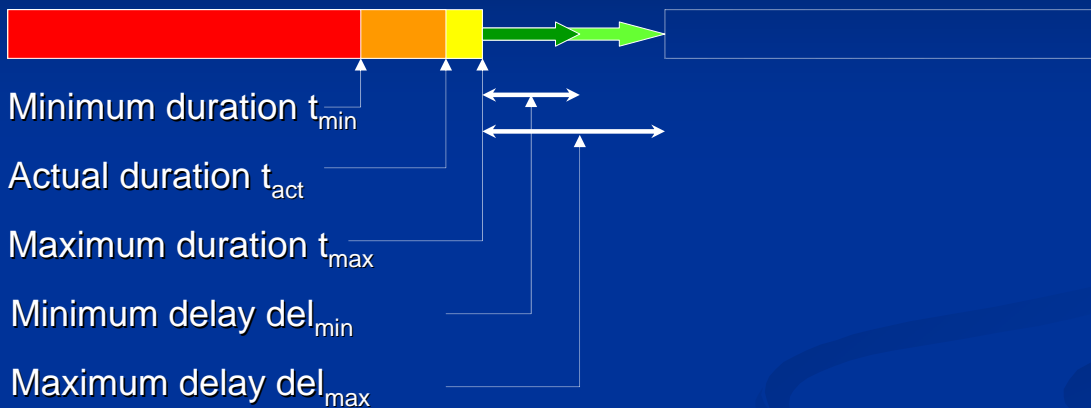


- Activities in a directed graph

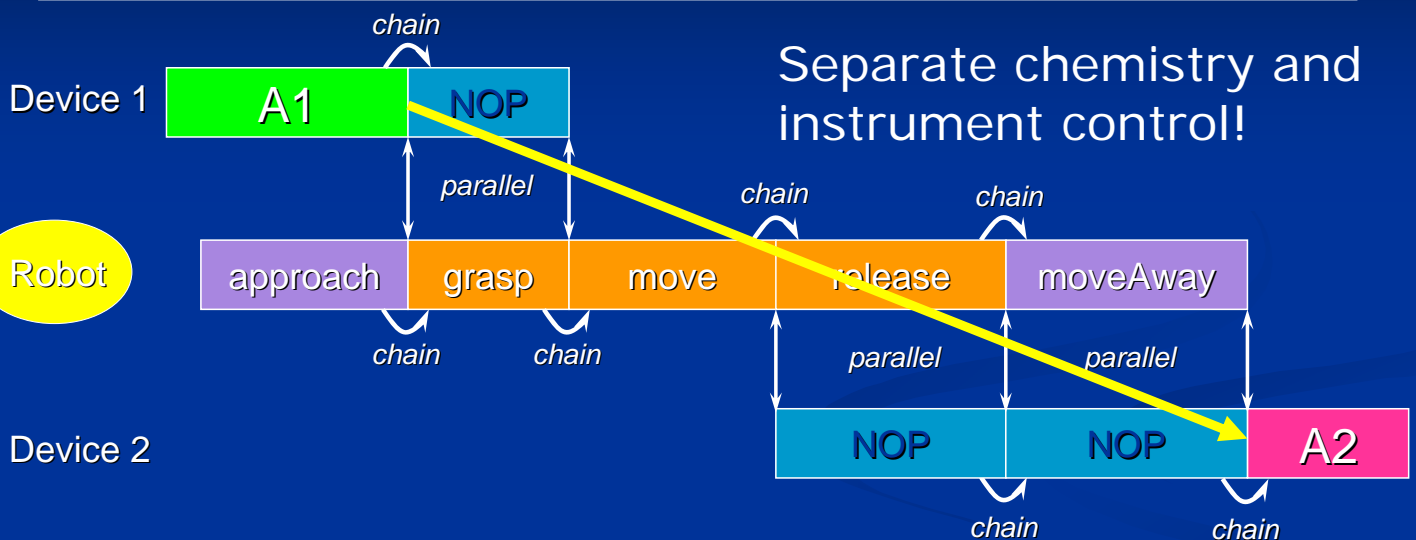


- (Data) flow diagram supplemented with certain special elements
- Editor to design the workflow and enrich it with necessary information

Timing of activities



Only experiment relevant activities: → Hidden transport

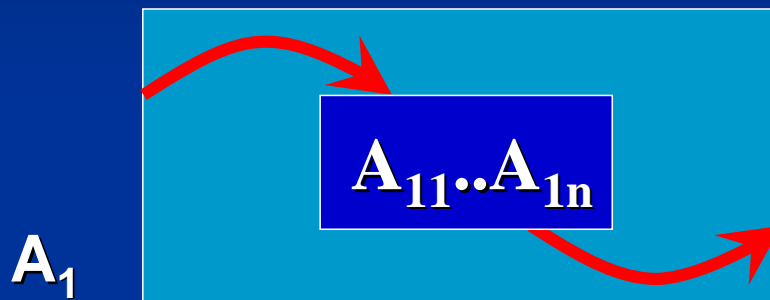


Legend:

- Colored activities are grouped to a transport macro.
- Arrows = constraints
- NOP = no operation



Inner structure of activities



To be transferred:

- Data
- Material
- Container(s)

→ **Functions**

→ Modularity of workflows

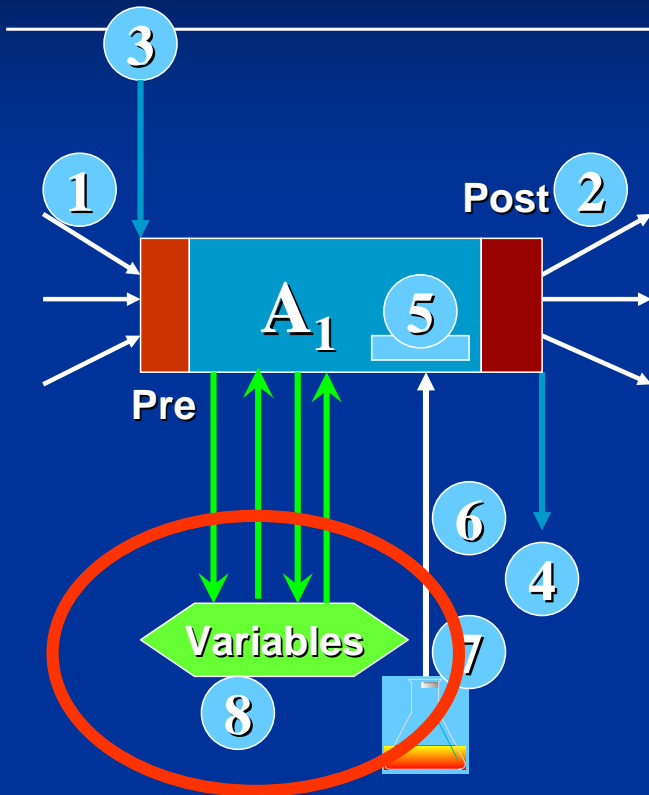


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Pseudo resources



Pseudo resources

(extended semantics)

- Calculator
- Storage manipulator
- Data mining component
- Statistics interface
- Database interface

Variables

- Results
- Calculation parameters

Routine evaluation to be integrated easily via workflows!

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Process elements (extended semantics)

- Activities
 - A piece of work that forms **one logical step** against a **virtual resource**.
- Control elements
 - IF, CASE, PARALLEL, LOOP, WHILE, UNTIL, SPLIT, MERGE, CAL, COND, OR
- Parameter operation
 - CREATE, ASSIGN, READ, UPDATE, DROP



Symbol for an activity in a GUI



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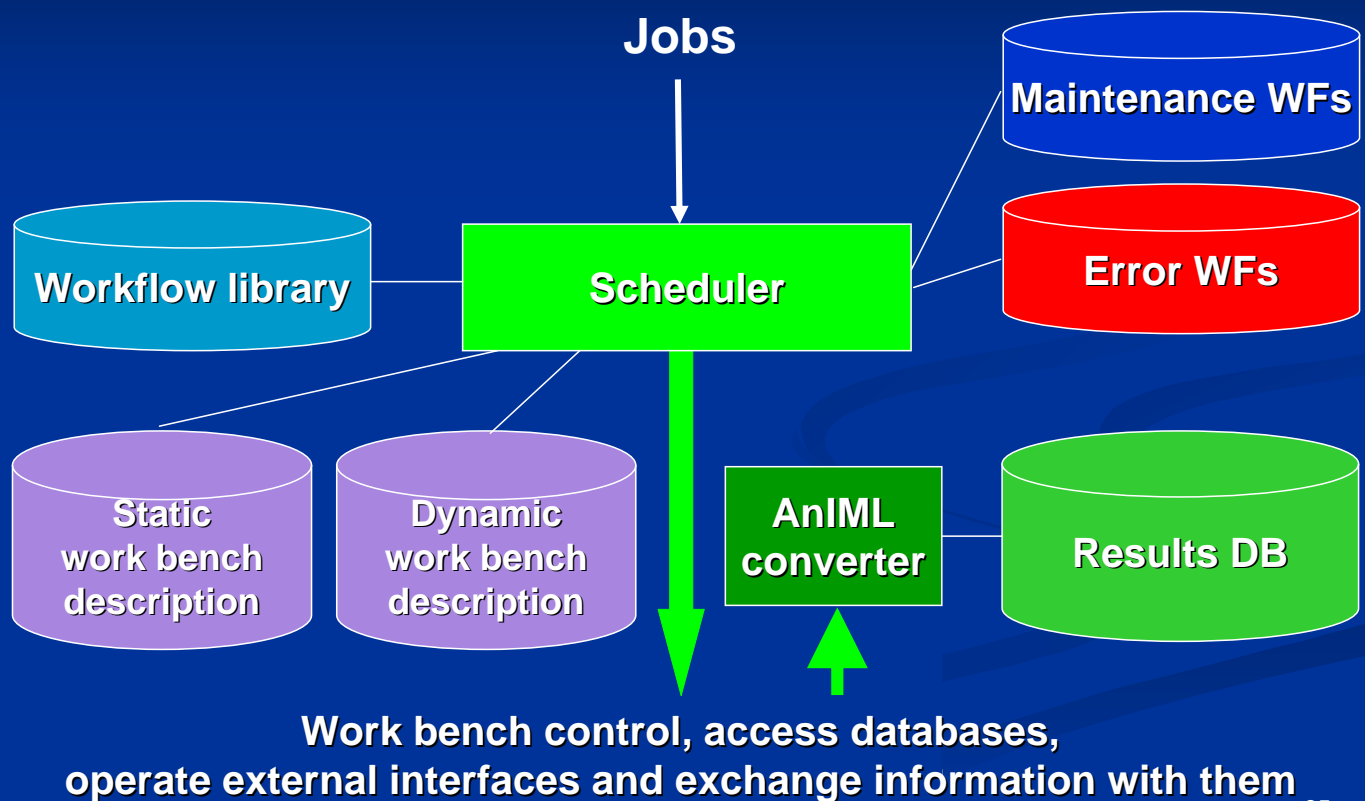
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More process elements

- Activities
 - A piece of work that forms one logical step within a process – manual or automated.
- Control elements
 - IF, CASE, PARALLEL, LOOP, WHILE, UNTIL, CALL, ONERROR
- Parameter operations
 - CREATE, ASSIGN, READ, UPDATE, DROP
- Converter to standard result format (AnIML)
- Storage operations
 - INSERT, SELECT, UPDATE, DELETE, Table operations
- Arithmetical operations

Workflow execution system



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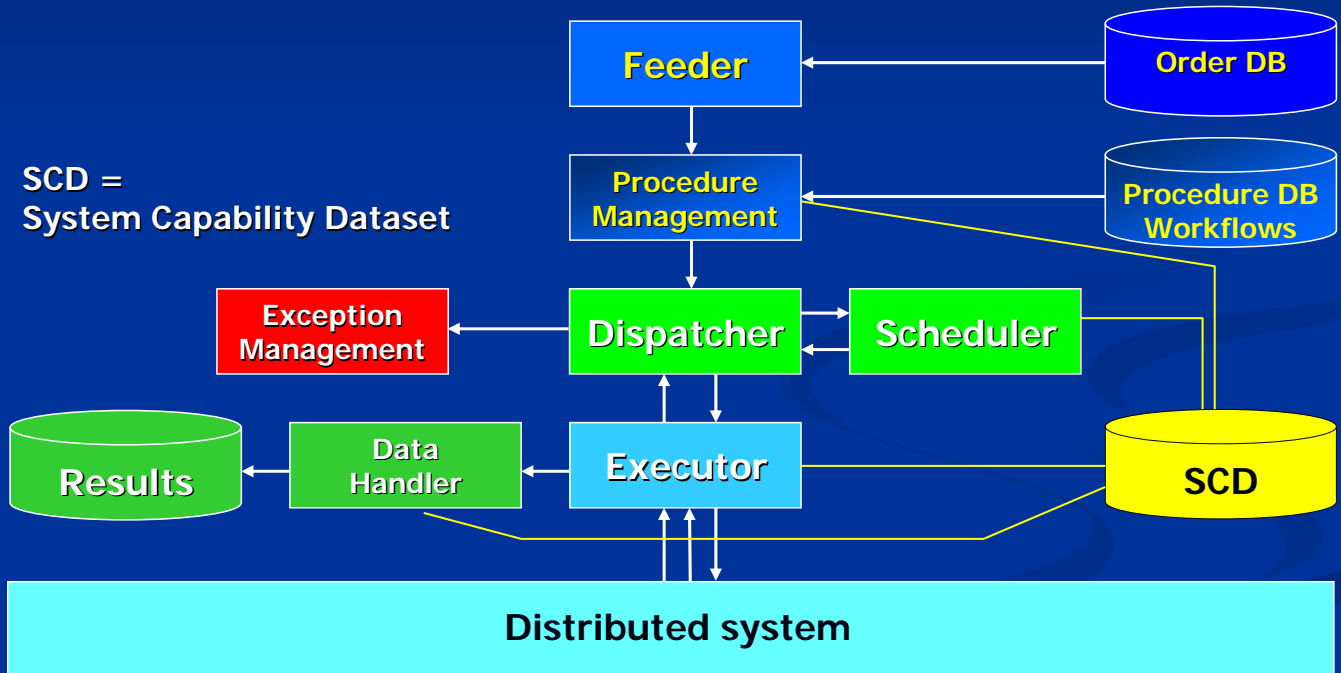
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System architecture (1)



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System architecture (2)



- Local variables for jobs
 - Storage operations
 - Control parameters
 - Calculations
 - ...
- Global variables
 - Resource management
 - Maintenance
 - ...



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Conclusions

- Workflows can support all steps in the laboratory
 - ➔ Automation with (almost) no human process interaction
- Describe resources in a System Capability Dataset
 - ➔ Plug-and-play
- Introduce AnIML as data standard
 - ➔ Compatibility between various different analytical methods

Conclusions (cont'd)

■ Major tasks

- Extend resources to virtual resources
- Add new workflow elements for program spawning and variable handling
- Provide a dynamic scheduler and a workflow processing engine
- Provide interfaces to external software



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