



7th of August 2018 at MPIKG in Potsdam Golm

Organizers: Dr. Baptiste Gault (MPIE) and Prof. Dr. Peter Fratzl (MPIKG)

Local coordinator: Dr. Lena Simon

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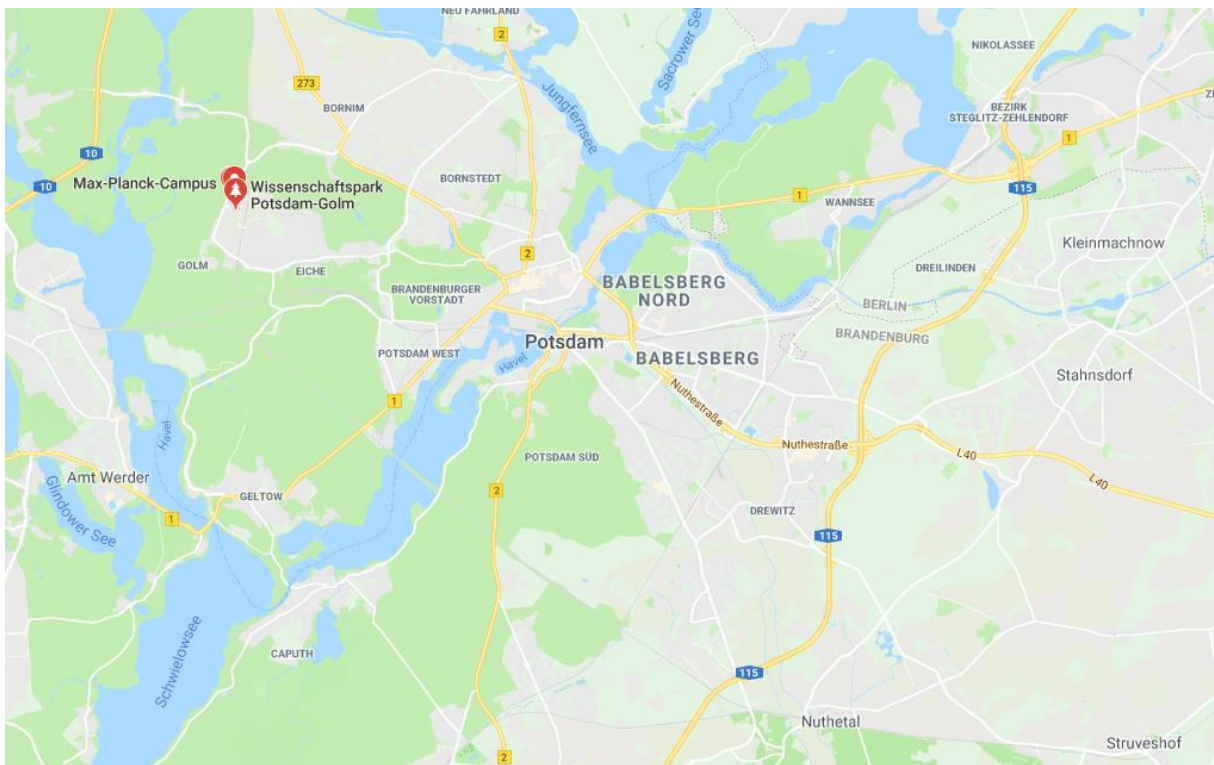
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Scope

The meeting will be focused on sharing best practices in collecting, processing of high amounts of data, storage, transfer, and try to define what is the best way to move forward on the integration of data from a variety of techniques (experimental & numerical) in data libraries, possibly come up with some kind of a roadmap, particularly for the techniques that are not as advanced as others in this regards.

Location

Max-Planck-Institut für Kolloid- und Grenzflächenforschung in Potsdam Golm



Program & discussions

7th of August 2018

		Topic	Speaker
11:00	11:15	Arrival	All
11:15	12:00	Introduction	Baptiste Gault
12:00	13:00	Lunch (MPI canteen)	All
13:00	13:40	RDA & MPCDF	Raphael Ritz
13:40	14:05	Deep Learning for FIB-SEM Data Processing	Luca Bertinetti
14:05	14:20	Imaging the structure of bone using x-ray scattering	Wolfgang Wagermaier
14:20	14:45	3D SAXS tomography	Paolino De Falco
14:45	15:10	NOMAD	Markus Scheidgen
15:10	16:10	Discussion and Coffee Break	All
16:10	16:35	Multidimensional photoelectron spectroscopy	Patrick Xian
16:35	17:00	EM, EELS, diffraction...	GD/TS/SZ (MPIE)
17:00	17:25	Atom probe data	Baptiste Gault
17:10	18:30	Discussion	All
19:00	20:00	Dinner and discussions	All
20:00	22:00	Wrap up discussion	All

The discussions were about issues related to data format, data extraction and processing, best practice for data sharing, inter-operability, integration of data / information from multiple techniques, with obviously the hope that we can later possibly get organized data with appropriate metadata into a repository etc.

The main focused points are the following:

- There clearly are commonalities in the problem that we face – in particular we all deal somehow with 3D data from which we need to extract information one way or another through segmentation first, maybe some coarse binning and then deploy what works?
- This aspect could really be an area on which we have a more focused-type discussion meeting at a later stage, i.e. how ML/DL can help extract info from 3D data, what can be efficiently done in this space...?
- The MPCDF has infrastructure to host data but also to process data and have an efficient implementation of tensorflow available for which they are looking to find partners – which may be coming from Peter’s department now that the connection has been established
- It seems clear that the software engineer position that has now been advertise will have work to do! There were many ideas that were discussed, and many early implementations of data processing and extraction methods that will benefit from an expert view.
- An area of interest would be the definition of appropriate metadata to store for a specific technique, how to store it, automate the extraction of “good data” and the reduction to the actual materials information...

Attendees

List of participants

<i>First Name</i>	<i>Last Name</i>	<i>Institution</i>
1-Gerhard	Dehm	Max-Planck-Institut für Eisenforschung (MPIE)
2-Tina	Scheu	Max-Planck-Institut für Eisenforschung (MPIE)
3-Baptiste	Gault	Max-Planck-Institut für Eisenforschung (MPIE)
4-Siyuan	Zhang	Max-Planck-Institut für Eisenforschung (MPIE)
5-Ralph	Ernstorfer	Fritz-Haber-Institut der Max-Planck-Gesellschaft (FHI)
6-Raphael	Ritz	Max Planck Computing and Data Facility (MPCDF)
7-Peter	Fratzl	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
8-Luca	Bertinetti	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
9-Mason	Dean	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
10-Paolino	De Falco	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
11-Richard	Weinkamer	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
12-Zhaoyong	Zou	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
13-Michaela	Eder	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
14-Markus	Scheidgen	Humboldt-Universität zu Berlin (HU)
15-Claudia	Draxl	Humboldt-Universität zu Berlin (HU)
16-Angelo	Ziletti	Fritz-Haber-Institut der Max-Planck-Gesellschaft(FHI)
17-Lena	Simon	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
18-Wolfgang	Wagermaier	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
19-Chenghao	Li	Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG)
20-Patrick	Xian	Fritz-Haber-Institut der Max-Planck-Gesellschaft (FHI)