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A Software Ecosystem for Remote Analysis of Mass Spectrometry Imaging Data

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In many areas of biomedical research, images are crucial for scientific progress. Interactive access to these images is essential, enhancing understanding and facilitating advancements, particularly in fields like pathology, radiology, and cellular biology. As imaging techniques continue to advance, generating ever more detailed datasets, the amount of data to be stored and processed will continue to grow. Consequently, data and computationally intensive processes are being increasingly relocated to centralized resources with substantial storage and processing capabilities. However, large, multidimensional and multi-modal biomedical images, such as those generated in experiments with mass spectrometry imaging, pose a major challenge for fast, comprehensive and interactive remote access. Processes as image data exploration, image analysis, the development of new image analysis methods, and interdisciplinary collaboration of domain experts can be hampered if data-intensive transfers to local systems are required, e.g. for processing of images with the interactive software the domain expert is familiar with. Current efforts to utilize remote resources focus on providing integrated environments for remote development and applications for execution of reproducible image analysis, while lacking comprehensive interactive capabilities to work with high-dimensional image data.

The first part of this work introduces advanced interactive access strategies for multi-modal 2D/3D mass spectrometry imaging (MSI) datasets. Concepts for fast, memory-efficient interactive access to imzML mass spectrometry imaging datasets are presented, which facilitate advanced interactive workflows such as multi-modal image fusion and 3D image reconstruction. The effectiveness of the concepts are demonstrated within the context of the novel and openly accessible desktop application called *Mass spectrometry imaging Applications for Interactive Analysis in MITK* (M²aia). Furthermore, concepts for a programming language-independent integration of third-party command-line applications via Docker (mitk-docker) into the interactive framework of M²aia are presented. Finally, concepts for an optimized MSI data access for deep learning are proposed and shown in combination with the data handling and processing capabilities of M²aia as part of a python package (pyM²aia).

The second part of this thesis proposes a versatile and efficient interactive remote working environment. It relies on interactive containerized applications that can be deployed with Docker and accessed using a web-browser. The effectiveness of the concept is demonstrated by applying it to a diverse set of biomedical image processing applications, M²aia for MSI data, MITK for clinical images, ImageJ for microscopy images, QuPath for manual segmentation of histology images, and ilastik for semi-automatic segmentation of a wide range of biomedical imaging modalities. Access to these remote-controlled applications facilitates a variety of interactive tasks on remote image data such as image analysis, method development and collaboration with experts.

In both parts of this work, diverse use-cases are elaborated to show the capabilities of the respective concepts. Use-cases demonstrate the advanced interactive capabilities of M²aia with respect to multimodal image fusion and 3D image reconstructions. A comprehensive set of MSI-based deep learning use-cases is realized to showcase the data access capabilities of pyM²aia. Furthermore, the seamless integration of Docker-based applications into the interactive environment of M²aia is demonstrated. Finally, capabilities of the interactive remote working environment are demonstrated.

In summary, this thesis introduces comprehensive concepts for processing and interactive analysis of multi-modal 2D/3D mass spectrometry image data as well as additional concepts for a general support of interactive remote working applying to a wide range of interactive biomedical image processing tasks.