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

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Brain & Behaviour


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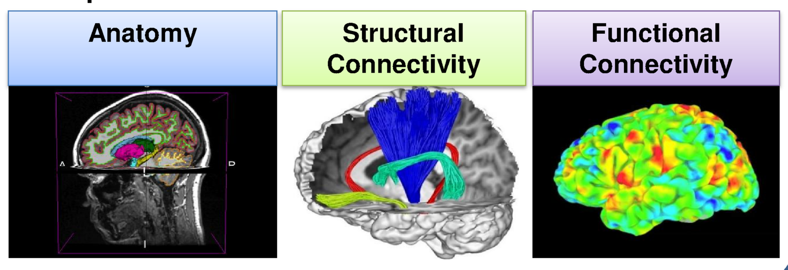
## Introduction

- 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 construct model networks based on the empirical structural connectivity (SC) and the simulation results are compared with empirical functional data.
- We consider two brain atlases and brain parcellations and evaluate 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 $\theta_n$ 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 |
|---|---|---|---|
| $\theta_i$ | 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 band-pass filtered 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

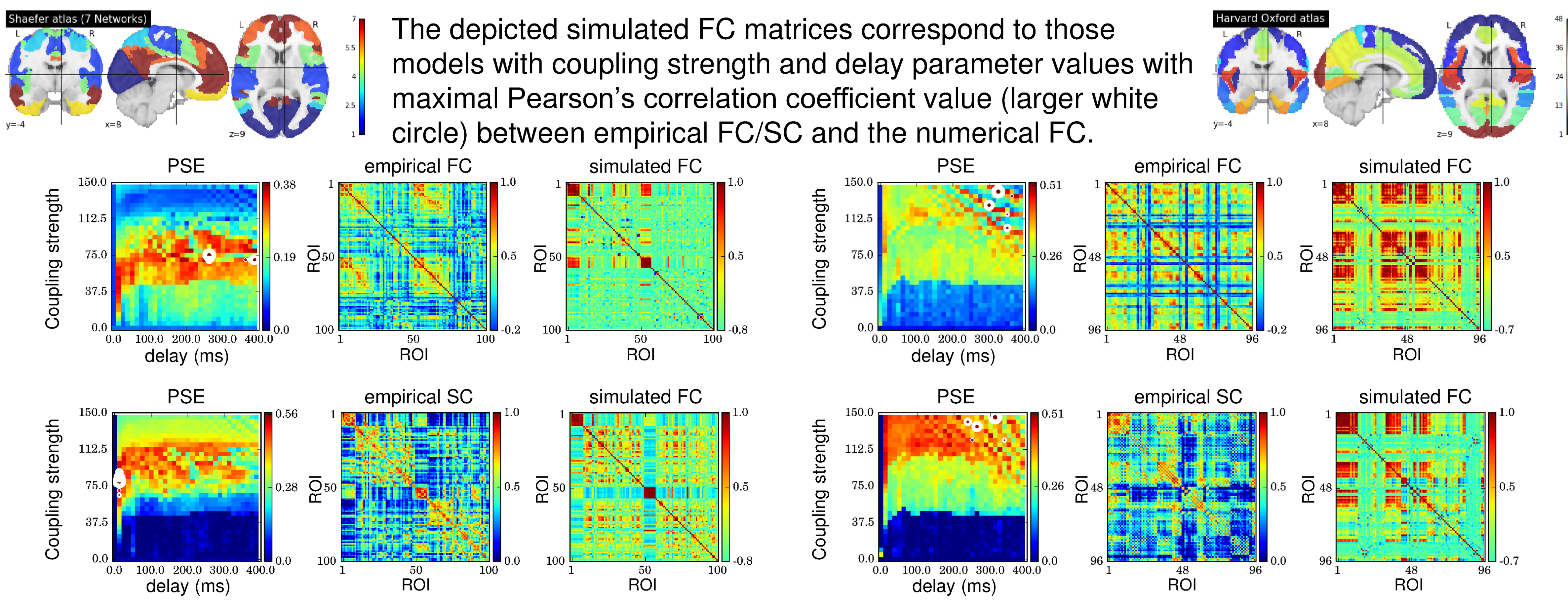
- Essential step in order to fit simulations with empirical data.
- Performed using **tvb-hpc** (CUDA) [7].
- TVB model kernels optimized for HPC on hybrid architectures.
- GPU code allows thousands of parameters to be explored in parallel: each parameter is assigned to a thread in the GPU.
- Global 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

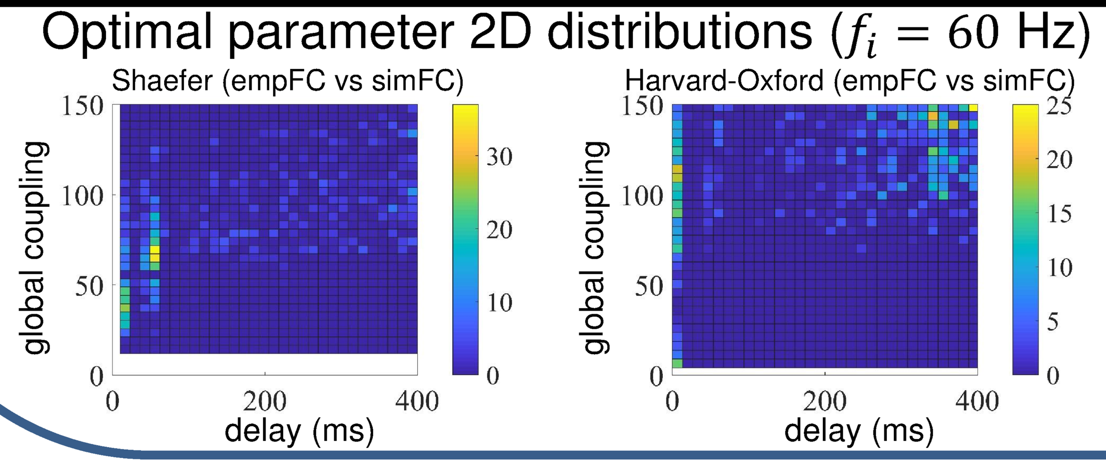
Parameter sweep exploration (PSE) for Shaefer and Harvard-Oxford atlases
($f_i = 60$ Hz – FC : mean over region – a case example)

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.

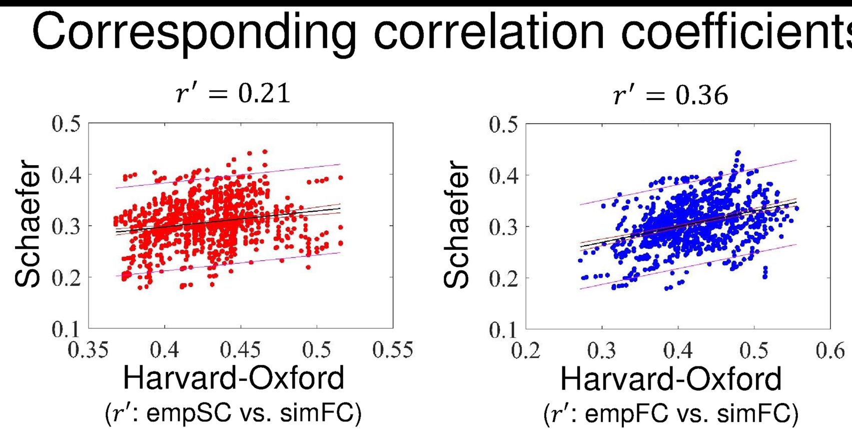



(white circles: 5 maximum Pearson's correlation coefficient values / 30s of simulated electrical activity)

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

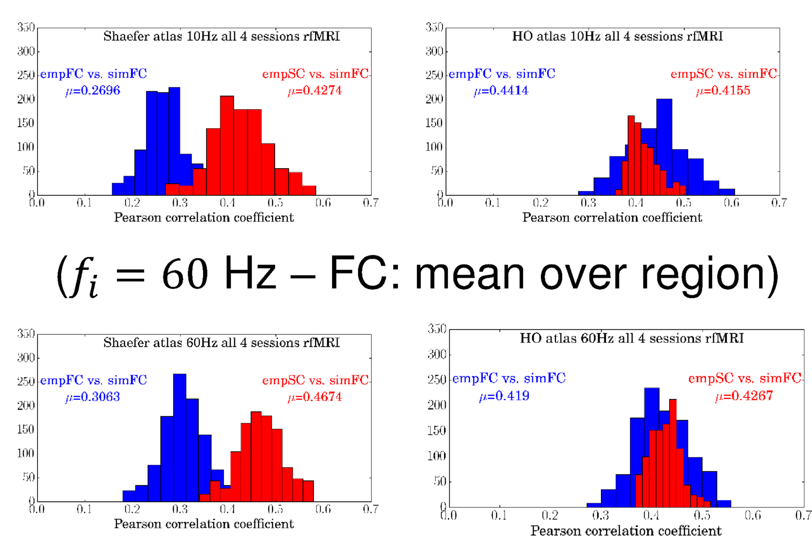



Corresponding correlation coefficients ($r'$)




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

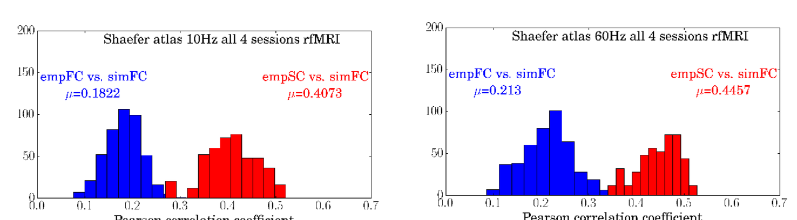
($f_i = 60$ Hz – FC: mean over region)




\# of subjects: 50
\# of sessions: 4

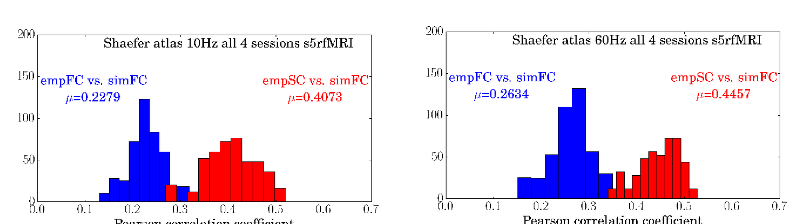
Using the 5 maximal Pearson's correlation coefficient values (4 sessions per subject) from the parameter sweep exploration analysis (white circles in the PSE figures)

Shaefer
($f_i = 10, 60$ 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

### References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