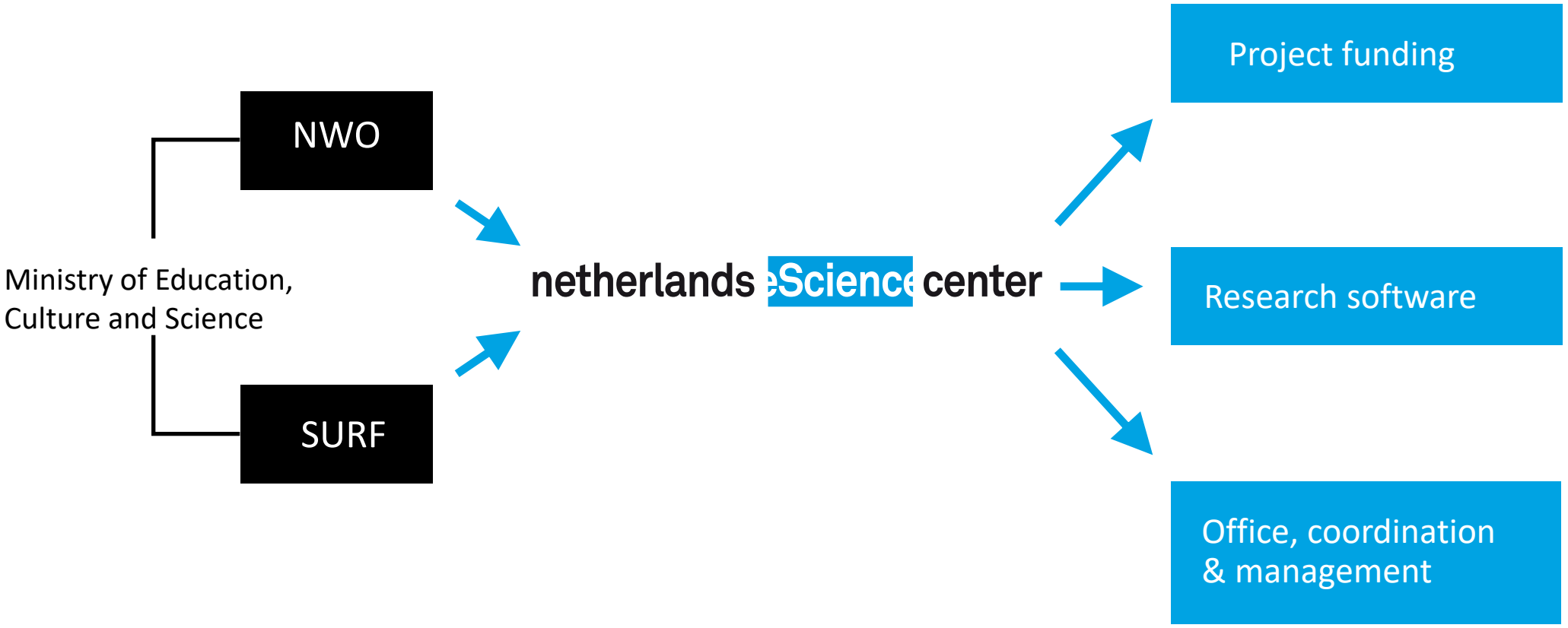
netherlands eScience center

Research and Software Engineering at the Netherlands eScience Center

Carlos Martinez-Ortiz
24th February 2021

What is the eScience center



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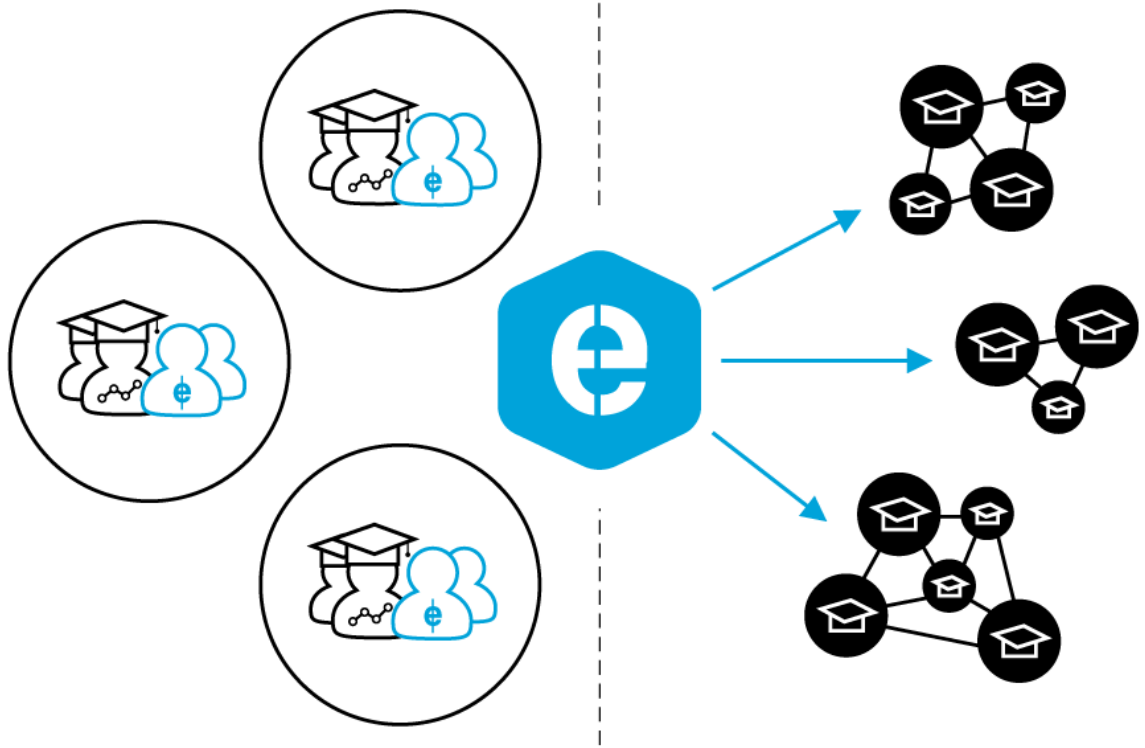
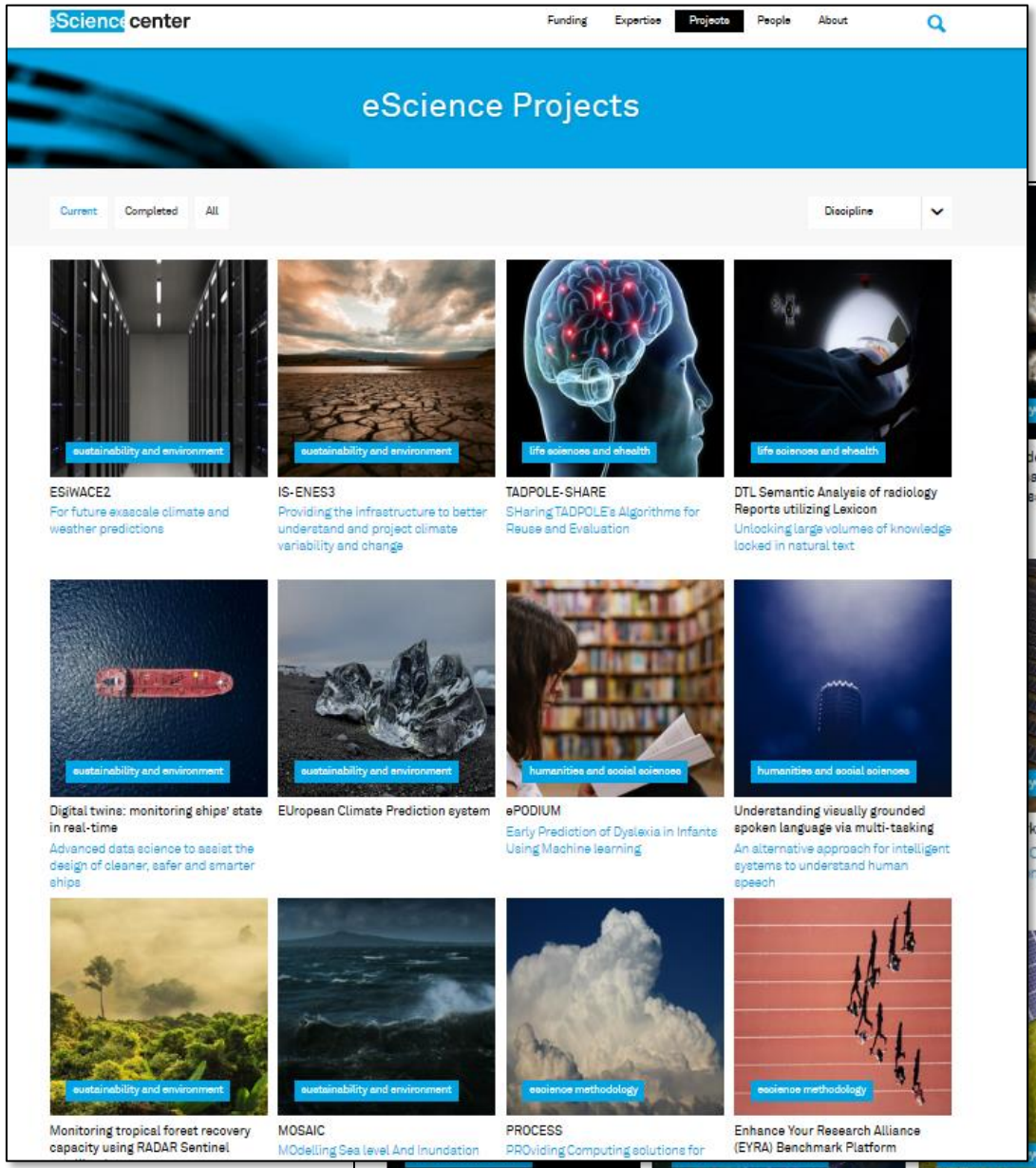
eScience Center main activities

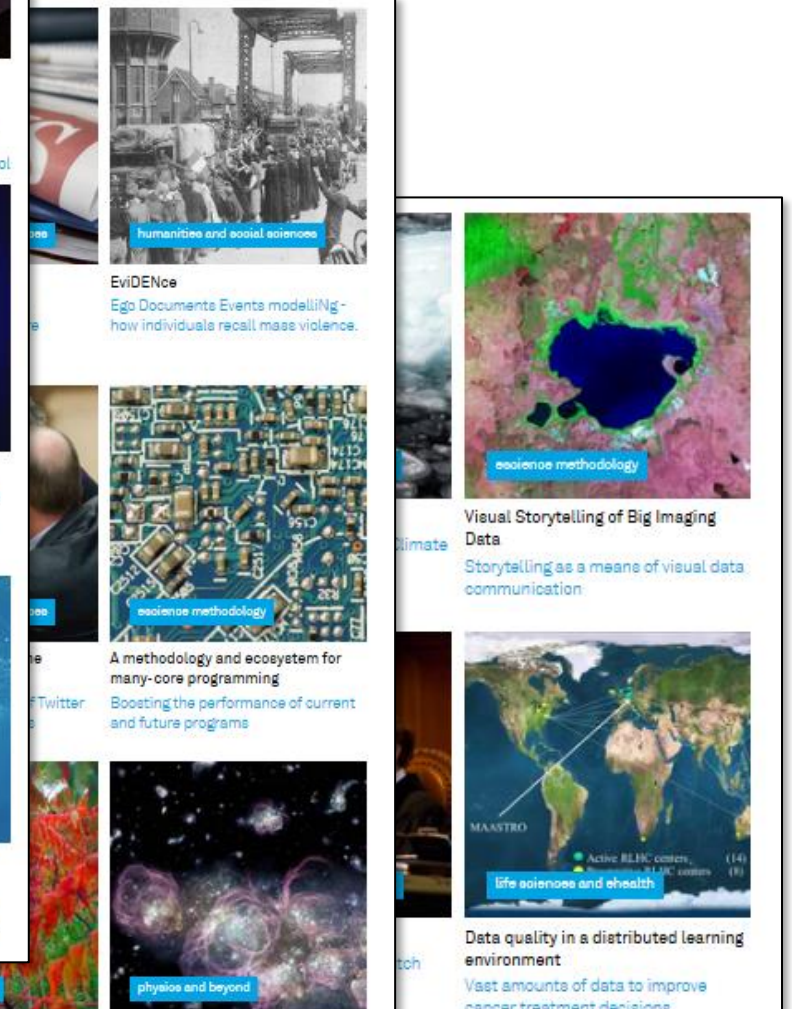
Collaborative projects
with selected academic researchers

Sharing expertise
with research communities



www.esciencecenter.nl/projects





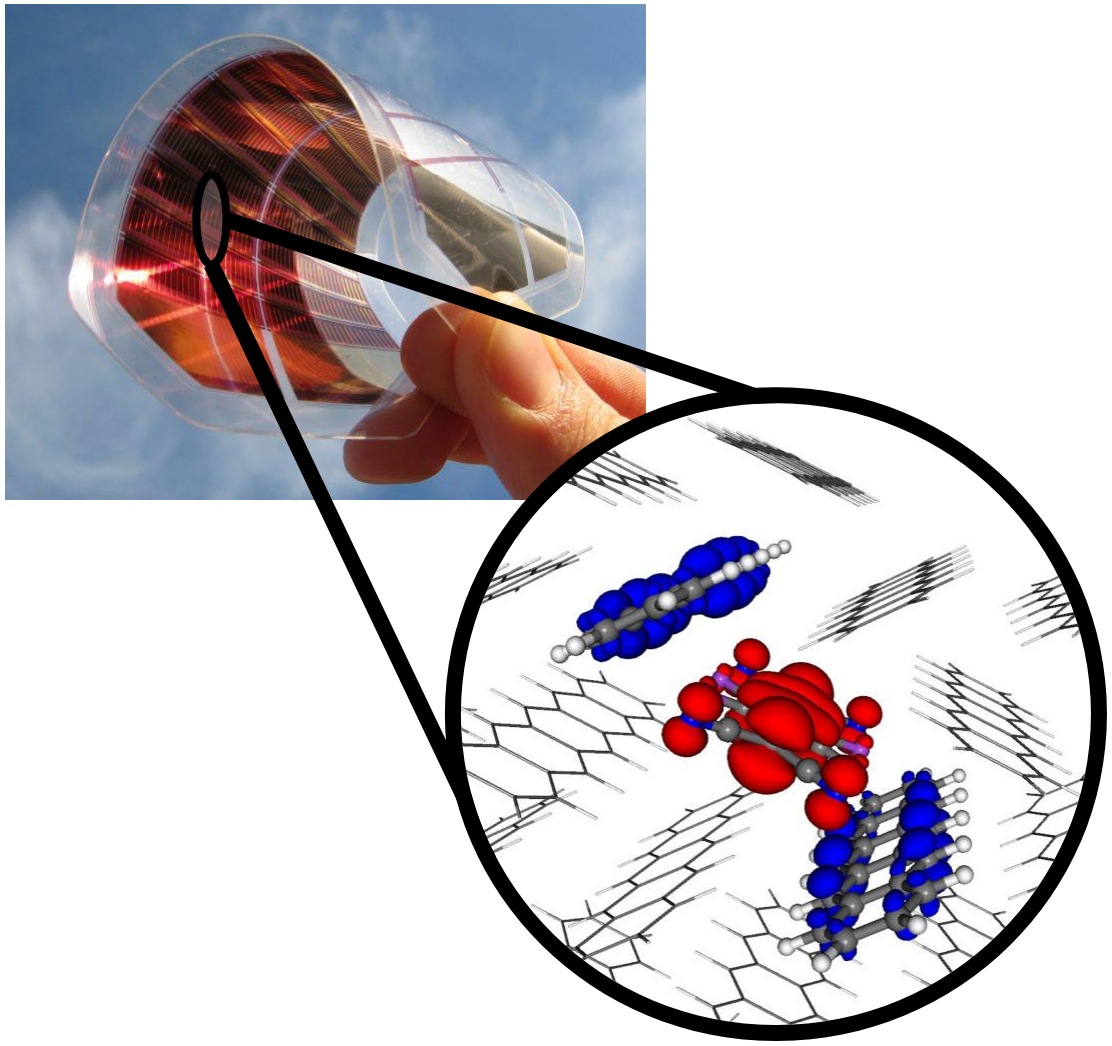
MULTIXMAS

Multiscale simulations of excitation dynamics in molecular materials for sustainable energy applications

Alexey Lyulin

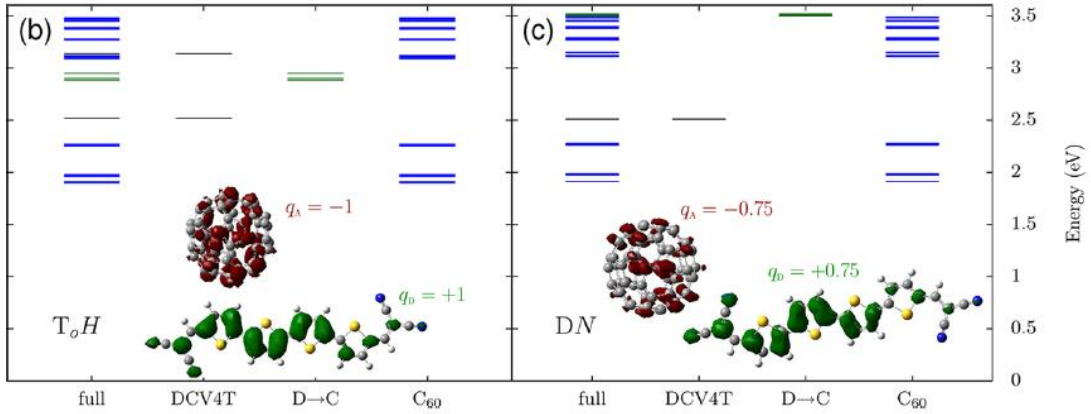
Bjoern Baumeier

- Understand how molecular systems harvest energy from the sun and how energy propagates in these materials
- Quantum Chemistry for energy applications



Harvesting solar energy in organic materials

Focus on the excited state properties of small molecular systems using GW-BSE



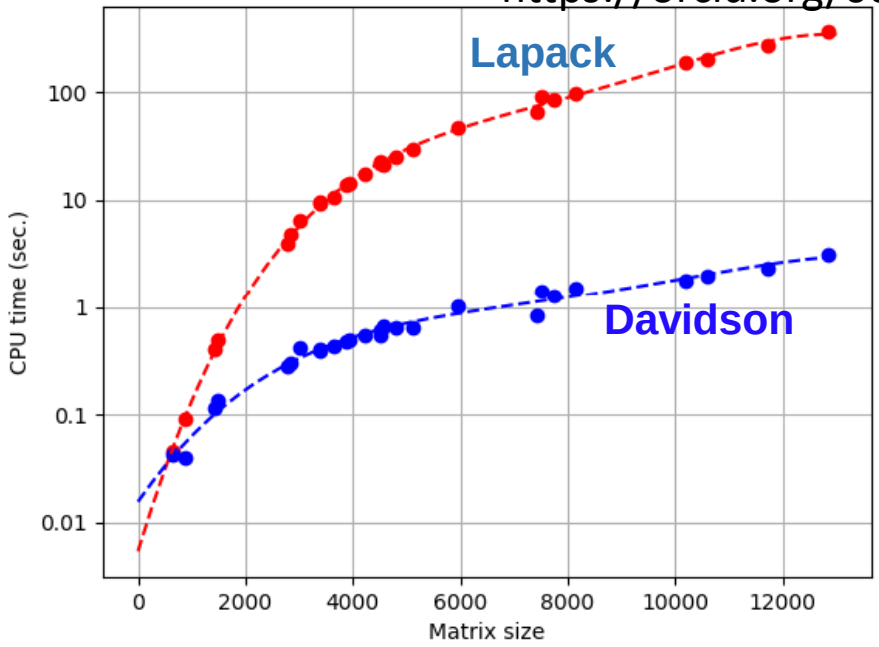
- ❑ **Reduce memory requirements**
- ❑ Accelerate diagonalization scheme
- ❑ **Off-load heavy calculation to GPU**

Diagonalization of large matrices

Nicolas Renaud

Development of matrix-free eigensolver (Jacobi-Davidson) and integration in the open source library Eigen

https://orcid.org/0000-0001-5565-7577



GPU programming

Felipe Zapata

Development of CUDA kernels for the calculations of tensor-matrix product Involved in 3-center integral calculations

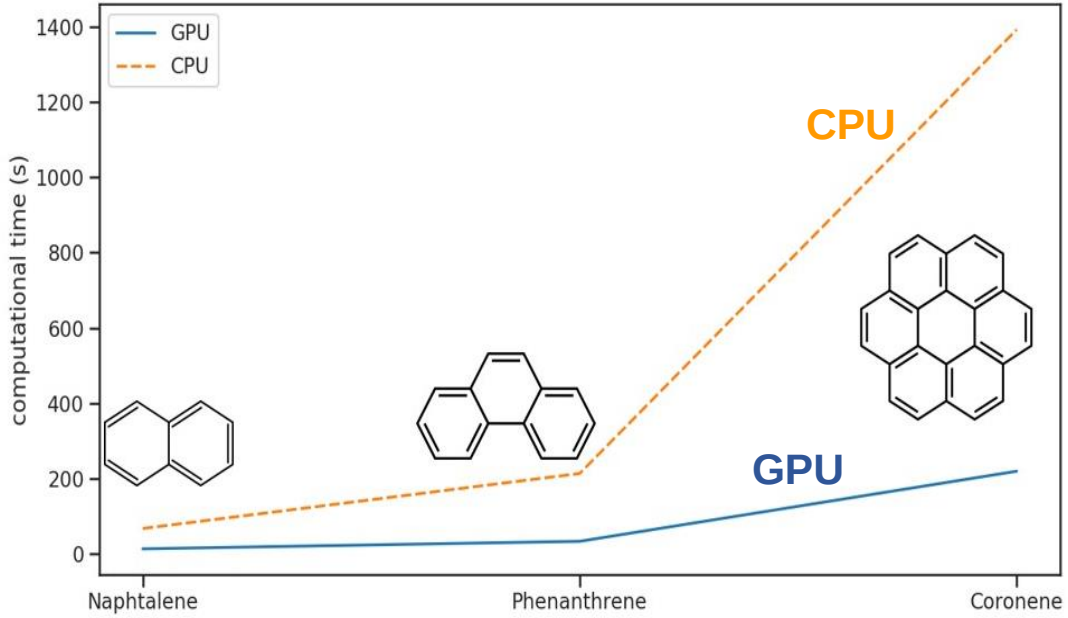


Photo by Hello I'm Nik on Unsplash

Retina COVID19

Real Time National Policy Adjustment and Evaluation on the basis of a computational model for COVID19

- Economic & social costs of social distancing measures

Prof. Martin Bootsma

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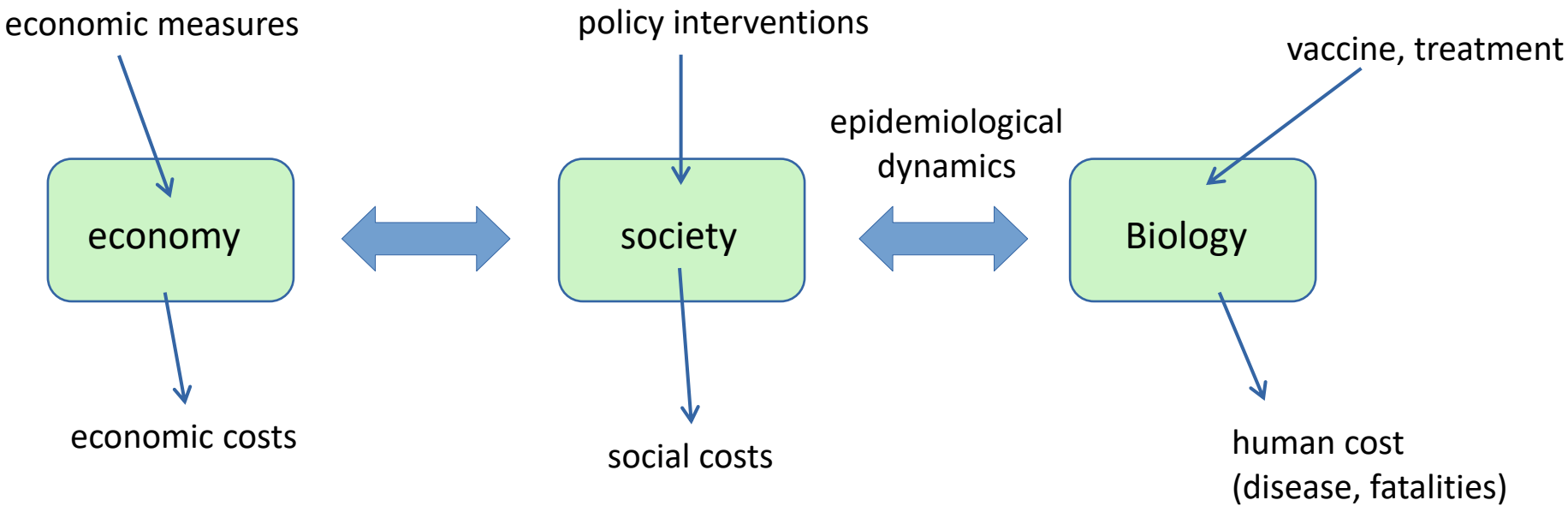
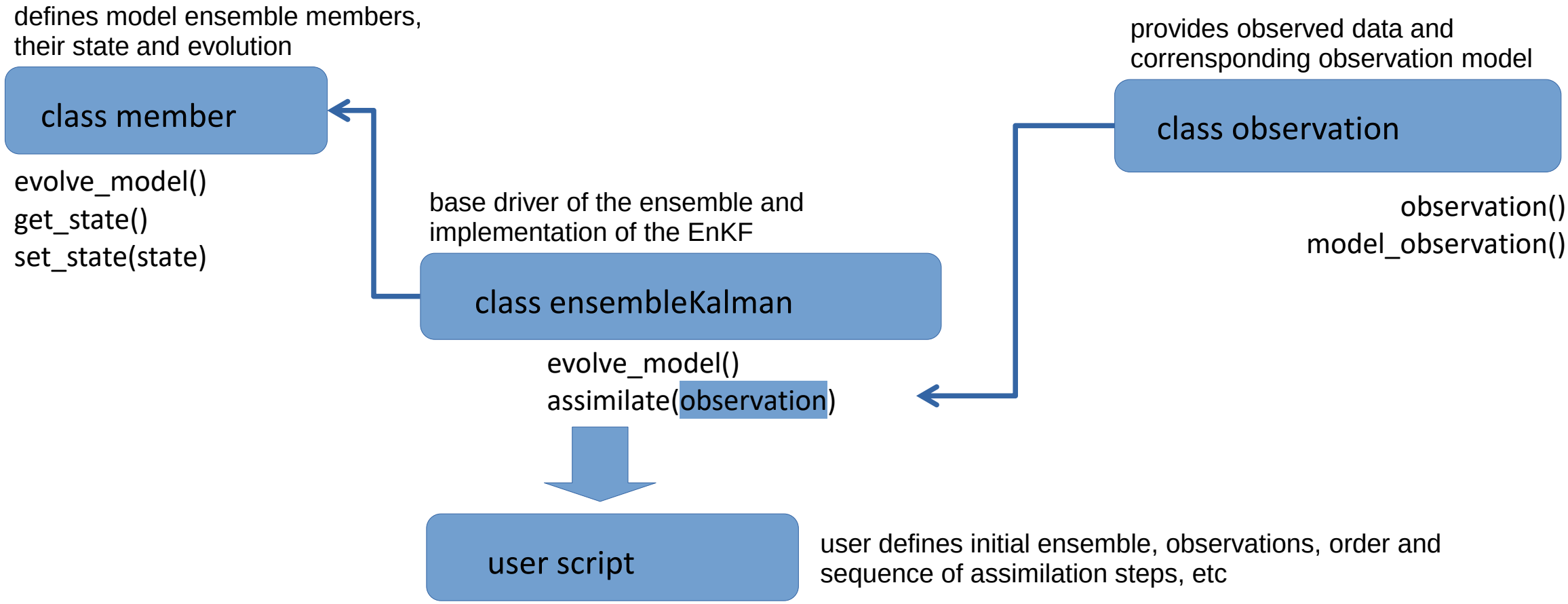
Real Time National Policy Adjustment and Evaluation on the basis of a computational model for COVID19



EnKF: Python implementation

– Python based implementation developed for OMUSE/HyMUSE
– based on driver class and a number user implementable classes



→the implementation and use of EnKF is easy, but the real devil is in the details of the choice of the state variables, observation function and the model for observation and state errors….

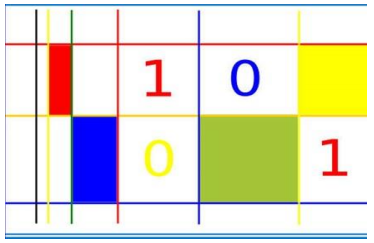
Special Interest Groups

- Stay up to date with the state of the art
- Coordinate use of technology in projects
- Recently: more external engagement
- Knowledge dissemination
  - workshops, hackathons, tutorials, etc.

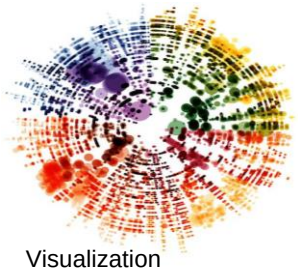
Natural Language Processing

Statistics / Data Mining

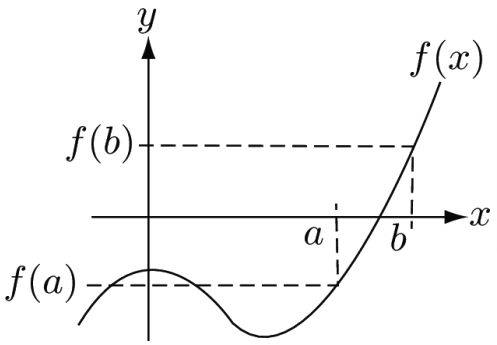
Data



Machine Learning /
Computer Vision



Visualization



Numerical Modelling
and
Efficient Algorithms

Workflows and Orchestration

Efficient Computing

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Research Software ~~Best~~ Good Practices, building expertise and knowledge sharing

Mateusz Kuzak

24th February 2021

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Questions that started it all

The Netherlands eScience Center is the National Expertise Center for Research Software Engineering.

That does not automagically make software developed at the Center better than that developed at other research institutions.

Q1. How do we know we know the software is of good quality?
Q2. What does it mean good quality software?

Answer: Software Quality Checklist

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Collaborations Workshop 2016 (CW16), Royal College of Surgeons of Edinburgh

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Lightning talk CW16

Mateusz Kuzak
eScience research engineer

nlesc
/estep-checklist

SoftDev4LS
/open-source-software
/good-enough-practices
/software-development-metrics

The checklist grew into a guide

https://guide.esciencecenter.nl/

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Checklist is still there

The **bare minimum** that every software project should do, from the start, is:

- Pick & include an open source license
- Use version control
- Use a publicly accessible version controlled repository
- Add a readme describing the project

We recommend that you also do the following (from the start of the project):

- Use code quality tools
- Testing
- Use standards

Additional steps depend on the goal of the software (zero or more can apply):

- I'm publishing a paper
- I'm expecting users
- I'm expecting contributors

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Guide in 2019

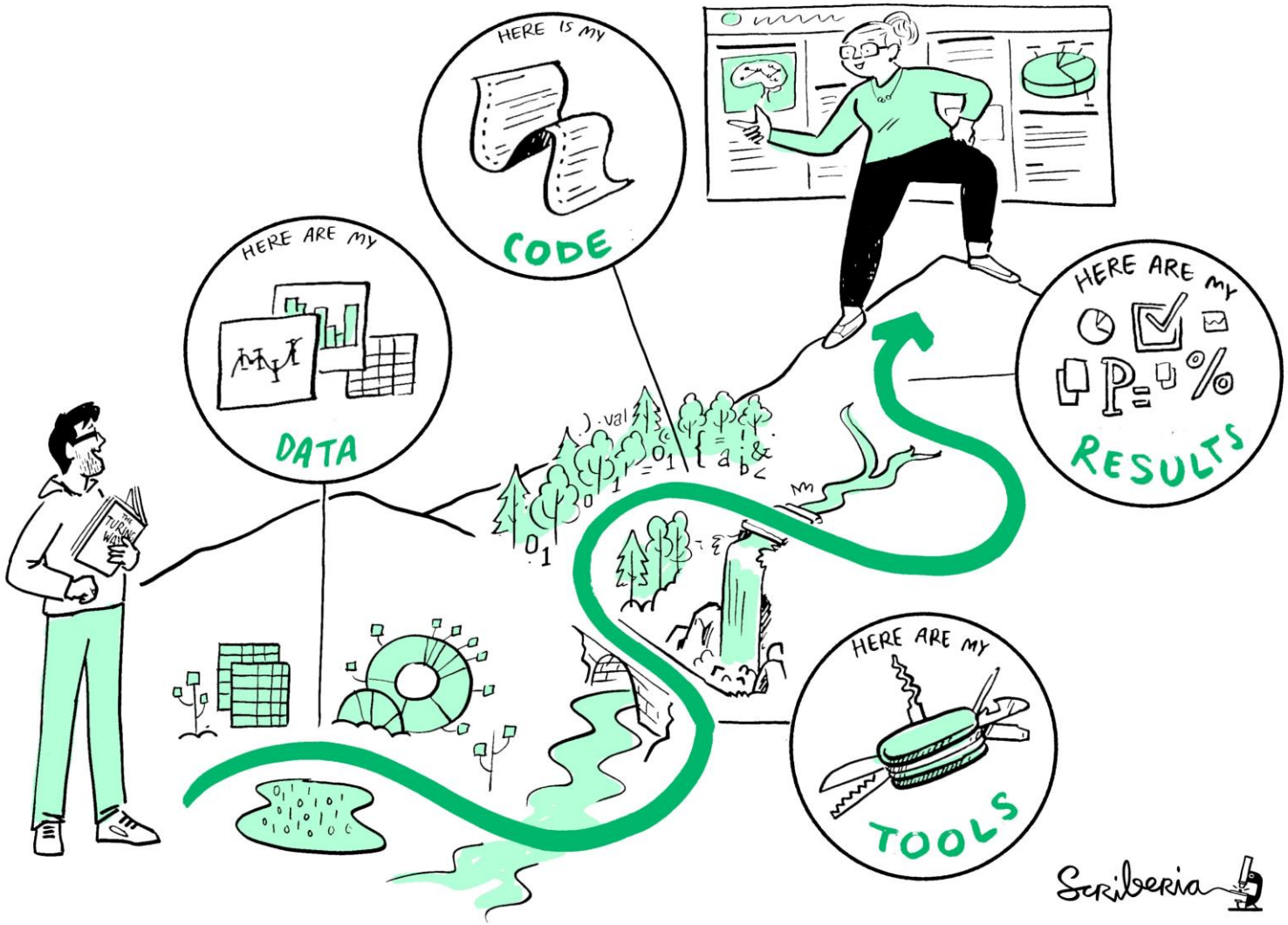
- Version Control
- Code Quality
- Code Review
- Licensing
- Communication
- Testing
- Releases
- Documentation
- Standards
- UX
- Specific language guides (Java, Python, C and C++, Fortran)
- Intellectual property
- … and more

Growing our own content

Vs

Referencing external content

The Turing Way



- largely similar content
- goes beyond research software
- large diverse international community of contributors
- opportunities for contributions by the Center, based on our expertise

Zenodo. http://doi.org/10.5281/zenodo.3332807

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What's in the Guide

How we do it at the Center
Internal Guide

Universal information
for all RSEs and researchers writing code

In 2019 we decided to the work

Guide

- How we do it at the Center
- Topics not covered by The Turing Way

The Turing Way Contribution

- Universal content

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How is the work organized?

- **Written by engineers, based on their expertise**
- **One Guide maintainer**
- **Coordinated by Software Sustainability SIG (Special Interest Group)**
- **Progress via sprints and async contributions**

Software Sustainability SIG

- Knowledge sharing on
  - Good practices
  - Sustainability
  - Reusability
  - Reproducibility
- Internal training (version control, CI/CD etc.)
- Developing guidelines
- Contribution to the Guide and the Turing Way

Work in small teams, project based in sprints.

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Zenodo. http://doi.org/10.5281/zenodo.3332807