

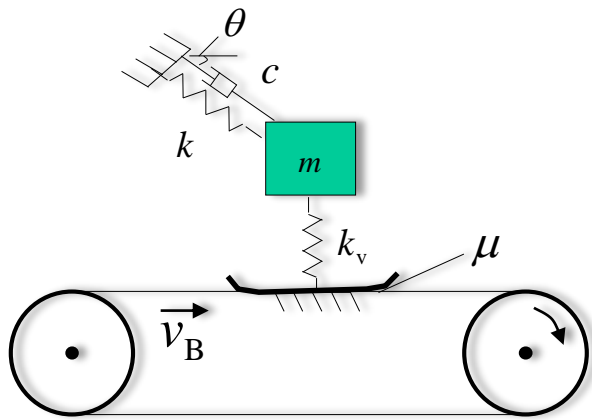
Documentation for FAIR Modelling

Sibylle Hermann

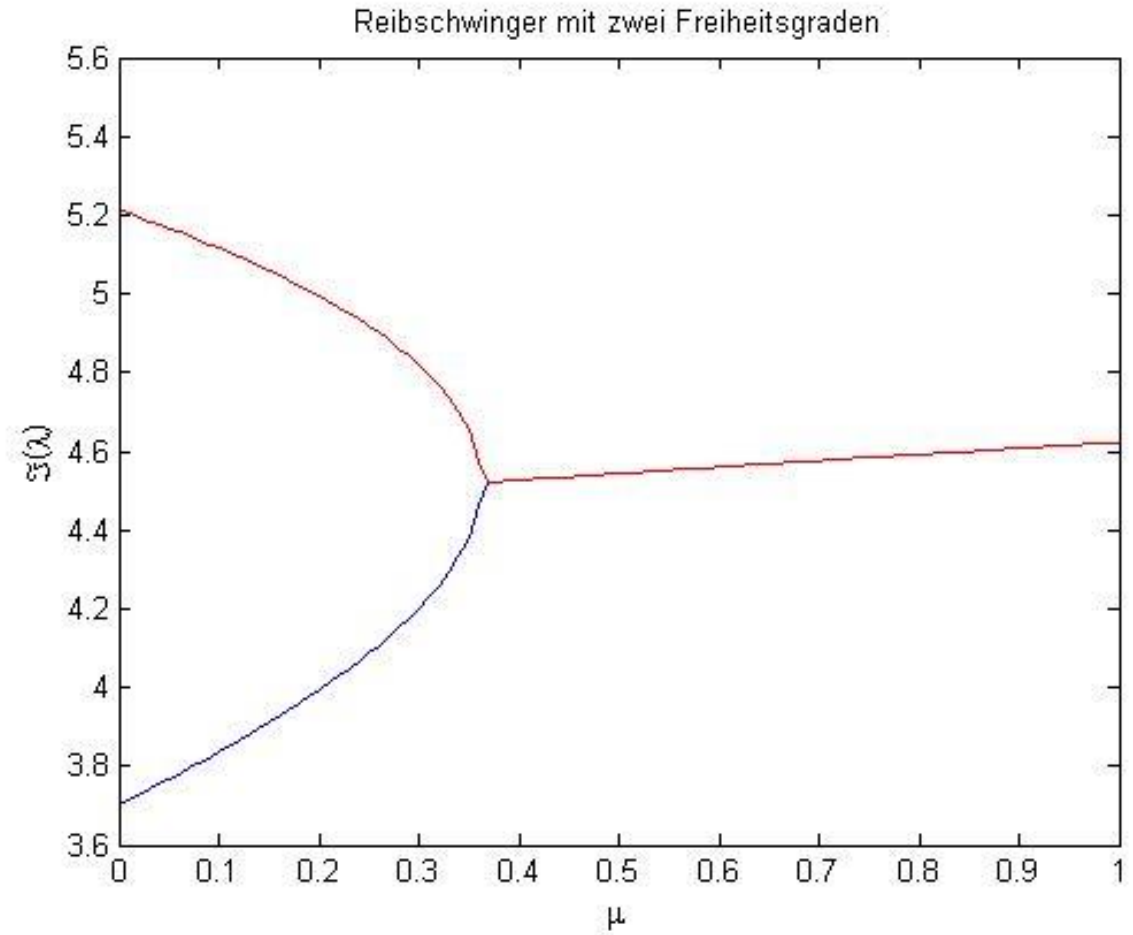
Institute of Engineering and Computational Mechanics, SimTech, University Library

Jörg Fehr, Andreas Baumann, Denis Pfeifer

My first RDM experience



$$\begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix} \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix} + \begin{bmatrix} c_{11} & -c_{12} \\ -c_{21} & c_{22} \end{bmatrix} \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} + \begin{bmatrix} k_{11} & -k_{12} \\ -k_{21} & k_{22} \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -F_R \\ 0 \end{pmatrix}$$



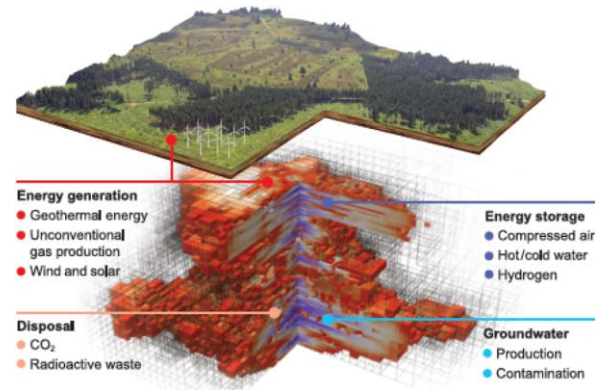
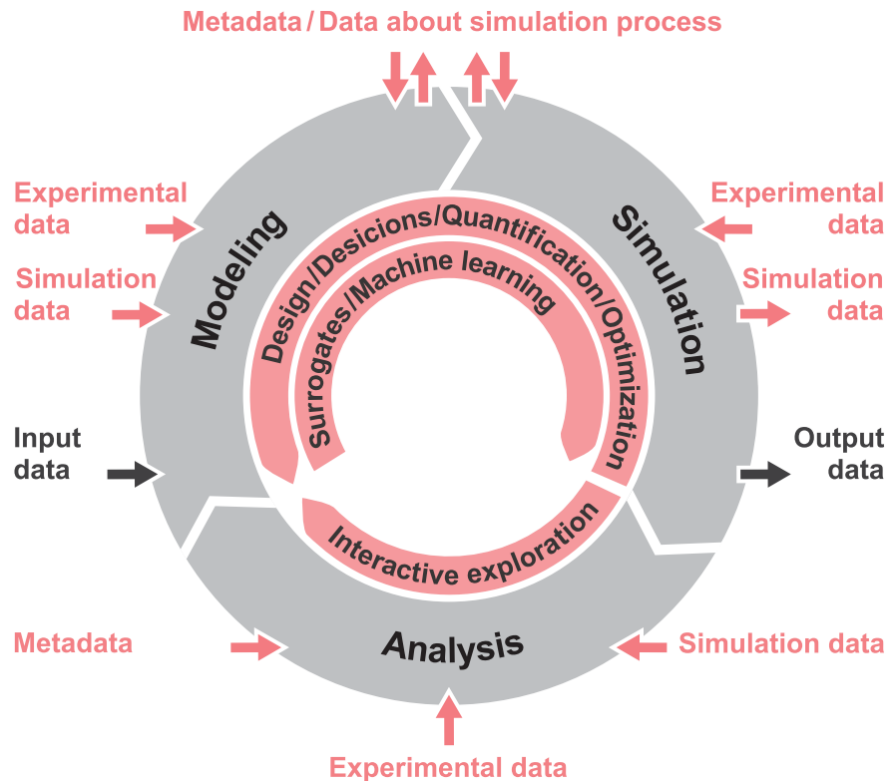
Lost in translation

```
opts.tol = 0.01 ;
[m n] = size(A) ;
x = ones (n,1) ;
y = A*x ;
[c R P info] = spqr (A, y, opts) ;
info
Rs = R (:, 1:m) ;
fprintf ('condest(Rs) %g\n', condest (Rs)) ;
xs = x (1:m) ;
xm = x (m+1:n) ;
A2 = -Rs \ R (:, m+1:n) ;
y2 = Rs \ c ;
norm(A2*xm + y2 - xs) % should be very small
nnz (A2) % should also be as small as possible
```

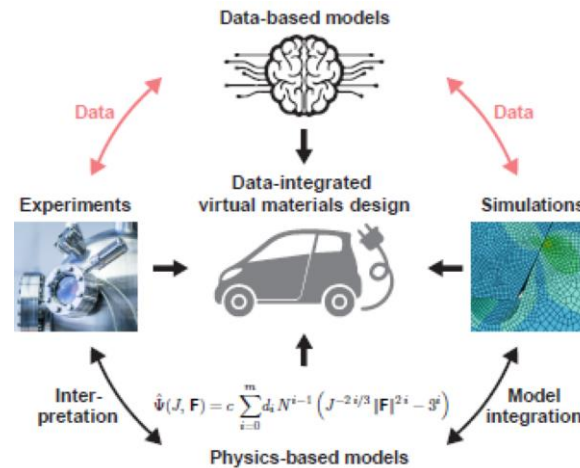
MSC Nastran™
Industry Leading Multidisciplinary FEA Solution

```
BEGIN BULK
$.....1.....2.....3.....4.....5.....6.....7.....8.....9.....10
MDLPRM,HDF5,1
PARAM,POST,0
PARAM PRTMAXIM YES
$.....1.....2.....3.....4.....5.....6.....7.....8.....9.....10
EIGRL 1 .1 30 0 MAX
CORD2C 1 0 0. 0. 0. 0. 0. 1.+FEMAPC1
+FEMAPC1 1. 0. 1.
CORD2S 2 0 0. 0. 0. 0. 0. 1.+FEMAPC2
+FEMAPC2 1. 0. 1.
```

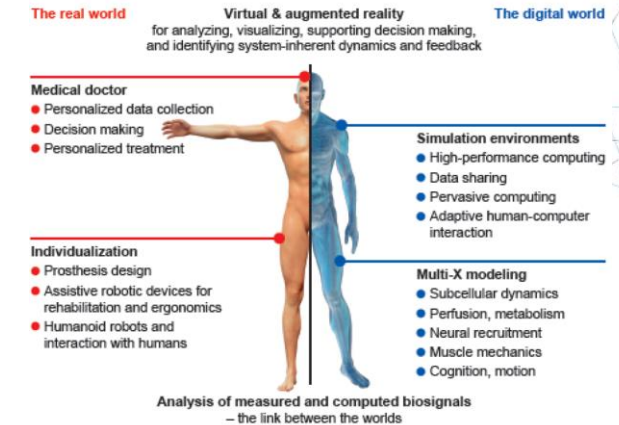
Modelling, simulation and analysis to solve visionary examples



Engineered Geosystems



Next-Generation Virtual Materials Design



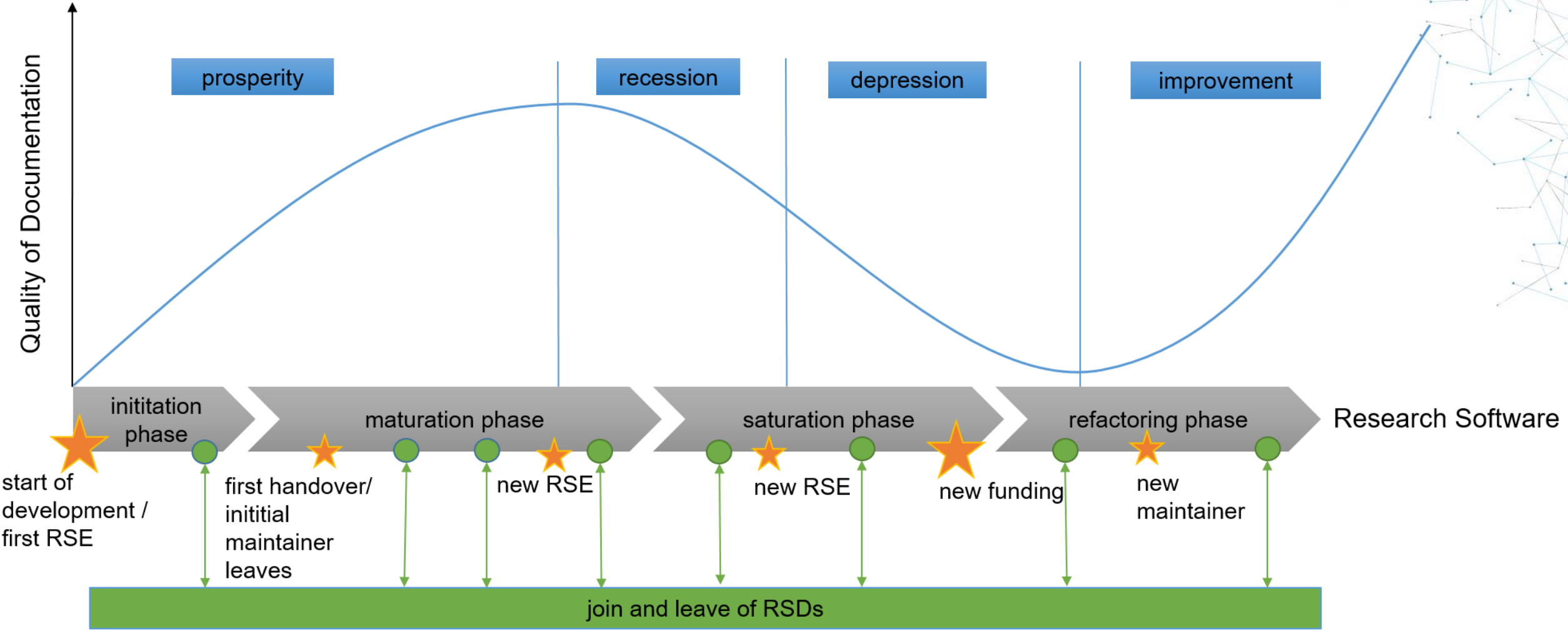
Digital Human Model

Example: Neweul-M²

- Written in Matlab
- Dynamic analysis of mechanical systems
- Multibody system method



Documentation has a history



<https://doi.org/10.1038/s41598-022-10376-9>

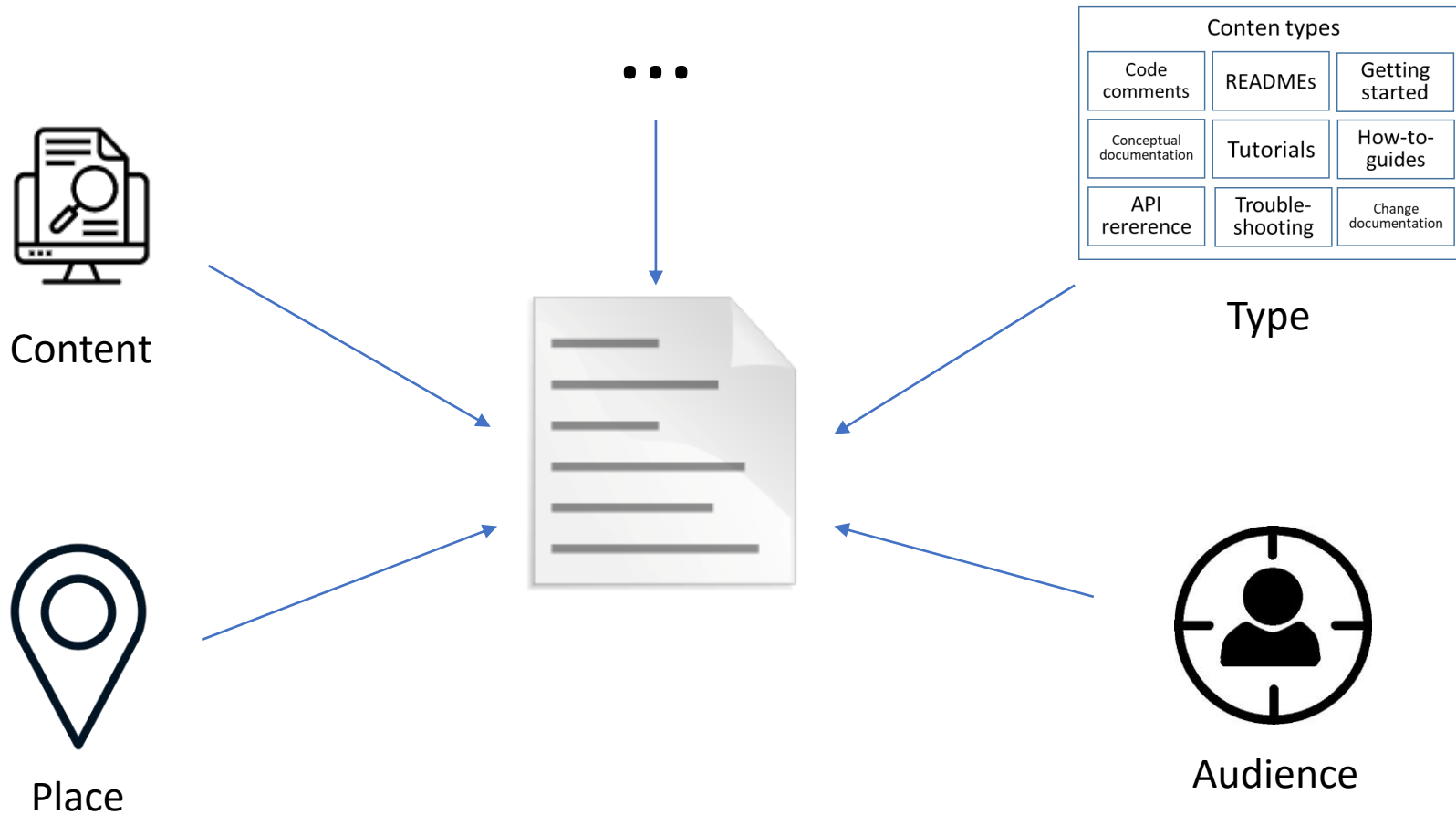
But how can we do better?



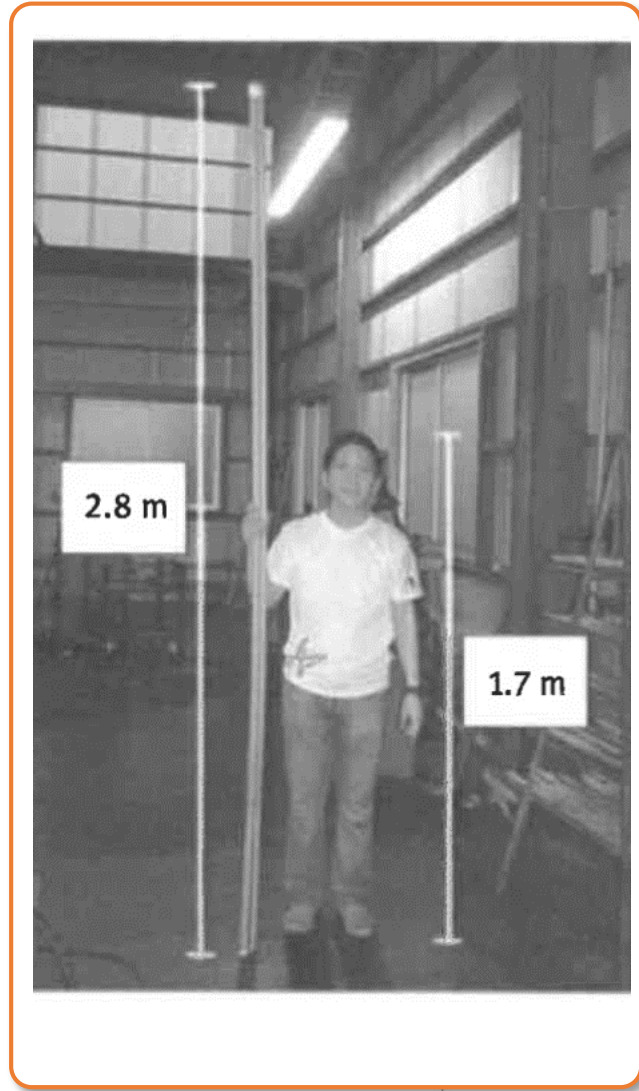
Tools



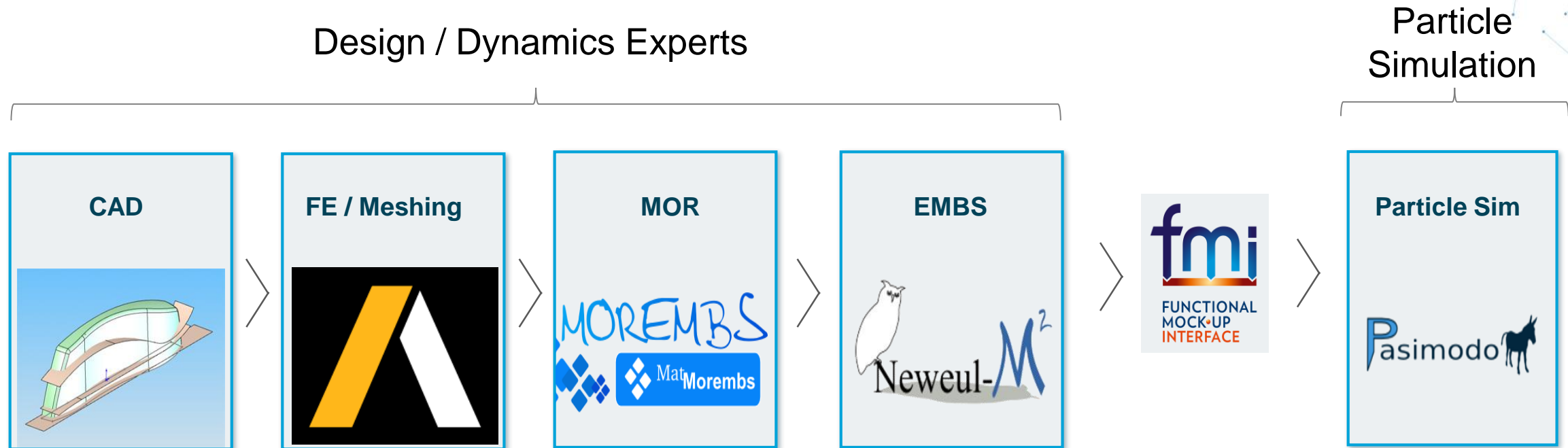
Different aspects of documentation



Research Andreas – Deep hole drilling

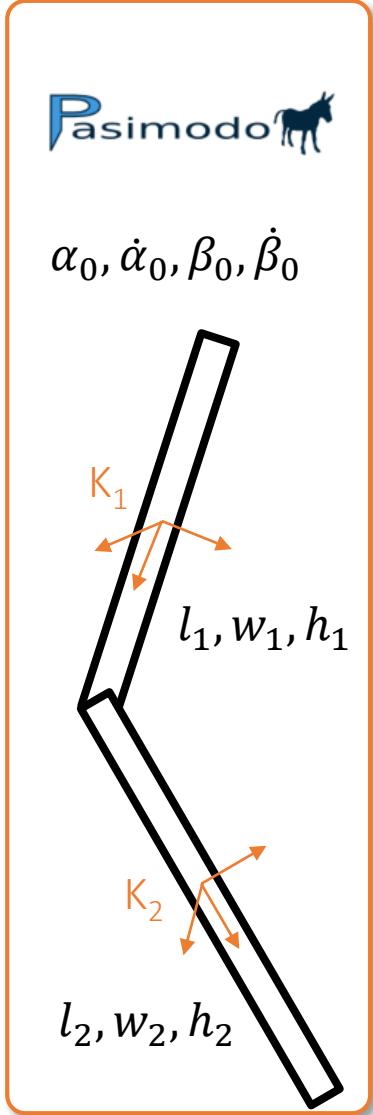
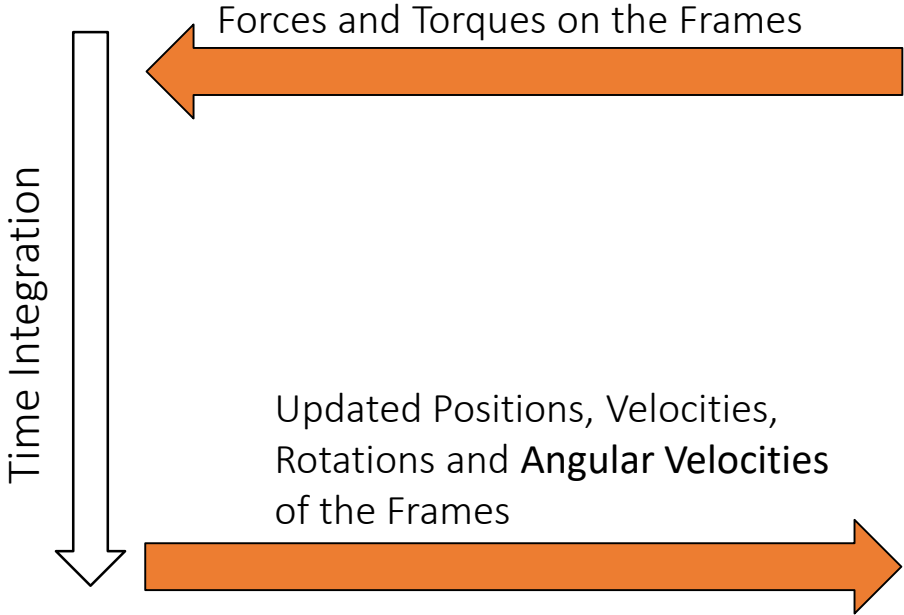
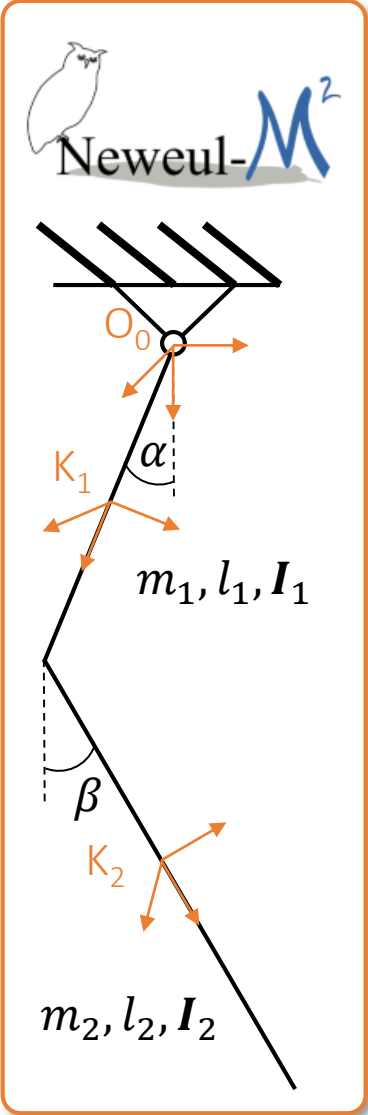


Toolchain Andreas



Toolchain to analysis of the cutting fluid behavior with a modified micro single-lip deep hole drilling tool [1]

Example from Andreas



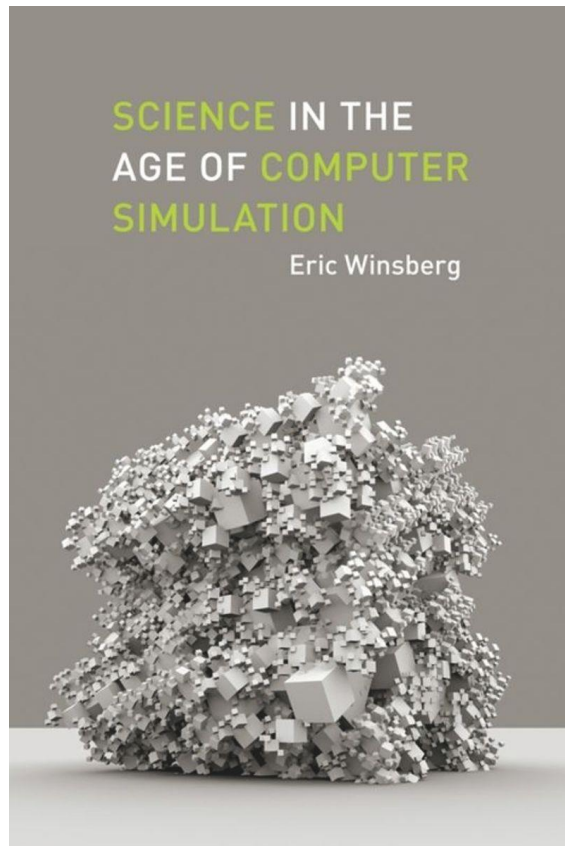
Software Engineering: Docs as code

Documentation as Code (Docs as Code) refers to a philosophy that you should be writing documentation with the same tools as code:

- Issue Trackers
- Version Control (Git)
- Plain Text Markup (Markdown, reStructuredText, AsciiDoc)
- Code Reviews
- Automated Tests

<https://www.writethedocs.org/guide/docs-as-code/>

Philosophy of Science

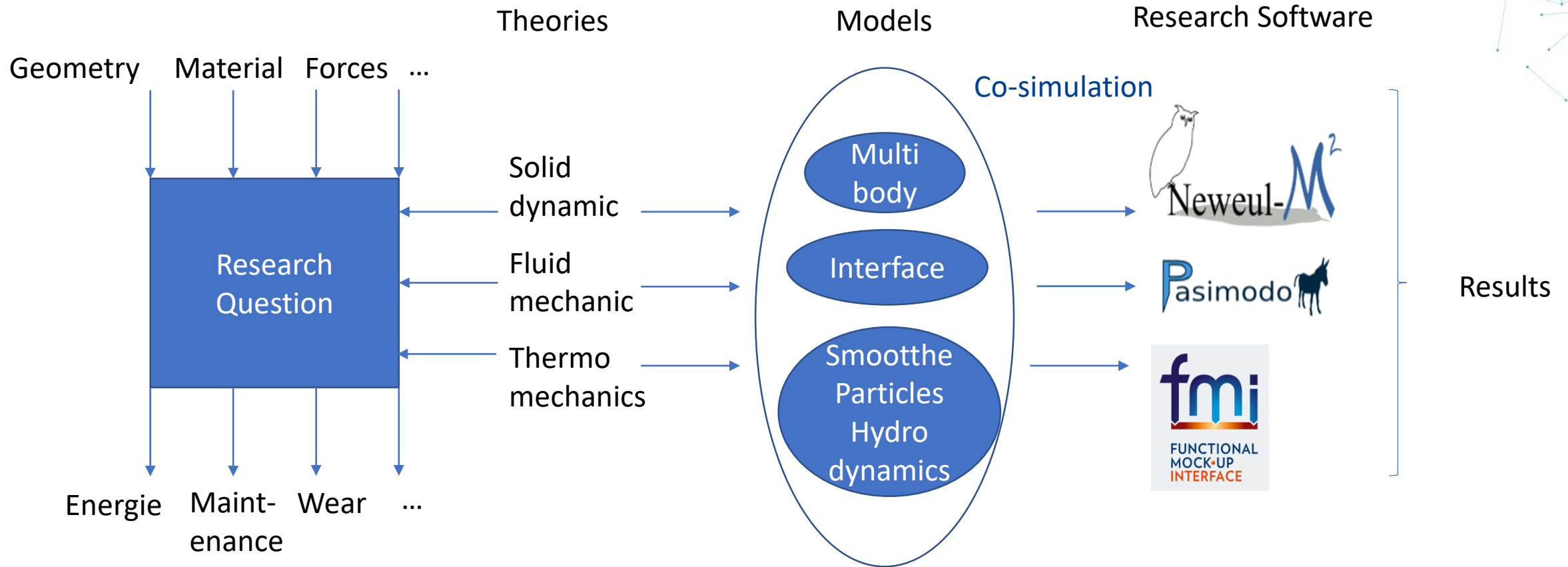


Science in the Age of Computer Simulation Eric Winsberg

“But simulations more often involve the application rather than the testing of scientific theories.”

<https://doi.org/10.7208/9780226902050>

Co-Simulation



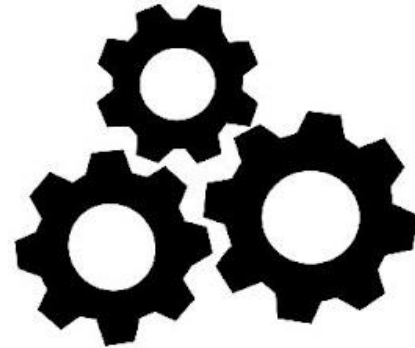
F
Findable



A
Accessible



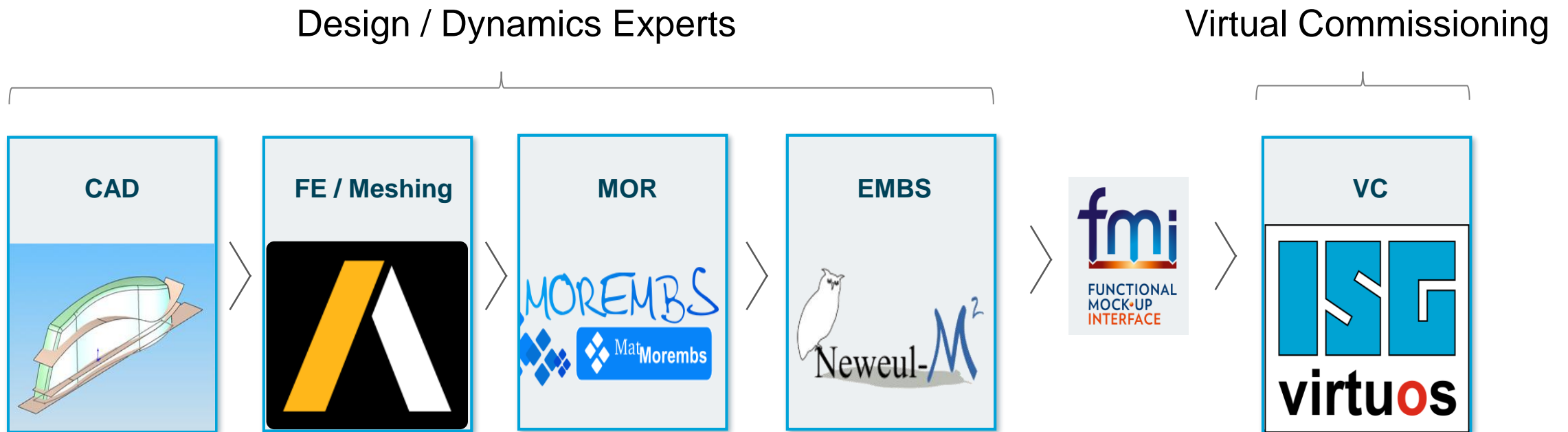
I
Interoperable



R
Reusable



Toolchain Denis



Toolchain for simulation of digital twins within a virtual commissioning approach

Verification and Validation

Software Engineering

Verification: solving the chosen equations correctly

Validation: choosing the correct equation

<https://doi.org/10.1016/j.jcp.2004.10.036>

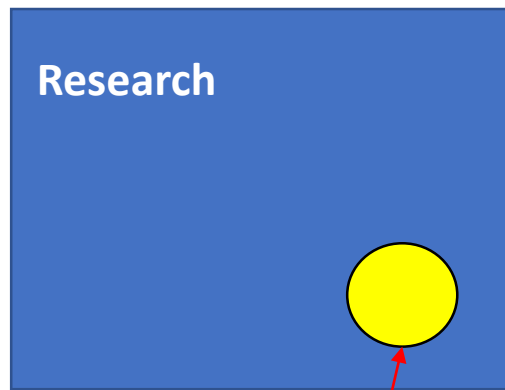
Philosophy of Science

Verification: transparency

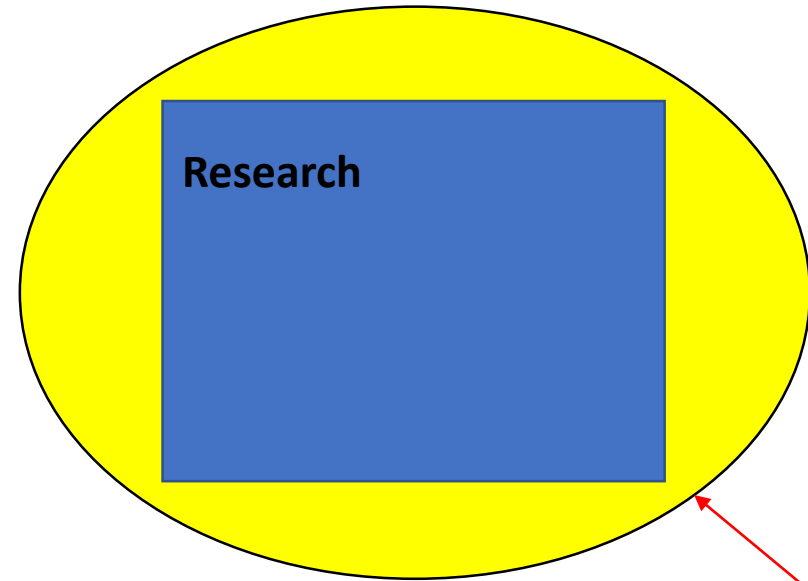
Validation: skill

<https://doi.org/10.1515/aot-2018-0066>

Micro vs. Macro Documentation



Detail



The whole

What to do

- Think about your own research and what is important to document
- Publish research results and document in a way others can understand it
- Think about your audience → who needs the documentation for what
- Think about the whole process

Conclusion

- Documentation is more complex than we would like to admit.
- Focus must be on the method not on tools, they change.
- Documentation happens at the end of the project and within the research process.
- Documentation is multidisciplinary.
- The research question determines the documentation.
- Micro and macro documentation is needed.