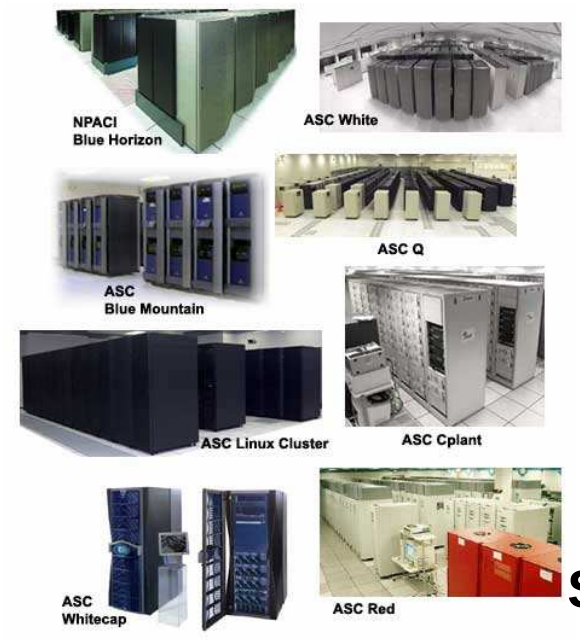
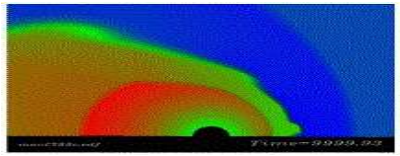
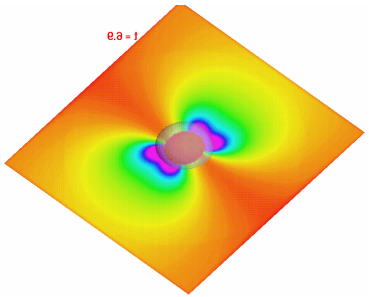
Computational Diagnostics & Biocybernetics Unit



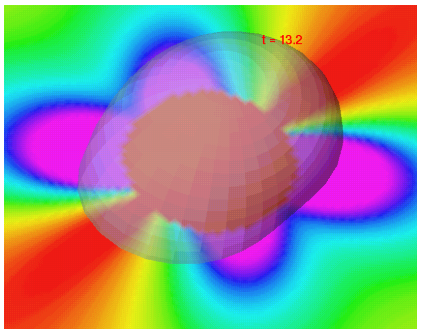


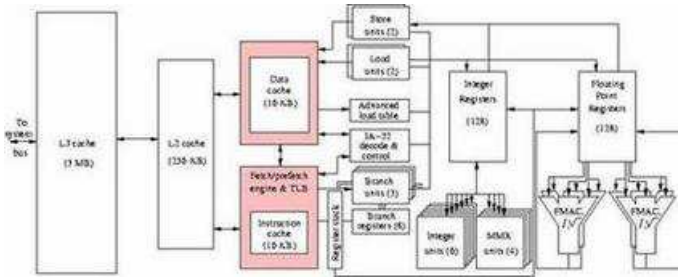


Neuro Signal Analysis and Modeling (BMT922)

Carlos Trenado

Saarland University of Applied Sciences





Review

-Derivative

The derivative of a function f at $x = a$ is $$f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}.$$

-Partial derivative

Definition. Suppose f is a function of x and y. Then we define

$$f_x(a,b) = \lim_{h \to 0} \frac{f(a+h,b) - f(a,b)}{h} \quad \text{and} \quad f_y(a,b) = \lim_{h \to 0} \frac{f(a,b+h) - f(a,b)}{h}.$$

$$\frac{\partial f}{\partial x} = f_x(x,y) \text{ and } \frac{\partial f}{\partial y} = f_y(x,y).$$

Review

Example. Suppose $f(x,y) = x^2 + xy + y^2$. Then

$$\begin{aligned} f_y(a,b) &= \lim_{h\to 0} \frac{f(a,b+h) - f(a,b)}{h} \\ &= \lim_{h\to 0} \frac{a^2 + a(b+h) + (b+h)^2 - (a^2 + ab + b^2)}{h} \\ &= \lim_{h\to 0} \frac{a^2 + ab + ah + b^2 + 2bh + h^2 - a^2 - ab - b^2}{h} \\ &= \lim_{h\to 0} \frac{ah + 2bh + h^2}{h} = \lim_{h\to 0} \frac{(a+2b+h)h}{h} = a + 2b. \end{aligned}$$

$$\frac{d}{dy}(x^2 + xy + y^2) = x + 2y,$$

Example. Suppose $z = x^3 + 4x^2y^2 + y^5$. Find: $\frac{\partial z}{\partial x}$ $\frac{\partial z}{\partial y}$ $\frac{\partial^2 z}{\partial x^2}$ $\frac{\partial^2 z}{\partial y \partial x}$

Review

Chain Rule

If $z = g(y)$ and $y = f(x)$ and then the chain rule is a formula for the derivative of z with respect to x. If we let $z = h(x) = g(f(x))$, the chain rule formula is

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx} \text{ or } h'(x) = g'(y)f'(x) \text{ where } y = f(x).$$

For example, if $T = T(x, y)$ is viewed as the temperature at (x, y) and $\vec{r}(t) = (x(t), y(t)$ is a path

then the temperature $T(x(t), (y(t))$ depends on t as the curve is traversed.

If x(t)=exp(-t+2) and y(t)=sin(t)

Then the rate of change of $T = (x(t), y(t))$ is **?**

Review

$$(x, y) = F(u, v, w)$$

e.g. x=F1(u,v,w) and y=F2(u,v,w)

T (x , y)=(T o F) (u ,v, w)=T (F (u ,v, w))

[(x,y)=F(u,v,w)=(F1(u,v,w),F2(u,v,w))]

Then,

$$\frac{\partial T}{\partial u} = \frac{\partial T}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial u} = (\frac{\partial T}{\partial x}, \frac{\partial T}{\partial y}) \cdot (\frac{\partial x}{\partial u}, \frac{\partial y}{\partial u})$$
$$\frac{\partial T}{\partial v} = \frac{\partial T}{\partial x}\frac{\partial x}{\partial v} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial v} = (\frac{\partial T}{\partial x}, \frac{\partial T}{\partial y}) \cdot (\frac{\partial x}{\partial v}, \frac{\partial y}{\partial v}$$
$$\frac{\partial T}{\partial w} = \frac{\partial T}{\partial x}\frac{\partial x}{\partial w} + \frac{\partial T}{\partial y}\frac{\partial y}{\partial w} = (\frac{\partial T}{\partial x}, \frac{\partial T}{\partial y}) \cdot (\frac{\partial x}{\partial w}, \frac{\partial y}{\partial w}).$$

or $$\begin{bmatrix} \frac{\partial T}{\partial u} & \frac{\partial T}{\partial v} & \frac{\partial T}{\partial w} \end{bmatrix} = \begin{bmatrix} \frac{\partial T}{\partial x} & \frac{\partial T}{\partial y} \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} & \frac{\partial x}{\partial w} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} & \frac{\partial y}{\partial w} \end{bmatrix}.$$

$$DF = F' = \begin{bmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} & \frac{\partial x}{\partial w} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} & \frac{\partial y}{\partial w}. \end{bmatrix}$$

[the Jacobian Matrix]

Setting $p = (u, v, w)$, this can be written in the form

$$D(T \circ F)(p) = DT(F(p))DF(p) \text{ or } (T \circ F)'(p) = T'(F(p))F'(p)$$

Review

Definition

A vector field is a mapping $F : X \subset \mathbb{R}^n \to \mathbb{R}^n$.

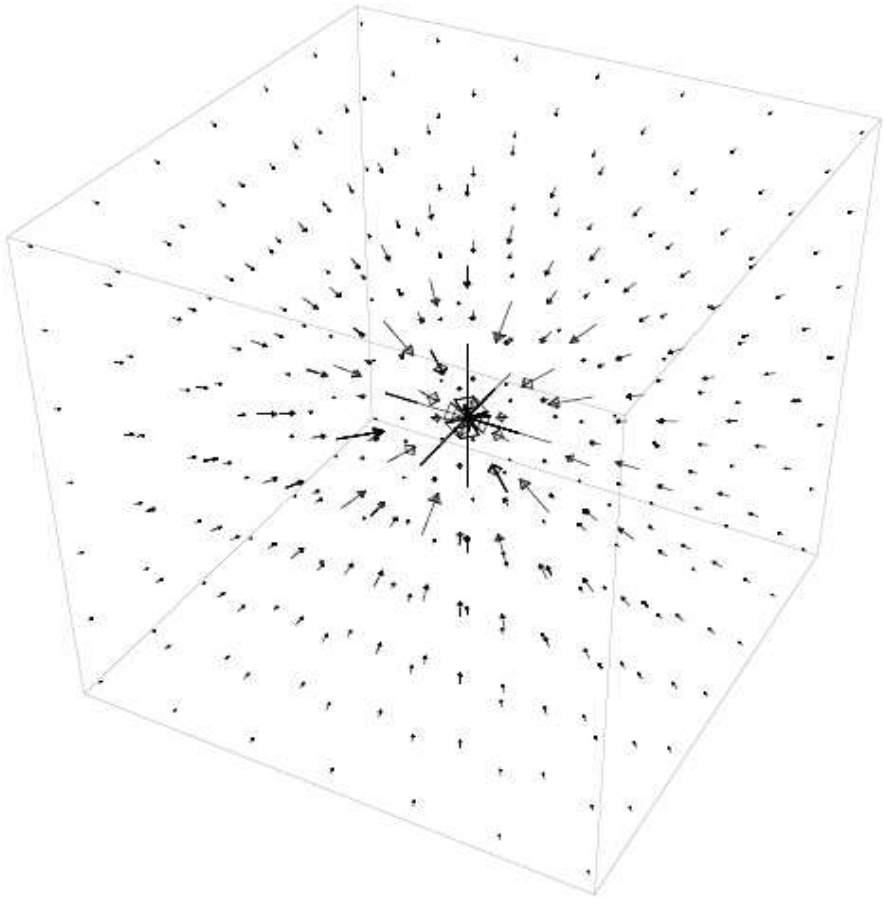
Problem

Sketch the following vector fields:

- $F(x, y) = (1, 1)$ *(constant field)*
- $F(x, y) = (y, -x)$
- $F(x, y) = (-x, -y)/\sqrt{x^2 + y^2}$

Review

A visualization of the gravitational vector field



Review

Definition

The del operator (in Cartesian coordinates) is expressed as

$$\nabla = \mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}$$

The del operator "acts" on a scalar function $f : \mathbb{R}^3 \to \mathbb{R}$ by

$$\begin{aligned}\nabla f &= \left(\mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}\right) f \\ &= \mathbf{i}\frac{\partial f}{\partial x} + \mathbf{j}\frac{\partial f}{\partial y} + \mathbf{k}\frac{\partial f}{\partial z},\end{aligned}$$

which is the gradient.

Review

Definition

A scalar function $f : \mathbb{R}^m \to \mathbb{R}$ is a potential for the vector field $F : \mathbb{R}^m \to \mathbb{R}^m$ if

$$F = \nabla f$$

Example

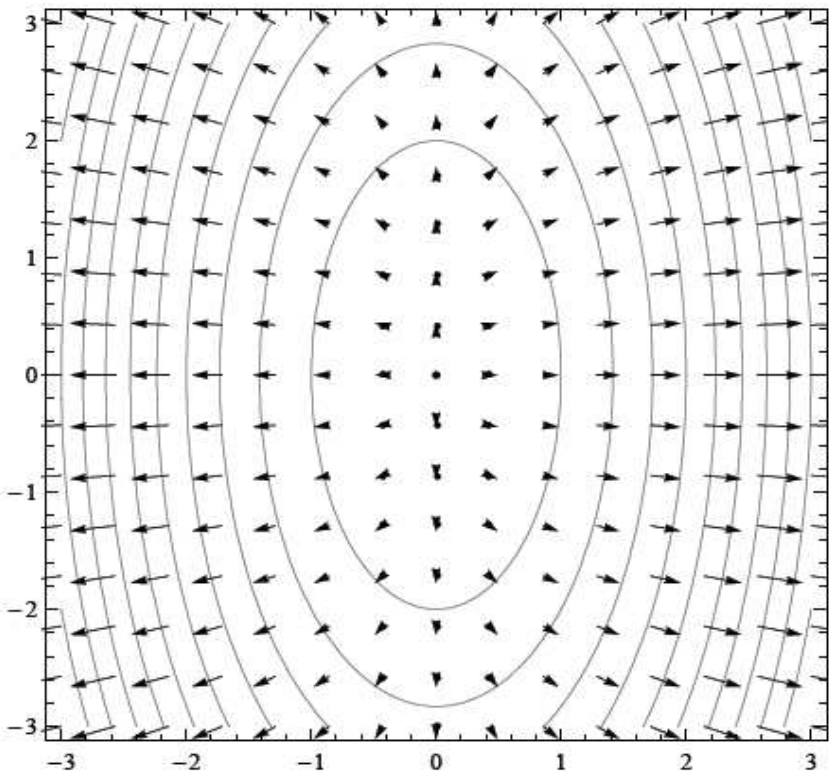
The vector field $F(x, y) = (y, x)$ has potential function $f(x, y) = xy$.

Definition

Let f be a potential function for the vector field F. The level curves (surfaces) of f are called equipotential lines (surfaces) of F. Observe that the vector field F is orthogonal to the equipotential lines or surfaces.

Review

The vector field of the potential function $f(x, y) = x^2 + y^2/4$. Notice that the field is orthogonal to the equipotential lines.



What is the vector field of this potential?

Review

Problem

Can you find a potential for the following fields:

- $F(x, y, z) = (x, -y, z)$
- $F(x, y) = (xy^2, 3x^2y)$

Definition

A flow line of a vector field $F : \mathbb{R}^n \to \mathbb{R}^n$ is a differentiable path $x : I \to \mathbb{R}^n$ such that

$$x'(t) = F(x(t)).$$

That is the velocity vector of x at any time is given by the value of the vector field at the point on x at any time.

Problem

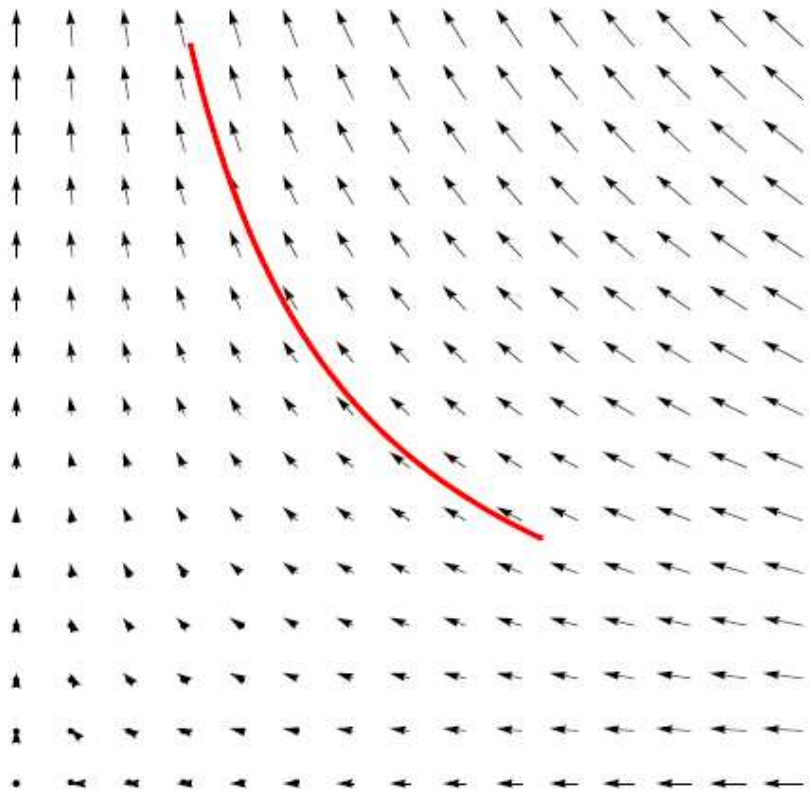
Show that $x(t) = (ae^t, be^t)$ is a flow line for the field $F(x, y) = (x, y)$.

Problem

Find a flow line for the field $F(x, y) = (-x, y)$ such that $x(0) = (2, 1)$.

Review

The flow line $x(t) = (2e^{-t}, e^{t})$ of the field $F(x, y) = (-x, y)$.



Review

Definition (The divergence)

Let $F : X \subset \mathbb{R}^n \to \mathbb{R}^n$ be a differentiable vector field. The divergence of F, denoted by $\mathrm{div}F$ or $\nabla \cdot F$ is the scalar function

$$\mathrm{div}F = \nabla \cdot F = \frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} + \cdots + \frac{\partial F_n}{\partial x_n}$$

where $(x_1, x_2, \cdots, x_n)$ are the Cartesian coordinates for $\mathbb{R}^n$ and $F_1, F_2, \cdots, F_n$ are the component functions of F.

Problem

Let $F(x, y, z) = (x^2 + y^2, xy^2z, y^3z)$. *Find* $\mathrm{div}F$.

Review

The "meaning" of the divergence

The divergence is a measure of the net mass flow through an infinitesimal region of space; thus,

- $\mathrm{div}F < 0$ corresponds to a sink
- $\mathrm{div}F > 0$ corresponds to a source
- $\mathrm{div}F = 0$ corresponds to a pure transfer.

Definition

A vector field F for which $\mathrm{div}F = 0$ everywhere is called incompressible or solenoidal.

Problem

Find divF in each case:

- $F(x, y, z) = \mathbf{i} + \mathbf{j} + \mathbf{k}$ *(a constant field)*
- $F(x, y) = (y, -x)$ *(a rotating field)*
- $F(x, y, z) = (-x, -y, -z)/(x^2 + y^2 + z^2)^{3/2}$ *(a gravitational field)*

Review

Definition (The curl)

Let $F : X \subset \mathbb{R}^3 \to \mathbb{R}^3$ be a differentiable vector field (note the dimension). The curl of F, denoted by $\text{curl}F$ or $\nabla \times F$ is the vector field

$$\text{curl}F = \nabla \times F = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_1 & F_2 & F_3 \end{vmatrix}$$

Problem

Let $F(x, y, z) = x^2yz\mathbf{i} + (y^2 + z^2)\mathbf{j} + (x + y)\mathbf{k}$ *and find* $\text{curl}F$.

Definition

A field F is said to be irrotational if $\text{curl}F = 0$.

Review

Prove the following:

Theorem

A potential field is irrotational.

Theorem

The curl of a vector field is an incompressible field.

Why bother to study PDE's?

- Most physical phenomena are described at a fundamental level by interactions between particles.

  – Quarks, nucleons, mesons in Nuclear physics
  – Atoms, molecules, electrons in Classical physics

- If we were to model a physical system, we would have to consider lots of particles such as 6.10^{23} per gram mole (per gram for Hydrogen). Unfortunately, It would not be efficient or even realistic (numerically speaking) to represent each particle by one equation.

PDE CONCEPT

DEFINITION. *An expression of the form*

$$F(D^k u(x), D^{k-1}u(x), \ldots, Du(x), u(x), x) = 0 \quad (x \in U) \tag{1}$$

is called a kth-order partial differential equation, *where*

$$F : \mathbb{R}^{n^k} \times \mathbb{R}^{n^{k-1}} \times \cdots \times \mathbb{R}^n \times \mathbb{R} \times U \to \mathbb{R}$$

is given, and

$$u : U \to \mathbb{R}$$

is the unknown.

Throughout $x \in U$, where U is an open subset of $\mathbb{R}^n$, and $t \geq 0$. Also $Du = D_x u = (u_{x_1}, \ldots, u_{x_n})$ denotes the gradient of u with respect to the spatial variable $x = (x_1, \ldots, x_n)$.

DEFINITIONS.

(i) *The partial differential equation* (1) *is called* linear *if it has the form*

$$\sum_{|\alpha|\leq k} a_\alpha(x) D^\alpha u = f(x)$$

for given functions a_α $(|\alpha| \leq k), f$. *This linear PDE is* homogeneous *if* $f \equiv 0$.

(ii) *The PDE* (1) *is* semilinear *if it has the form*

$$\sum_{|\alpha|=k} a_\alpha(x) D^\alpha u + a_0(D^{k-1}u, \ldots, Du, u, x) = 0.$$

(iii) *The PDE* (1) *is* quasilinear *if it has the form*

$$\sum_{|\alpha|=k} a_\alpha(D^{k-1}u, \ldots, Du, u, x) D^\alpha u + a_0(D^{k-1}u, \ldots, Du, u, x) = 0.$$

(iv) *The PDE* (1) *is* fully nonlinear *if it depends nonlinearly upon the highest order derivatives.*

A *system* of partial differential equations is, informally speaking, a collection of several PDE for several unknown functions.

PDEs

DEFINITION. *An expression of the form*

$$\mathbf{F}(D^k\mathbf{u}(x), D^{k-1}\mathbf{u}(x), \ldots, D\mathbf{u}(x), \mathbf{u}(x), x) = \mathbf{0} \quad (x \in U) \tag{2}$$

is called a kth-order system of partial differential equations, *where*

$$\mathbf{F} : \mathbb{R}^{mn^k} \times \mathbb{R}^{mn^{k-1}} \times \cdots \times \mathbb{R}^{mn} \times \mathbb{R}^m \times U \to \mathbb{R}^m$$

is given and

$$\mathbf{u} : U \to \mathbb{R}^m, \ \mathbf{u} = (u^1, \ldots, u^m)$$

is the unknown.

There is no general theory known concerning the solvability of all partial differential equations. Such a theory is extremely unlikely to exist, given the rich variety of physical, geometric, and probabilistic phenomena which can be modeled by PDE. Instead, research focuses on various particular partial differential equations that are important for applications within and outside of mathematics, with the hope that insight from the origins of these PDE can give clues as to their solutions.

Problem

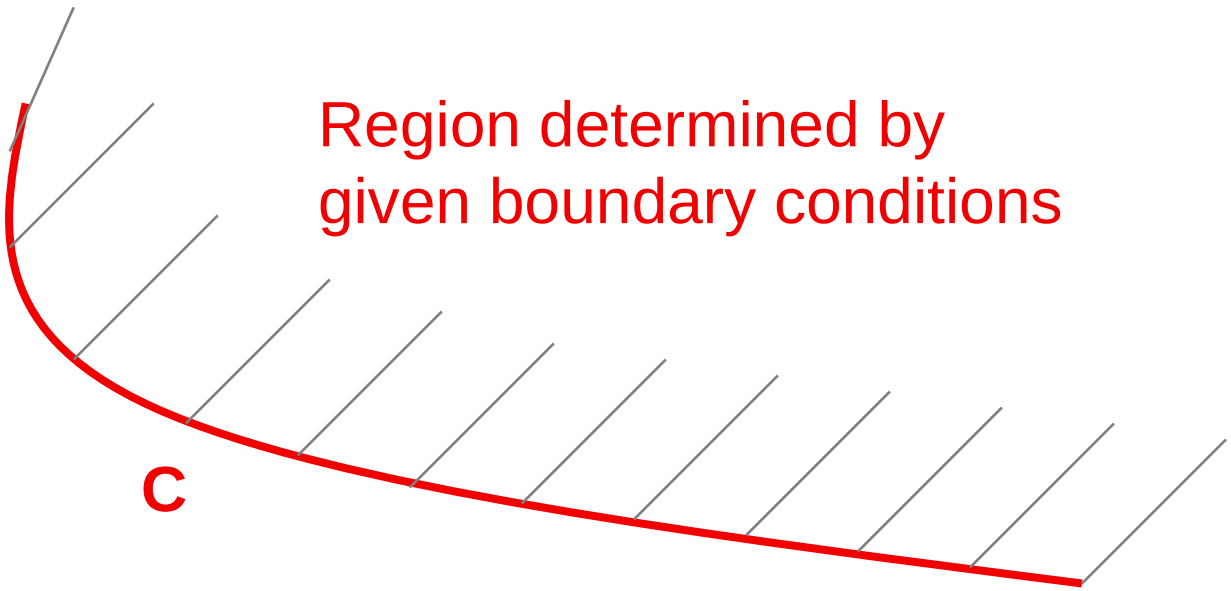
is the general solution of

$$x^2 u_{xx} - y^2 u_{yy} = 0$$

$$u = F(xy) + x\,G(\frac{y}{x}) \quad ?$$

Boundary Conditions for a PDE

- Cauchy Boundary Conditions are Ψ and $\partial\Psi / \partial n$ defined on a curve C where n is the normal direction to the curve. This is appropriate for hyperbolic equations



- **Dirichlet Boundary Conditions: Ψ given on closed a curve C**

- **Neumann Boundary Conditions: $\partial\Psi / \partial n$ given on closed curve C**

Examples of PDEs

a. Linear equations.

1. *Laplace's equation*

$$\Delta u = \sum_{i=1}^{n} u_{x_i x_i} = 0.$$

2. *Helmholtz's (or eigenvalue) equation*

$$-\Delta u = \lambda u.$$

3. *Linear transport equation*

$$u_t + \sum_{i=1}^{n} b^i u_{x_i} = 0.$$

4. *Liouville's equation*

$$u_t - \sum_{i=1}^{n} (b^i u)_{x_i} = 0.$$

PDEs

5. *Heat (or diffusion) equation*

$$u_t - \Delta u = 0.$$

6. *Schrödinger's equation*

$$iu_t + \Delta u = 0.$$

7. *Kolmogorov's equation*

$$u_t - \sum_{i,j=1}^{n} a^{ij} u_{x_i x_j} + \sum_{i=1}^{n} b^i u_{x_i} = 0.$$

8. *Fokker–Planck equation*

$$u_t - \sum_{i,j=1}^{n} (a^{ij} u)_{x_i x_j} - \sum_{i=1}^{n} (b^i u)_{x_i} = 0.$$

9. *Wave equation*

$$u_{tt} - \Delta u = 0.$$

PDEs

10. *Telegraph equation*

$$u_{tt} + du_t - u_{xx} = 0.$$

11. *General wave equation*

$$u_{tt} - \sum_{i,j=1}^{n} a^{ij} u_{x_i x_j} + \sum_{i=1}^{n} b^i u_{x_i} = 0.$$

12. *Airy's equation*

$$u_t + u_{xxx} = 0.$$

13. *Beam equation*

$$u_t + u_{xxxx} = 0.$$

b. Nonlinear equations.

1. *Eikonal equation*

$$|Du| = 1.$$

2. *Nonlinear Poisson equation*

$$-\Delta u = f(u).$$

3. *p-Laplacian equation*

$$\operatorname{div}(|Du|^{p-2}Du) = 0.$$

4. *Minimal surface equation*

$$\operatorname{div}\left(\frac{Du}{(1+|Du|^2)^{1/2}}\right) = 0.$$

5. *Monge–Ampère equation*

$$\det(D^2u) = f.$$

6. *Hamilton–Jacobi equation*

$$u_t + H(Du, x) = 0.$$

PDEs

7. *Scalar conservation law*

$$u_t + \operatorname{div} \mathbf{F}(u) = 0.$$

8. *Inviscid Burgers' equation*

$$u_t + uu_x = 0.$$

9. *Scalar reaction-diffusion equation*

$$u_t - \Delta u = f(u).$$

10. *Porous medium equation*

$$u_t - \Delta(u^\gamma) = 0.$$

11. *Nonlinear wave equations*

$$u_{tt} - \Delta u = f(u),$$
$$u_{tt} - \operatorname{div} \mathbf{a}(Du) = 0.$$

12. *Korteweg–de Vries (KdV) equation*

$$u_t + uu_x + u_{xxx} = 0.$$

Examples of PDEs systems:

a. Linear systems.

1. *Equilibrium equations of linear elasticity*

$$\mu\Delta\mathbf{u} + (\lambda+\mu)D(\operatorname{div}\mathbf{u}) = \mathbf{0}.$$

2. *Evolution equations of linear elasticity*

$$\mathbf{u}_{tt} - \mu\Delta\mathbf{u} - (\lambda+\mu)D(\operatorname{div}\mathbf{u}) = \mathbf{0}.$$

3. *Maxwell's equations*

$$\begin{cases} \mathbf{E}_t = \operatorname{curl}\mathbf{B} \\ \mathbf{B}_t = -\operatorname{curl}\mathbf{E} \\ \operatorname{div}\mathbf{B} = \operatorname{div}\mathbf{E} = 0. \end{cases}$$

PDEs

b. Nonlinear systems.

1. *System of conservation laws*

$$\mathbf{u}_t + \operatorname{div} \mathbf{F}(\mathbf{u}) = \mathbf{0}.$$

2. *Reaction-diffusion system*

$$\mathbf{u}_t - \Delta \mathbf{u} = \mathbf{f}(\mathbf{u}).$$

3. *Euler's equations for incompressible, inviscid flow*

$$\begin{cases} \mathbf{u}_t + \mathbf{u} \cdot D\mathbf{u} = -Dp \\ \operatorname{div} \mathbf{u} = 0. \end{cases}$$

4. *Navier–Stokes equations for incompressible, viscous flow*

$$\begin{cases} \mathbf{u}_t + \mathbf{u} \cdot D\mathbf{u} - \Delta \mathbf{u} = -Dp \\ \operatorname{div} \mathbf{u} = 0. \end{cases}$$

Well-posed problems, classical solutions. **(Conditions)**

(a) the problem in fact has a solution;

(b) this solution is unique;

and

(c) the solution depends continuously on the data given in the problem.

Partial Differential Equations

We can solve a PDE by:

A) Analytical Methods:

-Separation of variables;

-Green Functions

-Method of characteristics;

-Transformations: Laplace and Fourier transforms

B) Numerical Methods: Finite Element Method (FEM) (1D, 2D), Finite Difference Method (FDM), Finite Boundary Element.

2.0 Finite Element Method

- Two interpretations

1. Physical Interpretation:

   The continous physical model is divided into finite pieces called elements and laws of nature are applied on the generic element. The results are then recombined to represent the continuum.

2. Mathematical Interpretation:

   The differential equation representing the system is converted into a variational form, which is approximated by the linear combination of a finite set of trial functions.

Numerical Methods

In order to solve a PDE by FEM we need to:

a) Specify the type of solver (Stationary (linear/non linear), Time dependent, Eigenvalue, Parametric (Linear/non linear))
b) Specify the domain of the equation
c) Specify the Boundary conditions
d) Create a mesh

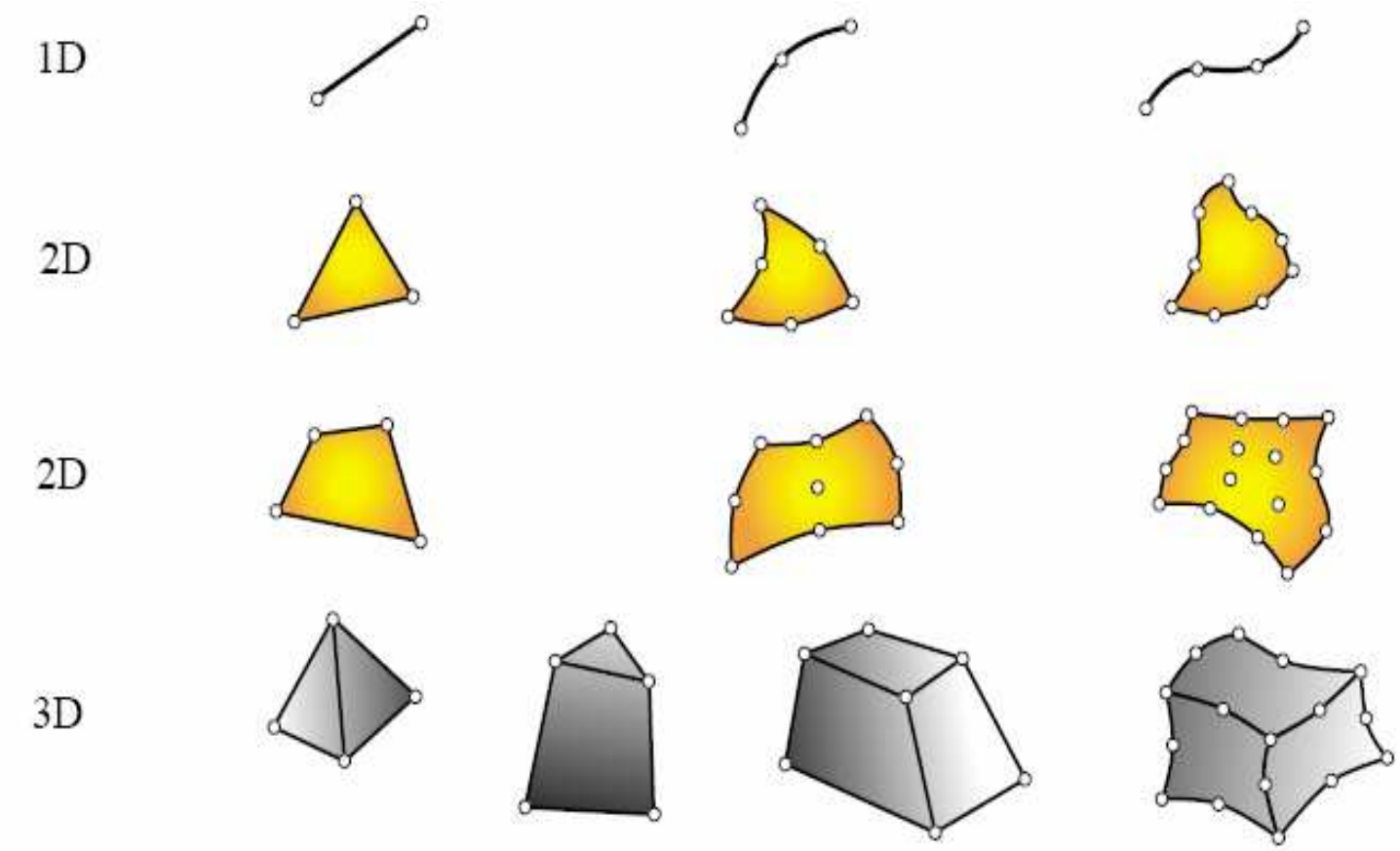
FEM Notation

Elements are defined by the following properties:

1. Dimensionality
2. Nodal Points
3. Geometry
4. Degrees of Freedom
5. Nodal Forces

   (Non homogeneous RHS of the DE)

Element Types



Open Source Software:

CalculiX is an Open Source FEA project. The solver uses a partially compatible ABAQUS file format. The pre/post-processor generates input data for many FEA and CFD applications Convergent Mechanical Solutions
Code Aster: French software written in Python and Fortran, GPL license
: Differential Equations Analysis Library using adaptive finite elements, written in C++, QPL open source license
DUNE, Distributed and Unified Numerics Environment GPL Version 2 with Run-Time Exception, written in C++
Febio, Finite Elements for Biomechanics, : GPL-licensed, general FEM library (2d), solver for stationary incompressible Navier-Stokes, linear elasticity, Poisson problem, allows shape optimisation
Elmer FEM solver: Open source Multiphysical simulation software developed by Finnish Ministry of Education's CSC, written in C, C++ and Fortran [7] : FEM software primarily for mechanical problems, GPL license, written in C
FEMM : Finite Element Method Magnetics
FEniCS Project : a LGPL-licensed software package developed by American and European researchers
: a GPL-licensed educational software
: a GPL-licensed software
: GPL-licensed software package
Hermes Project: Modular C/C++ library for rapid prototyping of space- and space-time adaptive hp-FEM solvers.
: Dynamic Finite Element Program Suite, for dynamic events like crashes, written in Java, GNU license
JFEM: 2D/3D C++ FEM codes developed for nanophotonics by Jeffrey M. McMahon,
: Framework for building multi-disciplinary finite element programs. Written in C++, open source, free for non-commercial purposes
: A framework for the numerical simulation of PDEs using arbitrary unstructured discretizations on serial and parallel platforms. Written in C++, LGPL license, developed at The University of Texas at Austin and Technische Universität Hamburg-Harburg.
OOFEM: Object Oriented Finite EleMent solver, written in C++, GPL v2 license
: General purpose, parallel, multi-physics FEM for Computational Fluid Dynamics, based on PETSc. Written in C++, GPL v2 license.
San Le's Free Finite Element Analysis, includes GUI, written in ANSI C, GPL license.
: a LGPL-licensed software package developed at Sandia National Laboratories
: Explicit/Impicit Finite Element Program with linear/nonlinear, elastic/hyperelastic/hypoelastic/plastic/visco, contact,thermal, fluid capabilities, written in C++, GPL license
Z88: FEM-software available for Windows and Linux/UNIX, written in C, GPL license

Commercial FEM Software

Abaqus: Franco-American software from SIMULIA, owned by Dassault Systemes SIMULIA
ACTRAN: Belgian software for aeroacoustics and vibroacoustics simulations ADINA R&D, Inc. See http://www.adina.com/
, Advance Design web page
ALGOR Incorporated ALGOR AMPS Technologies See http://www.ampstech.com/ampstech/Asp/index.asp
Analysis for Windows: Analysis for Windows
ANSYS: American software
: FEA software for piezoelectric vibroacoustic analysis mmech
: French software CASTEM
: geotechnics, tunnels, concrete & coupled analysis www.cesar-lcpc.com
COMSOL Multiphysics COMSOL Multiphysics Finite Element Analysis Software
: A SolidWorks module, owned by Dassault Systemes COSMOS
DIANA, See http://www.tnodiana.com/
Dytran: owned by MSC.Software, embedded into manufacturing simulation software Simufact.forming
by , Japan, also includes
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NEi Software: American software NEi Software
NISA: Indian software NISA
: Multiphysics CAE software developed and commercialized by OPEN ENGINEERING
: British Acoustic & Elastohyrodynamic FEA PACSYS
PAM: French software PAM
PERMAS: German software PERMAS

PDE
EXAMPLE

Example Laplace Equation

We consider the Laplace and Poisson Equation:

$$\Delta u = 0 \tag{1}$$

$$-\Delta u = f.^{*} \tag{2}$$

In both (1) and (2), $x \in U$ and the unknown is $u : \bar{U} \to \mathbb{R}$, $u = u(x)$, where $U \subset \mathbb{R}^n$ is a given open set. In (2) the function $f : U \to \mathbb{R}$ is also given. the *Laplacian* of u is $\Delta u = \sum_{i=1}^{n} u_{x_i x_i}$.

Now we look for analytical solutions of (1) and (2):

Let us therefore attempt to find a solution u of Laplace's equation (1) in $U = \mathbb{R}^n$, having the form

$$u(x) = v(r),$$

where $r = |x| = (x_1^2 + \cdots + x_n^2)^{1/2}$ and v is to be selected (if possible) so that $\Delta u = 0$ holds.

Examples

First note for $i = 1, \ldots, n$ that

$$u_{x_i} = v'(r)\frac{x_i}{r}, \quad u_{x_i x_i} = v''(r)\frac{x_i^2}{r^2} + v'(r)\left(\frac{1}{r} - \frac{x_i^2}{r^3}\right)$$

for $i = 1, \ldots, n$, and so

$$\Delta u = v''(r) + \frac{n-1}{r}v'(r).$$

Hence $\Delta u = 0$ if and only if

$$v'' + \frac{n-1}{r}v' = 0.$$

If $v' \neq 0$, we deduce

$$\log(v')' = \frac{v''}{v'} = \frac{1-n}{r},$$

Examples

and hence $v'(r) = \frac{a}{r^{n-1}}$ for some constant a. Consequently if $r > 0$, we have

$$v(r) = \begin{cases} b \log r + c & (n = 2) \\ \frac{b}{r^{n-2}} + c & (n \geq 3), \end{cases}$$

where b and c are constants.

DEFINITION. *The function*

$$\Phi(x) := \begin{cases} -\frac{1}{2\pi} \log |x| & (n = 2) \\ \frac{1}{n(n-2)\alpha(n)} \frac{1}{|x|^{n-2}} & (n \geq 3), \end{cases}$$

defined for $x \in \mathbb{R}^n$, $x \neq 0$, *is the* fundamental solution of Laplace's equation.

$\alpha(n)$ denotes the volume of the unit ball in $\mathbb{R}^n$.

Examples

For the Poisson Equation:

THEOREM *Define u by*

$$u(x) = \int_{\mathbb{R}^n} \Phi(x-y) f(y)\, dy$$

$$= \begin{cases} -\frac{1}{2\pi} \int_{\mathbb{R}^2} \log(|x-y|) f(y)\, dy & (n=2) \\ \frac{1}{n(n-2)\alpha(n)} \int_{\mathbb{R}^n} \frac{f(y)}{|x-y|^{n-2}}\, dy & (n \geq 3) \end{cases}$$

Then

(i) $u \in C^2(\mathbb{R}^n)$

and

(ii) $-\Delta u = f$ *in* $\mathbb{R}^n$.

Poisson Equation:

Let us consider in particular:

$-\nabla^2 u = 1$ within the unit circle

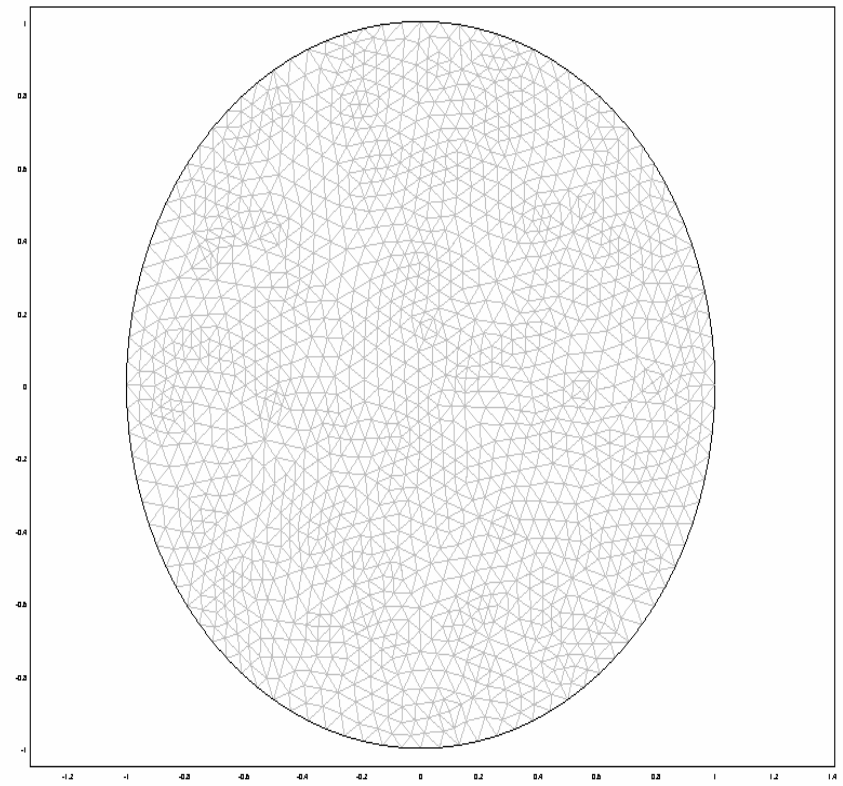
with boundary condition of Dirichlet type: $u = 0$

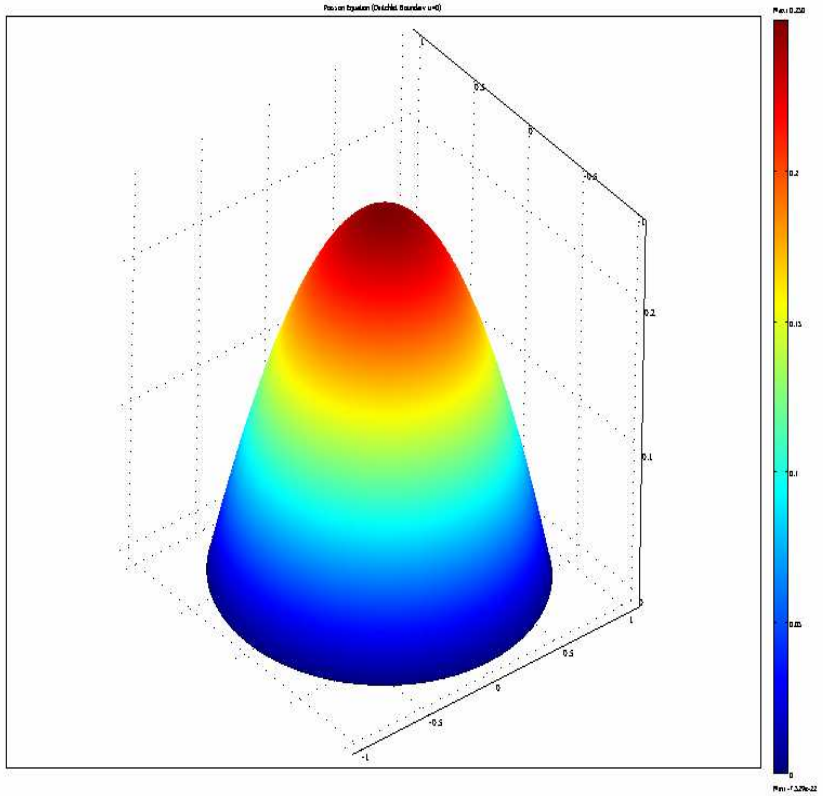
The analytical solution is given by:

Can you find (guess) the solution for this equation ?

Poisson Equation:

Now, we solve it with COMSOL

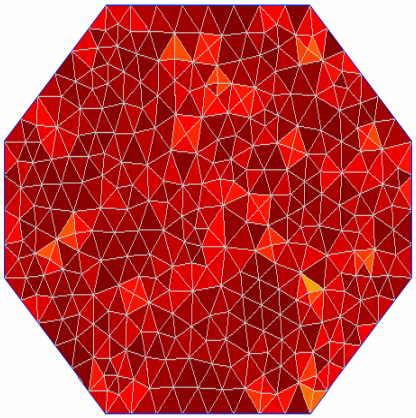


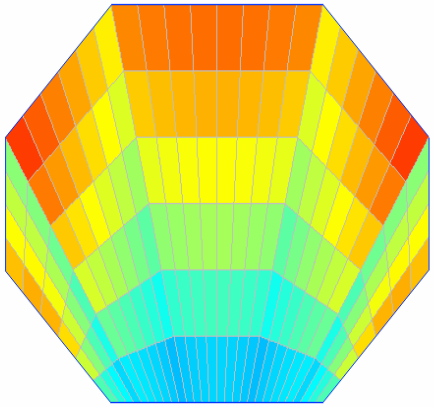


Circular domain with 3024 mesh elements

MESHES

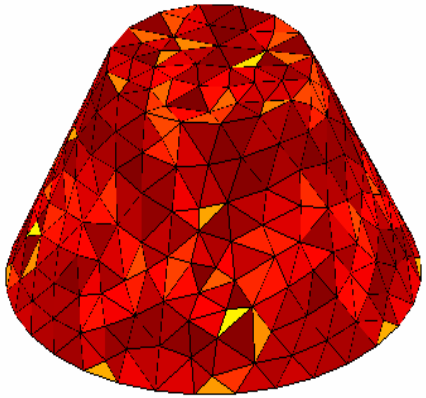
The geometric shapes of the elements can be triangular and quadrilateral in 2D and tetrahedral, hexahedral, and prismatic (with triangular base) in 3D.

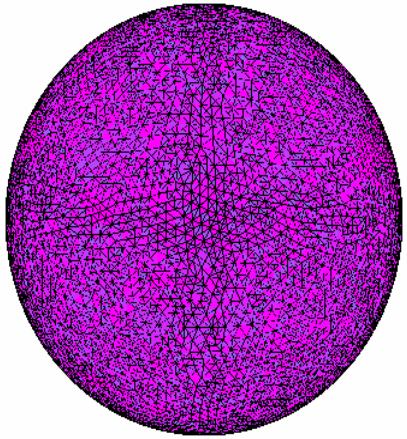




Two dimensional meshes

MESHES

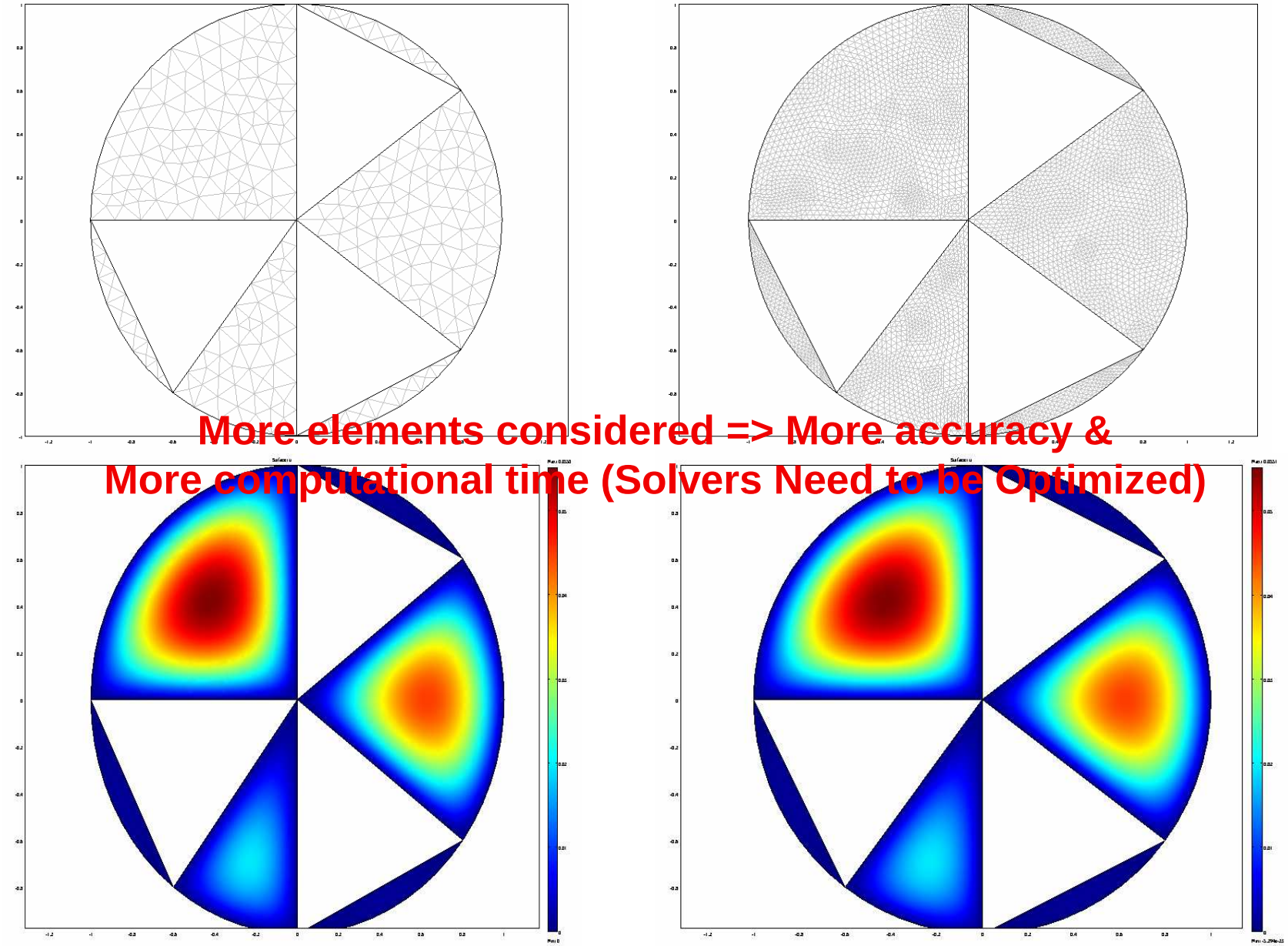




Three dimensional meshes

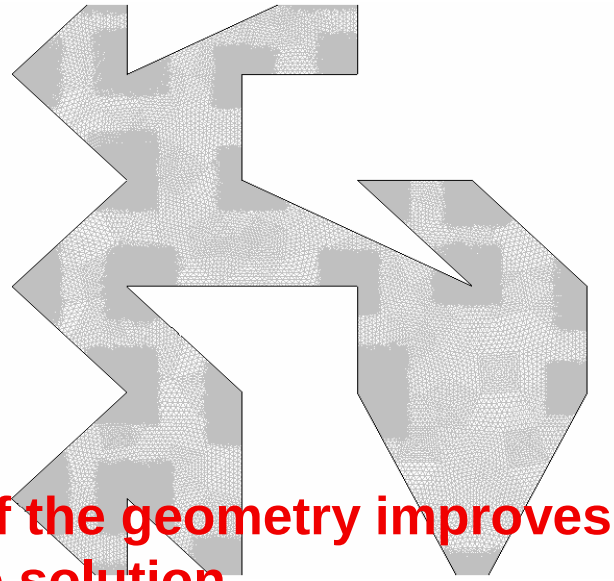
Computational Diagnostics & Biocybernetics Unit

Effect of Meshes in the Solution

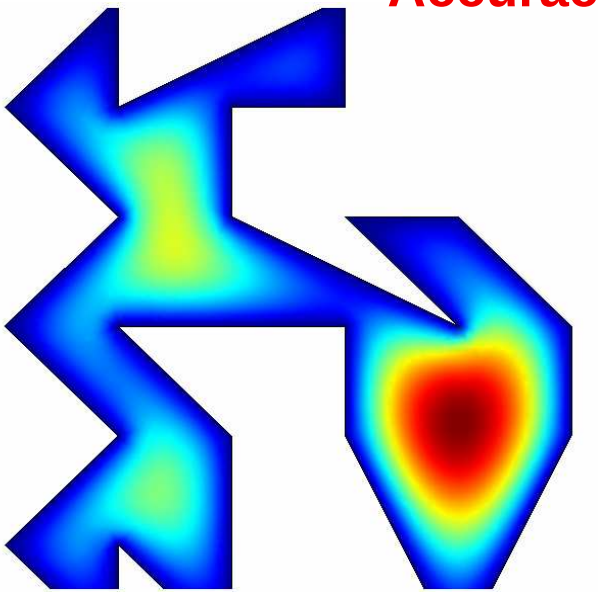


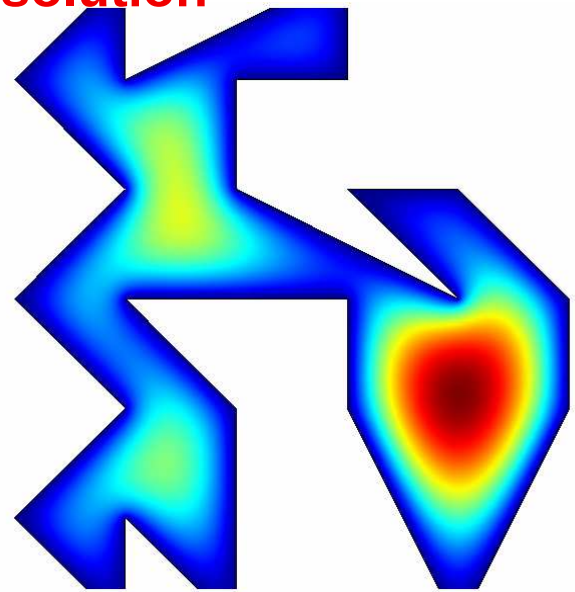
More elements considered => More accuracy & More computational time (Solvers Need to be Optimized)

Effect of Meshes in the Solution



Refinement in special places of the geometry improves Accuracy of the solution





UMFPACK:

Is a set of routines for solving unsymmetric sparse linear systems Ax=b.

(the Unsymmetric MultiFrontal method).

by Timothy A. Davis, University of Florida.

-A reorganization of spare Cholesky factorization based on eliminating column dependencies by partial factorization of dense and smaller sub-matrices called frontal matrices.

If A has real entries and is symmetric (or more generally, is Hermitian) and positive definite, then A can be decomposed as

$A=LL^*$

where **L is a lower triangular matrix with strictly positive diagonal entries, and L*** denotes the conjugate transpose of **L**

SPOOLES:

Sparse Object Oriented Linear Equations Solver

(developed by members of the Mathematics and Engineering Analysis Unit of Boeing Phantom Works)

a) Factor and solve square linear systems of equations with symmetric structure, with or without pivoting for stability.

b) Factor and solve overdetermined full rank system of equations using a Multifrontal QR factorization.

A QR factorization of a real square matrix A is a decomposition of A
where Q is an orthogonal matrix (meaning that $QTQ = I$) and R is an upper triangular matrix (also called right triangular matrix).

PARDISO

Was designed to solve large sparse symmetric and unsymmetric linear systems of equations on shared memory multiprocessors.

Olaf Schenk (Department of Computer Science, University Basel).

Unsymmetric, structurally symmetric or symmetric systems, real or complex, positive definite or indefinite, Hermitian.

LU with complete supernode. Parallel on SMPs. Automatic combination of iterative and direct solver algorithms to accelerate the solution process for very large three-dimensional systems.

CONJUGATE GRADIENTS (CG)

CG is the most popular iterative method for solving large systems

of linear equations of the form Ax=b.

where x is an unknown vector, b is a known vector, and A is a known, square, symmetric, positive-definite (or positive-indefinite) matrix.

(A matrix A is *positive-definite* if, for every nonzero vector x, $x^T A x > 0.$)

Classification

Physical Classification

-Stationary (steady state): Elliptic, Laplace and Poisson‘s equation

-Marching problems (solution depends on time): Parabolic, Hyperbolic.

Classification of Linear Second Order PDEs

Recall that a linear second order PDE in two variables is given by

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G$$

where all the coefficients A through F are real functions of the independent variables x, y.

Define a discriminant $\Delta(x, y)$ by

$$\Delta(x_0, y_0) = B^2(x_0, y_0) - 4A(x_0, y_0)C(x_0, y_0).$$

Partial Differential Equations

Definition 7. An equation is called hyperbolic at the point (x_0, y_0) if $\Delta(x_0, y_0) > 0$. It is parabolic at that point if $\Delta(x_0, y_0) = 0$ and elliptic if $\Delta(x_0, y_0) < 0$.

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G$$

Example.

$$u_{tt} - c^2 u_{xx} = 0$$

$$A = 1,\ B = 0,\ C = -c^2$$

Therefore,

$$\Delta = 0^2 - 4 \cdot 1(-c^2) = 4c^2 \geq 0$$

Thus the problem is hyperbolic for $c \neq 0$ and parabolic for $c = 0$.

Canonical form

Let ξ, η be twice continuously differentiable functions

$$\xi = \xi(x, y),$$
$$\eta = \eta(x, y).$$

Suppose also that the Jacobian J of the transformation defined by

$$J = \begin{vmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{vmatrix}$$

is non zero.

Partial Differential Equations

Use the chain rule to obtain all the partial derivatives required in

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G \qquad (*)$$

It is easy to see

$$u_x = u_\xi \xi_x + u_\eta \eta_x \qquad (1)$$

$$u_y = u_\xi \xi_y + u_\eta \eta_y. \qquad (2)$$

The second partial derivatives can be obtained as follows:

$$\begin{aligned} u_{xy} &= (u_x)_y = (u_\xi \xi_x + u_\eta \eta_x)_y \\ &= (u_\xi \xi_x)_y + (u_\eta \eta_x)_y \\ &= (u_\xi)_y \xi_x + u_\xi \xi_{xy} + (u_\eta)_y \eta_x + u_\eta \eta_{xy} \end{aligned}$$

By using (2)

$$u_{xy} = (u_{\xi\xi}\xi_y + u_{\xi\eta}\eta_y)\xi_x + u_\xi \xi_{xy} + (u_{\eta\xi}\xi_y + u_{\eta\eta}\eta_y)\eta_x + u_\eta \eta_{xy}.$$

Reorganize the terms

$$u_{xy} = u_{\xi\xi}\xi_x\xi_y + u_{\xi\eta}(\xi_x\eta_y + \xi_y\eta_x) + u_{\eta\eta}\eta_x\eta_y + u_\xi \xi_{xy} + u_\eta \eta_{xy}.$$

Partial Differential Equations

In a similar fashion we get u_{xx}, u_{yy}

$$u_{xx} = u_{\xi\xi}\xi_x^2 + 2u_{\xi\eta}\xi_x\eta_x + u_{\eta\eta}\eta_x^2 + u_\xi\xi_{xx} + u_\eta\eta_{xx}.$$

$$u_{yy} = u_{\xi\xi}\xi_y^2 + 2u_{\xi\eta}\xi_y\eta_y + u_{\eta\eta}\eta_y^2 + u_\xi\xi_{yy} + u_\eta\eta_{yy}.$$

one finds after collecting like terms in eq. (*)

$$A^*u_{\xi\xi} + B^*u_{\xi\eta} + C^*u_{\eta\eta} + D^*u_\xi + E^*u_\eta + F^*u = G^*$$

where all the coefficients are now functions of ξ, η and

$$\begin{aligned}
A^* &= A\xi_x^2 + B\xi_x\xi_y + C\xi_y^2 \\
B^* &= 2A\xi_x\eta_x + B(\xi_x\eta_y + \xi_y\eta_x) + 2C\xi_y\eta_y \\
C^* &= A\eta_x^2 + B\eta_x\eta_y + C\eta_y^2 \\
D^* &= A\xi_{xx} + B\xi_{xy} + C\xi_{yy} + D\xi_x + E\xi_y \\
E^* &= A\eta_{xx} + B\eta_{xy} + C\eta_{yy} + D\eta_x + E\eta_y \\
F^* &= F \\
G^* &= G.
\end{aligned}$$

Partial Differential Equations

We have that:

$$\Delta^* = (B^*)^2 - 4A^*C^* = J^2(B^2 - 4AC) = J^2\Delta$$

and since $J \neq 0$, the sign of Δ^* is the same as that of Δ.

Examples of Different Types of PDE's: Laplace and Poisson Elliptic Equations

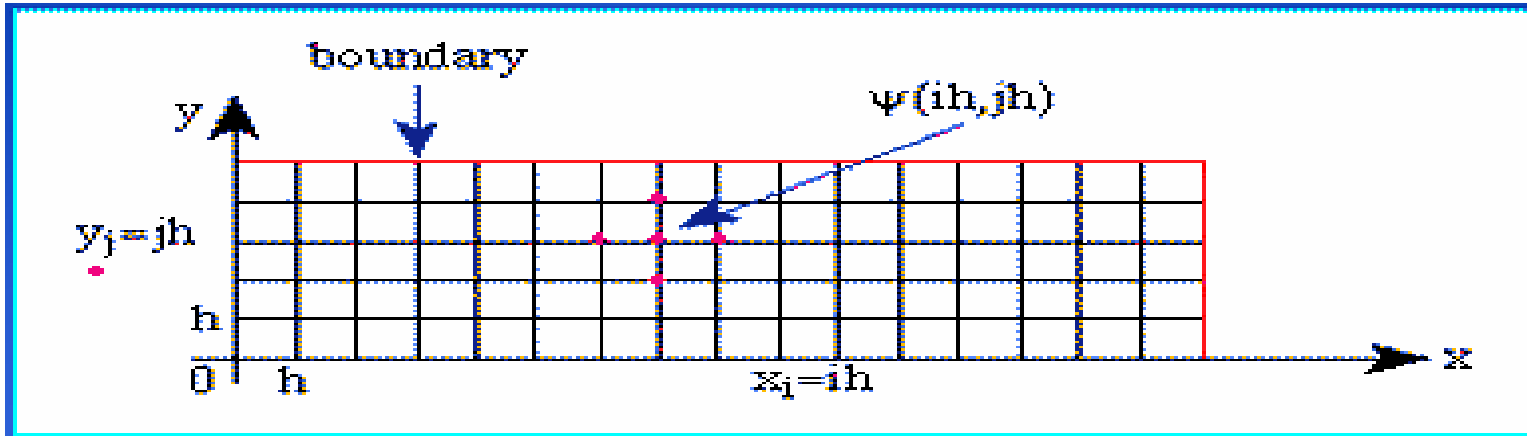
- Laplace's equation (elliptic): steady state in systems of electric or magnetic fields in a vacuum or the steady flow of incompressible non-viscous fluids

$$\nabla^2 \psi = 0$$

- Poisson's equation (elliptic): a variation of Laplace when an outside force, given by the function f, is applied to the system

$$\nabla^2 \psi = f(x, y)$$

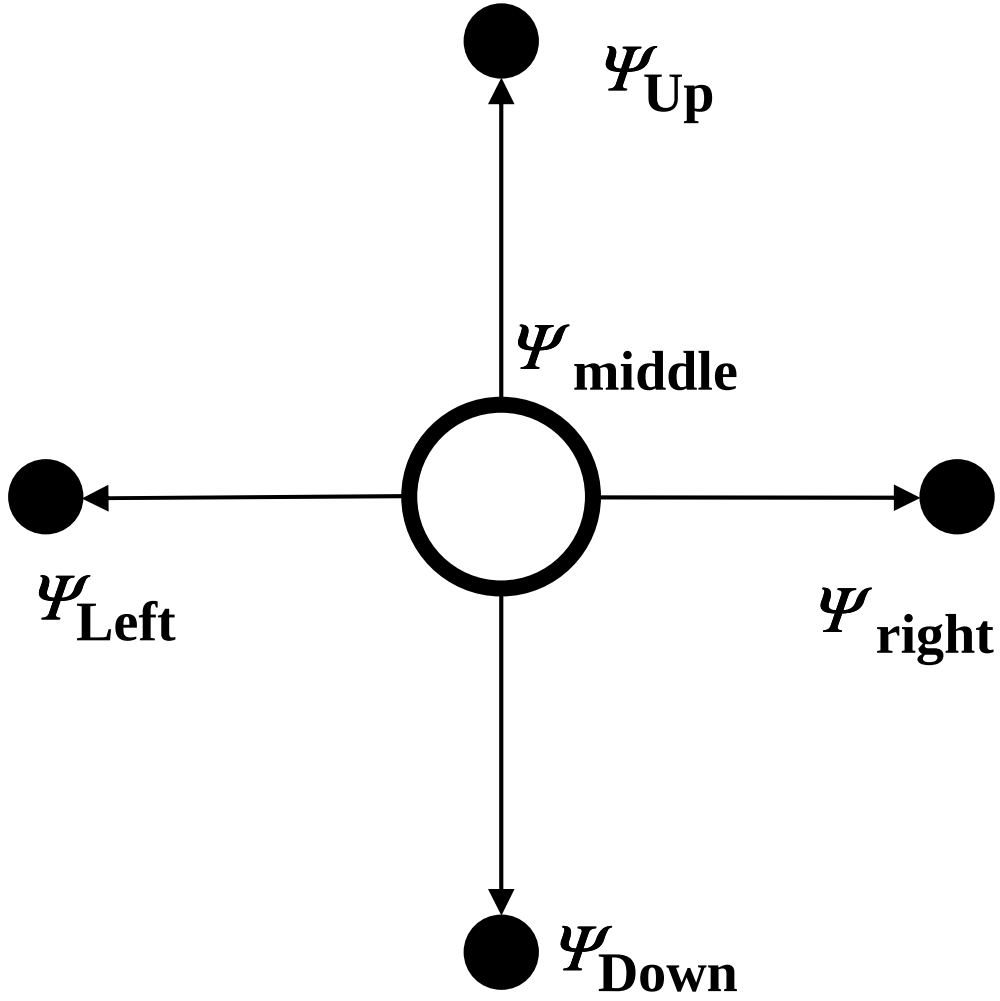
Solving Laplace's or Poisson's Equation



- We must convert continuous equations to a discrete form by setting up a mesh of points – finite difference method
- h is the step size of the grid
- N_x grid points in x ; N_y grid points in y

Basic Numerical Algorithm

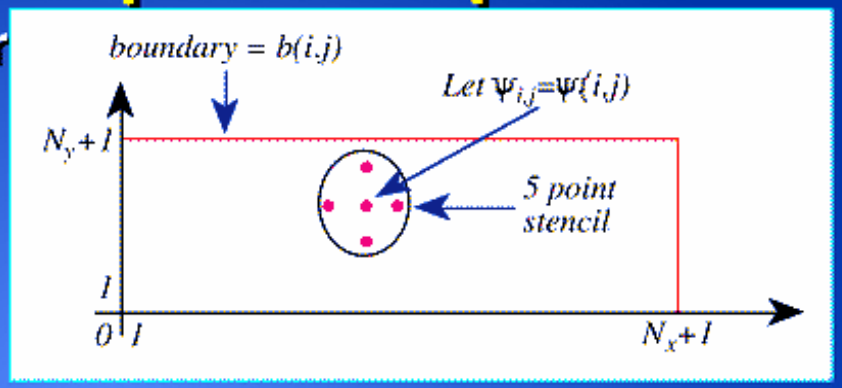
- Using standard "central differencing" techniques, one can approximate



$$\nabla^2 \Psi = (\Psi_{Left} + \Psi_{Right} + \Psi_{Up} + \Psi_{Down} - 4\,\Psi_{Middle}) / h^2$$

Difference Equation form of the Operator to solve Laplace's equation

- Use difference operator to solve for every interior point of grid



Since $\nabla^2 \psi = 0$,

$$\psi(x,y) = \frac{1}{4}\left(\psi(x+h,y) + \psi(x-h,y) + \psi(x,y+h) + \psi(x,y-h)\right)$$

- $N_x * N_y$ linear equations of the form

$$\psi_{ij} - \frac{1}{4}\left(\psi_{i+1j} + \psi_{i-1j} + \psi_{ij+1} + \psi_{ij-1}\right) = 0$$

The 12 by 12 Block Tridiagonal Equations Coming from Laplace's Equation on a Tiny 5 by 6 Grid

- Example equations to solve Laplace on a 5x6 grid with b labelling boundary and ψ internal points

$$
\begin{matrix}
b_{0,4} & b_{1,4} & b_{2,4} & b_{3,4} & b_{4,4} & b_{5,4} \\
b_{0,3} & \psi_{1,3} & \psi_{2,3} & \psi_{3,3} & \psi_{4,3} & b_{5,3} \\
b_{0,2} & \psi_{1,2} & \psi_{2,2} & \psi_{3,2} & \psi_{4,2} & b_{5,2} \\
b_{0,1} & \psi_{1,1} & \psi_{2,1} & \psi_{3,1} & \psi_{4,1} & b_{5,1} \\
b_{0,0} & b_{1,0} & b_{2,0} & b_{3,0} & b_{4,0} & b_{5,0}
\end{matrix}
$$

- System of 12 equations - block tridiagonal

$$
\begin{bmatrix}
1 & -1/4 & 0 & 0 & -1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1/4 & 1 & -1/4 & 0 & 0 & -1/4 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1/4 & 1 & -1/4 & 0 & 0 & -1/4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1/4 & 1 & 0 & 0 & 0 & -1/4 & 0 & 0 & 0 & 0 \\
-1/4 & 0 & 0 & 0 & 1 & -1/4 & 0 & 0 & -1/4 & 0 & 0 & 0 \\
0 & -1/4 & 0 & 0 & -1/4 & 1 & -1/4 & 0 & 0 & -1/4 & 0 & 0 \\
0 & 0 & -1/4 & 0 & 0 & -1/4 & 1 & -1/4 & 0 & 0 & -1/4 & 0 \\
0 & 0 & 0 & -1/4 & 0 & 0 & -1/4 & 1 & 0 & 0 & 0 & -1/4 \\
0 & 0 & 0 & 0 & -1/4 & 0 & 0 & 0 & 1 & -1/4 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1/4 & 0 & 0 & -1/4 & 1 & -1/4 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1/4 & 0 & 0 & -1/4 & 1 & -1/4 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/4 & 0 & 0 & -1/4 & 1
\end{bmatrix}
\begin{bmatrix}
\psi_{1,1} \\ \psi_{2,1} \\ \psi_{3,1} \\ \psi_{4,1} \\ \psi_{1,2} \\ \psi_{2,2} \\ \psi_{3,2} \\ \psi_{4,2} \\ \psi_{1,3} \\ \psi_{2,3} \\ \psi_{3,3} \\ \psi_{4,3}
\end{bmatrix}
= 1/4
\begin{bmatrix}
b_{0,1} + b_{0,1} \\ b_{2,0} \\ b_{3,0} \\ b_{4,0} + b_{5,1} \\ b_{0,2} \\ 0 \\ 0 \\ b_{5,2} \\ b_{0,3} + b_{1,4} \\ b_{2,4} \\ b_{3,4} \\ b_{4,4} + b_{5,2}
\end{bmatrix}
$$

General Form of Sparse Matrix Coming from Laplace's Equation - I

- We can write these equations

  $A\underline{\psi} = \underline{b}$

  $\underline{\psi}$ is a vector with $N_x N_y$ entries

A=

N_x

$$
\begin{matrix}
4 & -1 & 0 \ldots & & 0 & -1 & & \\
-1 & 4 & -1 & & 0 & 0 & -1 & \\
0 & -1 & 4 & -1 & 0 & 0 & 0 & -1 \\
\vdots & & & & & & & \\
0 & -1 & & & & & & \\
0 & 0 & -1 & 0 \ldots & -1 & 4 & -1 & & -1
\end{matrix}
$$

N_x

band

band

Diagonal

band

band

Iterative Methods (Stationary)

- There are many iterative methods which can be applied to solve any matrix equation but are particularly effective in sparse matrices as they directly exploit "zero structure"

- Here we look at three stationary methods - so called because iteration equation is the same at each iteration

Iterative Methods (Stationary)

- The Jacobi method is based on solving for every variable locally with respect to the other variables; one iteration of the method corresponds to solving for every variable once. The resulting method is easy to understand and implement, but convergence is slow.

- The Gauss-Seidel method is like the Jacobi method, except that it uses updated values as soon as they are available. In general, it will converge faster than the Jacobi method, though still relatively slowly.

- Successive Overrelaxation (SOR) can be derived from the Gauss-Seidel method by introducing an extrapolation parameter ϖ. For the optimal choice of ϖ, SOR converges faster than Gauss-Seidel by an order of magnitude.

Matrix Notation for Iterative Methods

$A\underline{x} = \underline{b}$

$$A = \begin{bmatrix} a_{11} \cdots & a_{1n} \\ & \\ a_{n1} & a_{nn} \end{bmatrix}$$

$$\underline{x} = \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

$$A = \begin{bmatrix} D & -U \\ -L & \end{bmatrix}$$

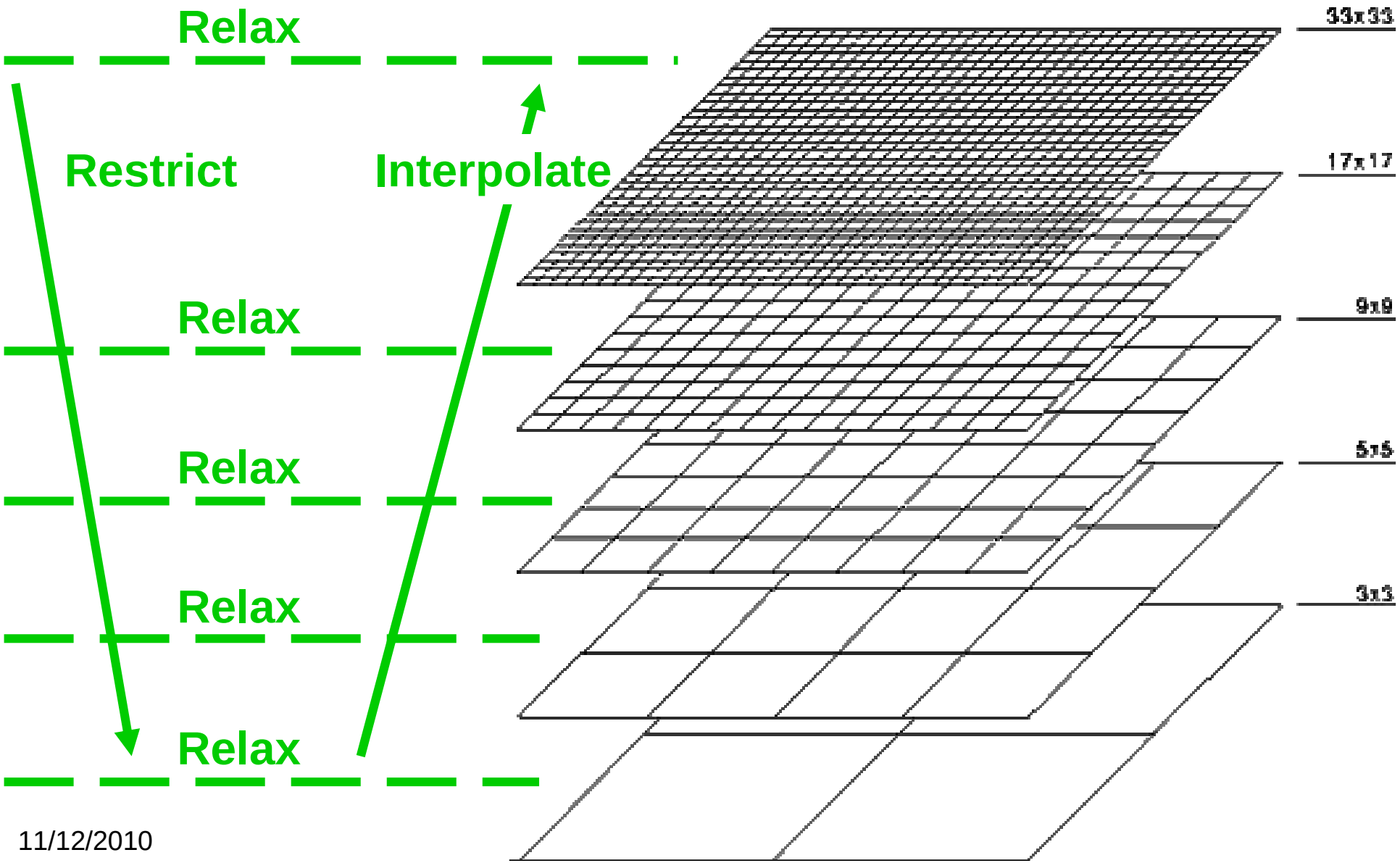
- Superfix k denotes iteration
- Write $A = D - L - U$
  - D = Diagonal
  - L = Lower Triangle
  - U = Upper Triangle

Multigrid Methods

- Basic idea in multigrid is key in many areas of science
  - Solve a problem at multiple scales

- We get coarse structure from small N and fine detail from large N
  - Good qualitative idea but how do we implement?

Multigrid Hierarchy



Simulation and Modelling
(Classical Point of View)

Concept of Math Model

- A **mathematical model** is a representation of the essential aspects of an existing system by means of mathematical language.

- Math models can take many forms: dynamical systems, statistical models, differential equations, or game theoretic models

Classifying Math Models

1) Linear vs. Non-Linear

2) Deterministic vs. Probabilistic

3) Static vs. Dynamic

4) Lumped parameters vs. Distributed parameters

5) Industrial vs. Scientific

A priori information

- **Black box models**
- **White box models**

} **Grey box models**

Modeling Examples:

- 1) Airflow over an airplane wing (**The Flow of an Evaporating Thin Film Liquid; PIMS Report (2002) Trenado et. al.**
- 2) Magnetic drug targeting (**Magnetic Nanoparticles for In Vivo Applications: A Numerical Modeling Study: Trenado and Strauss, 2007**)
- 3) Non-linear diffusion in image processing (**Mustaffa, Trenado, and Strauss, 2009**)
- 4) Modeling of Corrosion Protection Inhibitors Release (INM-Saarbruecken) **Trenado, Strauss, 2009.**

MODEL EXAMPLE: THIN FILMS

Thin Films

PROBLEM STATEMENT: Thin liquid films are ubiquitous. In geology, they appear as gravity currents under water or as lava flows. In biophysics, they appear as membranes, as linings in mammalian lungs or as tear films in the eye. They occur in Langmuir films and in foam dynamics. In engineering, thin films serve in heat and mass transfer processes to limit fluxes and to protect surfaces, and applications arise in paints, adhesives and membranes.

We develop a model that describes the development of thin film on a surface under constant shear. The model is then updated to account for evaporation when the bottom surface is heated. Parameters controlling the model are determined using real value data.

Thin Films

Airflow over an airplane wing

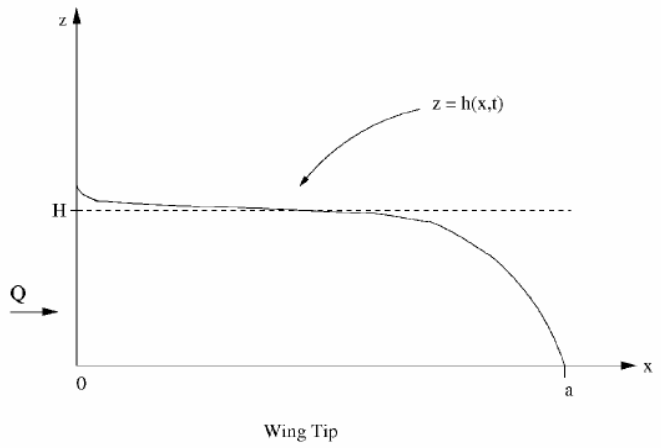
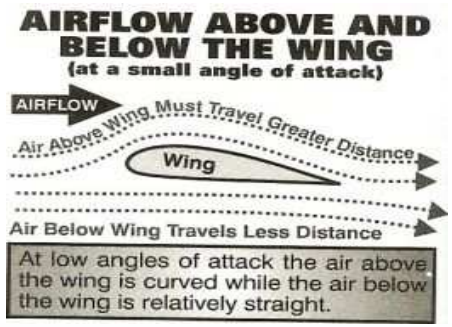


Figure 1.1: Half (due to the symmetry) of the wing tip.



Fluid is assumed to be flowing along a horizontal plane under the influence of interfacial continuous shear $\tau = \tau(x)$ and surface tension σ. The film has thickness h, the coordinates are such that x is directed down the plane, and z is perpendicular to the plane. The Navier-Stokes equations are assumed to govern the fluid flow. Using lubrication theory, these equations may be reduced to the following ones:

$$\left.\begin{aligned} &\textbf{(a)} \quad \frac{\partial^2 u}{\partial z^2} = \frac{1}{\mu}\frac{\partial p}{\partial x} \\ &\textbf{(b)} \quad \frac{\partial p}{\partial z} = 0 \end{aligned}\right\} \quad \textbf{(*)}$$

Thin Films

For an incompressible fluid the continuity equation is unaffected by lubrication theory:

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0$$

Here p is the fluid pressure, (u, w) is the velocity vector and μ is the fluid viscosity.

The boundary conditions for solving this problem are

(**) $u(x, z, t) = 0|_{z=0}$ no-slip condition

$w(x, z, t) = 0|_{z=0}$ no penetration through the bottom surface

Pressure difference across the free surface is taken to balance surface tension forces:

$$p - p_a = -\sigma \frac{\partial^2 h}{\partial x^2}$$

where p_a is the ambient pressure (which may vary over the fluid surface), and σ is the surface tension.

Another boundary condition at the interface is

(***) $$\left.\frac{\partial u}{\partial z}\right|_{z=h} = \frac{\tau}{\mu}$$

where τ is the shear stress caused by the air flow.

Thin Films

At the interface $z = h(x,t)$ the kinematic boundary condition is

$$\frac{D(z - h(x,t))}{Dt} = E$$

where E is the evaporation rate and

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + w\frac{\partial}{\partial z}$$

Then

$$\frac{D(z - h(x,t))}{Dt} = -h_t + u(-h_x) + w \cdot 1,$$

so the kinematic condition can be written as

$$w = E + h_t + uh_x$$

Integrate the continuity equation

$$0 = \int_0^{z=h(x,t)} \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z}\right) dz = \int_0^{z=h(x,t)} \frac{\partial u}{\partial x} dz + w|_{z=0}^{z=h(x,t)}$$

$$= \int_0^{z=h(x,t)} \frac{\partial u}{\partial x} dz + w(x,z,t)|_{z=h} - w(x,z,t)|_{z=0}.$$

Thin Films

Using the kinematic condition on the interface and zero normal velocity at $z = 0$, we have

$$0 = \int_0^{z=h(x,t)} \frac{\partial u}{\partial x} dz + E + \frac{\partial h}{\partial t} + \left(u(x,z,t) \frac{\partial h}{\partial x} \right) \Big|_{z=h(x,t)}.$$

Hence

$$\int_0^{z=h(x,t)} \frac{\partial u}{\partial x} dz = -E - \frac{\partial h}{\partial t} - \left(u(x,z,t) \frac{\partial h}{\partial x} \right) \Big|_{z=h(x,t)}.$$

Considering (*) we get pressure is the function of x alone: $p = p(x)$.

So by integrating (a) we obtain

$$\frac{\partial u}{\partial z} = z \frac{\partial p}{\partial x} + C_1$$

where the constant of integration C_1 can be found by using the boundary condition from the shear stress

(***)

Another integration gives $u(x,z,t) = \frac{z^2}{2} \frac{\partial p}{\partial x} + C_1 z + C_2$.

Thin Films

Using the no-slip condition **(**)** we get $C_2 = 0$.

Hence, the velocity profile is

$$u(x,z,t) = \frac{z^2}{2}\frac{\partial p}{\partial x} + \left(\frac{\tau}{\mu} - h\frac{\partial p}{\partial x}\right) z.$$

Consider rate of the change of the mass flux with respect to x.

$$\frac{\partial}{\partial x} Q(x,t) = \frac{\partial}{\partial x}\int_0^{z=h(x,t)} u(x,z,t)dz = -E - \frac{\partial h}{\partial t}.$$

$$\frac{\partial}{\partial x}\int_0^{z=h(x,t)} u(x,z,t)dz = \frac{\partial}{\partial x}\int_0^{z=h(x,t)} \left\{\frac{z^2}{2}\frac{\partial p}{\partial x} + \left(\frac{\tau}{\mu} - h\frac{\partial p}{\partial x}\right) z\right\} dz =$$

$$\frac{\partial}{\partial x}\left\{\frac{z^3}{6}\frac{\partial p}{\partial x} + \left(\frac{\tau}{\mu} - h\frac{\partial p}{\partial x}\right)\frac{z^2}{2}\right\}\Big|_0^{z=h(x,t)} =$$

$$\frac{\partial}{\partial x}\left\{\frac{h^3}{6}\frac{\partial p}{\partial x} + \left(\frac{\tau}{\mu} - h\frac{\partial p}{\partial x}\right)\frac{h^2}{2}\right\} = \frac{\partial}{\partial x}\left\{-\frac{h^3}{3}\frac{\partial p}{\partial x} + \frac{\tau}{\mu}\frac{h^2}{2}\right\}.$$

Thin Films

Therefore,

$$E + \frac{\partial}{\partial x}\left\{-\frac{h^3}{3}\frac{\partial p}{\partial x} + \frac{\tau}{\mu}\frac{h^2}{2}\right\} = -\frac{\partial h}{\partial t},$$

which represents the mass conservation of the fluid.

by using $p = p_a - \sigma\frac{\partial^2 h}{\partial x^2}$. Also we are mostly concerned with the film length at steady state. $\frac{\partial h}{\partial t} = 0$

so we get an ordinary differential equation on h

$$E + \frac{\partial}{\partial x}\left\{\frac{\sigma}{3}\frac{h^3}{\mu}\frac{\partial^3 h}{\partial x^3} + \frac{\tau}{\mu}\frac{h^2}{2}\right\} = 0.$$

by using the boundary condition

$$Q(x)|_{x=0} = Q_0 = \int_0^h u(z)\,dz = \int_0^h \frac{\tau}{\mu} z\,dz = \frac{\tau}{2\mu}h^2$$

$$Ex + \left(\frac{\tau}{\mu}\frac{h^2}{2} + \frac{h^3}{3\mu}\sigma h_{xxx}\right) = Q_0.$$

We can neglect the term with the high derivative of h since the surface tension is small to get an estimate for the height h

$$h \sim \sqrt{\frac{2\mu}{\tau}(Q_0 - Ex)}$$

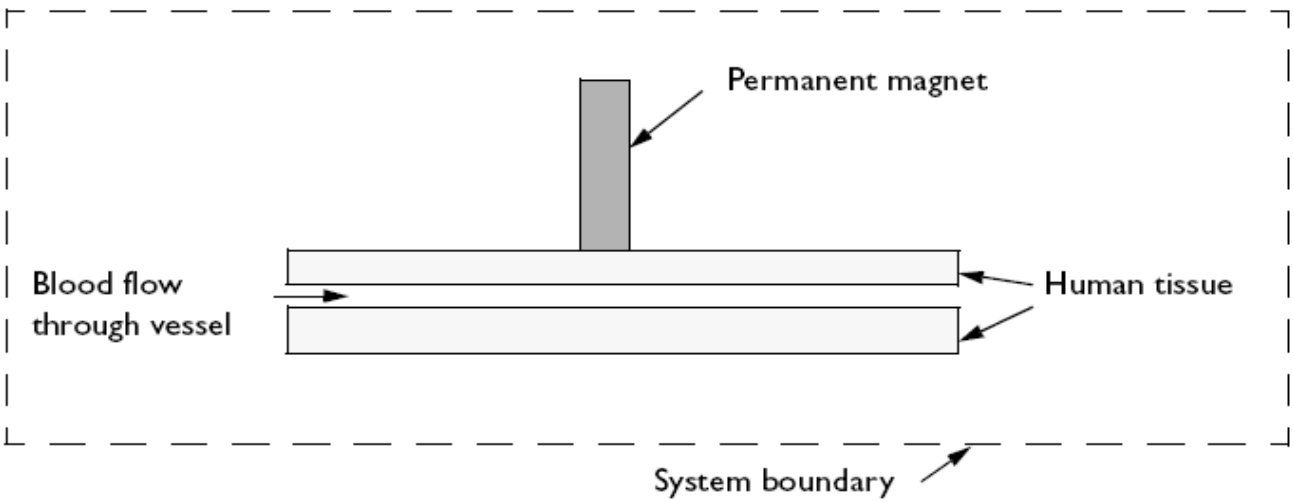
MODEL EXAMPLE: MAGNETIC DRUG TARGETING

Magnetic Drug Targeting

1. Background of the problem

Current research on methods to target chemotherapy drugs in the human body includes the investigation of bio-compatible magnetic nanocarrier systems. For example, magnetic liquids such as ferrofluids can play an important role as drug carriers in the human body (Ref. 1). As such, they can be used for drug targeting in modern locoregional cancer treatment. A remaining challenge for this medical application is the choice of clinical setting. Important parameters are optimal adjustment of the external magnetic field and the choice of ferrofluid properties.

2. Graphic idealization of the model



3. Actual Mathematical Model

MAGNETOSTATIC EQUATIONS

Maxwell-Ampere's law

$$\nabla \times \mathbf{H} = \mathbf{J} \qquad (1)$$

magnetic field $\mathbf{H}$ (A/m) and the current density $\mathbf{J}$ (A/m^2)

Gauss' law for the magnetic flux density $\mathbf{B}$ (Vs/m^2)

$$\nabla \cdot \mathbf{B} = 0 . \qquad (2)$$

The constitutive equations describing the relation between $\mathbf{B}$ and $\mathbf{H}$ in the different parts of the modeling domain read:

$$\mathbf{B} = \begin{cases} \mu_0 \mu_{r,\,mag} \mathbf{H} + \mathbf{B}_{rem} & \text{permanent magnet} \\ \mu_0 (\mathbf{H} + \mathbf{M}_{ff}(\mathbf{H})) & \text{blood stream} \\ \mu_0 \mathbf{H} & \text{tissue and air} \end{cases} \qquad (3)$$

Here μ_0 is the magnetic permeability of vacuum (Vs/(A·m)); μ_r is the relative magnetic permeability of the permanent magnet (dimensionless); $\mathbf{B}_{rem}$ is the remanent magnetic flux (A/m); and $\mathbf{M}_{ff}$ is the magnetization vector in the blood stream (A/m), which is a function of the magnetic field, $\mathbf{H}$.

Magnetic Drug Targeting

Defining a magnetic vector potential **A** such that

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \nabla \cdot \mathbf{A} = 0\,, \tag{4}$$

you finally, by substitution in Equation 1 through Equation 3, arrive at the following vector equation to solve:

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{A} - \mathbf{M} \right) = \mathbf{J}$$

Simplifying to a 2D problem with no perpendicular currents, this equation reduces to

$$\nabla \times \left(\frac{1}{\mu_0} \nabla \times \mathbf{A} - \mathbf{M} \right) = \mathbf{0}\,. \tag{5}$$

Note that this equation assumes that the magnetic vector potential has a nonzero component only perpendicularly to the plane, $\mathbf{A} = (0, 0, A_z)$.

Magetic Drug Targeting

the induced magnetization $\mathbf{M}_{\mathrm{ff}}(x, y) = (M_{\mathrm{ffx}}, M_{\mathrm{ffy}})$ of a ferrofluid

$$M_x = \frac{\chi}{\mu_0}\frac{\partial A_z}{\partial y}$$
$$M_y = -\frac{\chi}{\mu_0}\frac{\partial A_z}{\partial x} \qquad (6)$$

where $\chi = \alpha\beta$ is the magnetic susceptibility.

Magnetic Drug Targeting

FLUID FLOW EQUATIONS

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{F} \qquad (7)$$

$$\nabla \cdot \mathbf{u} = 0$$

where η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ the velocity (m/s), ρ the fluid density (kg/m^3), p the pressure (N/m^2), and $\mathbf{F}$ a volume force (N/m^3).

With the assumption that the magnetic nanoparticles in the fluid do not interact, the magnetic force $\mathbf{F} = (F_x, F_y)$ on the ferrofluid for relatively weak fields is given by $\mathbf{F} = |\mathbf{M}|\nabla|\mathbf{H}|$. Using Equation 3, Equation 4, and Equation 6 then leads to the expressions

$$F_x = \frac{\chi}{\mu_0 \mu_r^2}\left(\frac{\partial A_z}{\partial x}\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial A_z}{\partial y}\frac{\partial^2 A_z}{\partial x \partial y}\right)$$

$$F_y = \frac{\chi}{\mu_0 \mu_r^2}\left(\frac{\partial A_z}{\partial x}\frac{\partial^2 A_z}{\partial x \partial y} + \frac{\partial A_z}{\partial y}\frac{\partial^2 A_z}{\partial y^2}\right)$$

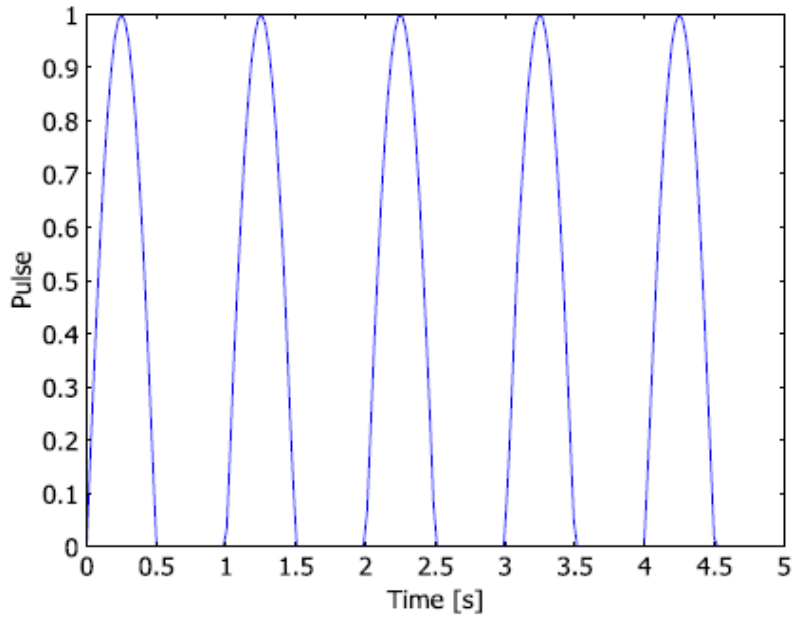
Magnetic Drug Targeting

Boundary Conditions

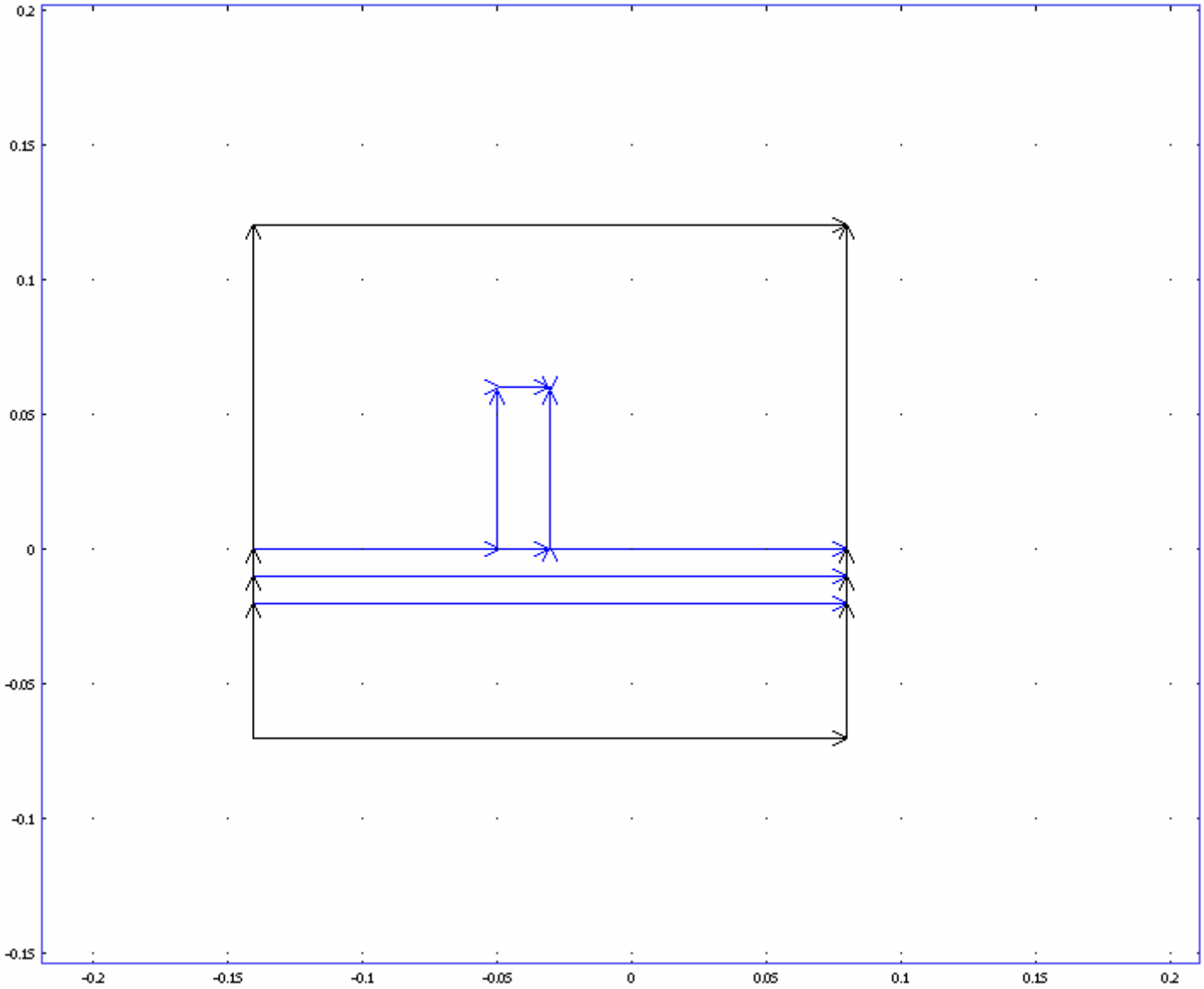
On the vessel walls, apply no-slip conditions, $u = v = 0$. At the outlet, you can set an outlet pressure condition, $p = 0$. At the inlet boundary, specify a parabolic flow profile on the normal inflow velocity according to $4U_m s(1-s)$, where s is a boundary segment length parameter that goes from 0 to 1 along the inlet boundary segment and U_m is the maximal flow velocity. To emulate the heart beat, the inflow velocity follows a sinusoidal expression in time:

$$U_0 = 2U_m s(1-s)(\sin(\omega t) + \sqrt{\sin(\omega t)^2})$$

Selecting the angular velocity ω to be 2π rad/s gives a heart beat rate of 60 beats per minute. Figure 2 displays the resulting expression (normalized to unity).

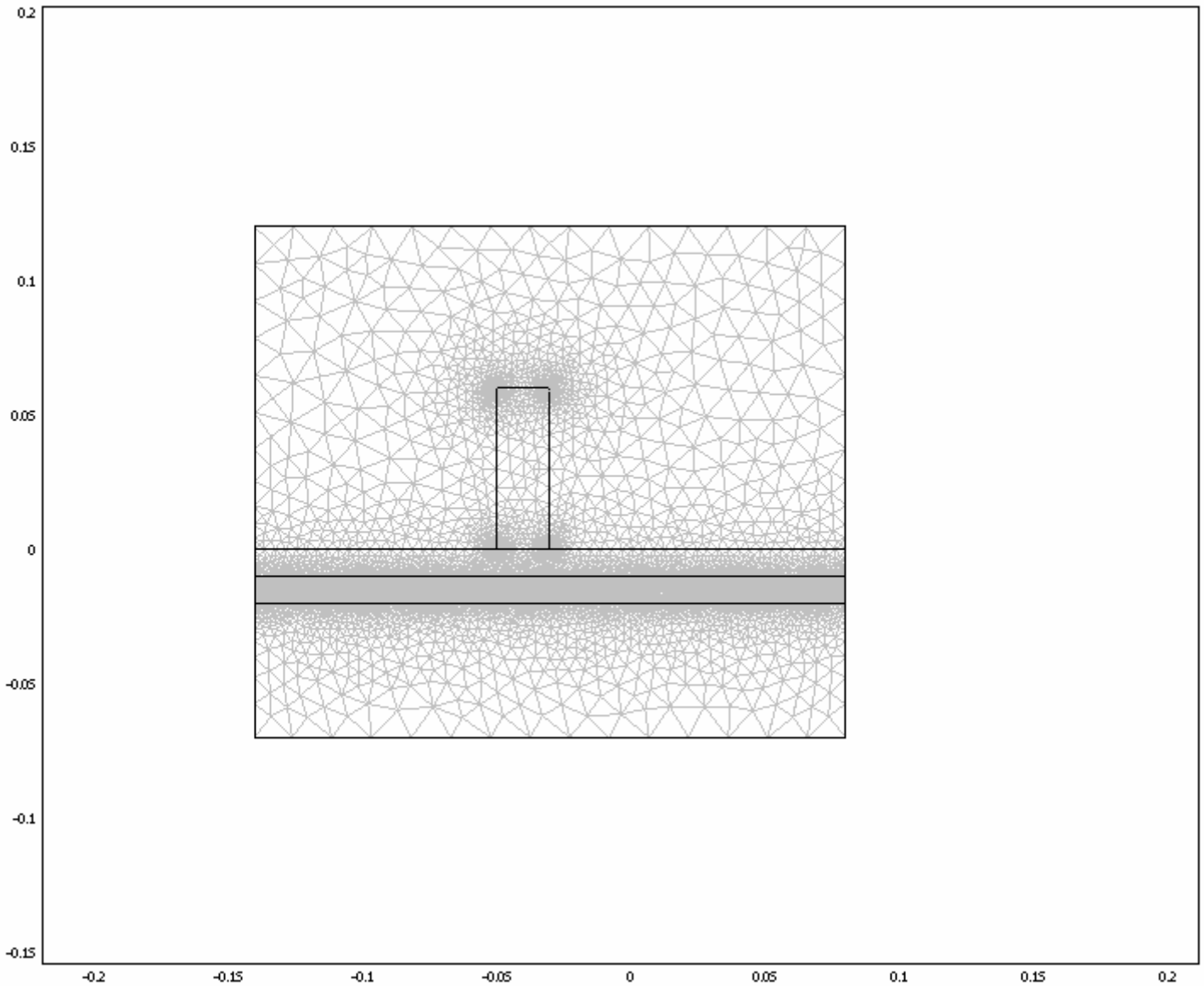


4. Domain definition and meshing



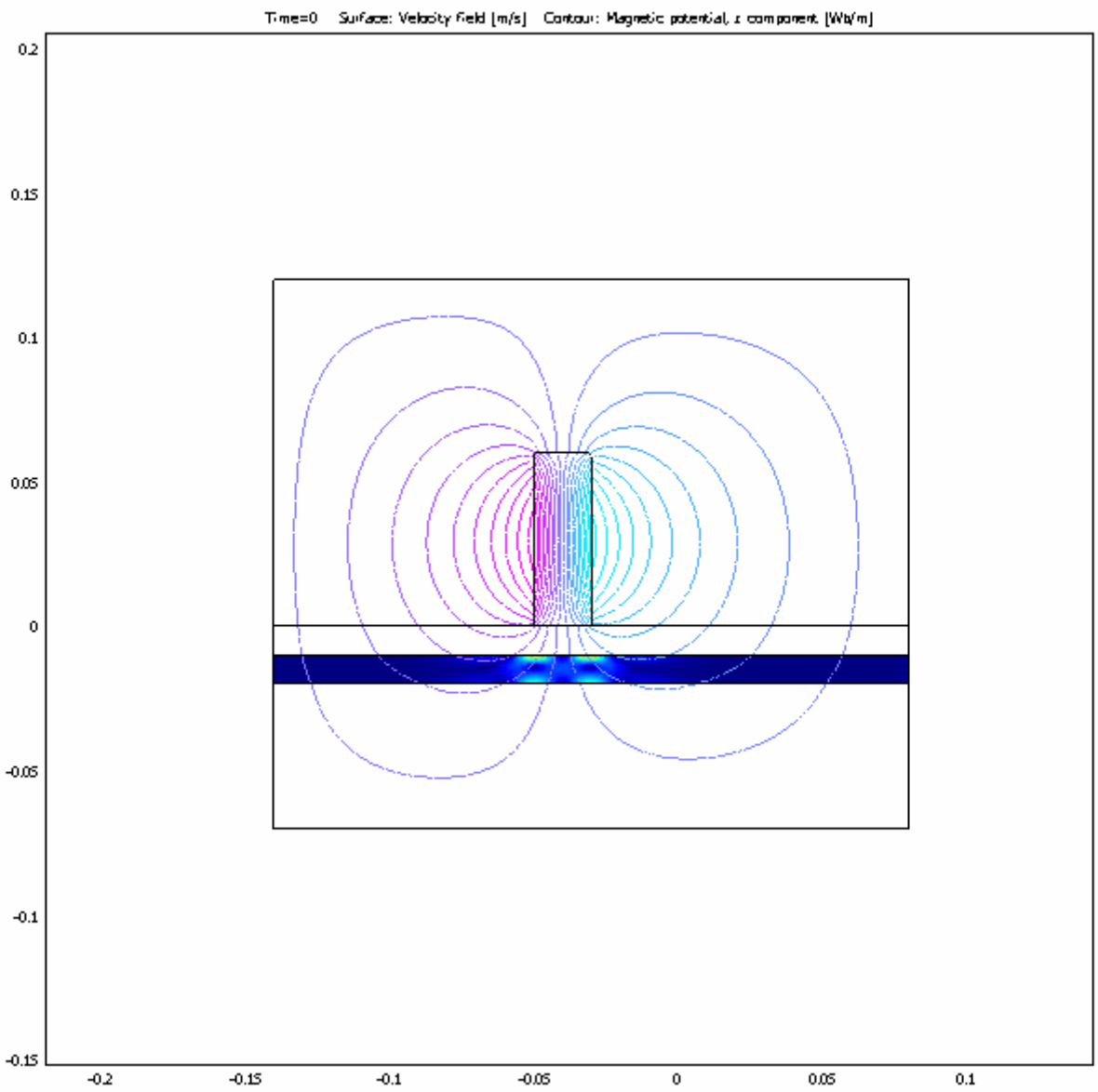
Computational Diagnostics & Biocybernetics Unit

Magnetic Drug Targeting



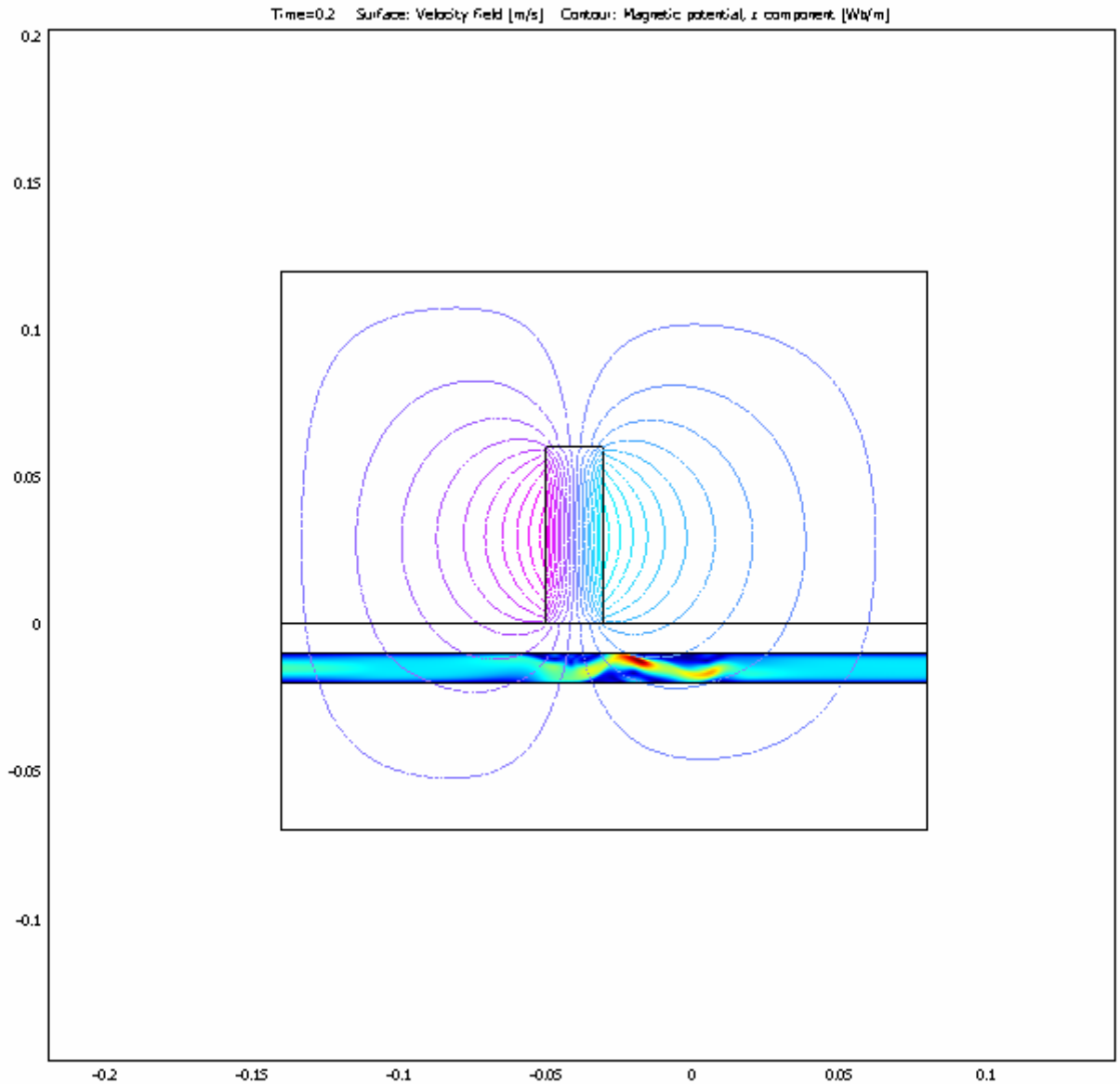
Computational Diagnostics & Biocybernetics Unit

Magnetic Drug Targeting



Computational Diagnostics & Biocybernetics Unit

Magnetic Drug Targeting



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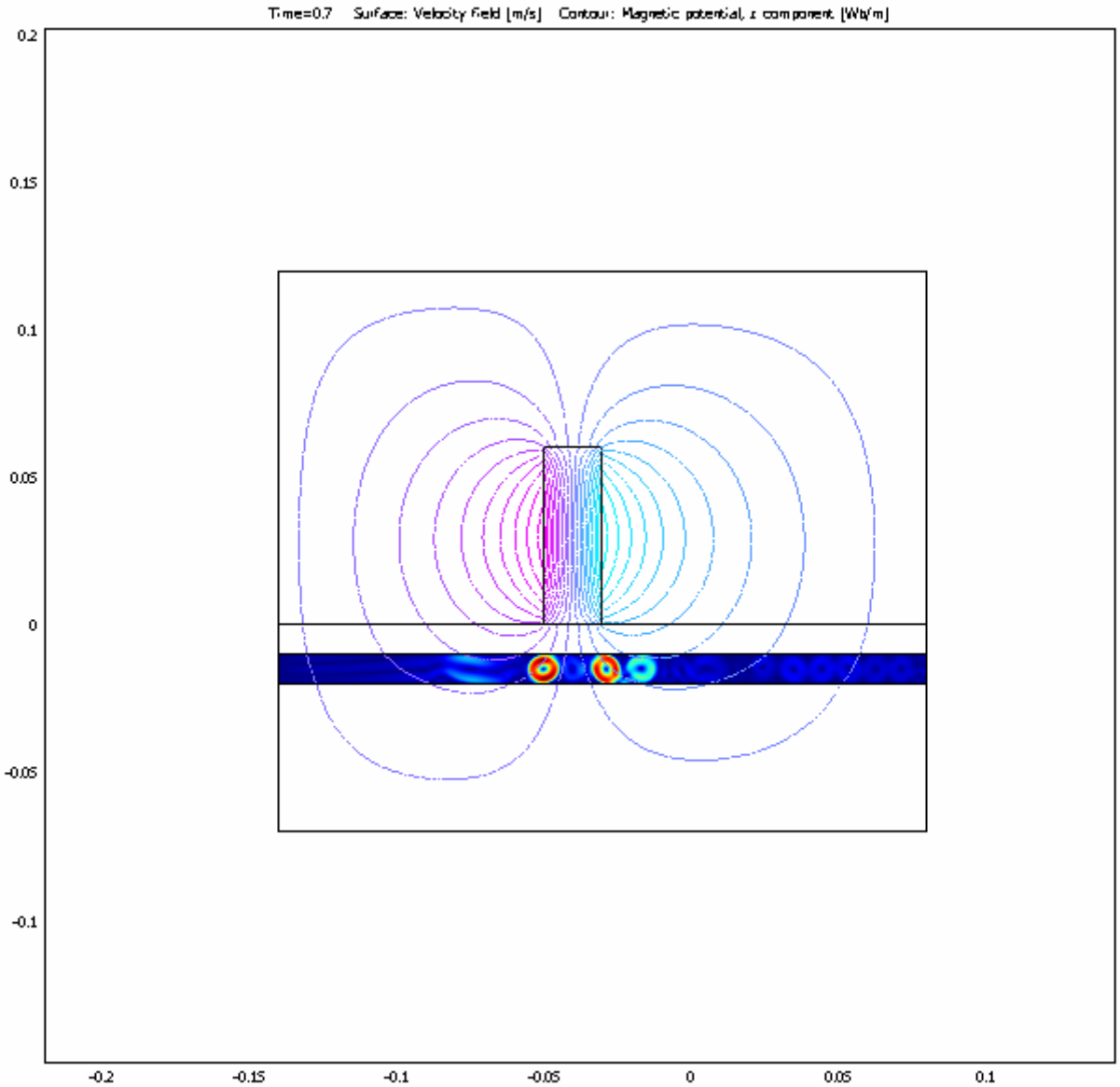
Magnetic Drug Targeting



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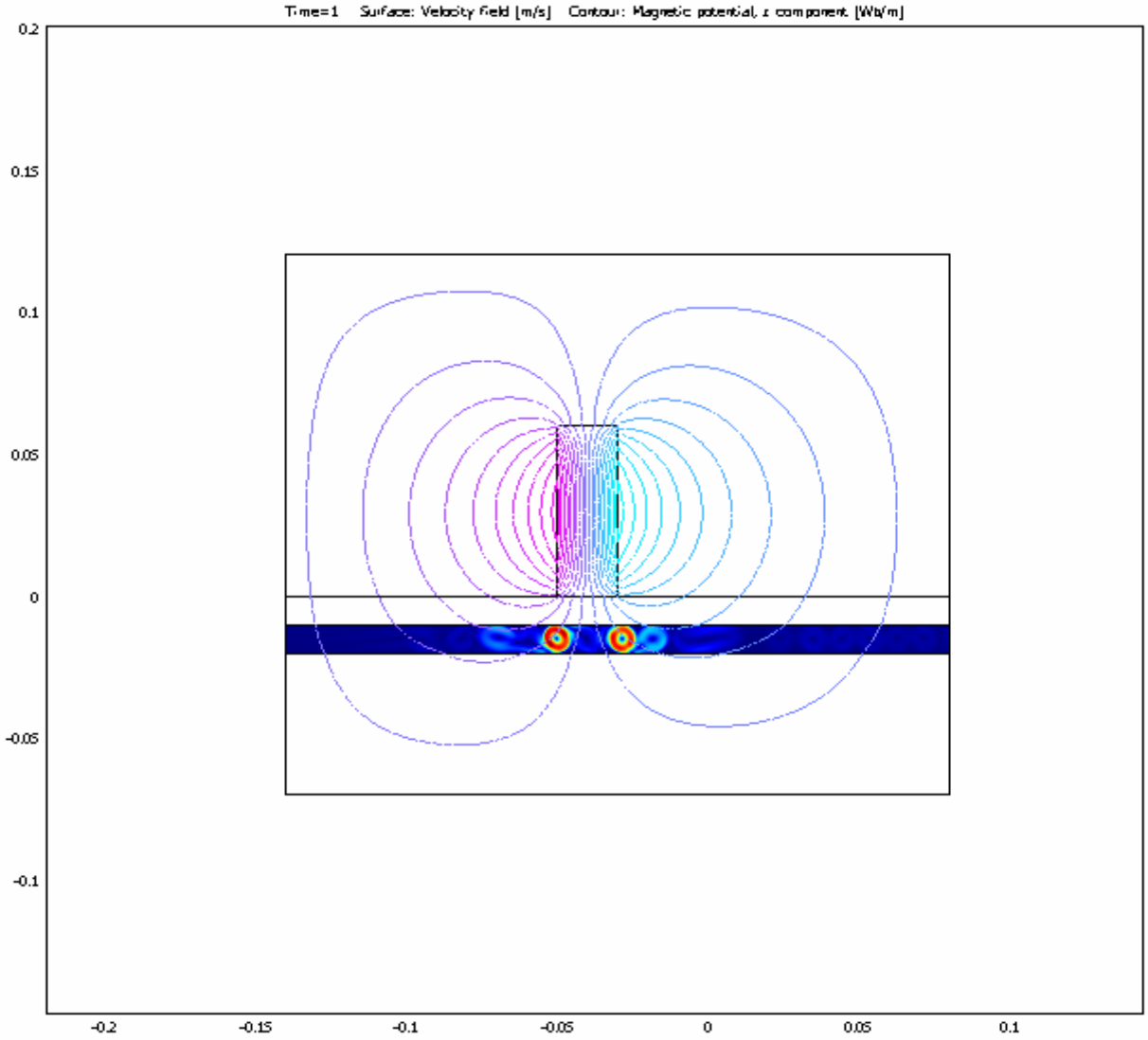
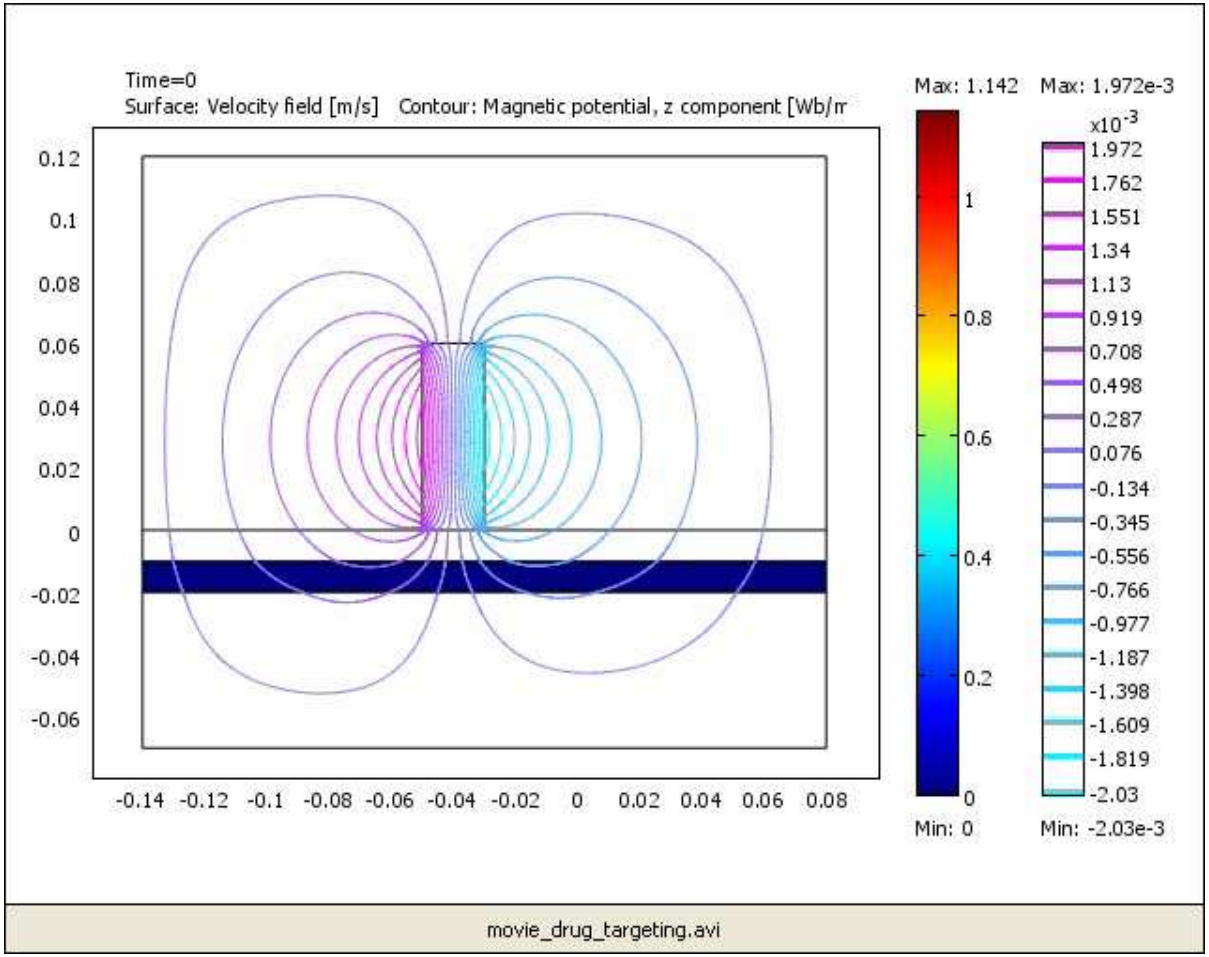
Magnetic Drug Targeting

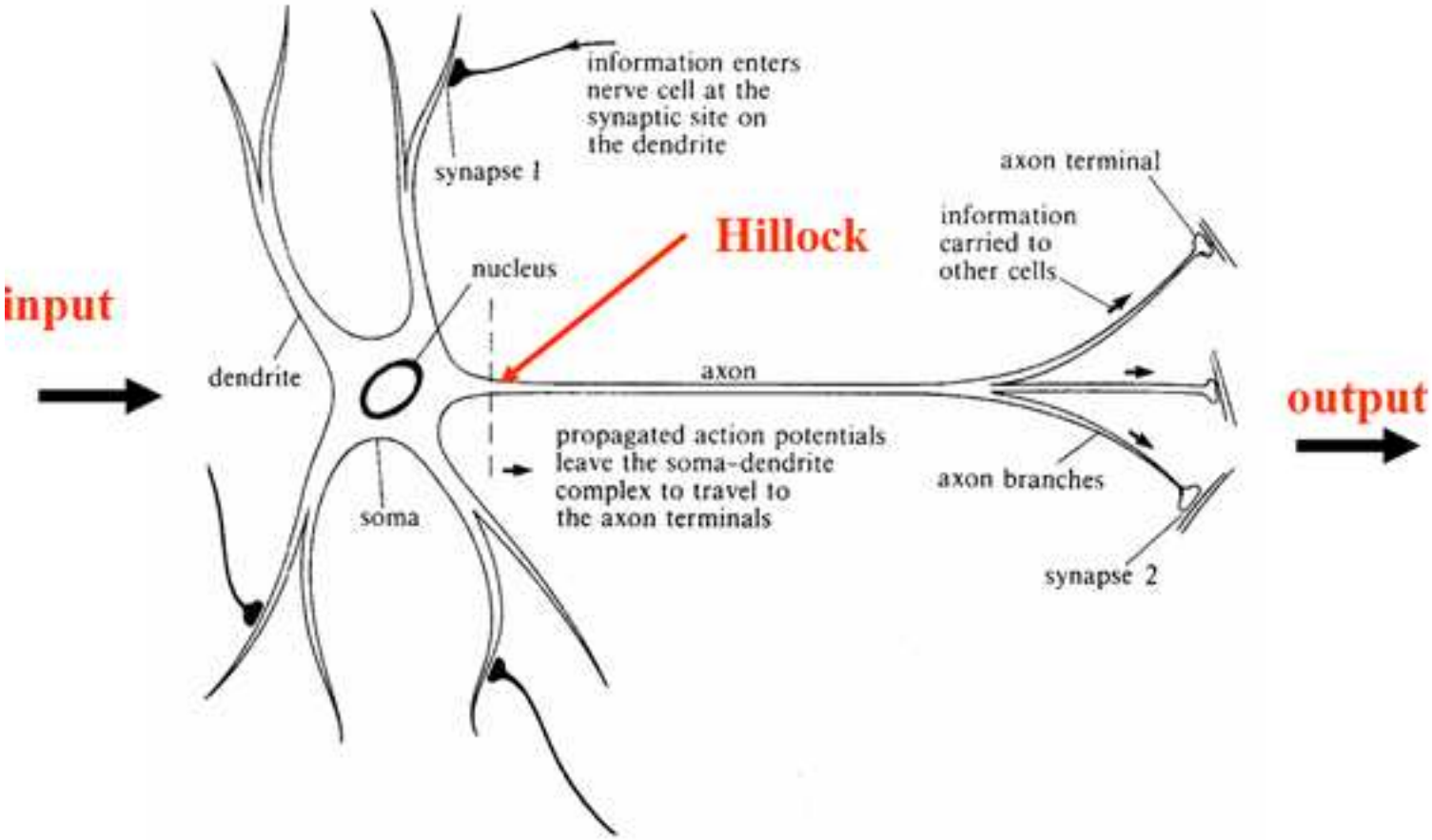


Magnetic Drug Targeting

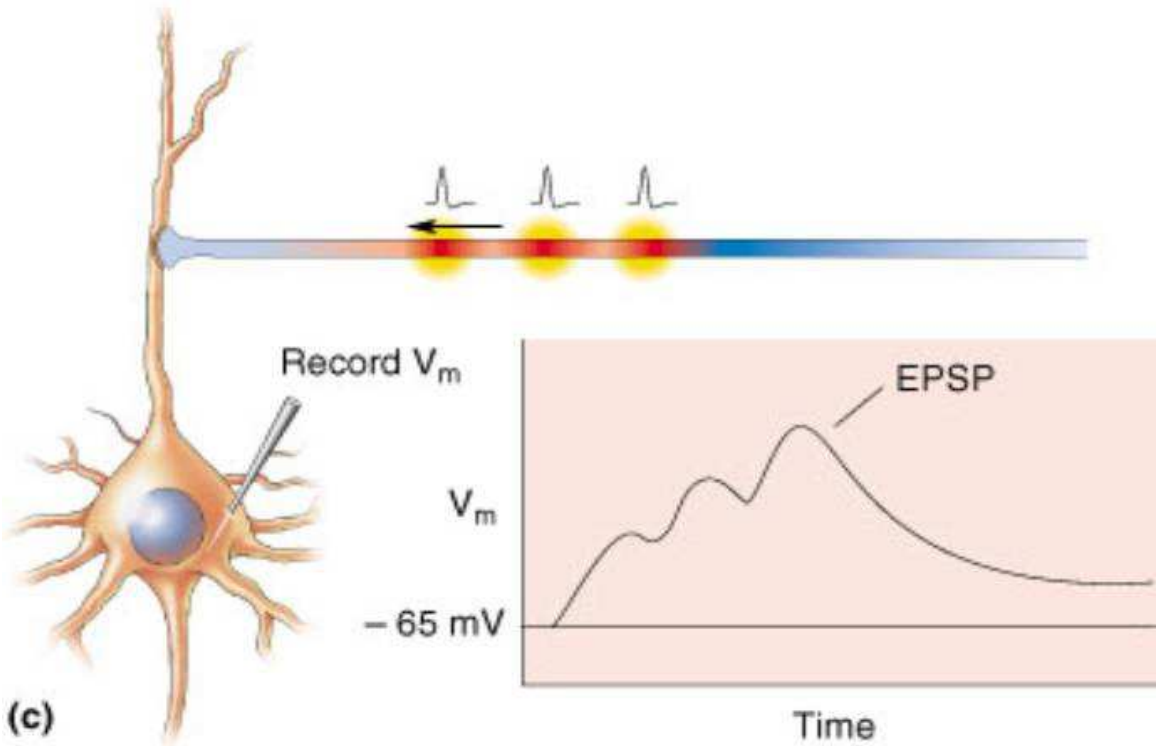


Modeling Example 3

Modeling in Neuroscience



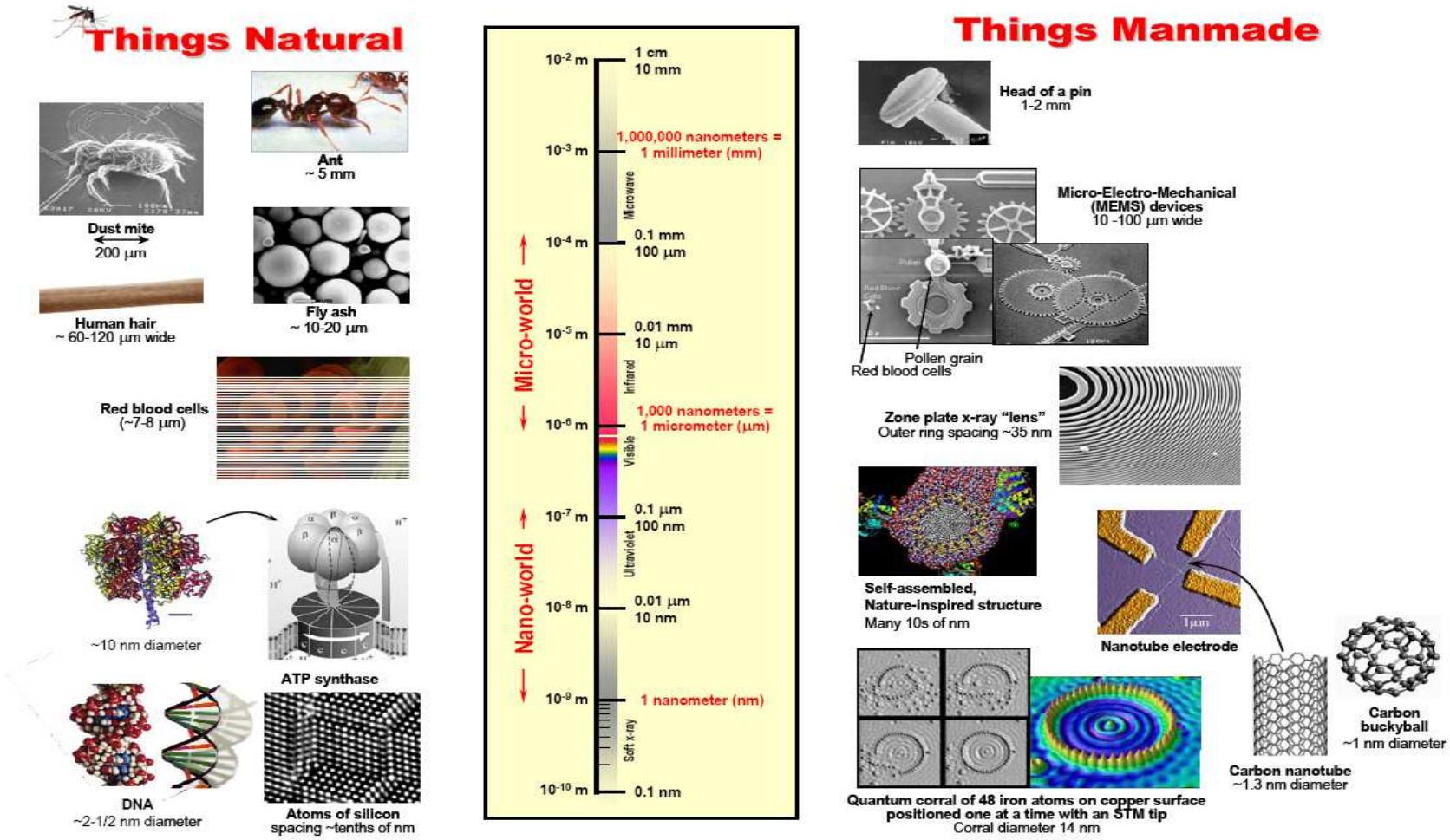
PDE's in Neuroscience



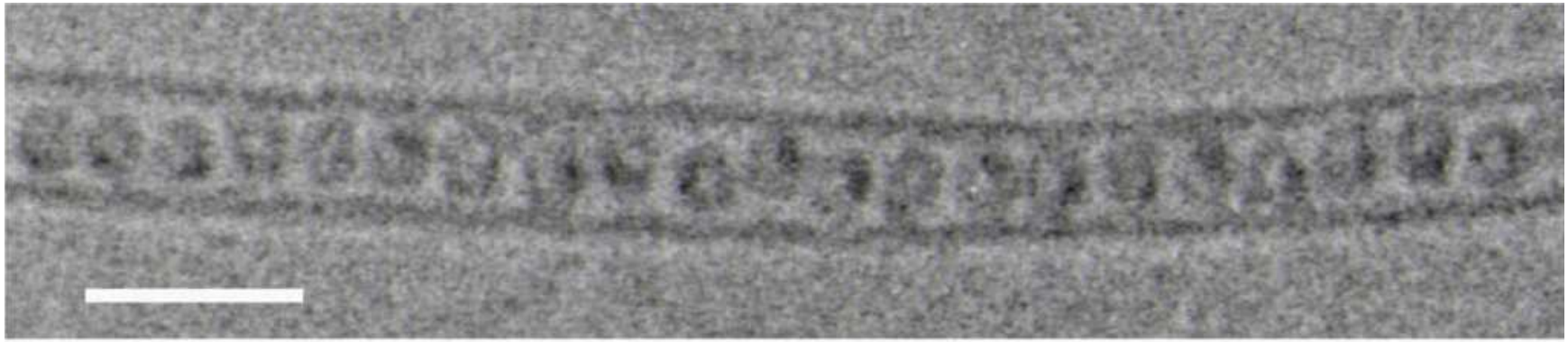
Propagation of axon potentials could be modeled by a partial differential equation, namely the cable equation:

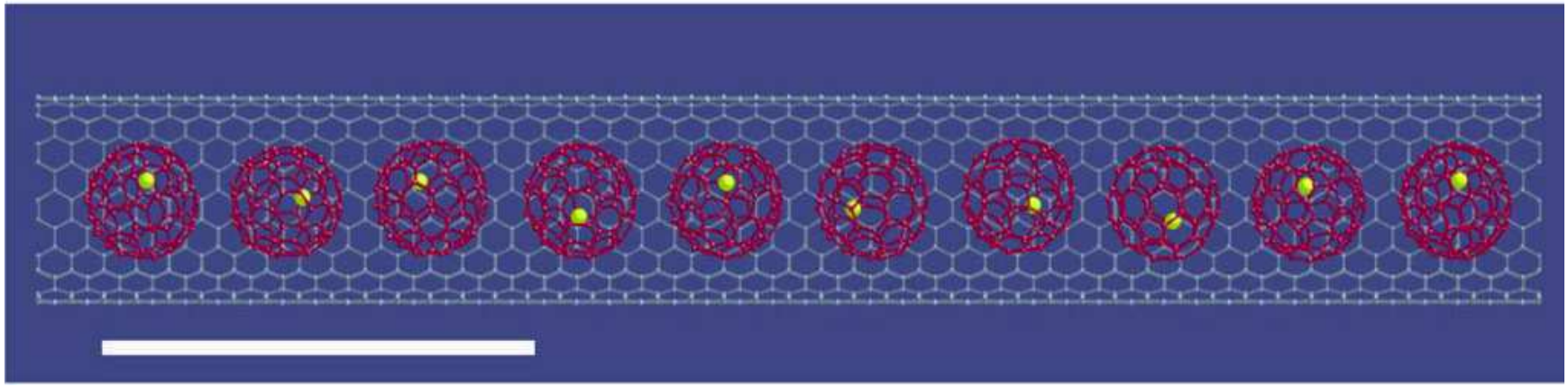
MULTISCALE MODELLING

Why Multiscale Modelling?



Nanotube with Gd–Metallofullerenes





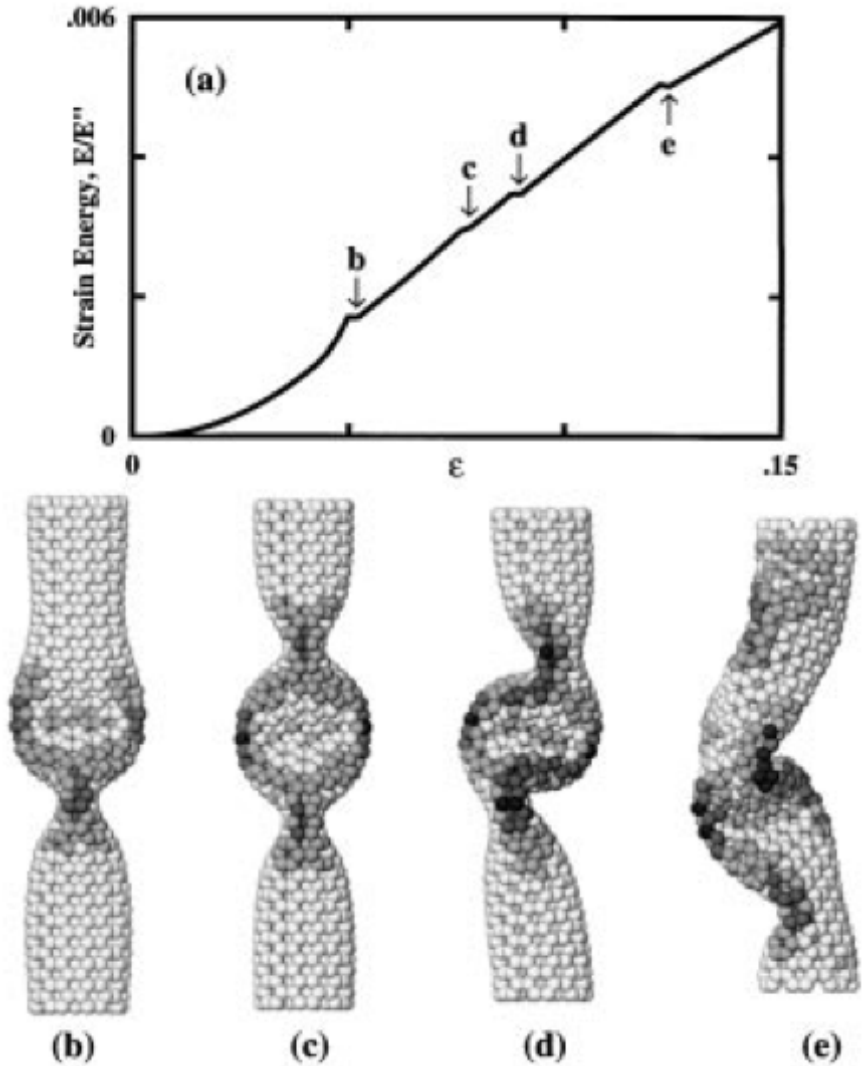
3 nm

K. Suenaga *et al.*, *Science* **290,** 2280 (2000)

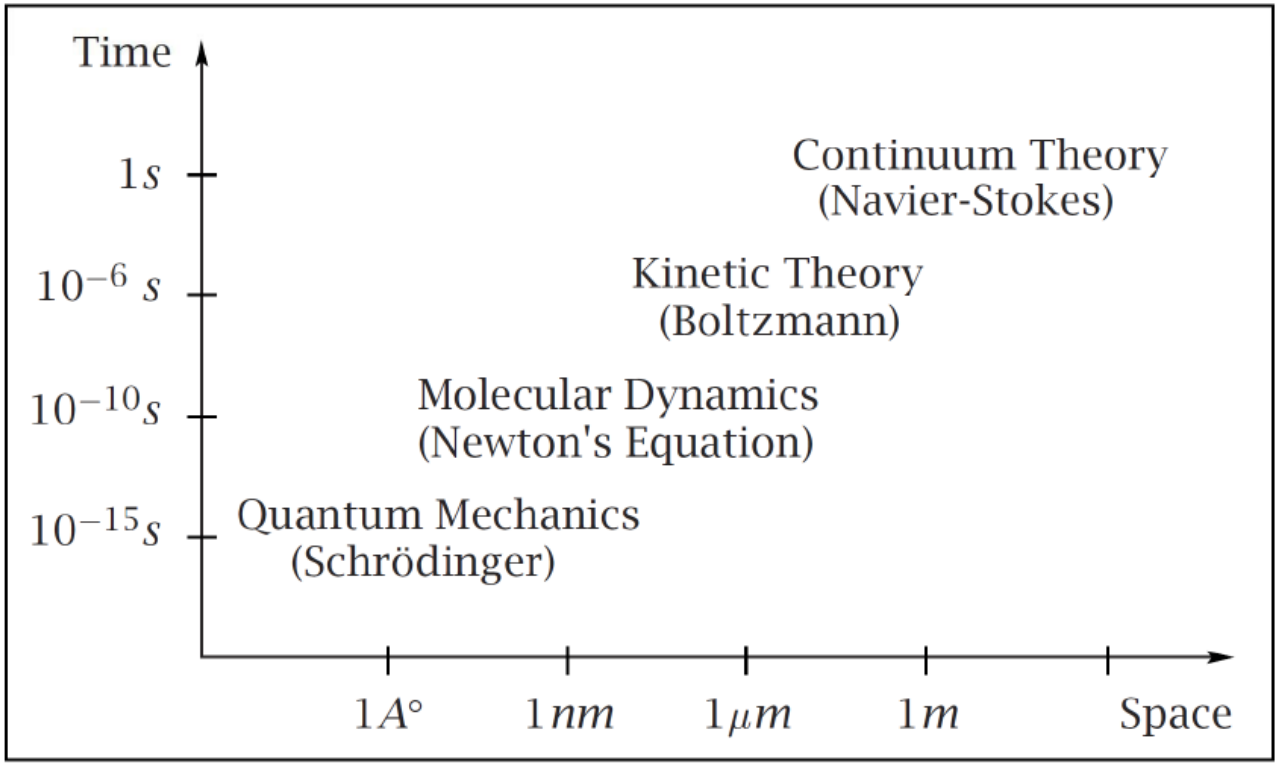
Deformation of Carbon Nanotubes

- axial compression
- Tersoff–Brenner potential

Yakobson *et al.*, *Phys. Rev. Lett.* **76**, 2511 (1996)



Different laws of physics:



What is the main challenge?

Methods for Multiscale Modelling

Sequential Methods

- Separation of length and time scales
- Parameter passing

Concurrent Methods

- Different length and time scales within hybrid scheme
- Typically DFT, MD, continuum (FE); Level set

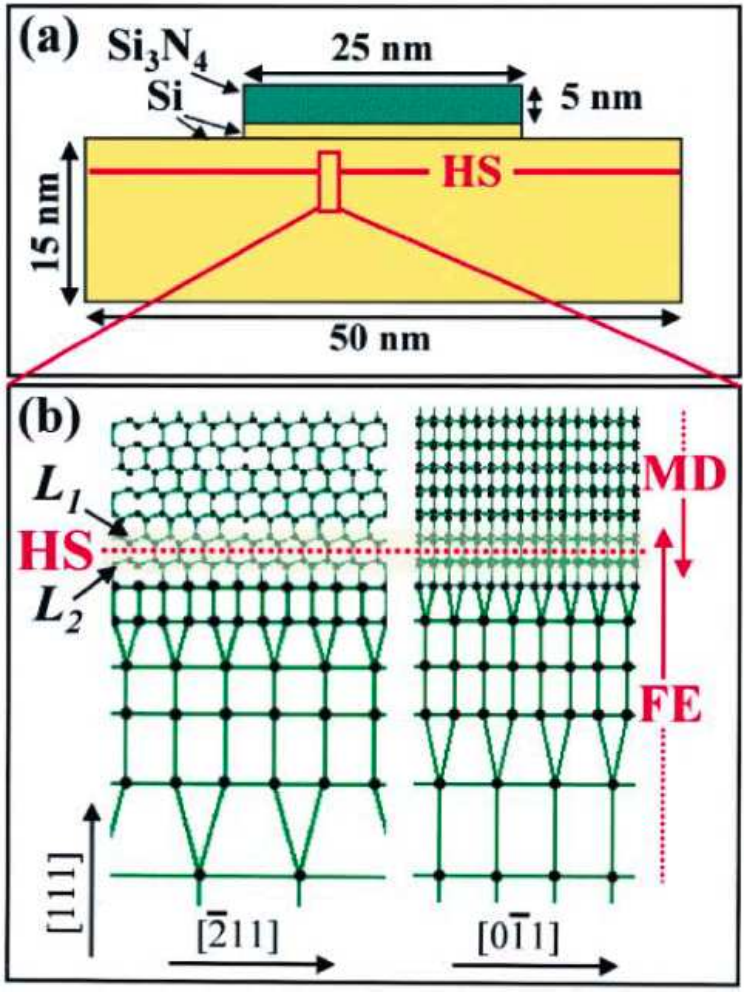
Coarse Graining

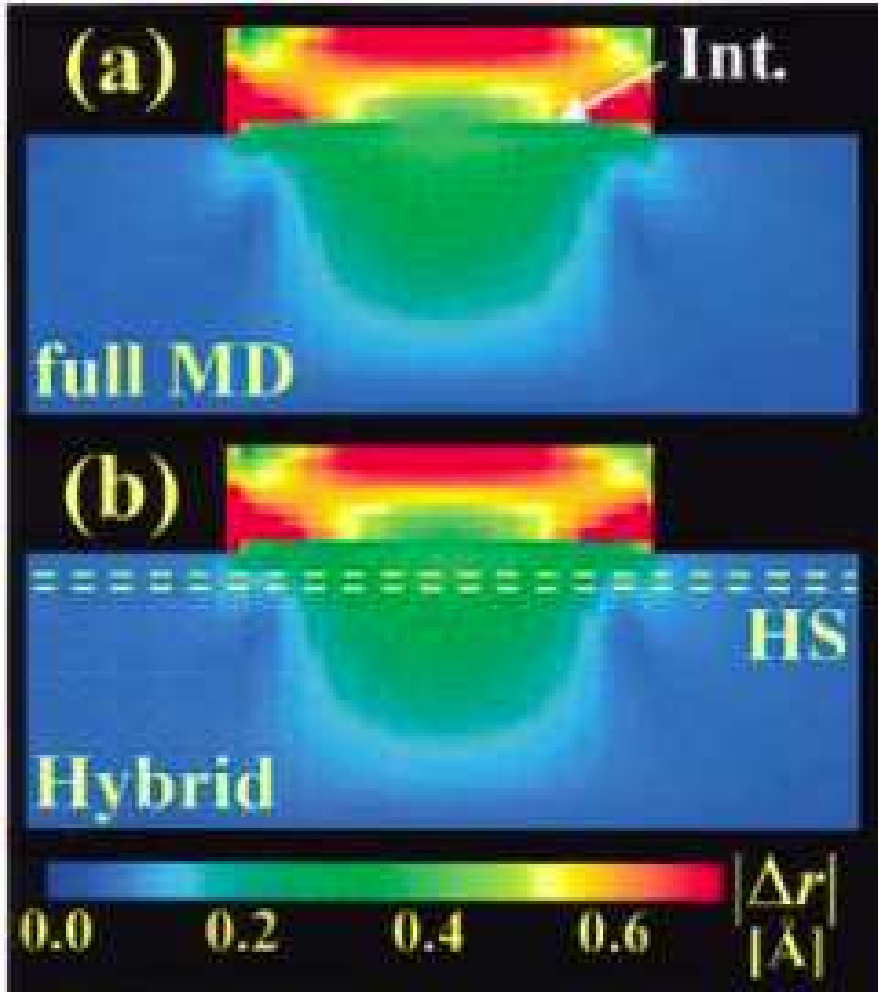
- Integration over fast time scales short length scales

CONCURRENT METHODS

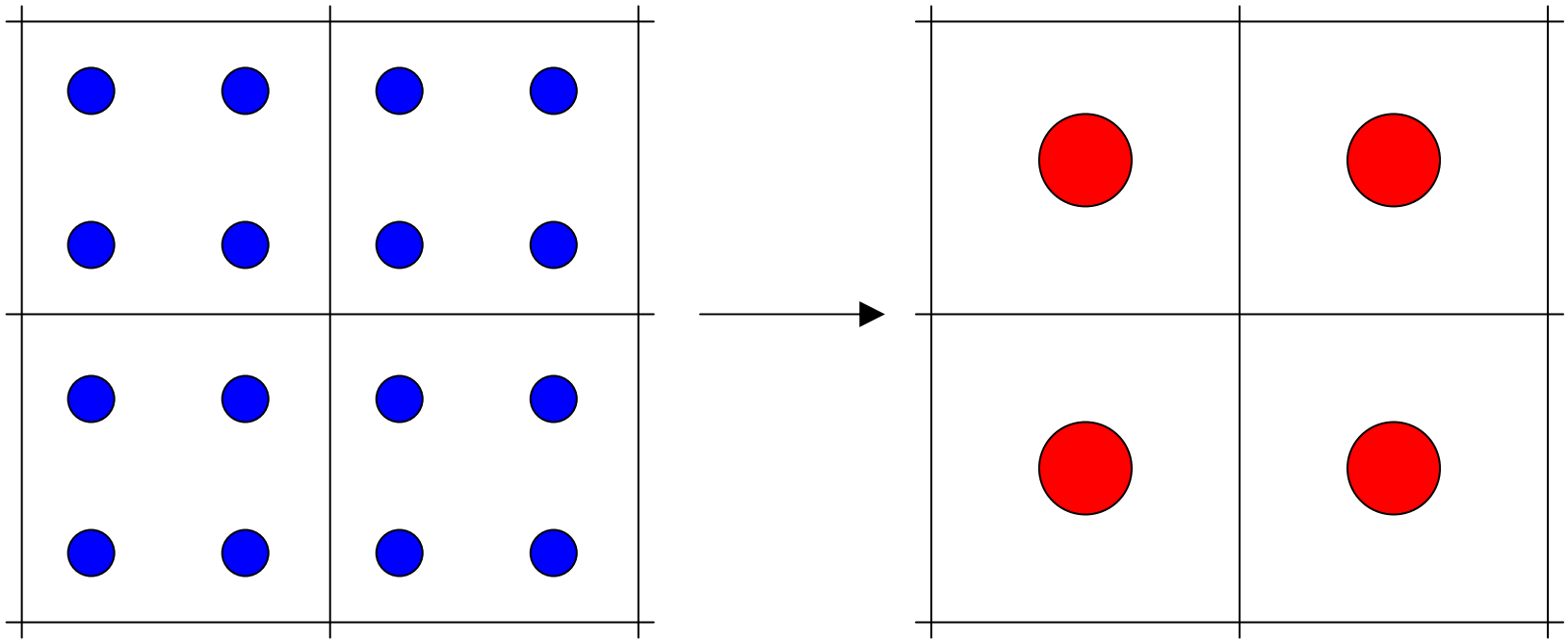
Molecular Dynamics–Finite Element Hybrid

E. Lidikoris *et al.*, *Phys. Rev. Lett.* **87**, 086104 (2001)



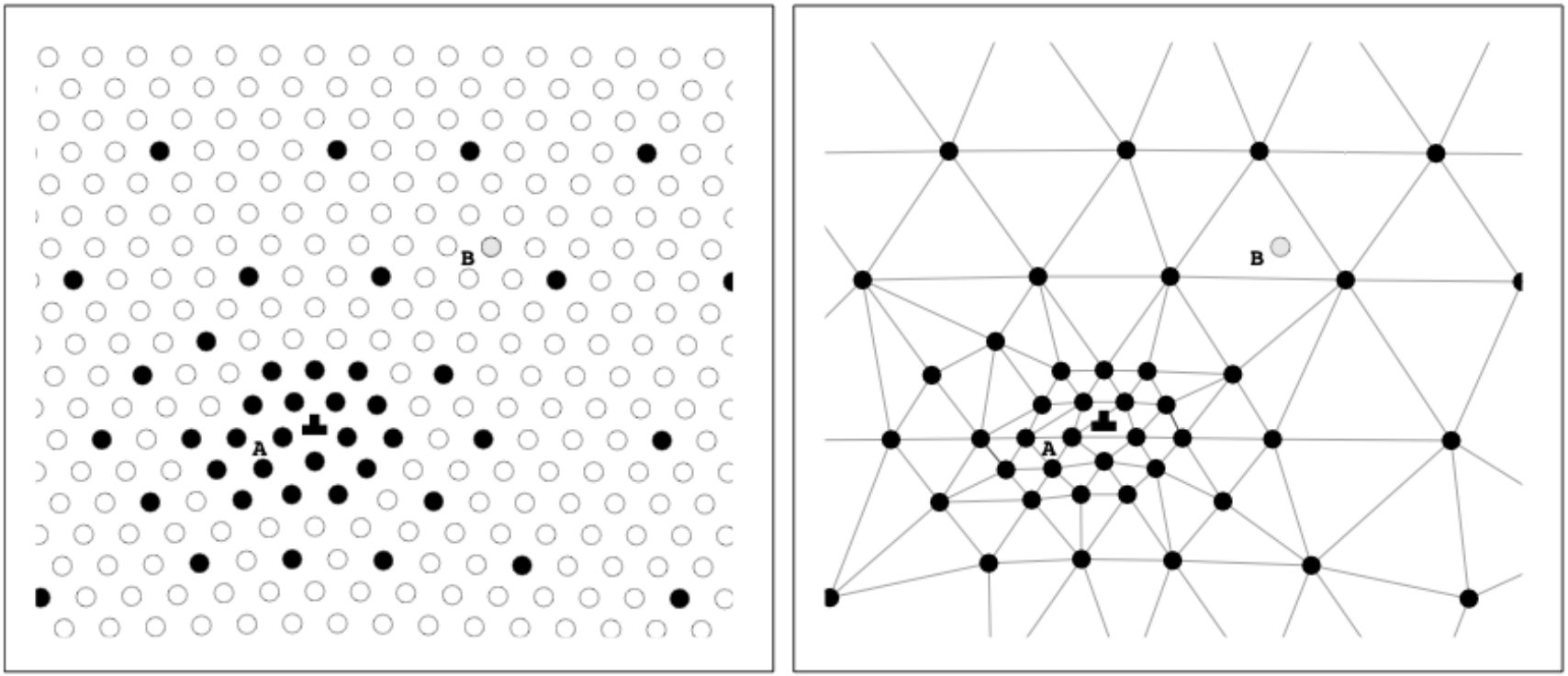


Coarse Graining



Quasicontinuum Method

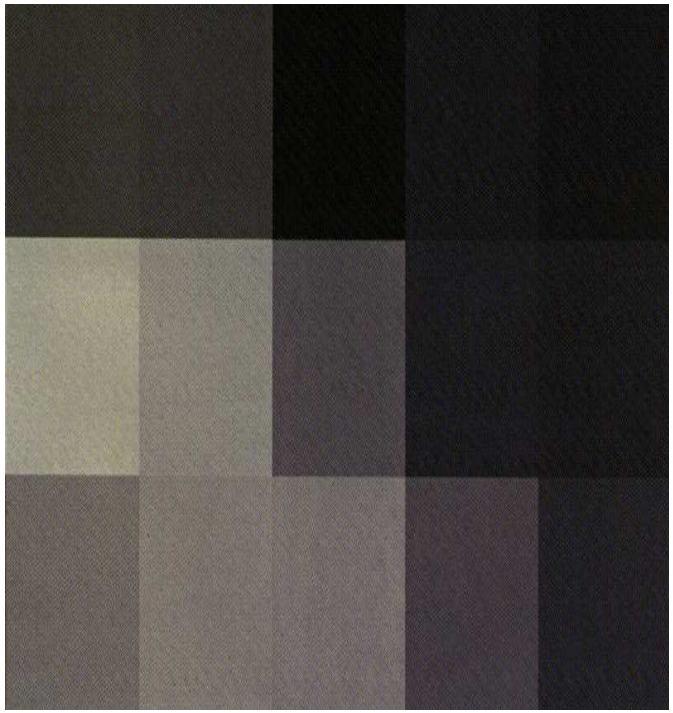
R. E. Miller and E. B. Tadmor, *J. Comput-Aided Mater*. **9**, 203 (2002)



Computational Diagnostics & Biocybernetics Unit

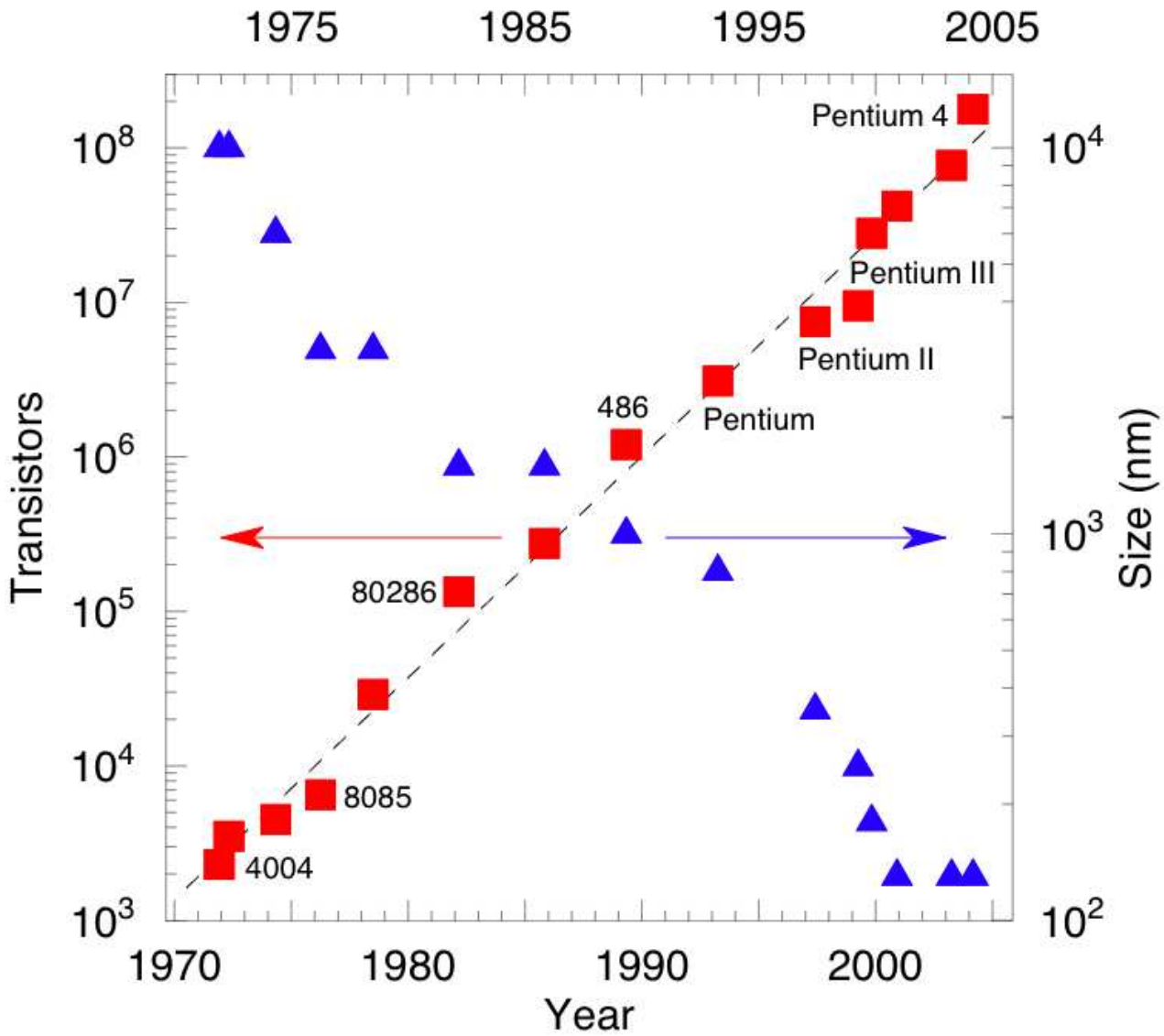
WEATHER MODELING

200 Km resolution



1.5 Km resolution

Satellite Image of the Golf of Mexico

Moore's Law for Computing Power

Source: www.intel.com