

Introduction

By means of the whole-brain dynamical models we investigate the impact of the neuroimaging data processing on the results of model validation against empirical data. In this study we considered the following data processing parameters:

- The functional Schaefer atlas [1] with 100 and 200 cortical parcels (S100 and S200) and anatomical Harvard-Oxford atlas [2] with 96 cortical parcels (HO96).
- Different frequency bands for the natural frequencies of the model oscillators, which were either randomly distributed or extracted from the empirical resting-state fMRI BOLD signals.

Aim: To find an optimal parameter setting for data-driven mathematical modeling of the resting-state brain dynamics and data analytics.

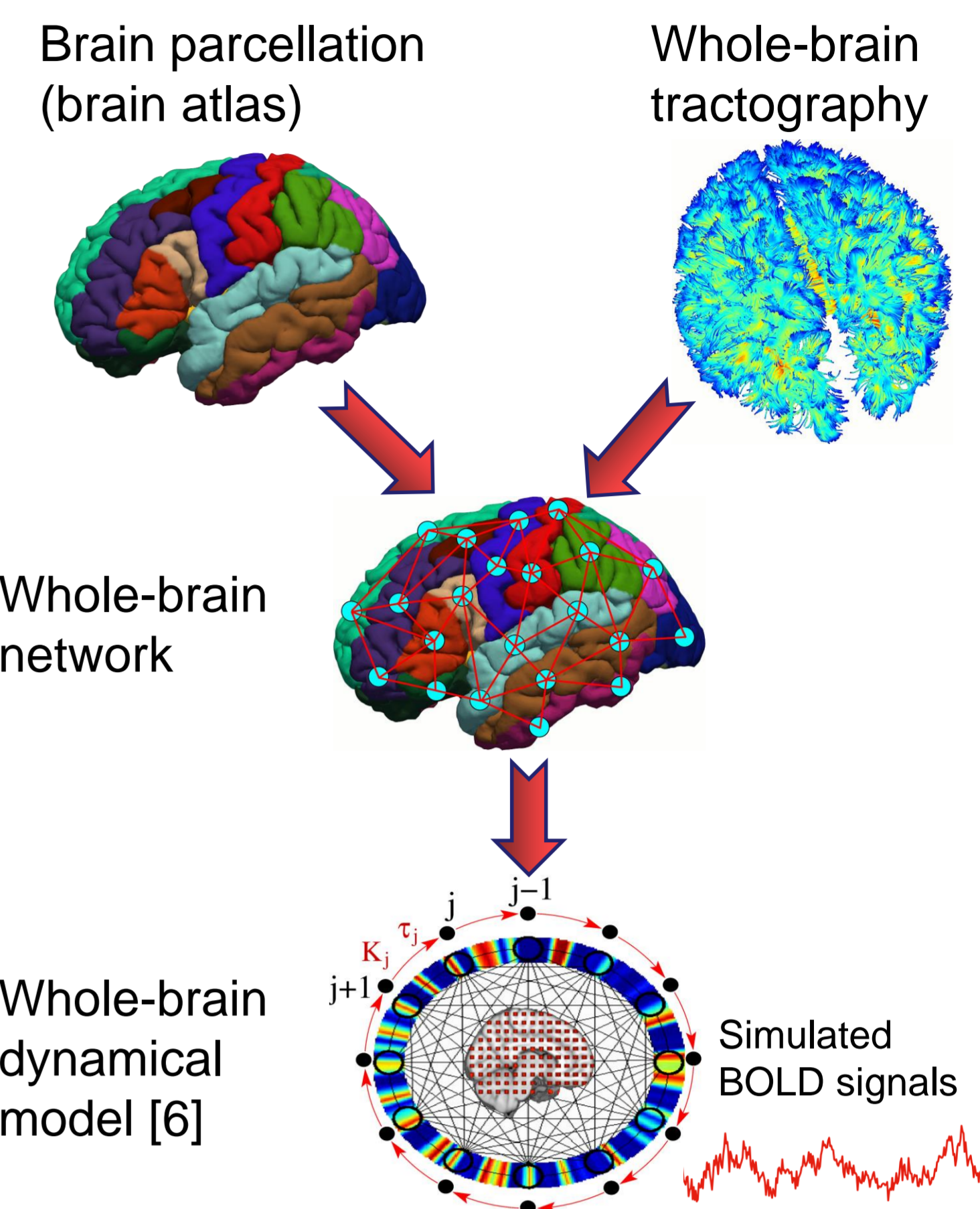
Methods

Computational model

Kuramoto model [3] of coupled phase oscillators was used to simulate the dynamics of the phases $\theta_i(t)$ of network nodes $i = 1, \dots, N$, which represent the mean resting-state dynamics of brain regions [4,5]

$$\frac{d\theta_i}{dt} = 2\pi f_i + \frac{C}{N} \sum_{j=1}^N k_{ij} \sin[\theta_j(t - \tau_{ij}) - \theta_i(t)] + \eta_i(t)$$

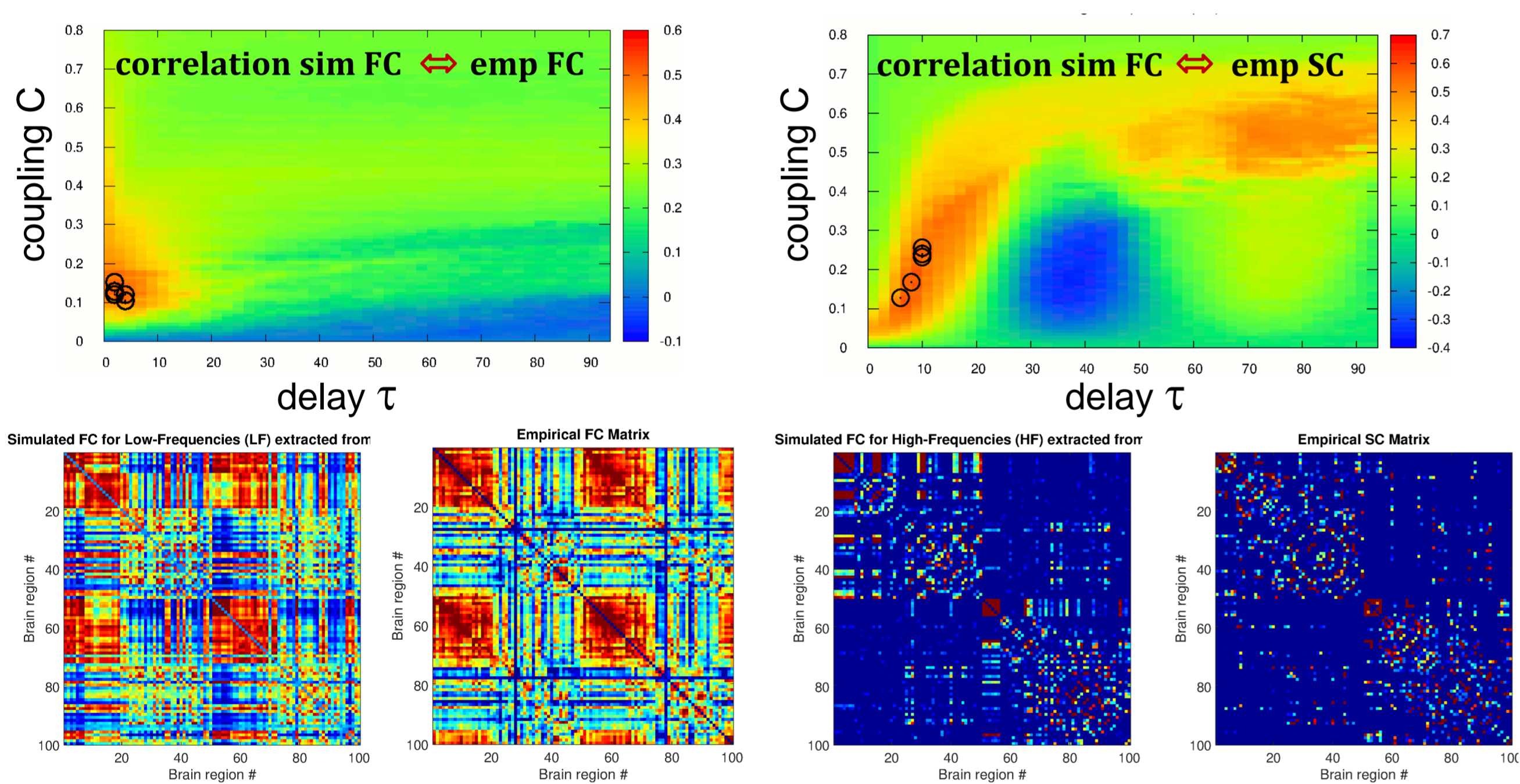
Model variables	Description	Model variables	Description
$\theta_i(t)$	phase of node i at time t	L_{ij}	average fiber path length of eSC from node j to node i
f_i	natural frequency of node i	V	mean conduction velocity
C	parameter of global coupling strength	$\tau = \langle L_{ij} \rangle / V$	parameter of global delay
$k_{ij} = n_{ij} / (n_{ij})$	relative number of streamlines in the empirical structural connectivity (eSC) from node j to node i	$\eta_i(t)$	independent noise
$\tau_{ij} = L_{ij} / V$ $= \tau \cdot L_{ij} / \langle L_{ij} \rangle$	coupling delay (signal conduction time) from node j to node i	$S_i = \sin[\theta_i(t)]$	simulated BOLD signals



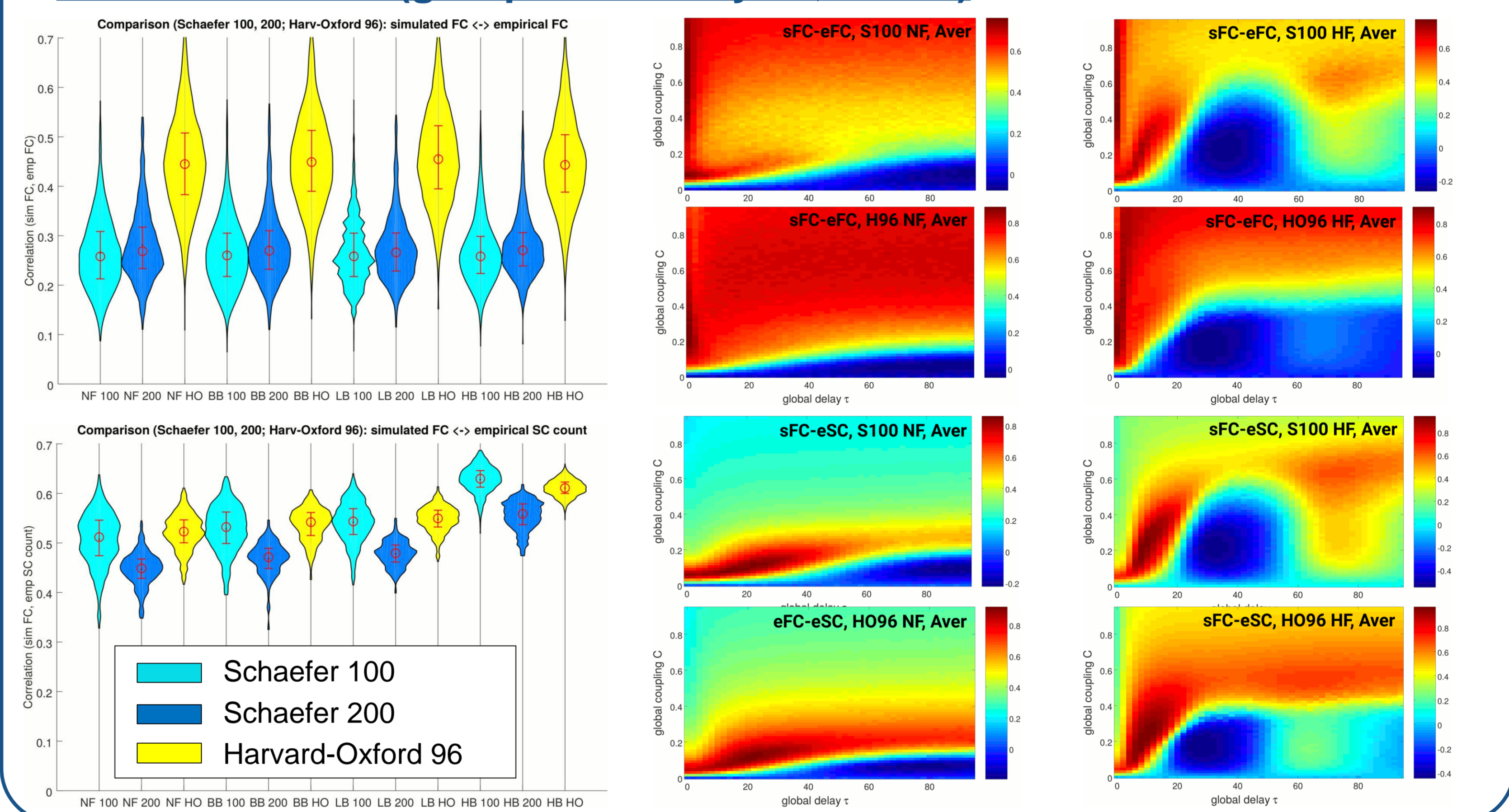
Results

Model validation (personalized simulations)

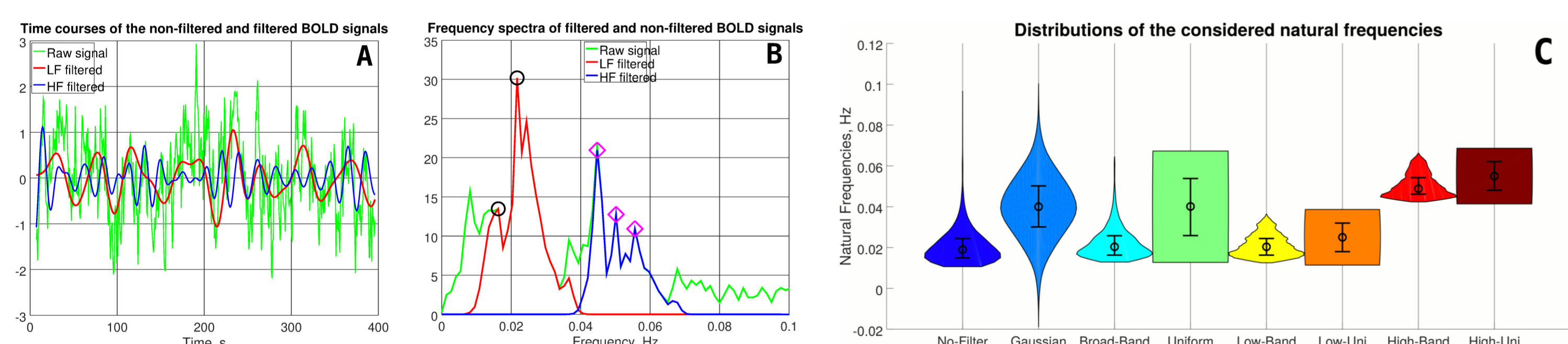
Simulated functional connectivity (sim FC) is compared with the empirical FC (emp FC) and structural connectivity (emp SC) for the best fitting Fit(sim FC, emp FC) and Fit(sim FC, emp SC).



Model validation (group-level analysis, n=272)

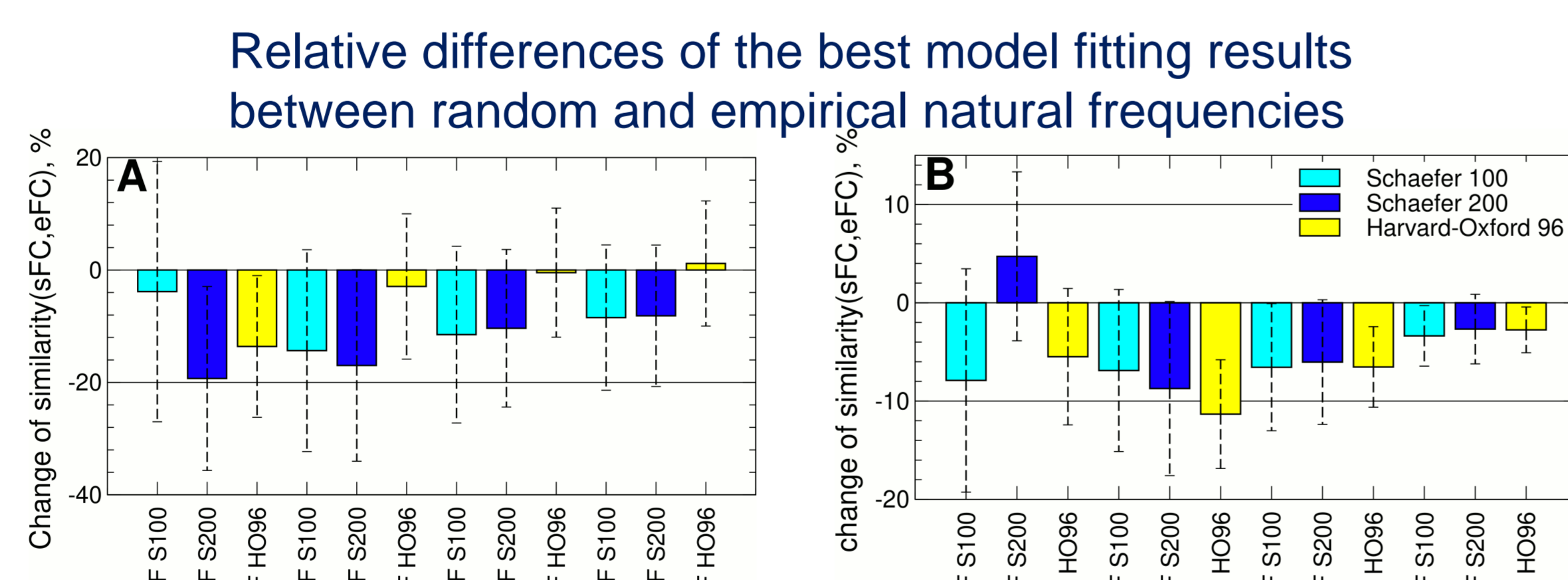


Natural frequencies

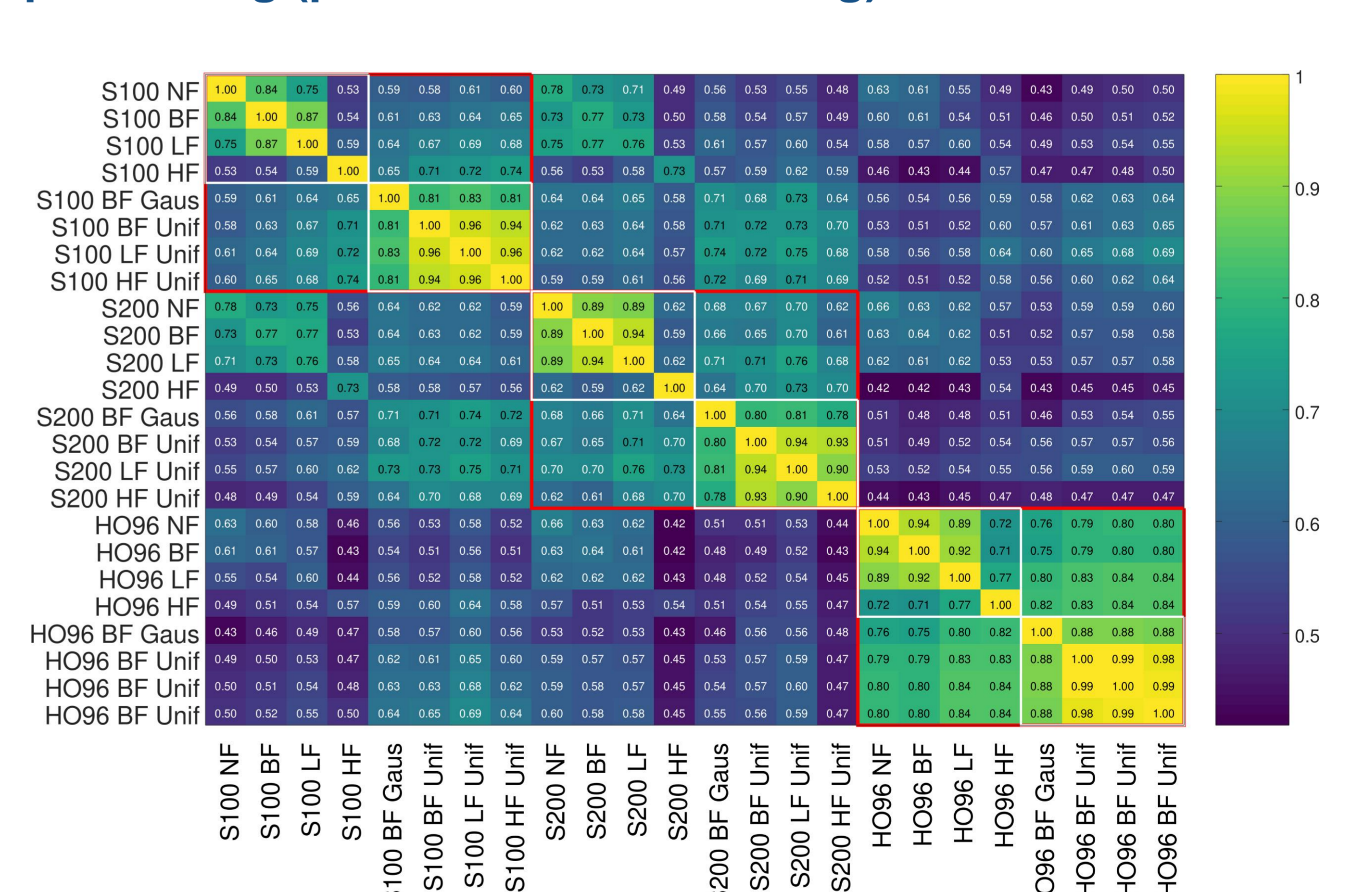


The natural frequencies f_i were extracted from the empirical BOLD signals filtered in the frequency bands: (LF) [0.01, 0.04] Hz, (HF) [0.04, 0.07] Hz, (BF) [0.01, 0.07] Hz as well as from non-filtered (NF) signals, or randomly distributed (Gaussian, uniformly) in these frequency ranges.

Empirical natural frequencies in most cases lead to a better correspondence between simulated and empirical data than randomly distributed ones



Compatibility of model validation for varying data processing (parcellation and filtering)



Conclusions

- A choice of a particular brain parcellation and frequency band of BOLD filtering can cause a significant impact on the quality of the model fitting and structure of the model parameter space.
- The main impact of the brain parcellation can be observed for the fitting quality of the simulated and empirical functional data: simFC to empFC.
- The frequency bands of the BOLD filtering mostly affect structure-function model validation modality, optimal model parameters and compatibility of the fitting results.