Research in CSE and Biocomputing at CSC

Michael Hanke

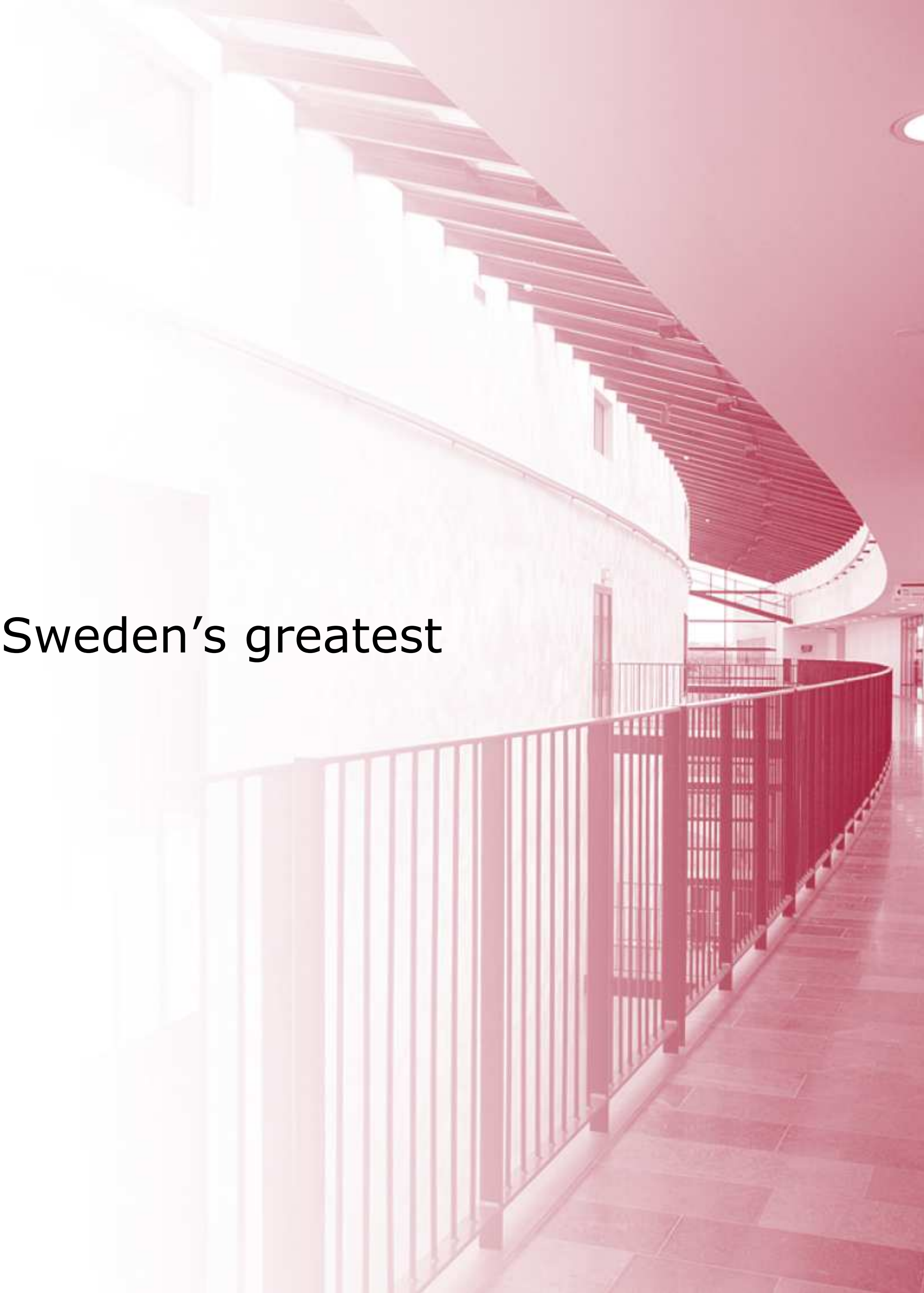
School of Computer Science and Communication
Royal Institute of Technology, Stockholm

Stockholm, February 8, 2011

ROYAL INSTITUTE OF TECHNOLOGY

About KTH

Facts and figures on Sweden’s greatest technical university



Premises for innovation

232 000 m² including beautiful, historical buildings.

ROYAL INSTITUTE OF TECHNOLOGY

KTH in Stockholm

KTH was founded in 1827 and is the largest of Sweden's technical universities. Since 1917, activities have been housed in central Stockholm, in beautiful buildings which today have the status of historical monuments.

KTH cooperates with Stockholm University in Kista, the primary Swedish resource centre of information technology, and in the new AlbaNova Centre, with its departments of physics and biotechnology.

ROYAL INSTITUTE OF TECHNOLOGY

KTH Schools

- School of Architecture and the Built Environment
- School of Biotechnology
- School of Chemical Science and Engineering
- **School of Computer Science and Communication**
- School of Electrical Engineering
- School of Information and Communication Technology
- School of Industrial Engineering and Management
- School of Engineering Sciences
- School of Technology and Health
- (Scientific Information and Learning)

Research-intensive staffing, CSC

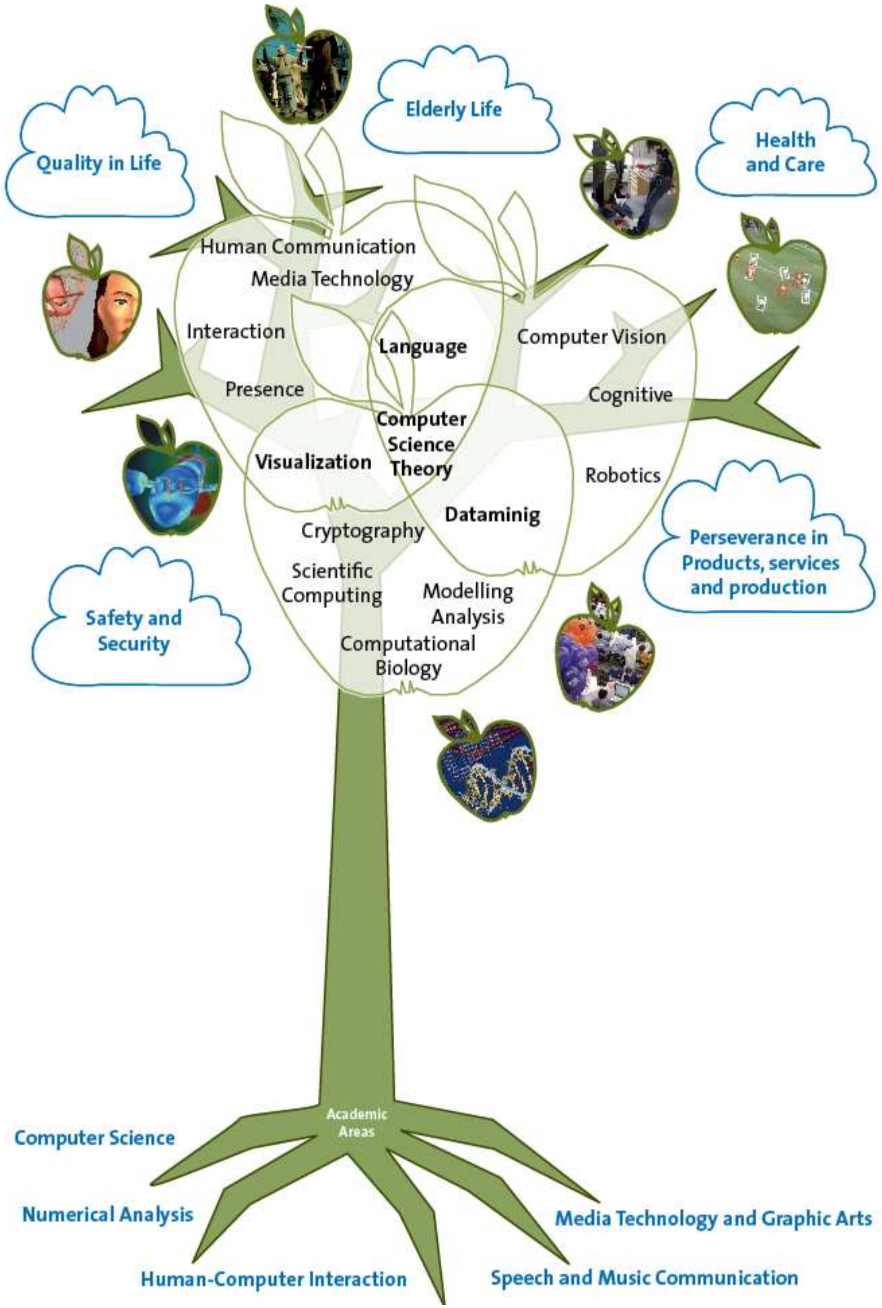
297 employees, including:

- 210 men
- 87 women
- 23 professors (3 of whom are women)
- 38 associate professors (9 of whom are women)
- 8 assistent professors (3 of whom are women)

Figures for 2010

Tree of Knowledge

Academic Areas;
The School of
Computer Science
and Communication



Research at Dept of Numerical Analysis

- Wave propogation: electromagnetism, gas dynamics, aeroacustics (Olof Runborg, Björn Engquist)
- Multiphase flows, particle and fiber flows (Anna-Karin Tornberg, Katarina Gustafsson)
- Fluid-structure interaction, biomechanics, biomedicin (Johan Hoffman, Johan Jansson)
- Turbulence, aerodynamics, geophysics (Johan Hoffman)
- Multiscale and multiphysics problems (Olof Runborg and others)
- Material science, chemistry (Schrödinger equation, molecular dynamics) (Anders Szeppessy)
- Computational systems biology (Michael Hanke)
- Optimal control, data assimilation (Anders Szepessy, Mattias Sandberg)
- Fast algorithms (all)

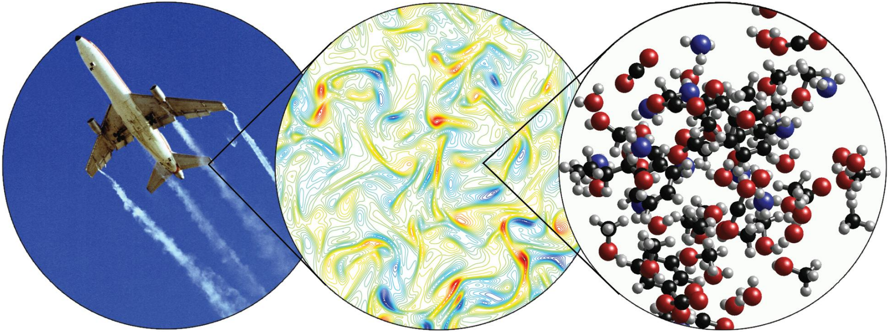
Research at Dept of Computational Biology

- Computational Neuroscience (memory, motor control, olfactory system, cell-cell signalling in insulin production)
- Neuroinformatics, Biological Physics/Systems Biology (mechanisms of gene regulation, non-coding RNA, complex networks)
- Bioinformatics (comparative genomics, modelling evolution, gene regulation, modelling cancer progression, mRNA editing)

Cooperation With KTH Centers

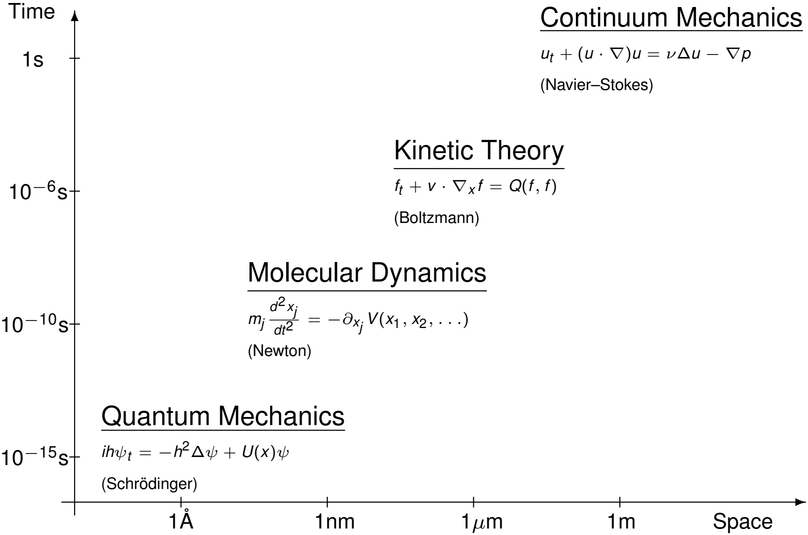
- SeRC: Swedish eScience Research Center
- KCSE: KTH Center for Computational Science and Engineering (Graduate School)
- Linné FLOW Center
- Simulation, Interactivity and Visualization Center at CSC
- PDC: National HPC Center
- Stockholm Brain Institute
- International Neuroinformatics Coordination Facility
- Stockholm Bioinformatics Centre
- KTH ACCESS Linnaeus Centre

Challenge of Multiscale Problems

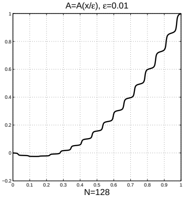
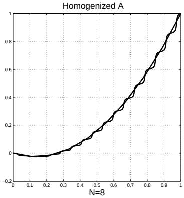


- Physical processes can be studied on widely different scales (in space and time).
- Different models derived for the different scales.
- Focus on problems where more than one scale/model is needed and where micro-scale model is too computationally costly.

Multiscale Problems – Fluid Mechanics



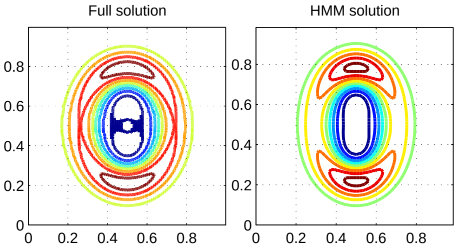
Multiscale Problems – Partial Differential Eqs.

Equation	*Solution*	*Computational cost*
$\nabla \cdot A(x/\varepsilon)\nabla u^\varepsilon = f,$		At least $\sim \mathcal{O}(\varepsilon^{-d})$ (Fine scales must be resolved.)
Homogenization $\Downarrow$ $\nabla \cdot \bar{A}\nabla \bar{u} = f.$ ($\bar{A}$ constant)		Independent of ε

Current work

- Wave propagation with HMM (Holst, Engquist)

$$u_{tt} = \nabla \cdot A^{\varepsilon}(\boldsymbol{x})\nabla u, \qquad \boldsymbol{x} \in \mathbb{R}^d,$$

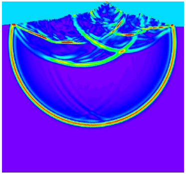


Algorithm development, analysis (error estimates), implementation

- Complex fluids (Arjmand, Di, Tornberg)
  + Mechanics within e-Science SRA

  Couple microscopic simulation of "stuff" in a fluid with macroscopic non-newtonian model

Wave Propagation Problems

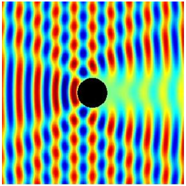


- Applications in e.g. optics, electromagnetics, geophysics, acoustics, quantum chemistry, ...
- Modeled by scalar wave equation

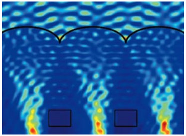
$$u_{tt} - c(\boldsymbol{x})^2 \Delta u = 0, \qquad (t, \boldsymbol{x}) \in \mathbb{R}^+ \times \mathbb{R}^d,$$

$$u(0, \boldsymbol{x}) = A(\boldsymbol{x}) e^{i\omega\phi(\boldsymbol{x})}, \qquad u_t(0, \boldsymbol{x}) = \omega B(\boldsymbol{x}) e^{i\omega\phi(\boldsymbol{x})},$$

where $c(\boldsymbol{x})$ (variable) speed of propagation and ω the angular frequency.



- Scattering problem
- Similar versions for elastic wave equation, Maxwell equations, Schrödinger equation, ...

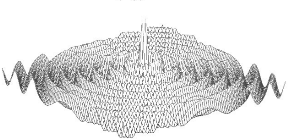


Computational challenges

- Simulation at high frequencies a major challenge.
  I.e., high relative to size of computational domain in time and space,

$$\omega \gg \frac{1}{T}, \quad \frac{\omega}{c} = k \gg \frac{1}{X}. \qquad \text{(When } 0 \le t \le T \text{ and } 0 \le x \le X\text{.)}$$

- High frequency $\rightarrow$
  short wave length $\rightarrow$
  highly oscillatory solutions $\rightarrow$
  many gridpoints.

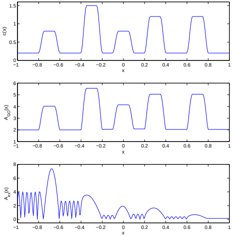


- Direct numerical solution resolves wavelength:
  #gridpoints $\sim \omega^d$ at least. Often unrealistic.
- Treatment of complicated geometry: boundaries and interfaces

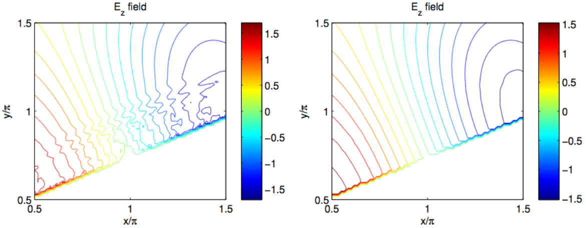
Current work

- Efficient direct numerical methods
  - Prescribed tolerance method for Helmholtz equation (Popovic)

    Algorithm development, analysis (cost and error estimate)

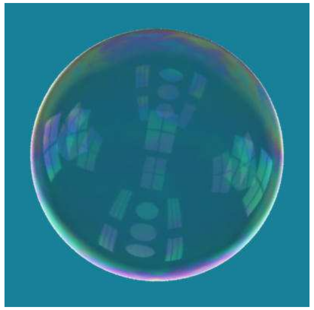


  - Improved boundary treatment in FDTD (Engquist, Häggblad)

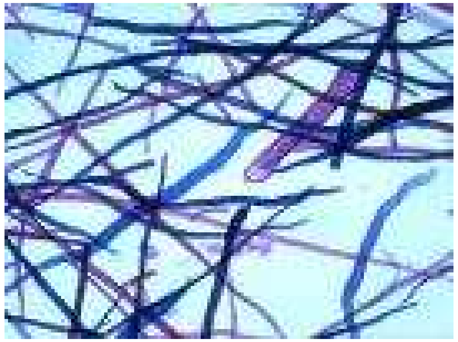


    Algorithm development, analysis (stability)

Multiphase and Particulate Flows

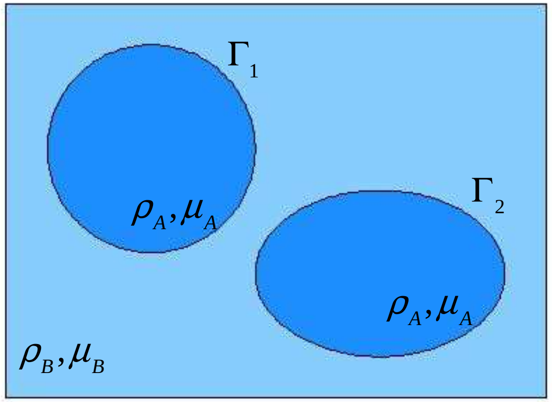


- Two-phase flow: Two immiscible fluids.
  Eg. Oil drops or air bubbles in water.
  Surface tension forces acting on interface between fluids.
- Particulate flow: Fluid with immersed solid or elastic particles.
- Suspension: Fluid with many immersed particles. Exhibits non-Newtonian behavior even though solvent is Newtonian.

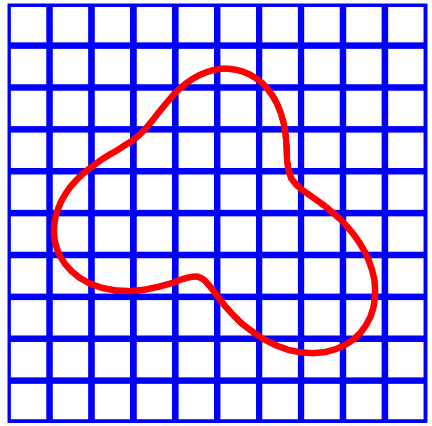


Interface tracking techniques

Immiscible multiphase flow



$$\Gamma = \bigcup_{j=1}^{M} \Gamma_j$$



Sketch in 2D:
Interface Γ cuts arbitrarily through background grid.

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \nabla\cdot(\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)) + \sigma\kappa\mathbf{n}\delta_\Gamma,$$

$$\nabla\cdot\mathbf{u} = 0 \qquad \text{(Velocity } \mathbf{u}(\mathbf{x}),\ \text{pressure } p(\mathbf{x}))$$

- Navier-Stokes equations discretized on grid not conforming to the interfaces.
- Density, viscosity and surface tension forces determined from the interface (surface or curve) representation.
- Discontinuous density, viscosity and singular surface tension forces often regularized.

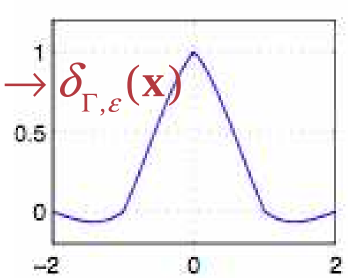
Interface tracking related research

Analysis of regularization of discontinuous and singular functions.

Quadrature errors and errors in solution of PDE.

Latest: work w Sara.

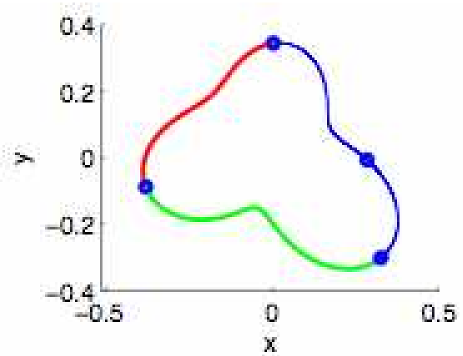
$\delta_{\Gamma}(\mathbf{x}) \rightarrow \delta_{\Gamma,\varepsilon}(\mathbf{x})$



Development of interface tracking technique,
Segment Projection Method, in new and improved framework.

With Dag.

Decomposing curve into segments



Curve segment is single valued function in local coordinate system

Boundary integral methods

- Applicable for linear PDEs, e.g. Stokes flow, elasticity.
- Stokes equations -> BIEs (with Stokeslet and Stresslet). Reduced dimension!
- Discretize integrals: surface representation + specially designed quadrature.

Reduced dimension:

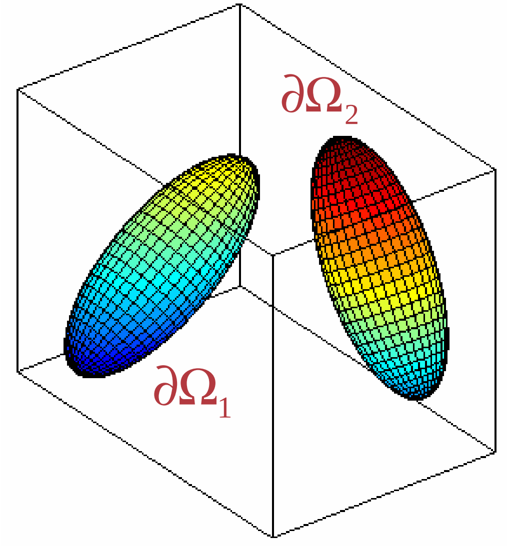
N discretization points.

Computational cost: $O(N^2)$.

- Yields dense system. All discretization points "interact" with each other.
- "Fast summation method" needed for truly efficient simulations.

Boundary integral equation (BIE) on "boundaries of domain":

Interfaces and outer boundaries.

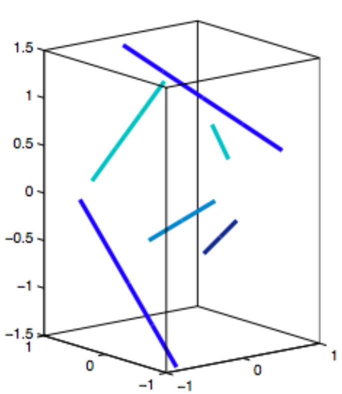


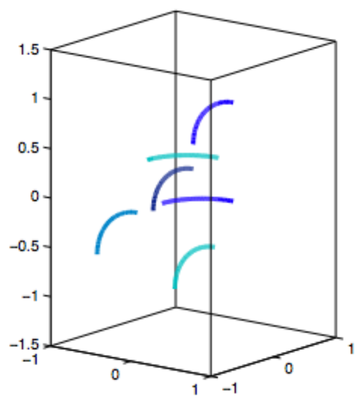
Stokeslet ($i, j = 1,2,3$) :

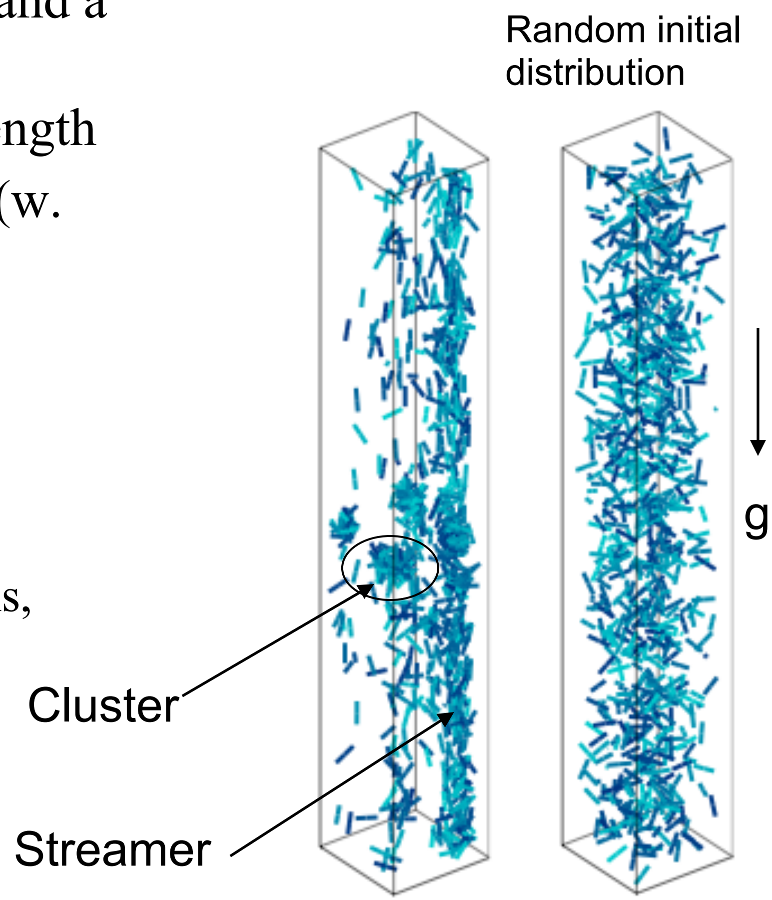
$$S_{ij}(\mathbf{x},\mathbf{y}) = \frac{\delta_{ij}}{|\mathbf{x}-\mathbf{y}|} + \frac{(x_i - y_i)(x_j - y_j)}{|\mathbf{x}-\mathbf{y}|^3}$$

Large scale simulations of slowly sedimenting slender fiber suspensions in Stokes flow

- Based on a boundary integral formulation and a *slender body approximation*
- Today all fibers are straight and of same length
- Extend model and numerical algorithm to (w. Jennifer Grünig, PhD stud.):
  - Multi-disperse fiber suspensions
  - Non-straight rigid fiber suspension
- Motivation
  - Fibers in paper pulp
  - Other kind of suspensions: micro organisms, bacteria







Simulations show good agreement to experimental data both on local and global levels

KTH Computational Technology Lab

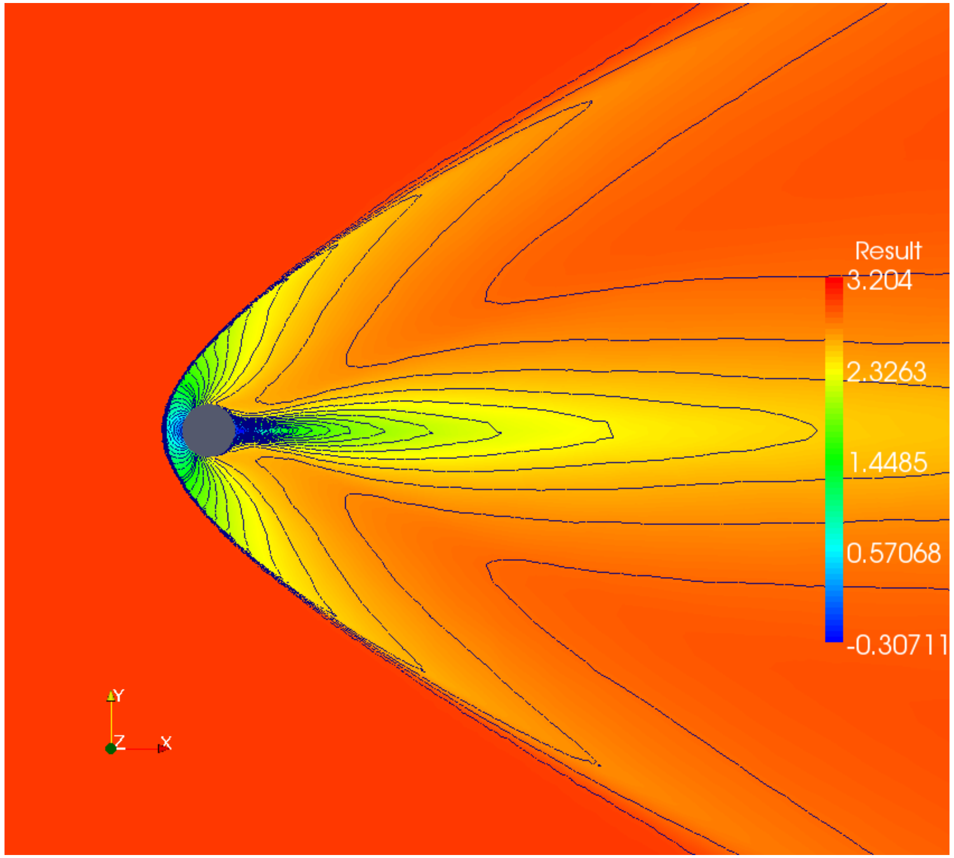
- Research group at KTH-CSC/NA
- www.csc.kth.se/ctl
- www.fenics.org

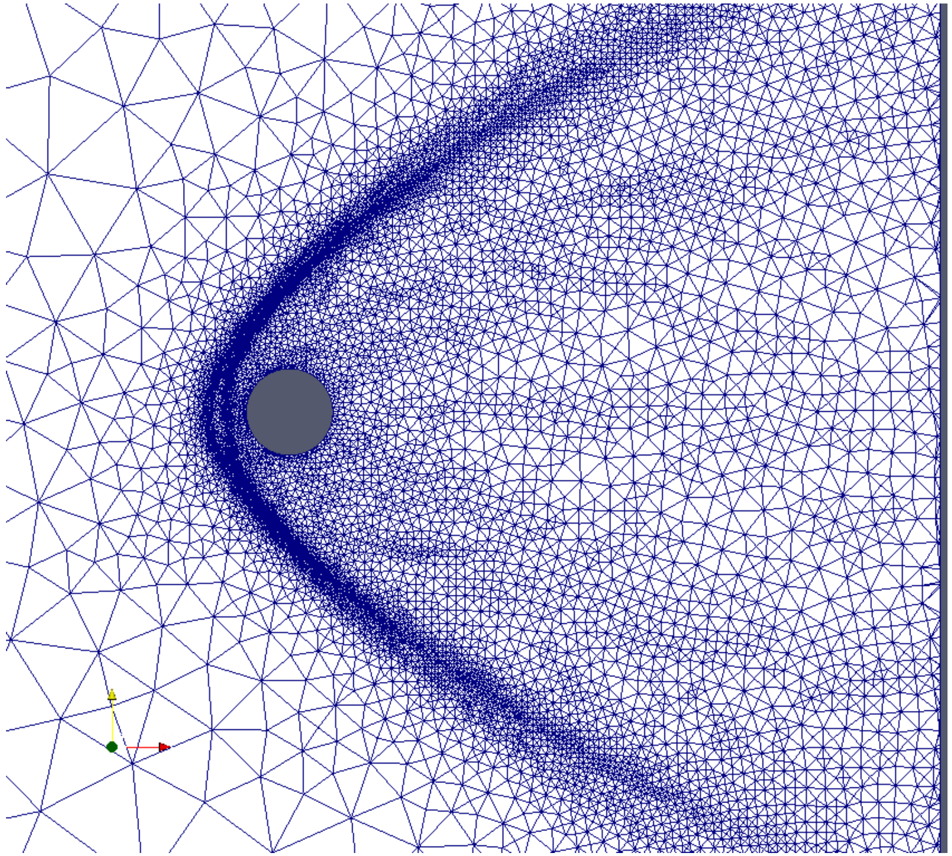
- Adaptive finite element methods
- High performance computing
- Incompressible/compressible CFD
- Fluid-structure interaction
- Aero-acoustics

Johan Jansson, Murtazo Nazarov, Niclas Jansson, Rodrigo Vilela, Jeannette Spühler, Cem Degirmenci, Ashraful Kadir, Peter Roman, Kenny Hedlund and Florian Rathgeber

Adaptive mesh: efficiency, reliability

- Ad hoc mesh refinement: local gradients etc.
- How is output of interest affected by local errors?





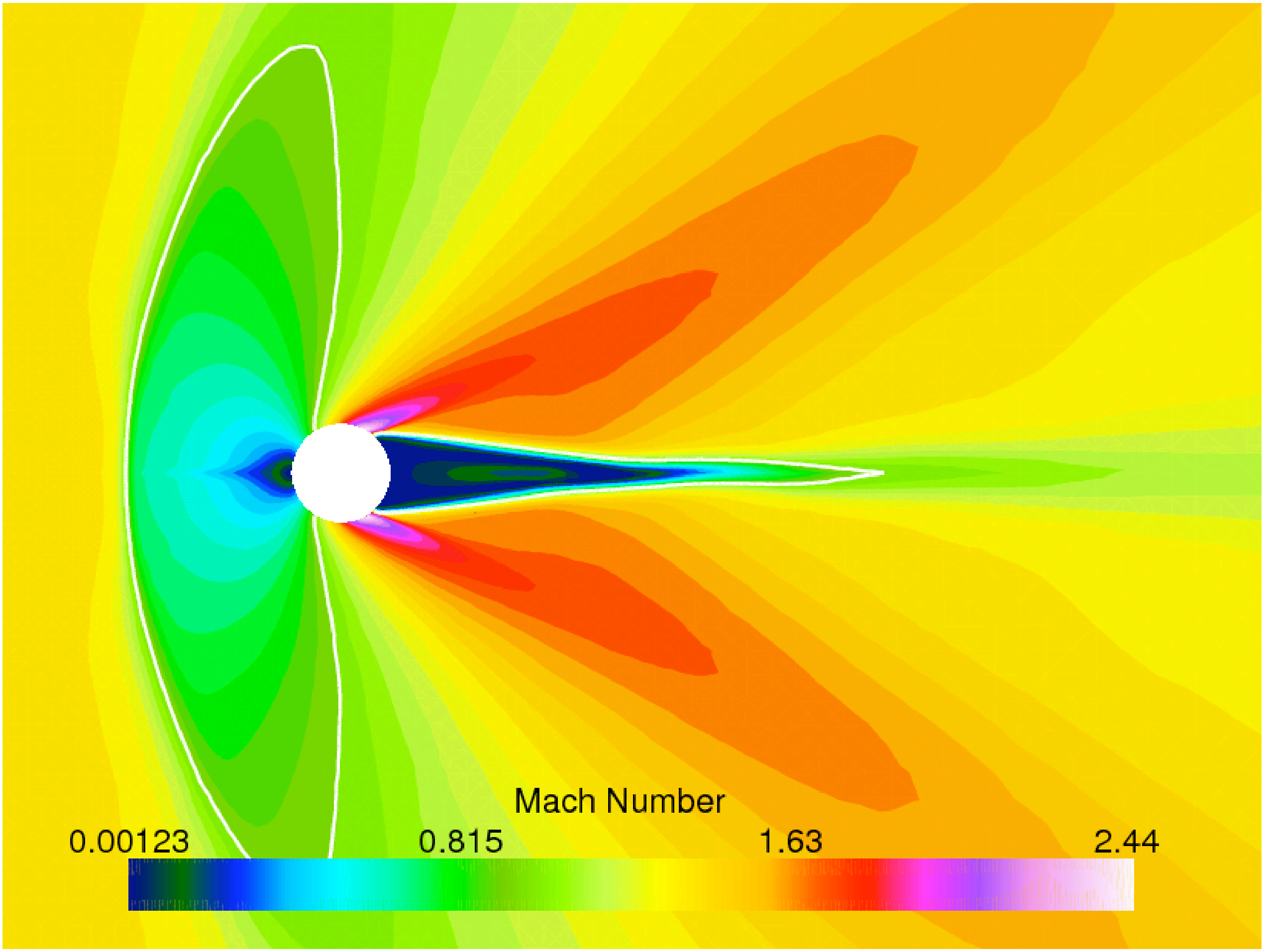
A posteriori error estimation

- General theory for PDE (FEM), the 1990s: Johnson (Chalmers), Rannacher (Heidelberg), Süli (Oxford), Barth (Nasa Ames), etc.
- Error control and mesh refinement from approximation U
- Quantity of interest M(u) of the solution u (forces, mean, etc.)
- How do local (residual) errors R(U) influence |M(u) - M(U)|?

- Error estimate: $|M(u) - M(U)| \leq \sum_K R_K(U)\, S_K$ (cells K)

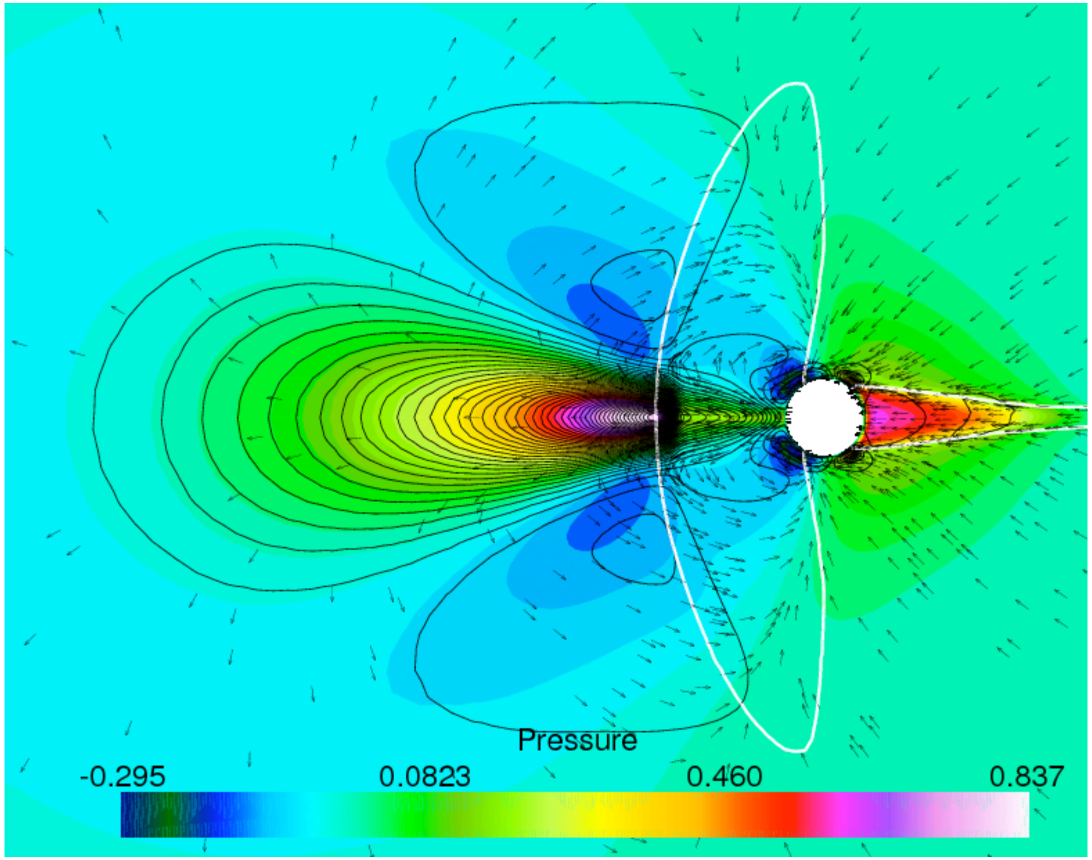
- S_K stability weight for cell K, computed from adjoint problem
- Optimal control problem: Find optimal mesh with minimal number of cells such that: $|M(u) - M(U)| < TOL$

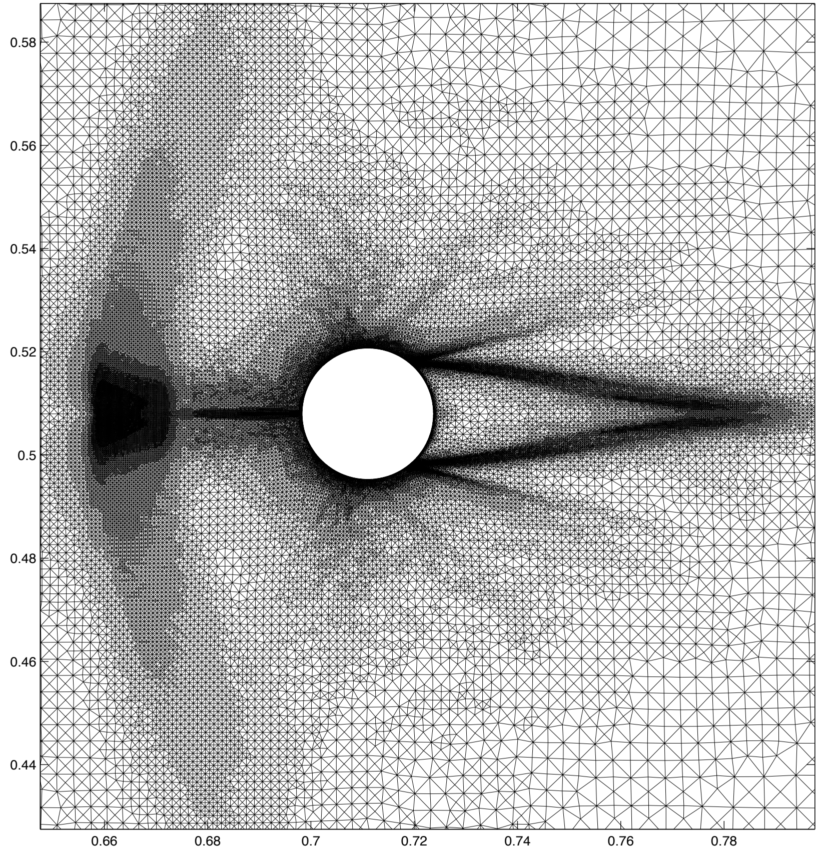
2D cylinder: Mach = 1.4



[M.Nazarov/J.Hoffman IJNMF 2010]

Dual solution and mesh (drag force)





[M.Nazarov/J.Hoffman IJNMF 2010]

Adaptive Turbulence Computation

- General Galerkin (G2) FE method: stabilized FEM/Implicit LES

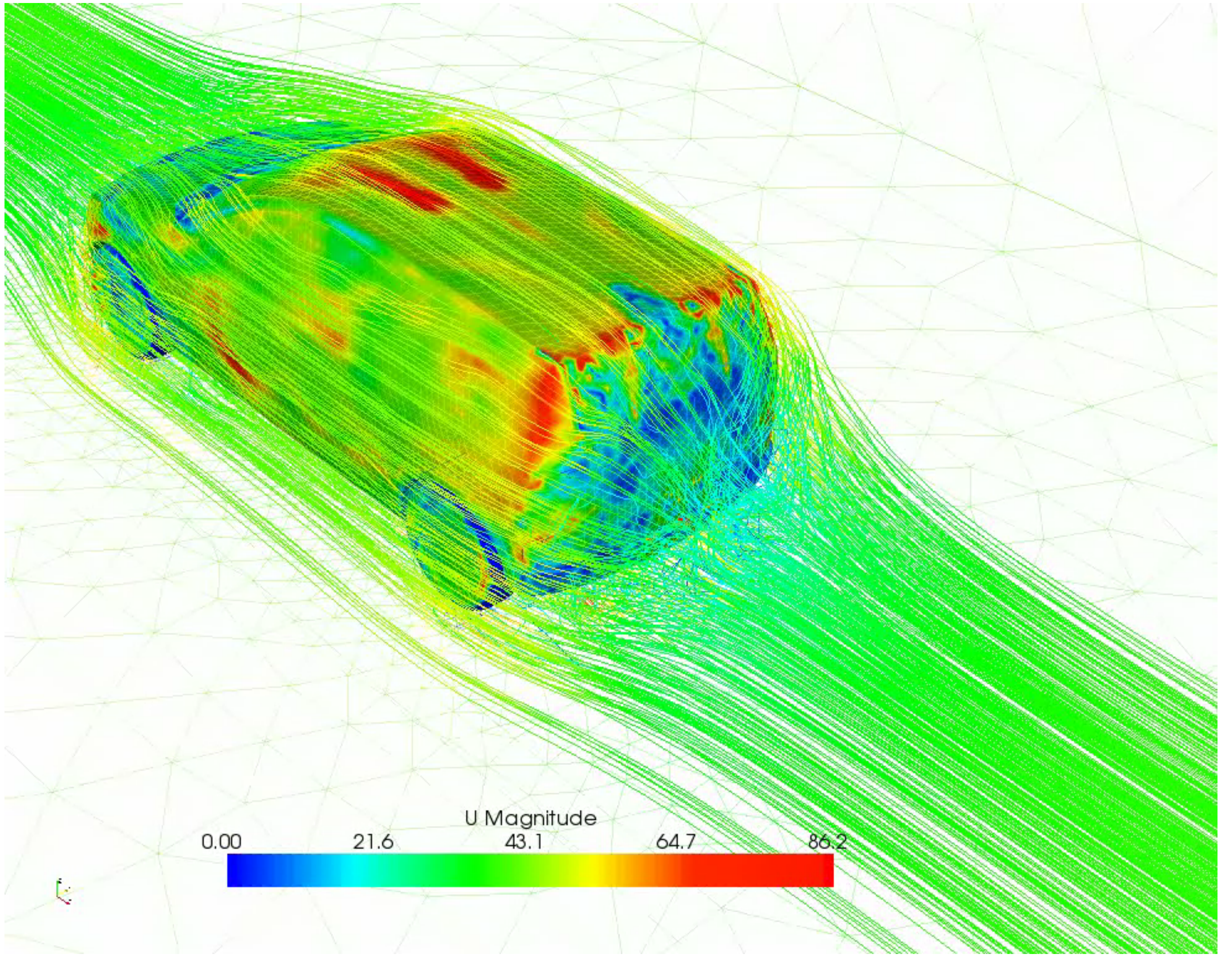
For all test functions (v,q) in W_h : find (U,P) in V_h :

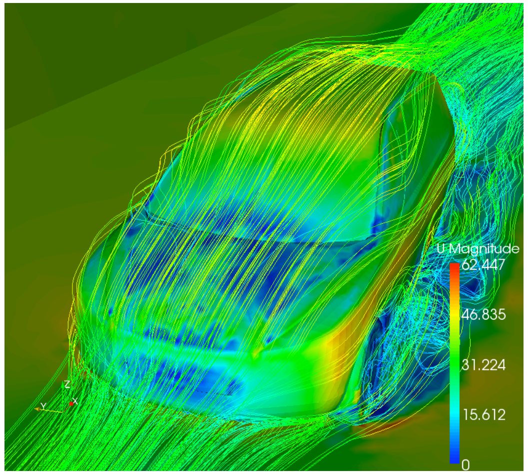
$$(U_t + U\cdot\nabla U, v) + (\delta(U\cdot\nabla U + \nabla P), U\cdot\nabla v + \nabla q)$$
$$+ (\nu\nabla U, \nabla v) - (P, \nabla\cdot v) + (q, \nabla\cdot U) = (f, v)$$

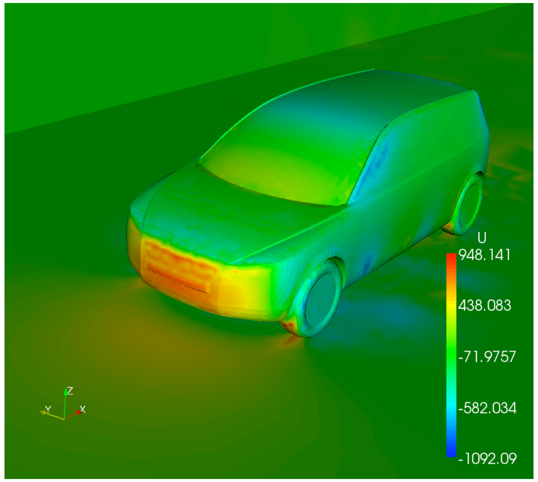
- Least squares stabilization of residual: $U\cdot\nabla U+\nabla P$, with $\delta \sim h$
- No explicit (physics based) subgrid model of unresolved scales
- Energy dissipation: $- dK/dt = ||\nu^{1/2}\nabla U||^2 + ||\delta^{1/2}(U\cdot\nabla U+\nabla P)||^2$
- For $\nu << h$: $- dK/dt \approx ||\delta^{1/2} (U\cdot\nabla U+\nabla P)||^2$

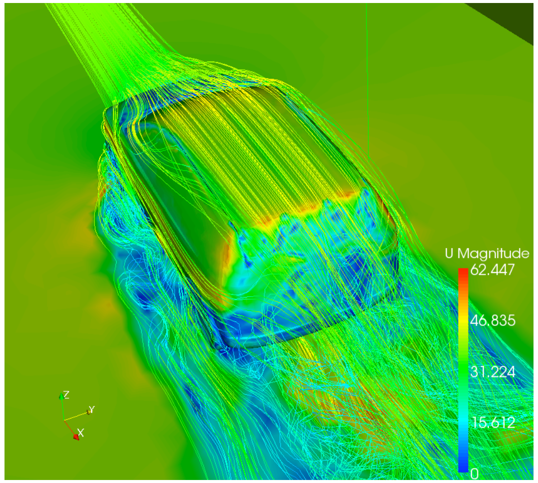
[J.Hoffman, SISC 05, JFM 06, IJNMF 08, J.Hoffman/C.Johnson, CMAME 06, Springer 07]

Turbulent boundary layer model: skin friction boundary conditions (geometry by Volvo Cars)



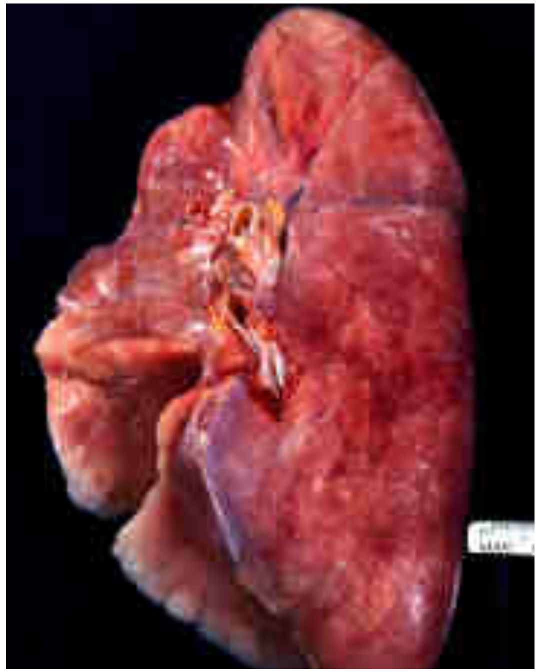






Fluid-structure interaction

- Robustness in coupling
- Specific discretizations
- Specific software
- Deforming meshes?
- Error analysis?



Unified Continuum Formulation

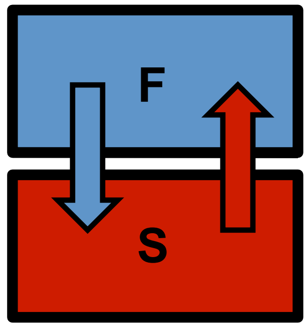
Conservation laws (in Euler coordinates):

$$\partial \rho/\partial t + \nabla\cdot(u\rho) = 0 \qquad \text{(Mass conservation)}$$

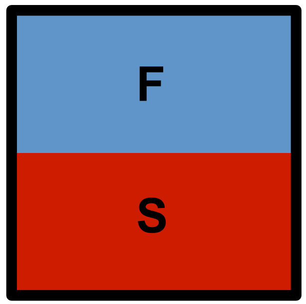
$$\partial m/\partial t + \nabla\cdot(um) = \nabla\cdot\sigma \qquad \text{(Newton 2}^{\text{nd}}\text{ law)}$$

$$\partial e/\partial t + \nabla\cdot(ue) = \nabla\cdot(\sigma u) \qquad \text{(Energy equation)}$$

$$\partial \phi/\partial t + (u\cdot\nabla)\phi = 0 \qquad \text{(Phase field)}$$



DD = F + S



UC = FS

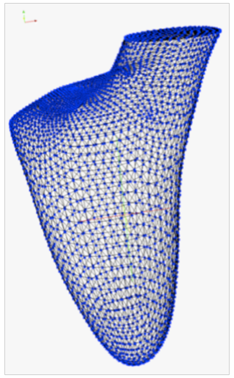
- Velocity u, density ρ, momentum $m=u\rho$, energy e
- Phase field ϕ (liquid/gas/solid)
- Constitutive law for the stress σ (for each phase)
- Treat FSI as a multiphase flow problem

[Hoffman/Jansson/Stöckli]

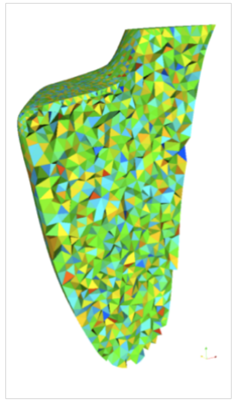
Human heart model

Ulf Gustavsson, Per Vesterlund, Matthias Aechtner, Jeannette Hiromi Spühler

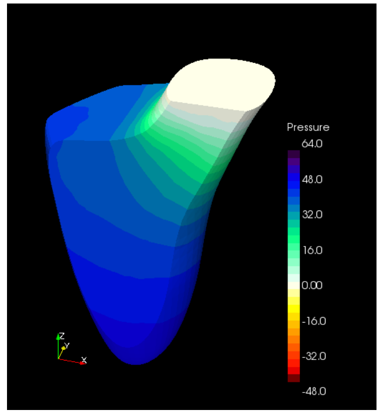
LiU/UmU

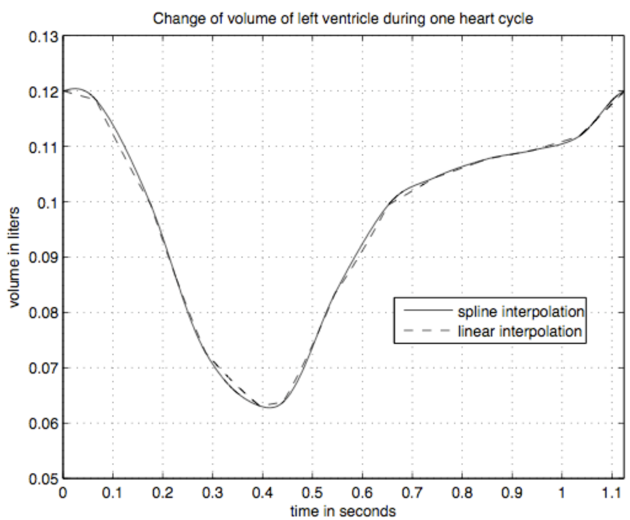


UmU



KTH





1. Image segmentation (ultra sound or MRI)
2. Mesh generation
3. Unicorn simulation

HPC Adaptive CFD implementation

- Unicorn solver: FEniCS open source project (www.fenics.org)

Hebb at PDC/KTH

- 1024 node Blue Gene/L system
- 2048 processors (virtual mode)
- 1 GB or 512 MB node memory

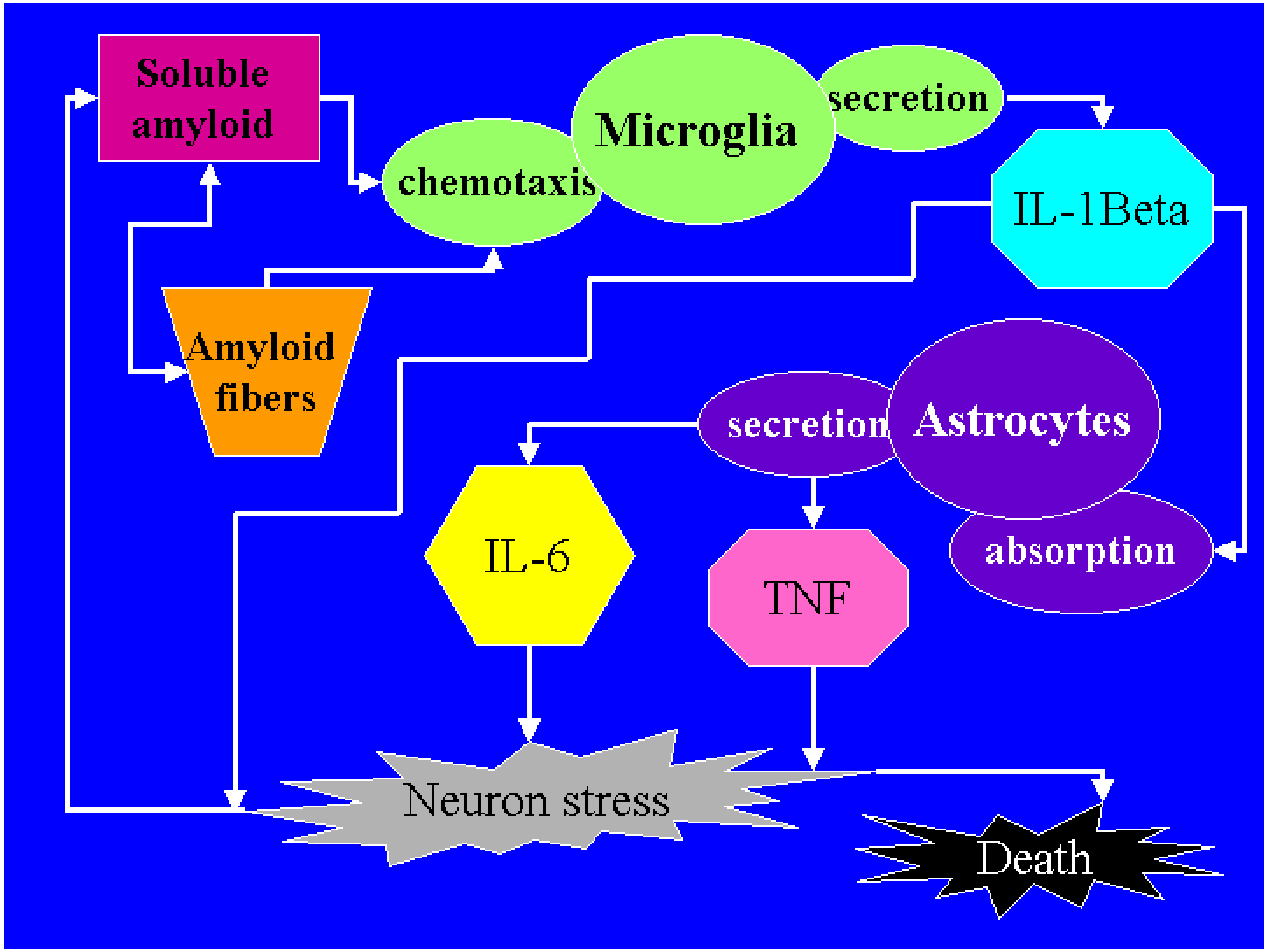
Neolith at NSC/LiU

- 805 node Linux cluster
- Dual quad core nodes, 6440 cores
- 16 GB or 32 GB node memory

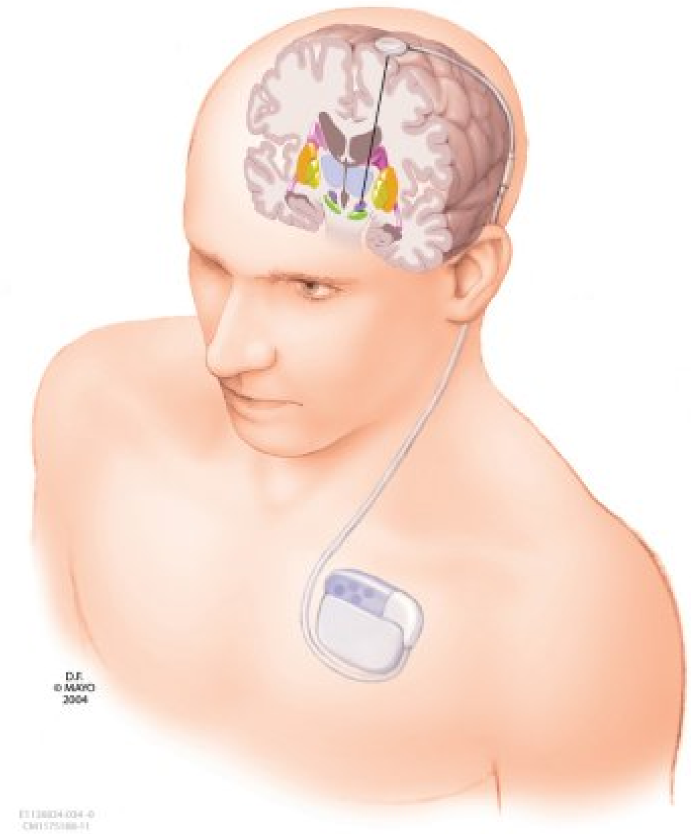
[N.Jansson/J.Jansson/Hoffman SIAM PP10 2010]

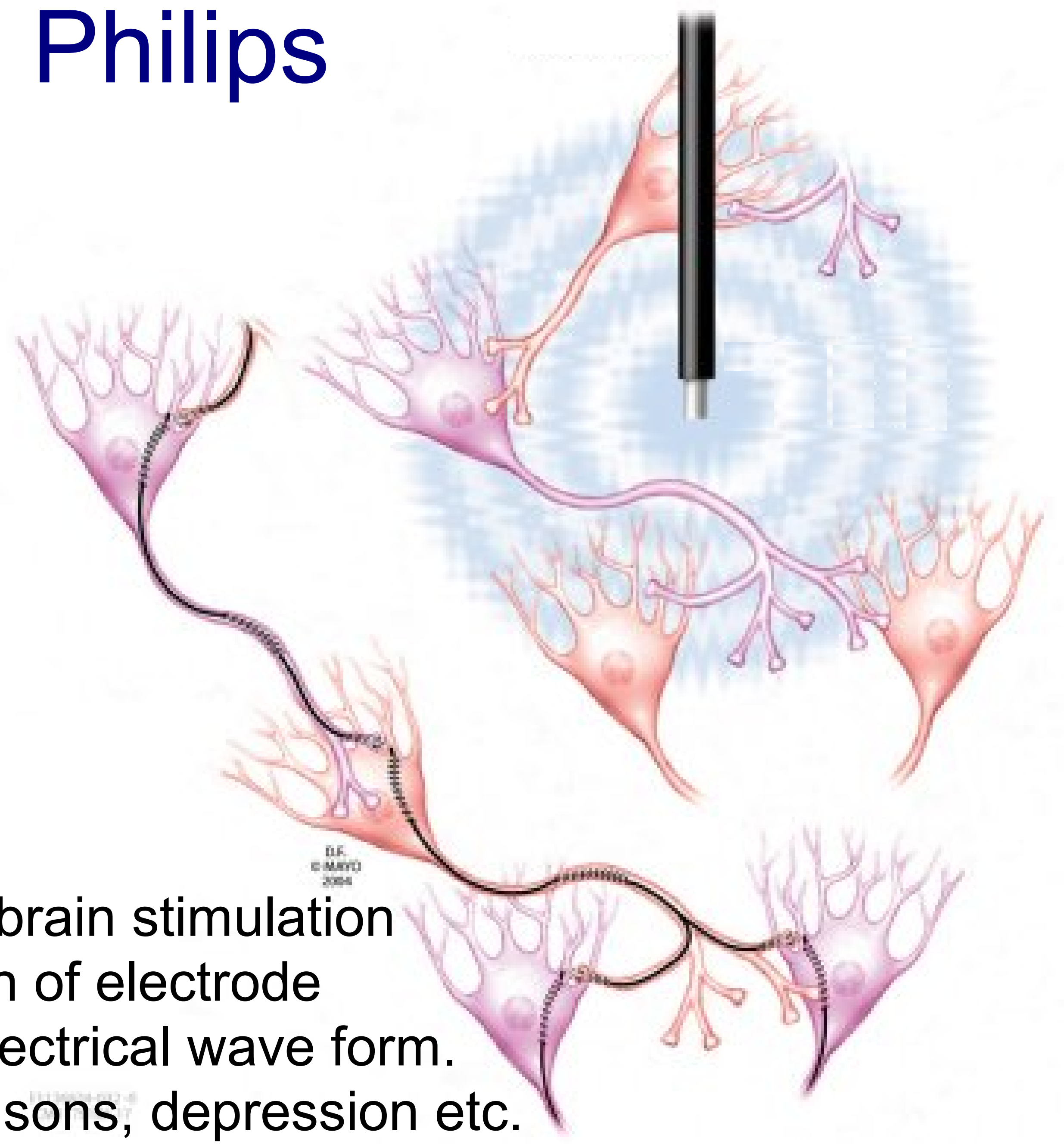
In Silico Biosciences

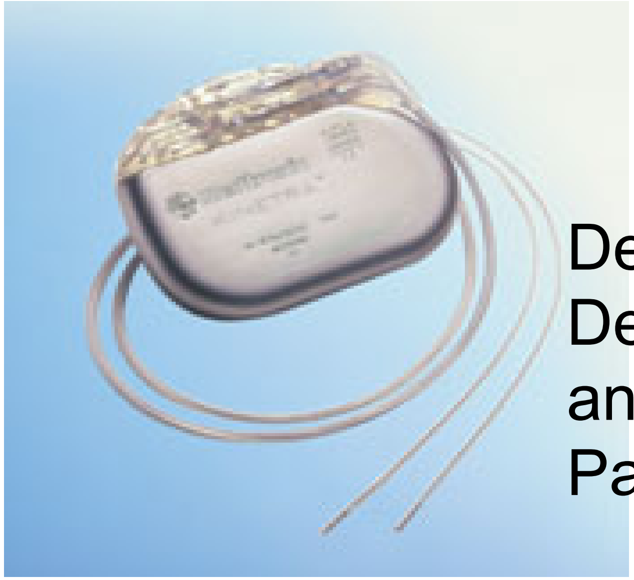
Simulation of the effect of new drugs
Alzheimer's disease



Philips





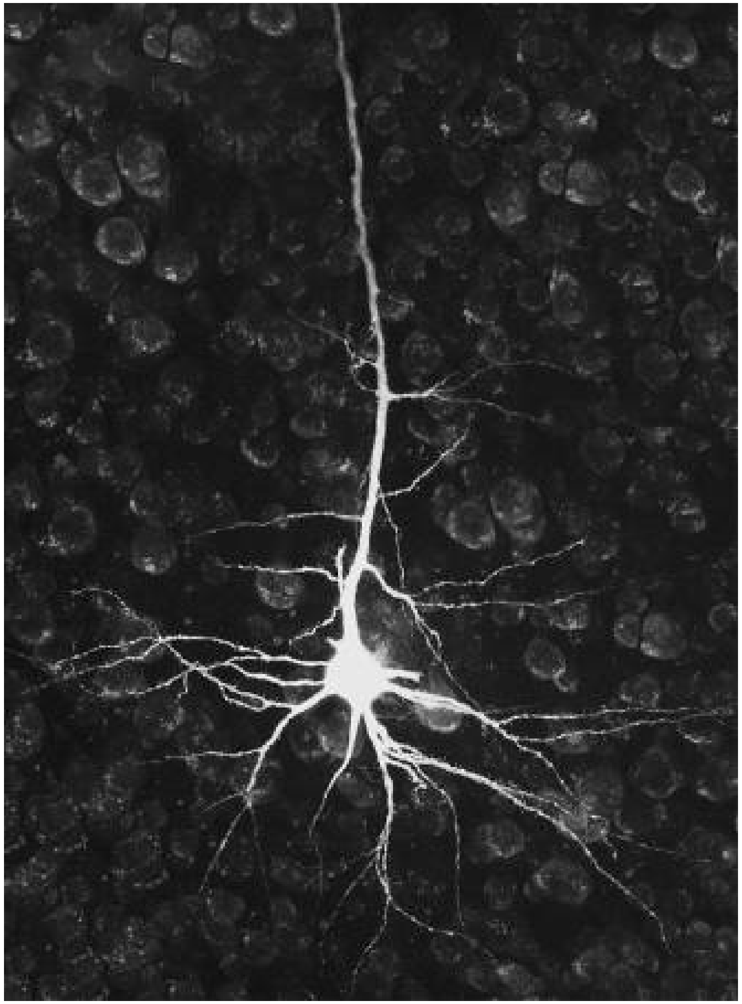


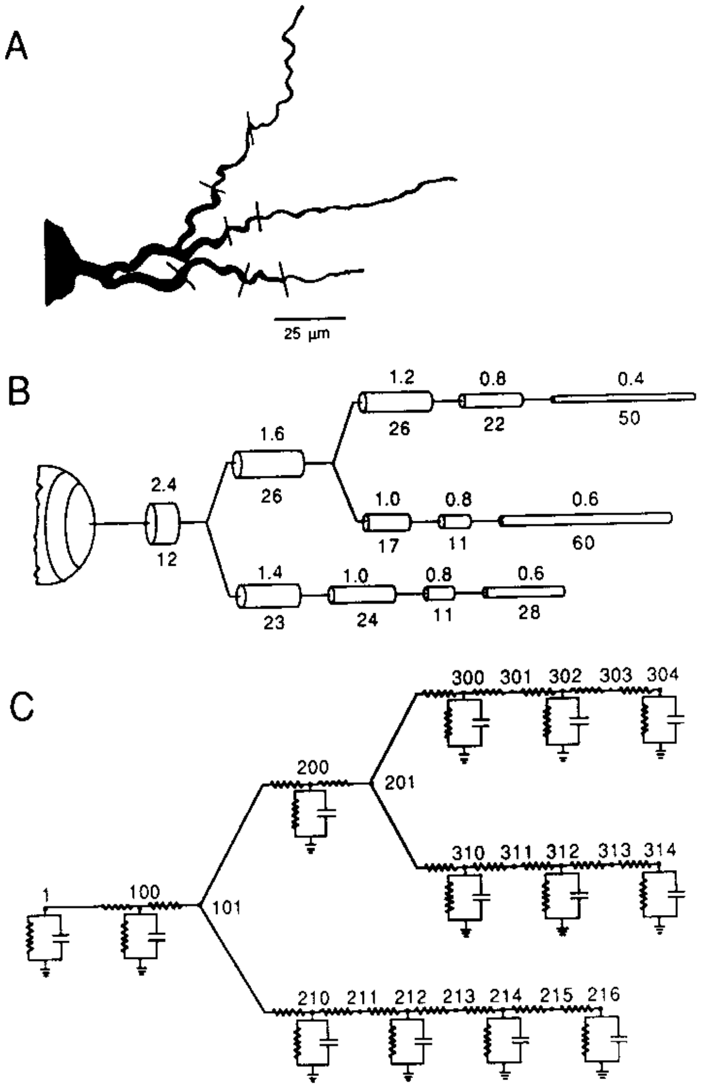
Deep brain stimulation
Design of electrode
and electrical wave form.
Parkinsons, depression etc.

The technique

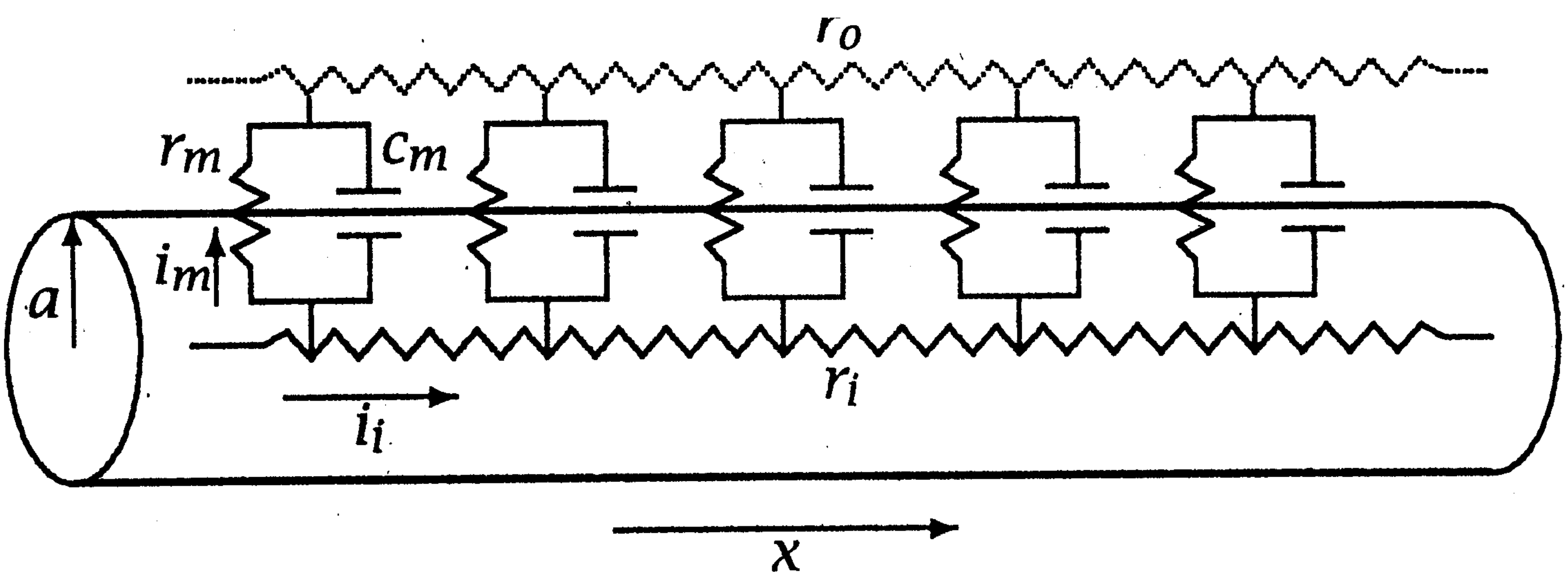
- Simulate
  - biochemical reactions
  - ion fluxes over membranes
  - diffusion inside or outside a cell
  - electrical signalling between neurons
  - activity in networks of neurons
  - activity in systems

Model for a whole neuron





Equivalent circuit of membrane



Assumes extracellular fluid has infinite conductivity, r_o=0

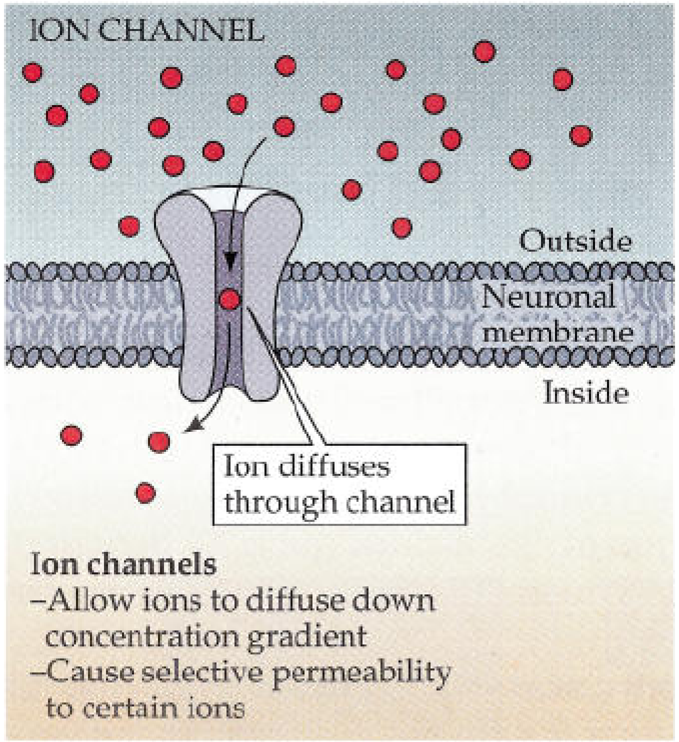
isotropic, r_m, r_i, c_m constant

i_i only axial

Solve dV/dt

Ion channels

- A pore in the cell membrane through which ions can flow
- Voltage dependent activation and inactivation



m: $C \underset{k_2}{\overset{k_1}{\rightleftarrows}} O$

$k_N = f(V)$

h: $I \underset{k_4}{\overset{k_3}{\rightleftarrows}} O$

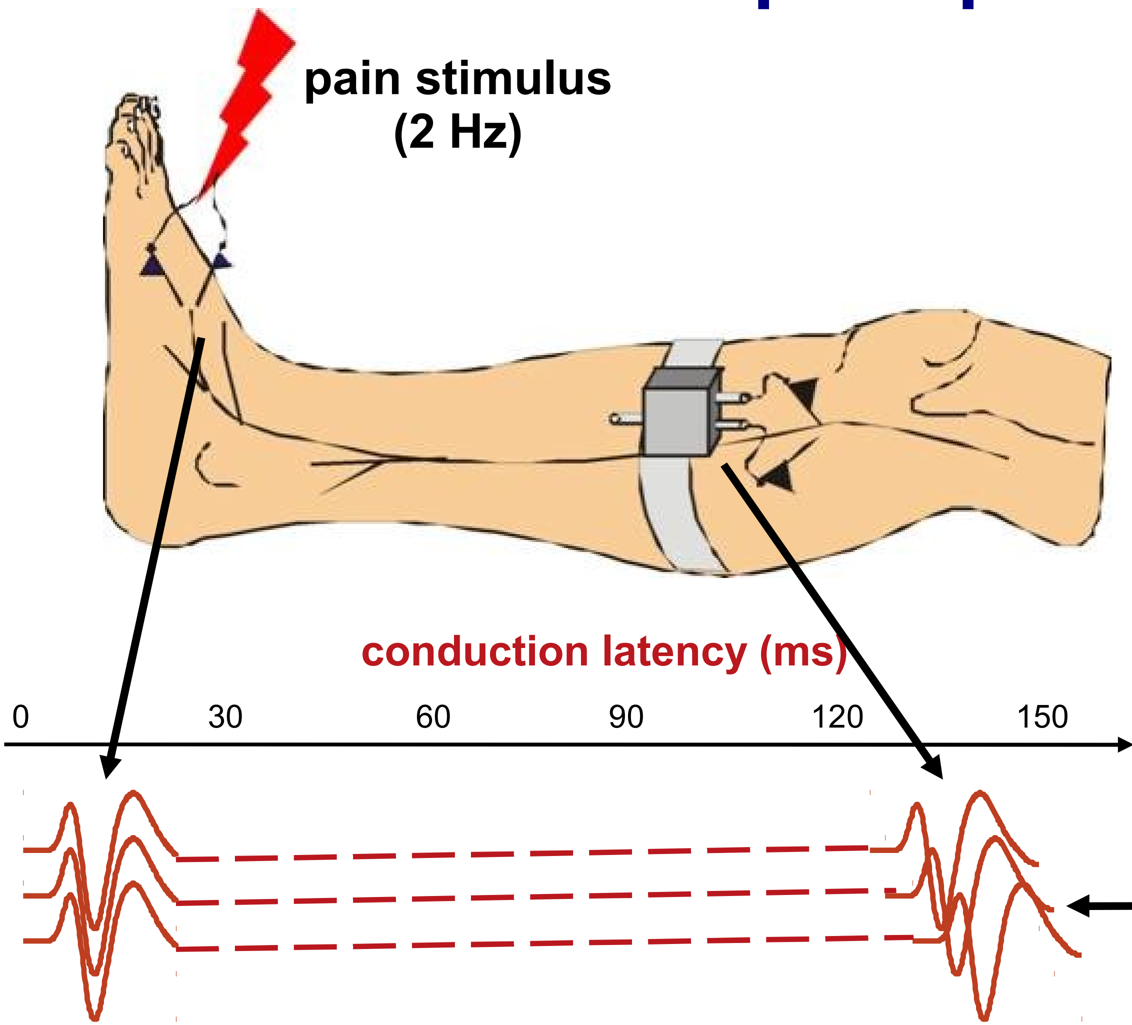
solve dm/dt and dh/dt

Biophysical simulation

- Discretize the neuron into 1-500 compartments
- Ion channel result in 1 or 2 ODEs / c
- Iso potential compartment results in 1 ODE / c
- In total a number of coupeled ODEs
- Initial value problem
- Compare simulation output to experimental data
- „Record“: 22 mill neurons, 11 bill synapses

ROYAL INSTITUTE OF TECHNOLOGY

Example from our research
Pain in peripheral nerves



micro-scale (ion channels)

MODEL!

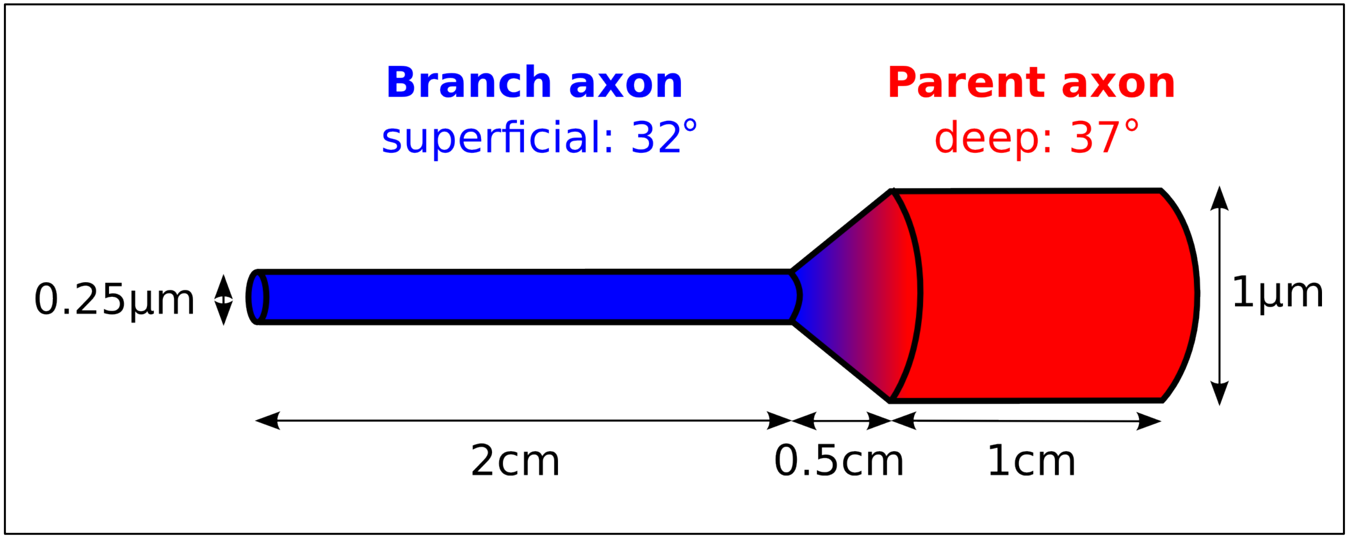
function (nerve impulse)

Activity-dependent slowing

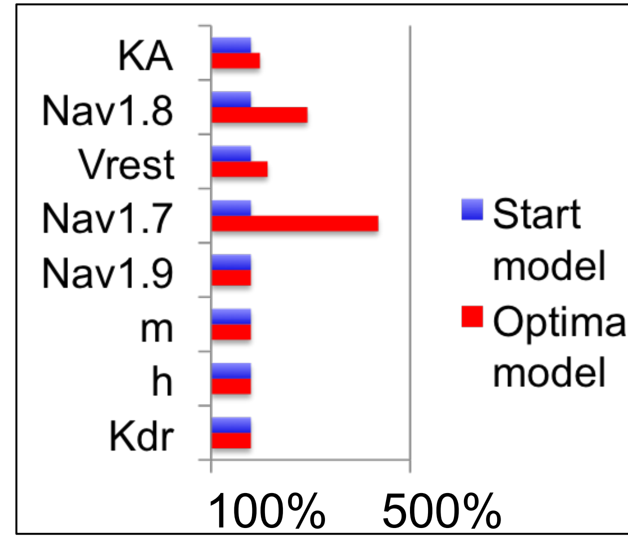
But why?

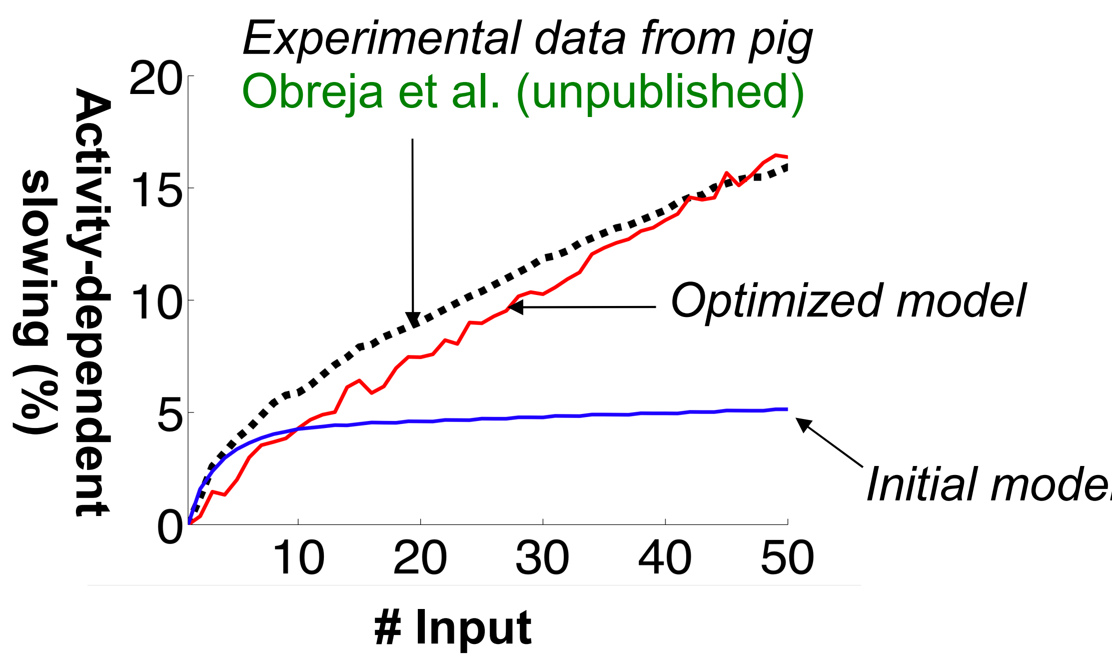
Model

Geometry and temperature

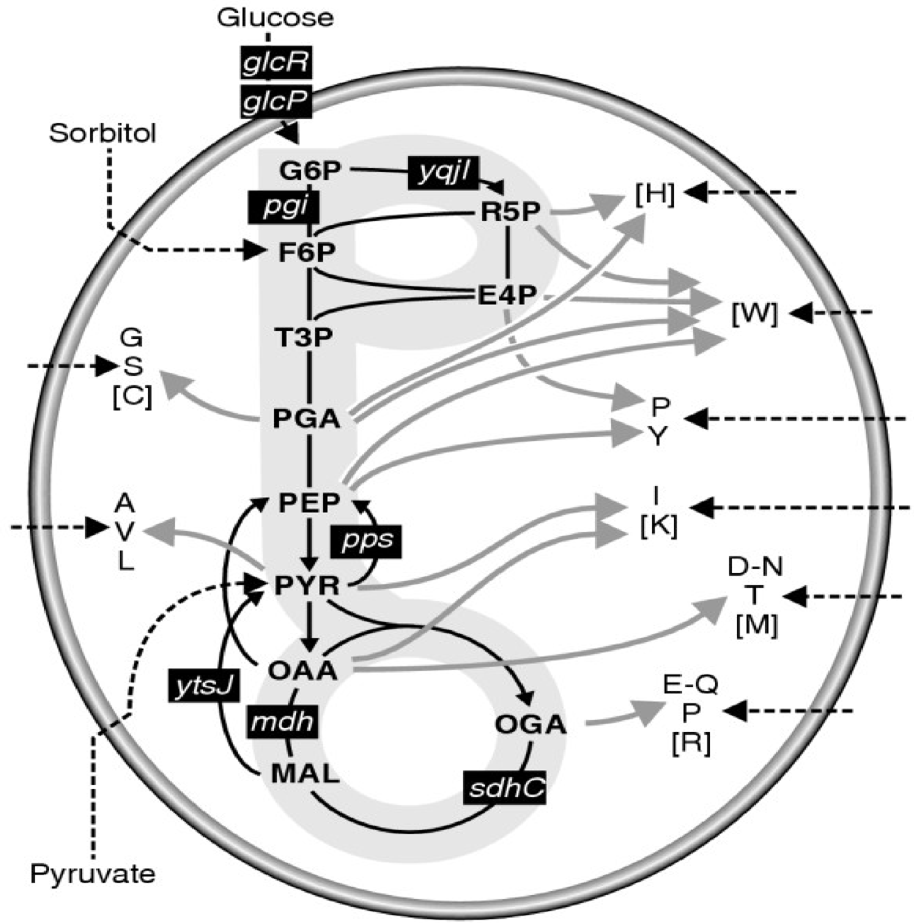


Parameter optimization





Intracellular signalling pathways sugar and fat metabolism, diabetes



Interaction between neural control and body mechanics