Impact of brain parcellation on parameter optimization of the whole-brain dynamical models

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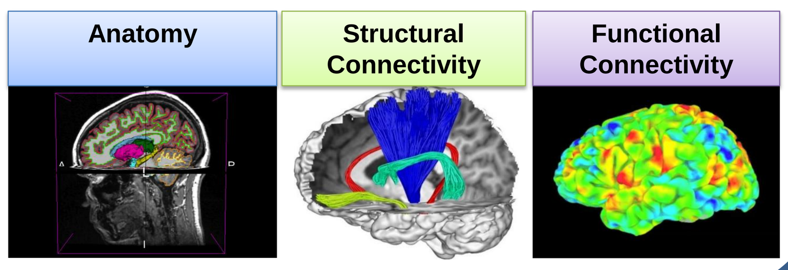
Introduction

- Resting-state (RS) functional connectivity (FC) analysis has brought new insights to the inter-individual variability and the pathophysiology of brain disorders [1,2].
- We constructed model networks based on the empirical structural connectivity (SC) and the simulation results are compared with empirical functional data.
- We considered two brain atlases and brain parcellations and evaluated their impact on the dynamics of the whole-brain models.



The computational model: Kuramoto

We use a computational Kuramoto model of coupled phase oscillators to simulate the dynamics of the resting-state (RS) brain networks [5]. The phase θ_n of node n at time t, obeys the following dynamical equation [6]:

$$\frac{d\theta_i}{dt} = \omega_i + K \sum_{j=1}^{N} C_{ij} \sin[\theta_j(t-\tau_{ij}) - \theta_i] + \eta_i(t), \quad i = 1, \dots, N.$$

Model variables	Description	Model variables	Description
θ_i	phase of node i at time t	$\eta_i(t)$	noise term
K	global coupling strength	$L_{ij}, \langle L \rangle$	relative, mean fiber length
C_{ij}	relative coupling strength from node j to node i	V	conduction speed
$\tau_{ij} = \frac{L_{ij}}{V} = \langle\tau\rangle L_{ij}/\langle L \rangle$	time delay between node j to node i	$\langle\tau\rangle$	mean time delay
$f_i=\omega_i/2\pi$	intrinsic frequency of node i on its limit cycle (f = 10 or 60 Hz)	$r_i = sin[\theta_i(t)]$	neural activity

Structural, Diffusion & Functional data preprocessing

We used 50 healthy subjects from the **Human Connectome Project** [3] database

CONNECTOME COORDINATION FACILITY

Magnetic Resonance Imaging protocol:

- Filtered blood-oxygen-level dependent (BOLD) time series are extracted from the FIX denoised RS data in MNI152 template space
- Parcellation-based empirical FC matrices: from the mean BOLD signals extracted for each brain regions after 5mm and without spatial smoothing (mean and 1st eigenvariate time series)

Structural pipeline [4]:

- Parcellation: Shaefer & Harvard-Oxford brain atlases
- Software method: Freesurfer
- Motion/eddy correction: ✓
- Intensity normalization: ✓
- Tractography: Probabilistic (MRTrix 3.0)
- SC Metric: Voxel pairs connected with 10^6 streamlines, ROI volume corrected

FreeSurfer MRtrix3

Parameter Sweep Exploration

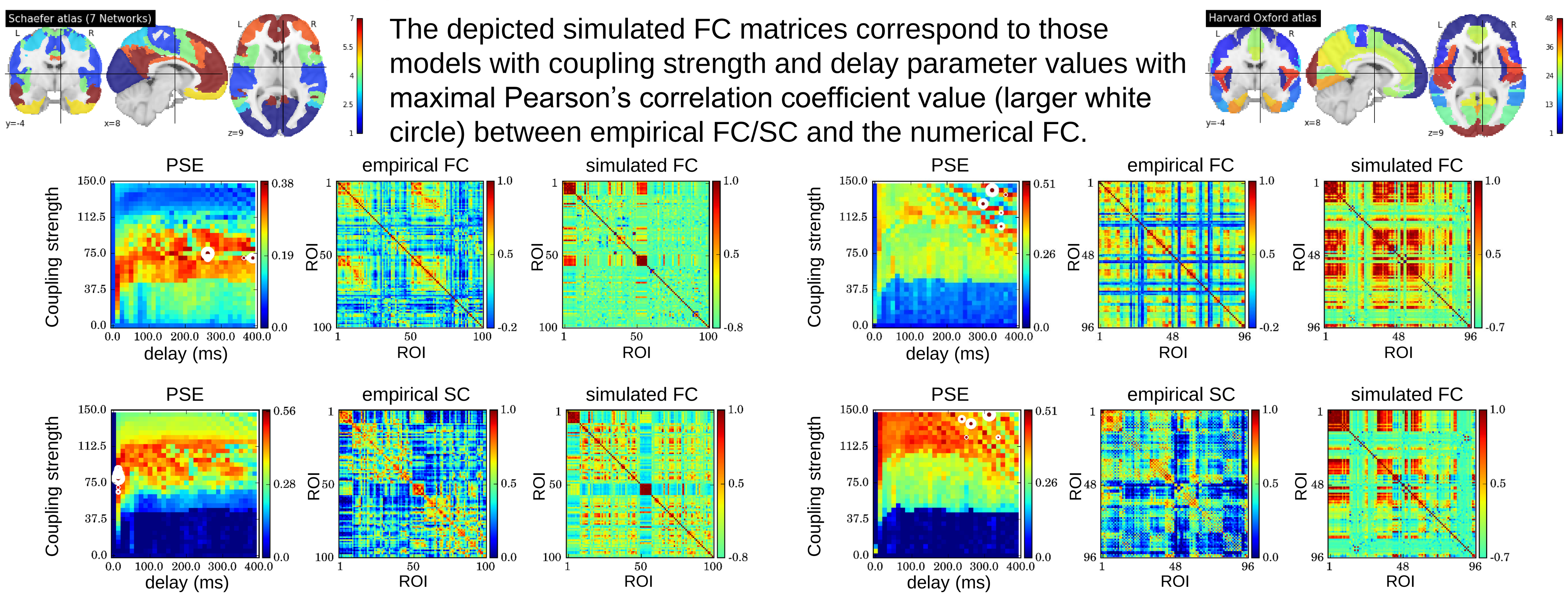
- Essential step in order to fit simulations with empirical data.
- Performed using **tvb-hpc** (CUDA) [7].
- TVB model kernels optimized for HPC on hybrid architectures.
- GPU code allows thousands of parameters to be explored in parallel: each parameter is assigned to a thread in the GPU.
- Global coupling (K) and mean time delay $\langle\tau\rangle$ are varied to maximize FC/SC correlation with simulated FC.
- Runs are performed on the JURECA GPU partition (Research Centre Jülich).

THEVIRTUALBRAIN.

Results: numerical simulations

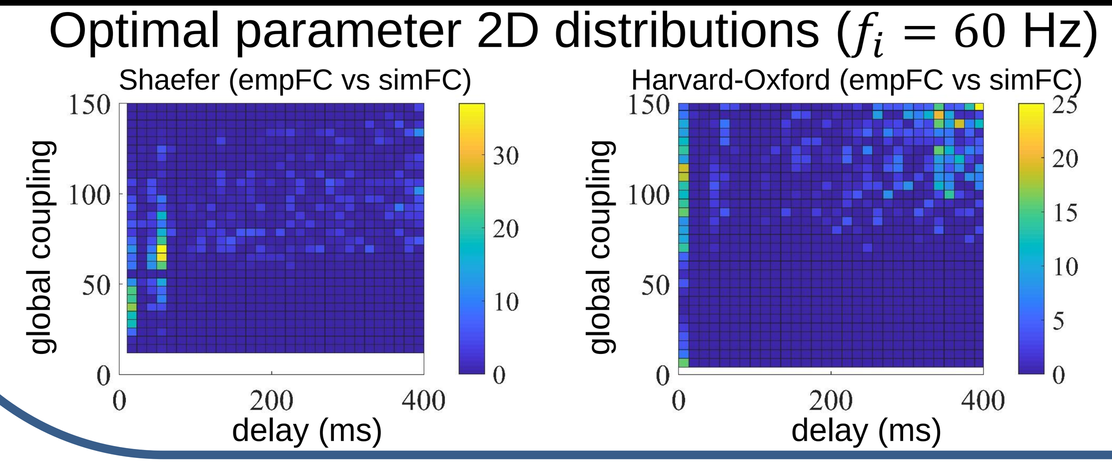
Parameter sweep exploration (PSE) for Schaefer and Harvard-Oxford atlases
($f_i = 60$ Hz – FC : mean over region – a case example)

The depicted simulated FC matrices correspond to those models with coupling strength and delay parameter values with maximal Pearson's correlation coefficient value (larger white circle) between empirical FC/SC and the numerical FC.

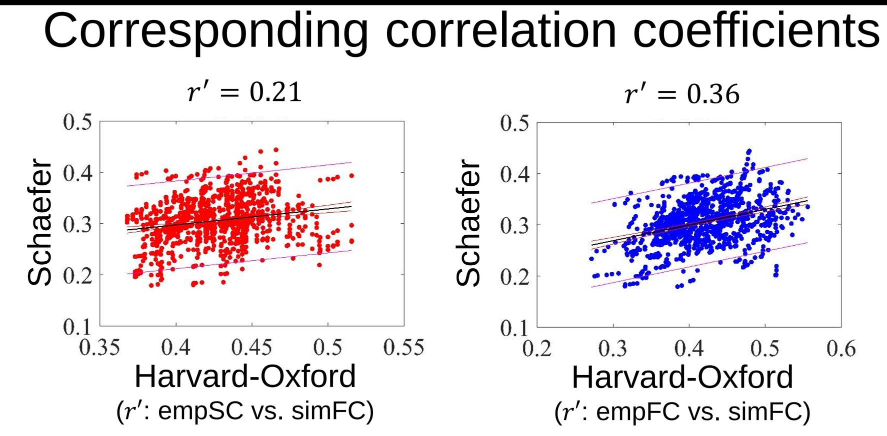


(white circles: 5 maximum Pearson's correlation coefficient values / 30s of simulated electrical activity)

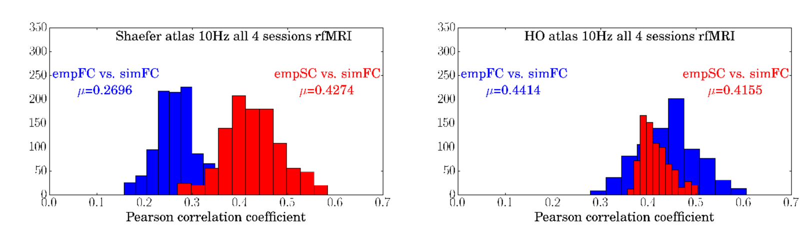
Optimal parameter 2D distributions ($f_i = 60$ Hz)



Corresponding correlation coefficients (r')

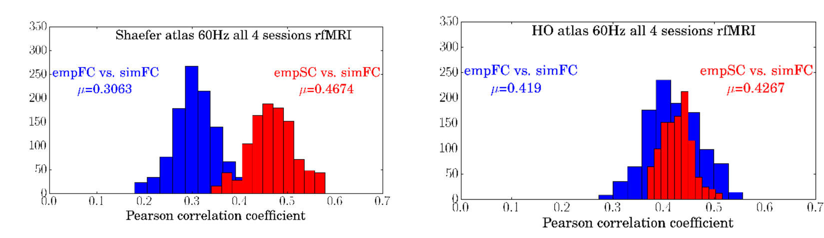


Schaefer vs Harvard-Oxford
($f_i = 10$ Hz – FC: mean over region)



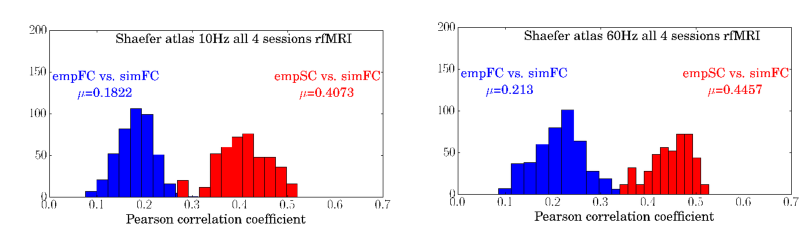
# of subjects: 50
# of sessions: 4

($f_i = 60$ Hz – FC: mean over region)



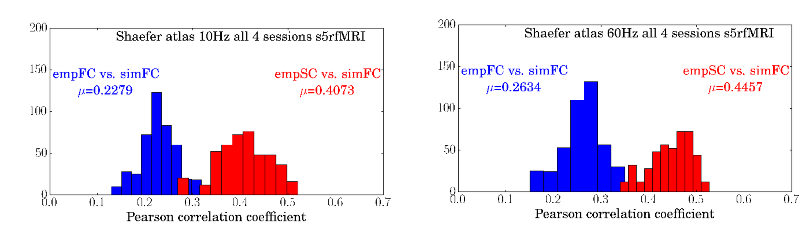
Using the 5 maximal Pearson's correlation coefficient values (4 sessions per subject) from the parameter sweep exploration analysis (white circles in the PSE figures)

Schaefer
($f_i = 10, 60$ Hz – FC: 1st eigenvariate without spatial smoothing)



# of subjects: 23
# of sessions: 4

($f_i = 10, 60$ Hz – FC: 1st eigenvariate with spatial smoothing)



Summary

- We calculated the SC matrices and FC matrices (mean and 1st eigenvariate over region with/without spatial smoothing) for 50 HCP subjects.
- We simulated resting-state network dynamics (mean node electrical activity) using the Kuramoto model (with $f_i = 10, 60$ Hz).
- We performed parameter sweep exploration for global coupling and mean time delay to maximize empirical FC/SC correlation with simulated FC.
- No observable advantage was found when using 1st eigenvariates instead of mean value from the BOLD time series.
- We produced 2D distributions for the optimal parameters for both atlases.
- We found relatively strong correlations ($r \gtrsim 0.35$) between emp. FC and sim. FC matrices, whereas the correspondence between emp. SC and sim. FC matrices is, however, weaker ($r \gtrsim 0.20$) for both atlases.

Outlook
- Add more subjects, atlases, models, refine parameter space intervals, explore different empirical to simulated measurements

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Acknowledgments

This study was supported by the Deutsche Forschungsgemeinschaft (DFG, EI 816/4-1, LA 3071/3-1), the National Institute of Mental Health (R01-MH074457), the Helmholtz Portfolio Theme "Supercomputing and Modelling for the Human Brain" and the European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement No. 7202070 (HBP SGA1), No.785907 (HBP SGA2), and No. 826421 (VirtualBrainCloud). This project has received funding from the German Federal Ministry of Education and Research project no. 01GQ1504B. Responsibility for the content of this publication belongs to the authors.