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Software Automation in Scientific Research Organizations

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IT in Science

- **Managing the software**
  - Science cannot be separated from the software used to support it
  - integration and interoperability, controlled evolution, configuration management, distribution and deployment
- **Managing the data**
  - Everything depends on the integrity of the data
  - Provenance, lineage, distribution
- **Managing the scientific process**
  - What are the activities undertaken in the discovery of new knowledge?
  - Processes must be repeatable - results must be reproducible
  - Managing may include: capture, document, archive, share, execute and reproduce processes

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Institute for Aerospace Research

Institute for Ocean Technology

- **NRC-IOT: support of Canada's ocean technology industries**
  - Offshore engineering basin
  - Towing tank
  - Ice tank
  - Cavitation tunnel
- **NRC-IAR: R&D related to the design, manufacture, performance, use, and safety of air and space vehicles.**
  - Wind tunnels
  - Jet engine testing
  - Chicken guns

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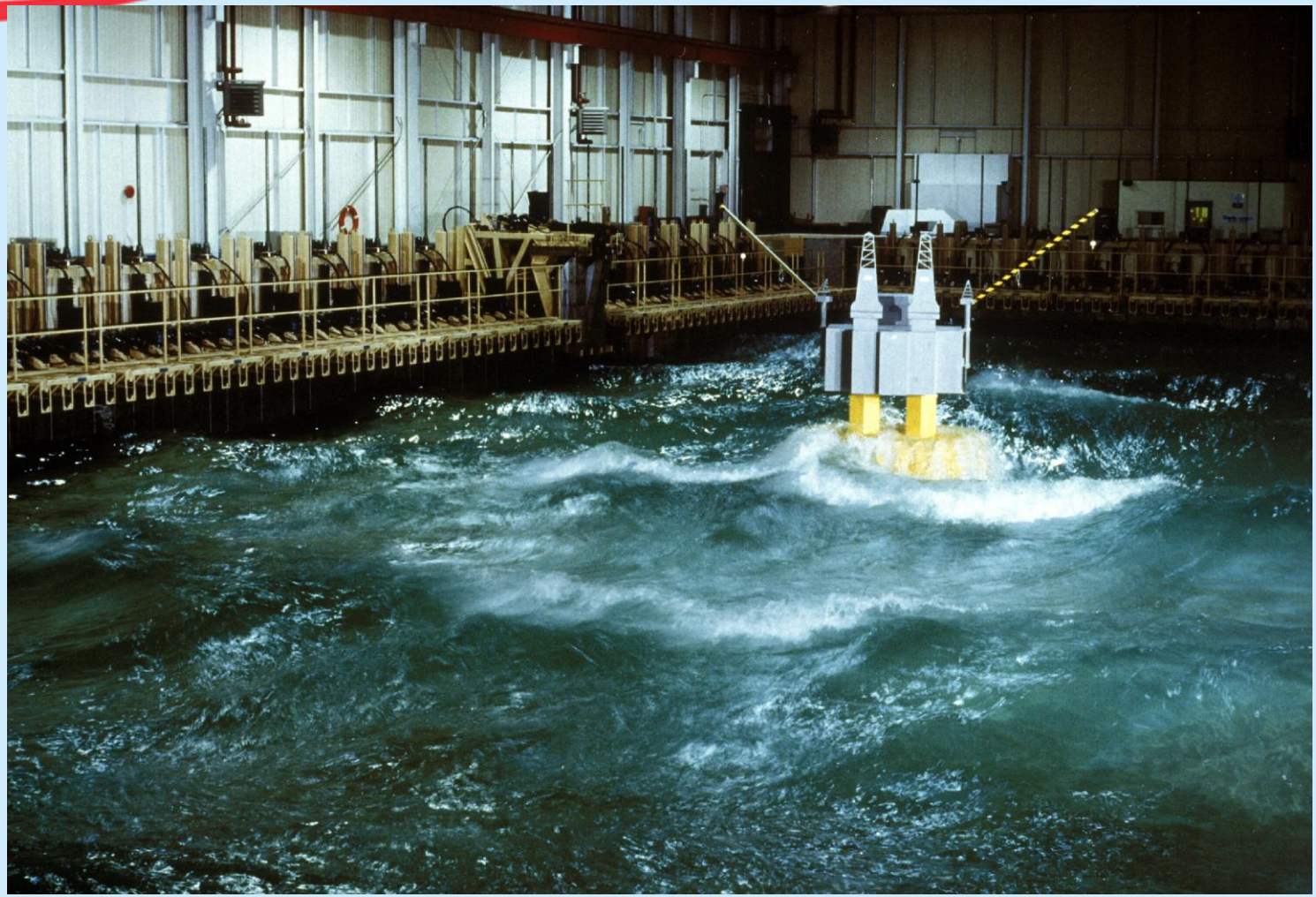
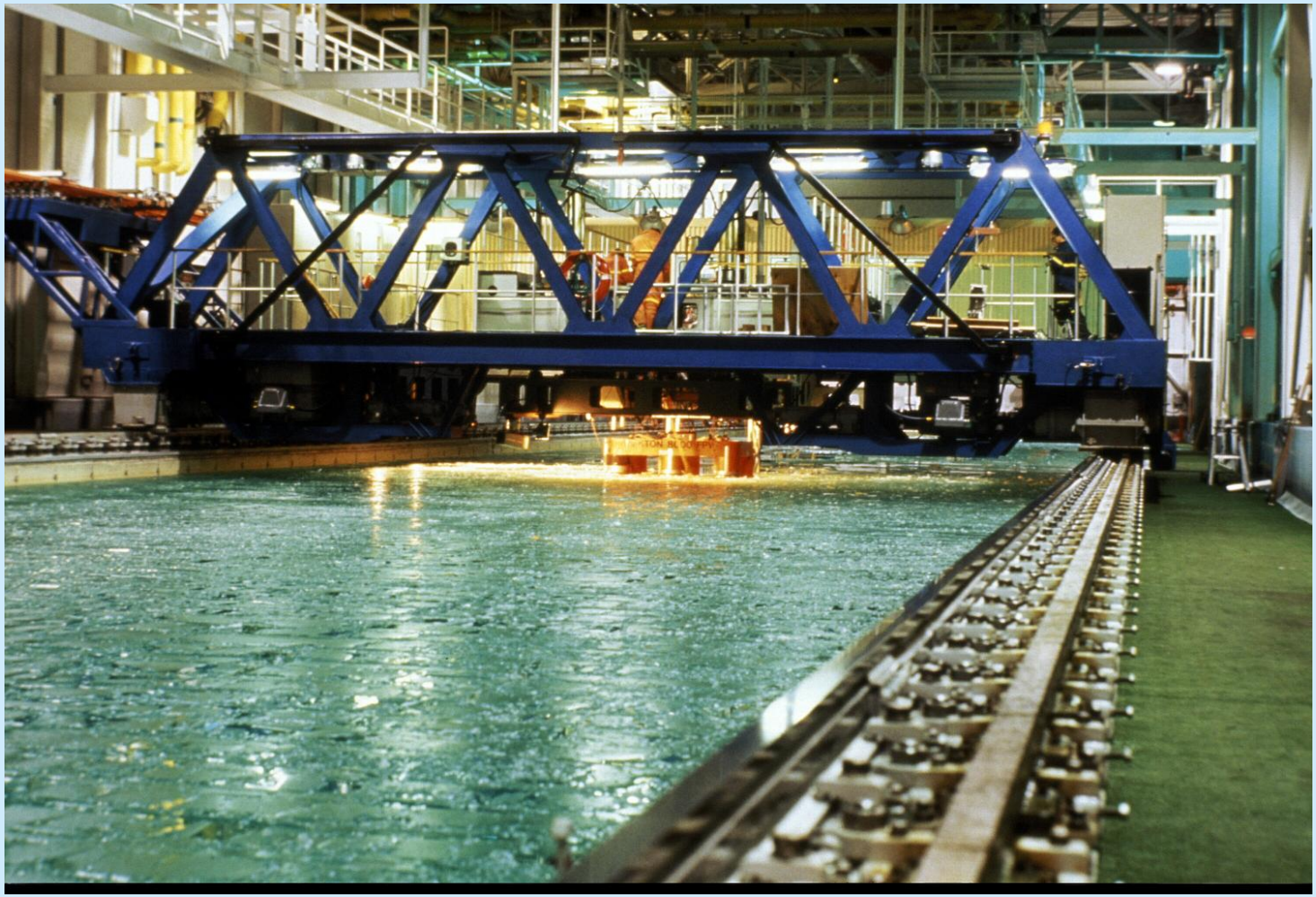
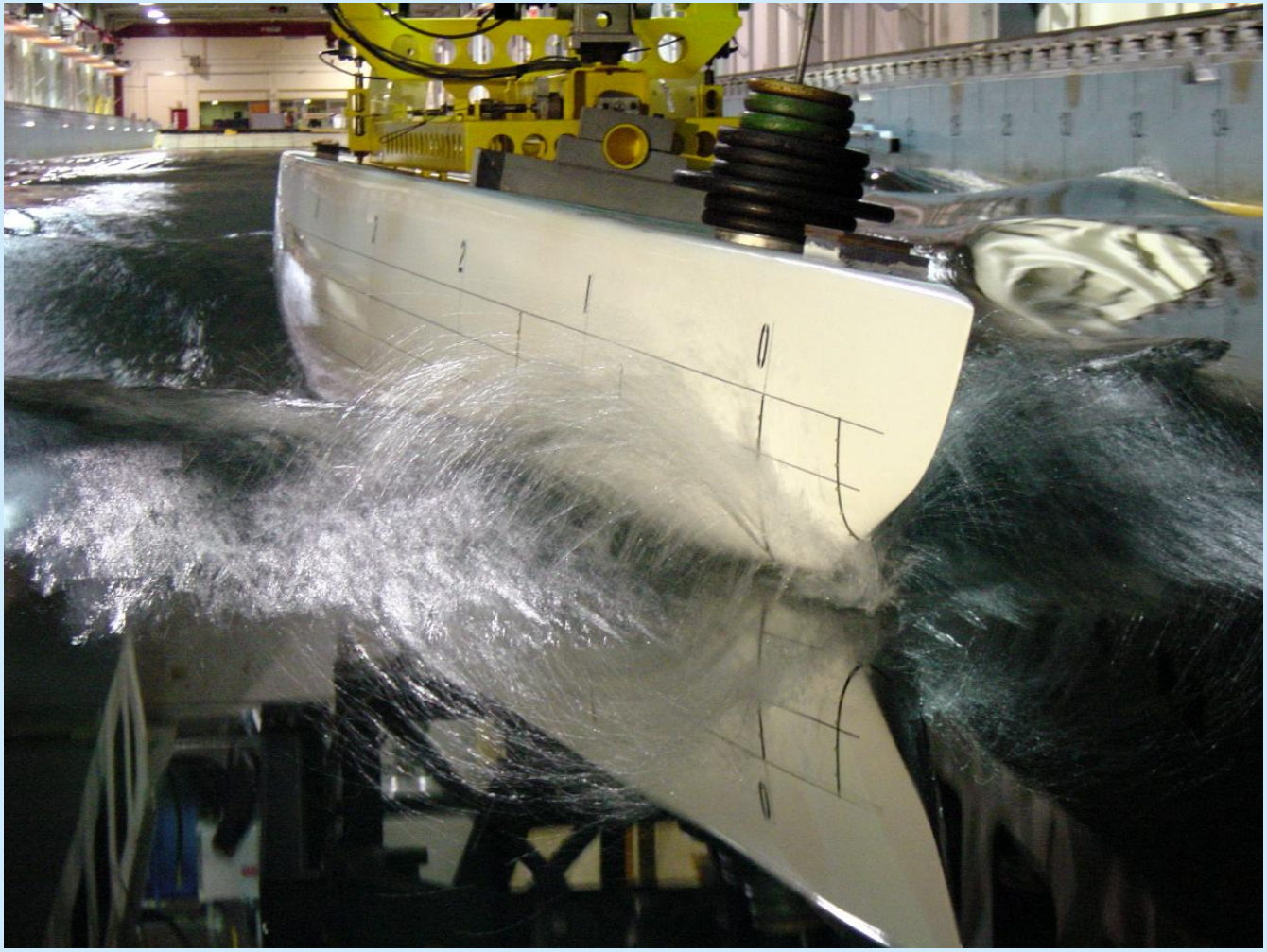
Hibernia



Ice Tank Carriage



Yacht



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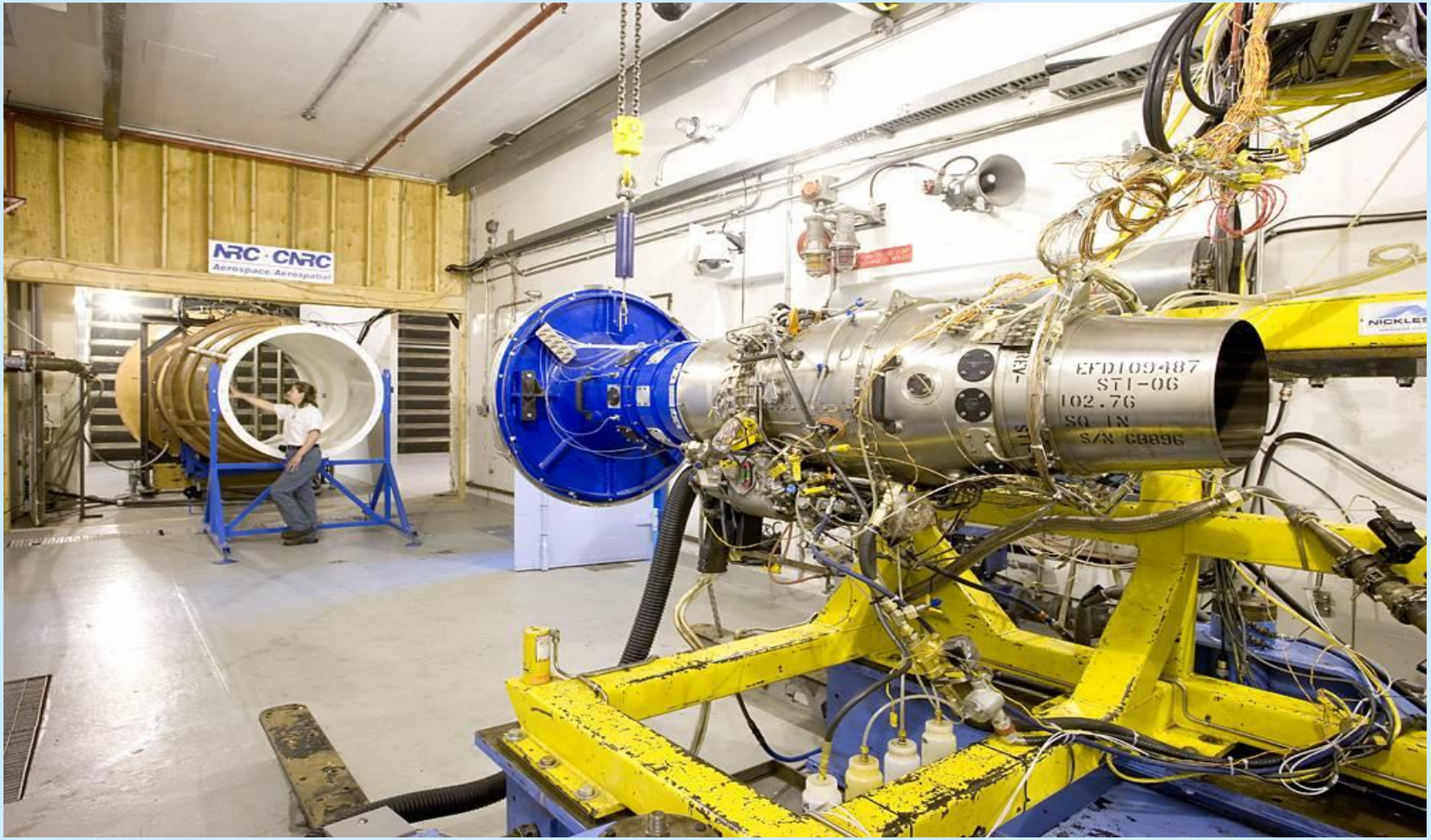
Turbofan



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IAR Control Room

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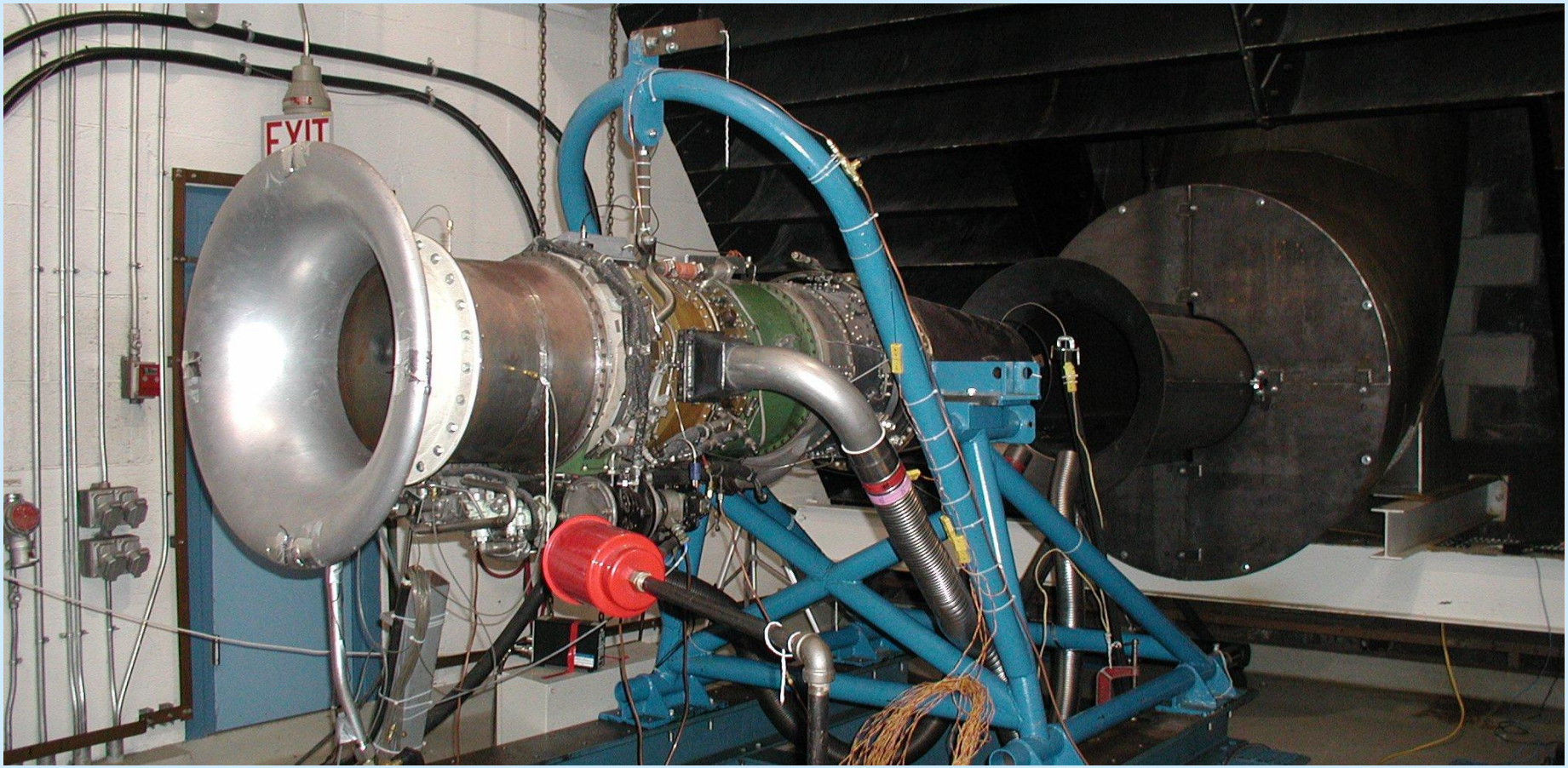
CF700 turbofan, data fusion development



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Framework for Scientists

- **Objective: build a software framework that supports some of the activities and processes of a research organization:**
  - Software tool integration
  - Workflow specification
  - Information management
- **An 'IDE' for scientific software tools**

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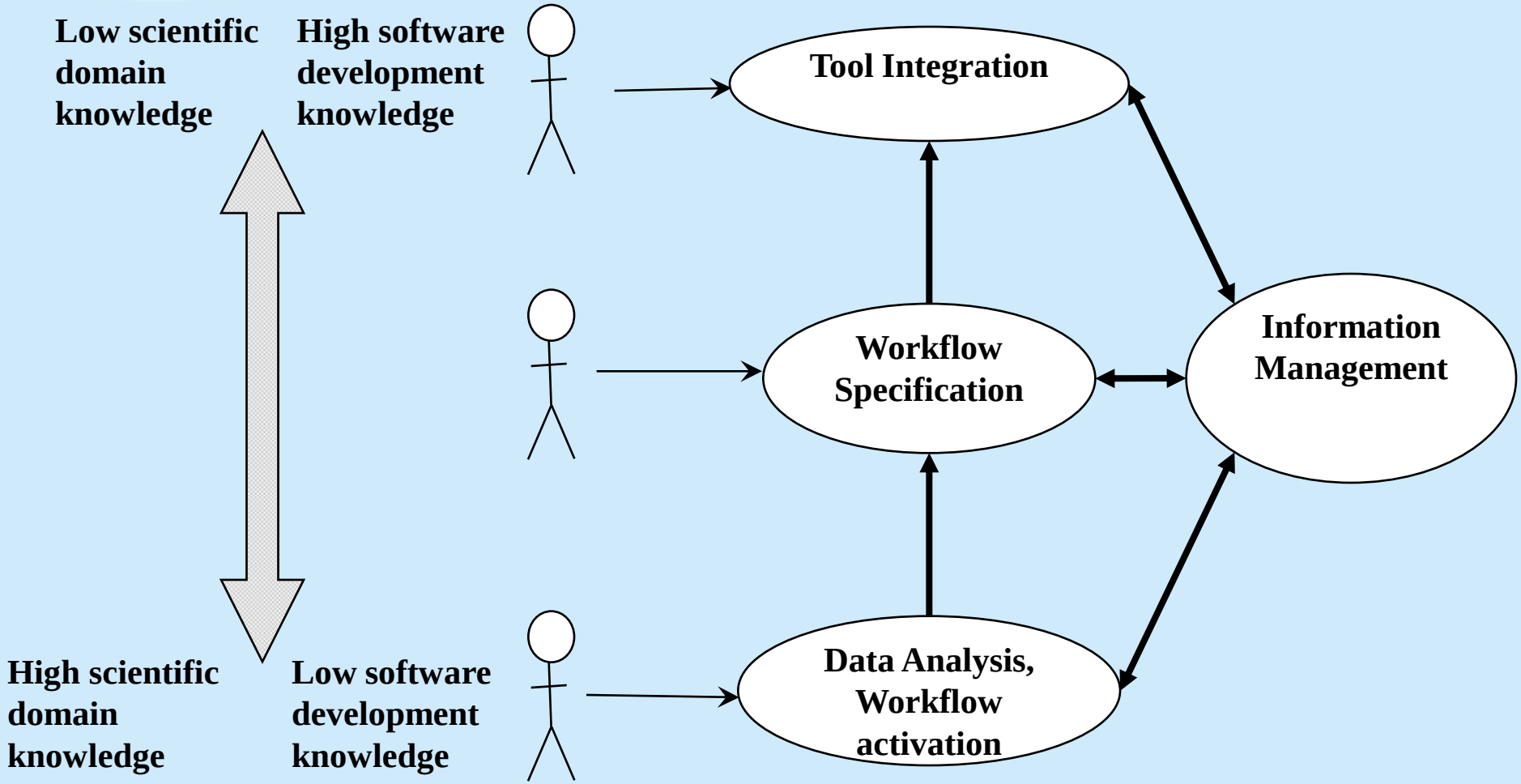
Goals of the Framework

- **Integration of the off-the-shelf software tools**
  - Common means for accessing different tools
  - Integration and interoperability between applications
- **Automate the workflows of the organization**
  - Identify and automate the standard activities and processes
  - Customization of the processes as needed
- **Technology refresh**
  - but bring along the legacy software
- **Improved data and information management**
  - Managing data: archiving, searching, provenance
  - Full configuration management
  - Reproducible

Software related activities

- **Data analysis activities**
  - Gathering, cleaning, transforming, reporting
  - Knowledge discovery from data
- **Tool integration**
  - Programmatic interfaces
  - Wrapping, adapting and extending applications
  - Data transfer between applications
- **Workflow specification**
  - Organize and execute the data analysis tasks in the proper sequence
  - Develop processes organizations use during analysis
- **Information and data management**
  - Archiving data, managing the archived data
  - Configuration Management

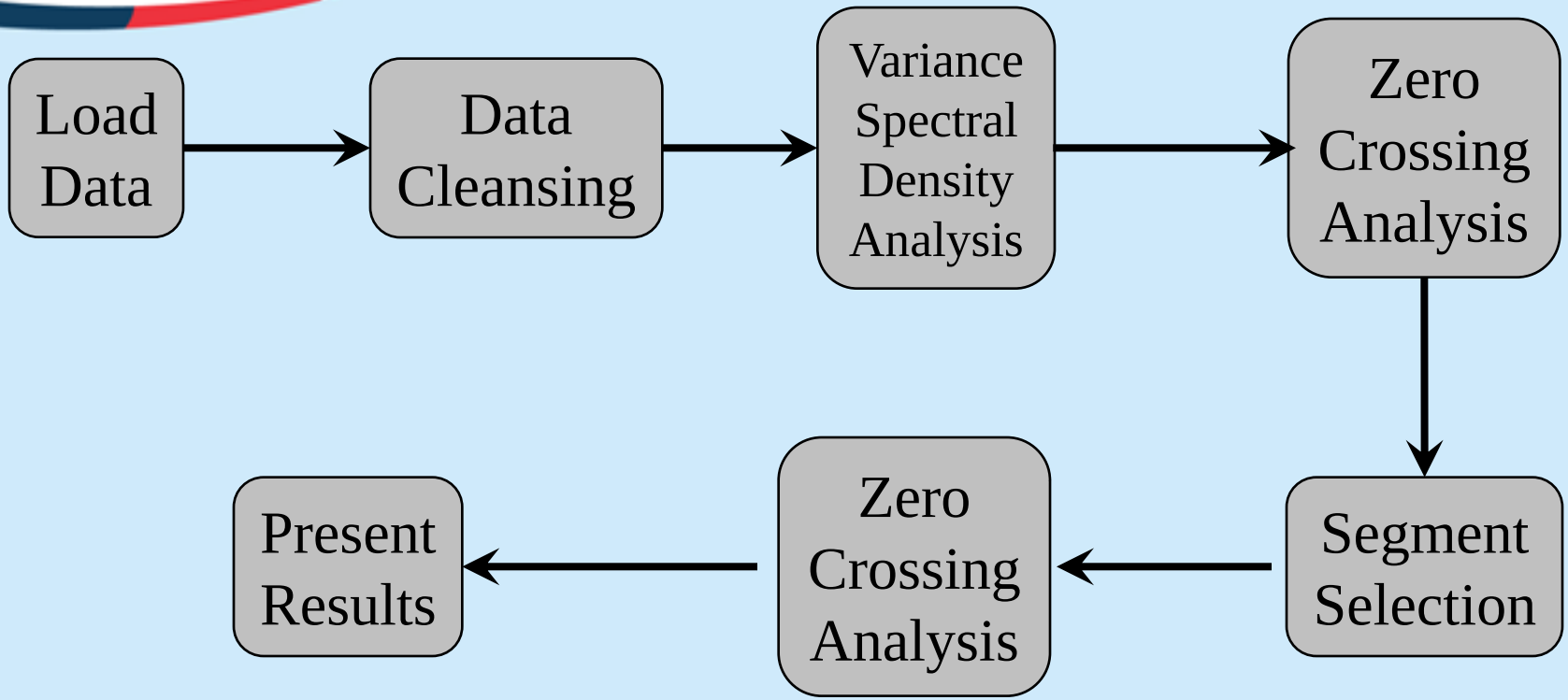
Organizational activities

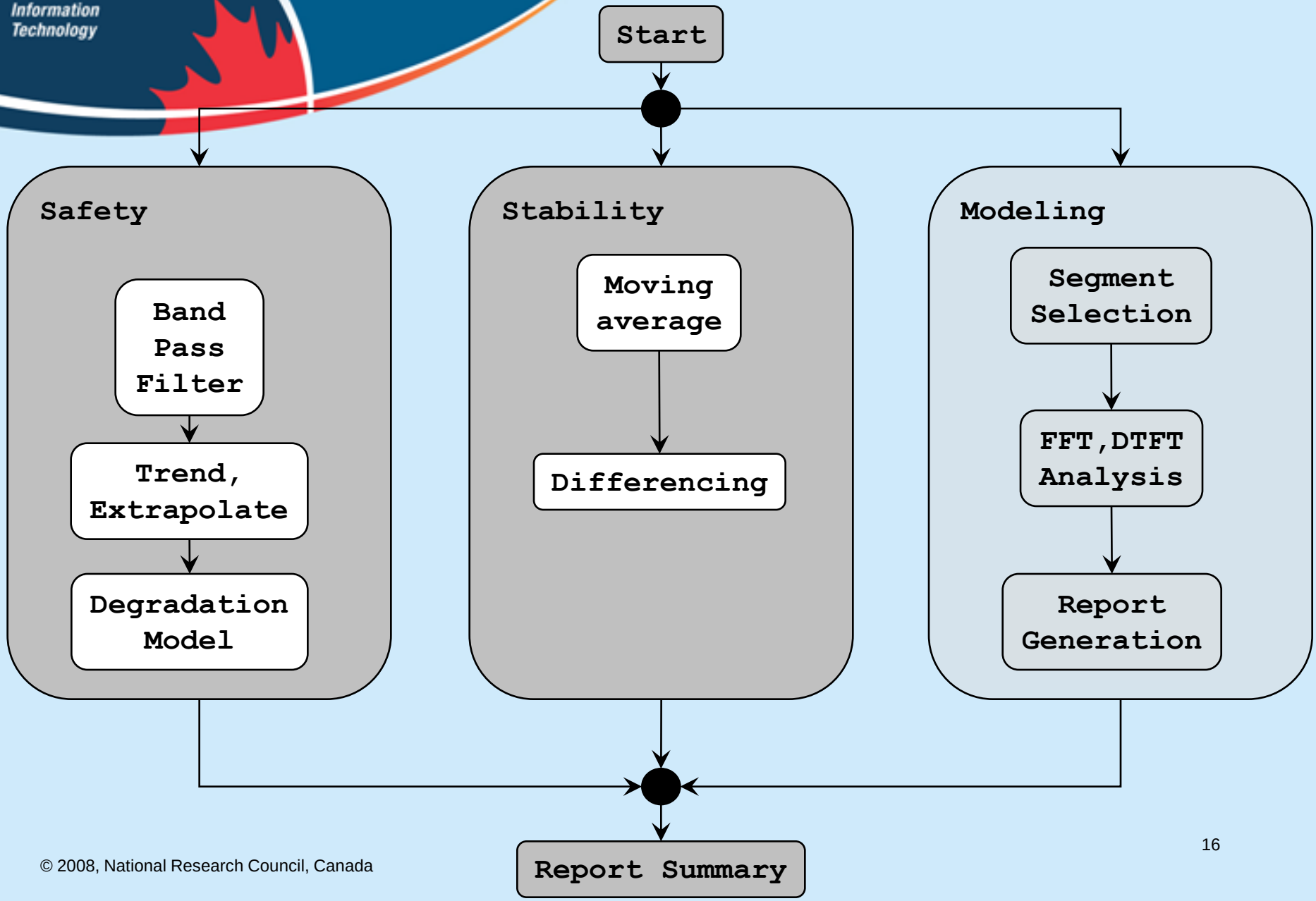


Scientific Workflows

- **Workflow: Movement of documents and/or tasks through a work process (Wikipedia)**
  - Structuring of tasks
  - Order and synchronization of tasks
  - Well established in business (BPEL)
- **Scientific workflows**
  - Throughput of data through various algorithms, applications and services
  - Use of multiple interconnected tools
  - Use of multiple data formats

Example workflow:
Regular wave calibration





End-user

- **End-users are the scientists and technicians**
- **Many cannot (or will not) write any software**
- **Must be able to:**
  - Find, select, configure workflows
  - Explore the data using different software tools
  - Manage the data generated, software versions used
- **For the end-user:**
  - Static variation points, presented in a dynamically generated GUI
  - Tools for entering data structures in variation points
  - Organizing and navigating workflow invocations

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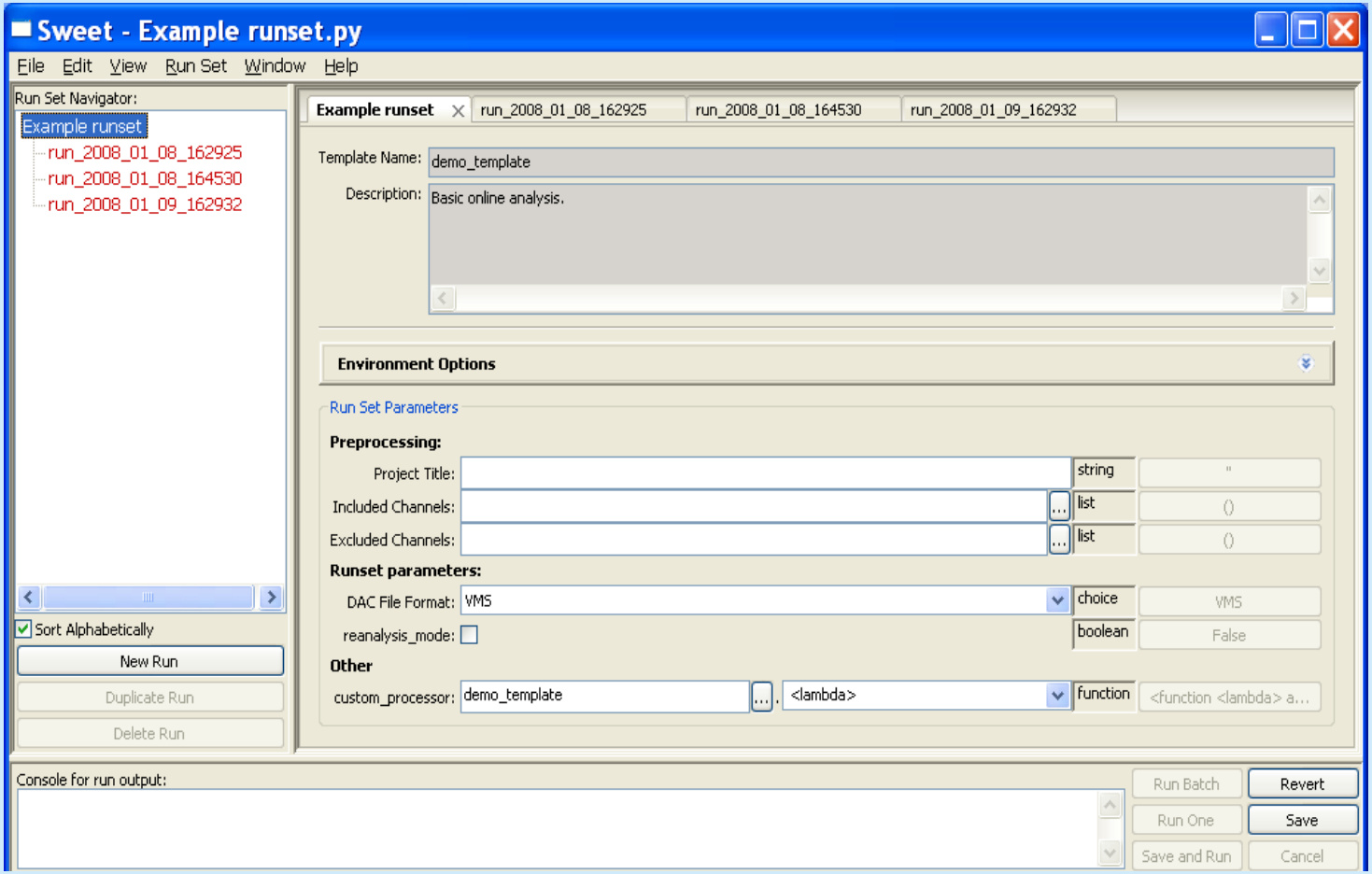
End-user

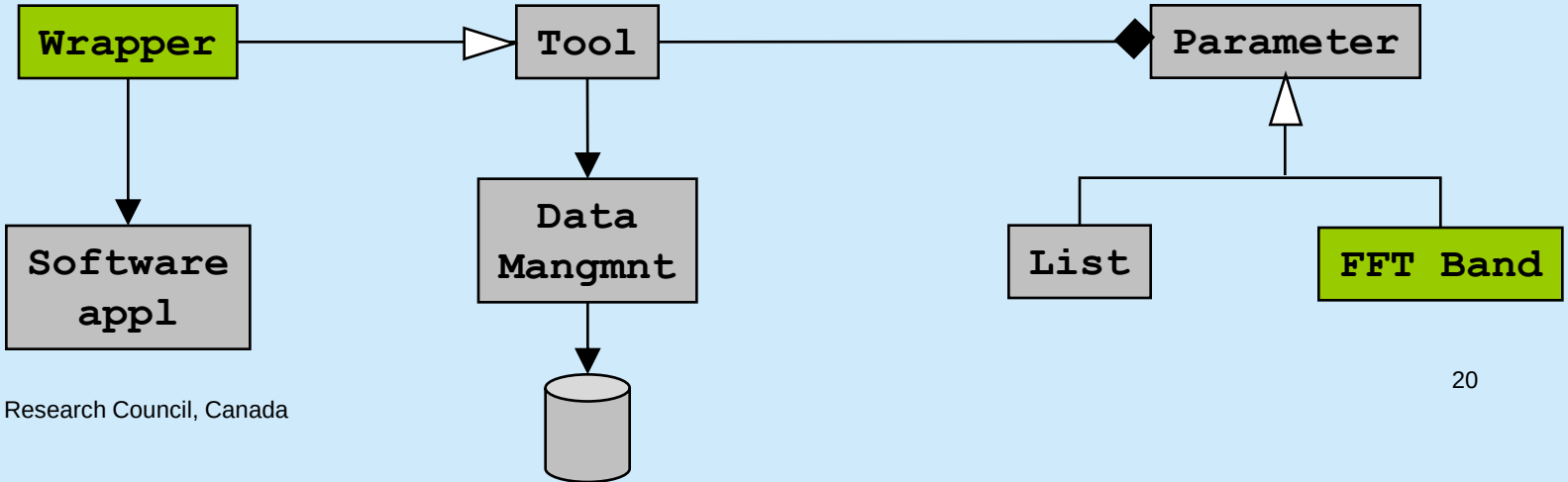


Workflow developer

- **Some software development knowledge required**
- **Accessible to knowledgeable end-users**
  - Written as simple scripts that invoke services
  - Full programming language capability (Python)
  - Tools gathered into a 'toolbox' and dynamically linked to the services are available to workflow developer
  - Workflows are represented as parameterized templates where the parameters represent the variation points
  - Metadata is used to describe the templates and dynamically build the GUI

Tool integrater

- **Develop wrappers for the tools**
- ***Warning: Nerds at work!***
  - Tools dynamically added to toolbox - can be customized to a domain
  - Parameter types understood by end-user - custom widgets can be added
  - Data management utilities
  - Logging, exception handling, other utilities...



Observations

- **Dynamically generated GUI's very successful.**
- **A great deal of the success was due to the strong software engineering group within IOT. IAR is more challenging**
- **Many of the standard software engineering techniques were introduced into the organization and were quickly adopted.**
- **Quick payback by automating easy tasks**

- **Questions?**

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Representing workflows

- **Automation**
  - Represent the workflow in an executable form
  - Engine for executing workflow
  - Invocation of software tools
  - Integration and interoperability of software
- **Re-usability**
  - Similar processes used in many experiments
  - Ease of customization by domain experts
  - Repository for storing, retrieving and managing workflow representations
- **Ease of creation**
  - Minimal software programming knowledge required

Template Metadata

```
def do(self,
        dac_file_name = "",
        target_wave_height = 0.0,
        target_wave_period = 0.0,
        analysis_segment_start_time = 0.0,
        analysis_segment_end_time = 0.0,
        best_cycles_segment_start_time = 0.0,
        best_cycles_segment_end_time = 0.0):

    """
    * dac_file_name = DAC File Name
    * target_wave_height = Target Wave Height (m)
    * target_wave_period = Target Wave Period (s)
    * analysis_segment_start_time = Analysis Segment Start Time (s)
    *
    *   Start time of the segment of wave probe data to be analyzed.
    *   Enter a time to bypass ramping. Enter 0 to interactively
    *   the segment.
    * analysis_segment_end_time = Analysis Segment End Time (s)
    *
    *   End time of the segment of wave probe data to be analyzed.
    *   Enter a time to bypass ramping. Enter 0 to interactively
    *   the segment.
    * best_cycles_segment_start_time = Best Cycles Segment Start Time (s)
    *
    *   Start time of the best cycles segment from a previous attempt.
    *   Used only for repeat attempts. Set to 0 for first attempt.
    * best_cycles_segment_end_time = Best Cycles Segment End Time (s)
    *
    *   End time of the best cycles segment from a previous attempt.
    *   Used only for repeat attempts. Set to 0 for first attempt.
    """
```

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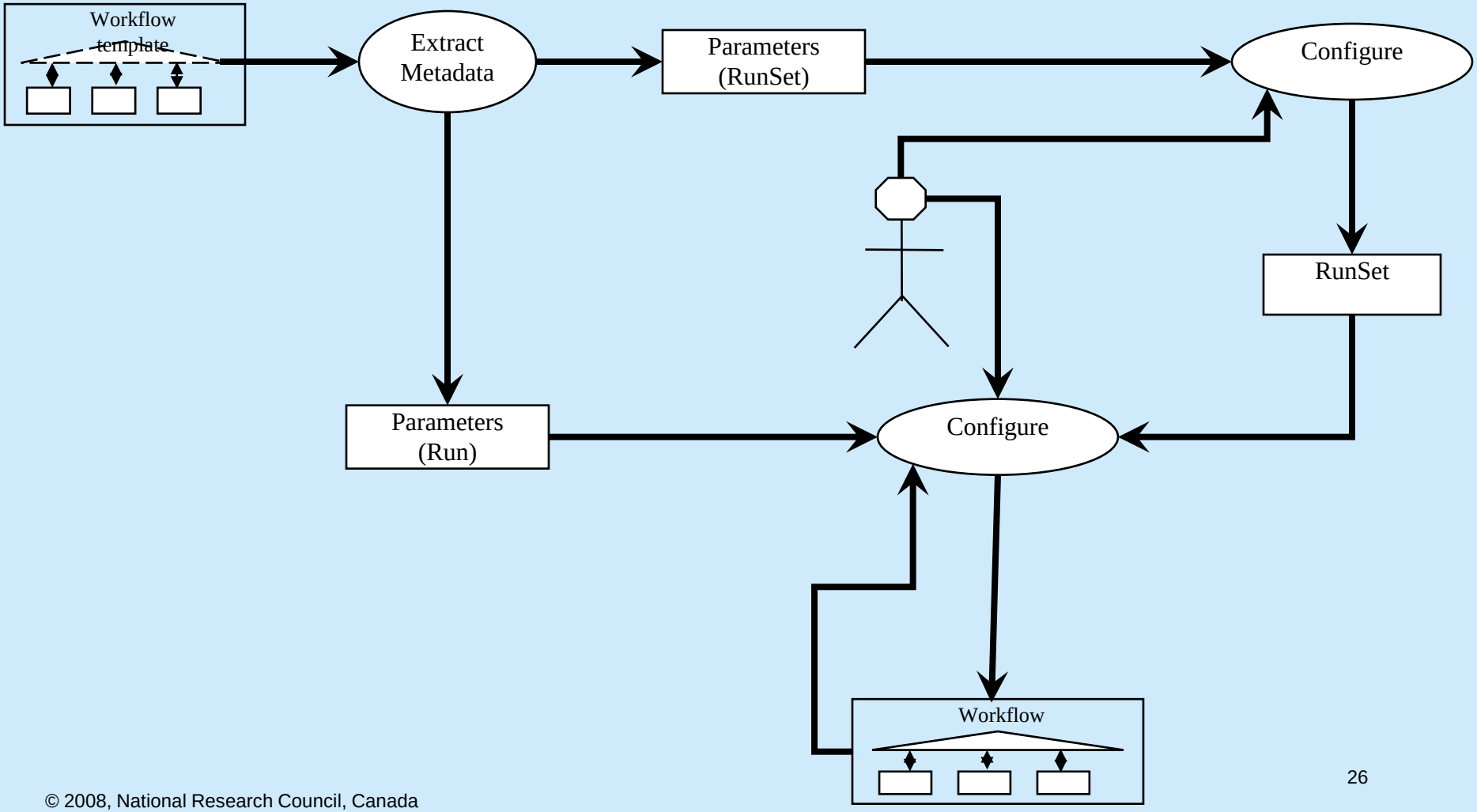
Managing RunSets and Runs



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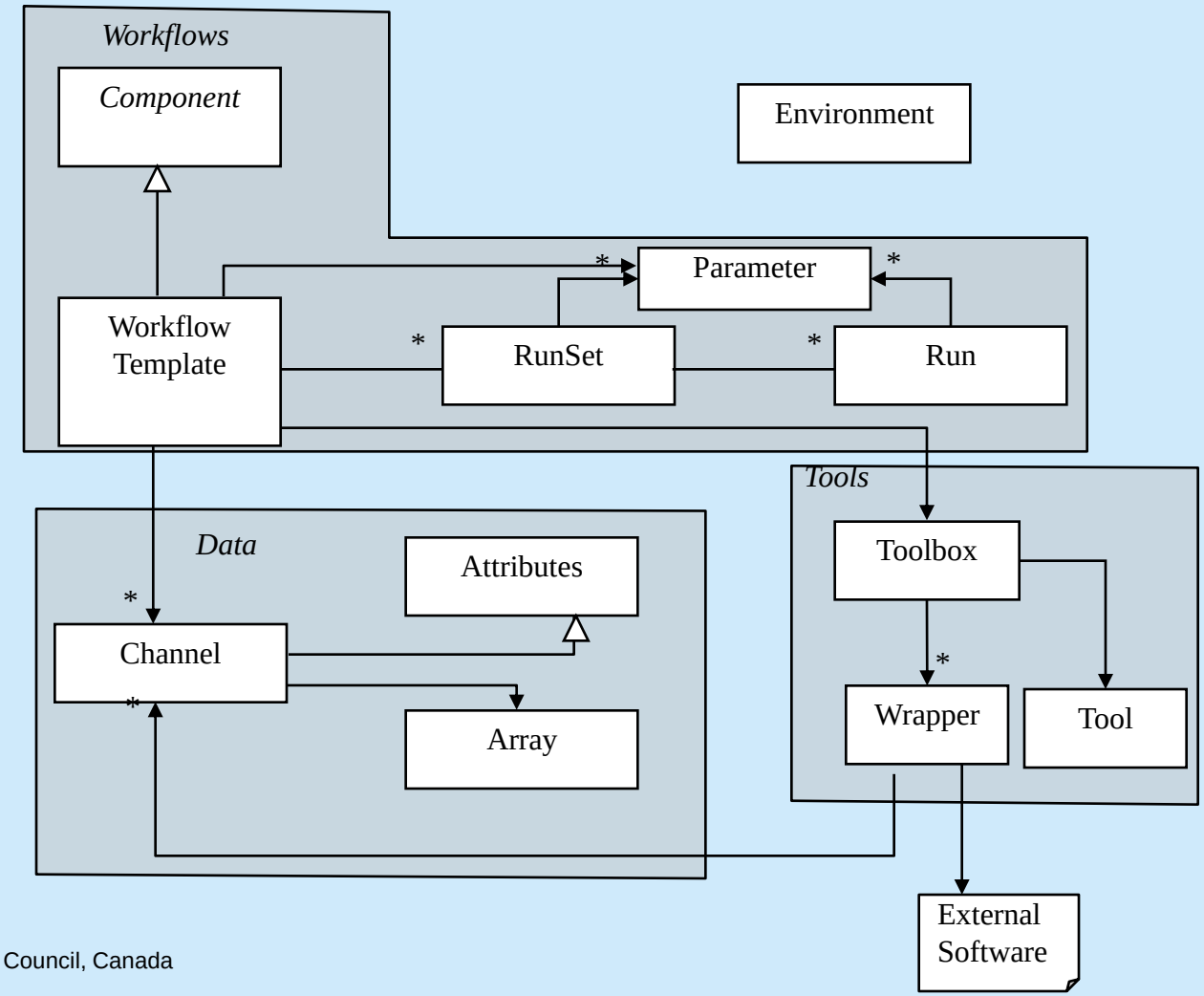
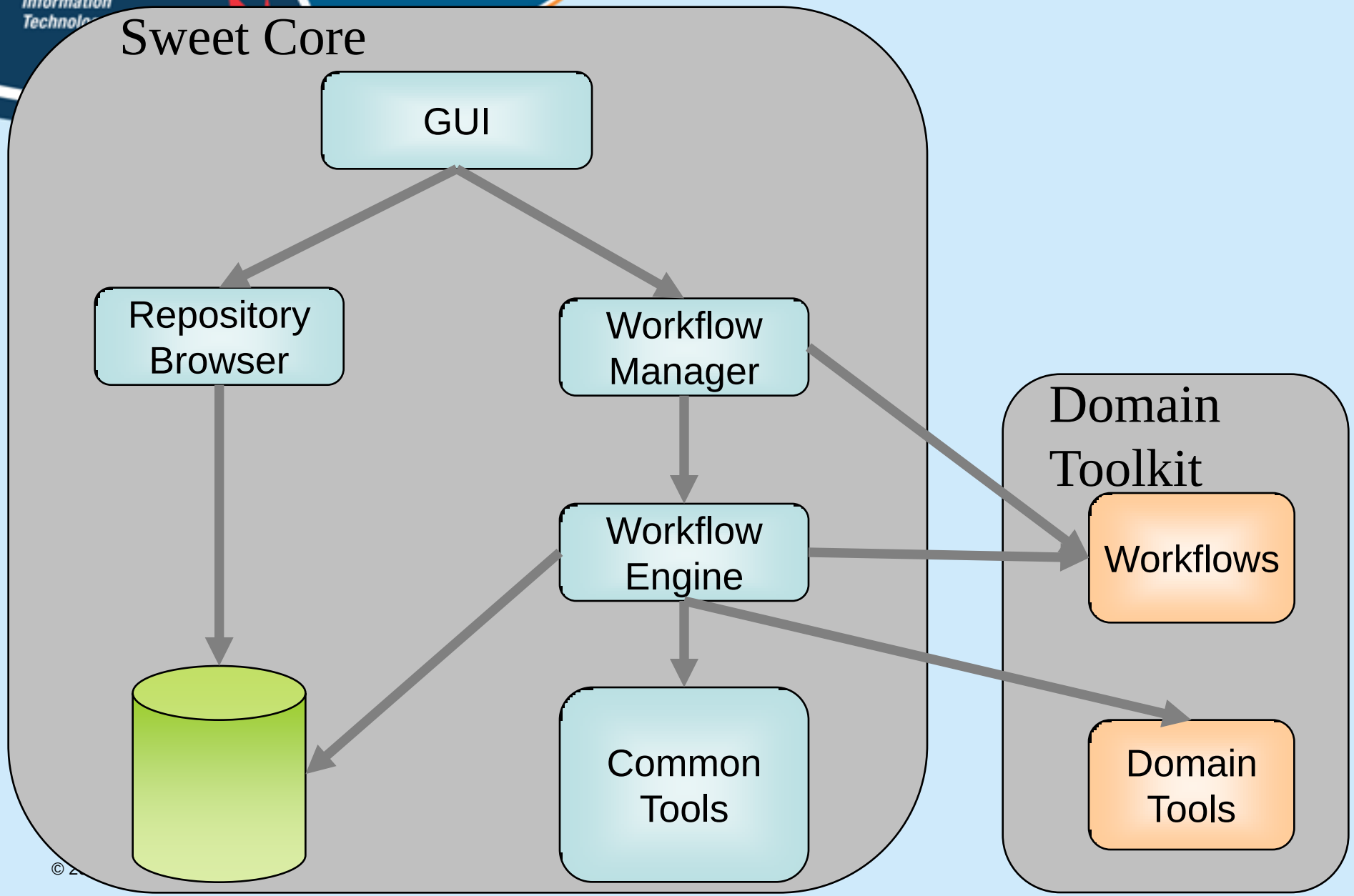
Sweet Design




Sweet Core
GUI
Repository Browser
Workflow Manager
Workflow Engine
Common Tools
Domain Toolkit
Workflows
Domain Tools