Scientific Computing in Würzburg

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Chair Mathematics IX - Scientific Computing

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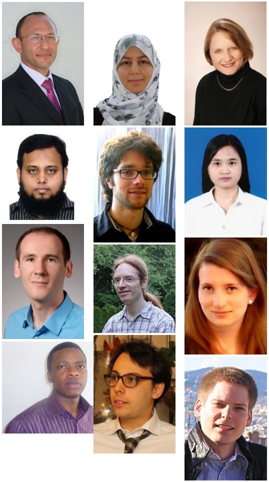

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Wissenschaftliches Rechnen - Scientific Computing

Scientific computing is the scientific discipline that deals with modelling and computer-based simulations of processes as they are investigated within natural, engineering or economical sciences.

The numerical simulation supplements the two classical pillars of knowledge acquisition in applied sciences, namely the theoretical investigation and the laboratory experiment.

Scientific computing has developed to a key technology for the understanding and handling of scientific and technical challenges.

Scientific computing as a key technology

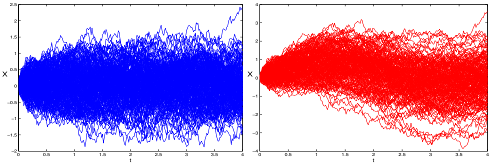
- Optimization and calibration of stochastic models in finance.
- Simulation of thermo-fluid-mechanical systems.
- Shape and topology optimization of mechanical structures.
- Modelling and visualization of physiological processes as the electrical activity of the brain.
- Optimal control of nanosystems in quantum optics and NMR.
- Development of fast algorithms for compressed sensing in tomography and particle tracking in microscope videos.
- Investigation of swarming and social behaviour using multi-particle systems.

Optimization and calibration of stochastic models

We consider continuous-time stochastic processes described by, e.g., Itō stochastic differential equations

$$dX_t = b(X_t, t; u_t)\, dt + \sigma(X_t, t)\, dW_t,$$

where $X_t \in \mathbb{R}^n$ is the state variable and $W_t \in \mathbb{R}^m$ is a multi-dimensional Wiener process, and determine a control $u(t) \in \mathbb{R}^\ell$ to drive the random process.



Our optimization strategy is based on the corresponding Fokker-Planck-Kolmogorov equation

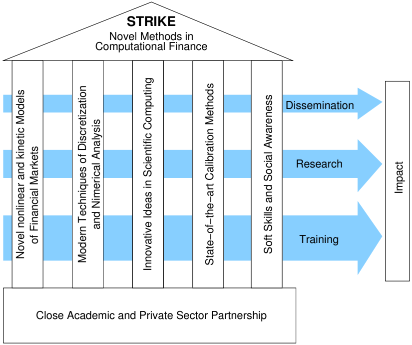
$$\partial_t f - \frac{1}{2} \sum_{i,j=1}^{n} \partial^2_{x_i x_j} \left(a_{ij}\, f \right) + \sum_{i=1}^{n} \partial_{x_i} \left(b_i(u)\, f \right) = 0$$

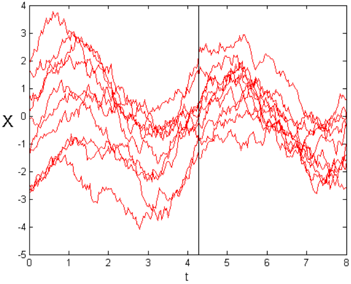
where $a = \sigma\sigma^\top$.

Novel methods in computational finance

$$dX_t = b(X_t, u)\, dt + \sigma(X_t)\, dW_t$$

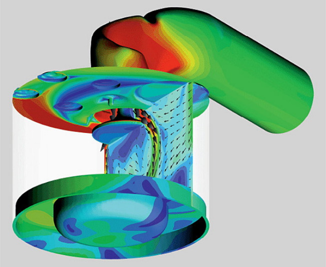
$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + r\frac{\partial V}{\partial S} S - rV = 0$$





Simulation of thermo-fluid-mechanical systems: combustion engines

Scientific computing is strongly linked to Industry through research and development projects in the field of high-performance computing of mechanical systems.



Simulation and optimization of an engine intake (collaboration with AVL List GmbH, Graz, Austria).

Simulation of thermo-fluid-biological systems: wine fermentation

Change of Sugar/glucose concentration

$$\frac{\partial S}{\partial t} = \sigma \Delta S + w \nabla S - X\, v_{ST}(S, E, T) + N_{ST}((N_{max} - N), X, T_{ucd}).$$

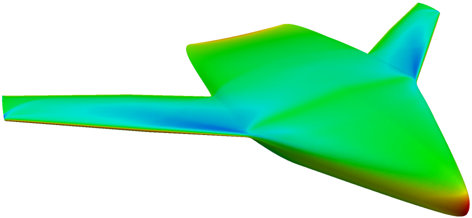
In addition, we have yeast X, nitrogen N, ethanol E, ...
The bio-chemical reaction-diffusion models are coupled with the Navier-Stokes equations for incompressible unsteady flow

$$\rho_f(T)\frac{\partial w}{\partial t} + \rho_f(T)\, w \cdot \nabla w - \eta \Delta w + \nabla p = f$$

$$\frac{\partial \rho_f(T)}{\partial t} + \rho_f(T) \cdot (\nabla \cdot w) = 0$$

Shape and topology optimization

Shape optimization is becoming a leading topic in engineering design. Scientific computing contributes to shape and topology optimization strategies with computing and modelling tools.



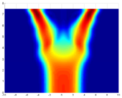
Simulation and optimization of VELA (courtesy of V. Schulz and DLR).
We develop fast multilevel shape and topology optimization schemes.

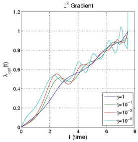
Optimal control of Bose-Einstein condensates

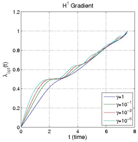
A Bose–Einstein condensate (BEC) is a state of matter of a dilute gas of bosons cooled to temperatures near absolute zero. A large fraction of the bosons occupy the lowest quantum state such that quantum effects become apparent on a macroscopic scale.
A BEC is modelled by the Gross-Pitaevskii equation

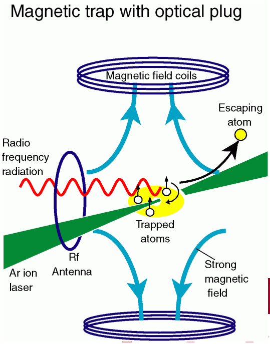
$$i \frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2}\nabla^2 + V(x,u(t)) + g\,|\psi(x,t)|^2\right)\psi(x,t)$$

We determine the optimal magnetic field $V(x,u(t))$ to drive the BEC to a desired configuration









Simulation and control of arrhythmia

The Aliev-Panfilov's model of cardiac excitation

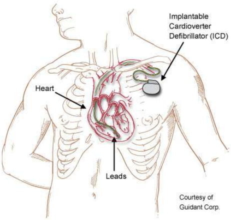
$$\frac{\partial y_1}{\partial t} = -ky_1(y_1 - a)(y_1 - 1) - y_1\, y_2 + \sigma\, \Delta y_1 + u$$

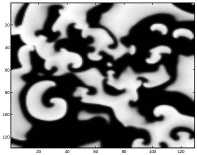
$$\frac{\partial y_2}{\partial t} = [\epsilon_0 + \frac{\mu_1 y_2}{\mu_2 + y_1}][-y_2 - ky_1(y_1 - b - 1)]$$

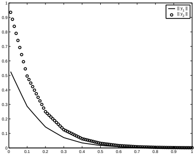
y_1 - transmembrane potential and y_2 - membrane conductance

The model evolves from an initial planar wave to a turbulent pattern.

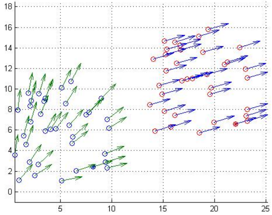
Determine a control response in the form of an electrical field to drive the system from a turbulent pattern to a uniform 'calm' pattern.







Swarming of self-propelled multi-particle systems

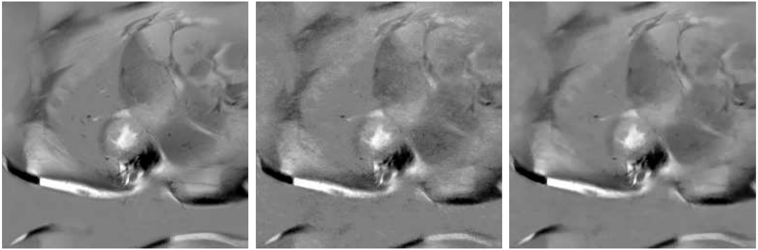


A dynamical system of N interacting agents

$$\begin{aligned}\frac{dx_b}{dt} &= v_b \\ \frac{dv_b}{dt} &= (\alpha - \beta \|v_b\|^2) v_b + F_b + F_b^0 + A_b \qquad \text{for} \quad b = 1, ..., N,\end{aligned}$$

Analysis of dynamic 3D medical images

Development of fast and accurate algorithms for image deblurring, detection, inpainting, registration, reconstruction, optical flow ...



(a) Original (b) FCSA (c) Fista-TV

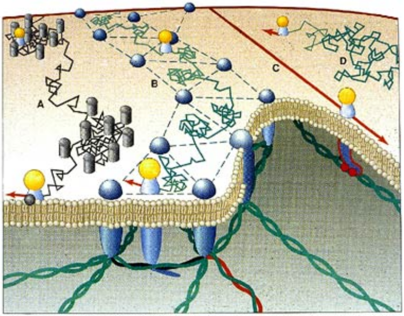
Figure : Reconstructed 3D heart images.

IZKF Würzburg

Julius-Maximilians-UNIVERSITÄT WÜRZBURG

A collaboration platform

Scientific computing provides an ideal ground for interdisciplinary projects.
New scientific initiative are starting in Würzburg, involving Biology, Informatics, Mathematics, Medicine and Physics ...



Lateral transport modes on the cell surface. **(A)** Transient confinement by obstacle clusters **(B)** or by the cytoskeleton, **(C)** directed motion, and **(D)** free random diffusion

Projects

1. EU Project Marie Curie Action 'Multi-ITN STRIKE - Novel Methods in Computational Finance'
2. DFG Project 'Controllability and Optimal Control of Interacting Quantum Dynamical Systems'
3. BMBF Project 'ROENOBIO: Robust energy optimization of fermentation processes for the production of biogas and wine'
4. IZKF Project 'Parallel Multigrid Imaging and Compressed Sensing for Dynamic 3D Magnetic Resonance Imaging'
5. ESF European Science Foundation OPTPDE Grants
6. Bayerisch-Französisches Hochschulzentrum (BFHZ) Exchange Grants
7. Bavarian Research Alliance (BayFOR) Grants

Thanks for your interest ☺