Hands-on with Research Data Management in Chemistry
-
Day 2 - afternoon

Alain Borel

Francesco Varrato

Research Data Team, EPFL Library

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Introduction

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Data as a snapshot *VS* data as a workflow:

- Not only “doing something with the data” but also knowing where the data is
- The state of your data will change along the workflow (raw, processed, sensitive, merged, open, etc.)

Hands-on for the whole afternoon

Hands-on 1: Data Workflow

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1. Discussion: RDM self-evaluation 2nd round
2. Select a data workflow to work with
3. Draw your data workflow
4. Feedback (in pairs)
5. Work and Q&A

1. Discussion: RDM self-evaluation 2nd round

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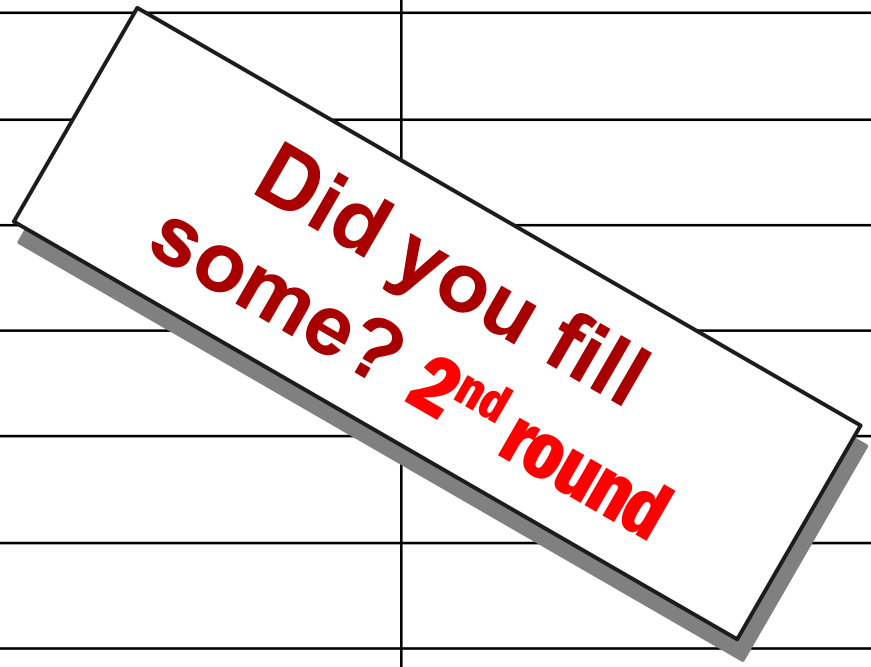
go.epfl.ch/**rdm-self**

Your results

Data actions in your project

ACTIVITIES	COLLEAGUE / PARTNER	TOOLS	TO-DO
FUNDING PLANNING			
CREATION			
ETHICAL CLEARANCE			
ACQUISITION			
STORING			
ANALYSIS			
LEGAL CLEARANCE			
SHARING			
PUBLISHING			
ARCHIVING			



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2. Select a data workflow to work with

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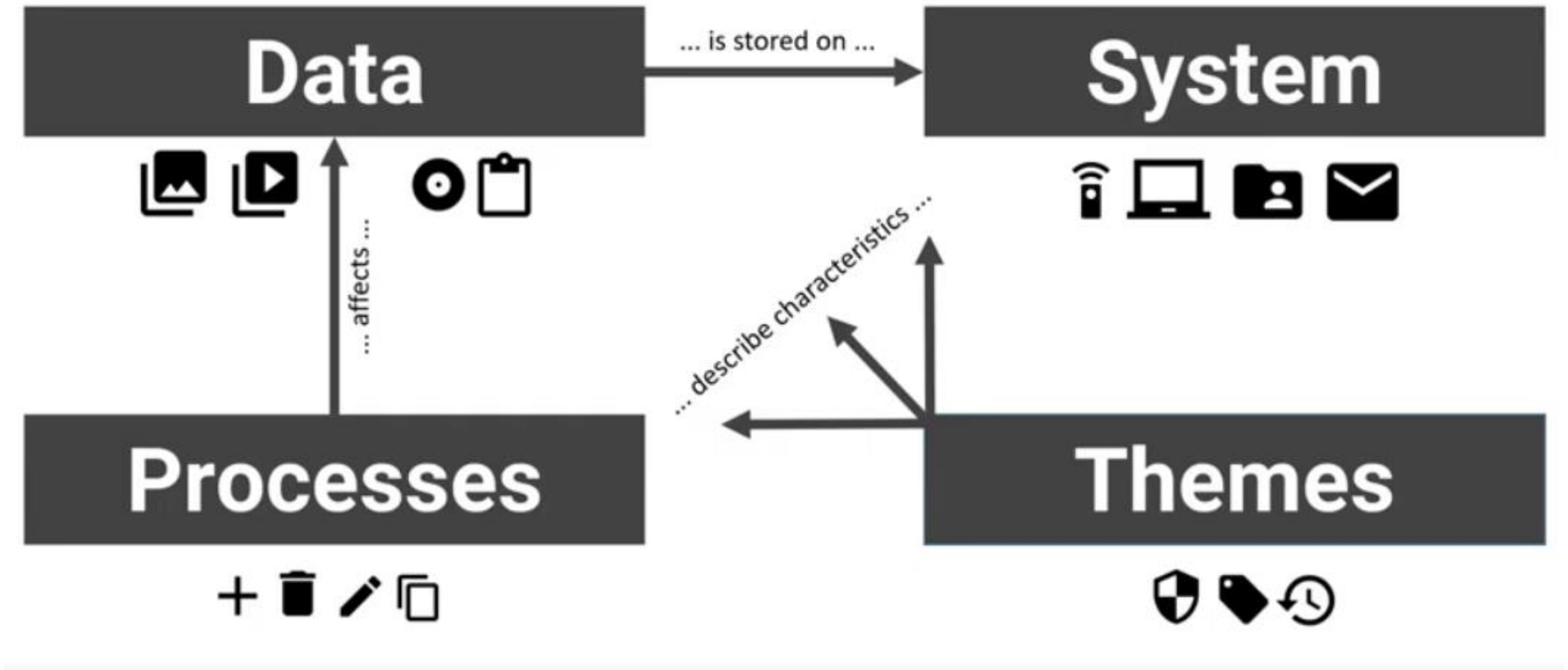
Criteria to choose the data workflow:

- If possible, choose a data workflow that includes:
  - data creation
  - data backup
  - data processing
  - data analysis
  - data sharing
  - data publication
- The more elaborated your workflow is, the more interesting the insights you will get from it
- It's OK if you don't know how everything will work at all stages of the workflow yet

[10'] Choose an actual process from your current PhD project and describe your data workflow with natural language

Example 1

Describe **data**, **processes,** and **systems** that are part of data workflows, categorized by theme



Source: Data Flow Tool Kit (https://dataflowtoolkit.dk/)

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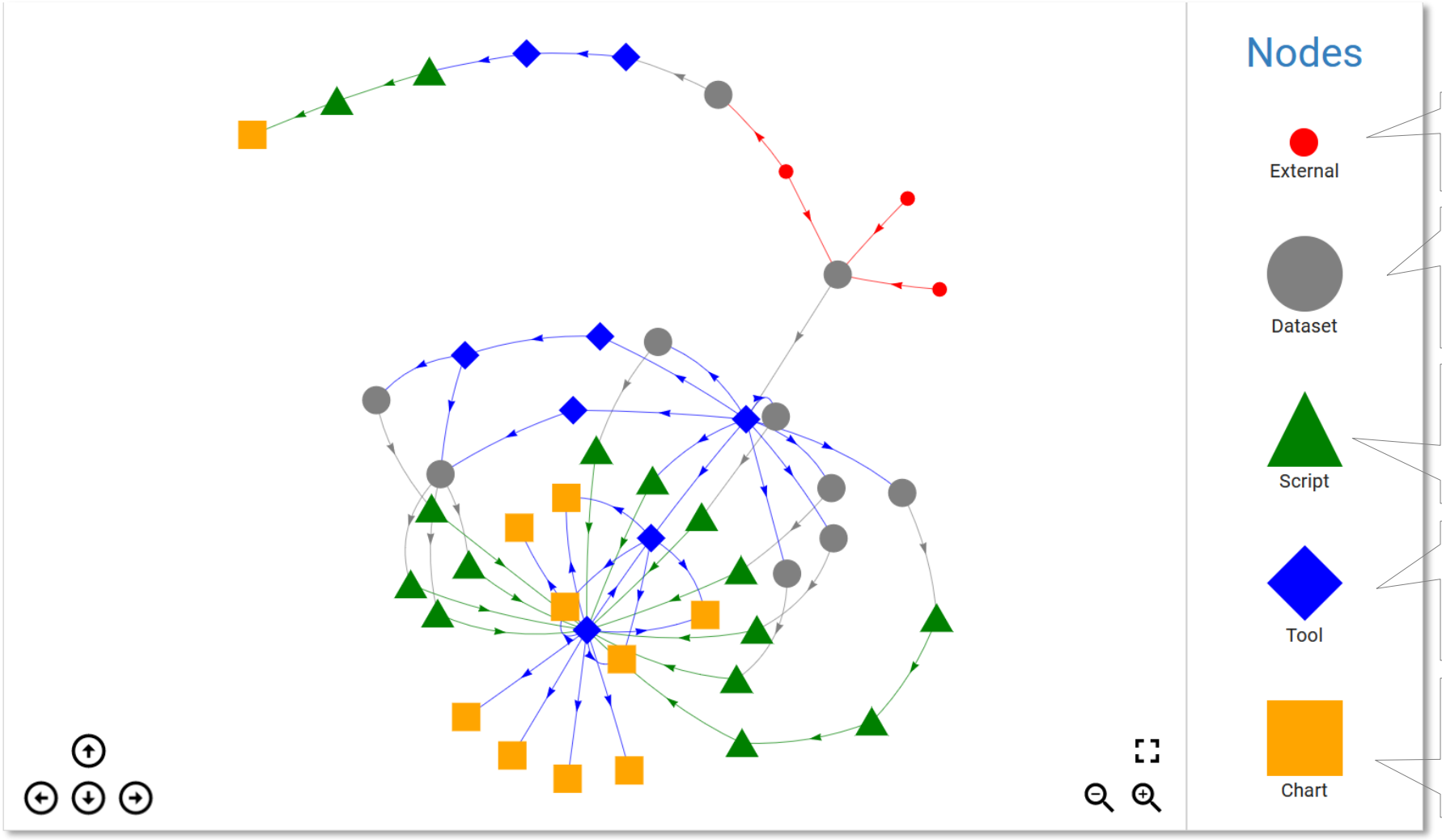
Example 2



Source: https://paperstack.uchicago.edu/paperdetails/5941869f1bd40fd44db0024a?server=https%3A%2F%2Fpaperstack.uchicago.edu
Related to article published in Chemistry of Materials 29, 2485 (2017)

Many others in Qresp.org's explorer section
(open source on Qresp GitHub repository)

3. Draw your data workflow

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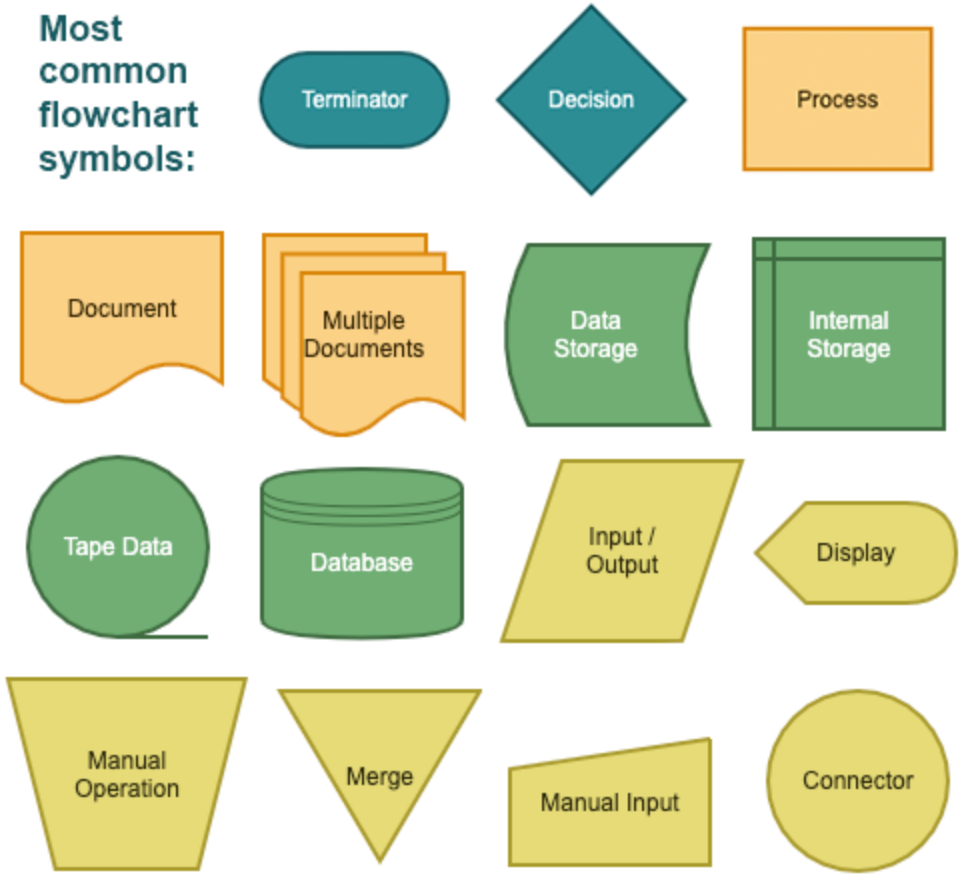
Conventions to draw a workflow schema:



Workflow drawing tools :

- www.drawio.com or similar
- MS Powerpoint or similar
- Pen and paper (digitally shared)
- ...

[45'] Draft your data workflow schema

Followed by peer-review

4. Feedback (in pairs)

Time for feedback ! You will be paired with another PhD student in a breakout room.

- **Exchange** workflow schemas

- **[10']** **Read** (i.e. try to understand) each other's schema and give feedback to your colleague.

  Look at these aspects:

  - **Comprehensiveness**: *are there steps that seem to be missing?*
  - **Understandability**: *as an "outsider" what don't you understand?*
  - **Thematic view**: *what aspects could be added to improve the schema or the workflow itself?*

- **[2' x workflow]** **Discuss** each workflow you reviewed

Next steps

1. Insert the feedback you have received today to improve your data workflow

2. Deposit your data workflow **via Moodle before** Wednesday **Mar. 12, 11:59:59 PM**

During *Day 3*, you will work with your data workflow again to work on the final report.

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5. Work and Q&A

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You can take your time to work on your workflow

&

Ask us any question