Centre for Computational
Personalised Medicine
International Research Foundation

We create computational technologies for optimised healthcare

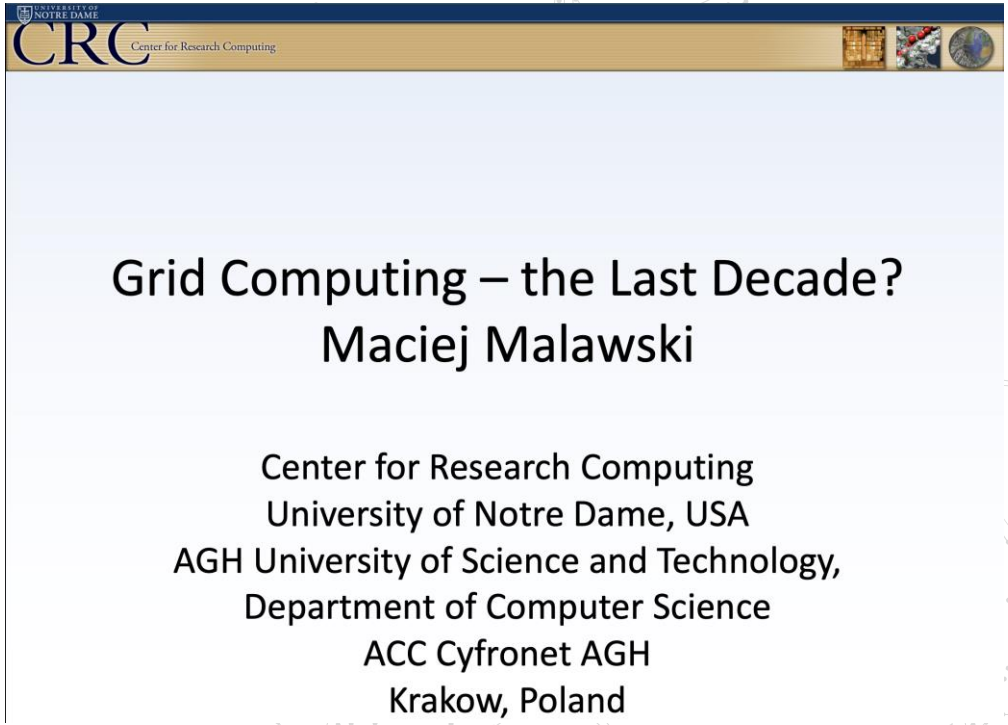
Digital Twins in Computational Medicine Large Scale Computing and Virtual Reality

Maciej Malawski
Sano Centre and AGH Krakow

21 December 2023 / Zakopane

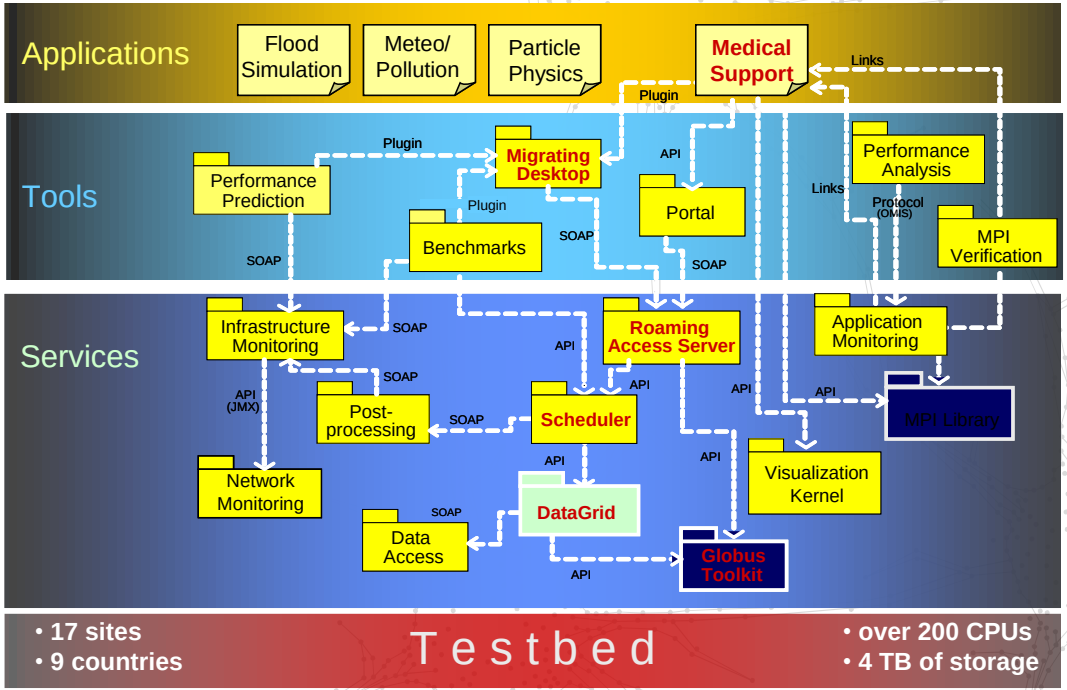
12 years ago

- From Grid to Cloud
- High levels of abstraction / programming -> Serverless computing



20 years ago - CrossGrid

- “Sister” project of GridLab
- “Interactive grid”
- Particle physics
- Medical applications

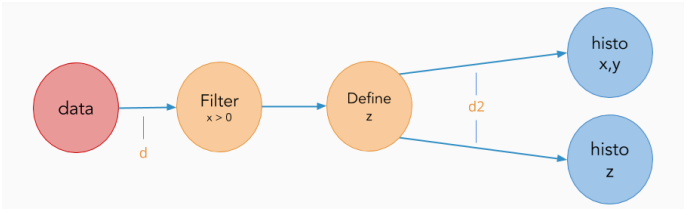


sano

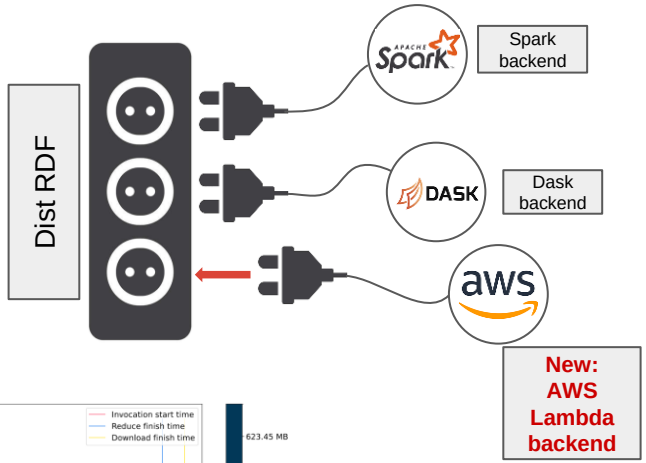
Serverless computing
High-level abstractions

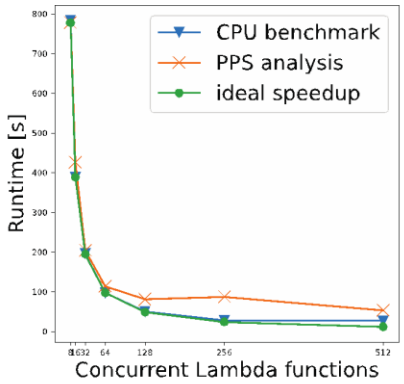
Serverless computing for High Energy Physics Speedup from hours to minutes + Jupyter interface = interactivity

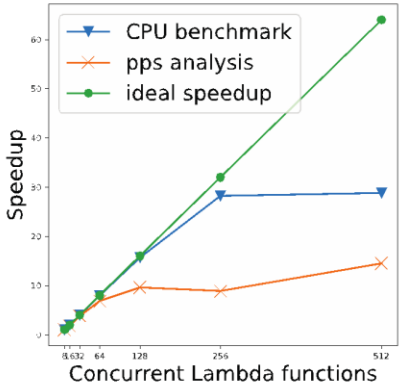
- ROOT C++ analysis framework https://root.cern
- RDataFrame in Python
- Experiments on data from CMS (Compact Muon Solenoid) experiment at CERN

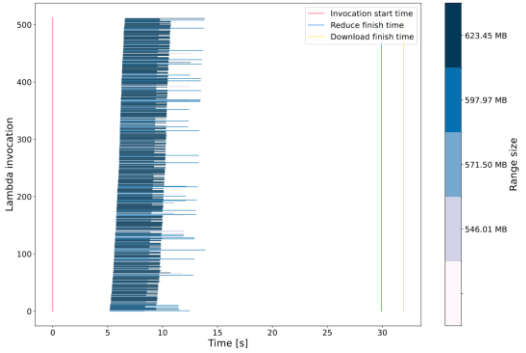



```
// d2 is a new data-frame, a transformed version of d
auto d2 = d.Filter("x > 0")
           .Define("z","x*x + y*y");
// make histograms out of it
auto hz = d2.Histo1D("z");
auto hxy = d2.Histo2D({"hxy","hxy",16,-1,1,64,-1,1},"x","y");
```









Jacek Kusnierz, Vincenzo Eduardo Padulano, Maciej Malawski, Kamil Burkiewicz, Enric Tejedor Saavedra, Pedro Alonso-Jordá, Michael Pitt, Valentina Avati: A Serverless Engine for High Energy Physics Distributed Analysis. CCGRID 2022: 575-584

Medical applications

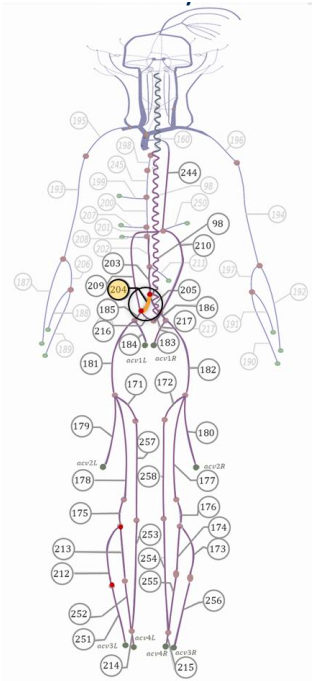
Computing

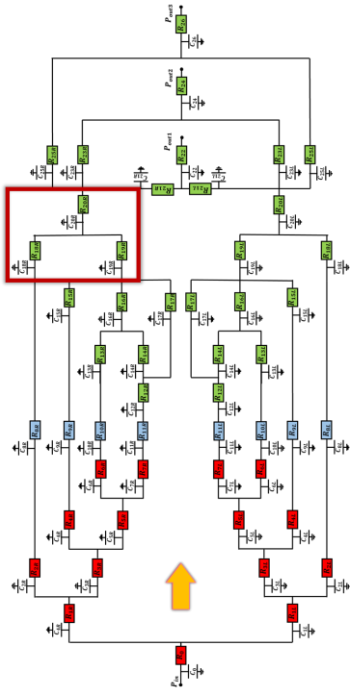
Sano – Centre for Computational Medicine

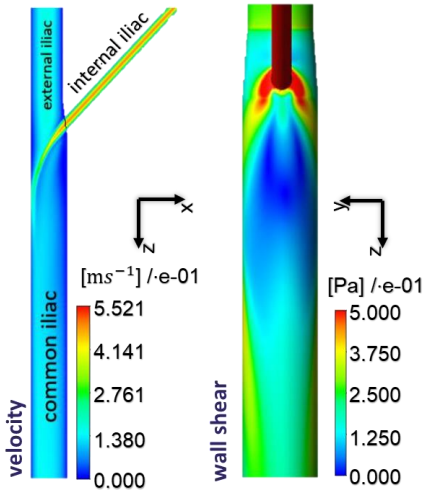
New research institution in Krakow
European Centre of Excelence
5 research Teams
100 People

Digital Twin / Virtual Human Twin (VHT)

- Digital, mathematical representation of human body
- VHT is an infrastructure that makes it easier to develop and validate digital twins.







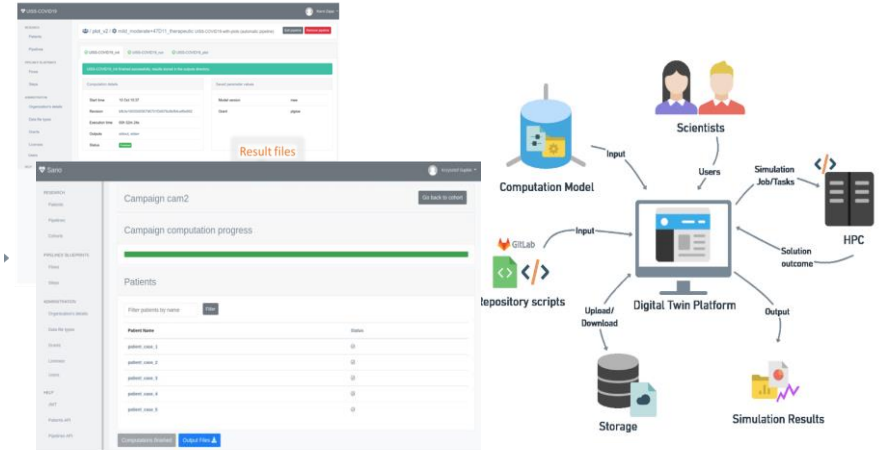
M. Otta – PhD Student

Platform for Simulations of Digital Twins
Model Execution Environment

Jan Meizner, Karol Zając, Adam Nowak, Krzysztof Gądek, Piotr Nowakowski

- Web-based system for management of multi-step computational pipelines on HPC systems
- Patient data-centered workflows:
  - Steps -> Pipelines -> Campaigns
  - Patients -> Cohorts
- Models implemented as software artifacts
  - Versioning: GitHub, GitLab
  - Comparison of results
  - **Reproducibility** -> Robust Science
- File management (HPC storage, Cloud storage)
- Usage in In Silico World EU Project
- Collaboration with Univ. Bologna, Univ. van Amsterdam, KU Leuven
- **Example campaign: 10 000 simulation runs** of BoneStrength application (osteoporosis)

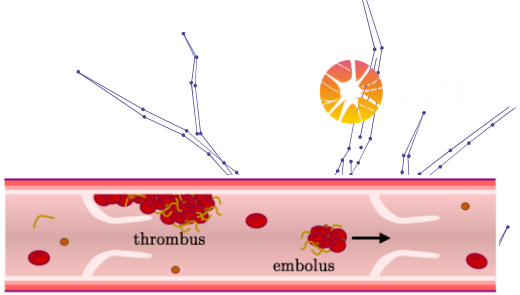
- https://mee.cyfronet.pl/



Marek Kasztelnik, Piotr Nowakowski, Jan Meizner, Maciej Malawski, Adam Nowak, Krzysztof Gadek, Karol Zajac, Antonino Amedeo La Mattina, Marian Bubak: Digital Twin Simulation Development and Execution on HPC Infrastructures. ICCS (2) 2023: 18-32

Verification, Validation, Uncertainty Quantification of simulation models

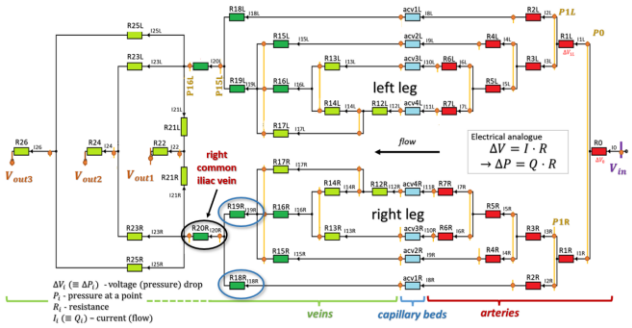
Magdalena Otta, Piotr Kica

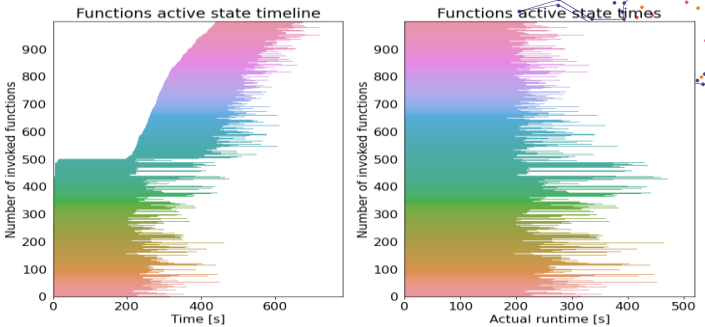


- 0D, 1D, 3D models of cardiovascular systems
- Example: Venous modelling to inform treatment of patients presenting with lower limb thrombosis (PhD project with University of Sheffield)
- VVUQ, Sensitivity analysis - required in the regulatory process of model certification
- Large parameter studies
  - 50 000 parameters -> tasks
- CloudVVUQ library using serverless computing, based on EasyVVUQ library
- Total time to compute locally ≈ **76.1h**
- Total time to compute using Google Cloud ≈ **12.5min**

- https://github.com/SanoScience/CloudVVUQ

Piotr Kica, Magdalena Otta, Krzysztof Czechowicz, Karol Zajac, Piotr Nowakowski, Andrew J. Narracott, Ian Halliday, Maciej Malawski: Serverless Approach to Sensitivity Analysis of Computational Models, CCGrid 2023





500 tasks running in parallel

AI and Virtual Reality

Medical applications

VR / AR

- On-line games
- Virtual „friends”

https://venturebeat.com/games/5-ways-to-build-the-mobile-gaming-metaverse/

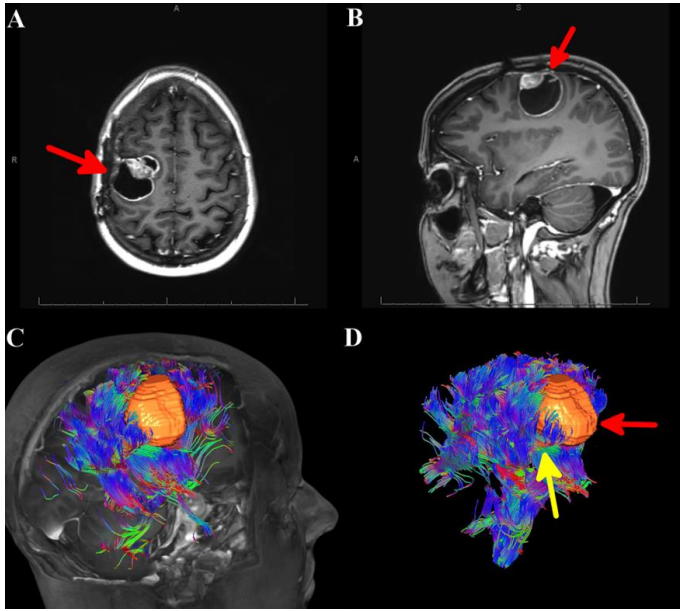
https://www.wired.com/story/what-is-the-metaverse/

https://replika.com/

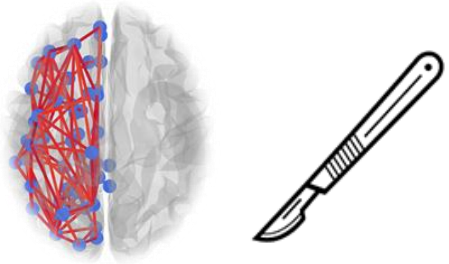
Brain tumor surgical planning and prediction

Joan Falco-Roget, Alex Crimi et al.

- A trained model is able to predict the brain connectivity of patients post-surgery and recovery
- Collaborations: University of Ghent for data, University of Messina and Padua for clinical support



"Bayesian Filtered Generation of Post-surgical Brain Connectomes on Tumor Patients" J. Roget Falco, F. Sambataro, A. Cacciola, A. Crimi
MICCAI 2022
https://link.springer.com/chapter/10.1007/978-3-031-21083-9_8
"Structural Reorganization Following a Brain Tumor: A Machine Learning Study Considering Desynchronized Functional Oscillations"
Nature Communication (to submit minor revision)
https://www.biorxiv.org/content/10.1101/2022.11.14.516248v2.abstract



Pre-surgery planning to avoid aphasia/motor deficict

Brain tumor surgical planning and prediction

Bartlomiej Ksiazek, Jan Argasinski, Alex Crimi et al.

Ongoing translation into clinical practice by the University Hospital of Palermo.

AR Data mapping of data and connectome prediction from J. Falco-Roget et al.

UNIVERSITÀ DEGLI STUDI DI PALERMO

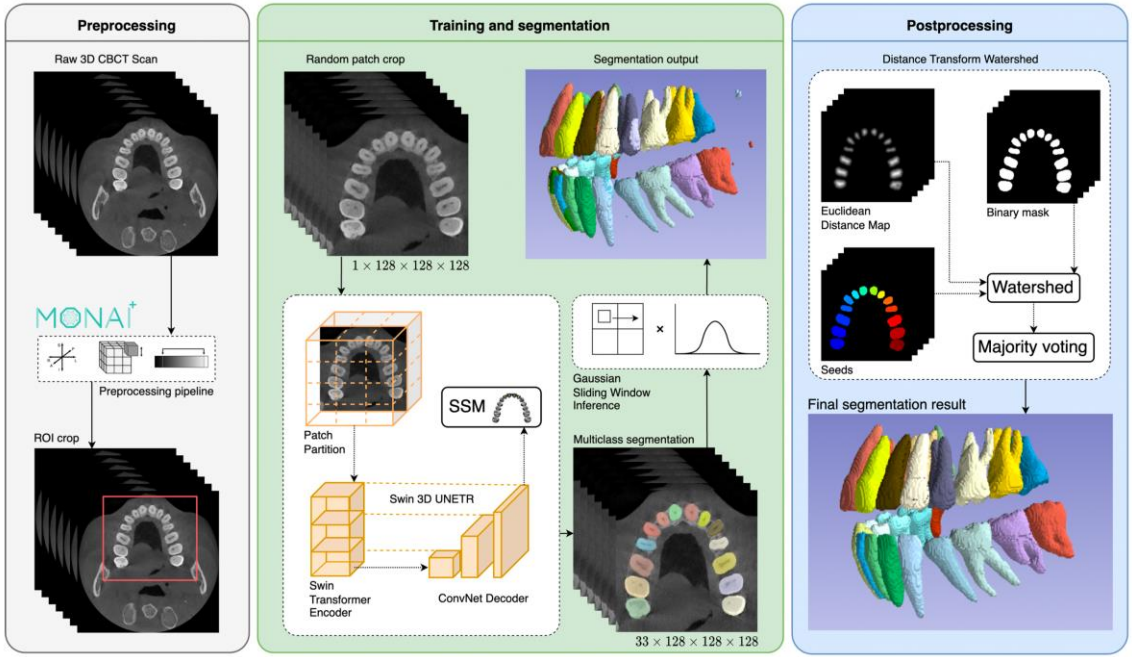
Orthodontic Treatment Planning

PhD Project by Tomasz Szczepański

Goal: Develop efficient automatic segmentation methods for CBCT scans to enhance orthodontic treatment planning due to the limitations of manual segmentation.

Research Results: Introduced a novel model for tooth segmentation and classification, utilizing global context and morphological insights from standard male and female dentition.

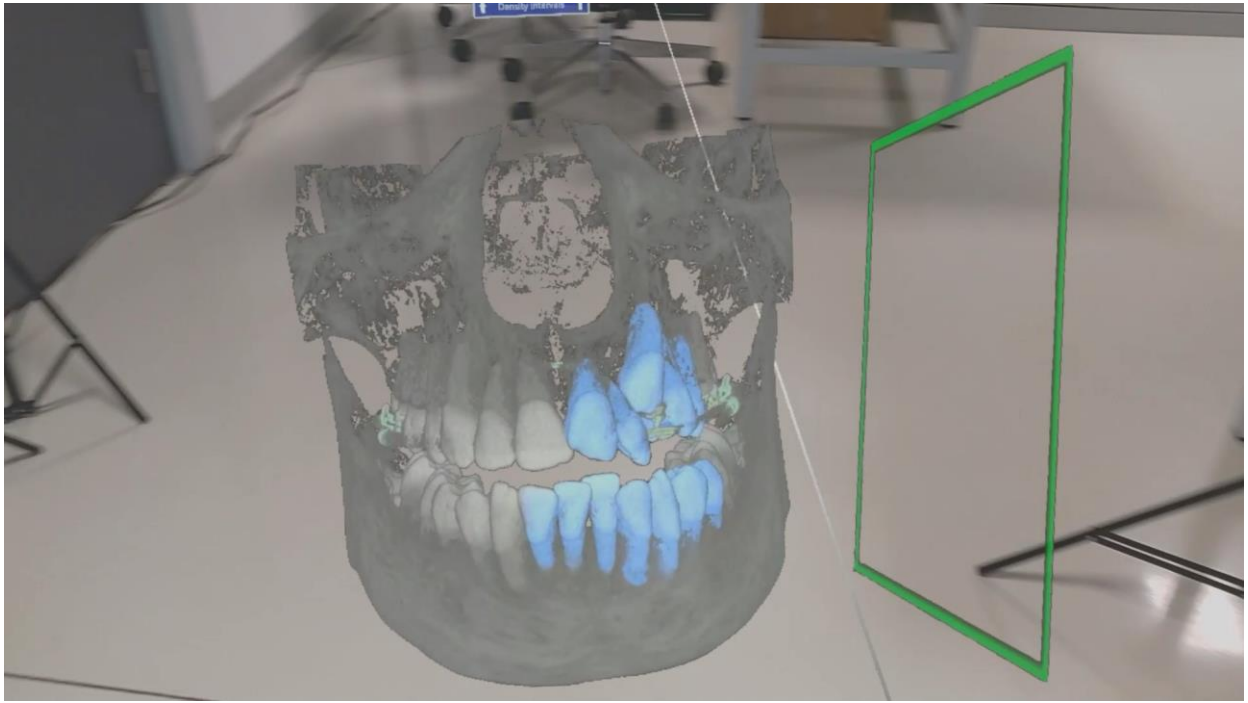
In cooperation with: Prof. Piotr Fudalej, President Elect of European Orthodontic Society, Collegium Medicum Jagiellonian University



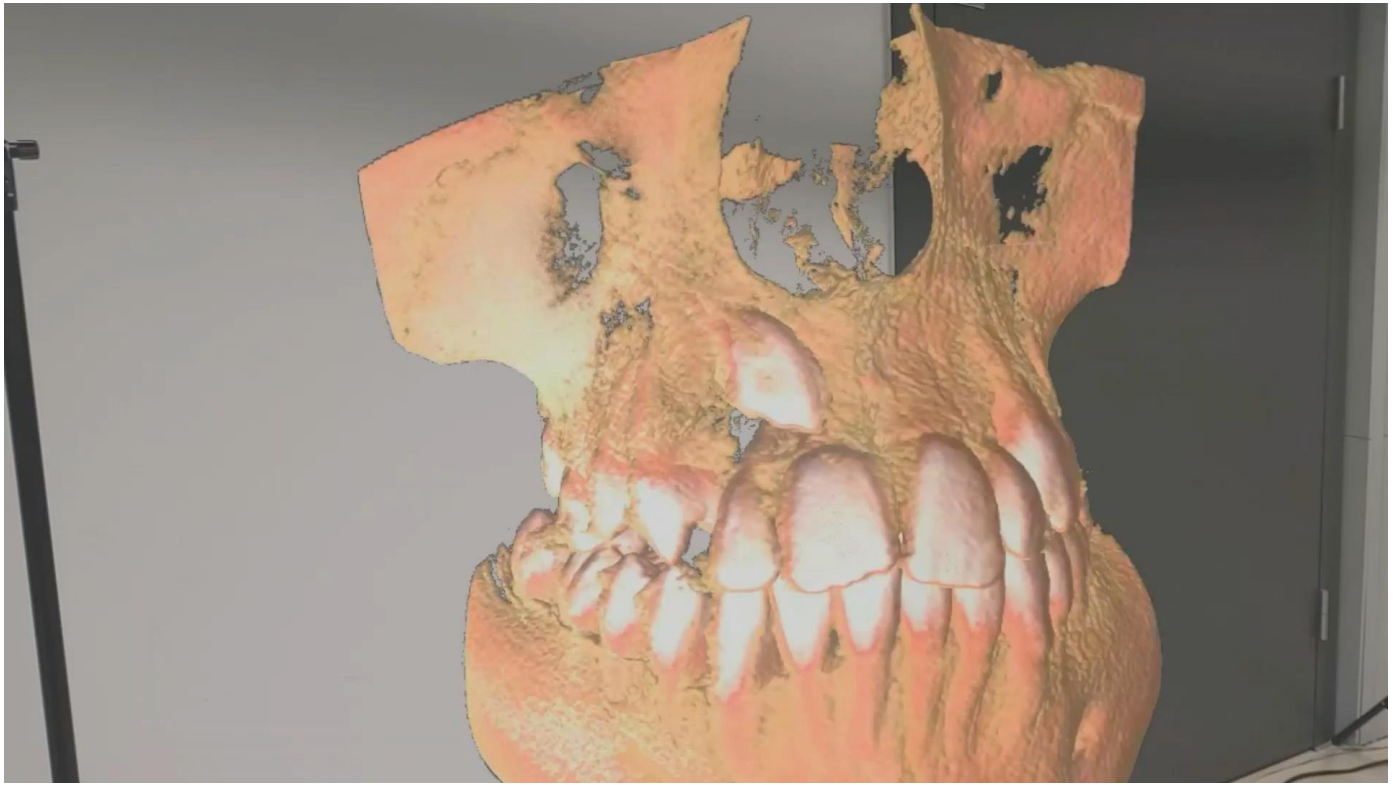
The overview of the proposed method. In pre-processing, we automatically extract teeth ROI from the CBCT scan. Then, we fed randomly cropped patches of ROI to the SwinUNETR, which is optimized with dentition-based loss leveraging a statistical shape model (SSM). In post-processing, we obtain the final segmentation result with watershed transform and majority voting.

Automatic tooth segmentation on CBCT using a machine learning algorithm, 24th Conference of Polish Orthodontic Society
Tooth Segmentation from CBCT Scans Using Dentition-Based Learning, Harvard Global Symposium on AI in Dentistry
DENTNet: 3D Tooth Instance Segmentation from CBCT Scans with Geometry Prior-Assisted Learning, 7th edition of ML in PL
Tomasz Szczepański, Szymon Płotka, Arleta Adamowicz, Piotr Fudalej, Przemysław Korzeniowski, Tomasz Trzciński, Arkadiusz Sitek

Example: tooth segmentation + AR



Example – orthodontic imaging



Virtual Reality Surgical Simulators

Przemysław Korzeniowski

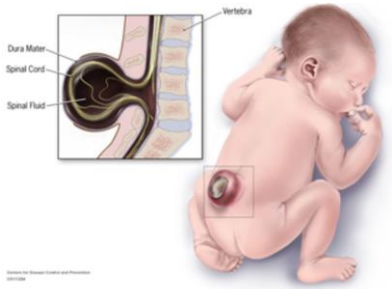
Goal: Given the challenges of fetoscopic Spina Bifida repair, there's a growing need for effective training. Computer-based VR simulation systems present a solution, offering a safe and adaptable training platform without ethical concerns.

Result: A simulation validation study, involving feedback from 14 clinicians, rated the system's realism at 4.07 out of 5. Its applicability for SB-repair training and laparoscopic skill acquisition received scores of 4.63 and 4.80, respectively.

Next Steps: There's an intent to refine the simulator based on clinician feedback and then pursue broader clinical research, such as skill transferability and construct validity evaluations.

In cooperation with: Dr Robert Biskupski-Brawura-Samaha, I Klinika Położnictwa i Ginekologii, Warsaw Medical University

Validation study participants



Spina Bifida

Simulator setup with haptic laparoscopic interface

Real (on the left) and simulated surgery (on the right)

Korzeniowski P, Plotka S, Brawura-Biskupski-Samaha R, Sitek A. *Virtual Reality Simulator for Fetoscopic Spina Bifida Repair Surgery*. IEEE/RSJ International Conference on Intelligent Robots and Systems 2022, CORE A

Fetoscopic Spina Bifida Repair Simulator

Predictions for the next decade

Predictions for the next decade

- Higher-level abstractions
  - Programming models
  - More elastic and dynamically autoscaling infrastructure
  - Serverless -> Cloudless computing (?)
- More interactivity
  - Shorter computing times
  - Faster response time
  - More capacity available locally
- Virtual reality - more real
  - HD Caves
  - VR/AR Goggles (Apple, Meta)
- AI
  - ?

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Centre for Computational Medicine

www.sano.science

Maciej Malawski
Sano Director
m.malawski@sanoscience.org

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Smart Growth

Republic of Poland

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