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Clinical Trials Use Case

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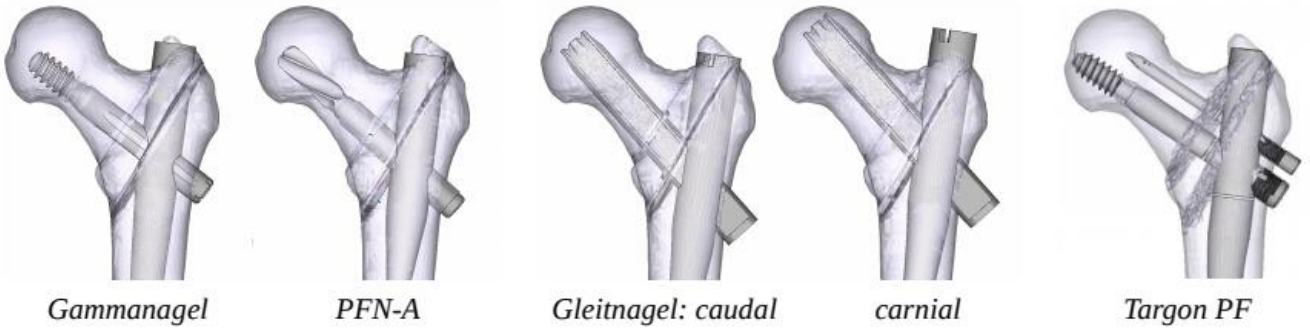
SODALITE Final Event

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 825480.

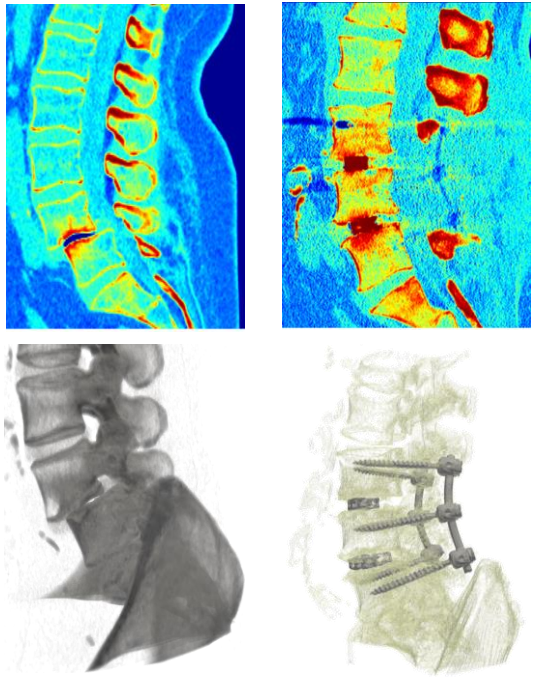
Virtual Clinical Trials

- Clinical trials with ***"real"*** patients are ***time-consuming and expensive***.
- Every patient is ***different and results can not be generalized***.
- Virtual clinical trials reproduce clinical trials by means of simulation.
  - Simulations are applied to virtual patient cohorts.
  - The UC represents research to advance this frontier.



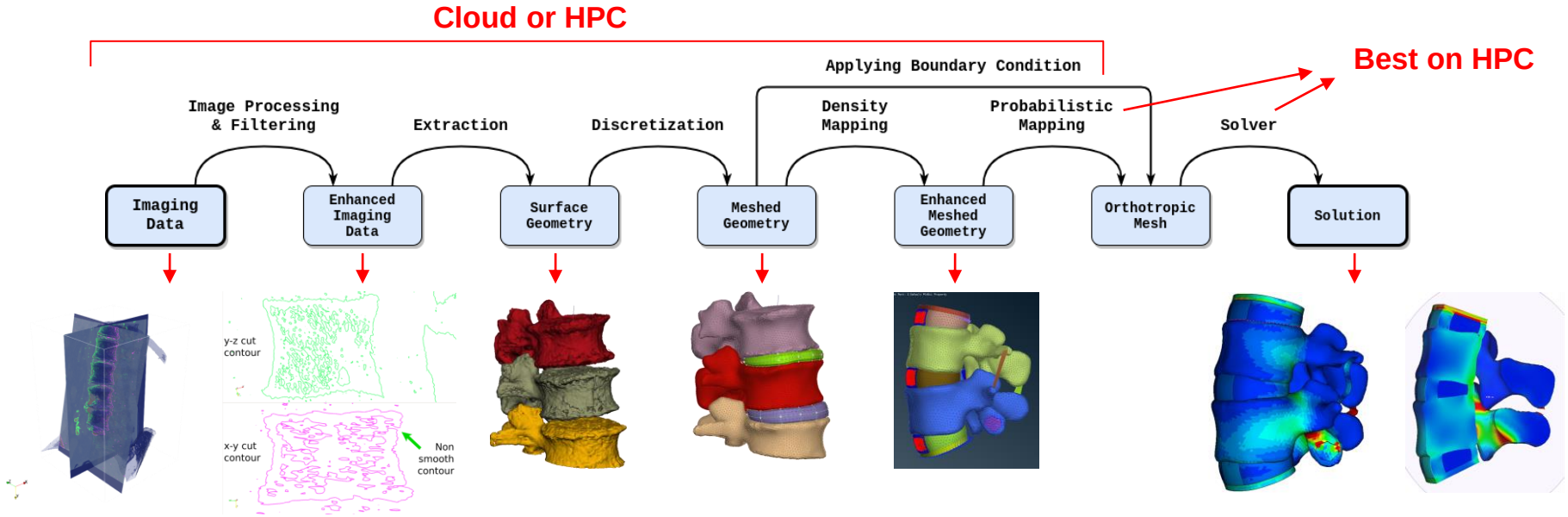
Medical Problem

- Some spinal conditions (e.g. disk displacement or prolapse) can only be treated ***operatively***. A common treatment is mono- or bisegmental ***fusion of the lumbar spine***.
- ***A screw-rod fixation bone implant system*** is used to fix parts of the lumbar spine.
- Biomechanical implant ***development*** is down to the present day ***done on empirical basis***
- Selection of type, size and placement position is done ***based on experience***
- ***Implant optimization is complicated***



Before and after the fixation

Workflow



CT-scan

Strain and stress distribution within the simulated structure

Requirements

A scientific workflow, composed of multiple integrated components, with ***efficient data processing*** over ***heterogeneous infrastructure***.
Efficient development and failure management. During a development cycle, a failed simulation should be ***debugged*** and ***restarted*** from the failed component, ***not running the whole chain*** again.
Data processing tasks are not finally defined and ***may change and get more complicated*** as the methodology of clinical virtual trials evolves: e.g. new data analytics component are likely to be introduced.
Efficient uncertainty quantification (currently done ***manually***), which is not only needed in this special case but is widely sought after nowadays.
Evaluation in terms of ***execution time/cost/power*** over ***various infrastructures and computing centers***.

Deployment problem

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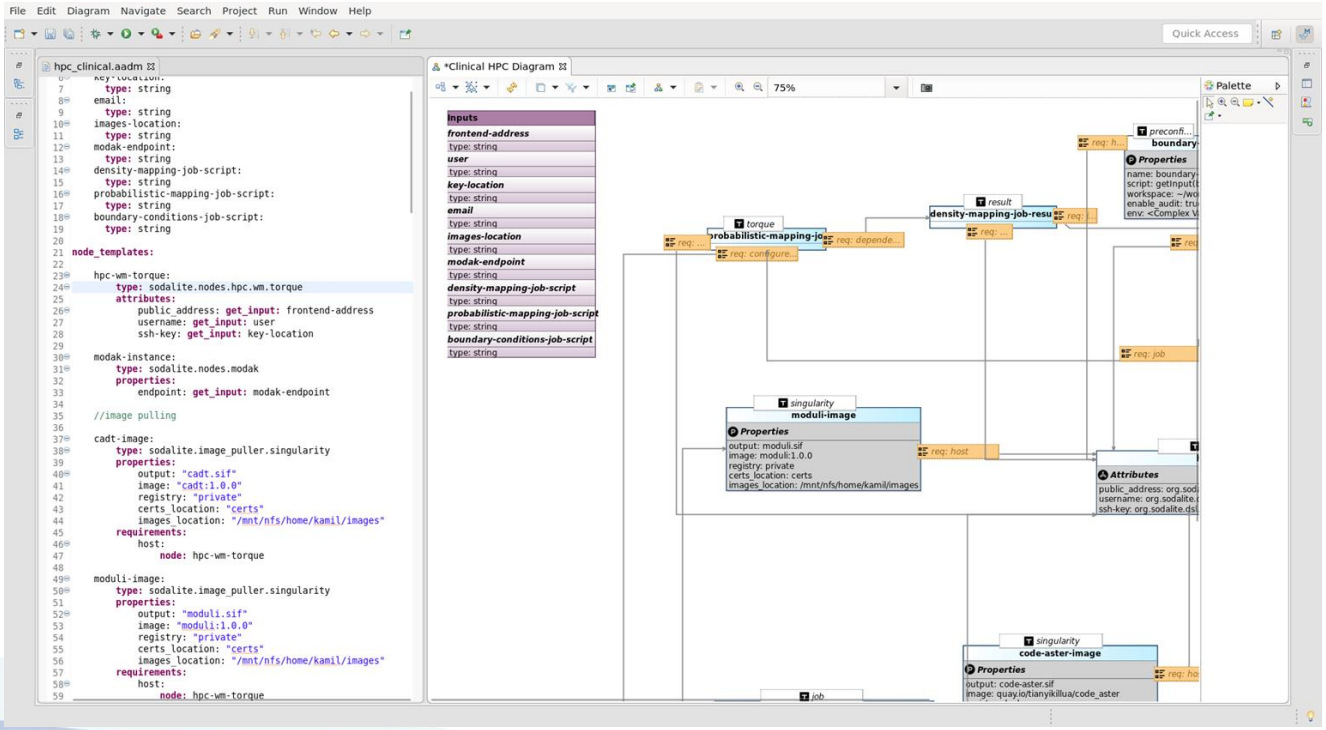
Current methodology of in-silico clinical trials in biomechanical simulations is not productive:

- Requires effectiveness in deployment, management and adaption to different IT-infrastructures (SC, Cloud, HW Heterogeneity)
- Requires ease-of-use for end users (medical device manufacturers or medical research institutes) and reduced effort of the developers.

→ DevOps practices shall be adopted: IaC-based abstraction, flexibility, portability, reduced cost and effort

Smart modeling



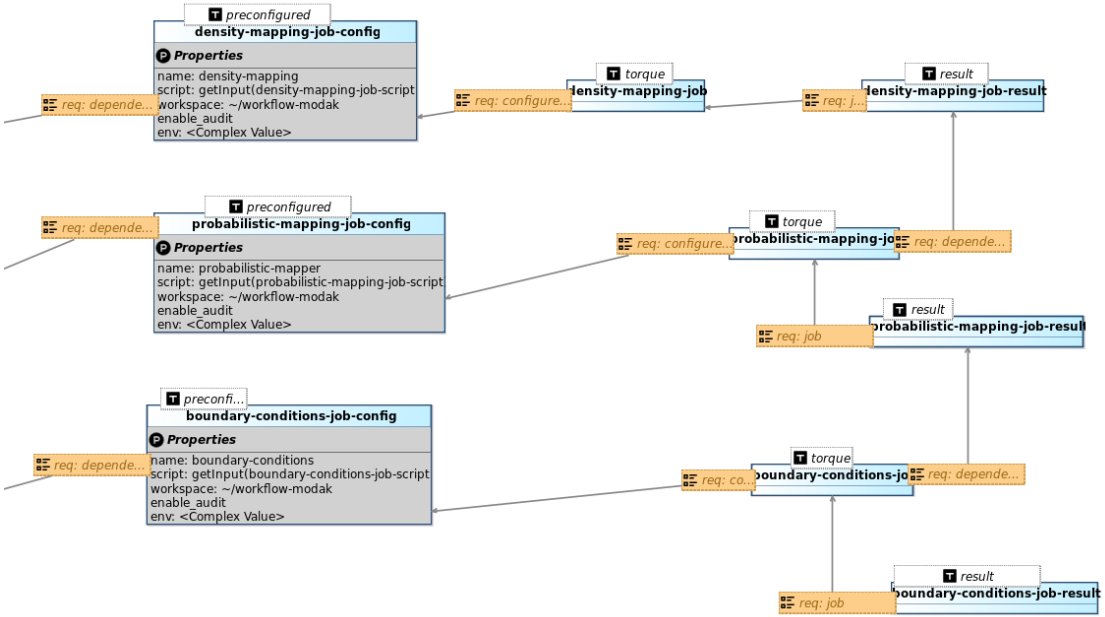
IDE demo: https://www.youtube.com/watch?v=8YC11JFSWC4

Workflow modeling

```yaml
density-mapping-job-config:
  type: sodalite.nodes.hpc.job.torque.preconfigured
  properties:
    name: "density-mapping"
    script: get_input: density-mapping-script
    workspace: "~/workflow"
    env:
      SINGULARITY_DIR: "/home/kamil/images"
  requirements:
    host:
      node: hpc-wm-torque

density-mapping-job:
  type: sodalite.nodes.hpc.job.torque
  requirements:
    host:
      node: hpc-wm-torque
    configured_job:
      node: density-mapping-job-config

probabilistic-mapping-job:
  type: sodalite.nodes.hpc.job.torque
  requirements:
    host:
      node: hpc-wm-torque
    configured_job:
      node: probabilistic-mapping-job-config
    dependency:
      node: density-mapping-job-result
```



Full description can be found in IDE GitHub [here]

Demo can be found - https://www.youtube.com/watch?v=5bj-gMfiirE

Improvements due to SODALITE

Modelling	Workflow execution	Optimisation
Simplified modelling	From single HPC target to multi-target	Traditional HPC optimization (Code_Aster Solver - 25% faster execution over baseline container available on github/dockerhub)
Effort reduction for deployment code development	PBS, Slurm, OpenStack, AWS	Adaptive optimization into different targets (Probabilistic Mapper can be deployed on different MPI implementations - OpenMPI and MPICH)

Exploitation Plan

- Developments will directly enter research activities in
  - Material model development
  - Development of contact models for screw fixations in bones
- Principles and Components with respect to data access will
  - be exploited in follow up projects and collaborations
  - ease data exchange with medical device manufacturers and hospitals
- Developments will be applied in the “Medical Solution Center”
  - Activity of HLRS & SICOS-BW to promote HPC to SMEs in the area of medical device manufacturing and medical engineering

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