Computer Simulations for Science and Engineering

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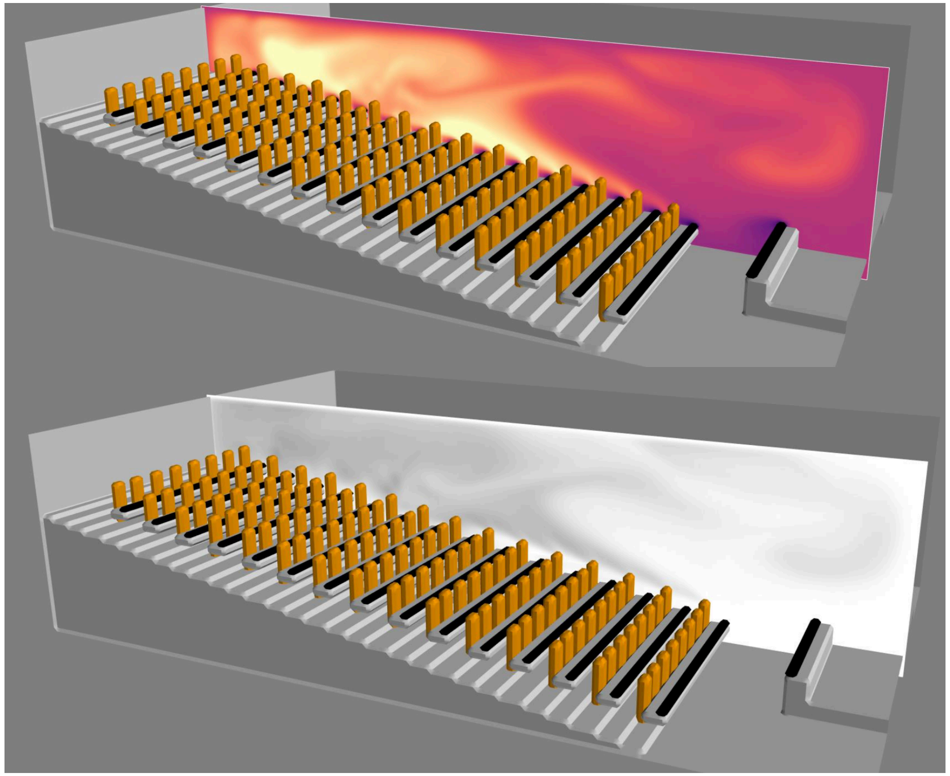

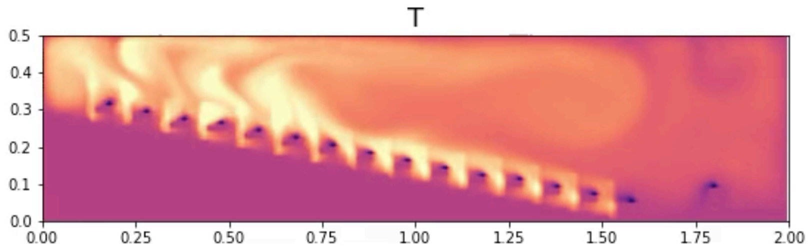
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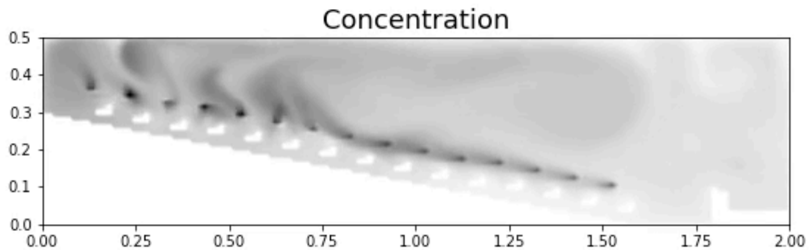
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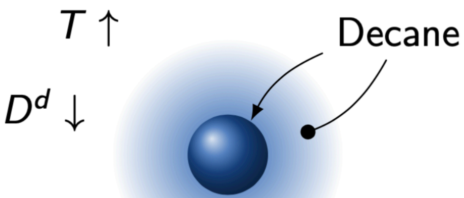
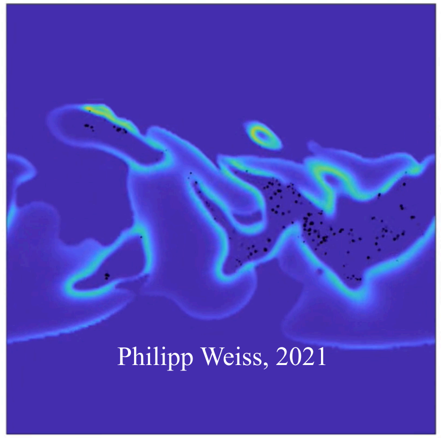
Outline

- Purpose and challenges of computational science
- Two major challenges illustrated on two examples
  - Pulverized Coal Combustion (PCC)

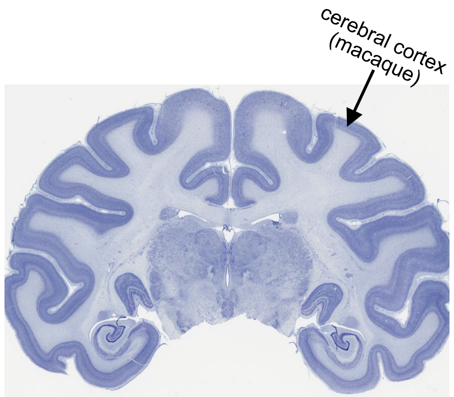


Heinrich Heinzer, 2021

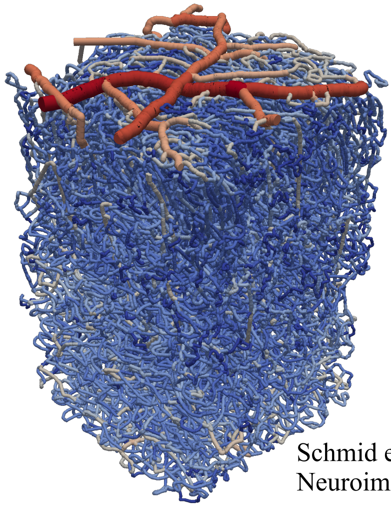


Philipp Weiss, 2021

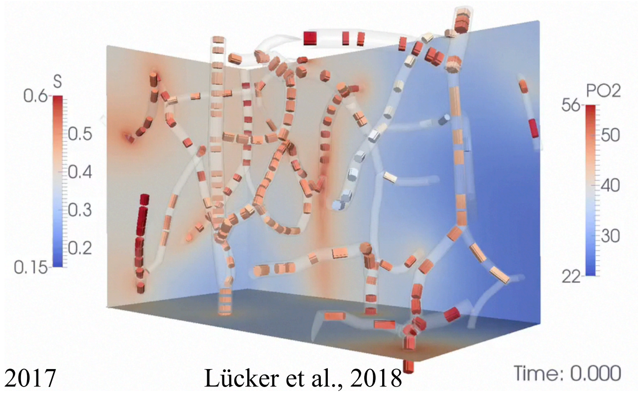
  - Cerebral Blood Flow (CBF)



brainmaps.org
by J.M.Garg (CC-BY-SA-4.0)



Schmid et al., 2017
Neuroimage



Lücker et al., 2018
Frontiers in Physiology

Purpose and Challenges of Computational Science

<u>Some application areas</u>

- chemistry and chemical engineering
- biology and medicine
- meteorology, climate and environment
- astronomy
- geology
- power generation
- finance
- aerospace and automotive
- …

Purpose and Challenges of Computational Science

Advantages compared to experiments

- often cheaper
- less time consuming
- suited for parameter studies
- suited for optimization
- systematic isolation of effects
- takes advantages of ongoing rapid development of computers and algorithms

Purpose and Challenges of Computational Science

Challenges

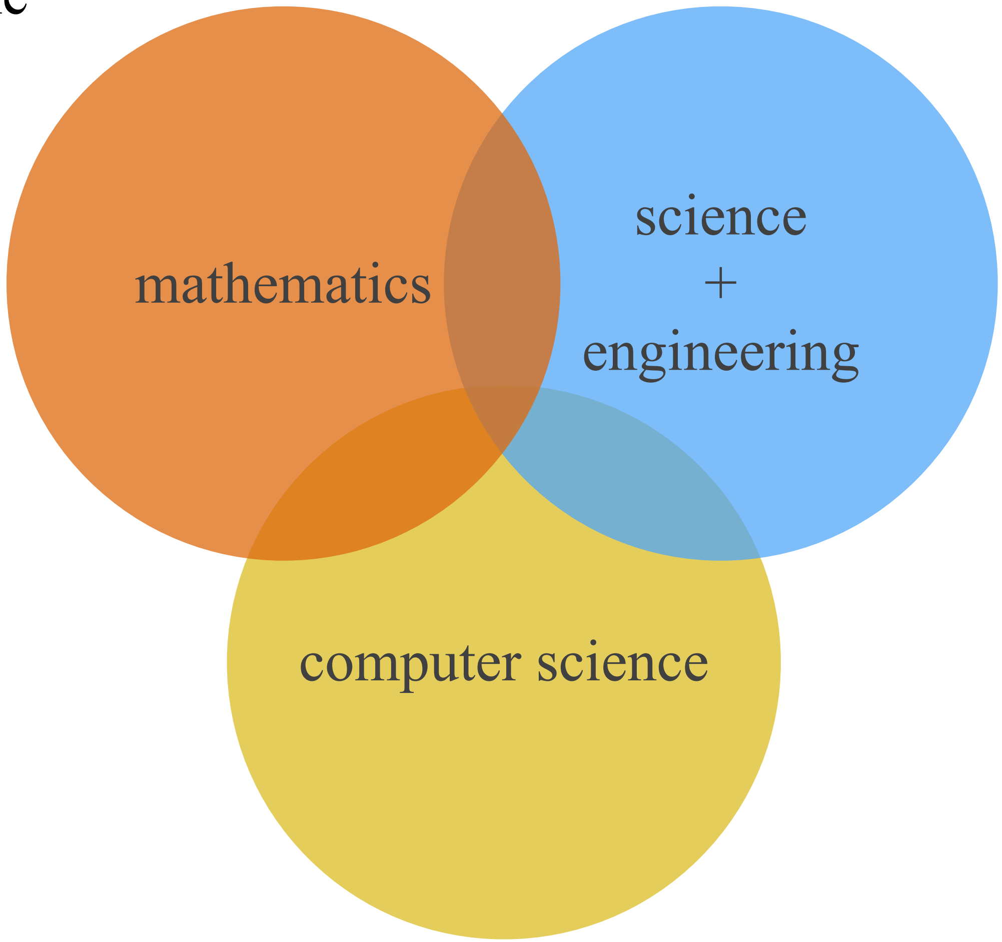
- multi-physics → tight coupling
- flexibility, e.g. complex and dynamic geometries
- data structure, implementation and parallelization

- closure of equations
- huge range of length and time scales → many degrees of freedom (DoF)
- uncertainty and inverse modeling
- …

Purpose and Challenges of Computational Science

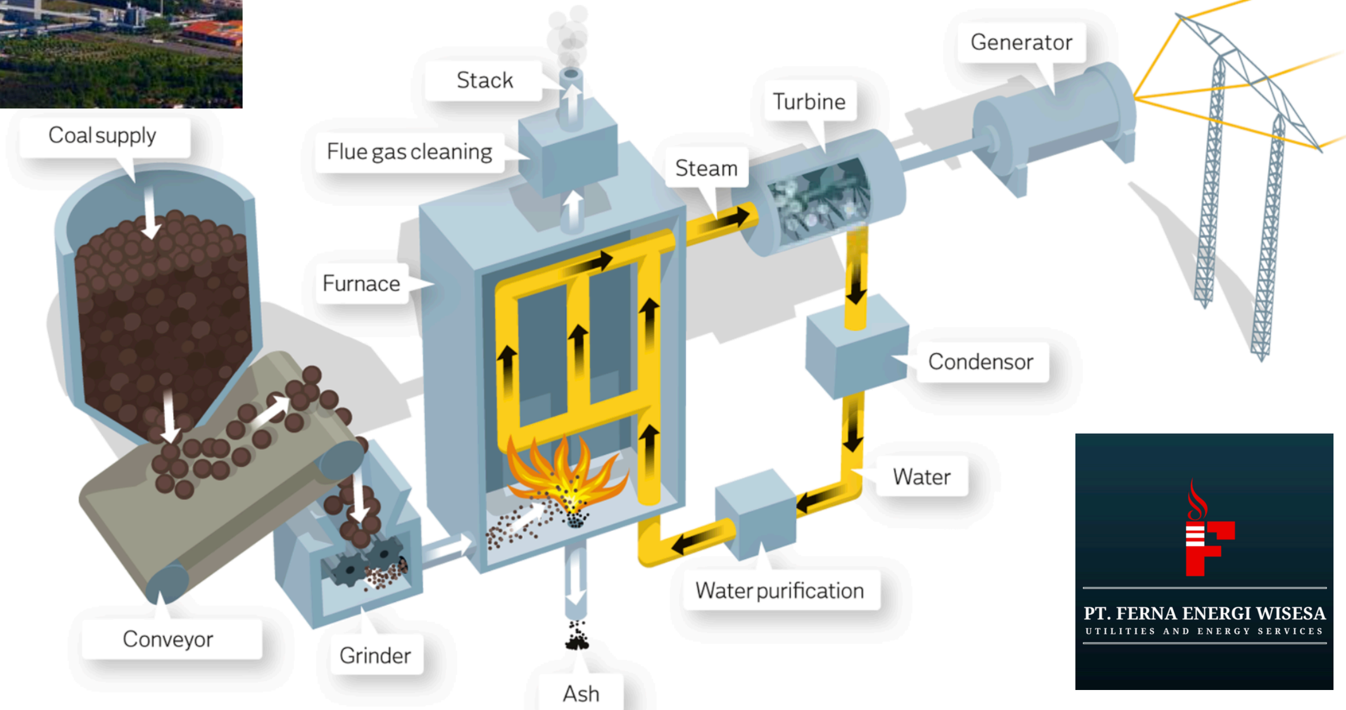
Basic requirements

- simulation time
- accuracy
- flexibility
- robustness



1st Example: Pulverized Coal Combustion (PCC)

<u>Why PCC?</u>



http://fernaenergi.com/2017/10/02/coal-power-plant/

1st Example: Pulverized Coal Combustion (PCC)

Why PCC?

- climate change is a global challenge

  → efforts to lower carbon emissions

- growing energy demand
- coal is abundant, cheap, and reliable

  → remains a main power source

- how to use it in a clean way?

  → oxy-fuel combustion + CO2 sequestration

- improvement

  → big impact

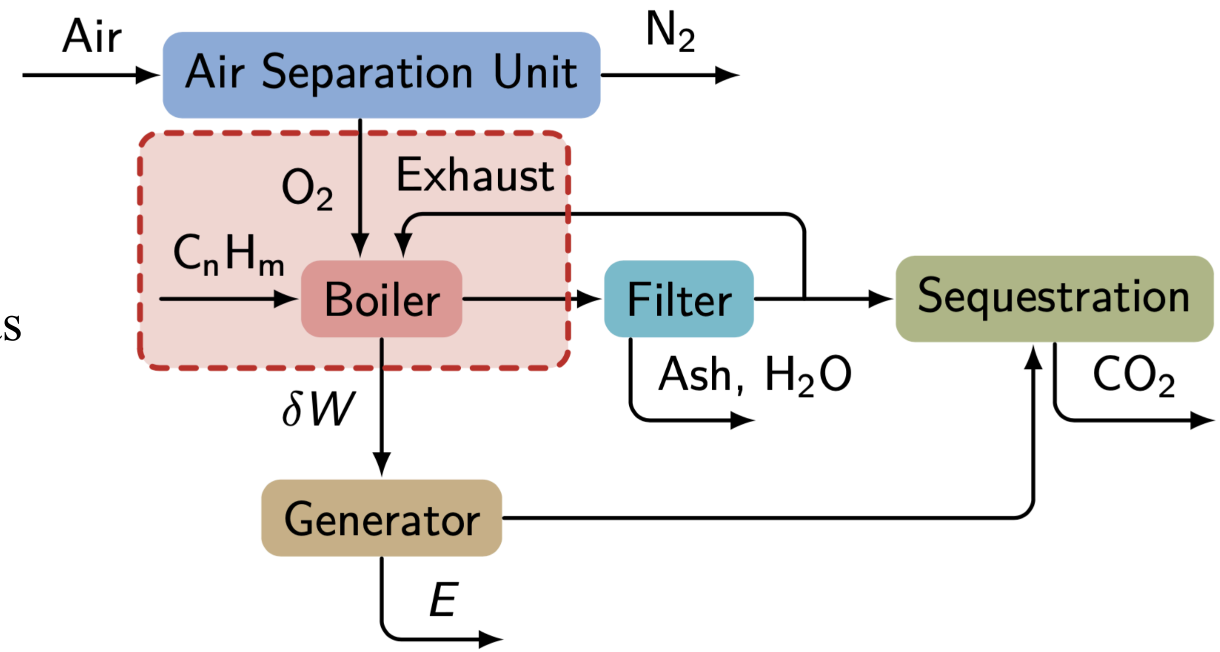
1st Example: Pulverized Coal Combustion (PCC)

Oxy-fuel combustion

- burn fuel in pure oxygen
  - → nitrogen in air not heated
  - → reduced fuel consumption
  - → higher flame temperatures
  - → reduced NOx production
  - → produce a CO2 rich flue gas
- CO2 capture and storage
- retrofit existing power plants

$$\text{Air} + \text{Fuel} \Rightarrow \text{Heat} + \text{Flue Gas}$$

$$O_2 + \cancel{N_2} + C_nH_m \Rightarrow \delta W + CO_2 + H_2O + \cancel{NO_x}$$



Heinrich Heinzer, 2021

1st Example: Pulverized Coal Combustion (PCC)

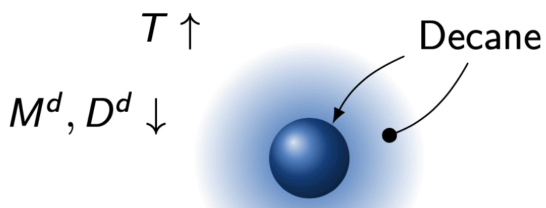
Particles

- release gas
- burn
- radiate

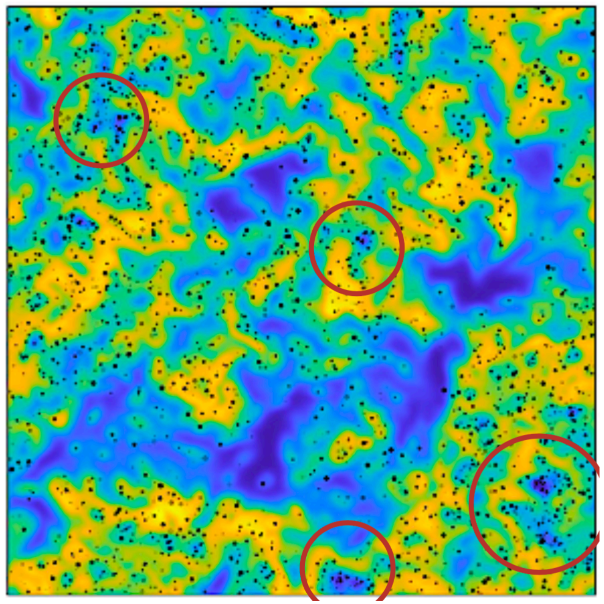
ordinary differential equation ⟷ partial differential equation

Gas phase

- convection
- diffusion
- mixing
- chemical reactions



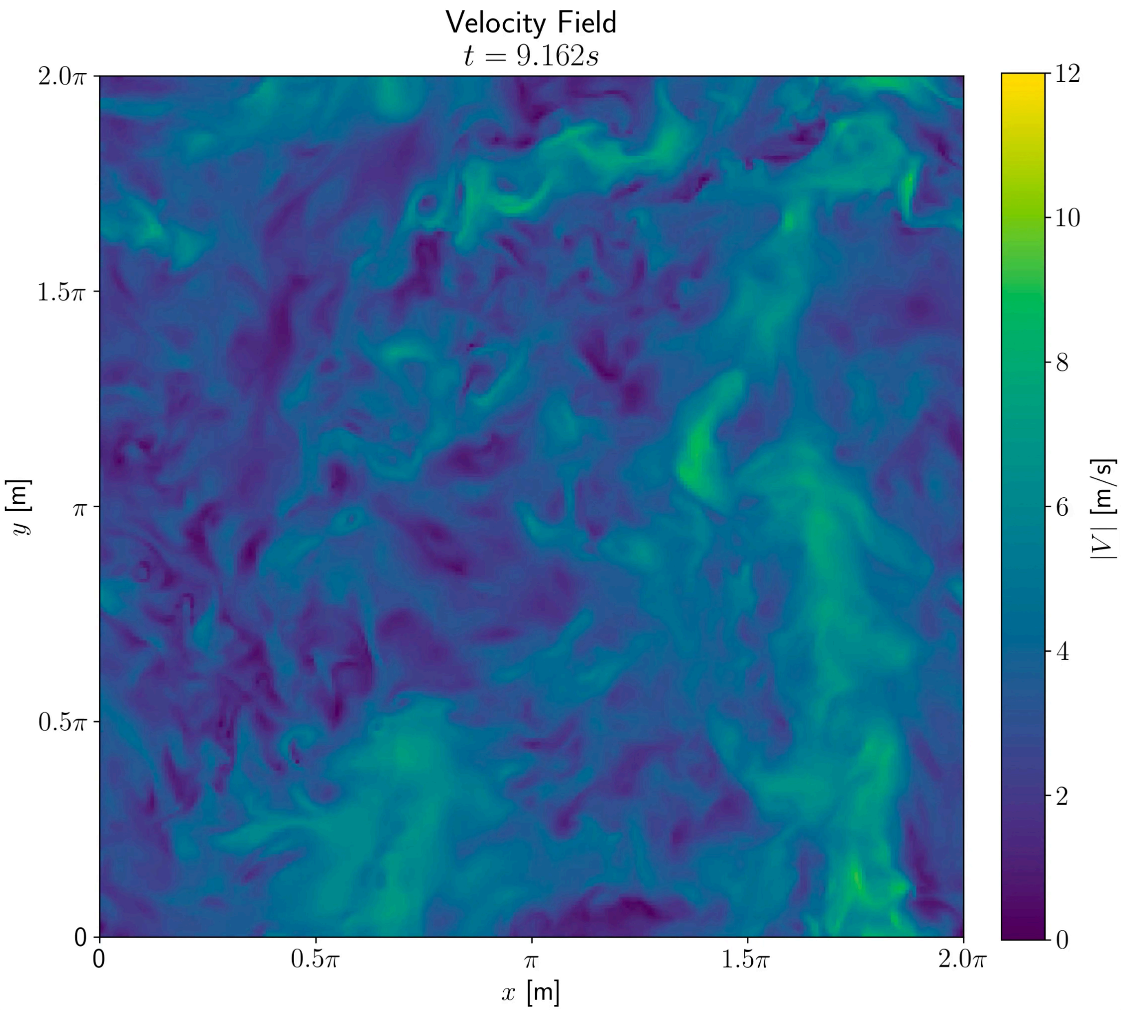
Heinrich Heinzer, 2021



Philipp Weiss, 2021

1st Example: Pulverized Coal Combustion (PCC)

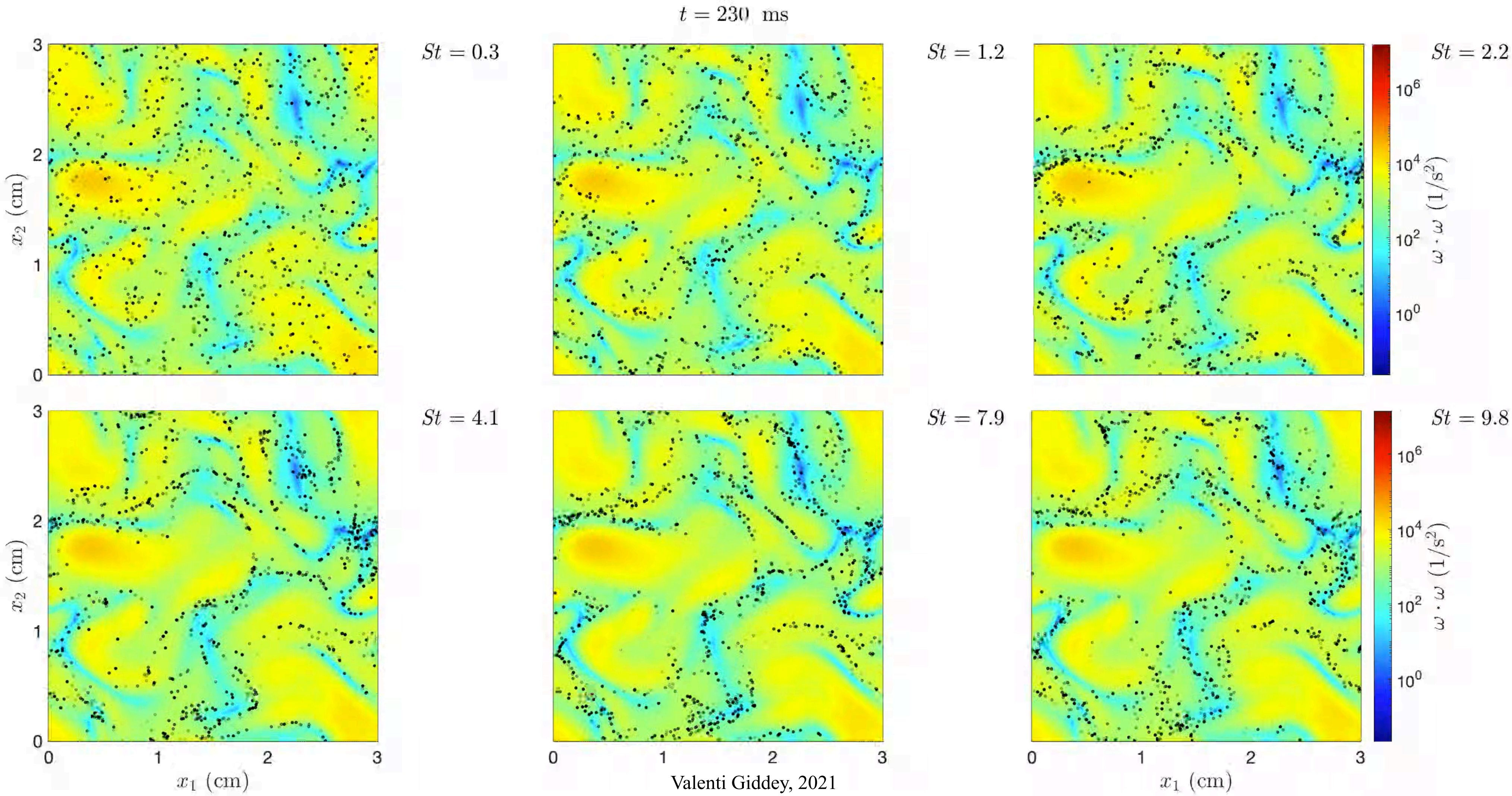
multiscale problem



Daniel Oberle, 2021

1st Example: Pulverized Coal Combustion (PCC)

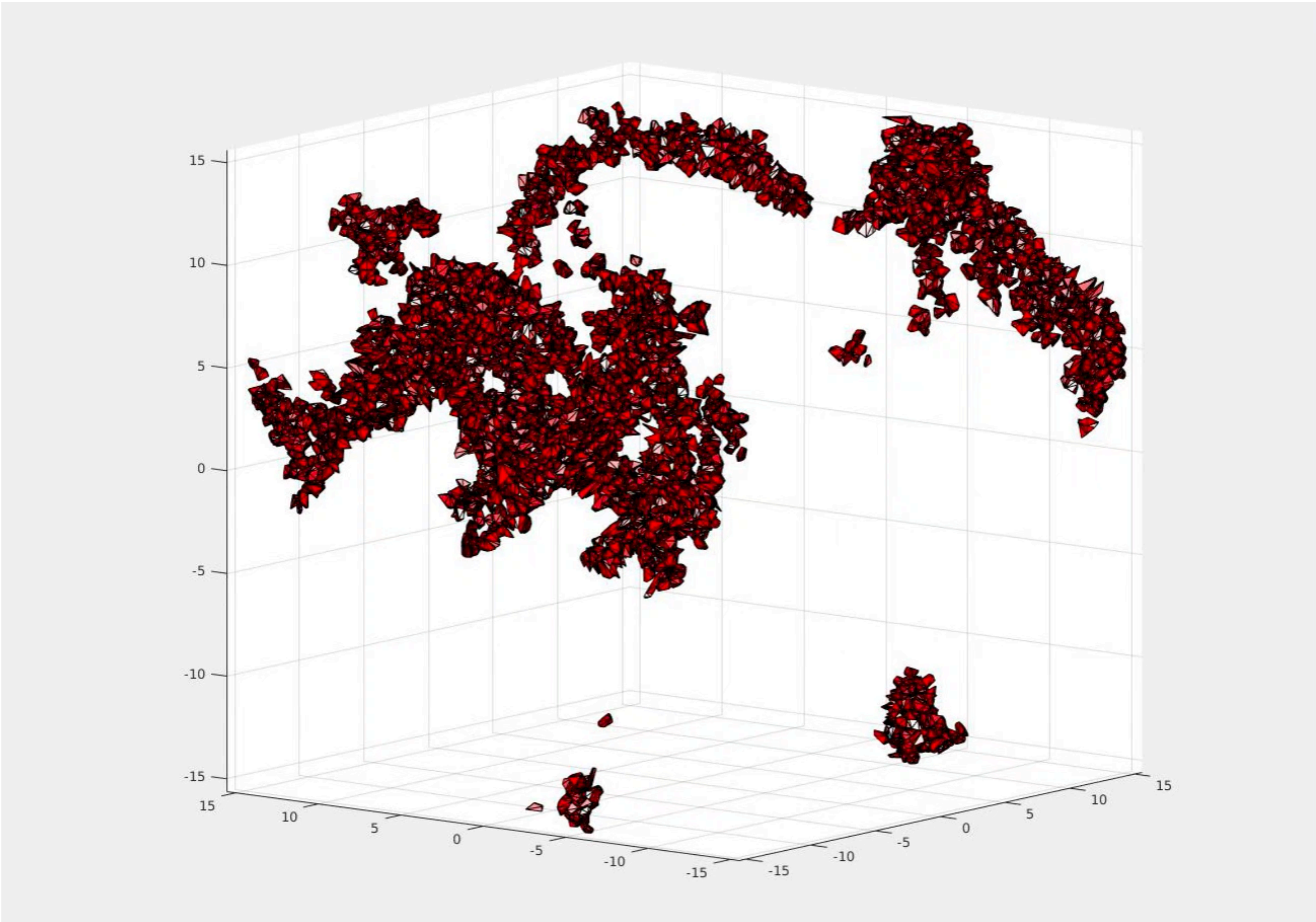
multiscale problem



Valenti Giddey, 2021

1st Example: Pulverized Coal Combustion (PCC)

multiscale problem

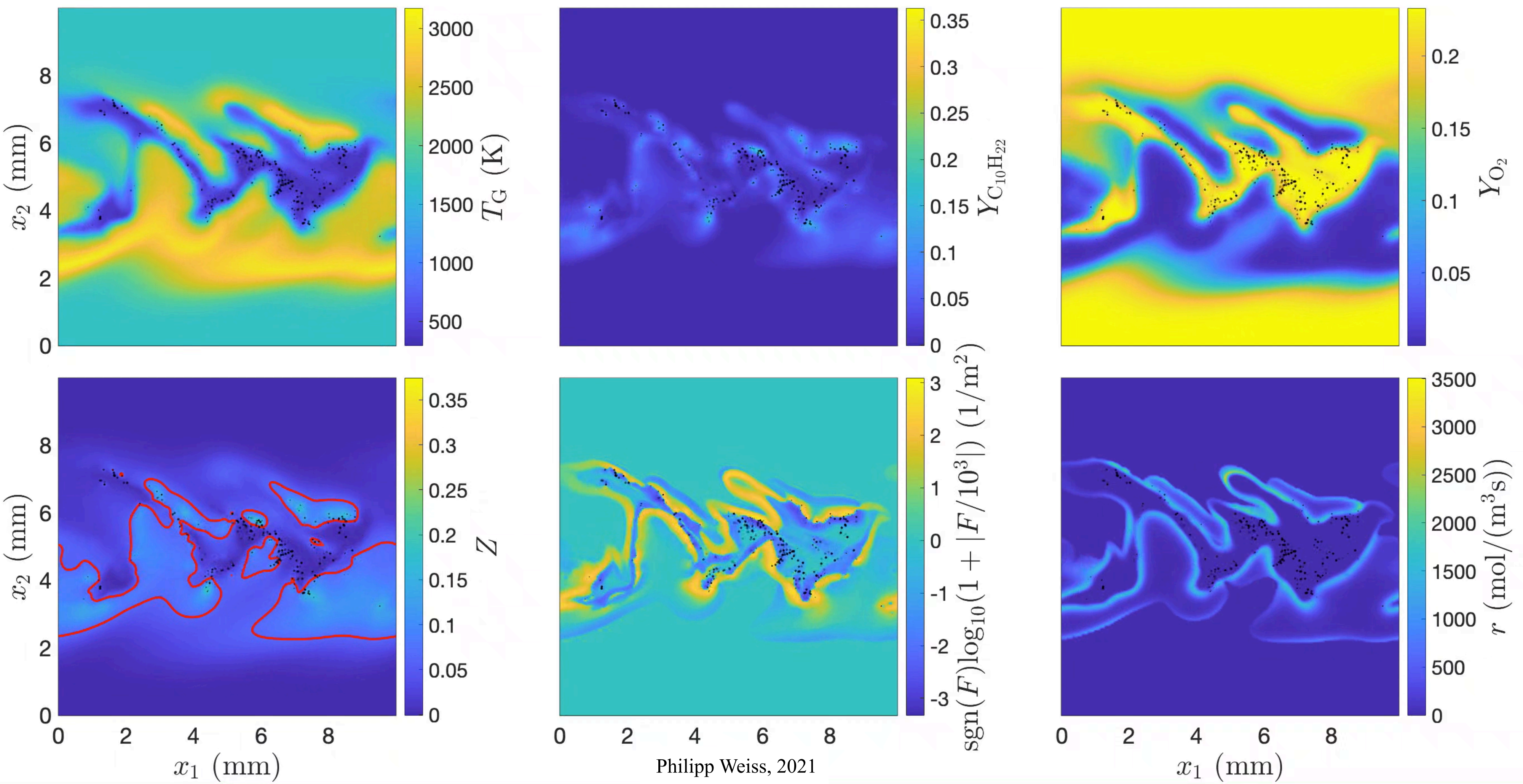


Valenti Giddey, 2021

1st Example: Pulverized Coal Combustion (PCC)

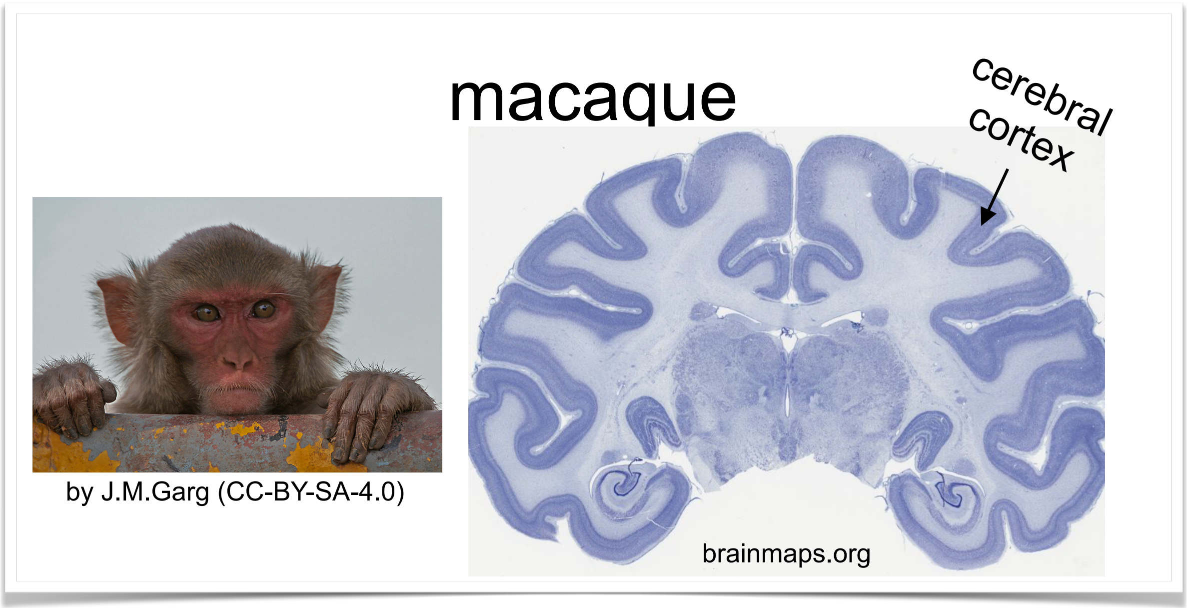
multiscale problem

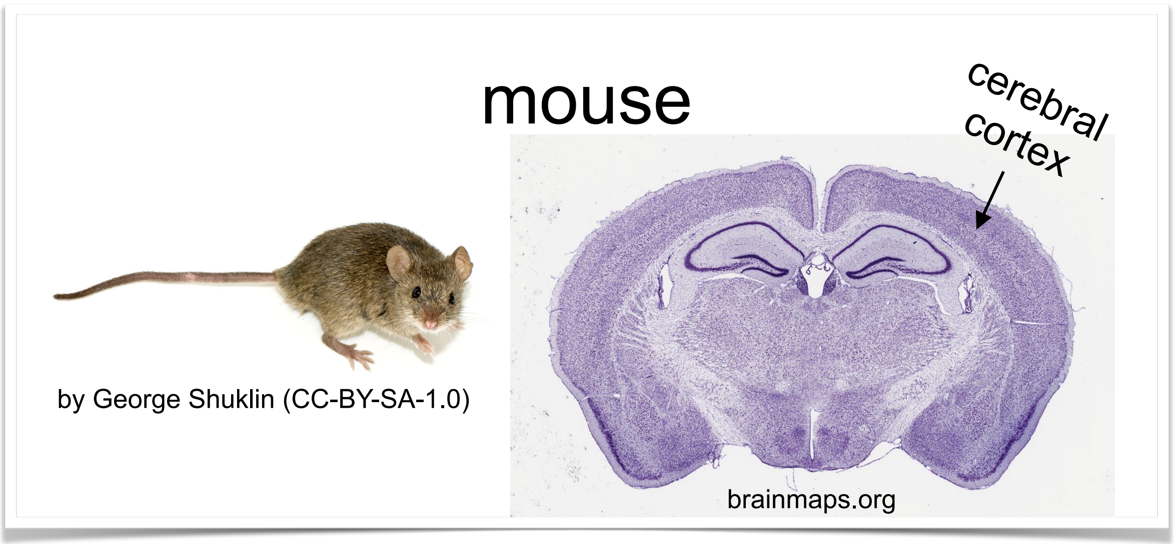
$t = 0.98$ ms



Philipp Weiss, 2021

2nd Example: Cerebral Blood Flow (CBF)





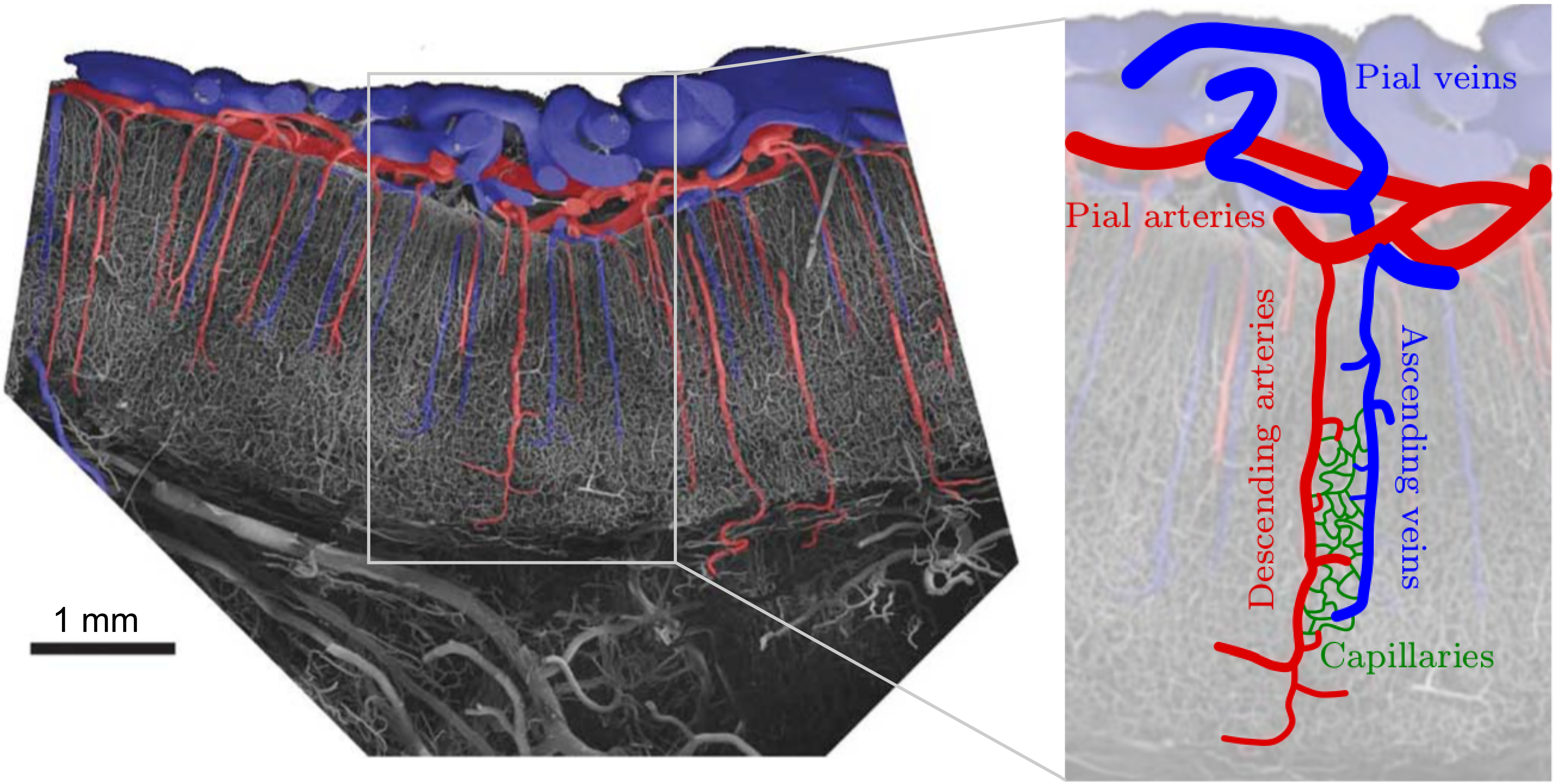
Main functions

- receiving and processing **sensory input**
- **controlling muscles** and movements

2nd Example: Cerebral Blood Flow (CBF)

vasculature of the monkey visual cortex

schematic of cortical vasculature

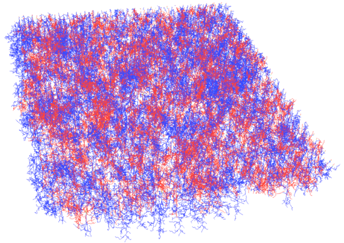


by Hirsch et al., JCBFM, 2012 [7]. Adapted by Schmid et al., Neuroimage, 2017 [1].

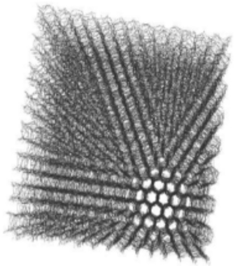
2nd Example: Cerebral Blood Flow (CBF)

Compound Network

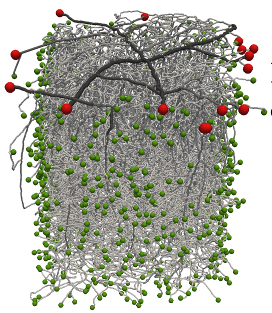
Network of penetrating trees



Artificial capillary bed



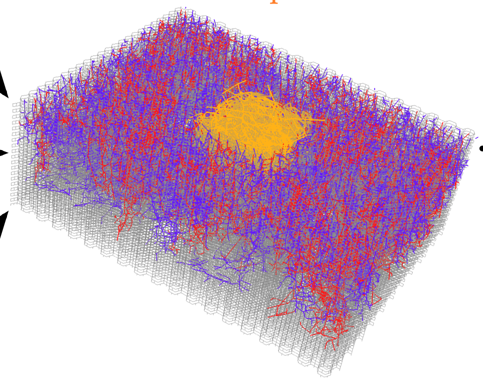
Realistic implant



Boundary conditions for:
- pial arterioles and venules
- capillaries

Steady state simulation

Full compound network with realistic implant

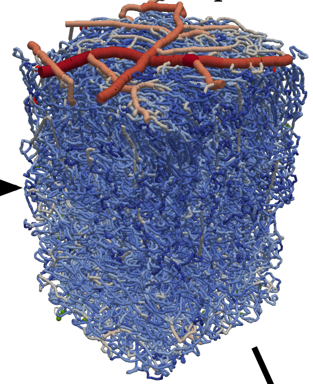


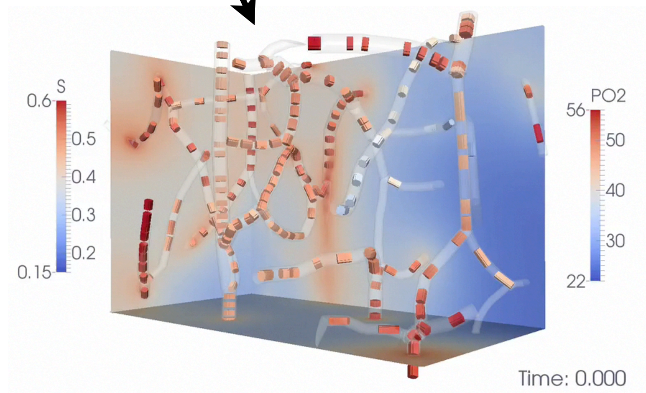
Schmid et al., 2017
Neuroimage

Boundary conditions

Discrete simulation

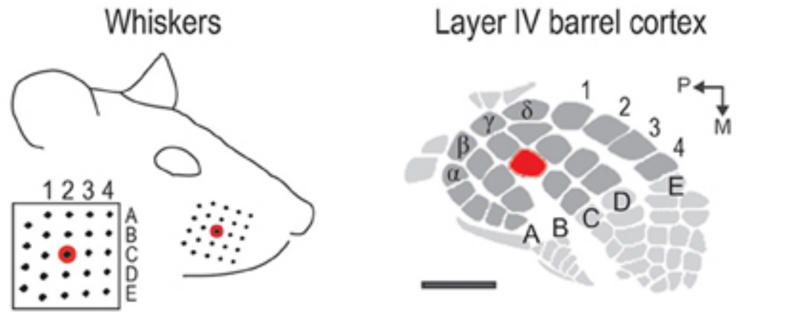
Realistic implant



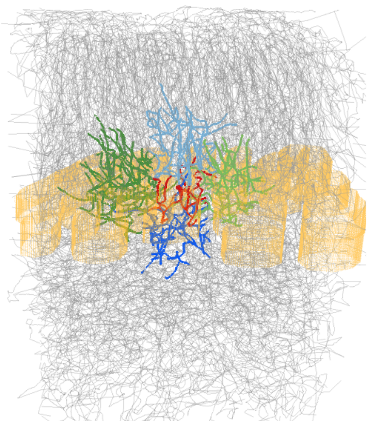


2nd Example: Cerebral Blood Flow (CBF)

The barrel cortex



From: Chen-Bee et al., *Frontiers in Neural Circuits*, 2012



Schmid et al., 2017
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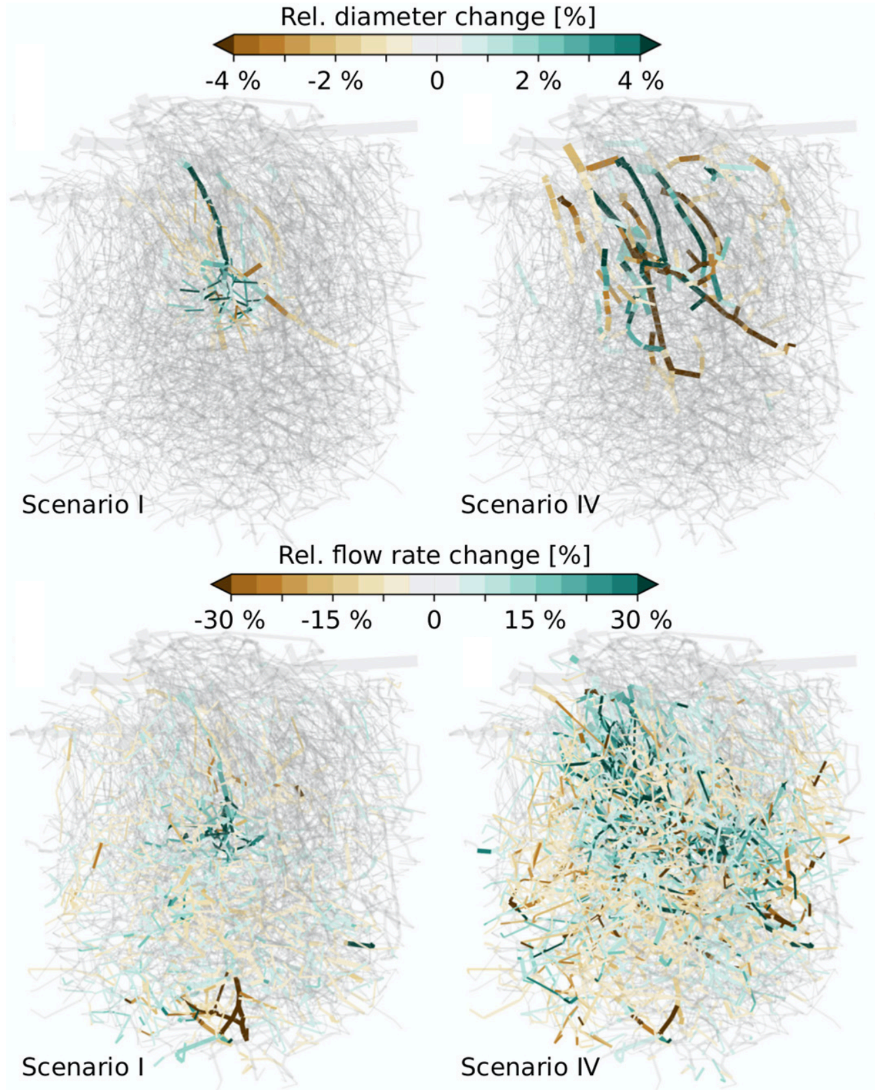
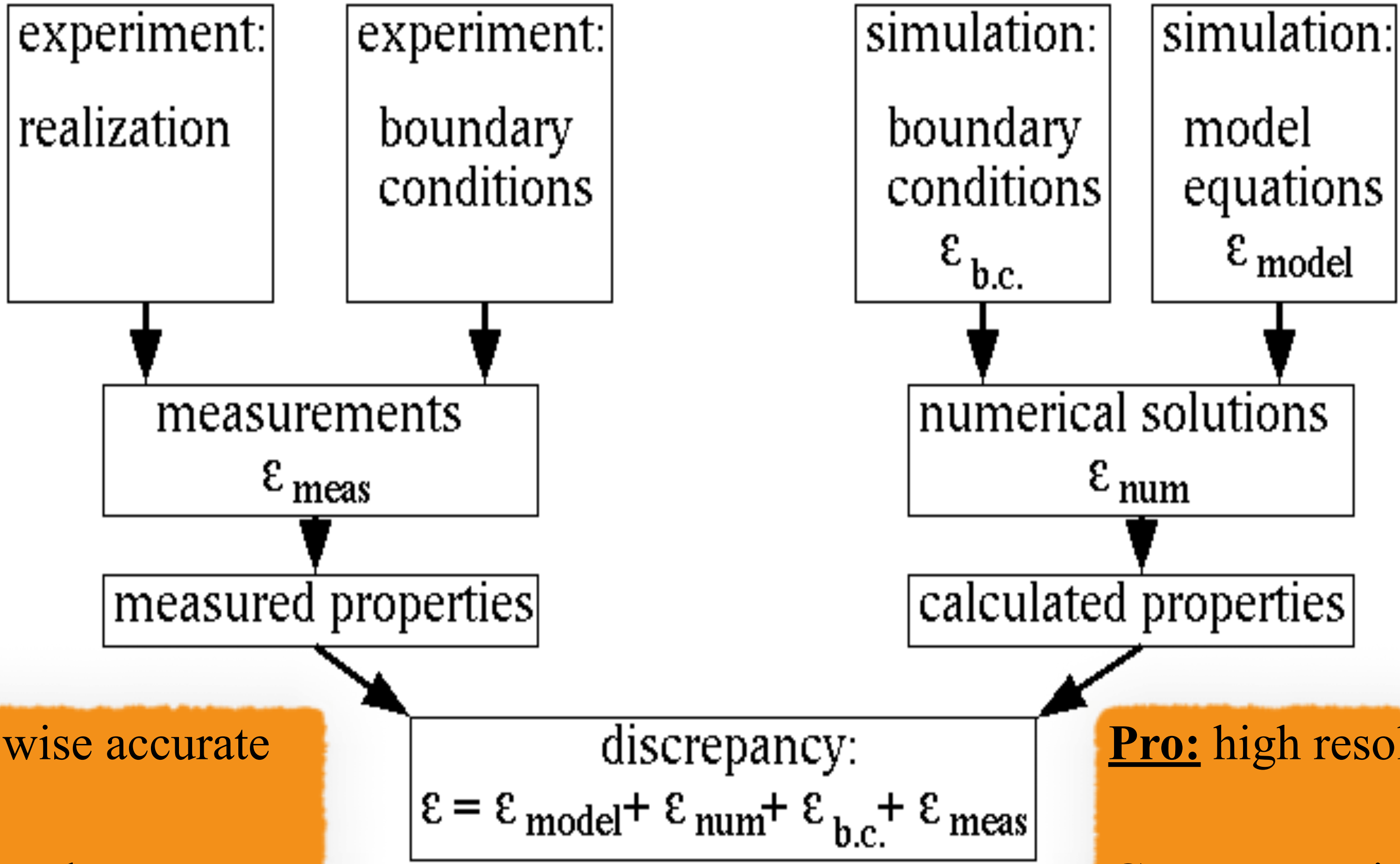


2nd Example: Cerebral Blood Flow (CBF)

<u>uncertainty problem → data assimilation → inverse modeling</u>



Pro: point wise accurate

Con: often only sparse

Pro: high resolution

Con: uncertain

Data Assimilation - Inverse Modeling - Optimization

non-linear forward problem $\mathcal{R}(\boldsymbol{V}, \boldsymbol{\alpha}) = \mathbf{0}$ with the solution $\boldsymbol{V}$ and parameters $\boldsymbol{\alpha}$

Problem: many parameters

goal: optimal point in parameter space to minimize a cost function $J(\boldsymbol{V}, \boldsymbol{\alpha})$

Data Assimilation - Inverse Modeling - Optimization

non-linear forward problem $\mathcal{R}(\boldsymbol{V}, \boldsymbol{\alpha}) = \mathbf{0}$

goal: optimal point in parameter space to minimize a cost function $J(\boldsymbol{V}, \boldsymbol{\alpha})$

Data Assimilation

Examples:

- meteorolgy
- computational fluid dynamics
- oil reservoir simulation
- optimization
- control
- …

Interpretations:

- inverse modeling
- optimization
- rigorous tuning
- empirical model correction
- uncertainty reduction
- learning
- physical inter-/extrapolation