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## Editorial for the Special Issue of “Computational Methods for Molecular Imaging” for Computerized Medical Imaging and Graphics

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Molecular imaging is an evolving clinical and research discipline enabling the visualization, characterization and quantification of biologic processes taking place at cellular and subcellular level (Weissleder and Pittet, 2008, Schroder et al., 2006, Beer et al., 2011, Clark et al., 2012). Computational methods are driving technical innovation in the field of molecular imaging. Since 2012, the guest editorial team has been organizing activities in molecular imaging computing, first tutorials and then workshops, as satellite events for MICCAI conferences. In the past years, world leading scientists and medical doctors were invited to participate in this unique event dedicated to molecular imaging during the computer science conference. The positive feedback was overwhelming and encouraged us to initiate this special issue advocating the methodology research for molecular imaging.

Molecular imaging acquires information based on the radioactive, magnetic or optical signals generated by injected molecules into the investigated organism. This special issue covers the topics of several classical and emerging molecular imaging modalities such as positron emission tomography (PET) (Lu et al., 2017, Paul et al., 2017, Karakatsanis et al., 2017), PET/CT (Bi et al., 2017), total internal reflection fluorescence microscopy (TIRFM) (Li et al., 2017) and PET/MR (Shi et al., 2017). Molecular imaging generates contrast between normal and abnormal tissues based on different metabolic properties of specific tracers or contrast agents and provides advanced information for many applications, such as elucidating basic

principles (Li et al., 2017), supporting early diagnosis (Lu et al., 2017), detecting lesions (Bi et al., 2017) and improving prognosis (Paul et al., 2017), which are addressed in this special issue.

Computational methods play an important role in the development of molecular imaging, from image synthesis to data analysis, and from clinical diagnosis to personalized therapy. They continuously increase the visualization depth, enhance the imaging resolution, extend the molecular scope, and improve the precision of interpretation.

Compared to anatomical imaging, molecular imaging often acquires signals emitted from the injected labeled molecules. The injected dose is usually restricted by pharmacological, physiological and radiation safety requirements. Therefore, molecular imaging usually has poor statistics and is affected by large dynamic effects due to tracer metabolism. The reconstruction and enhancement of molecular imaging also need to consider these barriers in addition to general medical imaging problems such as motion (Wang and Qi, 2015, Le Pogam et al., 2013). Karakatsanis et al. introduced an image-based motion-compensated image reconstruction approach for the reconstruction of static/dynamic PET data (Karakatsanis et al., 2017). Motion correction is performed within a maximum likelihood expectation maximization (MLEM) reconstruction framework using non-gated data and is accelerated using optimization transfer tools resulting in nested updates. In addition to the compensation of periodic motion, the proposed approach can be applied on bulk motion.

In the development of hybrid imaging techniques such as PET/MR, computational methods have also played a critical role in obtaining proper images. Classification methods or atlas based methods have been developed to obtain adequate attenuation maps from MRI images for precise imaging of PET/MRI (Hofmann et al., 2011). Shi et al. proposed an individual refinement method to improve the accuracy of classification-based attenuation correction methods without using external prior from atlas or database (Shi et al., 2017). This is achieved by a multi-resolution regional learning (MRRL) scheme to utilize the internal consistency inside the patient data. The improved segmented attenuation maps can consequently improve the accuracy of PET reconstructions of PET/MR.

The uptake of imaging agents of molecular imaging depends on many physiological factors, such as circulation, blood perfusion, interstitial pressure, endogenous competition, and others. Therefore, the acquired images of molecular imaging have larger physiological variations, which

make computer-aided diagnosis and therapy planning difficult (Thiele et al., 2013). Advanced computational methods are beneficial to extract meaningful characteristics to improve the clinical applications. Lu et al. developed a semi-supervised learning method to improve the feature representation for early diagnosis of mild cognitive impairment (MCI) (Lu et al., 2017). Regional features were pre-clustered using incomplete random forest and then the refined features were fed into a binary support vector machine (SVM) classifier. This method achieved better classification results to identify MCI from normal subjects. Another two-step feature selection method is proposed by Paul et al. based on Spearman correlation and genetic algorithm based on random forest for outcome prediction in oesophageal cancer (Paul et al., 2017). Both predictive and prognostic results show better performances with the improved feature selection. Refining feature selection can also assist the detection of abnormalities. A computational algorithm is developed by Bi et al for identifying sites of normal physiological FDG uptake and normal FDG excretion (sFEPUs) (Bi et al., 2017). A multi-scale superpixel-based encoding (MSE) was employed to group the individual sFEPUs fragments into larger regions. Then a class-driven feature selection and classification model (CFSC) was applied to avoid overfitting to the most frequently occurring classes during the classification of the regions into one of the sFEPUs classes.

The emerging technology of deep learning extends human power of perception for information from data (e.g. images) and has outperformed conventional machine learning methods in many applications such as image recognition and robotics (LeCun et al., 2015, Silver et al., 2016). It has already demonstrated advantages in computerized diagnosis on medical imaging (Roth et al., 2016, Suk et al., 2016). Convolutional neural networks (CNN) were applied to extract domain-transferred features to improve classifications (Bi et al., 2017). An approach was developed by Li et al. to identifying vesicle fusion events in time-lapse microscopy images of TIRFM based on CNN (Li et al., 2017). This hierarchical CNN can utilize the high-level time-series intensity change features and the visual appearance features to accurately classify candidate patch sequences.

In summary, computational methods actively contribute to almost every breakthrough of molecular imaging. We believe the publication of the selected papers in this special issue of Computerized Medical Imaging and Graphics can promote the exchange between computer science and the evolving molecular imaging activities as well as attract more interest in the computer science community to develop cutting-edge technologies for molecular imaging.

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