Universität Rostock Traditio et Innovatio

UNIVERSITEIT STELLENBOSCH UNIVERSITY

FAIRDOM

SEMS simulation experiment management system

SED-ML support in JWS Online

Using SED-ML and COMBINE archives to reproduce Simulation Results

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combine 2016

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Running a simulation by reading a paper

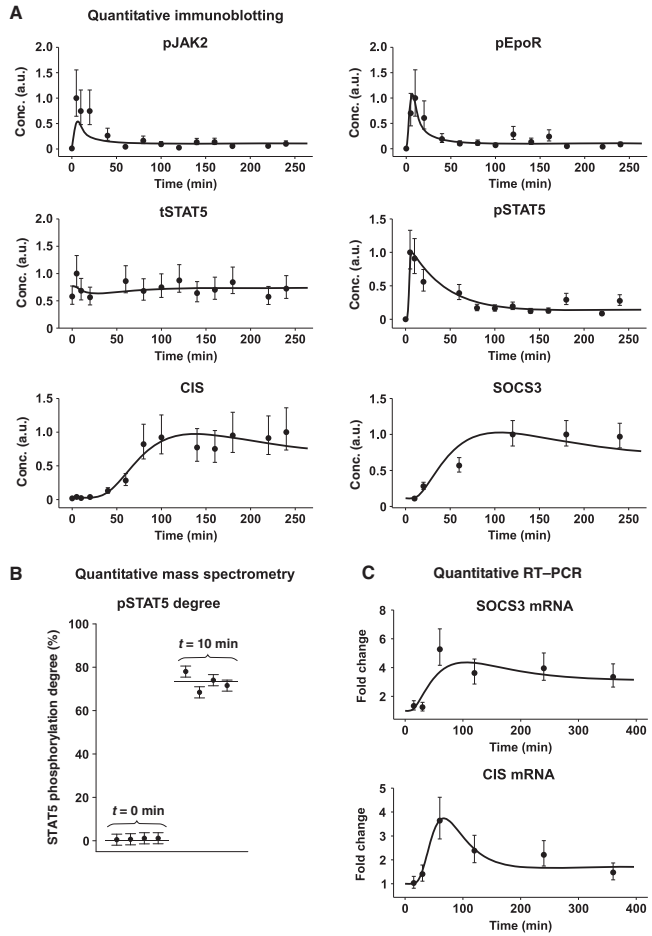


Figure 3 Model calibration with experimental data of JAK2-STAT5 signaling obtained by different experimental techniques. For all experiments, primary CFU-E cells were starved and stimulated with 5 U/ml Epo. At the indicated time points, samples were subjected to (**A**) quantitative immunoblotting, (**B**) mass spectrometry analysis or (**C**) qRT–PCR. Experimental data (black circles) with estimated standard errors and trajectories of the best fit (solid lines) are represented. Mass spectrometry data represent replicates of four independent experiments. (For additional experimental data used for the model calibration, see Figure 4 and Supplementary Figures S11–S23.) In total, 531 data points representing 18 different experimental conditions were used for model calibration. Source data is available for this figure at www.nature.com/msb.

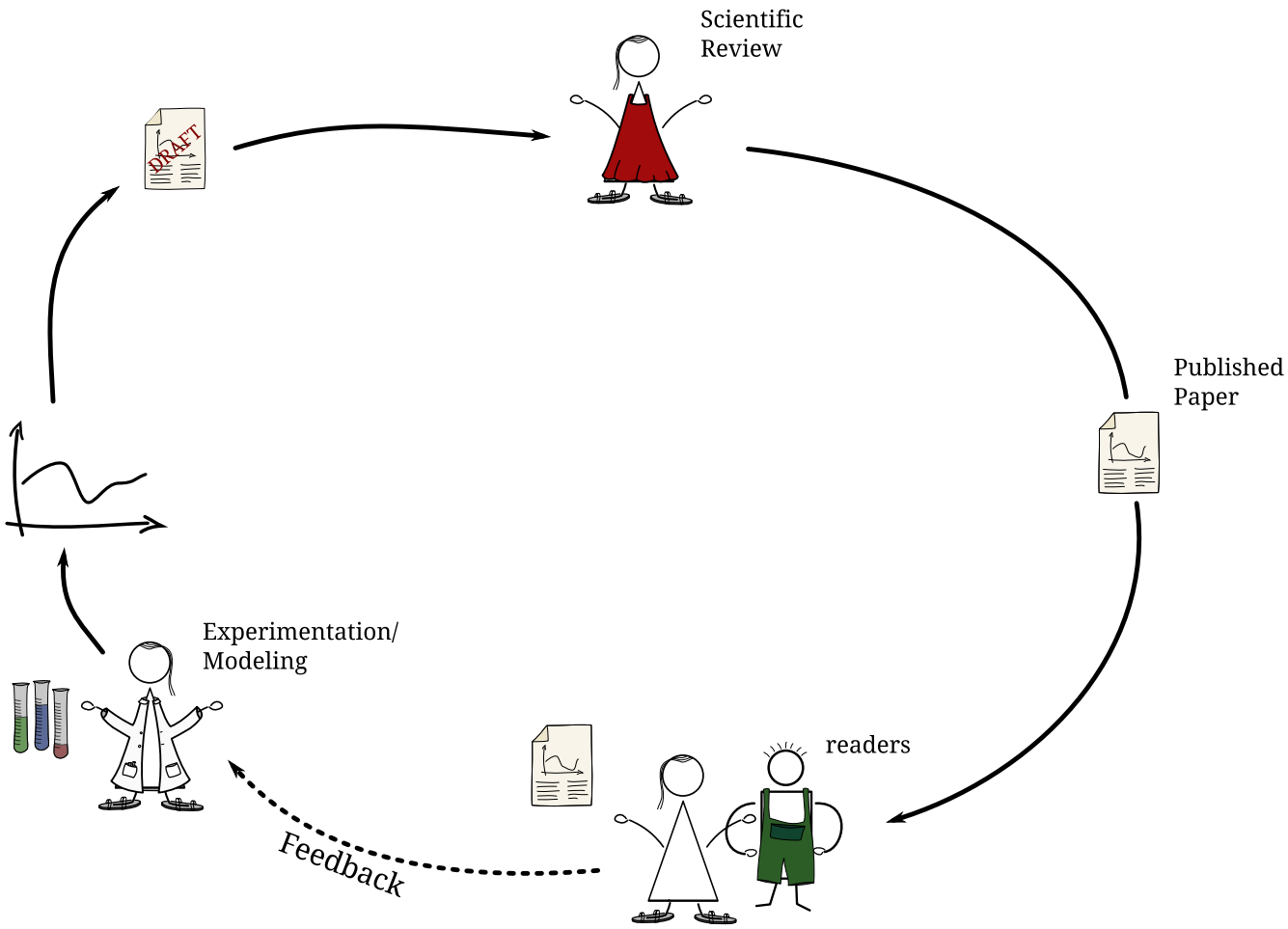
Reproducing Figures
Demonstrating the Magic

Demo shows experiment database in JWS Online in action.
Try it out here:

`https://jjj.bio.vu.nl/models/experiments/bachmann2011/simulate`

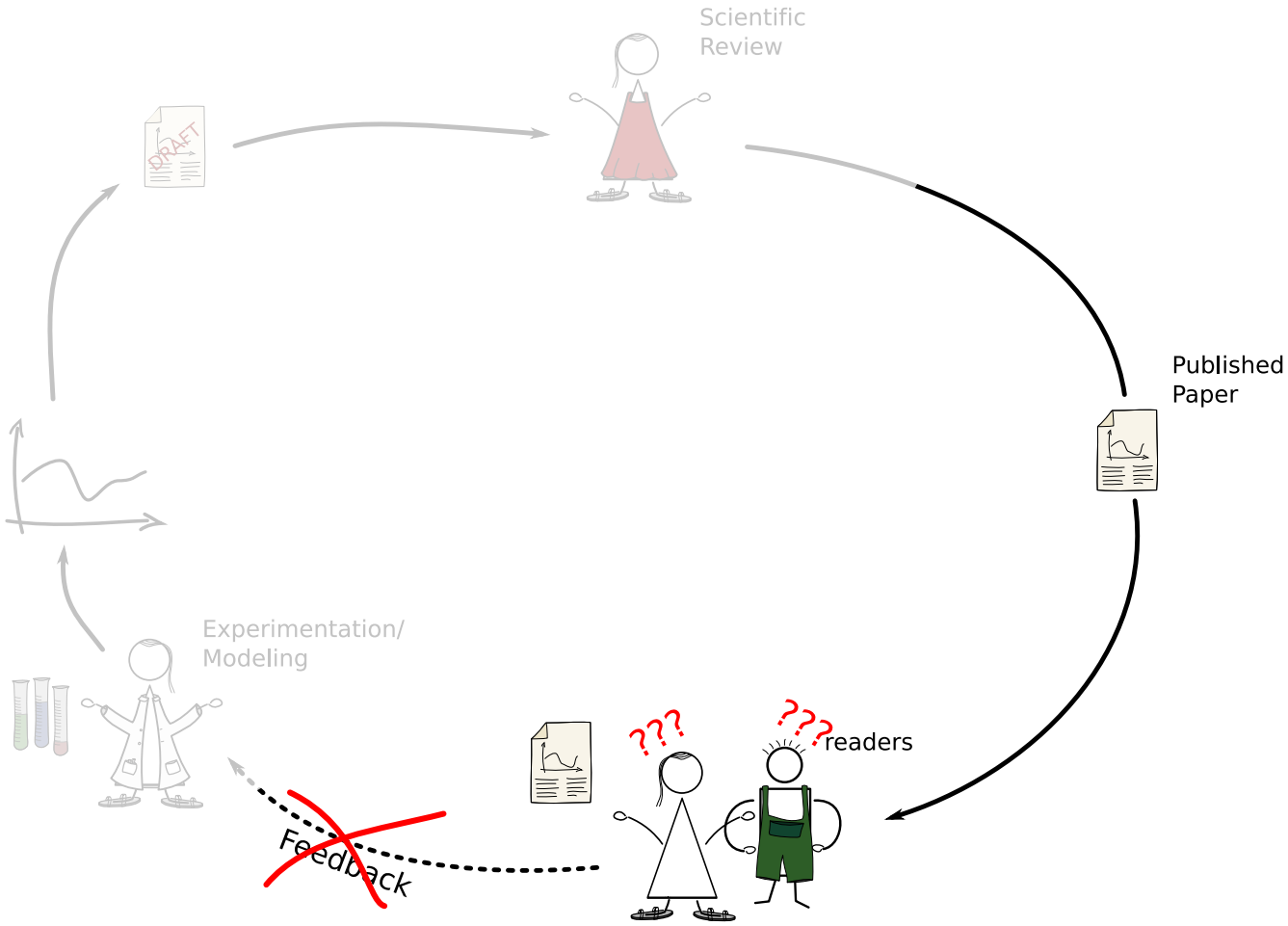
About JWS Online

and the circle of reproducibility



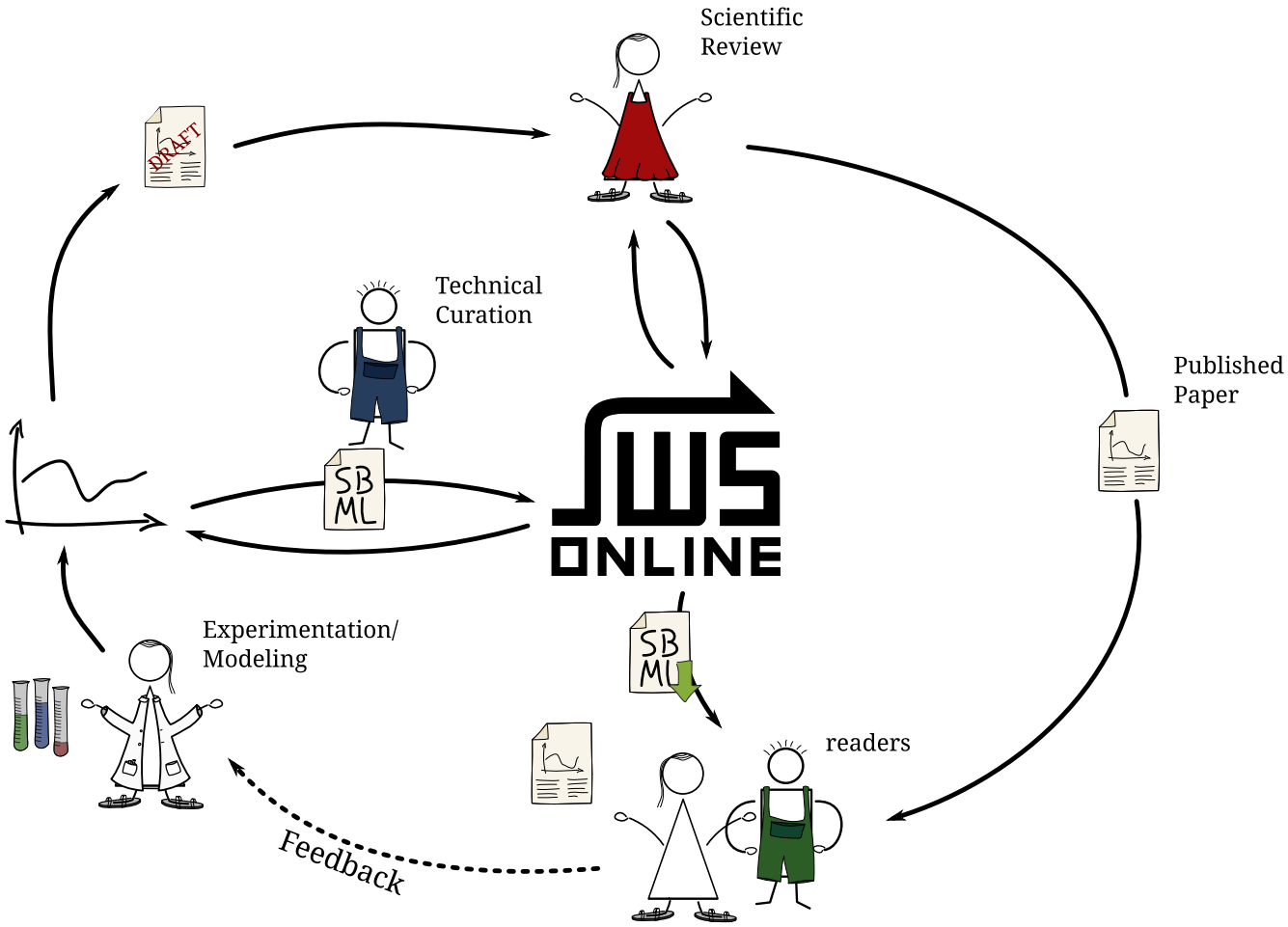
About JWS Online

and the circle of reproducibility



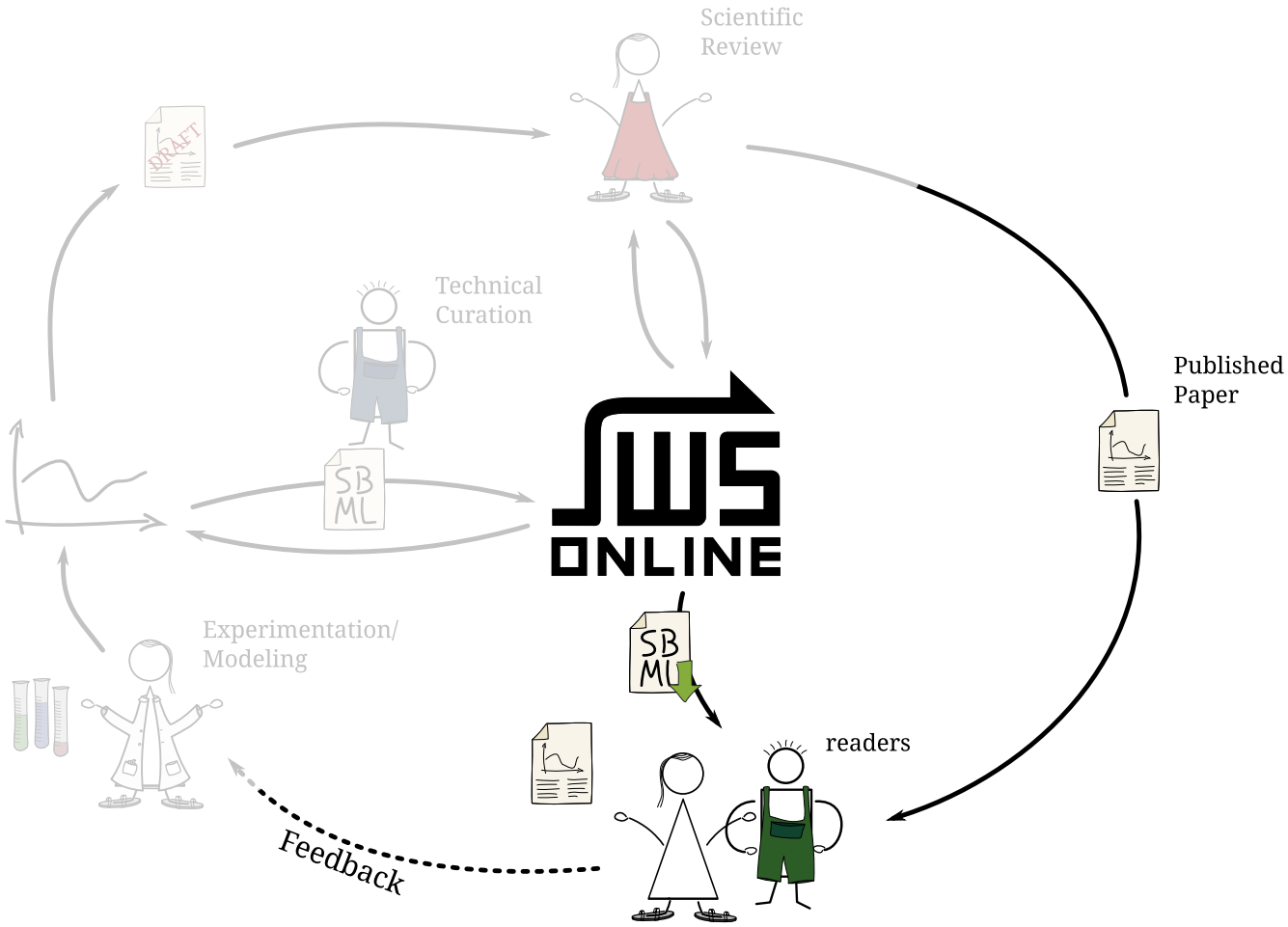
About JWS Online

a platform for curation and sharing



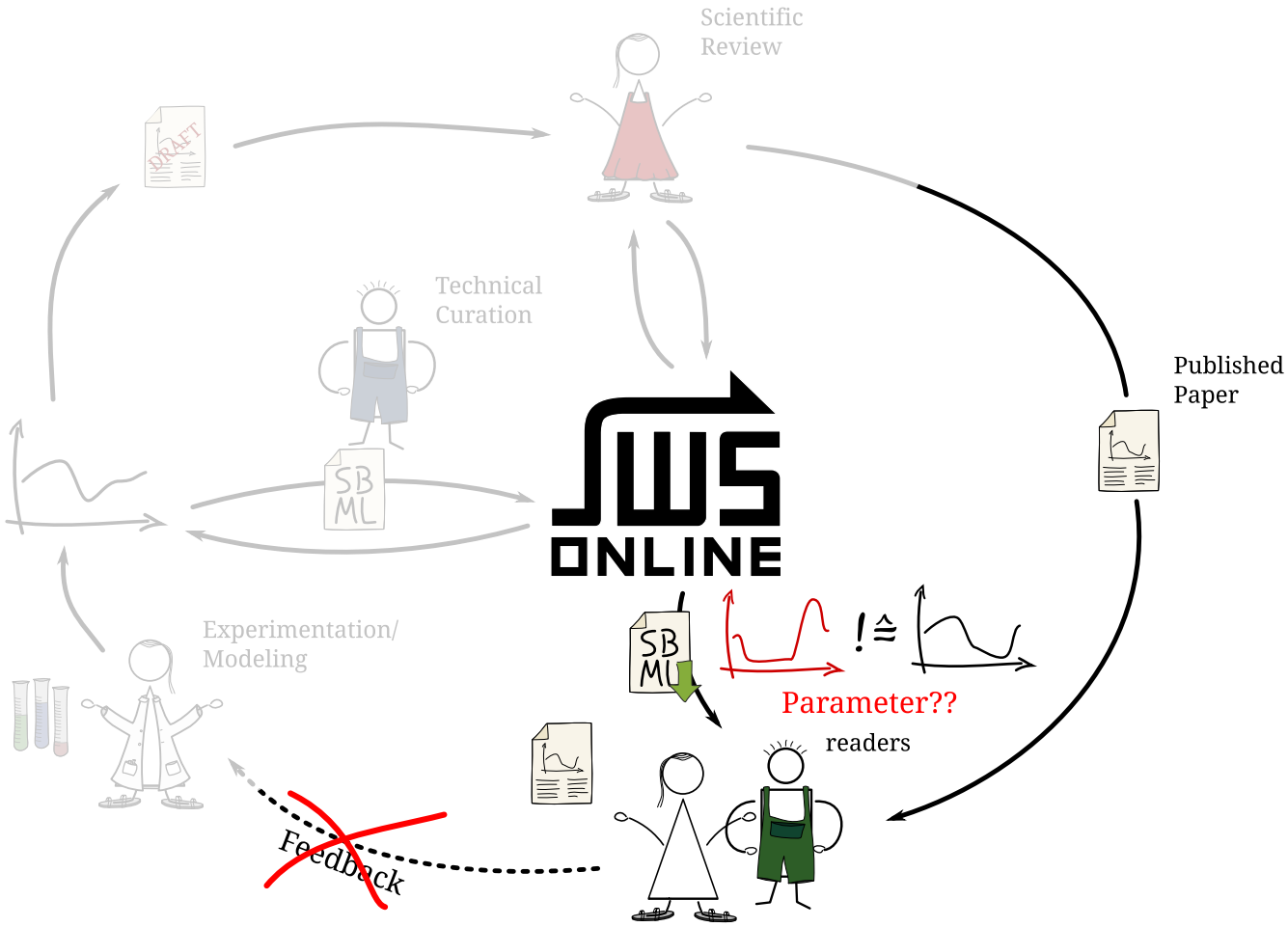
About JWS Online

a database for kinetic models



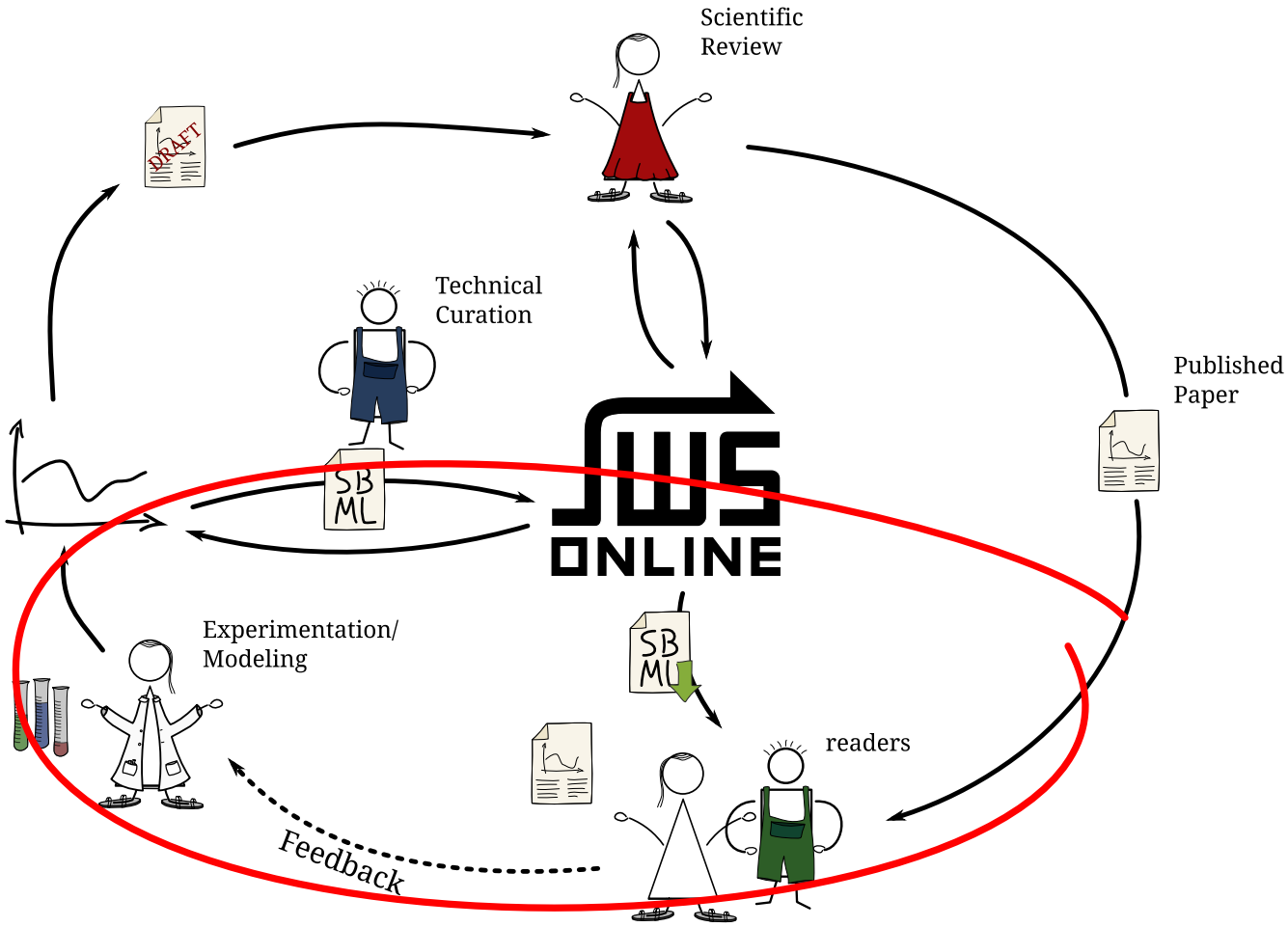
About JWS Online

a database for kinetic models

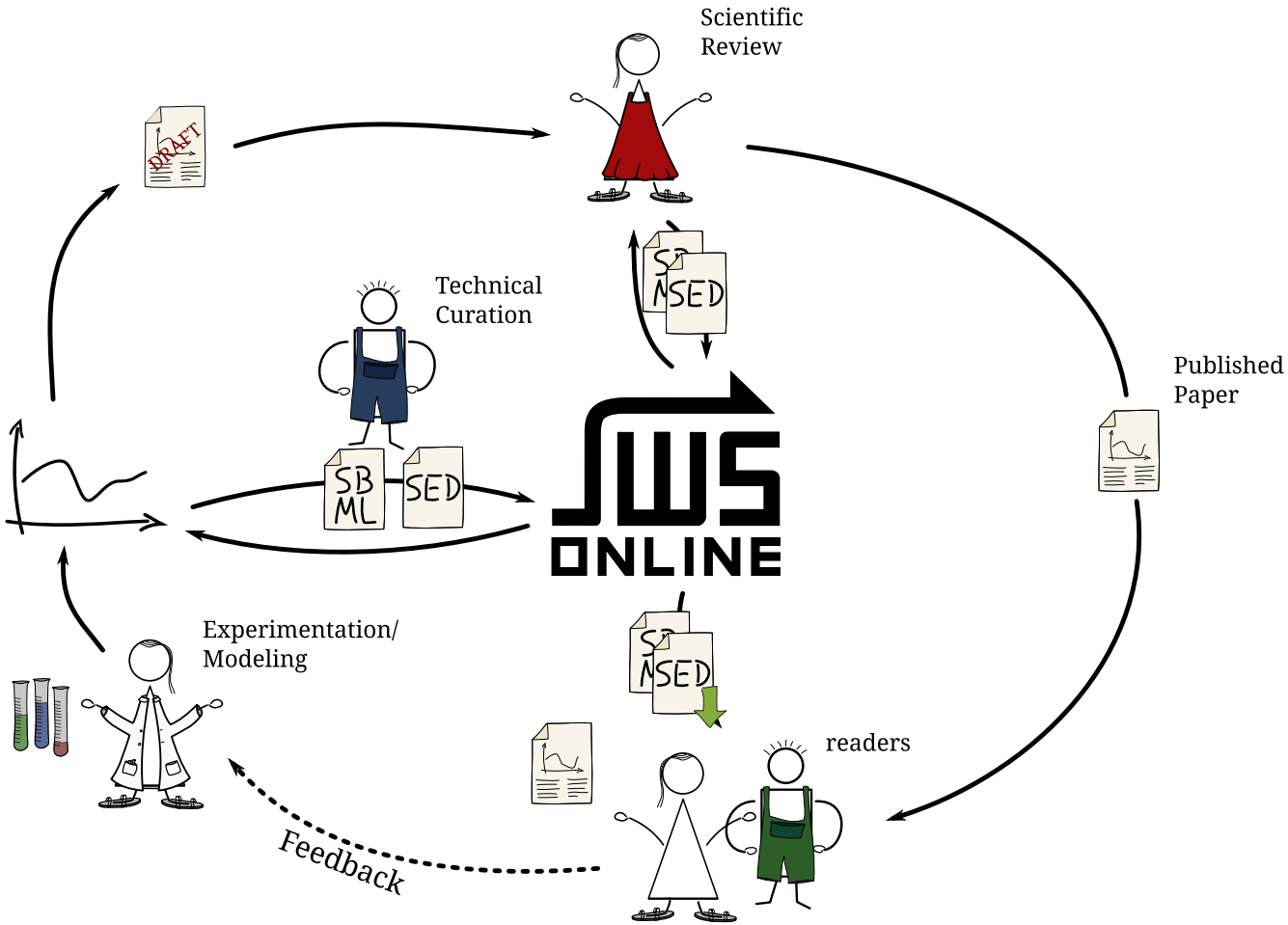


About JWS Online

and what we wanted to advance



About JWS Online
and SED-ML support

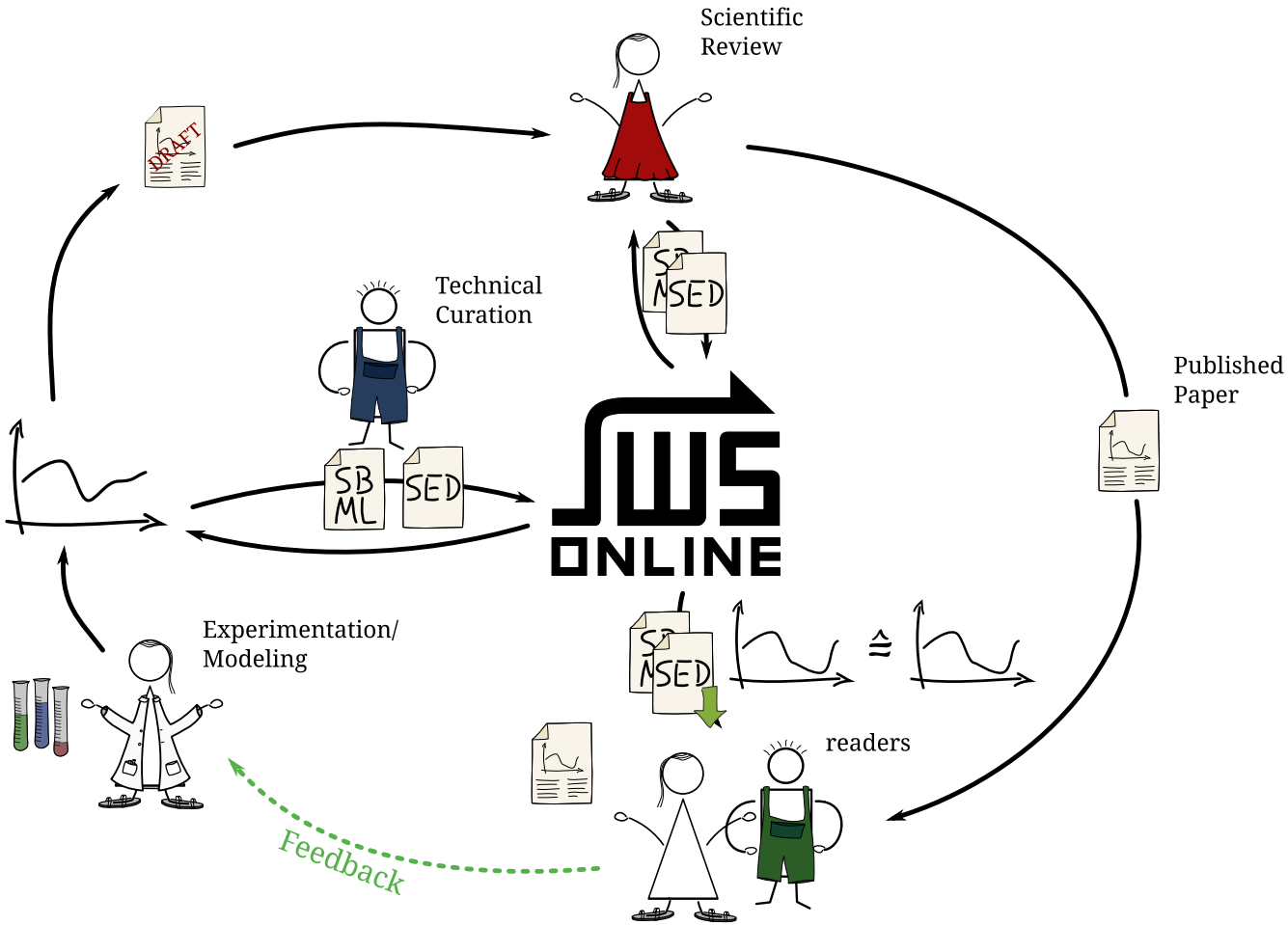


Introducing SED-ML
to JWS Online

- **S**imulation **E**xperiment **D**escription – **M**arkup **L**anguage
  `http://identifiers.org/combine.specifications/sed-ml.level-1.version-2`
- Enabling reproducible *in silico* experiments since 2007
- Sophisticated multi-model/multi-experiment setups
- Support for experimental data and post-processing

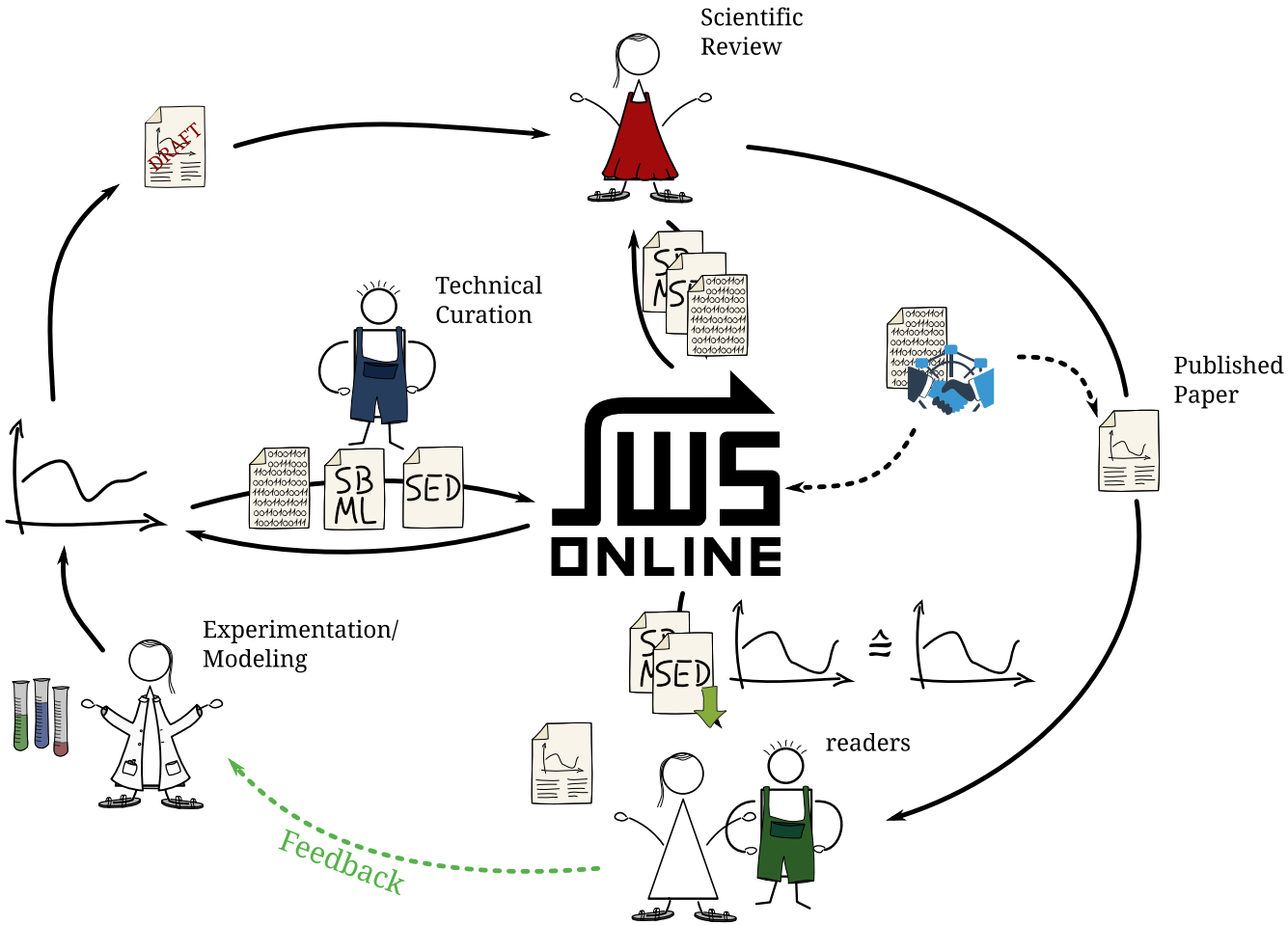
About JWS Online

and the single-click reproducibility

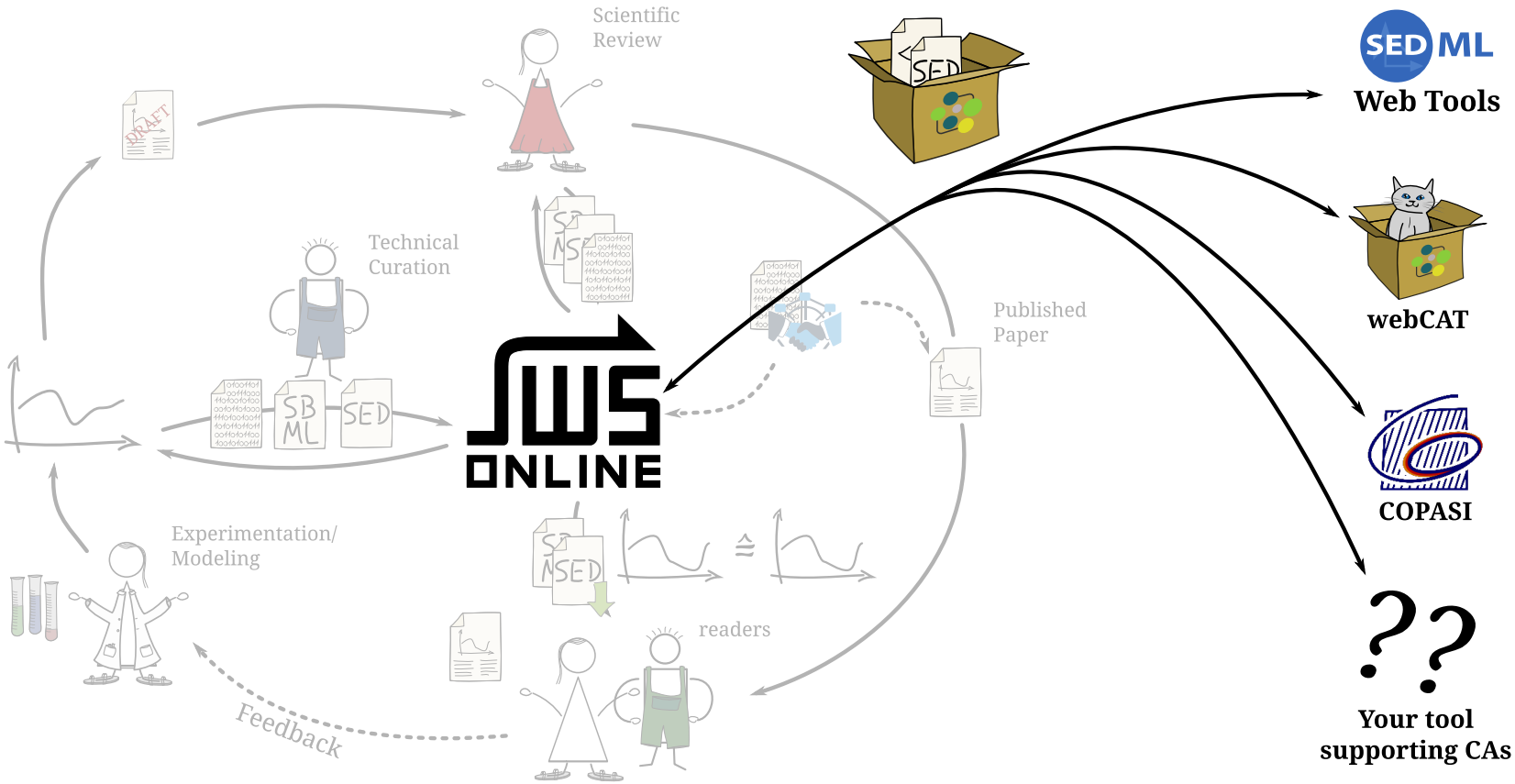


About JWS Online

and the single-click reproducibility



About JWS Online
and COMBINE Archive support



About COMBINE archives

one file to share them all

- Container format for bundling belonging to modeling or simulation experiment
- Enriched with meta information according to the *OMEX* standard
- Enable to bundle all necessary resources for reproduction
- `http://co.mbine.org/standards/omex`

Achievements
and all the other cool stuff

- Dockerized JWS Online
  `https://jws-docs.readthedocs.io/10_docker.html`
- Introduced a basic set of APIs into JWS Online
  `https://jws-docs.readthedocs.io/8_rest.html`
- Widely extended the handling of Manuscript meta information

- Implemented **SED-ML database** into JWS Online
  `https://jjj.bio.vu.nl/models/experiments/`
- Enabled import and export of **COMBINE Archives**
- Introduced **Reproduction of Simulation Experiments – by a single click**
  `https://jjj.bio.vu.nl/models/experiments/bachmann2011/simulate`

Limitations

and all the non-cool stuff

- Only Time-Course Simulations
- No Repeated-Tasks
- Excel Spreadsheets instead of NuML
- Only 2D Plots

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FAIRDOM

SEMS simulation experiment management system

That's it!

SEMS Task Force

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That's it!

Want to talk? Drop me a message!

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