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ExCAPE

Exascale Compound Activity Prediction Engine

Future and Emerging Technologies (FET)

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Topic: FETHPC-1-2014

Type of action: RIA

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Factsheet 2

Dissemination Factsheet

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Contributing Consortium Partners: All
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PU	Public	PU
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	



Document revision tracking

This page is used to follow the deliverable production from its first version until it has been reviewed by the assessment team. Please give details in the table below about successive releases.

Release number	Date	Reason of this release and/or validation	Dissemination of this release (task level, WP/ST level, Project Office Manager, Industrial Steering Committee, etc)
0	20.08.2018	A first draft	CO
1	05.10.2018	Final draft after compiling inputs from partners	PU

Glossary

No glossary is given.

Link to Tasks

Task number	Work from task carried out	Deviations from task technical content, with motivation and summary of impact
4.2	This fact sheet is the final fact sheet compiling dissemination actions by all partners	None

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Executive Summary

This fact sheet is the final fact sheet compiling dissemination actions by all partners.

It was late due to the desire to be as up-to-date as possible with activities that occurred late in the project.

Partner	Name	Date	DOI (Digital Object Identifier)	Activity
IMEC IT4I	Tom Ashby Jan Martinovič	2015-09-28 2015-10-01		Representing ExCAPE at EXDCI event (Rome) IT4I Newsletter: https://www.it4i.cz/wp-content/uploads/2015/10/newsletter-2015-01.pdf
RHUL	Fedorova, Valentina; Gammerman, Alexander; Nourtdinov, Ili; Vovk, Vladimir.	2015-12-01	http://dx.doi.org/10.1142/S0218213015600039	Hypergraphical conformal predictors. International Journal on Artificial Intelligence Tools, Vol. 24, No. 6, 01.12.2015.
UL	Thomas Unterthiner, Andreas Mayr, Günter Klambauer	2015-12-13		Poster: ELU-Networks - Fast and Accurate CNN Learning on ImageNet . ICCV 2015
RHUL	Alexander Gammerman, Iliia Nourtdinov and Paolo Toccaceli	2016-01-23		Invited Talk. Conformal Prediction in Bioinformatics* by Alex Gammerman, Iliia Nourtdinov and Paolo Toccaceli at International Conference on Pharmaceutical Bioinformatics, Pattaya, Thailand, January 2016 (ICPB2016).
RHUL	Paolo Toccaceli, Iliia Nourtdinov and Alex Gammerman	2016-01-23		Poster. at ICPB2016 (best poster award (2nd place)) - Applying Conformal Predictions on Public BioAssay Data by Paolo Toccaceli, Iliia Nourtdinov, Alex Gammerman. International Conference on Pharmaceutical Bioinformatics, Pattaya, Thailand, January 2016.
AU	Samuel Kaski	2016-02-25		Guest talk: Bayesian factorization of multiple data sources. University of Cambridge, Computer Laboratory.
AU	Samuel Kaski	2016-03-17		Guest talk: Modelling of multiple data sources: data integration and interactive retrieval. Frontiers in Digital Health. UCL Institute of Digital Health
AU	Kerstin Bunte, Eemeli Leppäaho, Inka Saarinen, Samuel Kaski	2016-04-16	https://academic.oup.com/bioinformatics/article/32/16/2457/2240476	Sparse group factor analysis for biclustering of multiple data sources. Bioinformatics 32(16), p. 2457-2463.
RHUL	Paolo Toccaceli	2016-04-16		Tutorial. Paolo Toccaceli on Venn-ABERS at Conformal and Probabilistic Predictions with Applications (COPA2016), Madrid, Spain, April 2016

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Partner	Name	Date	DOI (Digital Object Identifier)	Activity
RHUL	V. Vovk, V. Fedorova, I. Nourtdinov, and A. Gammerman.	2016-04-17	http://dx.doi.org/10.1007/978-3-319-33395-3_2	Criteria of efficiency for conformal prediction. In: Proceedings of COPA 2016 (Fifth Symposium on Conformal and Probabilistic Prediction with Applications) (ed. by A. Gammerman, Z. Luo, J. Vega, and V. Vovk), Lecture Notes in Computer Science, vol. 9653, pp. 23 - 39. Cham: Springer International Publishing Switzerland, 2016.
RHUL	G.Cherubin & I. Nourtdinov	2016-04-17	http://dx.doi.org/10.1007/978-3-319-33395-3_10	Hidden Markov Models with Confidence. Conformal and Probabilistic Prediction with Applications: 5th International Symposium, COPA 2016 Madrid, Spain, April 20-22, 2016 Proceedings. Springer, Vol. 9653, p. 128-144 (Lecture Notes in Computer Science; vol. 9653).
RHUL	Paolo Toccaceli, Iliia Nourtdinov and Alex Gammerman.	2016-04-17	http://dx.doi.org/10.1007/978-3-319-33395-3_4	Conformal Predictors for Compound Activity Prediction. Published in Conformal and Probabilistic Prediction with Applications; 5th International Symposium, COPA 2016 Madrid, Spain, Lecture Notes in Artificial Intelligence, Springer, 9653, 2016.
UL	Thomas Unterthiner	2016-05-02		Publication: Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs). International Conference on Learning Representations (ICLR 2016), San Juan, Puerto Rico, May 2-4, 2016
IMEC	Tom Ashby	2016-05-09		Representing ExCAPE at EXDCI/PRACE days event (Prague)
AU	Samuel Kaski	2016-06-02		Guest talk: Bayesian factorization of multiple data sources. Monash University
AU	Samuel Kaski	2016-06-07		Guest talk: Bayesian factorization of multiple data sources. Melbourne University
IMEC	Tom Ashby	2016-06-22		Overview presentation of ExCAPE project at the Intel booth at ISC 2016
AU	Samuel Kaski	2016-06-30		Guest talk: Bayesian factorization of multiple data sources. IBM Watson Research Center, Yorktown Heights, NY
RHUL	Alexander Gammerman	2016-07-01		Invited Talk. Conformal Prediction for big and imbalanced data sets* by Alex Gammerman. Summer School and Conference on Multivariate Statistical Analysis; July 2016, Armenia.
RHUL	V. Vovk and D. Pavlovic	2016-07-08	10.1007/978-3-319-33395-3_3	Universal probability-free conformal prediction. In: Proceedings of COPA 2016 (Fifth Symposium on Conformal and Probabilistic Prediction with Applications) (ed. by A. Gammerman, Z. Luo, J. Vega, and V. Vovk), Lecture Notes in Computer Science, vol. 9653, pp. 40 - 47. Cham: Springer International Publishing Switzerland, 2016.




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Partner	Name	Date	DOI (Digital Object Identifier)	Activity
AU	Samuel Kaski	2016-08-30		Guest talk: Modelling of multiple data sources: data integration and interactive retrieval. SciLifeLab, Stockholm, Sweden
IMEC	Tom Vander Aa	2016-09-12	10.1109/CLUSTER.2016.13	Publication and presentation of "Distributed Bayesian Probabilistic Matrix Factorization" at IEEECluster 2016
UL	Andreas Mayr, Thomas Unterthiner, Günter Klambauer	2016-09-28		Poster: Deep Learning for Drug Target Prediction. GPU Technology Conference (GTC) Europe 2016, Amsterdam. - Winner of GTC Best Poster Award
IMEC	Tom Vander Aa	2016-10-11		Presented MF methods at the Application Workshop with EXA2CT, EPIGRAM, INTERTWINE projects
AZ	Jiangming Sun, Lars Carlsson, Ola Engkvist, Hongming Chen	2016-10-20	http://niklasbjorn.github.io/	J. Sun et al. Exascale Compound Activity Prediction Engines: Big data in chemogenomics, 15th Swedish Bioinformatics Workshop. 2016, Linköping, Sweden
IT4I	Martin Palkovič, Vit Vondrák	2016-11-01		Yearbook HPC, Czech-ing into the world of HPC, Yearbook HPC 2016-2017 of Scientific Computing World, page 12.
IT4I	Stanislav Böhm, Jan Martinovič	2016-11-14		Poster at the IT4I booth at the SC16 - "Applying Exascale Machine Learning to problem in the Pharmaceutical industry"
IT4I	Jan Martinovič	2016-11-16		Rotated slides about ExCAPE project in the FET-HPC projects section at the ExDCI booth at SC16
UL	Thomas Unterthiner, Andreas Mayr	2016-12-05	https://openreview.net/pdf?id=S1uHfyyg	Speeding up Semantic Segmentation for Autonomous Driving: Poster/Publication at Workshop on Machine Learning for Intelligent Transport Systems, Neural Information Processing Systems (NIPS 2016), Barcelona, Spain
IMEC	Tom Vander Aa	2016-12-14		GASPI Forum attendance
IT4I	Jan Martinovič, Martin Palkovič	2017-01-23		Poster presentation at the HIPEAC 2017 conference with topic "ExCAPE: Exascale Compound Activity Prediction Engines"
RHUL	I.Nouretdinov	2017-02-02	http://dx.doi.org/10.1109/ICMLA.2016.0049	Distributed Conformal Anomaly Detection. Machine Learning and Applications (ICMLA), 2016 15th IEEE International Conference on. IEEE Computer Society, p. 1-6
AZ	Jiangming Sun, Lars Carlsson, Ola Engkvist, Hongming Chen	2017-02-15	https://doi.org/10.1101/116764	Paper under review: Applying Mondrian Cross-Conformal Prediction to Estimate Prediction Confidence on Large Imbalanced Cheminformatics Datasets
AZ	Jiangming Sun, Nina Jeliaskova, Hongming Chen, et al.	2017-03-01	10.1188/s13321-017-0203-5	Publish paper "ExCAPE-DB: an integrated large scale dataset facilitating Big Data analysis in chemogenomics" in J. Cheminfo.




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Partner	Name	Date	DOI (Digital Object Identifier)	Activity
IDEA	Nina Jeliaskova, Ivan Georgiev, Nikolay Kochev, Vedrin Jeliaskov	2017-03-01	10.1186/s13321-017-0203-5	Sun J, Jeliaskova N, Chupakin V, Golib-Dzib J-F, Engkvist O, Carlsson L, Wegner J, Ceulemans H, Georgiev I, Jeliaskov V, Kochev N, Ashby TJ, Chen H: ExCAPE-DB: an
AU	Xiangju Qin, Paul Blomstedt, Eemeli Leppäaho, Pekka Parviainen, Samuel Kaski	2017-03-02	arXiv:1703.00734	Under review paper: Distributed Bayesian Matrix Factorization with Minimal Communication, ArXiv e-prints arXiv:1703.00734.
RHUL	Vovk, V., Nouretdinov, I., Fedorova, V., Petej, I. and Gammerman, A.	2017-03-14	https://doi.org/10.1007/s10472-017-9540-3	Criteria of efficiency for set-valued classification, In : Annals of Mathematics and Artificial Intelligence
ALL	Everyone	2017-03-17		First ExCAPE board meeting
AU	Xiangju Qin, Paul Blomstedt, Eemeli Leppäaho, Pekka Parviainen, Samuel Kaski	2017-03-23		Poster: Massive-scale Recommendation Engines for Drug Discovery, Aalto Digi Matchmaking event, Aalto University, Computer Science building.
RHUL	Vovk, V.	2017-03-24	10.15330/ms.46.1.96-110	Purely pathwise probability-free Ito integral, in Matematychni Studii. 46, 1, p. 96-110
IMEC	Tom Vander Aa	2017-03-25		Provide ExCAPE data and be judge at the Pistoia Hackathon in London
RHUL	V. Vovk and D. Pavlovic.	2017-04-19	10.1007/s10472-017-9547-9	Universal probability-free prediction. Annals of Mathematics and Artificial Intelligence. Accepted for publication.
AU	Eemeli Leppäaho, Muhammad Ammad-ud-din, Samuel Kaski	2017-04-20	http://jmlr.org/papers/volume18/16-509/16-509.pdf	GFA: Exploratory Analysis of Multiple Data Sources with Group Factor Analysis. Journal of Machine Learning Research 18 (2017), p. 1-5.
UL	Günter Klambauer, Sepp Hochreiter	2017-04-27	doi.org/10.1002/humu.23237	panelcn.MOPS: Copy number detection in targeted NGS panel data for clinical diagnostics, Human Mutation, 38(7):889-897, 2017
RHUL	A. Gammerman	2017-04-28		Invited talk "Prediction and Testing" at Conference "Braverman's Readings in Learning Theory and Related Areas", Boston, USA.
RHUL	Vovk, V.	2017-04-28		Invited Talk, Conference "Braverman's Readings in Learning Theory and Related Areas", Boston, USA, April 2017. Title of the talk: Conformal predictive distributions.
RHUL	Vovk, V.	2017-05-02		Invited Talk, Fourth Bayesian, Fiducial, and Frequentist Conference, Boston, USA, Title of the talk: Conformal predictive distributions.
RHUL	Volkhonskiy, D., Burnaev, E., Nouretdinov, I., Gammerman, A. & Vovk, V.	2017-05-10	http://proceedings.mlr.press/v60/volkhonskiy17a.html	Inductive Conformal Martingales for Change-Point Detection, 6th Symposium on Conformal and Probabilistic Prediction with Applications (COPA 2017).

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Partner	Name	Date	DOI (Digital Object Identifier)	Activity	
RHUL	Vovk, V., Shen, J., Manokhin, V. & Xie, M.	2017-05-10	http://proceedings.mlr.press/v60/vovk17a.html	Nonparametric predictive distributions based on conformal prediction, presented at 6th Symposium on Conformal and Probabilistic Prediction with Applications (COPA 2017).	
RHUL	Noureddin, I.	2017-05-10	http://proceedings.mlr.press/v60/noureddinov17b.html	Improving reliable probabilistic prediction by using additional knowledge, presented at 6th Symposium on Conformal and Probabilistic Prediction with Applications (COPA 2017).	
RHUL	Noureddin, I.	2017-05-10	http://proceedings.mlr.press/v60/noureddinov17a.html	Reverse conformal approach for on-line experimental design, presented at 6th Symposium on Conformal and Probabilistic Prediction with Applications (COPA 2017).	
RHUL	Noureddin, I.	2017-05-10	10.25046/aj020335	Validity and efficiency of conformal anomaly detection on big distributed data, in Advances in Science, Technology and Engineering Systems Journal. 2, 3, p. 254-267	
RHUL	Paolo Toccaceli and Alex Gammerman	2017-05-10	http://proceedings.mlr.press/v60/toccaceli17a/toccaceli17a.pdf	Combination of Conformal Predictors for Classification, presented at 6th Symposium on Conformal and Probabilistic Prediction with Applications (COPA 2017).	
IT4I	Jan Martinovič	2017-05-19		Poster "HyperLoom" and representing ExCAPE at the HPCAFE workshop	
RHUL	Vovk, V.	2017-06-07	https://doi.org/10.1007/s00780-017-0336-4	The role of measurability in game-theoretic probability, in Finance and Stochastics.	
IMEC	Tom Vander Aa, Imec Chakroun, Tom Haber	2017-06-12	https://doi.org/10.1016/j.procs.2017.05.009	Paper: Distributed Bayesian Probabilistic Matrix Factorization at ICCS 2017	
IMEC	Imec Chakroun, Tom Haber, Tom Ashby	2017-06-12	https://doi.org/10.1016/j.procs.2017.05.082	Paper: SW-SGD: The Sliding Window Stochastic Gradient Descent Algorithm at ICCS 2017	
IMEC	Tom Ashby	2017-06-12	10.1016/j.procs.2017.05.024	Paper at ICCS 2017: Improving Operational Intensity in Data Bound Markov Chain Monte Carlo, Balazs Nemeth, Tom Haber, Thomas J. Ashby and Wim Lamotte.	
RHUL	Paolo Toccaceli, Ilia Noureddin and Alex Gammerman	2017-06-16	https://doi.org/10.1007/s10472-017-9556-8	"Conformal Prediction of Biological Activity of Chemical Compounds", Annals of Mathematics and Artificial Intelligence journal. Accepted for publication.	

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Partner	Name	Date	DOI (Digital Object Identifier)	Activity	
IT4I	Stanislav Böhm, Vojtěch Cima, Jiří Dvorský, Kateřina Janurová, Jan Martinovič, Tom Ashby, Vladimír Chupakhin, Jose Golib-Dzib	2017-06-17		Poster: Loom: A Platform for Defining and Executing Workflow Pipelines in a Distributed Environment, presented at (ISC 2017)	
IT4I	Jan Palkovič	2017-06-17		Representing ExCAPE at ISC 2017 (Frankfurt)	
AU	Xiangju Qin	2017-06-20			
UL	Sepp Hochreiter	2017-06-27		Self-normalizing Neural Networks and a Two Time-Scale Update Rule for GANs, Talk at Workshop on Deep Learning: Theory, Algorithms, and Applications, Berlin, Germany	
IMEC	Tom Ashby, Tom Vander Aa	2017-06-28		Organising a minisymposium on Scientific and High Performance Computing for Applied Life Sciences and Precision Medicine at PASC17	
IMEC	Tom Ashby, Tom Vander Aa	2017-06-28		Presentation of ExCAPE during the minisymposium on Scientific and High Performance Computing for Applied Life Sciences and Precision Medicine at PASC17	
IMEC	Tom Vander Aa	2017-06-30	(Not available)	Paper at INFOCOMP17: Machine Learning for Chemogenomics on HPC in the ExCAPE Project	
IT4I	Vojtěch Cima, Stanislav Böhm, Jan Martinovič, Jiří Dvorský, Thomas J. Ashby, Vladimír Chupakhin	2017-07-10	https://link.springer.com/chapter/10.1007/978-3-319-61566-0_36	Presentation: HyperLoom Possibilities for Executing Scientific Workflows on the Cloud, presented at Conference on Complex, Intelligent, and Software Intensive Systems (CISIS 2017)	
RHUL	Z. Luo	2017-07-14		Invited Talk "Machine Learning for Large-scale Compound Activity Prediction", Zhejiang University, China	
RHUL	A. Gammerman	2017-09-07		Invited talk Testing exchangeability" at Odessa National Mechnikov University, Ukraine.	
UL	Günter Klambauer, Thomas Unterthiner, Andreas Mayr, Sepp Hochreiter	2017-09-07	https://arxiv.org/pdf/1706.02515	Manuscript on Arxiv: Self-Normalizing Neural Network	
IT4I	Stanislav Böhm, Vojtěch Cima, Jan Martinovič, Jiří Dvorský, Kateřina Janurová	2017-09-12	https://cs.cz.facebook.com/IT4Inovations/	IT4I facebook article about HyperLoom	
IT4I	Jan Martinovič	2017-09-27		Poster: Hyperloom: A Platform for Defining and Executing Scientific Pipelines in Distributed environments, SOR 2017, Bled, Slovenia	

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IT4I	Karina Pešatová	2017-10-01	https://www.hipeac.net/assets/public/publications/newsletter/hipeacinfo52.pdf	End-to-end data processing on HPC systems made simple, article in HIPEAC newsletter vol. 52, pp. 11.
IT4I	Vojtěch Cima, Stanislav Böhm	2017-11-12		Presentation: HyperLoom: A Platform for Defining and Executing Scientific Pipelines in Distributed Environments, presented at Intel HPC Developer Conference 2017
IT4I	Thomas Ashby, Tom Vander Aa, Stanislav Bohm, Vojtech Cima, Jan Martinovic, Vladimir Chupakhin	2017-11-14	https://sc17.supercomputing.org/SC17%20Archives/tech_poster/tech_poster_pages/post193.html	Extended abstract "How To Do Machine Learning on Big Clusters" and poster "HyperLoom: A Platform for Defining and Executing Scientific Pipelines in Large-Scale Distributed Environments" presented at The International Conference for High Performance Computing, Networking, Storage and Analysis (SC 2017)
IT4I	Vojtěch Cima	2017-11-16		Lightning talk about HyperLoom possibilities, The International Conference for High Performance Computing, Networking, Storage and Analysis (SC 2017)
ALL	Everyone	2017-11-28		ExCAPE Flyer
IT4I	Vojtěch Cima	2017-11-29		Presentation: HyperLoom: A Platform for Defining and Executing Scientific Pipelines in Distributed Environments, presented at Intel® Nervana™ AI Academy Roadshow Fall/Winter 2017
IT4I	Karina Pešatová	2017-12-01	https://www.it4i.cz/wp-content/uploads/2018/01/Newsletter-Q4-2017-EN.pdf	Article: PARTICIPATION AT THE SUPERCOMPUTING CONFERENCE SC17 IN DENVER, USA, IT4Innovatins Newsletter Q4 2018
UL	Günter Klambauer, Thomas Unterthiner, Andreas Mayr, Sepp Hochreiter	2017-12-04	https://papers.nips.cc/paper/6698-self-normalizing-neural-networks.pdf	Self-Normalizing Neural Networks: Poster/Publication at Main Conference, Neural Information Processing Systems Foundation (NIPS 2017), Long Beach, USA
UL	Günter Klambauer, Thomas Unterthiner, Andreas Mayr, Sepp Hochreiter	2017-12-04	doi.org/10.1039/c8sc00148k	Large-scale comparison of machine learning methods for drug target prediction on ChEMBL, Chem. Sci., 9:5441-5451, 2018




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Partner	Name	Date	DOI (Digital Object Identifier)	Activity
UL	Günter Klambauer, Thomas Unterthiner, Andreas Mayr, Sepp Hochreiter	2017-12-05		Deep Learning Yields Virtual Assays: Poster at Workshop on Machine Learning for Molecules and Materials, Neural Information Processing Systems (NIPS 2017), Long Beach, USA
UL	Günter Klambauer, Thomas Unterthiner, Andreas Mayr, Sepp Hochreiter	2017-12-06		Toxicity Prediction Using Self-normalizing Networks: Poster at Workshop on Machine Learning for Molecules and Materials, Neural Information Processing Systems (NIPS 2017), Long Beach, USA
AU	Xiangju Qin, Paul Blomstedt, Eemeli Leppäaho, Pekka Parviainen, Samuel Kaski	2017-12-13		Poster: Large-scale Bayesian Matrix Factorization for Recommendation Engines, AI Day, Aalto University, Dipoli.
IMEC	Tom Vander Aa	2018-01-13		Invited Talk at the PARMA-DITAM workshop: Machine Learning for Chemogenomics on HPC in the ExCAPE Project
IT4I	Jan Martinovič	2018-01-21		Keynote: Accessible HPC Platform for Executing Scientific Pipelines on Supercomputing Facilities at 2nd International Conference on Data Management, Analytics & Innovation
IMEC	Tom Vander Aa	2018-01-24		Poster: Exascale Compound Activity Prediction Engines at the HIPEAC Conference
AU	Xiangju Qin, Paul Blomstedt, Eemeli Leppäaho, Pekka Parviainen, Samuel Kaski	2018-02-13	arXiv:1703.00734	Distributed Bayesian Matrix Factorization with Limited Communication, under review with ECML/PKDD journal track (minor revision)
IT4I	Stanislav Bohm	2018-02-23	10.1145/3183767.3183768	Paper: HyperLoom: A Platform for Defining and Executing Scientific Pipelines in Distributed Environments, PARMA-DITAM Workshop on HIPEAC 2018
IT4I	Stanislav Bohm	2018-02-23		Invited Talk: HyperLoom: A Platform for Defining and Executing Scientific Pipelines in Distributed Environments, HeLP-DC Workshop on HIPEAC 2018
IMEC/ALL	Tom Ashby	2018-03-01	https://vimeo.com/256141454	ExCAPE video released
IT4I	Karina Pešatová	2018-04-01	http://www.it4i.cz/wp-content/uploads/2018/03/1b_Review-2017_EN_preview.pdf	Project Description in IT4INNOVATIONS REVIEW 2017
IT4I	Karina Pešatová	2018-04-01	http://www.it4i.cz/wp-content/uploads/2018/04/Newsletter-Q1-2018-EN-preview.pdf	Article: HYPERLOOM: DATA PROCESSING USING HIGH PERFORMANCE COMPUTING SYSTEMS MADE SIMPLE, IT4Innovatins Newsletter Q1 2018

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Partner	Name	Date	DOI (Digital Object Identifier)	Activity
IMEC	Tom Vander Aa	2018-04-17	(Not yet available)	Paper: SMURFF: a High-Performance Framework for Matrix Factorization
IT4I	Vít Vondrák	2018-05-16	http://www.msmt.cz/v	Invited Talk: High Performance Computing in the Czech Republic at EuroHPC, Prague
IDEA	Nina Jeliázkova	2018-05-28	(Not available)	Poster: chem2vec : vector embedding of atoms and molecules
IMEC	Tom Vander Aa	2018-05-29	https://web.fe.up.pt/~specs/events/hpcafe2018/	Invited Talk at HPCAFE at the HPCSummit, Ljubljana
IT4I	Jan Martinovič	2018-05-29	(Not available)	Workshop: ALLScale, ANTAREX, READEX, and ExCAPE projects High-Performance Computing Approaches for Monitoring, Exploring, Optimizing and Autotuning, HPC Summit Week 2018, Ljubljana, Slovenia
IT4I	Václav Svatoň, Vojtěch Címa, Jan Martinovič, Nina Jeliázkova, Vedrin Jeliázkov, Luchesar Iliev, Vladimír Chupakhin	2018-06-03	https://submissions.pasc-conference.org/pasc18_program/views/includes/files/post180s2.pdf	Poster: HPC-as-a-Service for Driving Artificial Intelligence for Drug Discovery, PASC 2018, Basel, Switzerland
IT4I	Stanislav Böhm, Vojtěch Címa	2018-06-04	http://prace.it4i.cz/HyperLoom-06-2018	Prace Training Course: HyperLoom: A Platform for Executing Scientific Pipelines in Distributed Environments, Ostrava 2018, Czech Republic
RHUL	Vovk, V. and Bendtsen, C.	2018-06-13	(Not available)	Conformal Decision Making, COPA2018
RHUL	I.Nouretdinov, D.Volkhonskiy, P.Lim, P.Tocaceli, A.Gammerman	2018-06-13	(Not available)	Inductive Venn-Abers Predictive Distribution and its Application, PMLR 91:15-36
IT4I	Stanislav Böhm, Jan Martinovič	2018-06-13	(Not available)	Workshop: ExCAPE (Exascale Compound Activity Prediction Engine): HPC session, QSAR 2018, Bled, Slovenia
AU	Xiangju Qin, Paul Blomstedt, Samuel Kaski	2018-07-15	https://www.ijcai-boom.org/proceeding.html	Large-scale probabilistic non-linear matrix factorization for drug discovery. In the 3rd IJCAI International Workshop on Biomedical Informatics with Optimization and Machine Learning (BOOM 2018).
AZ	Noé Sturm, Jiangming Sun, Yves Vandriessche, Andreas Mayr, Günter Klambauer, Lars-Anders Carlson, Ola Engkvist, Hongming Chen	2018-08-15	https://doi.org/10.26434/chemrxiv.6969584.v1	Application of Bioactivity Profile Based Fingerprints for Building Machine Learning Models

Partner	Name	Date	DOI (Digital Object Identifier)	Activity
RHUL	Vladimir Vovk, Jieli Shen, Valery Manokhin, Min-ge Xie	2018-08-17	https://doi.org/10.1007/s10994-018-5755-8	Nonparametric predictive distributions based on conformal prediction
IDEA	Nina Jeliázkova, Nikolay Kochev	2018-08-20	10.1186/s13321-018-0295-6	Kochev N, Avramova S, Jeliázkova N: Ambit-SMIRKS: a software module for reaction representation, reaction search and structure transformation. J Cheminform 2018, 10:42.
RHUL	P. Tocaceli, A. Gammerman	2018-08-22	https://doi.org/10.1007/s10994-018-5754-9	Combination of inductive mondrian conformal predictors, MLJ, 2018
AU	Xiangju Qin, Paul Blomstedt, Samuel Kaski	2018-10-11	(Not yet available)	Poster: Large-scale probabilistic non-linear matrix factorization for drug discovery. Aalto CS Research Day.
AU	Xiangju Qin, Paul Blomstedt, Samuel Kaski	2018-10-20	(Not yet available)	Probabilistic non-linear matrix completion for massive-scale data. Manuscript in preparation.
AU	Jonathan Strahl, Hiroshi Mamitsuka, Jaakko Peltonen, Samuel Kaski	2018-11-10	(Not yet available)	Sparse Gaussian-Markov-random-field constrained EM algorithm for Bayesian matrix factorisation with graph side-information. Manuscript in preparation.
IT4I	Jan Martinovič, Václav Svatoň, Nina Jeliázkova, Vladimír Chupakhin	2018-11-13	(Not yet available)	Poster: HEAppE for Life Sciences, SC18, Dallas, USA

 Conference Attendance  					IMEC	IP	ITAI	AZ	UL	AAI/O	INTEL	IDEA	RHUL
Date	Organization and Co-Located Events	Place	Topics Covered by Event	Title (if presenting)	1	2	3	4	5	6	7	8	9
2015-05-02	ICLR 2015	San Juan, Puerto Rico	Machine learning	Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs)					Presenting, Paper				
2015-12-07	NIPS 2015	Montreal, Canada	Machine learning						Attending				
2016-04-20	5th Symposium on Conformal and Probabilistic Prediction with Applications	Madrid, Spain	Machine learning	Conformal prediction for biological activity									Presenting
2016-04-23	Machine Learning Prague 2016	Prague, Czech Republic	Machine learning				Attending						
2016-05-09	European HPC Summit Week 2016	Prague, Czech Republic	High Performance Computing	??	Presenting		Attending						
2016-05-18	Molecular Informatics Open Source Software	Hinxton, Cambridge, UK	cheminformatics	Making the data available with AMBIT cheminformatics platform								Invited talk	
2016-09-04	21th EuroQSAR conference	Verona, Italy	Chemoinformatics	Using Mondrian Cross-Conformal Prediction to Predict Properties of Large Imbalanced Cheminformatics Datasets				Presenting					
2016-09-12	IEEE Cluster Conference	Taipei, Taiwan	High Performacne Computing	Distributed Bayesian Probabilistic Matrix Factorization	Presenting								
2016-09-19	The Ninth Workshop on Information Theoretic Methods in Science and Engineering WITMSE 2016	Helsinki, Finland	Machine learning	Multiple output regression with latent noise						Invited talk			
2016-09-28	GPU Technology Conference 2016	Amsterdam, Netherlands	High Performacne Computing	Deep Learning for Drug Target Prediction (<i>Winner of GTC Best Poster Award</i>)					Presenting, Poster				
2016-10-13	The 15th International Symposium on Intelligent Data Analysis	Stockholm, Sweden	Machine learning	Bayesian factorization of multiple data sources						Invited talk			
2016-10-20	15th Swedish Bioinformatics Workshop	Linköping, Sweden	Bioinformatics	Exascale Compound Activity Prediction Engines: Big data in chemogenomics				Presenting					
2016-11-07	5th Annual Conference of IT4Innovations	IT4Innovations, Czech Republic	HPC	Task scheduling on HPC infrastructure			Presenting						
2016-11-14	SC16	Salt Lake City, USA	High Performance Computing, Networking, Storage and Analysis	Applying Exascale Machine Learning to problem in the Pharmaceutical industry			Presenting						
2016-12-05	NIPS 2016: Main conference	Barcelona, Spain	Machine learning				Attending		Attending				
2016-12-05	NIPS 2016: Workshop on Machine Learning for Intelligent Transport Systems	Barcelona, Spain	Machine learning	Speeding up Semantic Segmentation for Autonomous Driving					Presenting, Paper				
2017-01-23	HIPEAC Stockholm	Stockholm, Sweden	High Performance Computing	ExCAPE: Exascale Compound Activity Prediction Engines			Poster						
2017-05-15	European HPC Summit Week 2017	Barcelona, Spain	High Performance Computing		Attending		Poster						
2017-06-10	The 11th International Conference on Complex, Intelligent, and Software Intensive Systems	Torino, Italy	High Performance Computing	HyperLoom Possibilities for Executing Scientific Workflows on the Cloud			Presenting						



Conference Attendance



Date	Organization and Co-Located Events	Place	Topics Covered by Event	Title (if presenting)	IMEC	IP	ITAI	AZ	UL	AAI/O	INTEL	IDEA	RHUL
					1	2	3	4	5	6	7	8	9
2017-06-14	6th Symposium on Conformal and Probabilistic Prediction with Applications	Stockholm, Sweden	Machine learning	Combination of Conformal Predictors									Presenting
2017-06-17	ISC High Performance conference 2017	Frankfurt, Germany	High Performance Computing	Loom: A Platform for Defining and Executing Workflow Pipelines in a Distributed Environment			Poster						
2017-06-26	The Platform for Advanced Scientific Computing Conference 2017 (PASC)	Lugano, Switzerland	High Performance Computing				Attending						
2017-06-27	Workshop on Deep Learning: Theory, Algorithms, and Applications	Berlin, Germany	Machine learning	Self-normalizing Neural Networks and a Two Time-Scale Update Rule for GANs					Presenting				
2017-09-27	SOR 2017 The 14th International Symposium on Operations Research	Bled, Slovenia	High Performance Computing	Hyperloom: A Platform for Defining and Executing Scientific Pipelines in Distributed environments			Poster						
2017-11-11	Intel HPC Developer Conference 2017	Denver, USA	High Performance Computing	HyperLoom: A Platform for Defining and Executing Scientific Pipelines in Distributed Environments			Presenting						
2017-11-12	SC17: The International Conference for High Performance Computing, Networking, Storage and Analysis	Denver, USA	High Performance Computing, Machine learning	A Platform for Defining and Executing Scientific Pipelines in Large-Scale Distributed Environments			Poster - selected to set of 9 best posters...						
2017-12-04	NIPS 2017: Main Conference	Long Beach, USA	Machine learning	Self-Normalizing Neural Networks					Presenting, Paper				
2017-12-04	NIPS 2017: Workshop on Machine Learning for Molecules and Materials	Long Beach, USA	Machine learning	1) Deep Learning Yields Virtual Assays; 2) Toxicity Prediction Using Self-normalizing Networks					Presenting, Poster x2				
2018-01-19	2nd International Conference on Data Management, Analytics & Innovation	Pune, India	High Performance Computing	Accessible HPC Platform for Executing Scientific Pipelines on Supercomputing Facilities			Keynote						
2018-01-22	HIPEAC, PARMA-DITAM Workshop	Manchester, UK	High Performance Computing	HyperLoom: A Platform for Defining and Executing Scientific Pipelines in Distributed Environments			Invited talk and Paper Presentation						
2018-04-17	Exascale Applications and Software Conference	Edinburgh, Scotland	High Performance Computing	SMURFF: a High-Performance Framework for Matrix Factorization	Presenting								
2018-05-27	11th International Conference on Chemical Structures	Noordwijkerhout, NL	Cheminformatics, SAR, Virtual Screening, Analysis of Large Chemistry Spaces, Integration of Chemical Information with other Resources, Dealing with Biological Complexity	chem2Vec: vector embedding of atoms and molecules								Poster	



Conference Attendance



Date	Organization and Co-Located Events	Place	Topics Covered by Event	Title (if presenting)									
					IMEC	IP	ITAI	AZ	UL	AALTO	INTEL	IDEA	RHUL
					1	2	3	4	5	6	7	8	9
2018-05-28	European HPC Summit Week 2018	Ljubljana, Slovenia	High Performance Computing	ALLScale, ANTAREX, READEX, and ExCAPE projects High-Performance Computing Approaches for Monitoring, Exploring, Optimizing and Autotuning (HPCAFE)	Workshop		Workshop						
2018-06-11	QSAR, 18th International Conference on (QSAR in Environmental and Health Sciences	Bled, Slovenia	High Performance Computing	ExCAPE (Exascale Compound Activity Prediction Engine): HPC session			Workshop						
2018-06-11	COPA2018, 7th Symposium on Conformal & Probabilistic Prediction with Applications	Maastricht, The Netherlands	Machine learning	Inductive Venn-Abers Predictive Distribution and its Application								Presenting	
2018-07-02	PASC, The Platform for Advanced Scientific Computing (PASC) Conference	Basel, Switzerland	High Performance Computing	HPC-as-a-Service for Driving Artificial Intelligence for Drug Discovery			Poster						
2018-11-11	SC18: The International Conference for High Performance Computing, Networking, Storage, and Analysis	Dallas, USA	High Performance Computing	HEAppE for Life Sciences			Poster						
2018-07-15	BOOM 2018: 3rd IJCAI International Workshop on Biomedical informatics with Optimization and Machine learning	Stockholm, Sweden	Machine learning	Large-scale probabilistic non-linear matrix factorization for drug discovery						Presenting, Poster x2			
2018-11-10	Aalto CS Research Day	Aalto University, Dipoli, Helsinki	Machine learning	Large-scale Bayesian Matrix Factorization for Recommendation Engines						Poster			



Tutorial Matrix



Date	Place	Context	Number of Attendees	Tutorial Topic	Partner	How attendees will use what they learned
2016-09-25	Edinburgh, UK	EuroMPI Conference	40	Introduction to Machine Learning on HPC	IMEC	Implementing better communications routines for doing machine learning
2016-09-27	Hagenberg, Austria	PRACE Autumn school (RISC/JKU/Hagenberg)		Toxicity Prediction using Deep Learning	UL	Talk, attendees got information about deep learning for toxicity prediction (was more a talk than a tutorial)
2017-06-14	Stockholm, Sweden	COPA2017	15	Venn-ABERS Predictors	RHUL	Understanding a theoretically-backed technique for non-parametric probabilistic calibration of scoring classifiers
2018-06-04	Ostrava, Czech Republic	PRACE Training course	15	HyperLoom	IT4I	HyperLoom: A Platform for Executing Scientific Pipelines in Distributed Environments
2018-06-11	Bled, Slovenia	QSAR 2018	20	HyperLoom + HPC as a service for pharmaceutical industry	JPNV + IT4I	Workshop ExCAPE (Exascale Compound Activity Prediction Engine): Machine learning session

Dissemination
Tutorial Matrix

07/10/2018



Tutorial Matrix



Date	Place	Context	Number of Attendees	Tutorial Topic	Partner	How attendees will use what they learned
2018-06-11	Maastricht, The Netherlands	COPA2018	50	Probabilistic Prediction	RHUL	Calibrated probabilistic predictions using generic scoring ML methods
2018-06-11	Maastricht, The Netherlands	COPA2018	50	Conformal Predictors	RHUL	How to predict with guaranteed error rate
2018-08-28	ISG, Royal Holloway, UK	ISG Seminars	30	Conformal Predictors and Venn Predictors	RHUL	Introduction to prediction with confidence and calibrated probabilistic prediction

Dissemination
Tutorial Matrix

07/10/2018