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Izaro Fernandez-Iriondo, Antonio Jimenez-Marin, Naiara Aginako, Gorka Zamora-López, Asier Erramuzpe, Paolo Bonifazi & Jesus M. Cortes

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Modular structure–function coupling reveals different network reorganization for task performance

Izaro Fernandez-Iriondo^{1,2,3,*}, Antonio Jimenez-Marin², Naiara Aginako¹, Gorka Zamora-López^{4,5}, Asier Erramuzpe^{2,7}, Paolo Bonifazi^{2,7,8}, and Jesus M. Cortes^{2,6,7}

¹*Department of Computer Science and Artificial Intelligence, University of the Basque Country (EHU), San Sebastian, Spain*

²*Computational Neuroimaging Lab, Biobizkaia Health Research Institute, Barakaldo, Spain*

³*Informatics Engineering Doctoral Programme, University of the Basque Country (EHU), San Sebastian, Spain*

⁴*Department of Complex Systems, Institute of Computer Science of the Czech Academy of Sciences, Prague, Czech Republic*

⁵*Center for Brain and Cognition, Universitat Pompeu Fabra, Barcelona, Spain*

⁶*Department of Cell Biology and Histology, University of the Basque Country (EHU), Leioa, Spain*

⁷*IKERBASQUE: The Basque Foundation for Science, Bilbao, Spain*

⁸*Department of Physics and Astronomy, University of Bologna, Bologna, Italy*

*Correspondence: fernandeziriondo.izaro@gmail.com

Abstract

Understanding how structural and functional brain networks interact to support cognition remains a central challenge in systems neuroscience. Here, we investigated modular structure–function coupling (SFC) across cognitive tasks using multimodal neuroimaging data. We separated SFC into intra-modular coupling (SFC-INT), measuring alignment within structural modules, and inter-modular coupling (SFC-EXT), measuring alignment between each module and the rest of the brain. This decomposition revealed that between-module coupling was more sensitive to task demands than within-module coupling. Moreover, different tasks produced distinct rest-to-task displacement patterns in the SFC-INT vs. SFC-EXT representation, indicating task-specific reconfiguration of the same anatomical structure. Brain–behavior analyses further suggested that performance is better captured by coordinated SFC profiles across modules than by isolated module-level effects. Together, these results provide a modular framework for studying how task demands reshape the relationship between brain structure and function.

Introduction

Understanding the relationship between different types of brain connectivity is a key challenge in systems neuroscience [1]. Structural connectivity (SC), defined by white matter pathways, provides the foundation for neuronal communication, while functional connectivity (FC), measured by the statistical similarity of neural activity, reflects the brain’s dynamic interactions [2–5]. A central question in this field is how these two connectivity types interact to support cognitive processes and adapt to task demands [6–10]. Structural-functional coupling (SFC) measures the alignment between these two forms of connectivity and is emerging as a critical metric for understanding cognitive network dynamics [11, 12].

It is well established that SC constrains FC at rest, forming large-scale networks that remain stable across different states [13]; however, increasing evidence suggests that SC-FC relationships dynamically reorganize during cognitive tasks, reflecting the brain’s flexibility [14–16]. Although the extent and nature of this reorganization — particularly regarding the balance between network segregation and integration - remain open questions [17–21], recent studies leveraging structure-function coupling (SFC) have provided new insights into these dynamics. Specifically, brain SFC has been shown to offer robust signatures for cognitive task decoding primarily through global coupling patterns [22], while task-related SFC changes have been linked to intelligence, emphasizing the role of broader communication strategies [23].

Our study complements and extends previous research by introducing two key methodological inno-

variations. First, we systematically decompose structure-function coupling into intra-modular (SFC-INT) and inter-modular (SFC-EXT) components, quantifying the degree to which functional connectivity aligns with structural connectivity within modules and between modules, respectively. This distinction moves beyond a single global estimate of SFC and allows task-related coupling changes to be examined according to their anatomical context: within structural modules or between them. Second, we use this modular decomposition to characterize how cognitive tasks reshape structure-function coupling relative to rest.

Leveraging a high-resolution multi-modal dataset, we apply this framework to analyze how modular structure-function coupling differs across cognitive tasks at two key levels: globally, we assess how task execution impacts overall SFC patterns; and, at the modular level, we examine how different cognitive tasks induce distinct patterns of coupling reorganization across brain modules relative to resting state.

Altogether, this modular SFC framework offers a complementary lens for studying task-related structure-function coupling. By separating within-module from between-module alignment, it provides a simple way to examine how cognitive demands reshape functional communication over the same anatomical structure.

Results

We analyzed $\mathcal{P} = 163$ healthy participants with quality-assured anatomical MRI, diffusion MRI, resting-state fMRI, and task fMRI acquired during emotion anticipation, emotion matching, gender Stroop, and visual working memory (quality-control details in Figures S2 and S1). Population-level pSC and pFC^{rest} matrices had dimensions 2035×2035 . Before modular decomposition, pFC^{rest} was thresholded by progressively removing the weakest $|\text{pFC}^{\text{rest}}|$ values until its density matched pSC, yielding a final density of 9.71%. Hierarchical agglomerative clustering of pSC identified $M = 9$ non-overlapping structural modules at the dendrogram level with maximal modularity ($Q = 0.71$). As summarized in Figure 1, modular structure-function coupling was then computed separately for within-module links (SFC-INT) and between-module links (SFC-EXT), allowing task-induced changes to be tested at the level of global task separation, module-wise rest-to-task displacement, and behavior.

The nine structural modules were mapped onto interpretable anatomical and functional systems (Supplementary Tables S11 and S12). Modules m6 and m7 were predominantly visual/occipital (Yeo visual overlap: 57.4% and 62.7%; occipital overlap: 72.7% and 56.5%, respectively), whereas m8 was mainly parietal and dorsal-attention related (89.0% parietal; 34.9% dorsal attention). Modules m1, m4, and m5 were frontal-dominant (79.7%, 78.7%, and 71.4% frontal overlap), with m5 showing the strongest frontoparietal contribution (25.1%). Modules m2 and m9 were temporal/limbic-DMN

systems (m2: 74.0% temporal, 33.8% limbic; m9: 84.7% temporal, 27.6% DMN and 26.6% limbic), while m3 combined parietal and temporal territories (60.1% and 30.7%) with somatomotor, dorsal-attention, and DMN components.

At the descriptive level, task modulation was stronger for between-module than within-module coupling (Figure 2). The task/rest ratio distributions in Figure 2A were more compact for SFC-INT and more dispersed for SFC-EXT, indicating that between-module alignment changed over a wider dynamic range. The task-similarity matrices in Figure 2B showed the same organization from a second perspective: distances between task-specific modular profiles were larger and more structured for SFC-EXT than for SFC-INT. Thus, the global visualization suggested that task identity was expressed most strongly in how structural modules coupled to the rest of the brain, rather than in the coupling preserved within modules.

We tested this pattern using subject-level task-induced changes, $\Delta\text{SFC} = \text{SFC}_{\text{task}} - \text{SFC}_{\text{rest}}$. First, a repeated-measures ANOVA on inter-task variability showed a strong main effect of coupling type, with greater variability for SFC-EXT than SFC-INT ($F(1, 162) = 190.96, p < .001, \eta_G^2 = 0.272$), together with a module effect ($F(8, 1296) = 30.99, p < .001, \eta_G^2 = 0.030$) and a coupling type $\times$ module interaction ($F(8, 1296) = 18.62, p < .001, \eta_G^2 = 0.016$; Supplementary Table S1). Second, task-pair distances in ΔSFC space were markedly larger for SFC-EXT than SFC-INT ($F(1, 162) = 1020.98, p < .001, \eta_G^2 = 0.451$), with a significant task-pair effect ($F(5, 810) = 76.49, p < .001, \eta_G^2 = 0.167$) and coupling type $\times$ task-pair interaction ($F(5, 810) = 43.30, p < .001, \eta_G^2 = 0.047$). This result was unchanged when module distances were weighted by edge count (coupling type: $F(1, 162) = 1087.56, p < .001, \eta_G^2 = 0.460$; coupling type $\times$ task pair: $F(5, 810) = 37.65, p < .001, \eta_G^2 = 0.043$; Supplementary Table S2). Third, SFC-INT and SFC-EXT followed different task-modulation profiles, as shown by the coupling type $\times$ task modality interaction ($F(3, 486) = 102.54, p < .001, \eta_G^2 = 0.030$; Supplementary Table S3). FDR-corrected post-hoc comparisons confirmed reliable pairwise task differences for both coupling types, with the largest separation between Emotion Matching and Gender Stroop (SFC-INT: $d = -0.924, p_{\text{FDR}} < .001$; SFC-EXT: $d = -1.333, p_{\text{FDR}} < .001$; Supplementary Table S4).

The EXT > INT effect was stable across the main robustness checks. Split-half recomputation of the structural partition yielded above-chance agreement between independently derived module solutions (mean ARI = 0.43 ± 0.07 , range 0.29–0.56; Supplementary Table S5). The EXT/INT variability ratio remained greater than 1 at all tested FC densities: 1.594 at 4.91% density, 1.380 at the main 9.82% density, and 1.255 at 14.73% density (Supplementary Table S6). Alternative HAC linkage strategies also preserved the qualitative result despite producing different partitions: weighted/correlation linkage yielded 9 modules ($Q = 0.7072$, EXT/INT ratio 1.380), complete/correlation linkage yielded

10 modules ($Q = 0.6691$, $ARI = 0.337$, ratio 1.070), and Ward/Euclidean linkage yielded 10 modules ($Q = 0.1990$, $ARI = 0.029$, ratio 2.294; Supplementary Table S7). Split-half reliability of SFC profiles was uniformly high across rest and all tasks (SFC-INT: 0.995–0.997; SFC-EXT: 0.996–0.998; Supplementary Table S8). Finally, the $EXT > INT$ pattern generalized across structural dendrogram resolutions, with EXT/INT ratios of 1.394 ($M = 500$), 1.672 ($M = 250$), 3.374 ($M = 100$), 3.251 ($M = 50$), and 1.380 ($M = 9$; Supplementary Table S9).

At the module level, Figure 3 shows the rest-to-task displacement of each structural module in the SFC-INT/SFC-EXT plane. Figure 3A displays these displacements by task, whereas Figure 3B reorganizes the same information by module, making it possible to compare the four task trajectories within each structural system. Emotion anticipation produced heterogeneous module-specific displacements, consistent with a mixed coupling configuration. Emotion matching and visual working memory generally shifted modules toward reduced SFC-EXT with more variable SFC-INT changes, indicating weaker alignment of between-module functional interactions with the direct structural scaffold. Gender Stroop showed the opposite tendency, with a broad shift toward increased SFC-INT and SFC-EXT, consistent with stronger structure–function alignment during cognitive control. These module-wise trajectories indicate that the same structural architecture supports distinct task-specific SFC fingerprints.

We finally tested whether modular SFC related to behavioral performance in the three tasks with comparable behavioral measures: Emotion Matching, Gender Stroop, and Visual Working Memory. After two-sided BH-FDR correction across the module-wise tests, higher SFC-INT in module 2 during Emotion Matching was associated with faster responses ($r = -0.228$, $p_{FDR} = 0.030$). One-sided correction recovered the same module 2 association ($p_{FDR} = 0.015$) and an additional Emotion Matching association for SFC-INT in module 9 ($r = -0.181$, $p_{FDR} = 0.047$). Reduced-dimensional analyses indicated that mean SFC-INT during Emotion Matching was also associated with faster response time ($r = -0.170$, $p_{FDR} = 0.046$), and that the full 9-module SFC-EXT profile during Gender Stroop predicted accuracy after correction ($F(9, 153) = 3.48$, $p_{FDR} = 0.0019$). Thus, corrected brain–behavior evidence was modest at the single-module level but stronger for distributed SFC profiles, particularly for between-module coupling during cognitive control (Supplementary Table S10).

Discussion

This study asked how structure–function coupling is reconfigured when the brain moves from rest to task engagement. We introduced a modular SFC framework that separates alignment within structural modules (SFC-INT) from alignment between each module and the rest of the brain (SFC-EXT). Across

four tasks, the dominant result was that task identity was expressed more strongly in SFC-EXT than in SFC-INT. This finding was visible in the population-level ratio space, confirmed in subject-level analyses of Δ SFC, preserved after edge-count weighting, and robust to alternative density thresholds, linkage strategies, split-half reliability tests, and modular resolutions.

The interpretation is that task engagement does not simply increase or decrease global structure–function coupling. Instead, it changes how functional interactions between structural systems follow the anatomical scaffold. Within-module coupling was comparatively stable, consistent with the idea that local or module-internal communication remains more tightly constrained by structural architecture. Between-module coupling was more flexible and more task-specific, suggesting that cognitive demands are implemented partly by changing the degree to which distributed functional interactions are anatomically aligned. This extends previous work showing that SFC carries information about cognitive state and inter-individual differences [11, 22, 23] by showing that the between-module component is the most sensitive axis of task reconfiguration.

Importantly, SFC-INT and SFC-EXT should not be read as direct graph-theoretical measures of segregation and integration. They quantify SC–FC alignment within and between structural modules. A high SFC-INT value means that within-module functional connectivity follows the pattern of within-module structural connectivity; a high SFC-EXT value means that functional connectivity between a module and the rest of the brain follows the corresponding structural connectivity pattern. Thus, the framework does not replace classical segregation or integration metrics. It provides a complementary way to ask whether segregated and distributed functional interactions are constrained by the underlying anatomical network.

The module-wise displacements add anatomical specificity to this result. Gender Stroop shifted modules toward stronger SFC-INT and SFC-EXT, suggesting that cognitive control favors functional interactions that are more closely aligned with structural pathways. Emotion matching and visual working memory showed reduced SFC-EXT with more heterogeneous within-module changes, consistent with task states in which distributed functional interactions deviate more from direct anatomical connectivity. Emotion anticipation showed a mixed profile, plausibly reflecting the combined contribution of affective anticipation, sensory processing, and predictive components. The anatomical annotations further clarify that these trajectories involved systems with distinct biological profiles, including visual/occipital modules, parietal attention-related modules, frontal/frontoparietal modules, and temporal limbic-DMN modules.

The behavioral results support a cautious interpretation. After correction for multiple comparisons, single-module associations were present but modest, with the clearest local effect linking higher SFC-INT in temporal/limbic module m2 during Emotion Matching to faster responses. The stronger signal

emerged from reduced-dimensional or multivariate summaries: mean SFC-INT related to Emotion Matching response time, and the full 9-module SFC-EXT profile predicted Gender Stroop accuracy. This pattern suggests that behavior is unlikely to be explained by one isolated structural module. Rather, performance appears to depend on distributed SFC configurations, especially when the task requires cognitive control across systems.

Several methodological points follow from the robustness analyses. HAC was retained because it is deterministic, matches the structural-partition framework used in previous analyses of this dataset [24, 25], and provides a full dendrogram that can be interrogated across resolutions. The 9-module structural partition was reproducible above chance in split-half data and anatomically interpretable, but the key $\text{EXT} > \text{INT}$ result did not depend on that exact partition. It remained present across FC density thresholds, alternative HAC linkage strategies, and finer structural resolutions. This matters because external coupling contains more edges than internal coupling; the edge-count weighted task-distance analysis showed that the stronger task separation for SFC-EXT was not a trivial consequence of dimensionality. The split-half reliability results also indicate that the SFC profiles were stable enough to support subject-level inference rather than reflecting noisy estimates.

The study also has limitations. First, the task set sampled affective processing, cognitive control, and working memory, but not the full space of cognitive states. The results should therefore be interpreted as evidence for task-dependent SFC reconfiguration within the domains tested here, not as a universal law of cognition. Second, diffusion MRI tractography is an indirect estimate of anatomical connectivity and remains sensitive to false positives, false negatives, and endpoint assignment errors. Third, the present framework measured direct SC-FC alignment, whereas functional connectivity may also arise through indirect polysynaptic communication over the structural network. Network communication models such as search information and path transitivity can predict functional connectivity beyond direct structural links [26], and could be integrated with modular SFC in future work. Fourth, both SC and FC are constrained by brain geometry; geometry-preserving null models [27] will be important for determining how much of the observed SFC reconfiguration reflects topology beyond spatial embedding.

In summary, separating structure-function coupling into within-module and between-module components provides an interpretable framework for studying task-related brain reconfiguration. Across the present task set, between-module coupling was the most task-sensitive component, cognitive demands produced distinct modular SFC fingerprints, and behavior was better captured by coordinated SFC profiles than by isolated module effects. This framework can be extended to broader task batteries, lifespan cohorts, and clinical populations to test whether altered between-module SFC flexibility is a general marker of cognitive state, development, aging, or disease.

Methods

Participants

A total of 216 participants from the Amsterdam Open MRI Collection (AOMIC) dataset [28] were initially considered in this study accompanied by demographic and psychometric information. This data is freely accessible via OpenNeuro data-sharing platform and specifically here, we made use of the PIOP1 dataset which includes T1w, DWI, resting-state fMRI and fMRI images while performing several cognitive tasks per each participant [29]. For this study, we selected the following tasks: emotion matching, working memory, emotion anticipation, and gender stroop. After data quality assurance (see Figures S1 and S2), the final number of included participants was $\mathcal{P}=163$ with ages ranging from 18.25 to 26.25 years (mean 22.38, standard deviation 1.73).

The present study involved a secondary analysis of de-identified, publicly available data and did not involve new participant recruitment or data acquisition. For the original AOMIC data collection, all participants provided written informed consent. The study protocols were approved by the Ethics Review Board of the Faculty of Social and Behavioural Sciences at the University of Amsterdam (PIOP1 EC number: 2015-EXT-4366). All ethical regulations relevant to human research participants were followed.

Cognitive tasks

In this study, four task-related functional data sessions were performed per participant. The emotion anticipation task examined the ability to anticipate and respond to emotions, focusing on curiosity and prediction; participants were initially given cues predicting the likelihood of viewing an emotionally negative or neutral image, followed by the actual presentation of the image, testing anticipatory emotional responses through 30 unique images. The emotion matching task, inspired by earlier paradigms from Hariri et al. [30], assessed facial emotion processing by requiring participants to match the emotional expression of a target face to one of two probe faces. The gender stroop task measured cognitive conflict and control using a face-gender variant of the stroop test, where participants were presented with congruent or incongruent face-label pairs and asked to identify the gender of the face while disregarding the distractor word. Lastly, the working memory task aimed to assess how participants maintained and manipulated visual information in both active and passive conditions, responding to orientation changes or maintaining attention according to specific cues, encompassing various stages of working memory processing. For a detailed description of the methodologies see the full article [28].

Imaging data acquisition

Anatomical data:

A high-resolution T1-weighted image was acquired with a 3D magnetization prepared rapid acquisition gradient echo (3D MPRAGE) with parameters: TR/TE (ms) = 8.5/3.9, voxel size = $1 \times 1 \times 1 \text{ mm}^3$, field of view (FOV) = $188 \times 240 \times 220$ (RL $\times$ AP $\times$ FH; mm; RL: right-left, AP: anterior-posterior, FH: feet-head), flip angle = 8° and a duration of 6 min 3 sec.

Diffusion weighted imaging (DWI):

A spin-echo diffusion weighted imaging (SE-DWI) sequence was acquired with the following parameters: TR/TE = 7456/86, voxel size = $2 \times 2 \times 2 \text{ mm}^3$, slice thickness = mm, field of view (FOV) = $224 \times 224 \times 120$ (RL $\times$ AP $\times$ FH; mm), number of b_0 images = 1, number of diffusion-weighted directions = 32, DWI b-value = 1000 s/mm^2 , matrix size = 112×112 , number of slices = 60, slice gap = 0 mm, flip angle = 90° and a duration of 5 min 27 sec.

Resting functional data:

Acquired with a gradient echo EPI scan technique using the following parameters: TR = 750 ms, TE = 28ms, FOV (RL $\times$ AP $\times$ FH; mm) = $240 \times 240 \times 118 \text{ mm}^3$, voxel size = $3 \times 3 \times 3 \text{ mm}^3$, matrix size = 80×80 , number of slices = 36, slice gap = 0.3mm and flip angle = 60° .

Task functional data:

Acquired with a gradient echo EPI scan technique using the following parameters: TR/TE = 2000, FOV (RL $\times$ AP $\times$ FH; mm) = $240 \times 240 \times 122 \text{ mm}^3$, voxel size = $3 \times 3 \times 3 \text{ mm}^3$, matrix size = 80×80 , number of slices = 37, slice gap = 0.3mm and flip angle = 76.1° .

Imaging data preprocessing

Diffusion images

Preprocessed using a custom pipeline making use of brain-extracted T1 images [31, 32], MRtrix3 (v3.0.RC3) [33], FSL (v6.0.1) [34], and ANTs (v2.3.1). Our DWI pipeline involved cleaning the raw images using *DWIdenoise* [33, 35–37] and *DWIpreproc* [33, 38–40] tools. Next, we performed whole-brain probabilistic tractography using the iFOD2 [41] tracking algorithm in MRtrix3 [33]. The tractography was initiated from seeds located at the gray matter-white matter interface, with a selection of 3 million fibers based on an angle threshold of $<45^\circ$ and a length threshold of $<200 \text{ mm}$, following the

recommendations in the MRtrix3 documentation. The tool *SIFT2* [42] was used to correct for the effect of crossing and disconnection of fibers on the quantification of the total number of streamlines.

Functional images

Preprocessed with our pipeline previously used in [31,32] including slice-time correction, and alignment of volumes for head-motion artifact correction with MCFLIRT (FSL 6.0.1) [43–45]. Movement time-courses obtained from MCFLIRT were used as an input of ICA-AROMA tool [46], a data-driven method used to identify motion-related independent components (IC) in fMRI data. After intensity normalization, time-courses of the motion-related ICs, the 5 PCA components of the cerebrospinal fluid and the 5 components of the white matter signals with more variance explained, and linear and quadratic trends were removed together with a 0.01–0.08 Hz band-pass. In the case of the task fMRI, the design event matrix was also removed. Finally, images were normalized to the MNI152 brain template ($3 \times 3 \times 3$ mm³ voxel size) and spatially smoothed with a 6 mm full width at half maximum isotropic Gaussian kernel.

Parcellation of neuroimaging data

In our approach, we first delineated a functional partition comprising a large number of micro-regions (> 2000), that lately will represent the different nodes in SC and FC. We employed an unsupervised clustering method that groups voxels into the same region based on voxel-level dynamics similarity [47]. In an effort to integrate anatomical constraints among these micro-regions, our previous work involved various, independent, functional partitions across various macro-regions [25]. Here, we considered the following eight macro-regions: *frontal lobe*, *parietal lobe*, *occipital pole*, *temporal pole*, *insula*, *brain stem*, *cerebellum*, and *subcortical structures* (the latter achieved by pooling together the thalamus, caudate, putamen, pallidum, amygdala and hippocampus). Therefore, although we used a functional partition, our approach ensures that the derived functional partition is informed by, and reflective of, the brain’s intrinsic anatomical macro-organization.

Population connectomes

In our methodology, we obtained subject-specific SC and FC matrices. Subject-level SC matrices were obtained by counting the number of white matter streamlines connecting all possible pairs of micro-regions. For FC, we computed a time series for each of the micro-regions, by averaging within micro-region voxel time-series, and then assessed the statistical dependence between all pairs of micro-regions using the Pearson correlation coefficient. The next step is to build population pSC and pFC matrices, that here was done by calculating for each link in pSC and pFC, the median value of all

links across all individuals. Finally, out of the original number of micro-regions, we removed those exhibiting null connectivity values to any other region in the pSC. For details on code to generate these steps, see <https://github.com/compneurobilbao/bha2>.

Assessing modular organization

We identified modules or communities in the population structural connectome (pSC). The structurally defined partition was used as the main analytical framework, because SFC-INT and SFC-EXT quantify structure–function alignment within and between structural modules, respectively.

While it is true that the most celebrated method for community detection is modularity maximization [48], it has been acknowledged by previous authors that modularity maximization encounters a variety of serious conceptual flaws [49, 50]. The most problematic one is that it always finds high-modularity partitions in networks sampled from its own null model [49], providing a hard interpretation to the communities found at the maximum of modularity. A different strategy to modularity maximization that sorts out this problem is Bayesian Stochastic Block-Modeling [51], but this alternative needs prior information before Bayesian Inference, which is also unknown for many practical situations.

Here, and following previous work [24, 25], we performed hierarchical agglomerative clustering on pSC, and then calculated Newman’s modularity Q at all levels of the tree [52]. The final list of structural modules was chosen at the dendrogram level with highest Q . Therefore, we do not search for the optimal partition that maximizes Q ; instead, among different hierarchical partitions, we use the representation with highest Q .

To aid interpretation, each structural module was annotated by its voxel overlap with Yeo 7 resting-state networks and anatomical lobe masks in 3 mm MNI space. These annotations were used only to describe the modules, not to define them or compute SFC, and are reported in Supplementary Tables S11 and S12.

Assessing Modular Structure–Function Coupling

The strength of structure–function coupling (SFC) for each module was quantified using Pearson’s correlation coefficient r between structural and functional connectivity patterns (see bottom panel in Figure 1). Mathematically, for module m , we compute:

$$\begin{aligned} SFC_m &= r_m \left(\overrightarrow{SC_m}, \overrightarrow{FC_m} \right) \\ &= \frac{\sum_i (SC_{m,i} - \overline{SC_m})(FC_{m,i} - \overline{FC_m})}{\sqrt{\sum_i (SC_{m,i} - \overline{SC_m})^2 \sum_i (FC_{m,i} - \overline{FC_m})^2}}. \end{aligned} \quad (1)$$

where $\overrightarrow{SC_m}$ and $\overrightarrow{FC_m}$ are the vectorized connectivity values for module m (with i indexing each connection). This correlation value lies in the range $[-1, 1]$, capturing the degree of alignment between functional and structural connectivity patterns.

Each brain module m comprises a set of n nodes (regions). Its structural (SC_m) and functional (FC_m) connectivity matrices include two components: An internal (within-module) sub-matrix of size $n \times n$ describing the connections among nodes within the module (diagonal block) together with an external (between-module) sub-matrix of size $(N - n) \times n$ capturing the connections between module m and the remaining brain regions (N is the total number of regions).

Accordingly, we compute two module-specific SFC metrics: SFC-INT: Pearson r between the internal SC and FC vectors, reflecting structure–function alignment within the module. SFC-EXT: Pearson r between external SC and FC vectors, capturing alignment in inter-modular connectivity. This decomposition on internal and external connectivity aligns with prior approaches in the literature [31, 53–55].

Task-related SFC modulation

At the global level, task-related SFC modulation was summarized using task vs. rest SFC ratios. For each module m and task t , the ratio was defined as $SFC_{m,task}/SFC_{m,rest}$. These ratio values were used to compute the global task-similarity matrices shown in Figure 2. At the modular level, task-related changes were quantified as rest-to-task displacements in the original SFC space. For each module m and task t , we defined $\Delta SFC_{m,task} = SFC_{m,task} - SFC_{m,rest}$. This difference-based measure preserves the direction and magnitude of each module’s movement from rest to task in the SFC-INT vs. SFC-EXT plane and was used for Figure 3.

Statistics and Reproducibility

Sample size, repeated measurements, and replicates. The participant was the independent observational unit. A total of 216 participants were initially considered, and 163 participants were retained after the quality-assurance procedure described above and in the Supplementary Information. Each retained participant contributed repeated measurements from one resting-state condition and four task conditions; these within-participant conditions were not treated as independent biological replicates. All subject-level statistical analyses therefore used the same final sample of 163 participants unless otherwise indicated. Behavioral analyses were restricted to Emotion Matching, Gender Stroop, and Visual Working Memory because the Anticipation task did not provide a comparable response-time or accuracy measure.

Subject-level inferential statistics. Subject-level statistical analyses were performed using task-induced coupling changes, defined as $\Delta\text{SFC} = \text{SFC}_{\text{task}} - \text{SFC}_{\text{rest}}$, computed separately for SFC-INT and SFC-EXT. We tested three hypotheses. First, to test whether SFC-EXT changed more across tasks than SFC-INT, we compared the inter-task variability of ΔSFC between SFC-INT and SFC-EXT using repeated-measures ANOVA. Second, to test whether tasks were more clearly separated by SFC-EXT than by SFC-INT, we computed Euclidean distances between all task pairs using module-wise ΔSFC profiles and compared these distances between SFC-INT and SFC-EXT; this analysis was also repeated after weighting modules by edge count. Third, to test whether SFC-INT and SFC-EXT followed different task-specific profiles, we compared ΔSFC across the four tasks separately for SFC-INT and SFC-EXT. Post-hoc pairwise comparisons were then used to identify which specific task pairs differed within SFC-INT and within SFC-EXT. Greenhouse–Geisser correction was applied when required, generalized eta-squared (η_G^2) was reported for ANOVAs, and post-hoc p -values were corrected using Benjamini–Hochberg false discovery rate correction.

Robustness and sensitivity analyses. We performed robustness analyses to test whether the observed difference in task-related SFC variability between SFC-INT and SFC-EXT depended on analytic choices. First, we assessed the stability of the 9-module structural partition using split-half resampling and quantified agreement between independently derived partitions with the adjusted Rand index (ARI). Second, we repeated the analysis across FC density thresholds, alternative HAC linkage criteria, and different structural dendrogram resolutions ($M = 9, 50, 100, 250$, and 500 modules).

Because participants were scanned in a single session, direct test–retest reliability could not be estimated. Instead, we assessed split-half reliability of the group-level SFC profiles by repeatedly dividing the sample into two halves, computing mean SFC-INT and SFC-EXT profiles in each half and condition, and correlating the resulting profiles. Full robustness and reliability results are reported in Supplementary Tables S5–S9.

Data Availability

The neuroimaging and behavioral data analysed in this study are publicly available through the Amsterdam Open MRI Collection PIOP1 dataset on OpenNeuro (dataset ds002785, version 2.0.0; <https://doi.org/10.18112/openneuro.ds002785.v2.0.0>) [28]. Additional information about the data is available from the corresponding author upon reasonable request.

Code Availability

No new standalone software was developed specifically for this study. The analyses used established open-source neuroimaging software and the procedures, software versions, and parameters required for reproduction are described in the Methods and Reporting Summary. Implementation details for connectome construction are available at <https://github.com/compneurobilbao/bha2>. Additional information about the analysis implementation is available from the corresponding author upon reasonable request.

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Author Contributions

I.F.-I., J.M.C., and P.B. conceived the main idea and designed the study. I.F.-I. performed the formal analyses, prepared the figures, and wrote the original draft of the manuscript. J.M.C. wrote the draft of the manuscript. A.J.-M., N.A., G.Z.-L., A.E., P.B., J.M.C. reviewed and edited the manuscript. All authors read and approved the final version of the manuscript.

Competing interests

The authors declare no competing interests.

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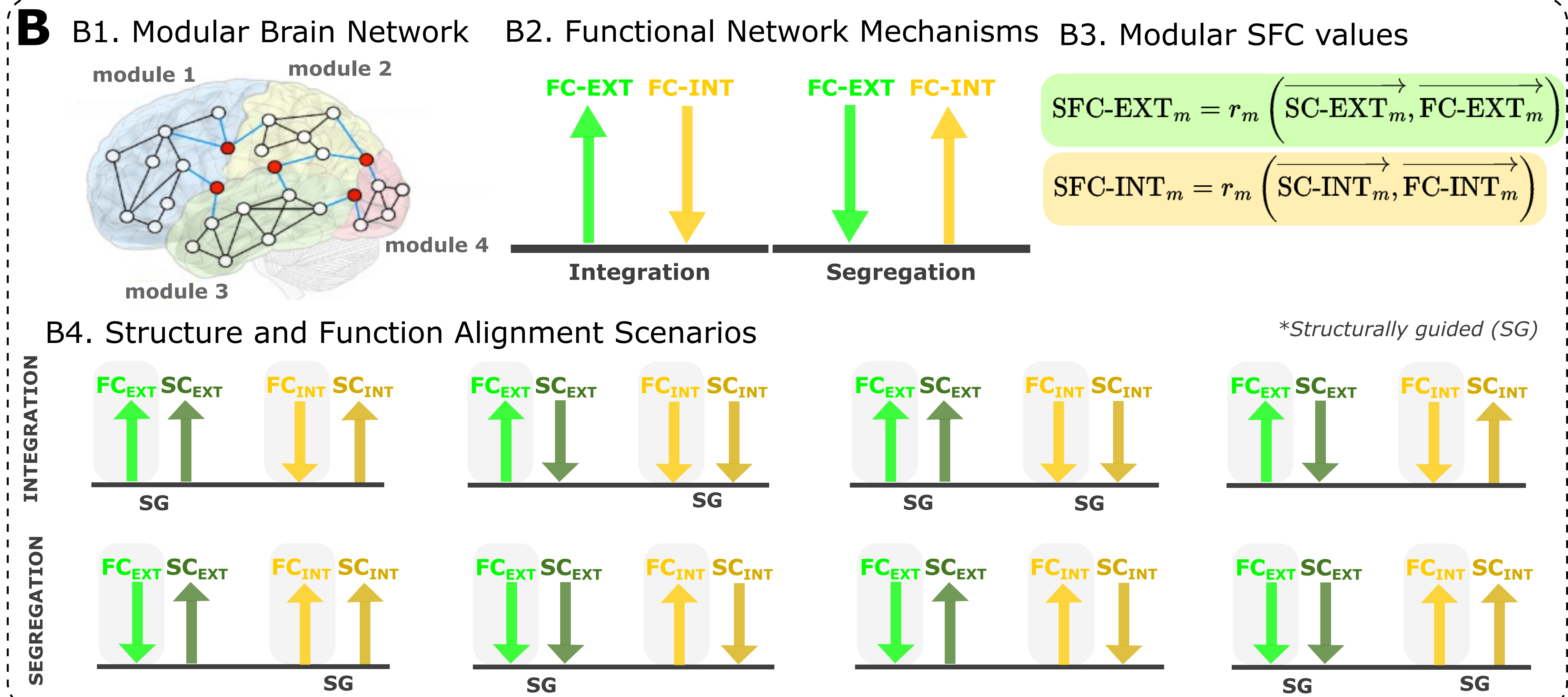
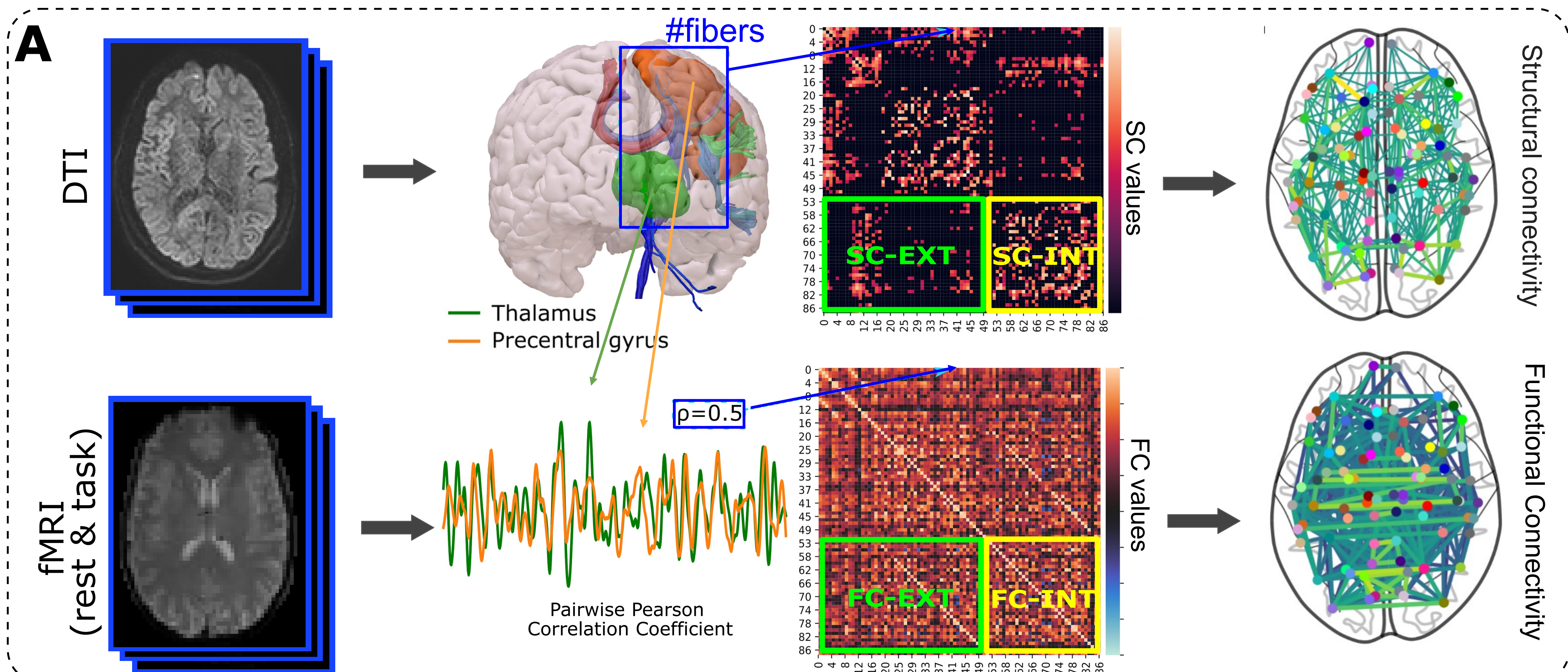
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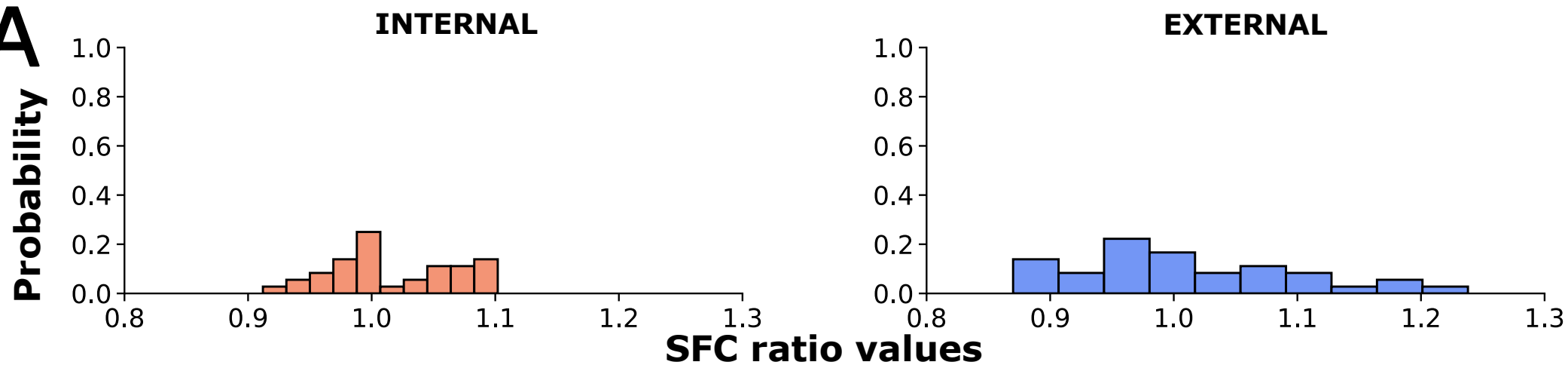
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Figure 1: **Methodological pipeline. A. Brain connectivity matrices calculation.** Multi-modal neuroimaging data were used to construct structural and functional brain connectivity matrices. Diffusion MRI data were used to estimate anatomical fibers and derive the structural connectivity (SC) matrix, whereas resting-state and task-based fMRI data were used to extract regional BOLD time series and compute functional connectivity (FC) matrices through pairwise Pearson correlations. For each connectivity matrix, links were separated according to the structurally defined modular partition into intra-modular connections (INT, within modules) and inter-modular connections (EXT, between modules). This yielded SC-INT, SC-EXT, FC-INT, and FC-EXT components for each module. **B. Assessing modular structure–function coupling (SFC).** **B1.** Modular brain network representation, illustrating the distinction between internal and external connections for a given module. **B2.** Schematic representation of internal and external functional network interactions. **B3.** Modular SFC values were computed separately for external and internal connections as the Pearson correlation between the corresponding structural and functional connectivity vectors: SFC-EXT between SC-EXT and FC-EXT, and SFC-INT between SC-INT and FC-INT. **B4.** Structure–function alignment scenarios illustrate how increases or decreases in functional connectivity may either follow or deviate from the underlying structural connectivity pattern. This framework allows task-related changes in structure–function alignment to be assessed separately within modules and between modules.

Figure 2: **Distribution of SFC ratios and task similarity for the structurally driven partition.** **A) Distribution of SFC ratios for internal and external connectivity.** The histograms represent the probability distribution of task/rest SFC ratio values for internal coupling (SFC-INT, left) and external coupling (SFC-EXT, right). Ratios are used here as a normalized descriptive measure of relative task modulation with respect to rest. **B) Global task similarity based on SFC ratio profiles.** Each element in the heatmaps represents task similarity between pairs of tasks. Similarity was computed from the Euclidean distance between the module-wise task/rest SFC ratio profiles of two tasks, with $SFC_{m,task}/SFC_{m,rest}$, and expressed so that higher values indicate greater similarity. The left heatmap shows intra-modular SFC similarity, whereas the right heatmap shows inter-modular SFC similarity.

Figure 3: **Task-induced SFC displacements from resting state.** **A) Task-wise SFC displacements.** Structure–function coupling (SFC) space defined by intra-modular coupling (SFC-INT, x-axis) and inter-modular coupling (SFC-EXT, y-axis) for the structurally defined modules. Each panel corresponds to one cognitive task: Anticipation, Emotion Matching, Visual Working Memory, and Gender Stroop. Filled circles indicate the resting-state position of each module, open diamonds indicate the task-state position, and arrows show the displacement from rest to task. Rightward displacements indicate increased within-module structure–function alignment, whereas upward displacements indicate increased between-module alignment. **B) Module-wise SFC displacements.** The same rest-to-task displacements are reorganized by module (M1–M9), with all four tasks shown together for each module. This representation highlights module-specific coupling profiles and task-dependent changes in SFC-INT and SFC-EXT. Brain maps on the right show the anatomical location of each structural module.



A**B**