Enrichment of data analytics by whole-brain computational models

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Introduction

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

- The functional Schaefer atlas [1] with 100, 200 and 400 cortical parcels (S100, S200 and S400) and anatomical Harvard-Oxford atlas [2] with 96 cortical parcels and several thresholds of the maximal probability (HO96 0% - HO96 45%) .

We investigated the impact of the brain atlases and a few data variables on the model fitting and showed that these conditions may strongly influence the modeling results.

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

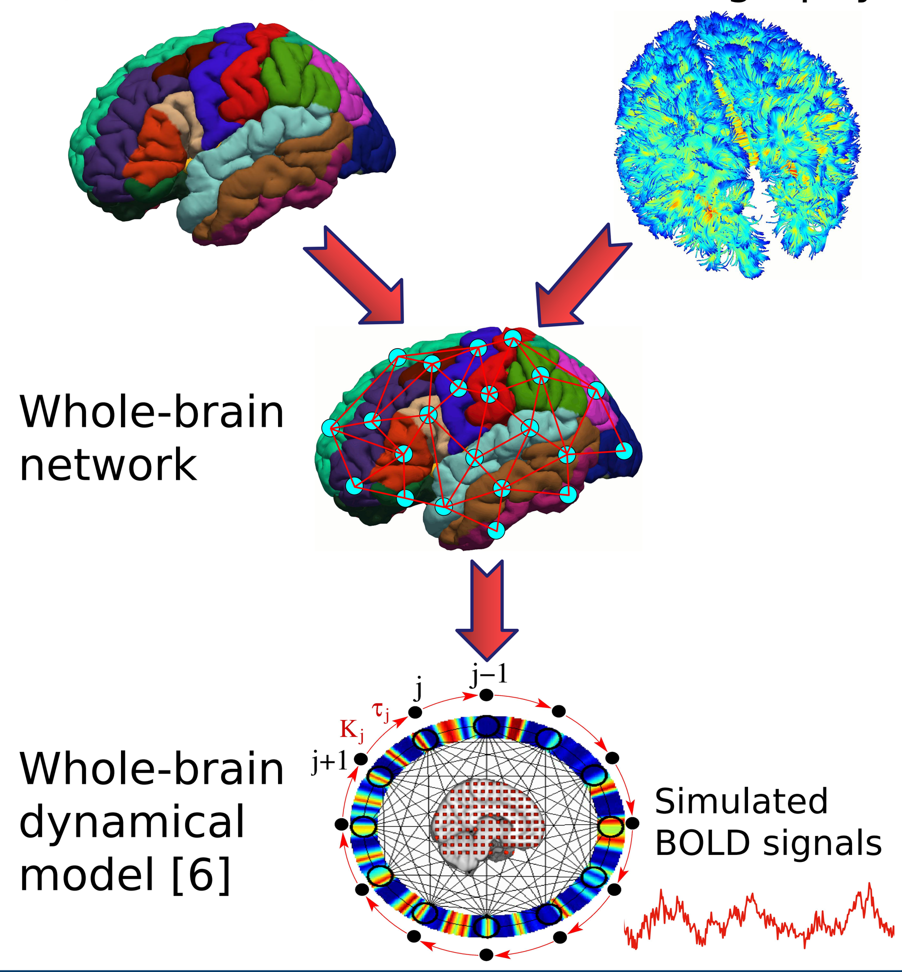
Methods

Computational model

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

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

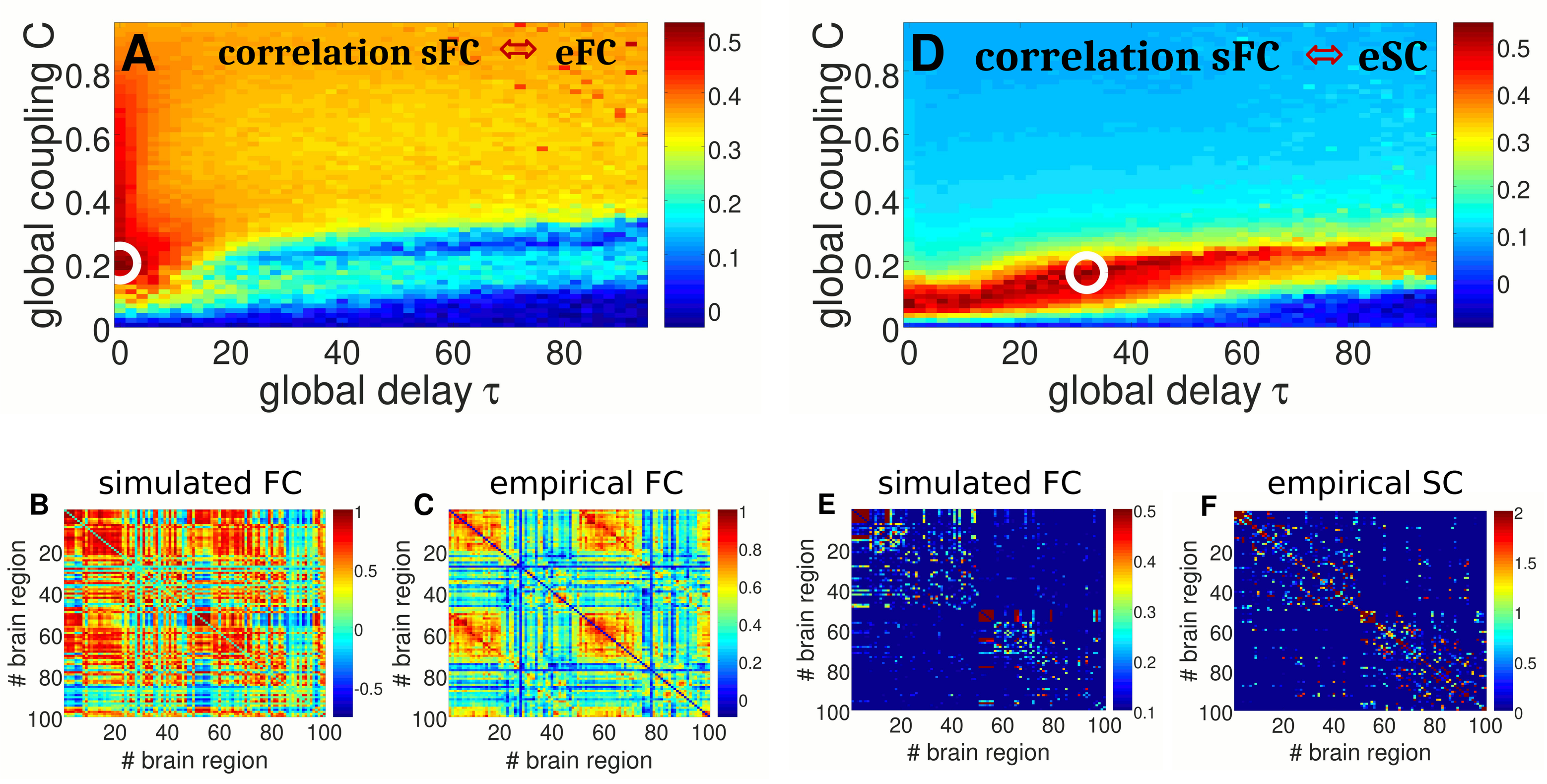
Model variables	Description	Model variables	Description
$\theta_i(t)$	phase of node i at time t	L_{ij}	average fiber path length of eSC from node j to node i
f_i	natural frequency of node i	V	mean conduction velocity
C	parameter of global coupling strength	$\tau = \langle L_{ij}\rangle / V$	parameter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



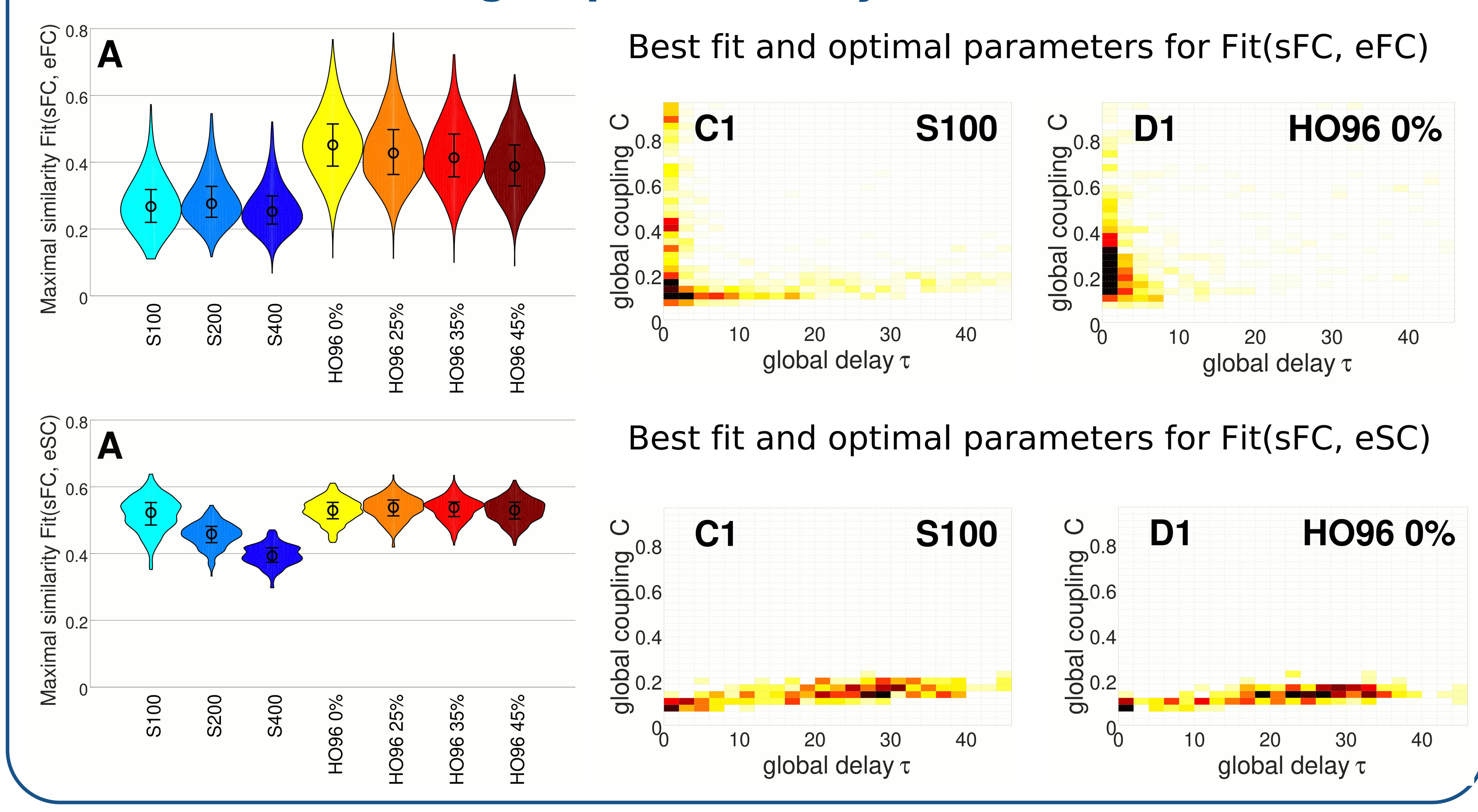
Results

Model validation (personalized simulations)

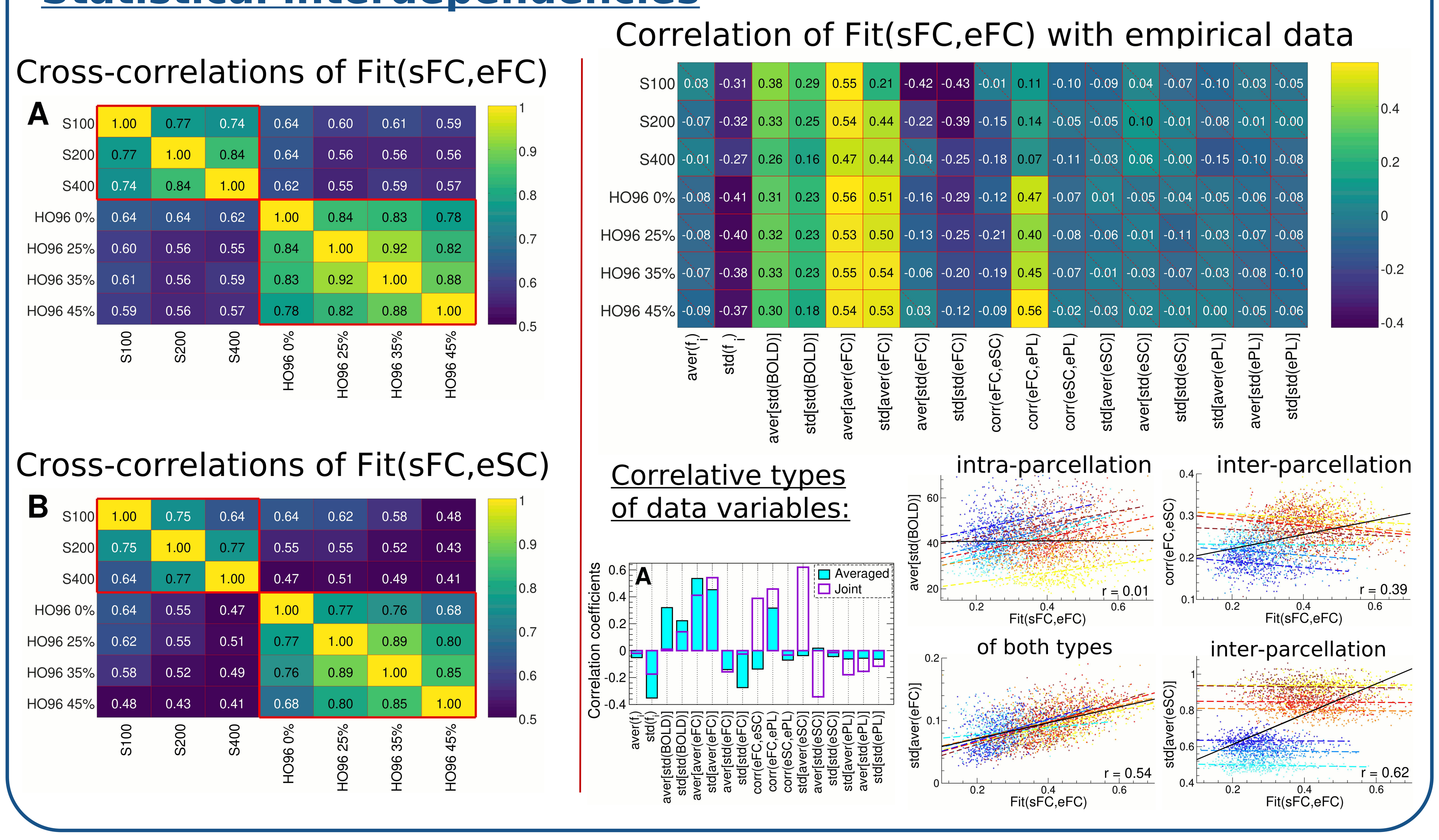
Simulated functional connectivity (sFC) is compared (by Pearson's correlation) with empirical FC (eFC) and structural connectivity (eSC) for the best fitting Fit(sFC, eFC) and Fit(sFC, eSC).



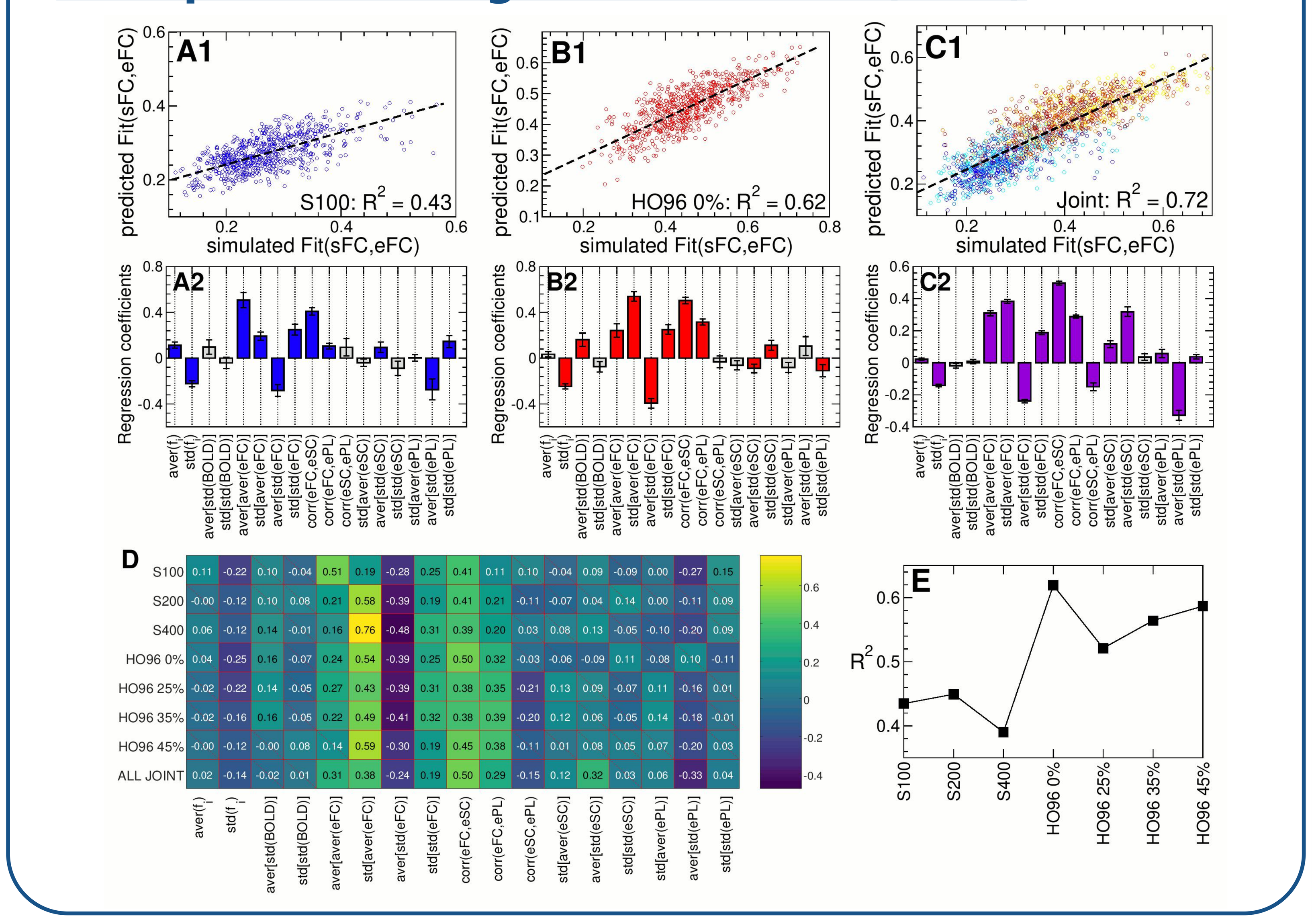
Model validation (group-level analysis, n=272 HCP)



Statistical interdependencies



Multiple linear regression model (MLR)



Conclusions

- A choice of a particular brain parcellation can cause a strong impact on the quality of the model validation and structure of the model parameter space, which may deviate for different fitting modalities.
- The variation of Fit-values across subjects and parcellations can be accounted for by data variables of different correlative types: intra-parcellation variables, inter-parcellation variables and of both types.
- The results of MLR modeling showed that up to 70% of the variance of modeling results (Fit-values) can be explained by the properties of empirical data used for model derivation and validation.

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