

Questions and answers are in data – the development of elnfrastructure and Digital Health technologies

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Institute of Bioorganic Chemistry Polish Academy of Sciences

- The Institute of Bioorganic Chemistry of the Polish Academy of Sciences (IBCh PAS) is a unique research unit in Europe, which carries out interdisciplinary research in chemistry, biology, bioinformatics and computer science
- Together with its affiliated Poznań Supercomputing and Networking Center (PSNC) it is one of the largest institutes of Polish Academy of Sciences, employing in total over 750 people
- The core mission of PSNC is to foster scientific excellence by providing reliable and cutting-edge e-Infrastructure such as communication networks, data and supercomputing systems, as well as highly-specialized laboratories





- The core mission of PSNC is to foster scientific excellence by providing reliable and cuttingedge e-Infrastructure such as communication networks, data and supercomputing systems, as well as highly-specialized laboratories
- We achieve this goal particularly through extensive R&D activities related to information and communication technologies and their innovative applications.
- In collaborative project teams we draw from the synergy of science, technology, business, and education to tackle the greatest challenges for our future.
- It is our highest objective to ensure steady growth of the competencies of our people. They
 are the pillar for the successful exploration of new technologies and the development of
 scientific and engineering innovations, and ultimately the winning deployment of our
 services.



Locations



Focus on Digital Transformation based on advanced einfrastrucutre

• Continuous R&D activities related to information and communication technologies and their innovative applications



Networking: GEANT and PIONIER (NREN in Poland operated by PSNC)







PIONIER – Polish Optical Internet



High Performance Computing: PRACE/EuroHPC and PRACE-LAB I/II in 2021







High Performance Computing @PSNC in 2021

- All major HPC services are provided by two systems: Eagle (since 2016) and Altair (since 2021), which deliver conventional power and a specialized accelerating environment GPGPU for AI and big data analysis.
- The remaining cloud services are delivered for specific requirements at universities (dedicated resources, higher availability and critical services), industry and administration entities.
- PSNC computing systems have defined 200 grants and 5,000 computing accounts in both HPC and clouds.
- Access is provided for national and international users based on the contracts signed for the exchange of computing power under:
 - Partnership for Advanced Computing in Europe (PRACE),
 - nuclear physics—Worldwide LHC Grid Computing (WLCG),
 - Low-frequency Array for radio astronomy (LOFAR),
 - number of international flagship ESFRI projects.





High Performance Computing @PSNC in 2021 – core-hours/disciplines



PRACE (Partnership for Advanced Computing in Europe) grant:

Prof. Agnieszka Kaczor (Medical University of Lublin)

"Molecular simulations of drug targets involved in the central nervous system diseases (NERVOMOLSIM)"



National Data Storage and HPC Infrastructures in Poland in 2021 and 2022





Polish Rodmap for Research Infrastructures 2020 – PSNC projects

01 – 01 PIONIER-LAB National Platform for Integrating Research Infrastructures with Ecosystems of Innovation

02 - 02 National Laboratory for Photonics and Quantum Technologies - NLPQT

03-02 PRACE - Cooperation in the field of advanced computing in Europe

 $04-03\ \text{PRACE-LAB2}$ - Cooperation in the field of advanced computing in Europe

05 – 03 NEBI - National Centre for Advanced Analysis of Biological and Biomedical Imaging

06 – 04 Digital Research Infrastructure for Arts and Humanities DARIAH-PL

- 07 04 National Laboratory for Advanced 5G
- 08 04 National Data Storage
- 09 04 National Supercomputing Infrastructure for EURO HPC PL

10 – 04 ECBIG - The European Center for Bioinformatics and Genomics – MOSAIC





R&D Activities, Projects, People



Healthcare – our emphasis on data management and integration towards better diagnosis and treatment

- ICT
 - ADMIRE Adaptive multi-tier intelligent data manager for Exascale (Brain Super-resolution imaging)
 - INSENSION Personalized intelligent platform enabling interaction with digital services to individual with PMLD (Profound and multiple learning disabilities)
 - GlaucomAI Multimodal Advanced Glaucoma Diagnosis Model
 - medVC Real-time audio-video collaboration for doctors
- AAL
 - PELOSHA: Personalizable services for supporting healthy ageing
 - Fit4Work: Self-management of physical and mental fitness of older workers
- eInfrastrucutre
 - NEBI National Imaging Centre for biological and biomedical sciences
 - MOSAIC AI Platform to integrate and analyze multiomics and clinical data for new insights and tools for broadly accessible, personalized prevention, diagnosis and medical therapy



Digital Transformation: Shaping the future of European healthcare – Deloitte report (2020)

Top challenges facing HC organizations in implementing digital technologies

Europe





Source: Deloitte research and analysis, 2020

Common European Data Spaces

 The medicine of today is increasingly employing IT technologies to better understand the observed processes and support diagnostic and individual therapeutic procedures based on digital models



https://digital-strategy.ec.europa.eu/en/library/building-data-economy-brochure



Glaucoma is a progressive optic neuropathy which is the most common cause of irreversible vision loss in the world.

Its pathomechanism is associated with a change in lamina cribrosa phenotype under the influence of excessive mechanical forces, which leads to neurotrophic deprivation and subsequent accelerated process of retinal ganglion cell apoptosis.

Loss of retinal ganglion cells leads to disruption of the functional visual pathway continuity which leads to the development of specific (depending on the architecture of the retina and optic nerve) defects in the visual field.

Those defects appear clinically when at least 30 to 50% of the ganglion cells of a given area of the retina is lost.



Multimodal Advanced Glaucoma Diagnosis

Data collected from SENSIMED Triggerfish®



Multimodal Advanced Glaucoma Diagnosis

Data collected from SOMNOtouchTM NIBP









Atributes

Feature engineering during reference periods:

- Sum of areas under the TF curve
- The slope angle of the linear regression straight line for TF measures
- The total pace of change in TF
- Power and frequency of the main FFT components of the TF signal
- Correlations of TF and cardiovascular sensor signal (SAP, DAP, HR, SpO₂)
- Discrete convolution product of TF with HR, SAP for short periods after sleep (1-1.5h)
- Additional attributes: clinical metadata describing eyeball biomechanical properties (CH, CRF),



I 2021: 100 subjects, 8-fold cross-validation Model #3: CH i sensor attribiutes, {NORM, POAG | <u>NTG</u>} (*GLM*)

ROC CURVE - CROSS VALIDATION METRICS , AUC = 0.779101



		Screening s	etpoint			Optimal RO	C knee setpo	int		
		Specificity	Sensitivity	PPV	F-measure	Specificity	Sensitivity	PPV	F-measure	AUC
Single source	Genome information (G)	0.850	0.543	0.143	0.227	0.744	0.760	0.122	0.183	0.810
	Retinal fundus image features (I)	0.850	0.420	0.115	0.180	0.720	0.662	0.101	0.166	0.722
	Personal data (P)	0.850	0.197	0.057	0.089	0.596	0.554	0.060	0.108	0.561
Combined source	Genome information + retinal image features (G+I)	0.850	0.647	0.166	0.264	0.764	0.812	0.139	0.192	0.856
	Personal data + genome information (P+G)	0.850	0.639	0.164	0.261	0.750	0.824	0.134	0.186	0.853
	Personal data + retinal image features (P+I)	0.850	0.454	0.123	0.193	0.714	0.718	0.107	0.171	0.753
	AGLAIA-MII: Personal data + genome information + retinal fundus image features (P+G+I)	0.850	0.671	0.171	0.273	0.786	0.816	0.153	0.201	0.866
Current glauco	ma screening using IOP	0.850	0.304	0.086	0.134	0.614	0.560	0.064	0.118	0.604

Table 3 Key diagnostic metrics (specificity, sensitivity, PPV, F-measure, AUC) as a result of using the various individual and combined sources

For specificity, sensitivity and PPV, two conditions are considered: screening setpoint by setting specificity constant at 0.85, and at the optimal ROC knee point. The best results are highlighted in italics.

AGLAIA-MII, automatic glaucoma diagnosis through medical imaging informatics; AUC, area under the (ROC) curve; IOP, intraocular pressure; PPV, positive predictive value; ROC, receiver operating characteristic.



Challenges and future plans

- Number of cases to analyze the disproportion between the parameters and the size of the set to analyze
- Data mining to determine the parameters of the case description strictly controlled by the physician's expertise
- Feedback effect model building based on medical knowledge and interpretation of physiology based on work with data and model
- Assessment of model reliability and validation of results
- Transition from the level of the diagnostic model to the proposal of therapeutic intervention for doctors



Result: Data Analytics App - patient classification



Medical Diagnostic Hypothesis Refinement Through Data Analysis

Predict diagnosis for u_125

Data analysis method: 🔿 Time series summary 🔿 Data distribution summary 🔿 Gradient Boosting Machine model 🧿 Diagnosis assessment								
Enter time (hh:mm)			Select raw Triggerfish CSV file for patient	Select cardio record in zip file for patient	Select classification model			
TF start 11:33	Sleep from 23:05	Wake at 07·18	File selected 3-u_1	File selected 3-u_1	basic TF/Somno model			
11.00			Run conversion of the .CSV file	Run conversion of the .zip file				
Enter CH ((numeric)							

Zip file conversion has been successful. Now you can check classification.

Conlusions – Challenges for Digital Health solutions

- A multidisciplinary approach in medicine no longer means only medical teams working together
- For data-driven solutions, it is crucial to have access to sufficient number of records to avoid imbalances between numer of parameters and the size of the set to analyze
- Data mining leading to determination of the crucial parameters which characterize the case and disease should be strictly supervised by the physician's expertise
- Feedback loop for improved understanding modeling based on medical knowledge and physiology cross-referencing while working with data and model
- Advancing beyond diagnosis support towards specific therapeutic interventions suggested for physicians

7th European Laryngological Live Surgery Broadcast 23rd November 2022 | 9.00 16.00 (GMT+1)

Save the date els.livesurgery.net





Thank you!

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