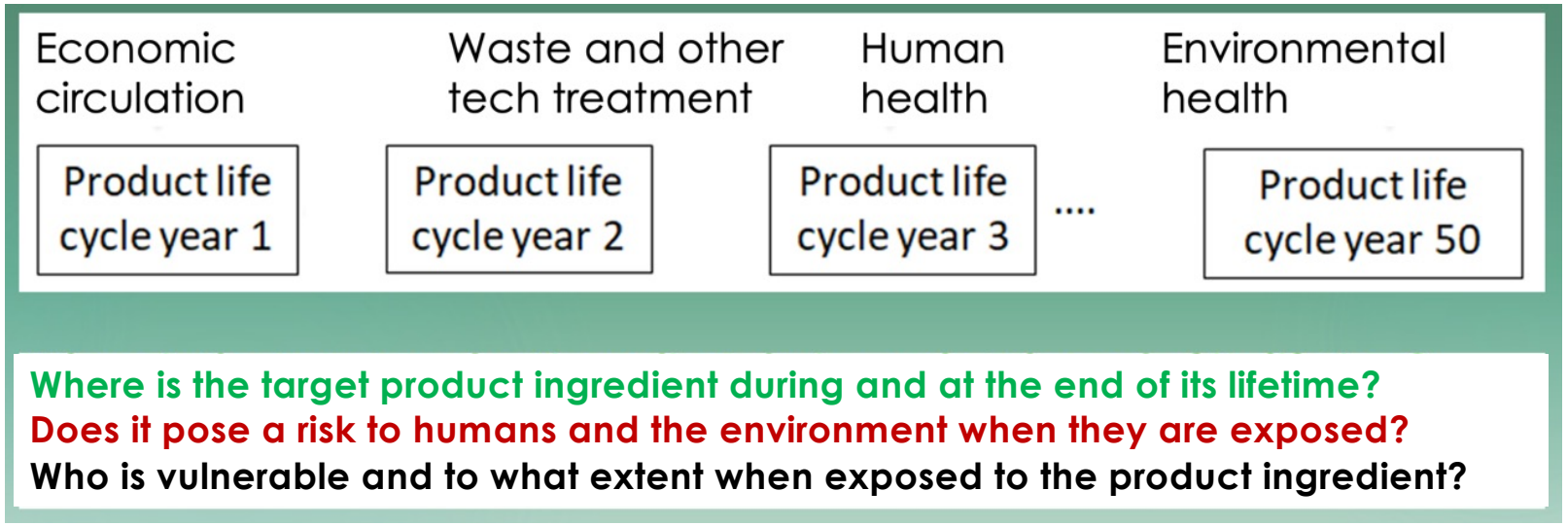
PERST (prospective early risk screening tool)

Nanorigo Deliverable 2.3

Fadri Gottschalk, Michael Steinfeldt, Bernd Giese, Sebastian Purker, Carina R. Lalyer, Isabel Rodriguez

This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.

… answers three questions (in green, in red … and in the contexts shown)



This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.

- … by stochastically-probabilistically predicting product ingredient's risks for humans and environment
- including, but not exclusively, emerging engineered nanomaterials
- in a life cycle monitoring when they stay/migrate through environmental (human) and technical (disposal) systems
- by comparing exposure concentrations of environmental media and human and other bodies (bioaccumulation) to their (eco)toxic sensitivity
- the same is done with vulnerability that is found when organisms and other creatures could be potentially (theoretically) negatively affected in the future when exposure concentrations would have reached toxic levels

This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.

- considers *air, freshwaters, marine waters, groundwater, saline groundwater, freshwater sediments, marine water sediments, soil, soil treated with sewage treatment sludge, flora fresh water, flora marine water, fauna fresh water, fauna marine water, humans (children), and humans (adults)*
- provides long term predictions (100 years) and a large range of results for optimistic to worst cases
- may be conducted for different target geographic regions covering all EU member states, CH and UK
- could become the base for a risk prediction service easy to make use when a database in the background is constructed and linked to its services

This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.

- comes from this without any use of predefined (theoretical and other) probability distributions
- but produces them himself even if data is highly sparse
- its output distinguishes
    - 3D graphics of various kinds of probability results
    - boxplots that reveal a summary of these output distributions
    - line charts visualizing a time series possibly in the future and
    - (a PERST risk etiquette for labelling the risk of an evaluated product (material))

This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.

- its methodologies very freely originate ideally and partly in its objective from earlier risk prediction approaches shown below, however:

- it vastly differs from them having its own stochastic concept and development strongly focused on probabilities of target material's (product ingredient's) location and transformation over its life cycle and beyond, no longer mass flow focused

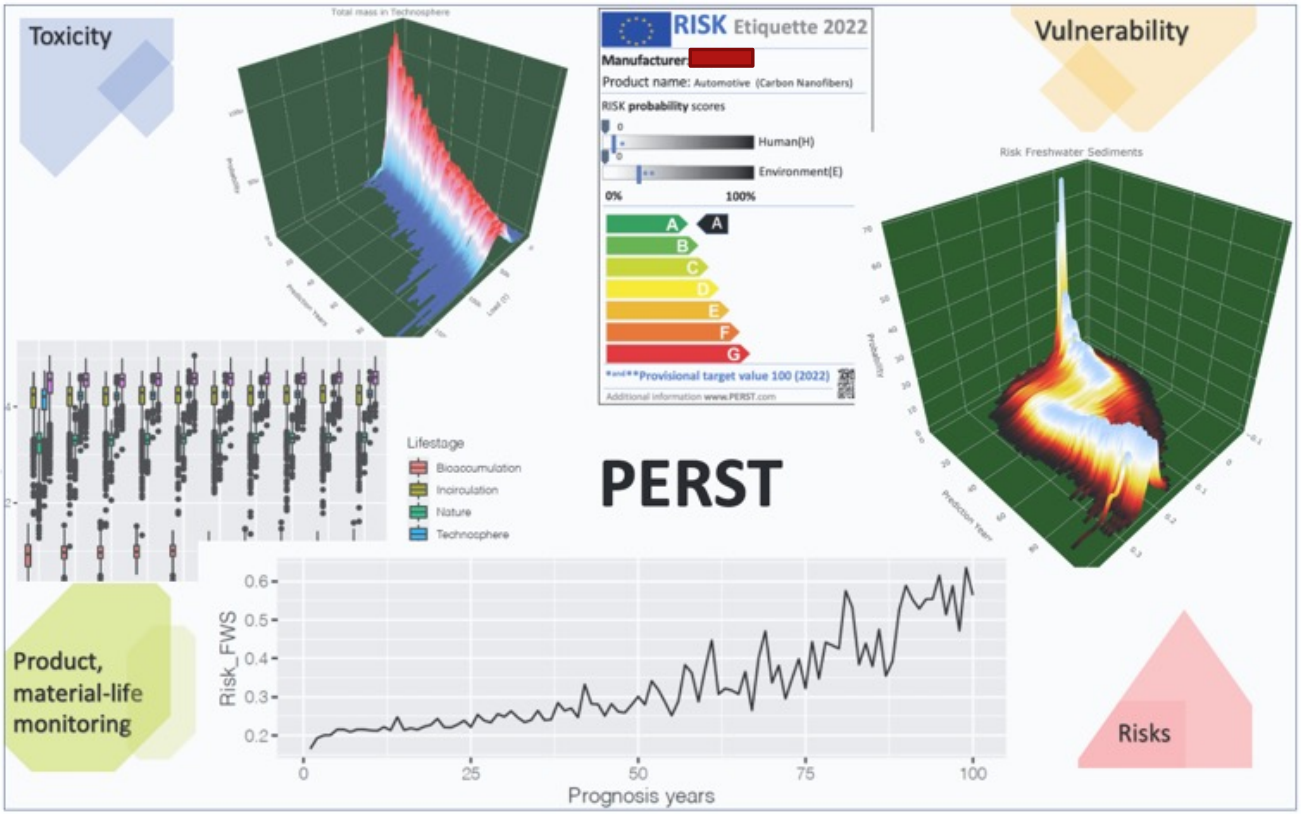
- newly, also suitable for long-rem predictions possible (100 years and more)

- again, in contrast to compared approaches, PERST performs without any use of predefined (theoretical and other) probability distributions but generates those distributions itself

- the tool is developed in R (R Development Core Team 2021) with its arithmetic operations embedded on their part and to different extents into multiple developed Monte Carlo, Bayes and combinations of these and other fundamental computing operations

Gottschalk, F., T. Sonderer, R. W. Scholz, and B. Nowack. 2009.Environmental Science and Technololgy 43:9216-9222.
Gottschalk, F., E. Kost, and B. Nowack. 2013. Environmental Toxicology & Chemistry 32:1278-1287.
Giese, B., F. Klaessig, B. Park, R. Kaegi, M. Steinfeldt, H. Wigger, A. von Gleich, and F. Gottschalk. 2018. Scientific Reports 8:1565.
R Development Core Team. 2021. R version 4.1.2 (2021-11-01)

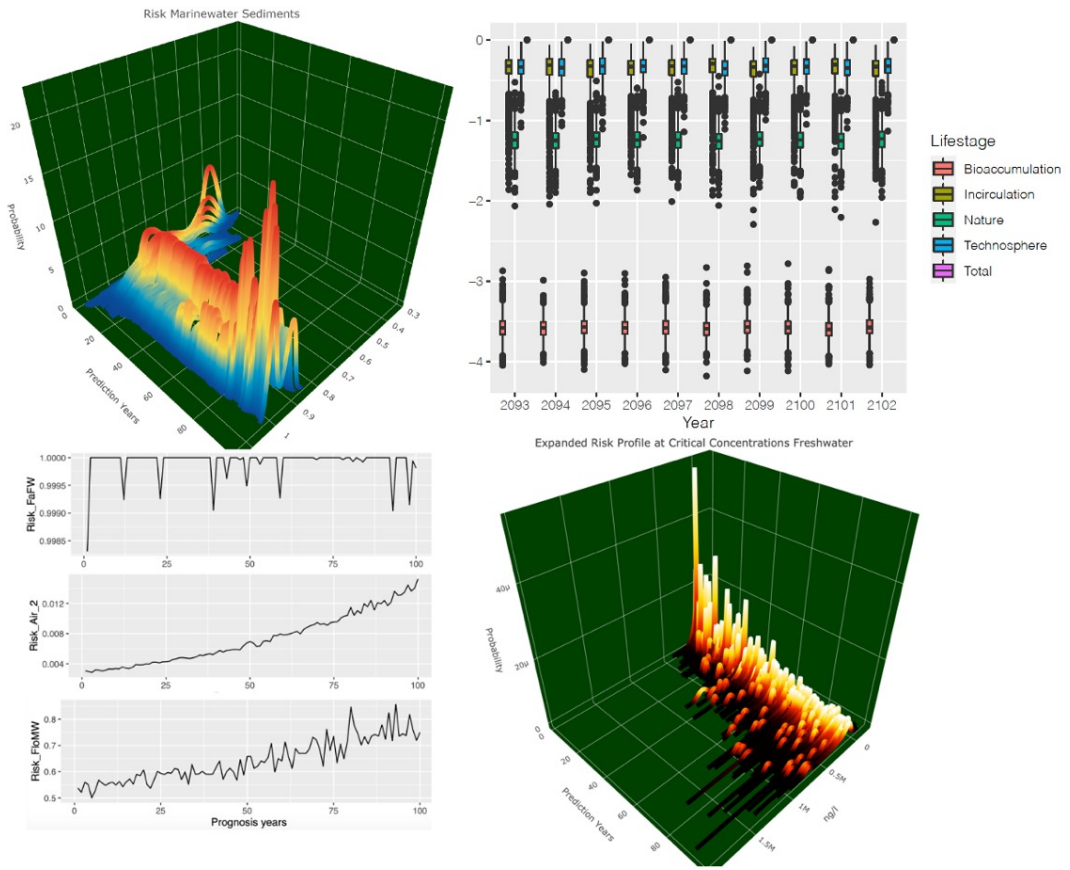
This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.



- Finally, a PERST output
- Test examples are visualized on the last slide

All symbols (graphic parts)
of a potential risk etiquette are of course in this exercise taken from widely known similar or identical labels, and only shown for test purposes, for check out possible symbols (graphic layouts) and are only
of an exemplary nature as in use in other contexts,
PERST currently does not produce any labels and does not claim any rights on them of course,
PERST only produces the scores to be taken!

This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.



- 3D graphics (probability is used synonymously with density [z-axis])
- boxplots summarizing over time output distributions, and
- line charts visualizing the evolution of a particular target variable

This project has received funding from The European Union's Horizon 2020 Research and Innovation Programme under Grant agreement 814530.