netherlands eScience center

Portable HPC workflows & software re-use

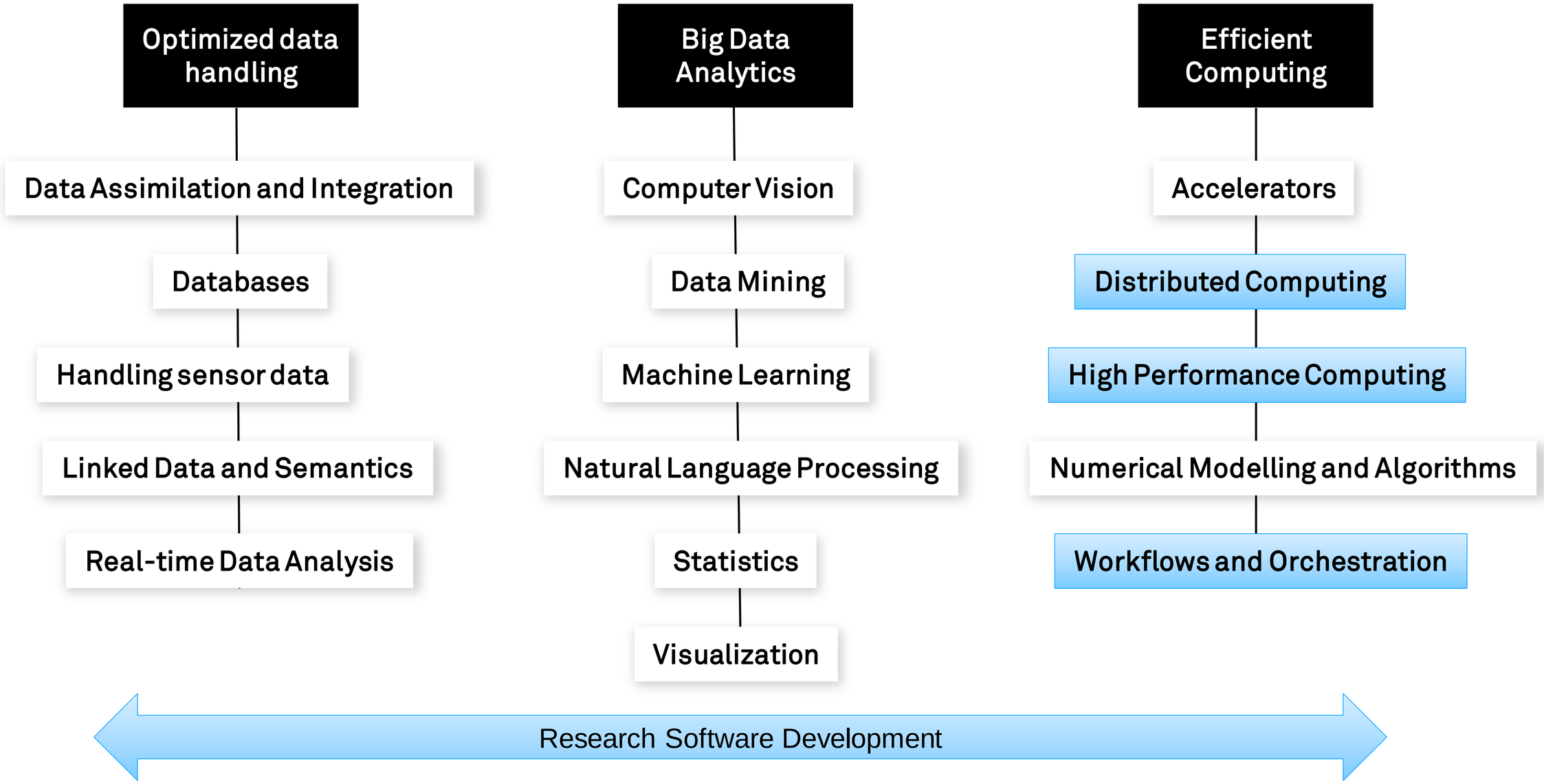
Arnold Kuzniar
eScience research engineer

a.kuzniar@esciencecenter.nl

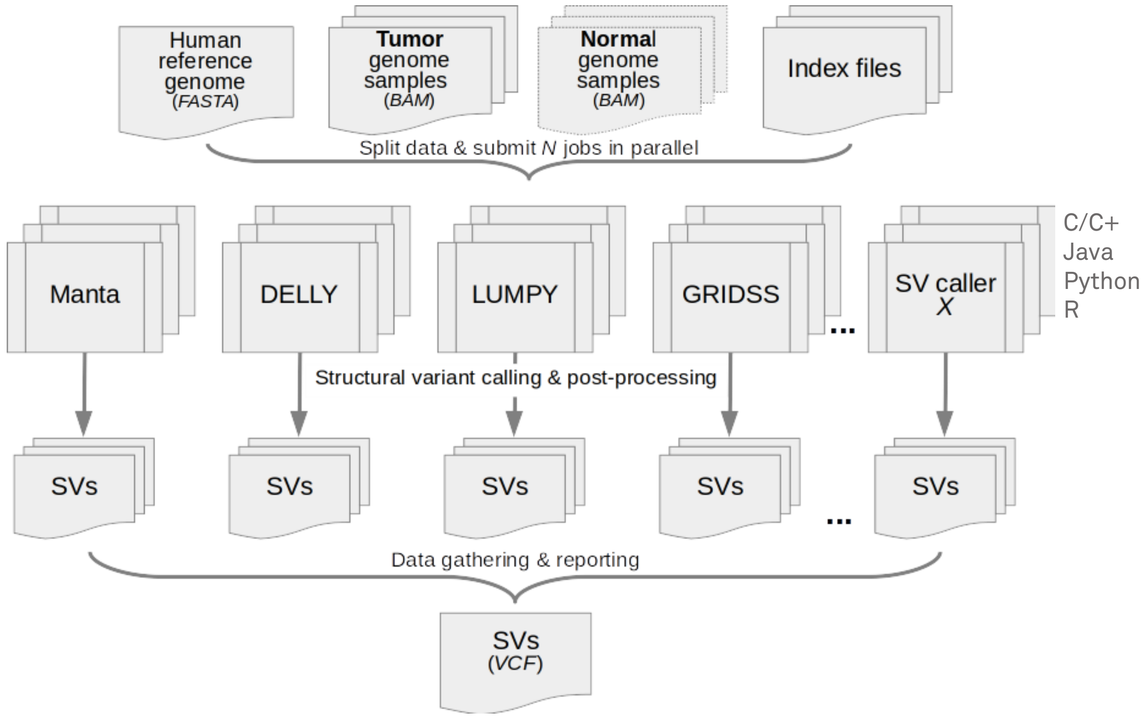
www.esciencecenter.nl

19/06/2019

Our expertise in collaborative research



Example from Life Sciences | Highly portable genomics workflow



Big challenge!

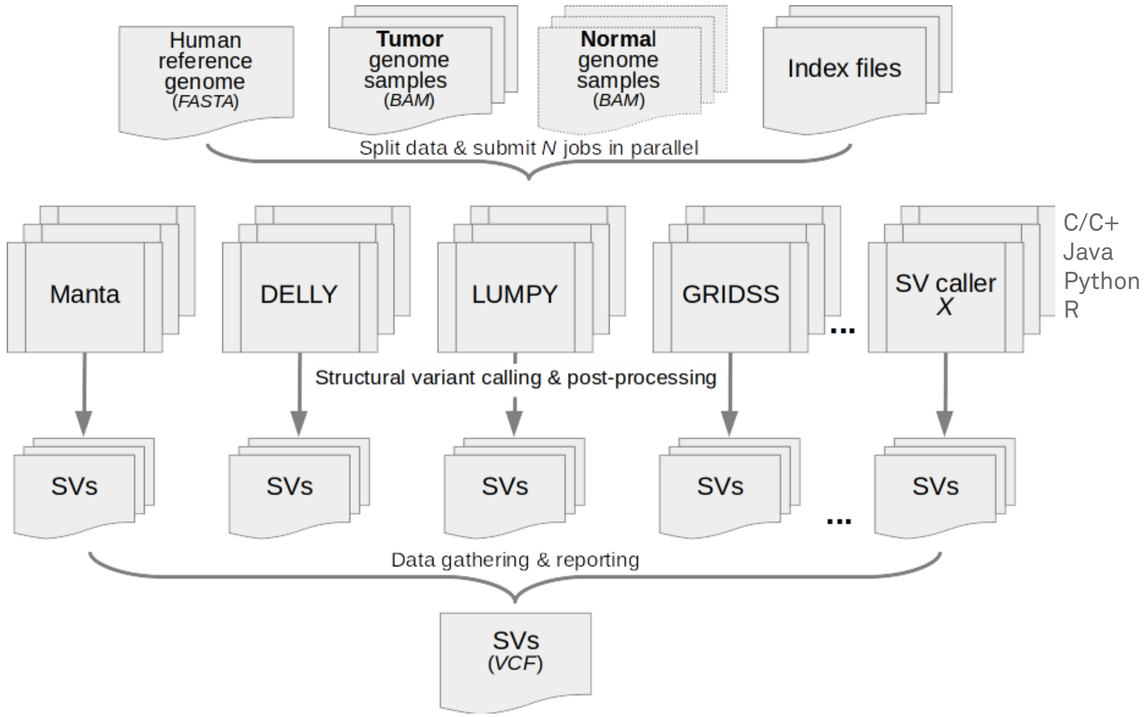
supercomputer / HPC cluster / cloud

SURF SARA

DAS 5

Utrecht Bioinformatics Center

Example from Life Sciences | Highly portable genomics workflow



Snakemake (CWL)

CONDA

XENON

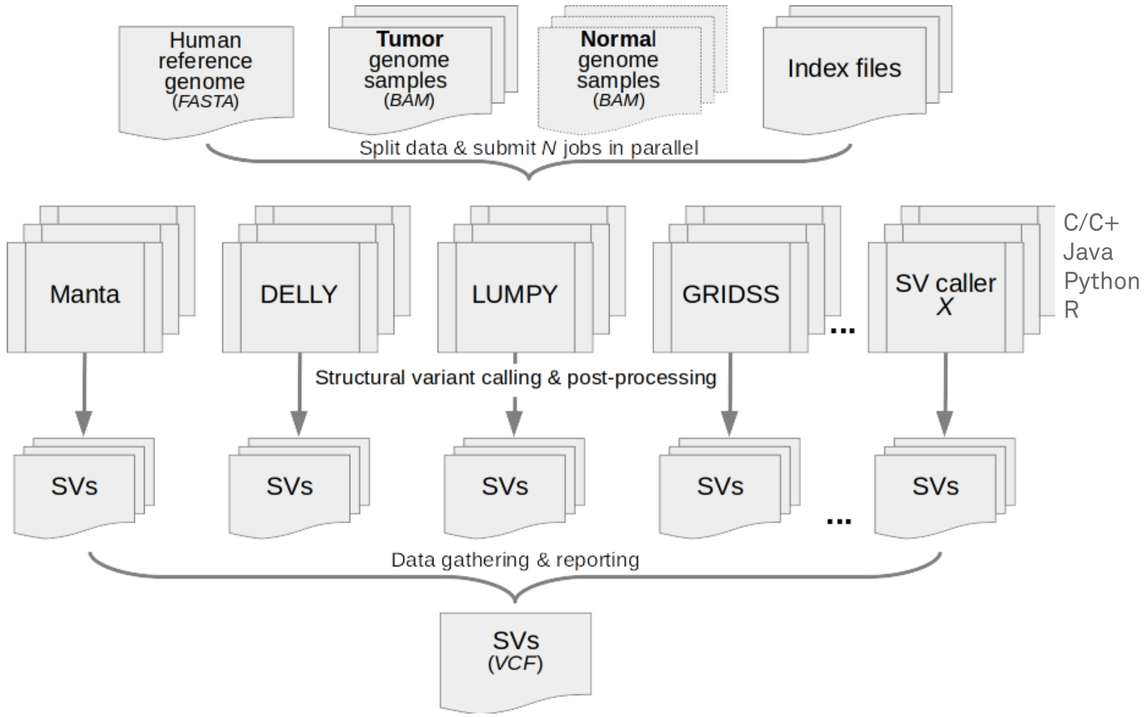
supercomputer / HPC cluster / cloud

SURF SARA

DAS 5

Utrecht Bioinformatics Center

Example from Life Sciences | Highly portable genomics workflow



- Enabling portable & reproducible analyses
- Making tools easy to use / extend / deploy
- Following SWE best practices

Snakemake (CWL)

CONDA

XENON

supercomputer / HPC cluster / cloud

SURF SARA

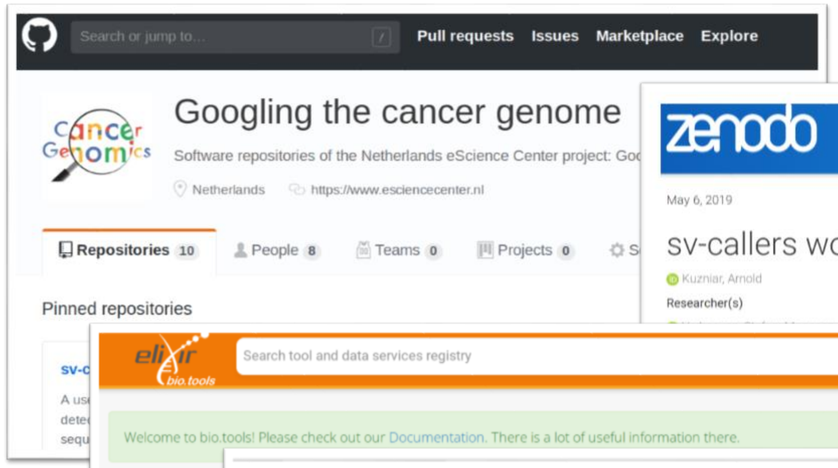
DAS 5

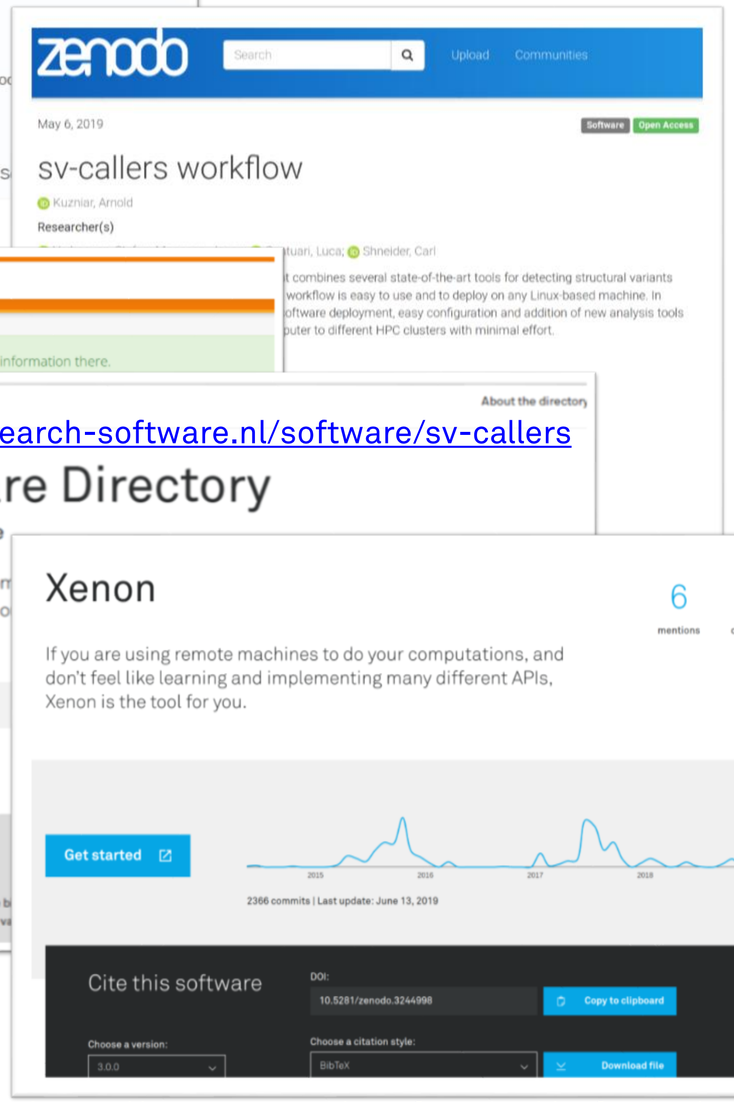
Utrecht Bioinformatics Center

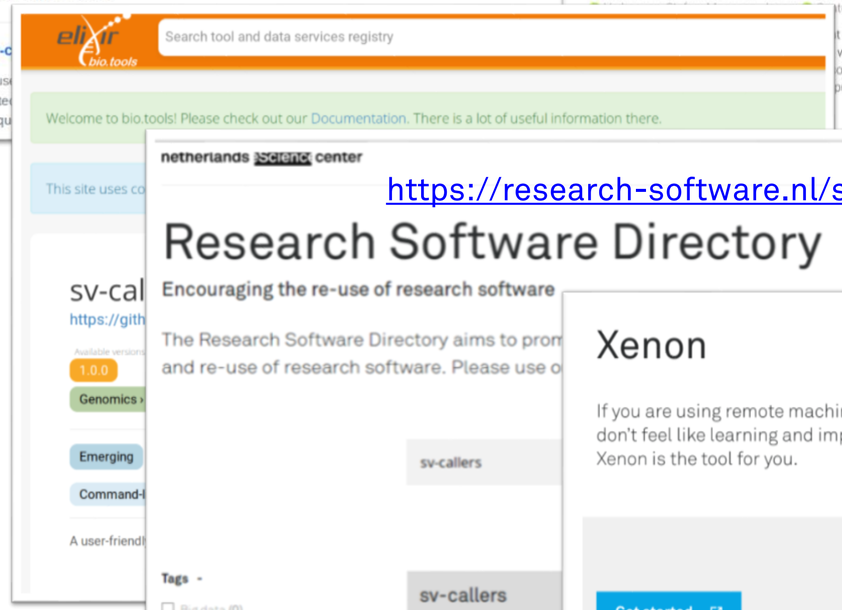
Googling the cancer genome — UMC Utrecht
Chemo-informatics for metabolite identification — WAGENINGEN UR For quality of life
The evolution of start clusters — Universiteit Leiden
Predicting sea level changes — Utrecht University
Mapping the Via Appia in 3D — VU University Amsterdam
. . .

Software re-use @eScience center

It's Open Science...

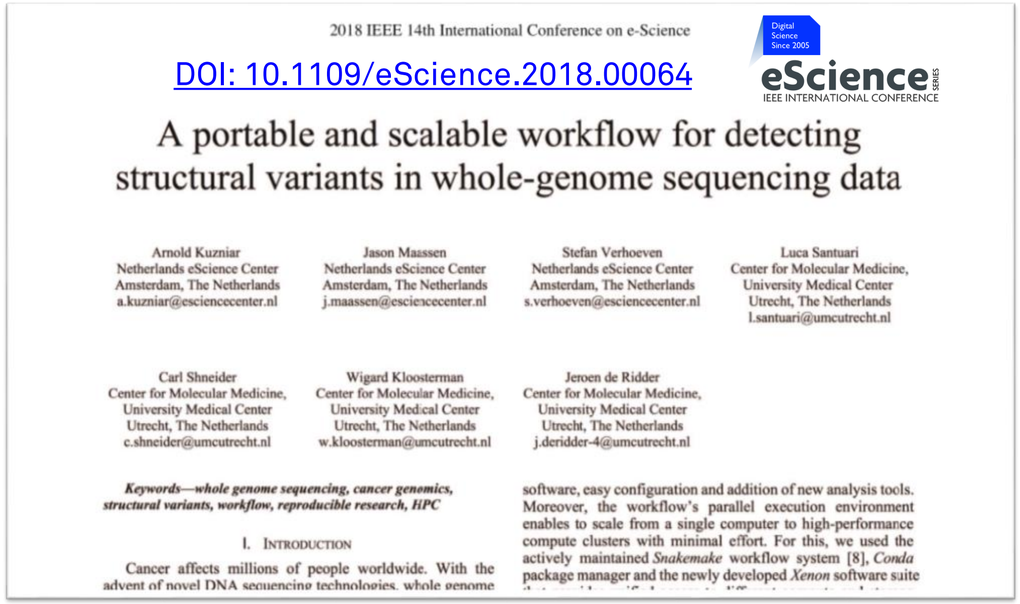






https://research-software.nl/software/sv-callers

https://www.research-software.nl/software/xenon



https://blog.esciencecenter.nl/