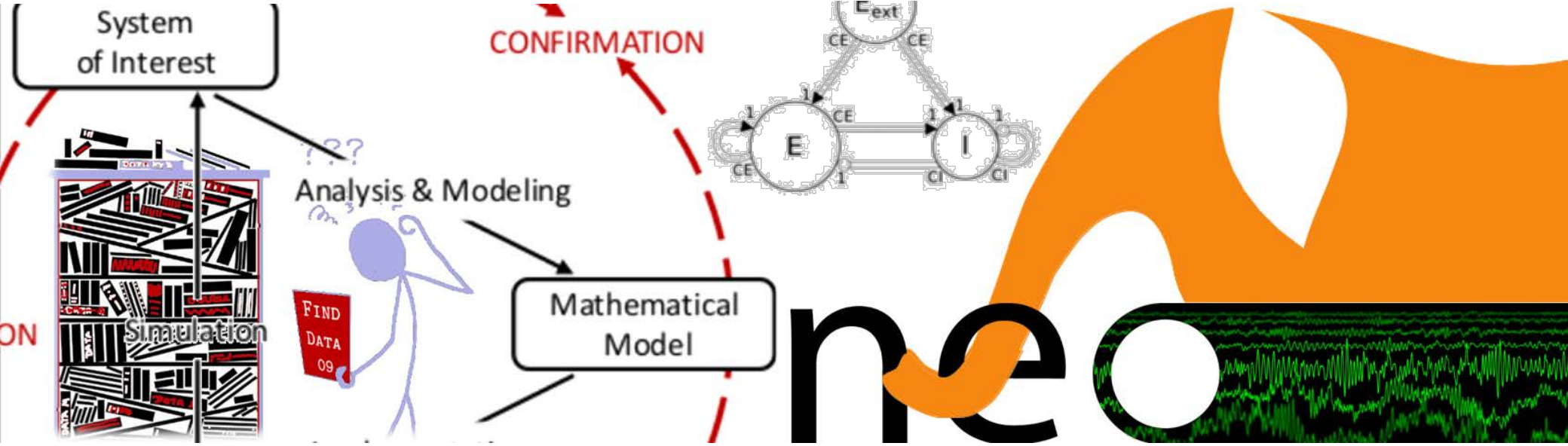



Stick Figure Image: Lyuba Zehl
web.gin.g-node.org/lzehl/ExperimenTales

# Task Area 3

# Computational Neuroscience

NFDI Neuroscience Virtual Community Workshop | July 1, 2020

Michael Denker
Sonja Grün

Stefan Rotter

JÜLICH Forschungszentrum

Bernstein Center Freiburg

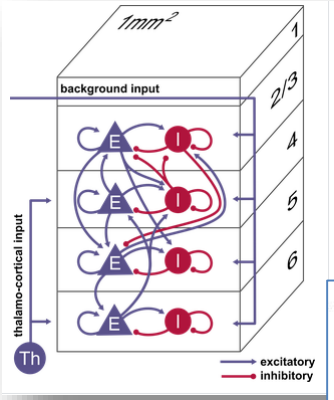
NFDI Neuroscience

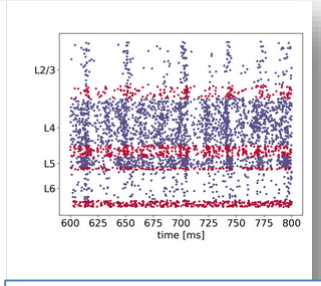
# Core Areas of Task Area Computational Neuroscience

Computational neuroscience is centered on understanding the **principles of information processing** in the brain.

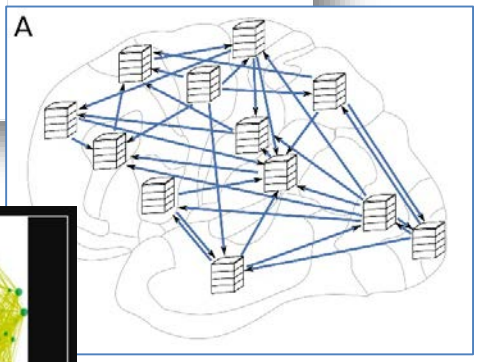
This involves the development of **theories** and **models** of the brain, as well as **analysis methods** to probe for signatures of these theories and models in the data…

- …on various scales and levels of observation.
- …related to many neuroscience systems or concepts.
- …at various levels of abstraction.

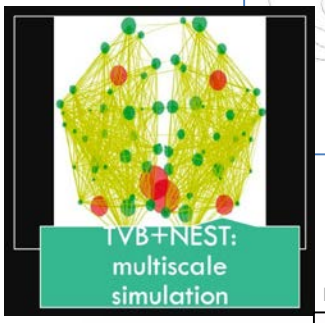



Potjans and Diesmann, 2014
https://github.com/nest/nest-simulator/tree/master/pynest/examples/Potjans_2014



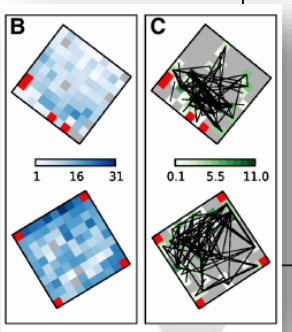

Schmidt M et al., 2018
https://github.com/INM-6/multi-area-model




TVB Multi-scale simulation
http://ebrains.eu
https://www.thevirtualbrain.org

This poses **challenges** for data management and processing:

- Sharable, standardized, comparable model descriptions and simulation outcomes (on-disk, between-tools)
- Reproducible execution of complex, multi-scale, large brain simulations
- Standardization of complex analysis methods and analysis processes across models and experiments
- Validation of models and simulation outcomes




Courtesy:
Alexa Riehle

Torre et al., 2016

NFDI
Neuroscience

# Three **examples for actions** in three planned focus areas of Task Area Computational Neuroscience

**Focus I:** Best practices for network model descriptions and simulation outcomes

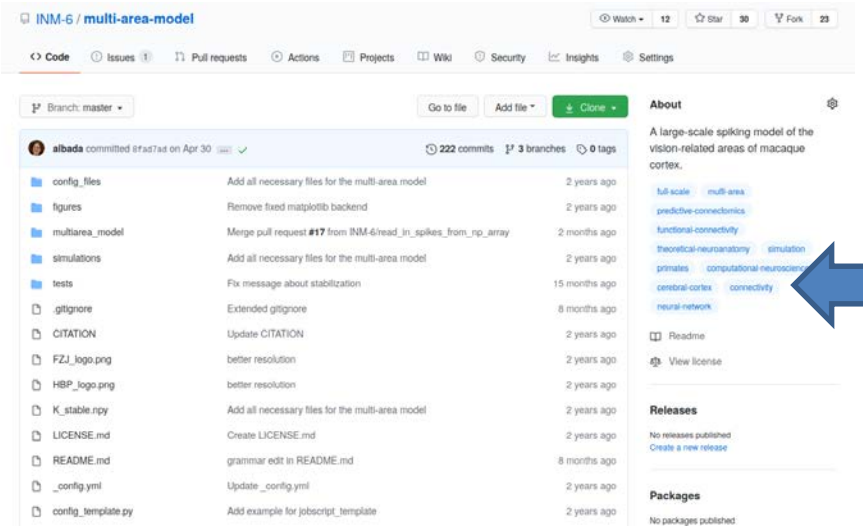
**Focus II:** Simulation, analysis, validation workflows and provenance

**Focus III:** Simplifying model validation and verification of simulations

# **Focus I:** Best practices for network model descriptions and simulation outcomes

Model descriptions

- are in general not reproducible from papers
- are in heterogeneous types of formats:
  - as executable code
  - via common abstracted APIs, e.g., PYNN
  - via description languages, e.g., NESTML, NEUROML
  - text documents
  - equations
  - tables
  - illustrations
  - code





https://github.com/INM-6/multi-area-model

http://www.opensourcebrain.org/projects/ca3-pyramidal-cell/

NFDI Neuroscience

# **Focus I:** Best practices for network model descriptions and simulation outcomes

*"**Authors should use diagrams** to illustrate their model structure and to specify relations between the different model parts.*
*A good model description should use at least one diagram, showing the overall structure of the model.*
*Further diagram can then be given to elaborate on details and different aspects of the model."*

Nordlie, E., Gewaltig, M.-O., Plesser, H.E. (2009) Towards reproducible descriptions of neuronal network models. PLoS CB

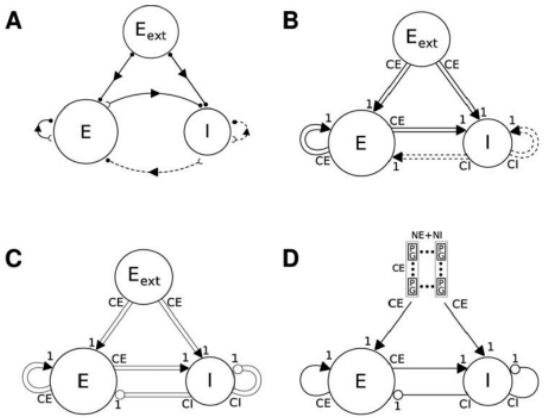



Figure 6 of Nordlie et al. (2009)

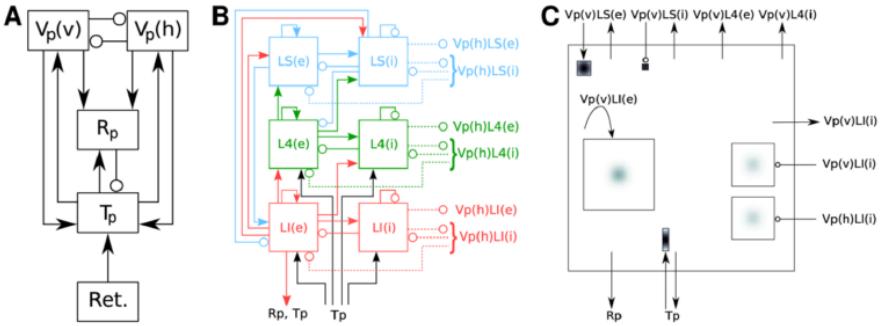


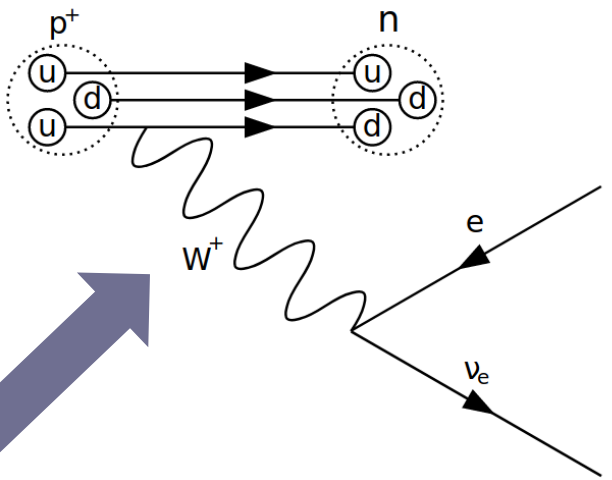

Figure 9 of Nordlie et al. (2009)

NFDI Neuroscience

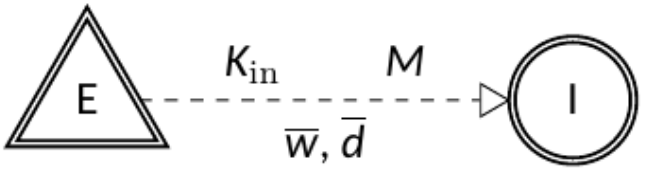
# **Focus I:** Best practices for network model descriptions and simulation outcomes

What if Feynman diagrams were so unstandardized?

Standardization of the
representations of neuronal network models






Johanna Senk, Birgit Kriener, Hans-Ekkehard Plesser, Mark-Oliver Gewaltig, Markus Diesmann, Mikael Djurfeldt, Nicole Voges, Lisa Schüttler, Gabriele Gramelsberger. Sacha van Albada, in prep.

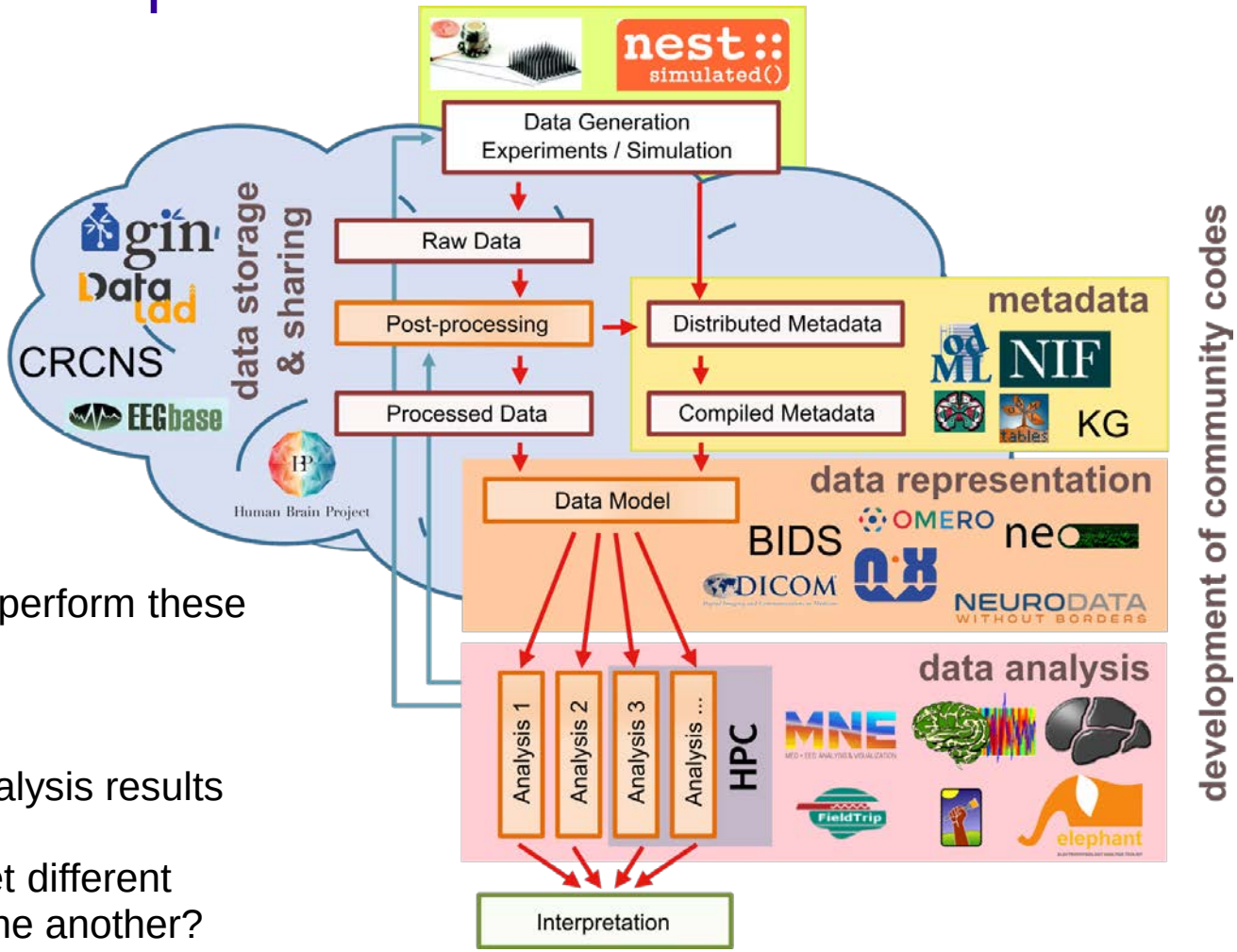
TA3 could support by:

- Promoting community standardization efforts and emerging solutions, internationally
- Establishment of a working group to ensure that standardization is practical and generic
- Support interfaces of model definitions to existing brain simulation tools

# **Focus II:** Simulation, analysis, validation workflows and provenance

Individual workflows developed for
- data ingestion
- data annotation
- data pre-processing
- data analysis
- data publication

for multiple scales, data sources, paradigms,…

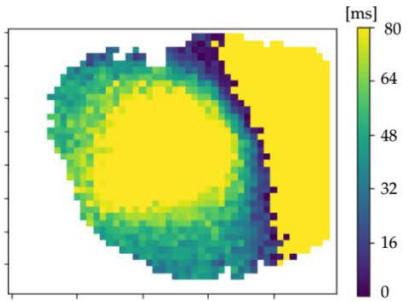



Many tools and services emerge to perform these data processing steps.

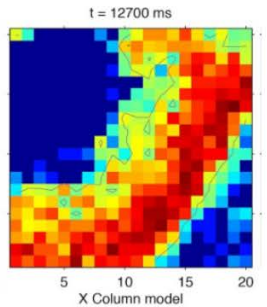
However:
- How to make processing and analysis results comparable between tools?
- How to relate complementary, yet different methodological approaches to one another?
- How to incorporate and validate models based on these findings?

# **Focus II:** Simulation, analysis, validation workflows and provenance

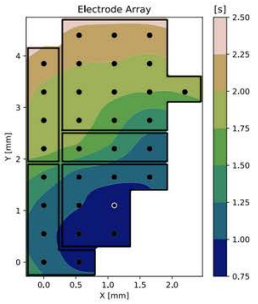
**Example:**
Periodic transitions between Up and Down state (0-5Hz) in sleep and anaesthesia…
…are seen at multiple spatio-temporal scales and across measurement modalities
…can be characterized using diverse complementary methods
…provide a robust experimental phenomenon to validate network simulations against




Celotto et al., 2020



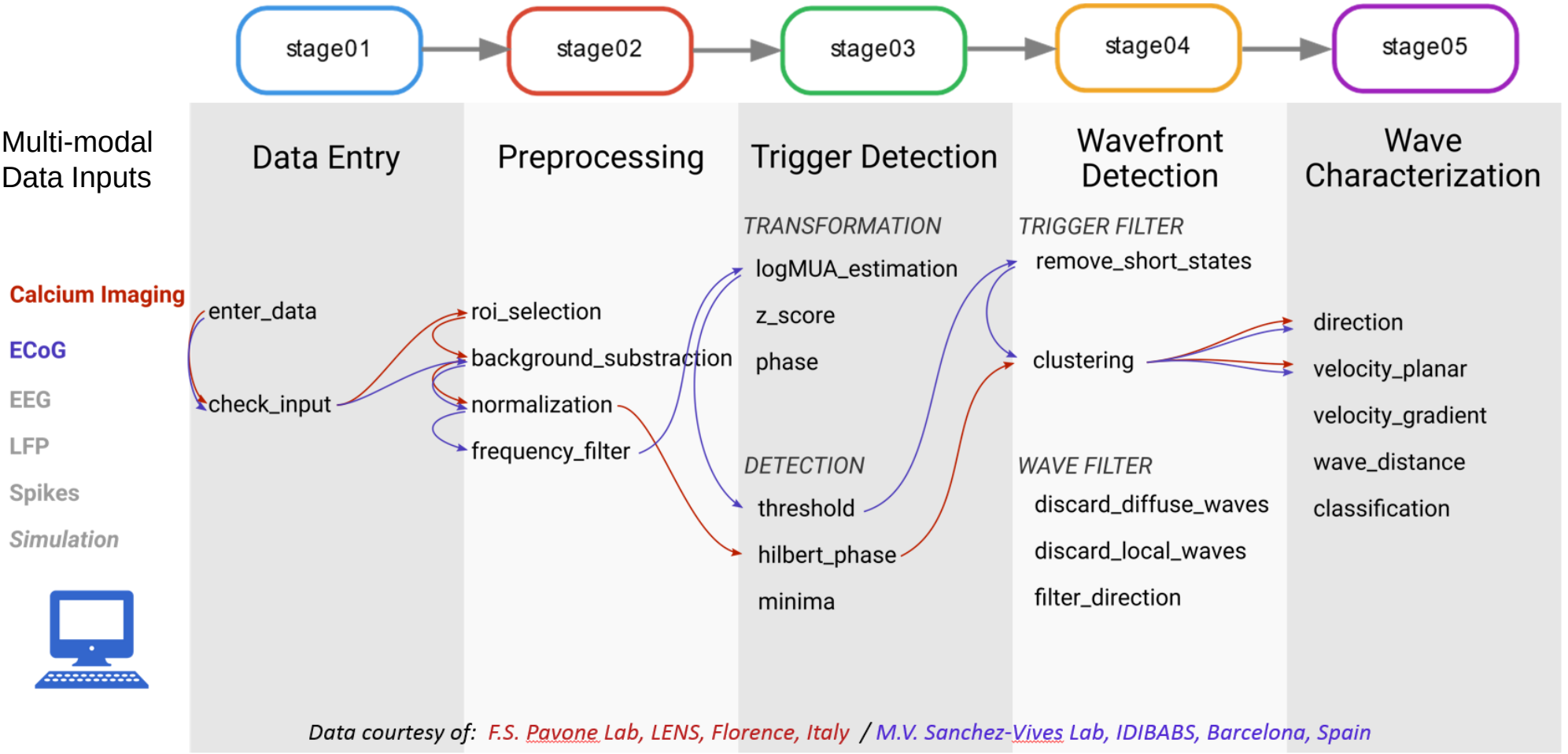

Pastorelli et al., 2019




De Bonis et al., 2019

Calcium Imaging ⟷ **Simulation** ⟷ ECoG

# **Focus II:** Simulation, analysis, validation workflows and provenance




**Challenge:** Build universal workflows to jointly analyse and compare data sets, models, and methods

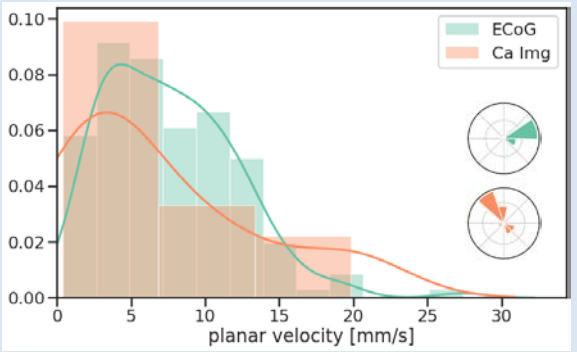
NFDI Neuroscience

# **Focus II:** Simulation, analysis, validation workflows and provenance

Anna Letizia Allegra Mascaro
Francesco Resta
Francesco Saverio Pavone
Maria-Victoria Sanchez-Vives
Giulia De Bonis
Elena Pastorelli
Cristiano Capone
Chiara De Luca
Pier Stanislao Paolucci
Robin Gutzen
Yann Zerlaut
Glynis Mattheis
Andrew Davison
Michael Denker
Sonja Grün

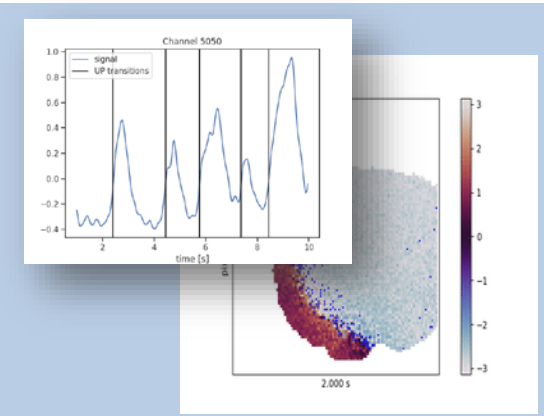
https://www.youtube.com/watch?v=uuAiY6HScM0

Calcium Imaging / ECoG

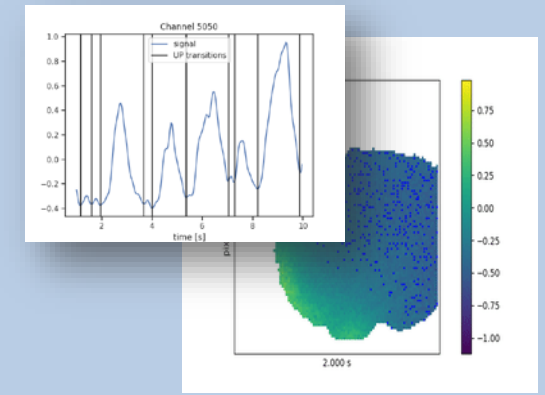



Different modalities

via Hilbert tf.

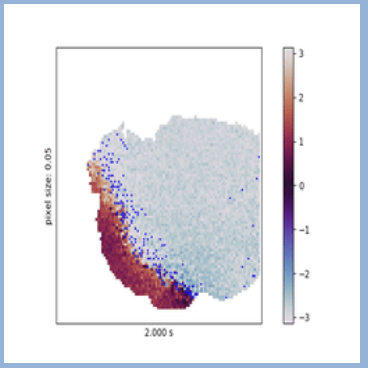



via minima

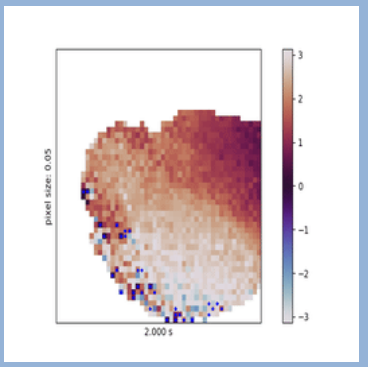



Different methods

recorded




simulated



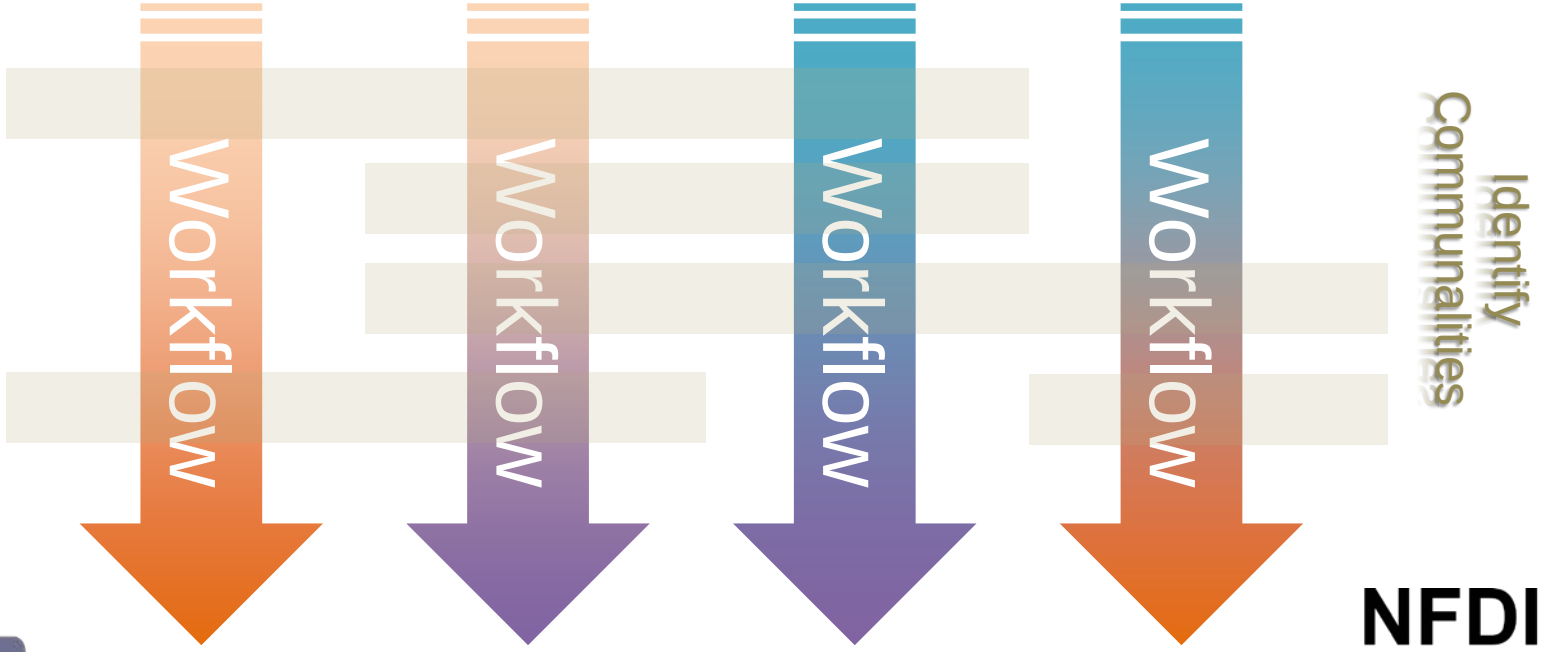

Validate models

NFDI Neuroscience

# **Focus II:** Simulation, analysis, validation workflows and provenance

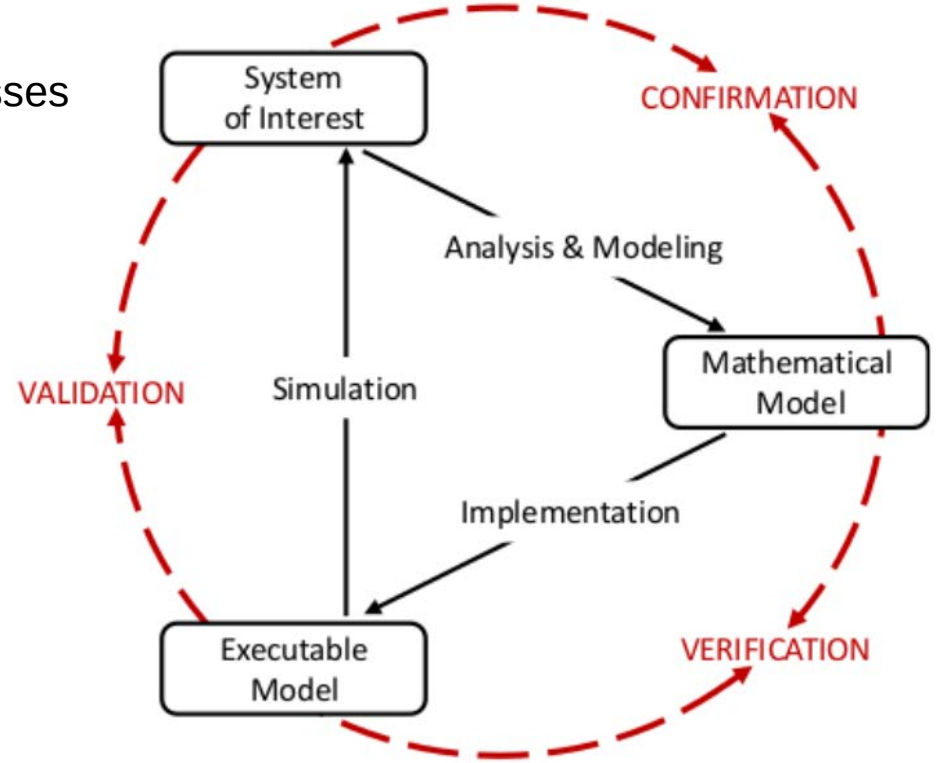
TA3 could support by:

- Teaching and coaching in the use of community infrastructure for data analysis
- Organization, collection, curation and provision of workflows built on these tools and creating links and communalities to foster interoperability (“*Marketplace for tools*”)
- Organization of common interest workgroups to
  - standardize workflows for defined areas
  - increase tool interoperability through connectors (e.g., Neo and MNE)



# **Focus III:** Simplifying model validation and verification of simulations

- Need to define terminology and formal processes for validation in computational neuroscience
- Must take into account multiple validation scenarios:
  - **Model to experiment** vs **model to model**
  - **Network level** vs **low-level components**
  - Different degrees of **acceptable agreement**

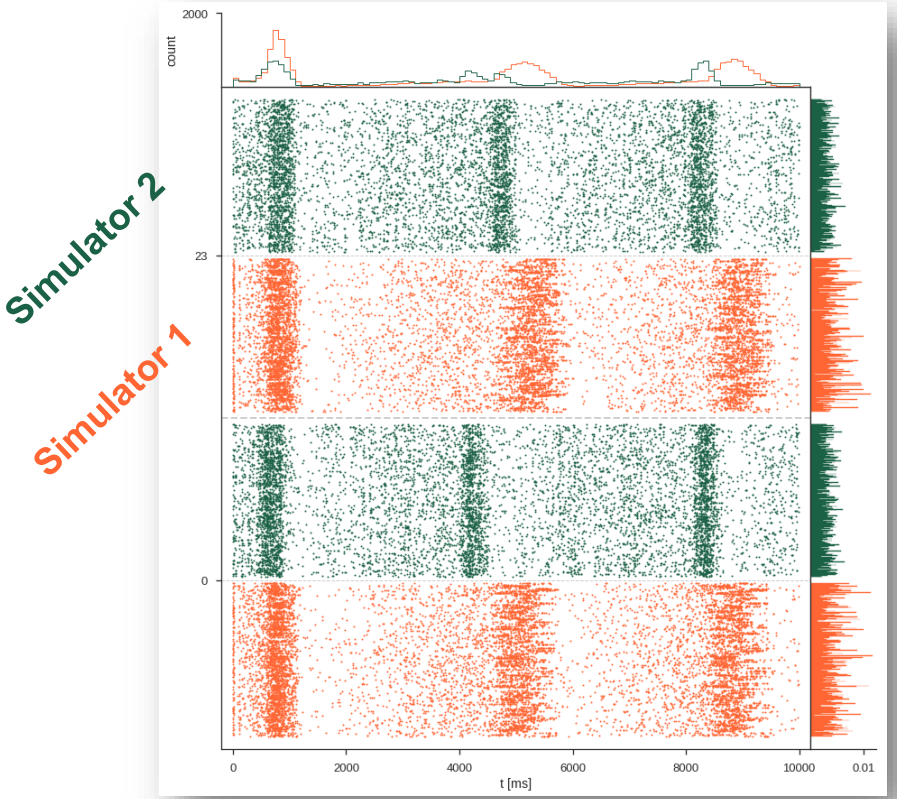



Schlesinger et al. (1979); Thacker et al (2014)
Trensch, Gutzen, Blundell, Denker, Morrison (2018)
Gutzen, von Papen, Trensch, Grün, Denker (2018)

# **Focus III:** Simplifying model validation and verification of simulations

TA3 could support by:

- Lead working groups to establish and promote best practices for reproducible simulation environments and verification
- Define standard validation tests for cross-simulation scenarios




Courtesy of Robin Gutzen

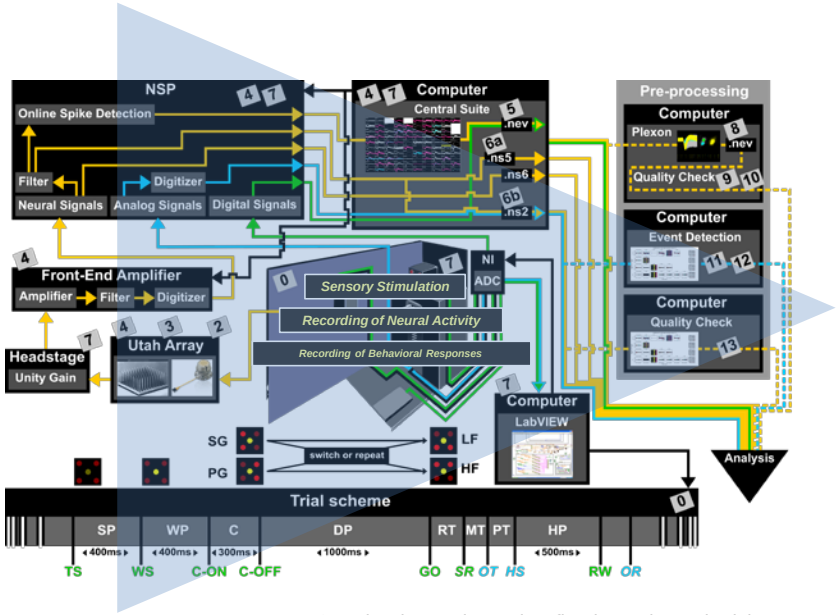
NFDI Neuroscience

# **Focus III:** Simplifying model validation and verification of simulations

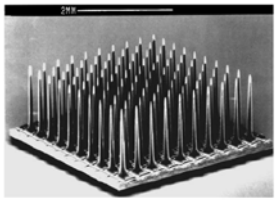
How to effectively (automatically?) compare common metadata descriptions for experiment and models with experimental data?

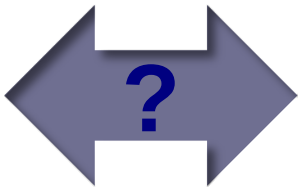
TA3 in conjunction with TA2 could support by:

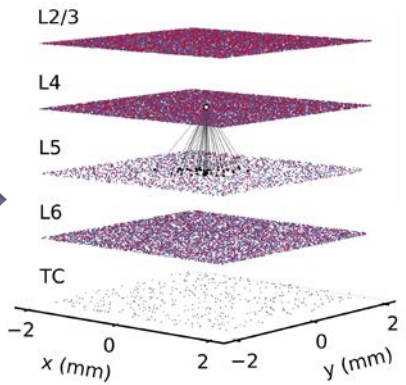
- Establish guidelines for compatible output formats (models and data)
- Promote off-the-shelf protocols for comparing model outputs to experimental data
- Support development for automated comparisons based on available metadata




Complex data and metadata flow in an electrophysiology setup
modified from *Zehl et al., 2016*






Senk, Hagen, van Albada, Diesmann (2018)
https://arxiv.org/abs/1805.10235

NFDI Neuroscience

# Building bridges to computational neuroscience infrastructure across the globe

EBRAINS

incf

OPEN SOURCE BRAIN

NSG NEUROSCIENCE GATEWAY
A Portal for Computational Neuroscience

ALLEN INSTITUTE

Related communities
Robotics
BMI
...

Tool Communities, e.g., Simulation Engines

arbor

THEVIRTUALBRAIN.

nest ::

NEURON

STEPS

LFPy

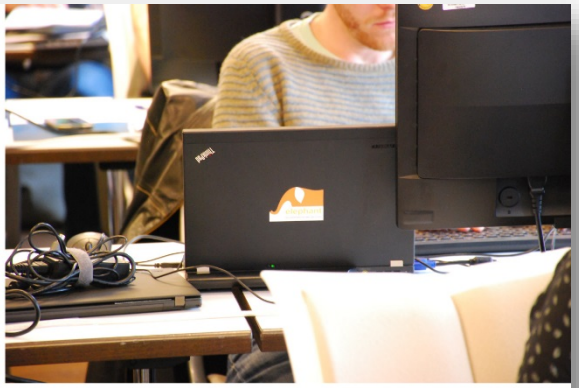
...

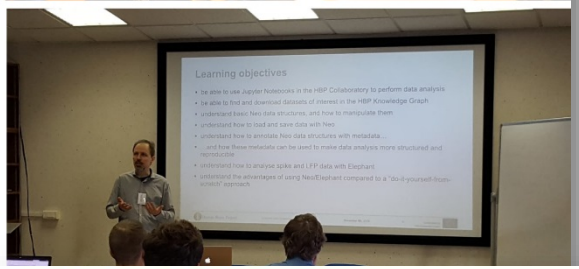

NFDI
Neuroscience

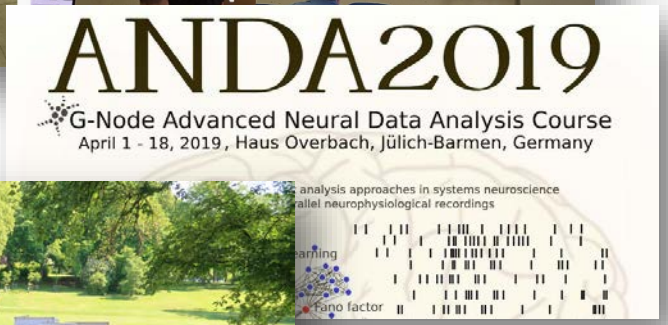
# Teaching Offers

Build and sustain existing offers to promote better research data management, e.g.,:

- Advanced neuronal data analysis (ANDA) course: Spring school on neuronal data analysis incorporating modules on good RDM practices
- NEST Conference: Promoting RDM at the yearly conference and hackathon on advancing NEST simulation technologies
- Elephant User Workshop: Emerging yearly offer for hands-on support in designing data analysis workflows
- *"-thonification"* of activities, e.g.:
    - Hackathons
    - Curatathons






**Sustain = Community + Interopability**

NFDI Neuroscience

# How participants and supporting community members profit in practice: some examples

➔ Identify, collect and make available suitable analysis workflows and tools for specific analysis problems and scenarios

➔ Manage a work group to define the best practices and metadata templates for storing and curating specific types of models

➔ Help in making a lab software development compatible with existing simulation engines and data formats

➔ Introduce emerging community developments into the workflows of laboratories and research consortia in the spirit of co-design


**Become an NFDI-Neuro participant, bring your needs, and help shape the community:**

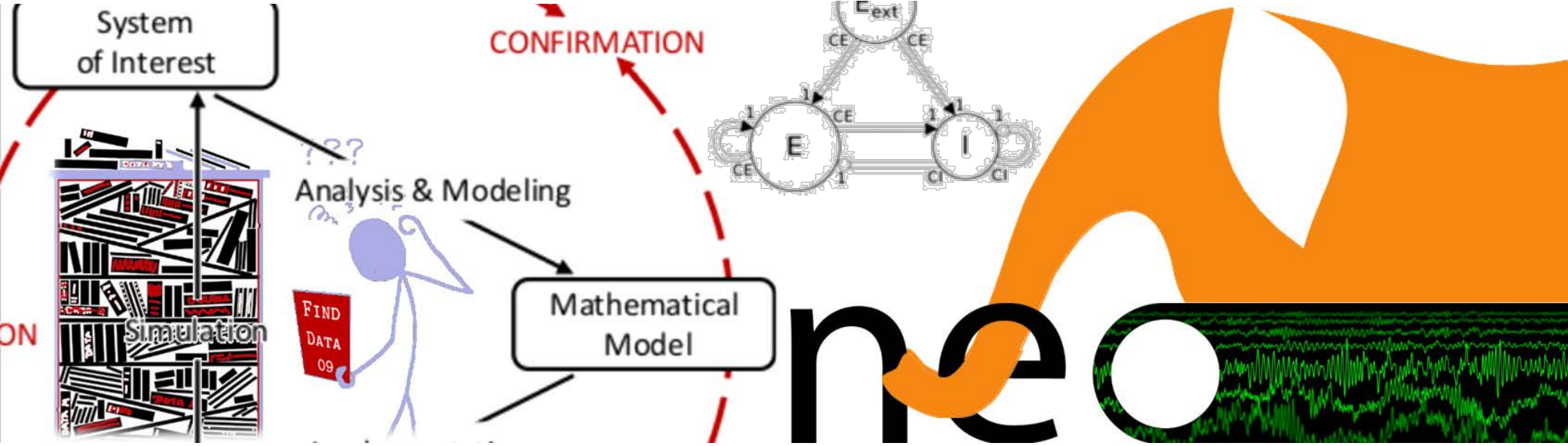
- individuals or institutions
- sustained contribution to the NFDI-Neuro community and its work program through work groups, shaping developments, and providing use cases
- Transfer teams, instruments, and the community support participant contributions

https://nfdi-neuro.de

https://tinyurl.com/nfdi-compneurosci



NFDI Neuroscience




Stick Figure Image: Lyuba Zehl
web.gin.g-node.org/lzehl/ExperimenTales

# Task Area 3
# Computational Neuroscience

# Discussion

NFDI
Neuroscience