
Scaling Cascades in Complex Systems

SCCS

A DFG Collaborative Research Center initiative

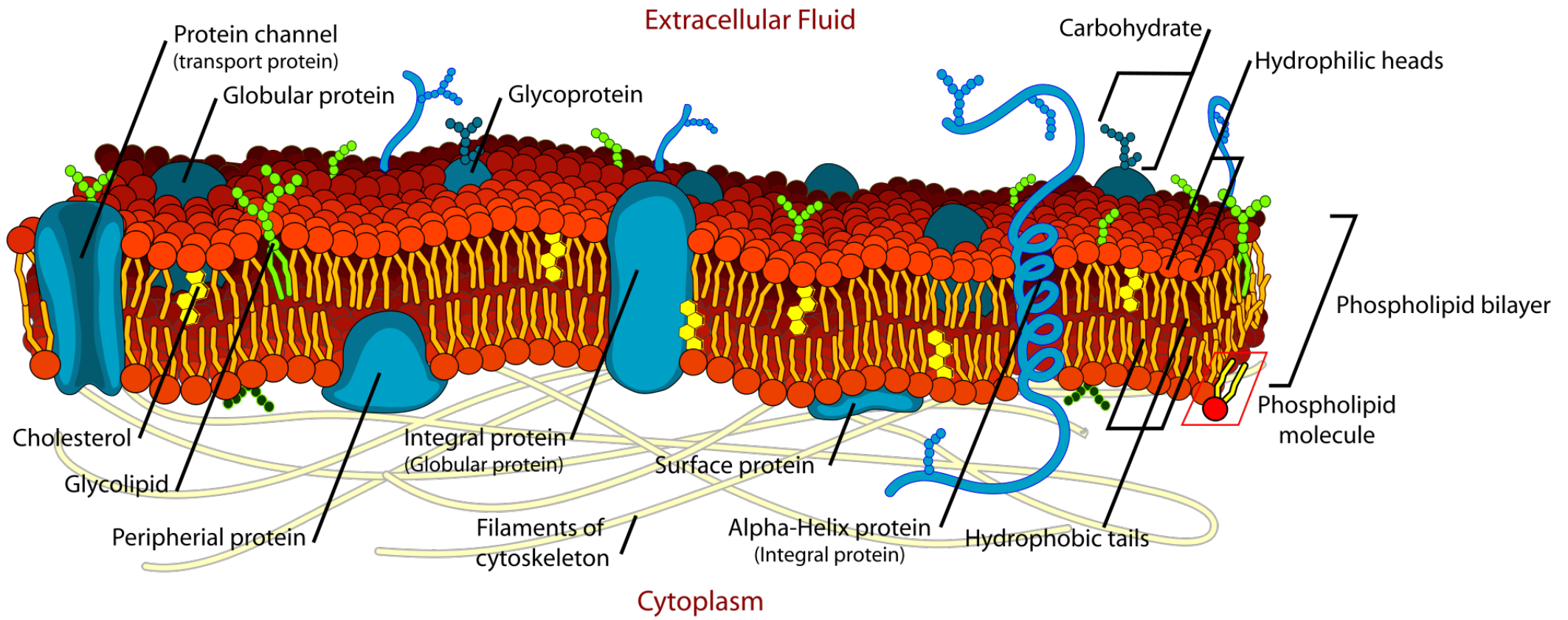
[Place all the logos here]

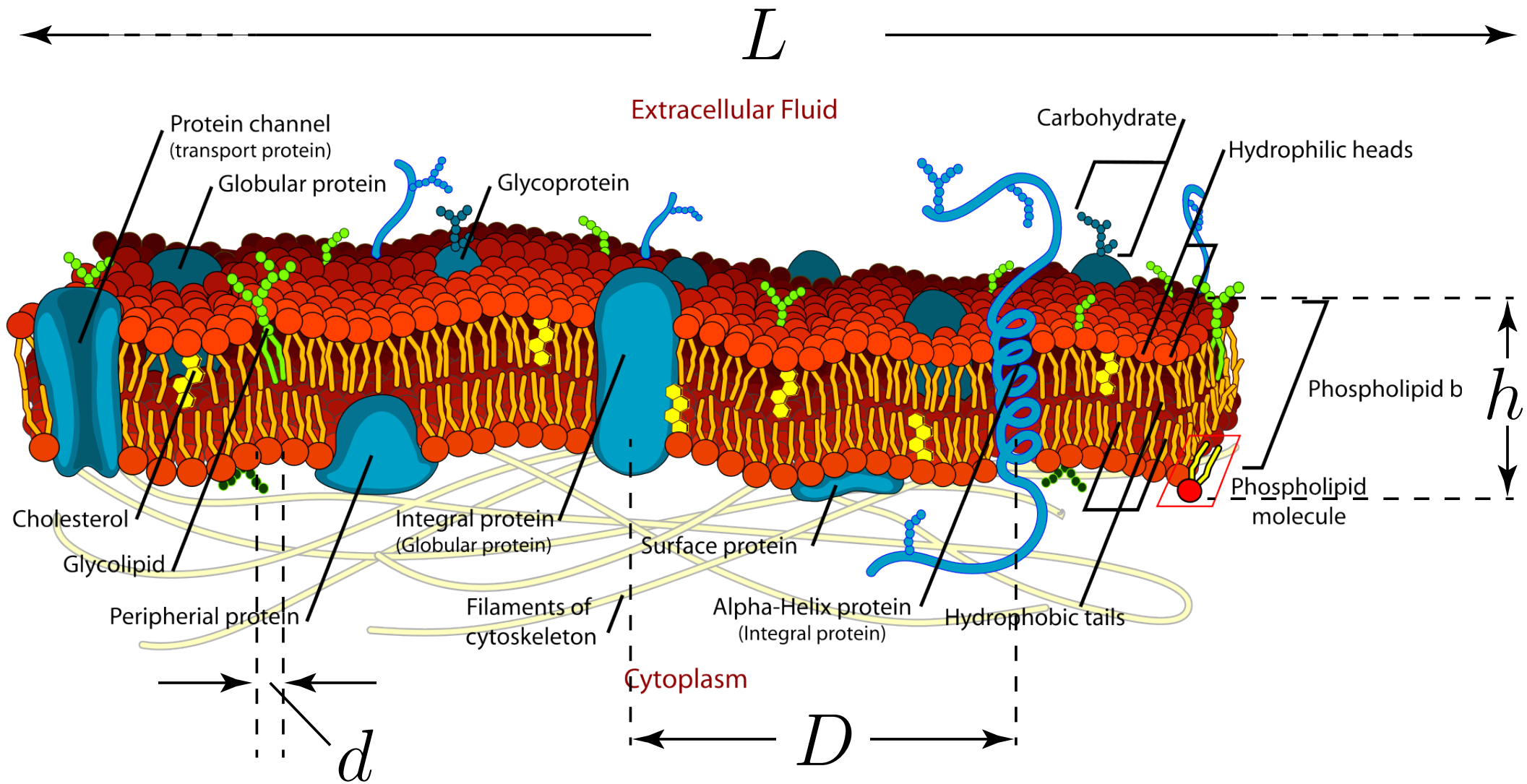
Motivation

Conceptual framework

Research directions

Research areas





$$d \ll h \ll D \ll L$$

No. of **Protein** Molecules \ll No. of **Lipid** Molecules

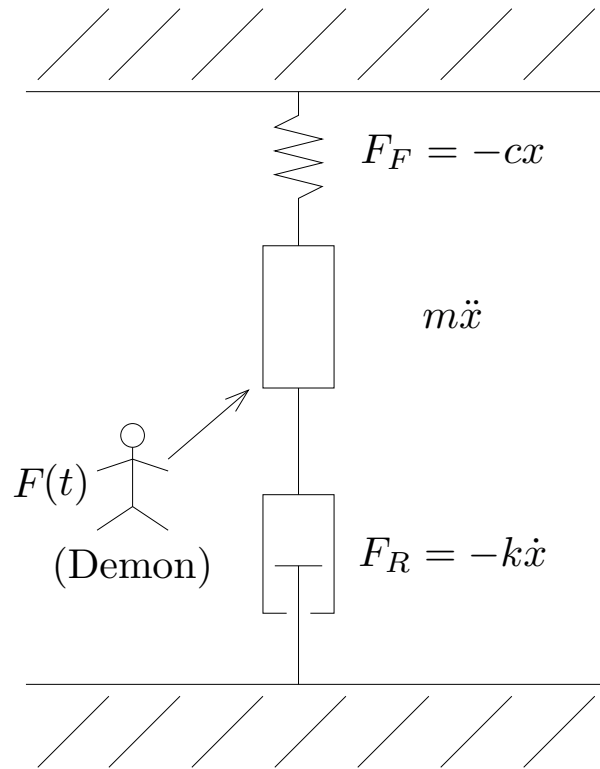
Motivation

Conceptual framework

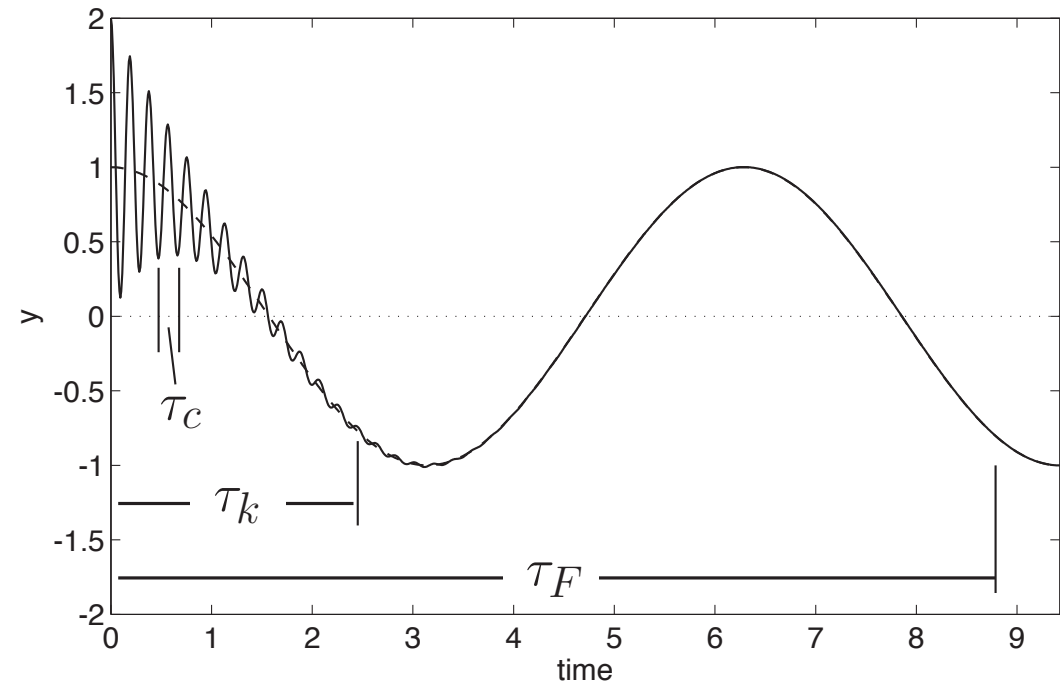
Research directions

Research areas

Linear Oscillator



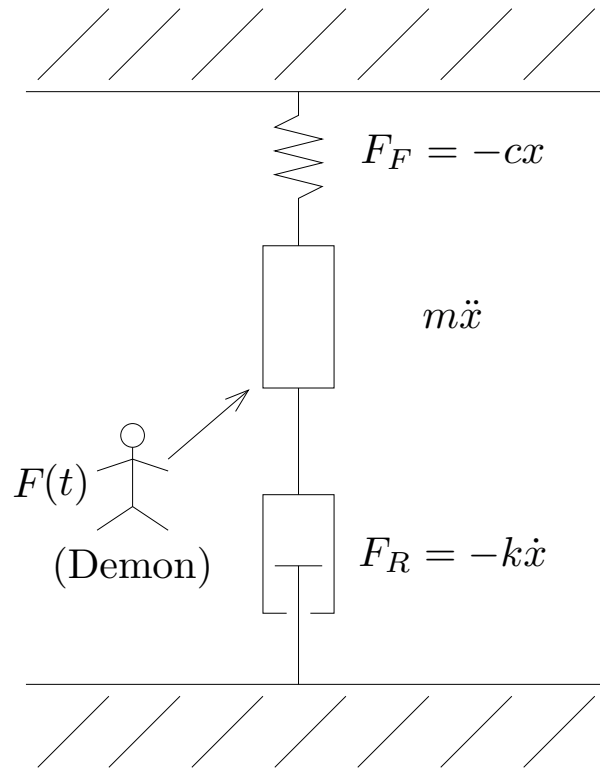
$$m\ddot{x} + k\dot{x} + cx = F_0 \cos \Omega t$$



Time scales

$$t_c = \sqrt{\frac{m}{c}}, \quad t_k = \frac{k}{c}, \quad t_F = \frac{1}{\Omega}$$

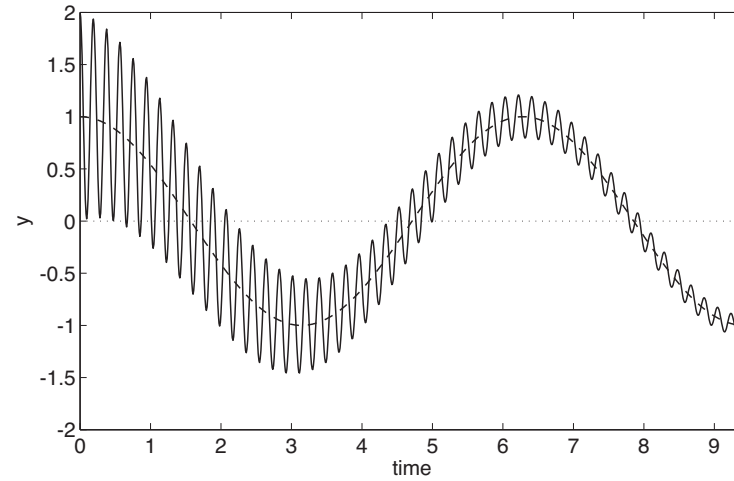
Linear Oscillator



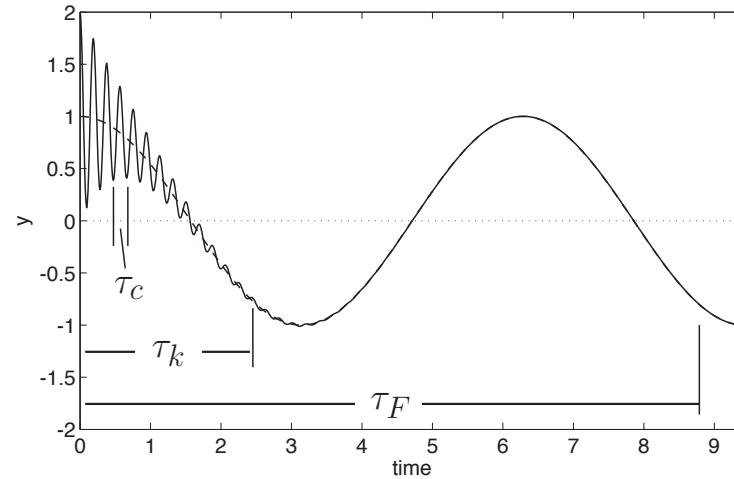
$$m\ddot{x} + k\dot{x} + cx = F_0 \cos \Omega t$$

Time scales

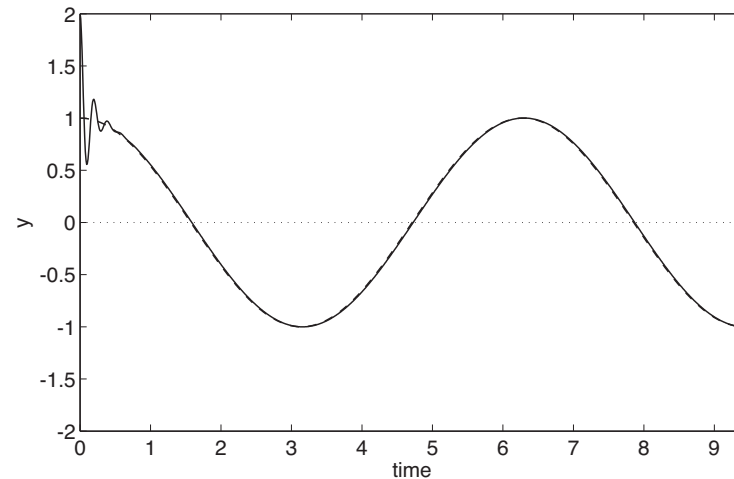
$$t_c = \sqrt{\frac{m}{c}}, \quad t_k = \frac{k}{c}, \quad t_F = \frac{1}{\Omega}$$



$$t_c \ll t_k \sim t_F$$



$$\underline{t_c \ll t_k \ll t_F}$$



$$t_c \sim t_k \ll t_F$$

Linear Oscillator

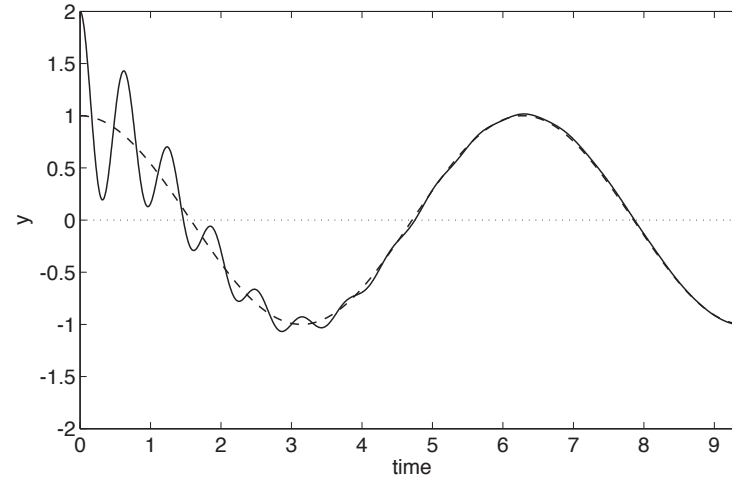
$$m \ddot{x} + k \dot{x} + c x = F_0 \cos \Omega t$$

Dimensionless parameters

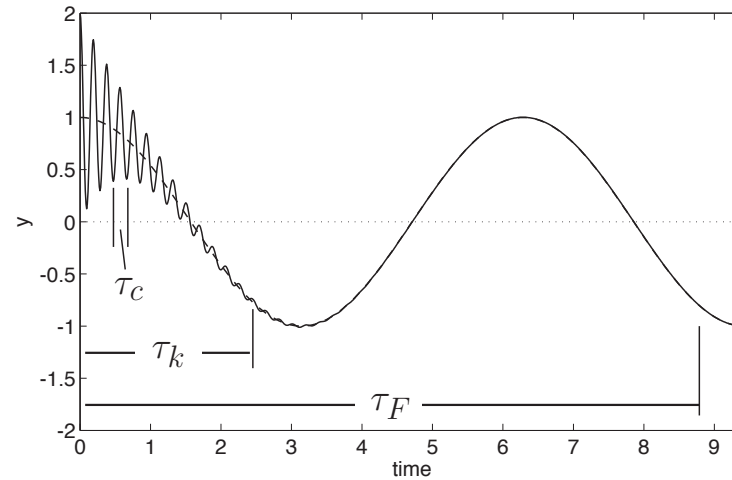
$$\frac{t_c}{t_F} = \sqrt{\frac{m\Omega^2}{c}} \equiv \epsilon,$$

$$\frac{t_k}{t_F} = \frac{k\Omega}{c} = \frac{1}{2} \epsilon^{\frac{3}{2}},$$

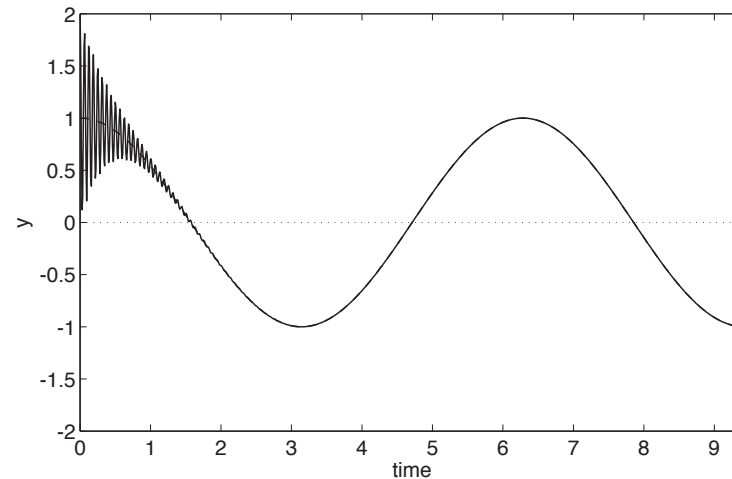
Three
asymptotically separated
time scales



$$\epsilon = 1 \cdot 10^{-2}$$



$$\epsilon = 1 \cdot 10^{-3}$$



$$\epsilon = 1 \cdot 10^{-4}$$

Root Model

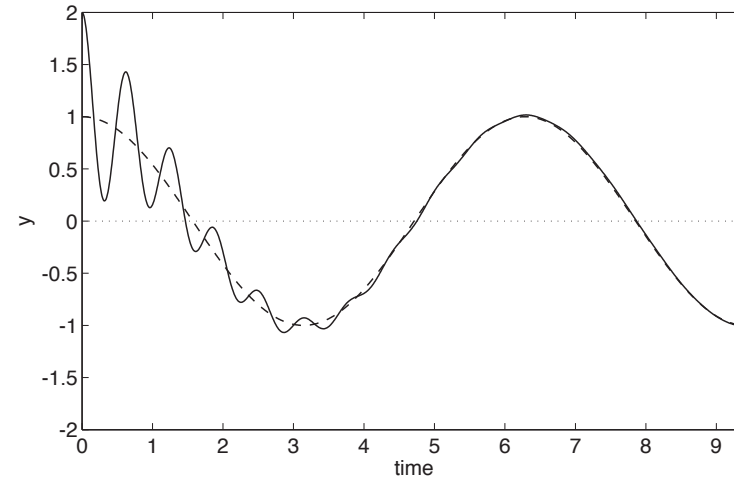
$$m \ddot{x} + k \dot{x} + c x = F_0 \cos \Omega t$$

Measure of scale separation

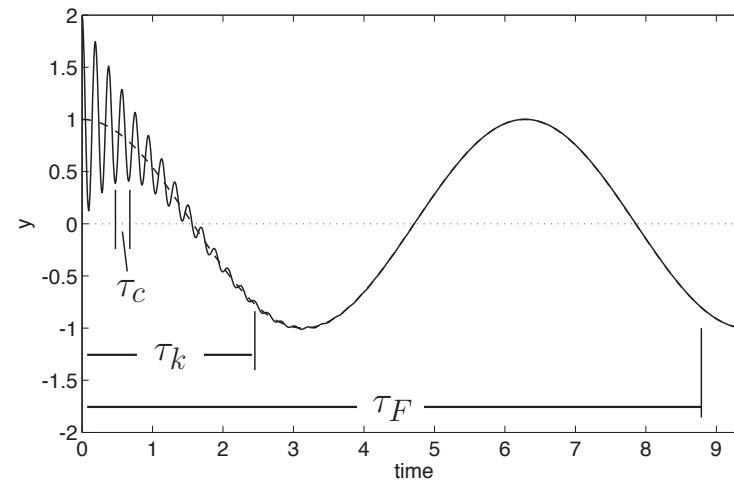
$$\frac{t_c}{t_F} = \sqrt{\frac{m\Omega^2}{c}} \equiv \epsilon,$$

$$\frac{t_k}{t_F} = \frac{k\Omega}{c} \equiv \delta = \frac{1}{2} \epsilon^{\frac{3}{2}},$$

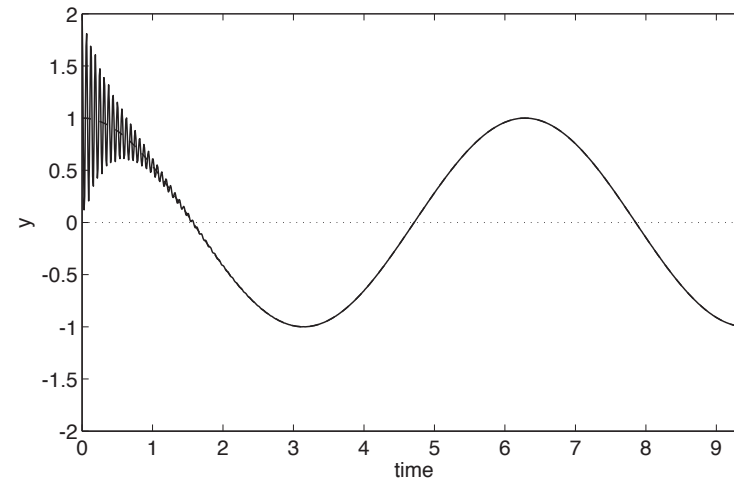
More than two
asymptotically separated
time scales



$$\epsilon = 1 \cdot 10^{-2}$$



$$\epsilon = 1 \cdot 10^{-3}$$



$$\epsilon = 1 \cdot 10^{-4}$$

Root Model (dimensionless)

$$\epsilon^2 \ddot{y} + \kappa \epsilon^{\frac{3}{2}} \dot{y} + y = \cos \tau$$

Reduced models

rapid oscillation

$$\frac{d^2 y}{d\vartheta^2} + y = 0 \quad (\vartheta = \tau/\epsilon)$$

damping of the envelope

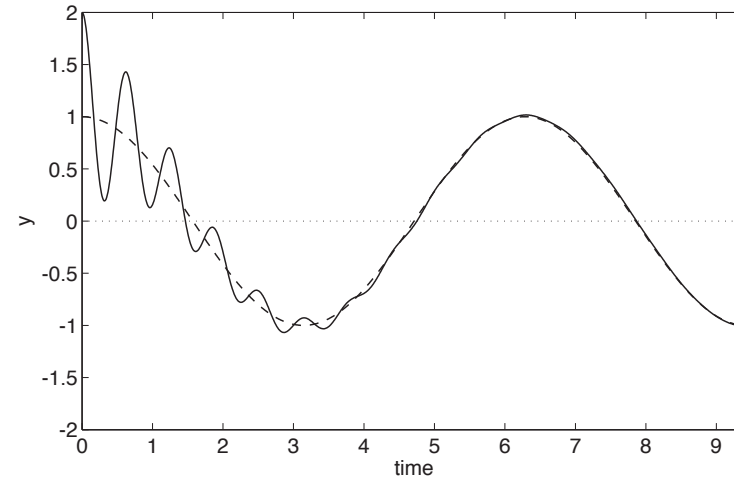
$$\frac{d\hat{y}}{d\theta} + \frac{\kappa}{2} \hat{y} = 0 \quad (\theta = \tau/\sqrt{\epsilon})$$

long-time force balance

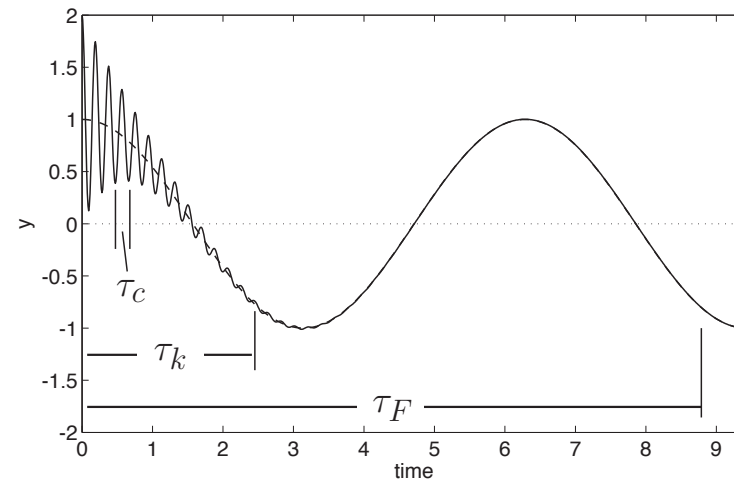
$$Y(\tau) = \cos(\tau) \quad (\tau = \Omega t)$$

Coupled model solution

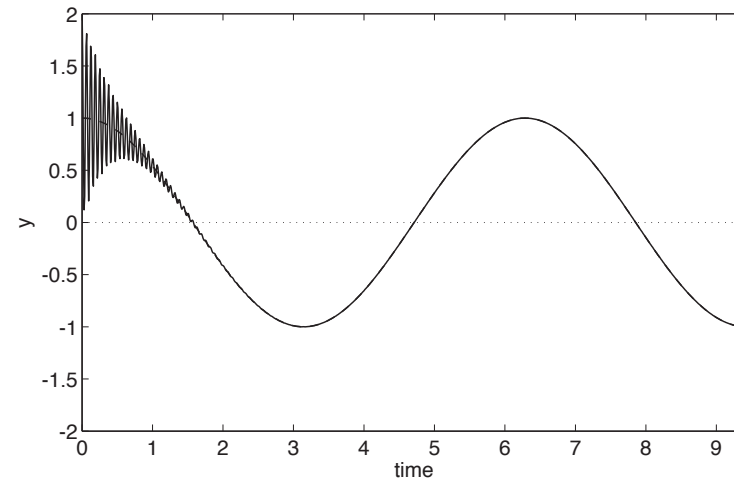
$$y(\tau; \epsilon) = \cos(\tau) + e^{-\kappa\tau/2\sqrt{\epsilon}} \cos(\tau/\epsilon)$$



$$\epsilon = 1 \cdot 10^{-2}$$



$$\epsilon = 1 \cdot 10^{-3}$$



$$\epsilon = 1 \cdot 10^{-4}$$

Key Notions

Root Model

Asymptotically Emerging Multiple* Scales

Solution concepts that survive the limit

* generally more than two

Motivation

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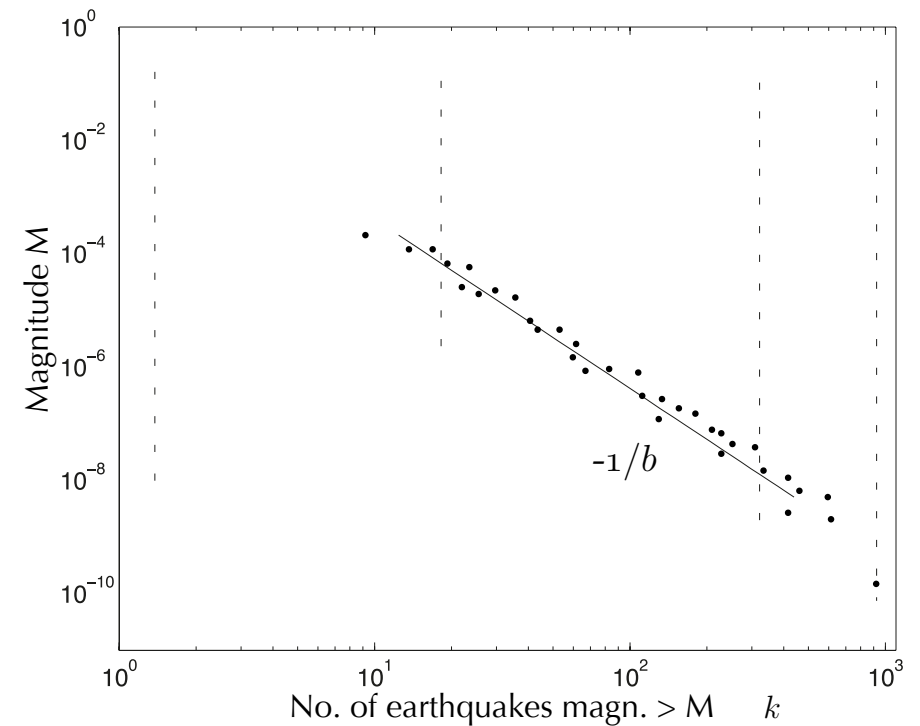
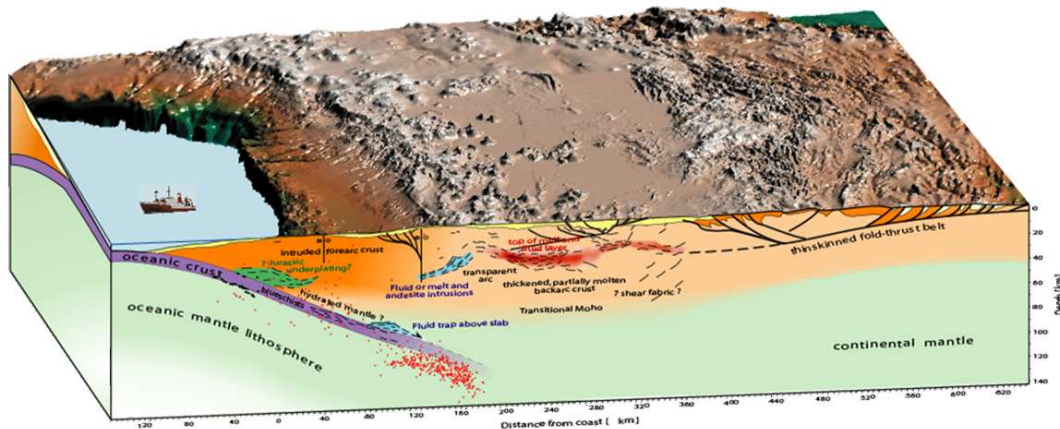
Research areas

Research directions

First Principles explanations

Analysis of complex simulation systems

Efficient, robust computational techniques

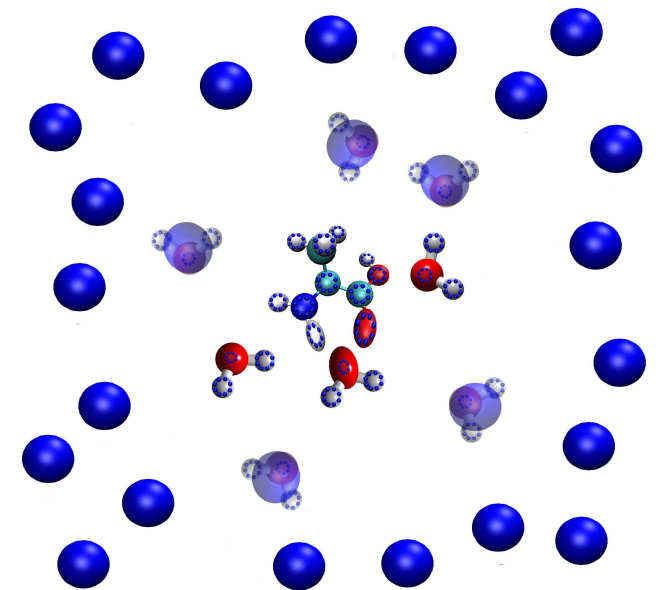
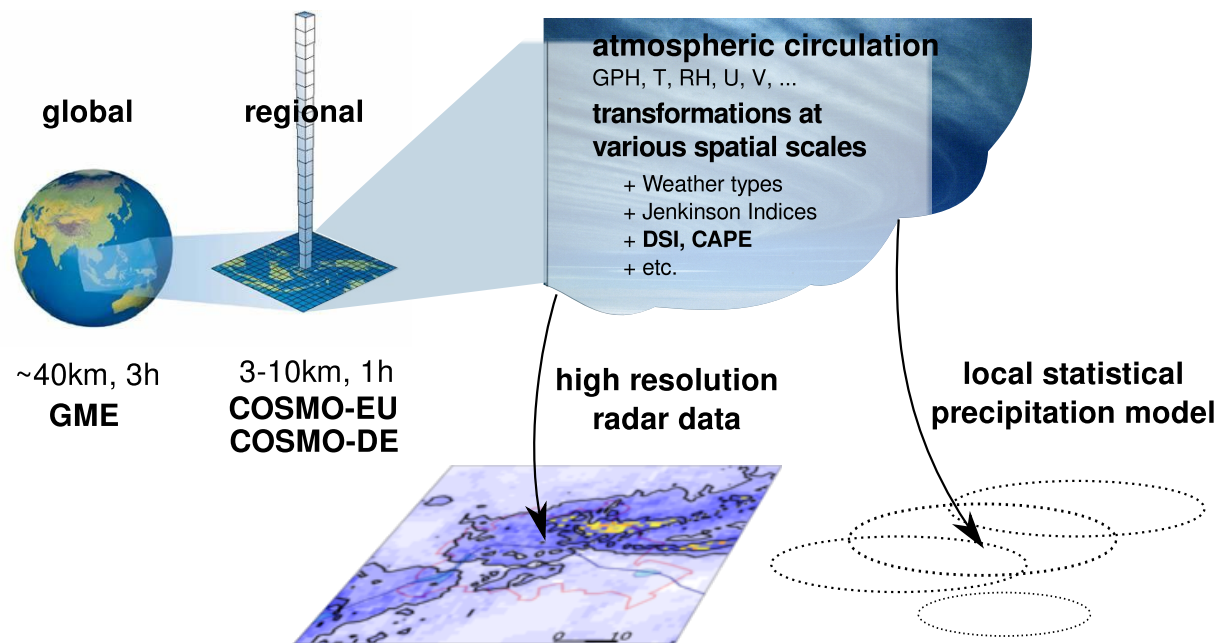


Research directions

First Principles explanations

Analysis of complex simulation systems

Efficient, robust computational techniques

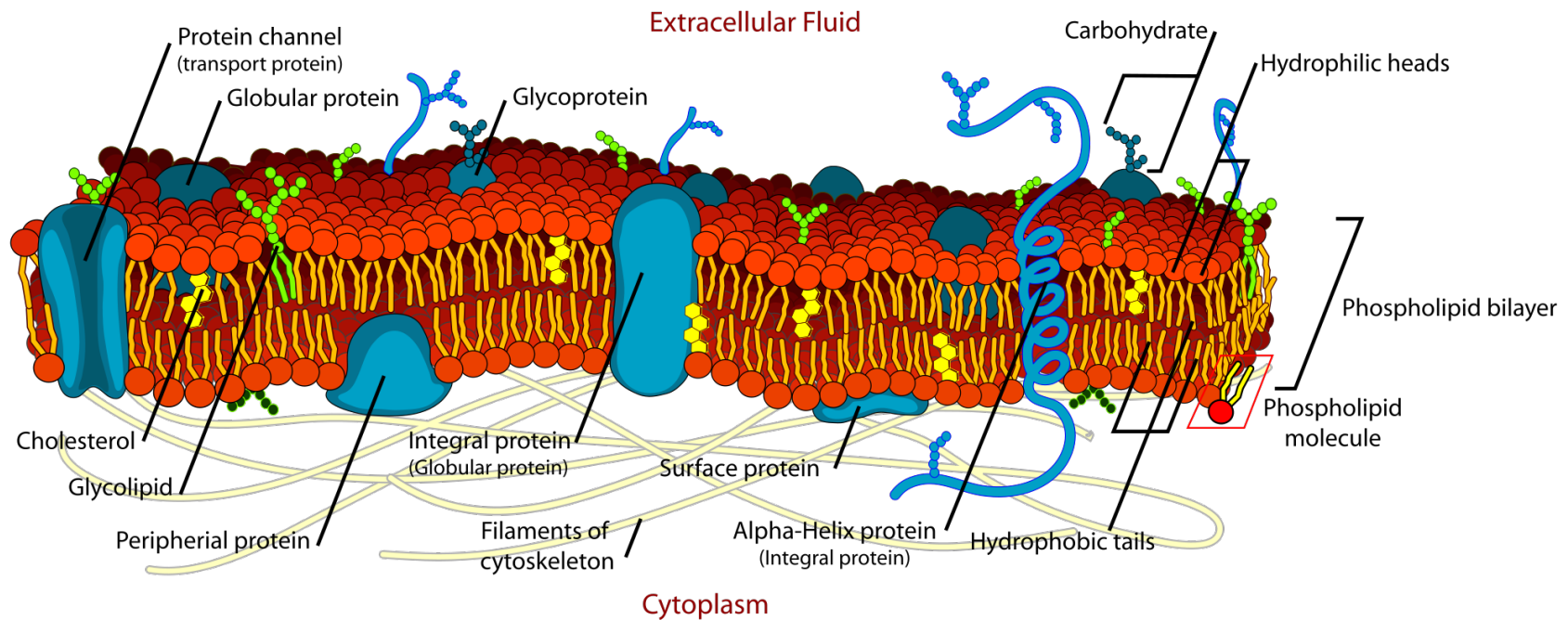


Research directions

First Principles explanations

Analysis of complex simulation systems

Efficient, robust computational techniques



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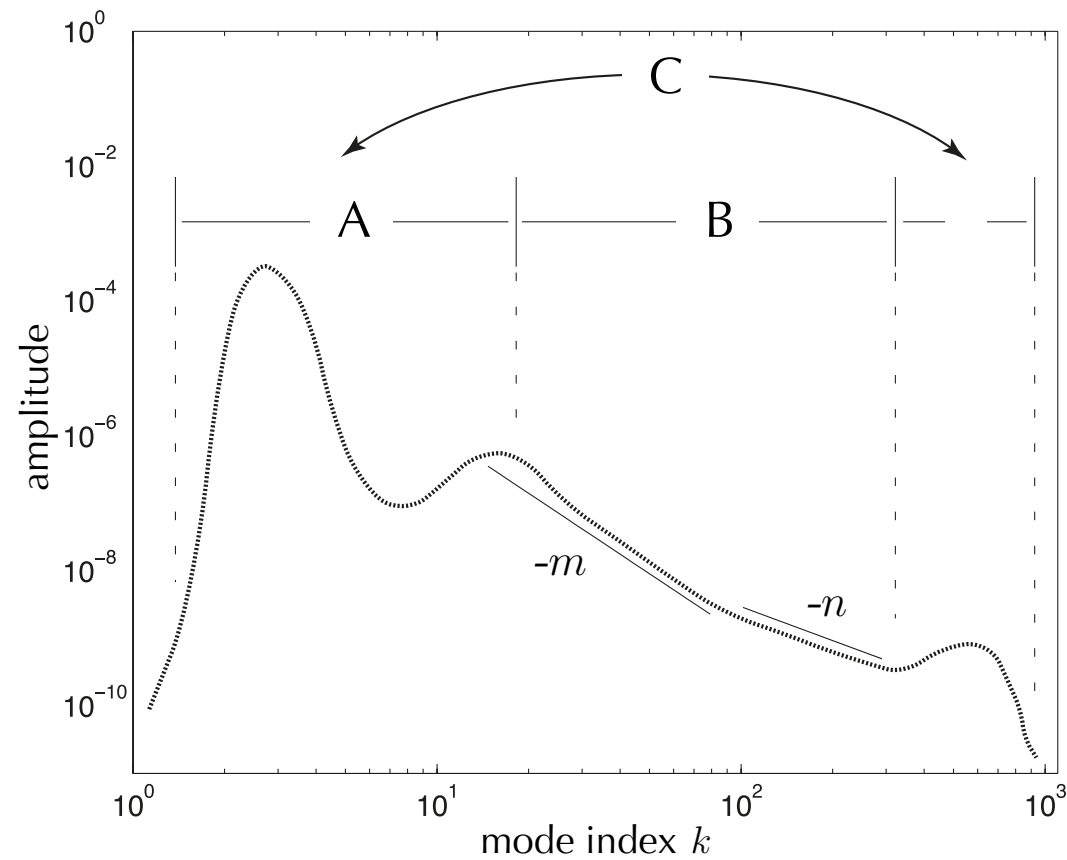
Research directions

Research areas

A: Efficient modelling of macro scales

B: Uniform meso scale behavior in scaling cascades

C: Bridging the micro-macro scale range



Prj.	PIs	Title	Research Area
A: Efficient modelling of macro scales			
A01	Rust, Ulbrich, Névir, Schartner	Optimal use of regional climate models (RCMs) for small scale extreme precipitation	Meteorology
A02	Reich, Klein	Efficient multiscale filtering and prediction for complex systems subject to measurements	Meteorology
A03	John, Patterson	Complex particles in turbulent flows	Fluid Dynamics
A04	Noé, Weigl	Equilibrium molecular expectations from multi-ensemble simulations	Molecular Dynamics
A05	Weber, Fackeldey, Hartmann, Schütte	Driving into non-equilibrium / Non-equilibrium fluctuation relations for multiscale processes	Molecular Dynamics

Prj.	PIs	Title	Research Area
B: Uniform meso scale behavior in scaling cascades			
B01	Klein, Sander, Oncken, Rosenau	Fault networks in plate boundary zones	Geophysics
B02	Klein	A multilevel approach to Large-Eddy-Simulation of turbulence	Fluid Dynamics
B03	Netz et al.	Protein folding free energy landscapes, Markov state models, and polymer dynamic theories	Molecular Dynamics
B04	Schütte, Hartmann, Kornhuber, Koksch	Multilevel coarse graining of multi-scale problems	Biochemistry
B05	Kornhuber, Schneider, Yserentant	Multiscale decomposition methods	Applied Mathematics

Prj.	PIs	Title	Research Area
C: Bridging the micro-macro scale range			
C01	delle Site	Adaptive coupling of scales in molecular dynamics	Molecular Dynamics
C02	Netz et al.	Water diffusion at biological molecules: from a stochastic to a hydrodynamic description	Molecular and Fluid Dynamics
C03	Schütte, Noé	Multiscale modelling and simulation for spatio-temporal master equations	Biochemistry
C04	Kornhuber, Hartmann	Diffusing particles in lipid bilayers	Surface Physics
C05	Knees, Mielke	Effective models for interfaces with microstructure	Surface Physics
C06	Scheffler et al.	From molecular dynamics to kinetic Monte-Carlo methods on catalytic surfaces	Surface Physics
