

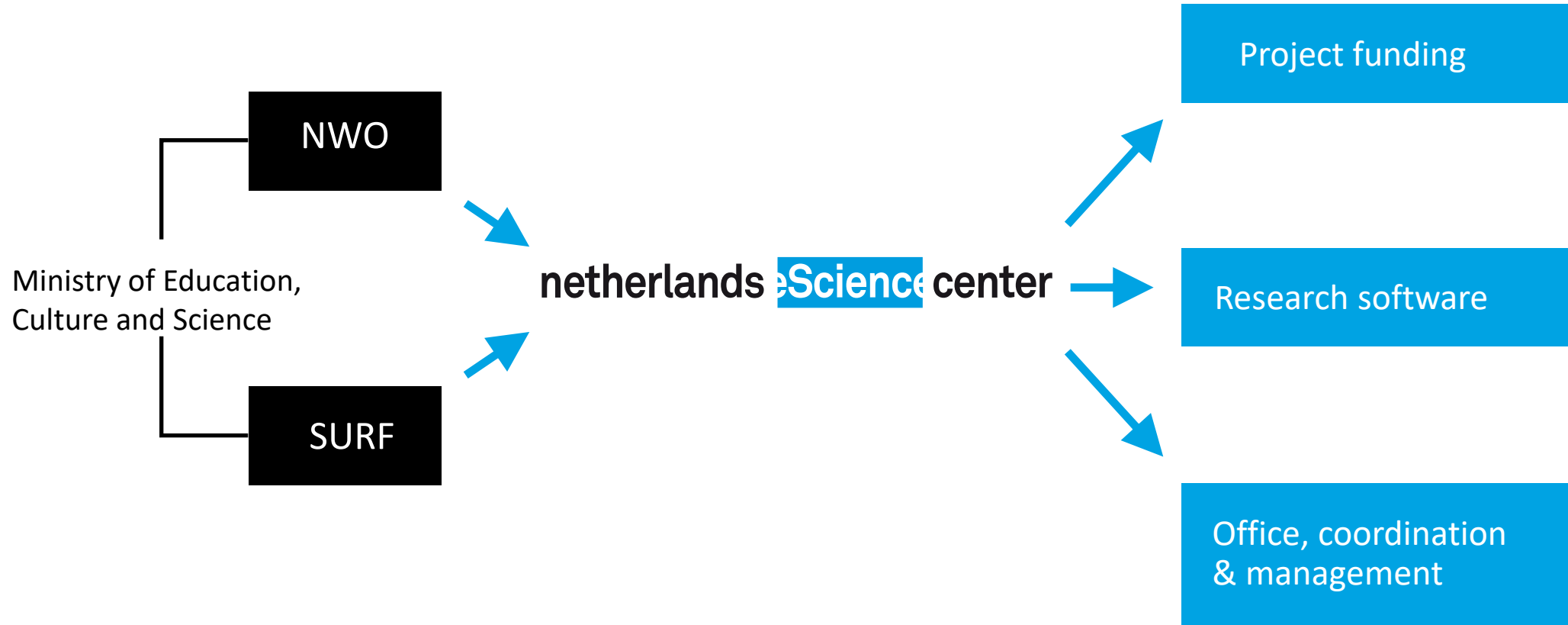
netherlands

eScience center


Research and Software Engineering at the Netherlands eScience Center

Carlos Martinez-Ortiz
24th February 2021

What is the eScience center

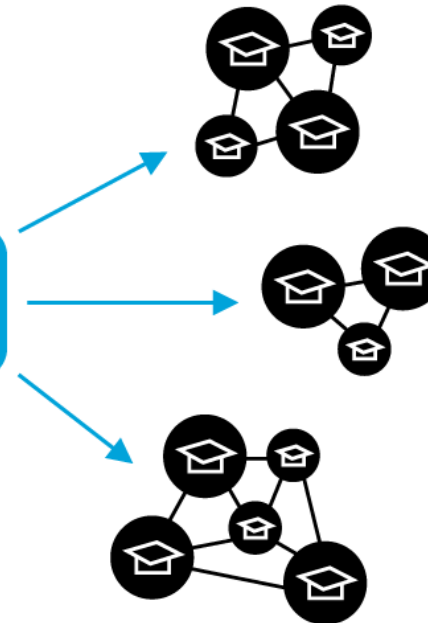


eScience Center main activities

 **Collaborative projects**
with selected academic
researchers



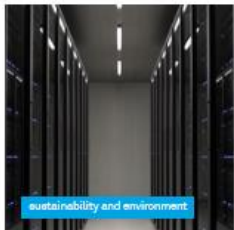
 **Sharing expertise**
with research communities



eScience Projects

Current Completed All

Discipline



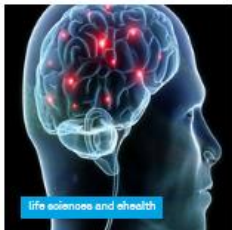
sustainability and environment

ESIWACE2
For future exascale climate and weather predictions



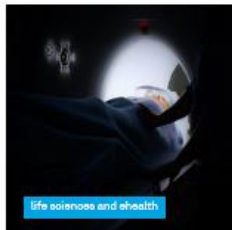
sustainability and environment

IS-ENES3
Providing the infrastructure to better understand and project climate variability and change



life sciences and health

TADPOLE-SHARE
SHaring TADPOLE's Algorithms for Reuse and Evaluation



life sciences and health

DTL Semantic Analysis of radiology Reports utilizing Lexicon
Unlocking large volumes of knowledge looked in natural text



sustainability and environment

Digital twins: monitoring ships' state in real-time
Advanced data science to assist the design of cleaner, safer and smarter ships



sustainability and environment

European Climate Prediction system



humanities and social sciences

ePODIUM
Early Prediction of Dyslexia in Infants Using Machine learning



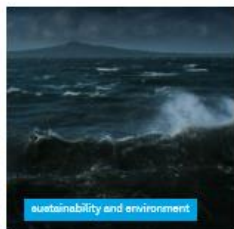
humanities and social sciences

Understanding visually grounded spoken language via multi-tasking
An alternative approach for intelligent systems to understand human speech



sustainability and environment

Monitoring tropical forest recovery capacity using RADAR Sentinel



sustainability and environment

MOSAIC
MOdelling Sea level And Inundation



science methodology

PROCESS
PROviding Computing solutions for



science methodology

Enhance Your Research Alliance (EYRA) Benchmark Platform

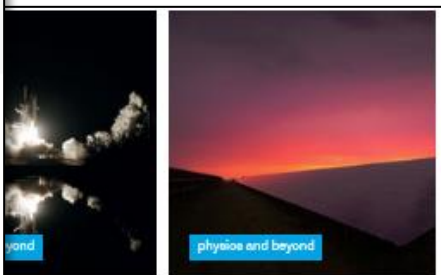
A phase field model to guide the development and design of next generation solid-state-batteries
Safer batteries with higher energy densities

Integrated omics analysis for small molecule-mediated host-microbiome interactions
Advancing our understanding of molecular mechanisms of health and

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

Stochastic Multiscale Climate Models
Coupling an implicit low-resolution model to an explicit high-resolution ocean model

www.esciencecenter.nl/projects



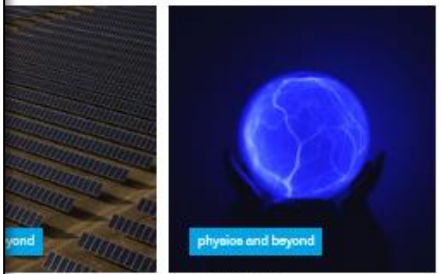
yond

Velocity simulations of phase flows at sea level



physics and beyond

Computation of the Optical Properties of nano structures
Accurate and Efficient Computation of the Optical Properties of Nanostructures for Improved Photovol



yond

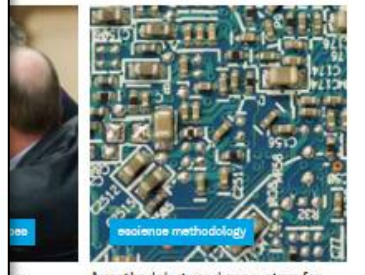
physics and beyond

Passing XSAMS
New tools for researchers in plasma, combustion and chemical reactor science



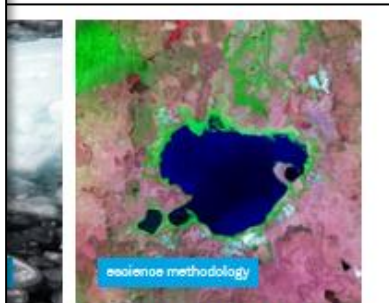
science methodology

EviDENce
Ego Documents Events modelling - how individuals recall mass violence.



science methodology

A methodology and ecosystem for many-core programming
Boosting the performance of current and future programs



climate

Visual Storytelling of Big Imaging Data
Storytelling as a means of visual data communication



Twitter

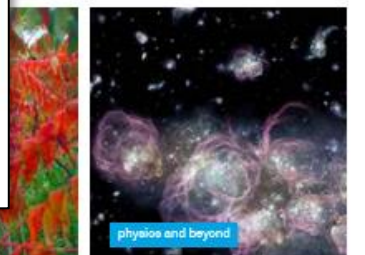
science methodology

Data quality in a distributed learning environment
Vast amounts of data to improve cancer treatment decisions



yond

sustainability and environment



science methodology

Data quality in a distributed learning environment
Vast amounts of data to improve cancer treatment decisions

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

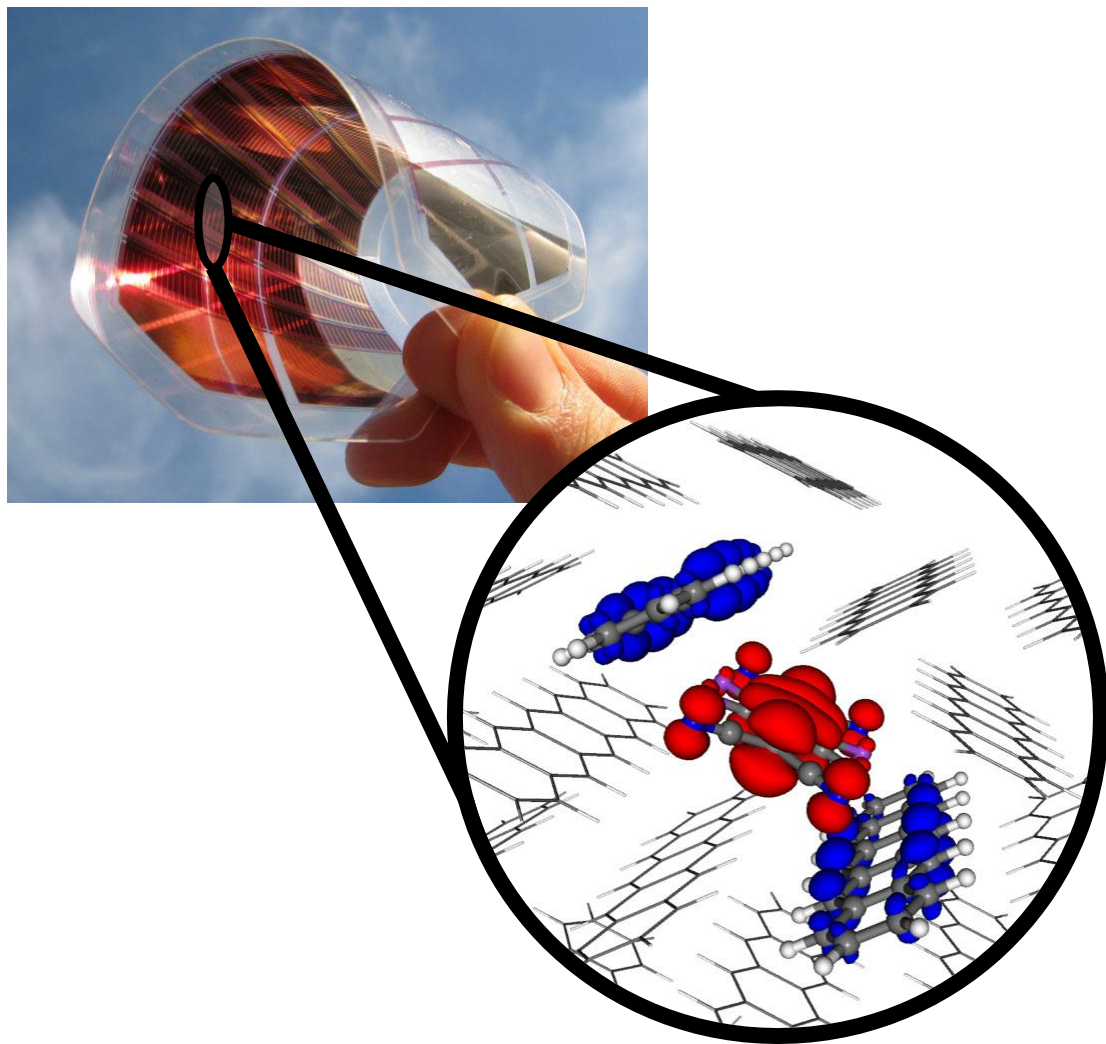
- Understand how molecular systems harvest energy from the sun and how energy propagates in these materials
- Quantum Chemistry for energy applications



Alexey Lyulin

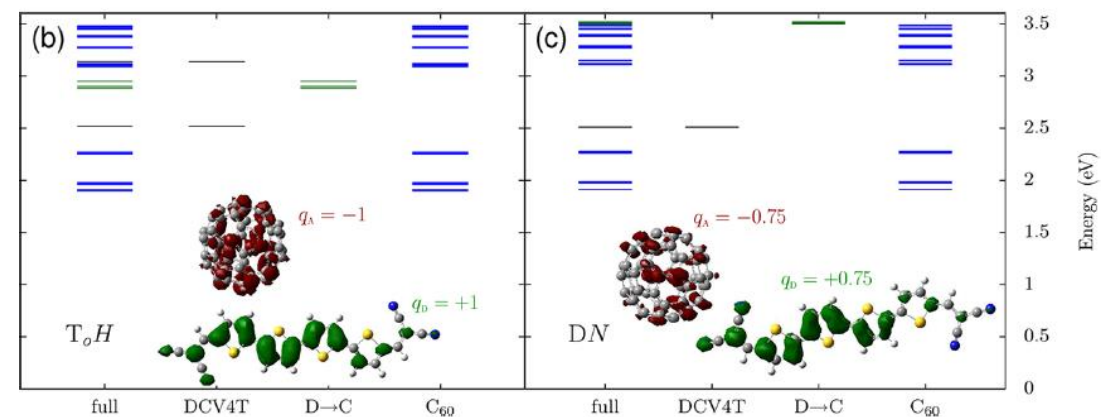


Bjoern Baumeier



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



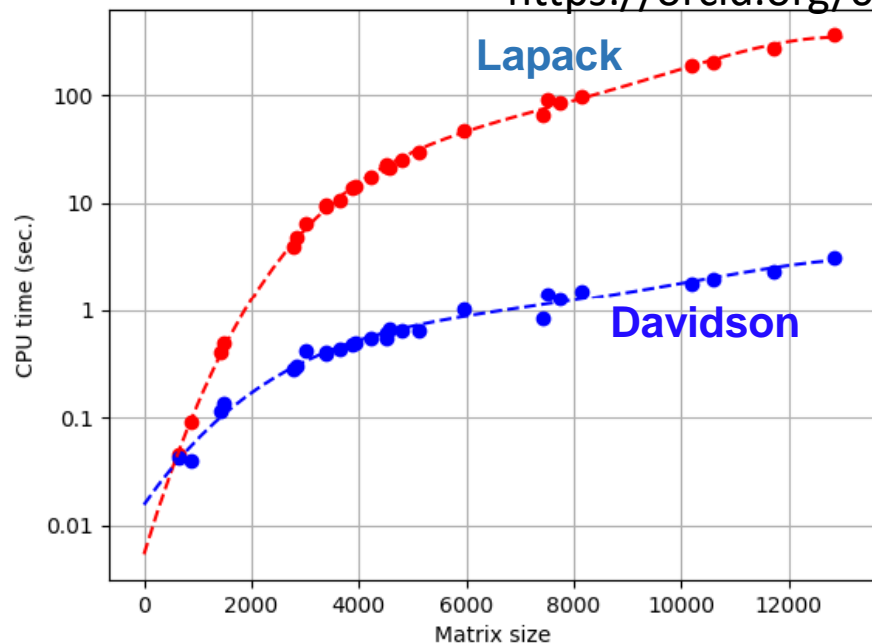
Diagonalization of large matrices

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

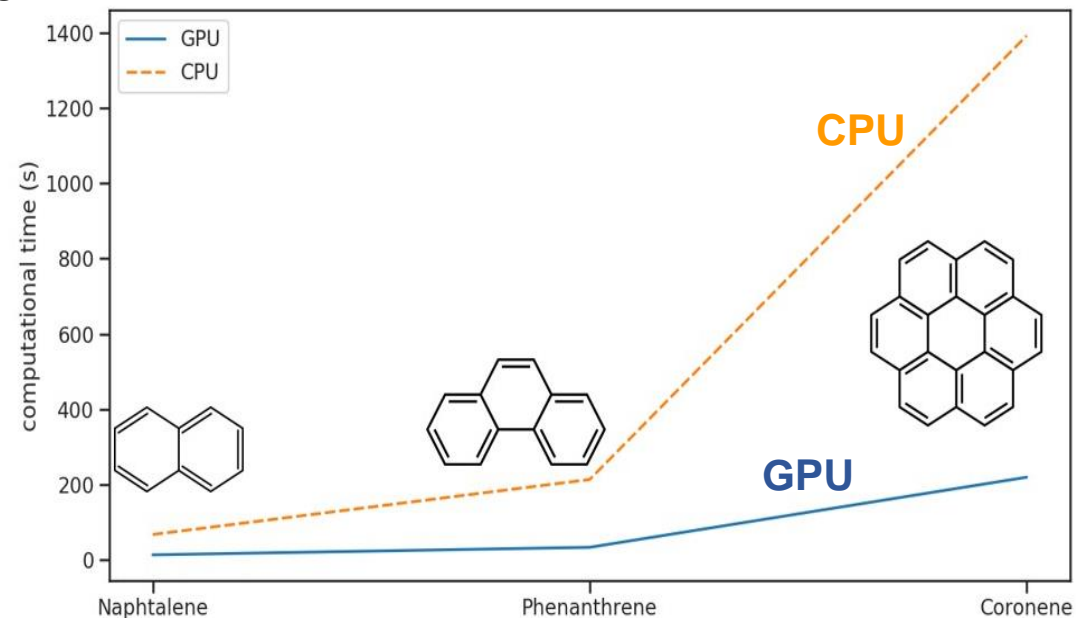




Photo by [Hello I'm Nik](#) on [Unsplash](#)

Retina COVID19

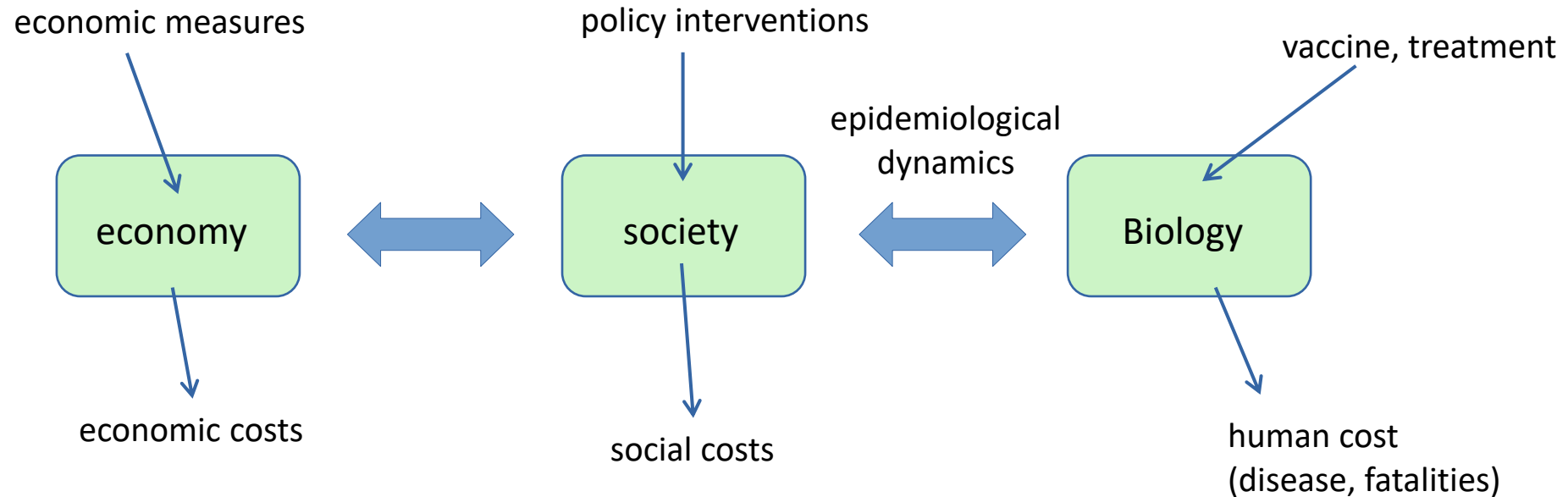
Real Time National Policy Adjustment and Evaluation on the basis of a computational model for COVID19

- Economic & social costs of social distancing measures



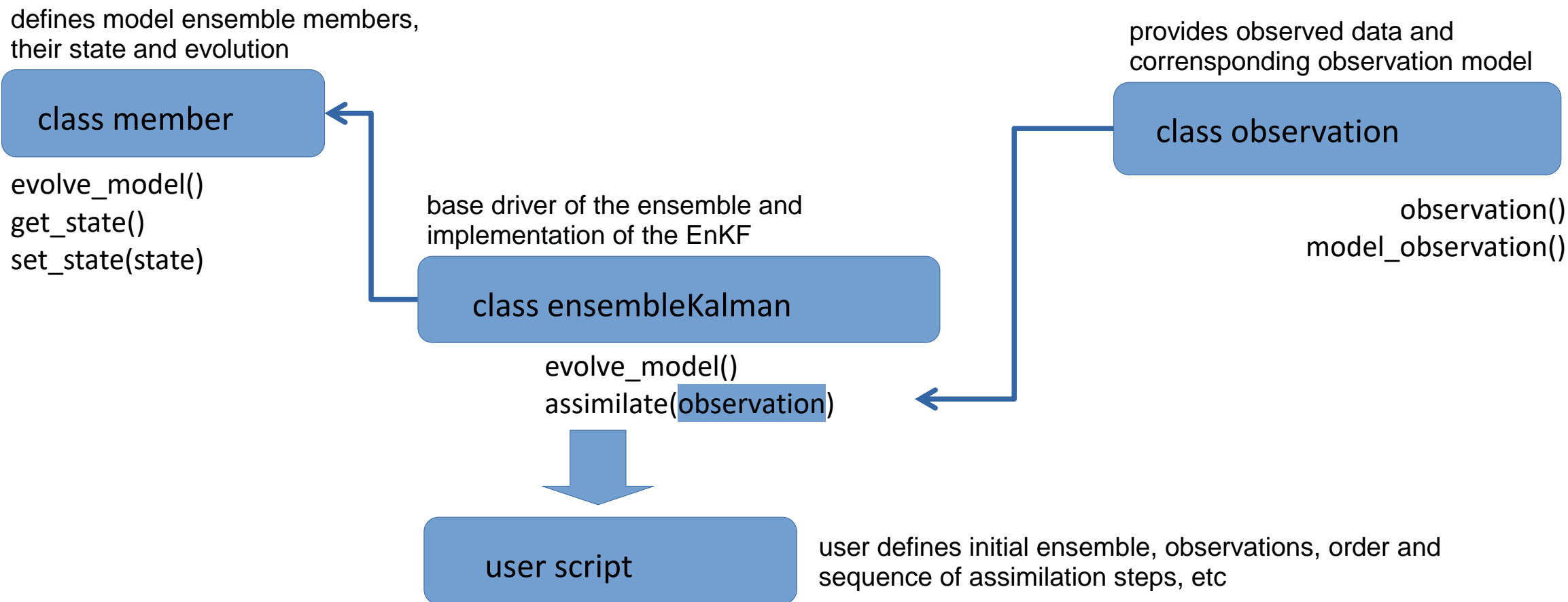
Prof. Martin Bootsma

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

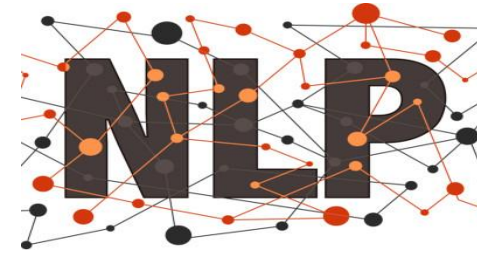


→the implementation and use of EnKF is easy, but the real devil is in the details of the choice of the state variables, observation function and the model for observation and state errors....

Special Interest Groups

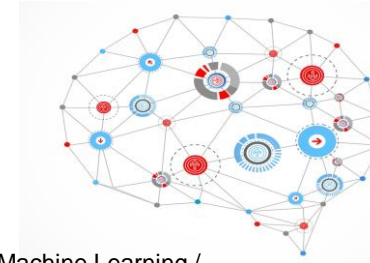
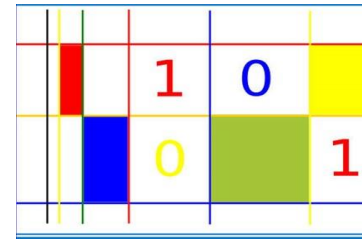
- Stay up to date with the state of the art
- Coordinate use of technology in projects
- Recently: more external engagement
- Knowledge dissemination
 - workshops, hackathons, tutorials, etc.

Natural Language Processing



Statistics / Data Mining

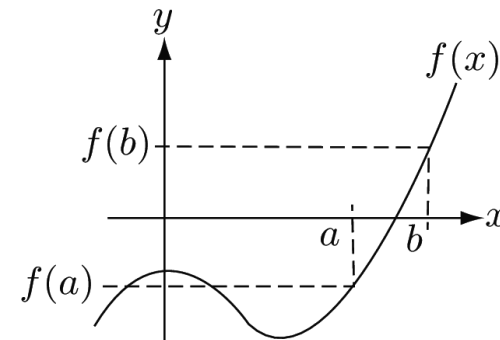
Data



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

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



Mateusz Kuzak
eScience research engineer



nlesc
/estep-checklist



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

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The checklist grew into a guide



<https://guide.esciencecenter.nl/>

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](#)

- **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

Scriberia 

What's in the Guide

**How we do it at the Center
Internal Guide**

**Universal information
for all RSEs and researchers writing code**

Guide

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

The Turing Way Contribution

- **Universal content**

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**

- **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.

