WI4014TU – Numerical Analysis for PDE's

Lecture 1
Course Structure and Mathematical Preliminaries

Course Structure

WI4014TU

1. 16 weeks, 1 lecture per week
2. 5 assignments, approximately 4 weeks per assignment
3. **Deadlines for each assignment, see Brightspace. Late uploads will result in point deductions**
4. **Identical parts of reports and codes will be considered plagiarism, and points will be deducted**
5. Assignments should be typeset in LaTeX (use Overleaf), converted to PDF and uploaded on Brightspace
6. Python code should also be uploaded
7. Adhere to the code structure suggested in the assignment
8. Feedback and grade per assignment
9. Deductions are made for all mathematical errors, no matter how small, and for the missing derivations and discussions
10. Course grade is the average grade of all 5 assignments, minimum 5.8

Course materials

1. Main book: J. van Kan, A. Segal, and F. Vermolen, *Numerical Methods in Scientific Computing*, TU Delft Open Textbook, 2023, `https://textbooks.open.tudelft.nl/textbooks/catalog/book/70`
2. Basic numerical analysis book: C. Vuik, F.J. Vermolen, M.J. Vuik, *Numerical Methods for ordinary differential equations*, TU Delft Open Textbook, 2023 `https://textbooks.open.tudelft.nl/textbooks/catalog/book/57`
3. Calculus: J. Stewart, *Calculus: Early Transcendentals*
4. Assignments 1–5 (Brightspace)
5. Additional reading: *The FEniCS Tutorial*, `https://fenicsproject.org/tutorial/`
6. These slides are linked to at Brightspace
7. Install a working Python 3 environment with `numpy`, `scipy`, `matplotlib`, FEniCS package `https://fenicsproject.org`)
8. Consider using Linux (virtual environment or dual-boot)
9. LaTeX environment (Overleaf)

Creating a numerical PDE solver

1. Get your physics, PDE's, and BC's right. Decide 1D, 2D, or 3D?
2. Choose between FD, FV, and FE methods
3. Discretization on paper (required details depend on software choices): matrix elements (FDM, FVM); weak form of PDE's, choice of basis/test functions (FEM)
4. Software implementation:
   - Choose: package (COMSOL, ANSYS), high-level library (FEniCS, Matlab), low-level library (OpenFOAM), from scratch (Python, Matlab, C/C++, FORTRAN)
   - Geometry, materials, mesh, refinement (use software tools)
   - System matrices (automated in packages, difficult from scratch)
   - Non-linear and/or time-domain solver, linear-algebraic solver, preconditioning (use existing libraries)
5. Debug, calibrate, compare with others (difficult, tedious)
6. Study something new, make predictions (have fun)

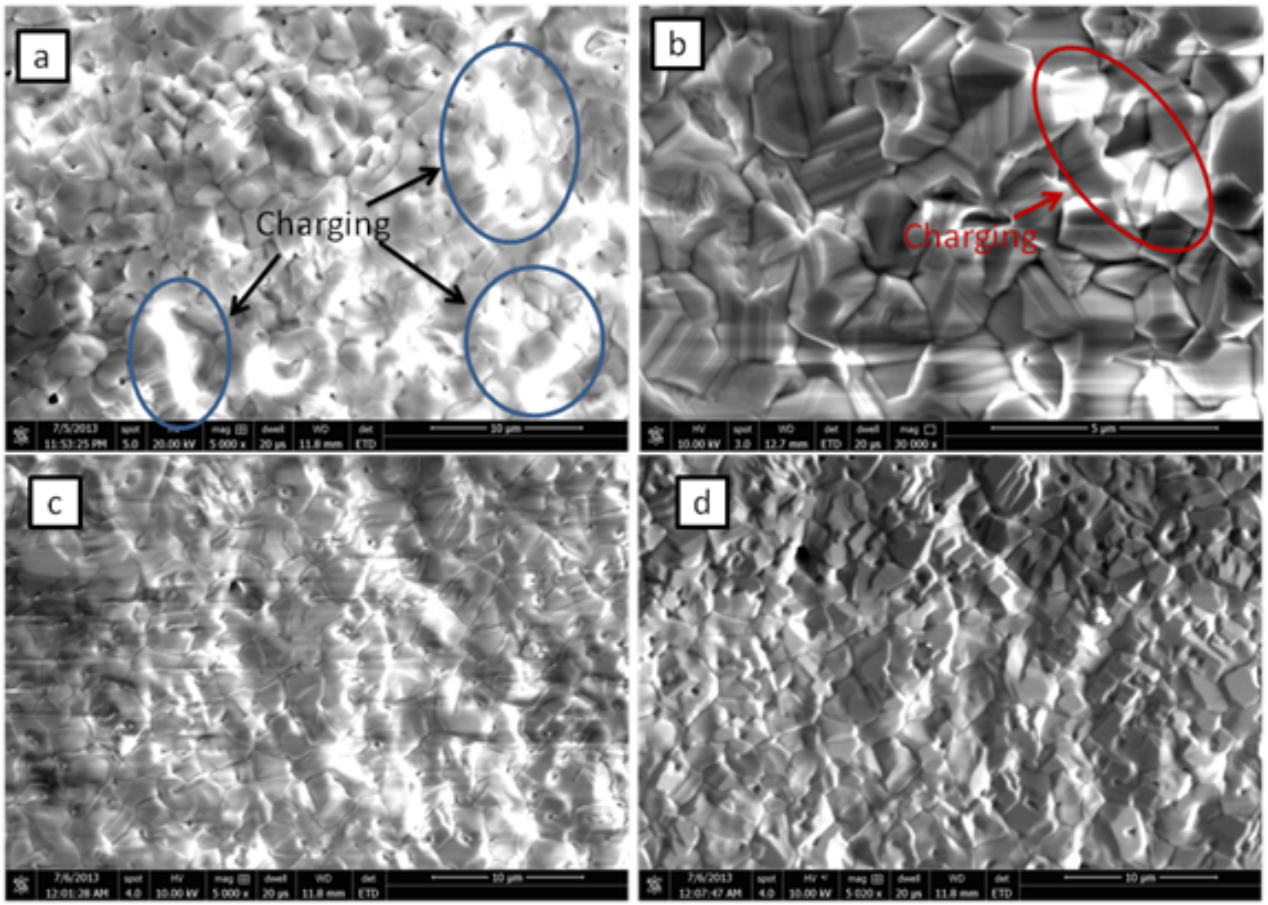
Numerical Analysis of PDE's: A Case Study

Charge injection and transport in insulating materials

B Raftari, NV Budko, C Vuik, Self-consistent drift-diffusion-reaction model for the electron beam interaction with dielectric samples *Journal of Applied Physics*, 118 (20), 2015.

B Raftari, N Budko, K Vuik, A modified and calibrated drift-diffusion-reaction model for time-domain analysis of charging phenomena in electron-beam irradiated insulators *AIP Advances*, 8 (1), 2018.

Understand the problem



Write down your PDE's

$$\partial_t n + \nabla \cdot \boldsymbol{J}_n = G_n - R_n + S_n$$
$$\partial_t p + \nabla \cdot \boldsymbol{J}_p = G_p - R_p + S_p$$
$$\boldsymbol{J}_n = -D_n \nabla n + \mu_n n \nabla V$$
$$\boldsymbol{J}_p = -D_p \nabla p - \mu_p p \nabla V$$
$$\nabla \cdot (\varepsilon \nabla V) = -\frac{e}{\varepsilon_0}(p + C - n - n_T)$$
$$\partial_t n_T = (R_n - G_n) - (R_p - G_p)$$
$$R_n = \sigma_n v_{th} n (N_T - n_T), \quad R_p = \sigma_p v_{th}\, p\, n_T$$
$$G_p = \sigma_p v_{th} n_i (N_T - n_T), \quad G_n = \sigma_n v_{th} n_i n_T$$
$$S_{n/p} = g_{n/p}(\boldsymbol{x}) f(t)$$

Specify initial and boundary conditions

- At $t = 0$: $n_0 = p_0 = n_i$ and $n_T = N_T/2$ (steady-state)
- Isolated interfaces: $\boldsymbol{J}_n \cdot \boldsymbol{\nu} = \boldsymbol{J}_p \cdot \boldsymbol{\nu} = 0$ (no current)
- Ohmic contacts: $n = p = n_i$
- At least at one interface: $V = V_0$ (and fully coupled approach)
- Sample-vacuum interface? Assumed isolated in semiconductor device modeling

Sometimes, invent your own boundary conditions

Sample-vacuum interface with tertiary current:

$$\boldsymbol{J}_n \cdot \boldsymbol{\nu} = \begin{cases} v_e(n - n_i) + \alpha \frac{\partial V^-}{\partial \vec{\nu}}, & n > n_i \\ 0, & \text{otherwise} \end{cases}$$

$$\boldsymbol{J}_p \cdot \boldsymbol{\nu} = 0$$

Spatial distribution is governed by the attractive force:

$$\left.\frac{\partial V^-}{\partial \vec{\nu}}\right|_\Sigma = \begin{cases} \left.\frac{\partial V}{\partial \vec{\nu}}\right|_\Sigma, & \text{if } \frac{\partial V}{\partial \vec{\nu}} < 0 \\ 0, & \text{otherwise} \end{cases}$$

Choose discretization method, solver, software

1. Finite Volume or Finite Element Methods are better for this type of problems
2. Finite Volume: OpenFOAM
   - Advantages: free, powerful, fast
   - Disadvantages: poorly documented, did not support specific boundary conditions at the time, need to be good at C++
3. FEM: COMSOL
   - Advantages: well-documented, supports general BC's, adaptive grids, GUI-based, Matlab-type language
   - Disadvantages: commercial, not flexible, memory hungry

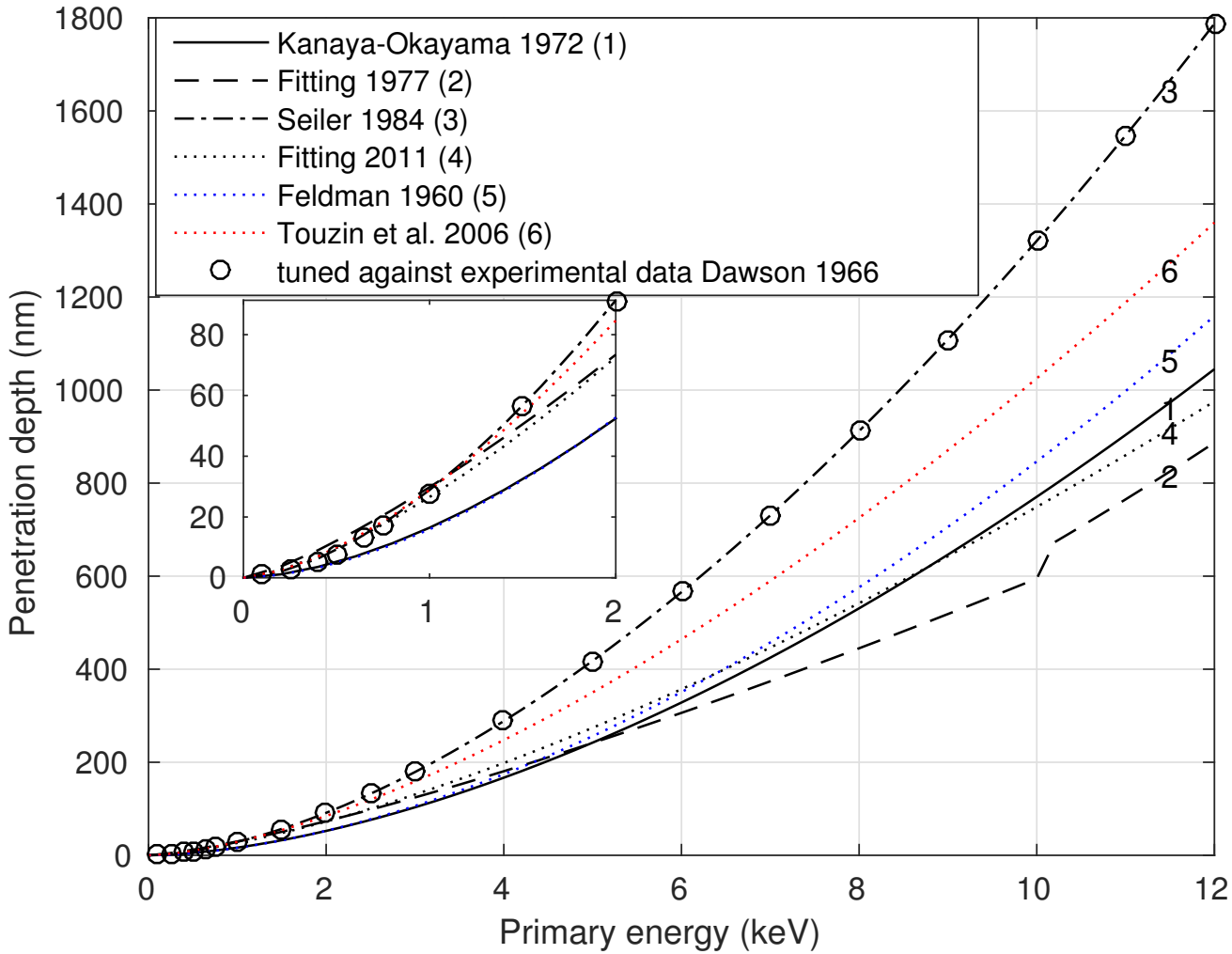
Software implementation

- We skip it for the moment...

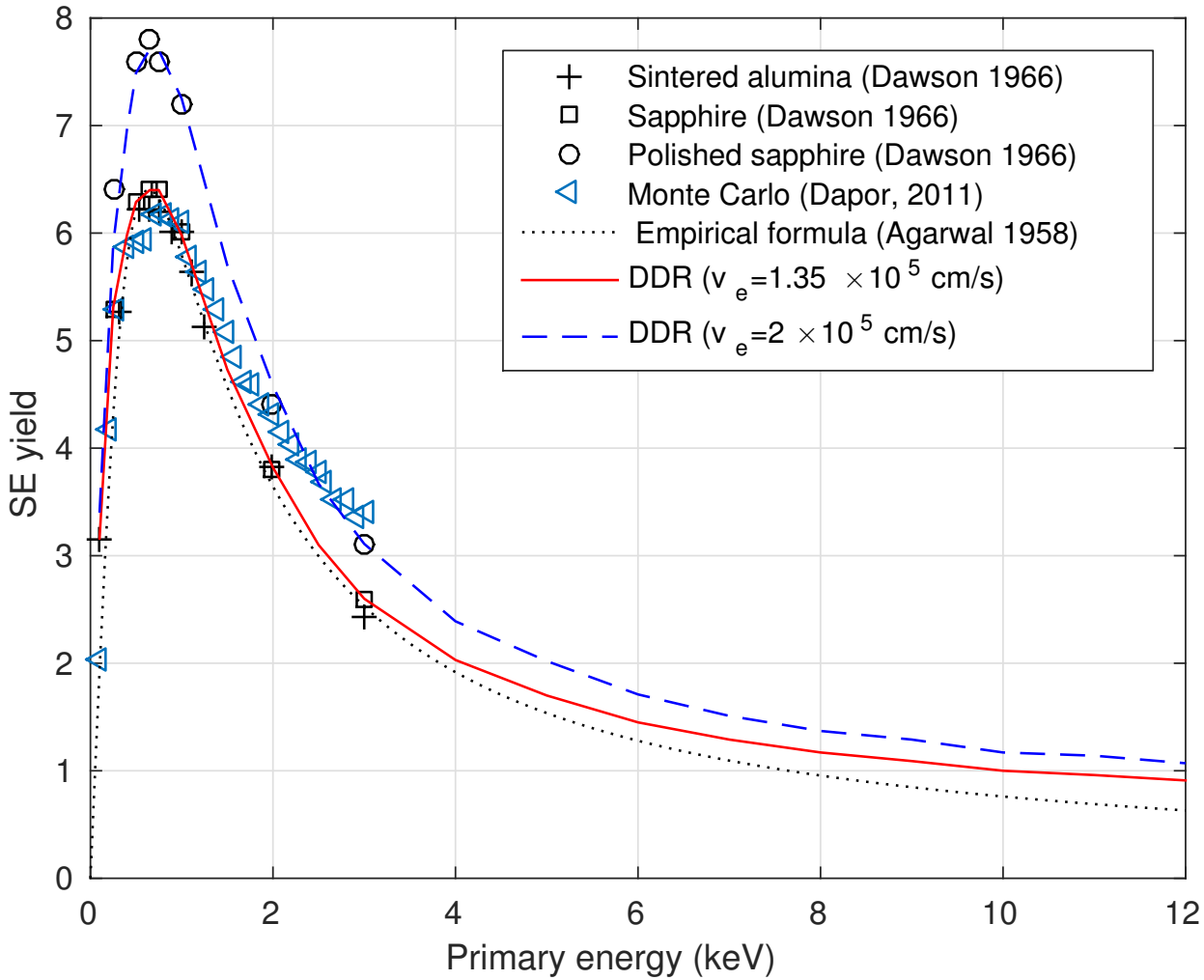
Calibration: search literature for material parameters

Parameter	SiO_2	Al_2O_3	Unit
ε	3.9	10	
μ_n	20	4	$cm^2V^{-1}s^{-1}$
μ_p	0.01	0.002	$cm^2V^{-1}s^{-1}$
σ_n	10^{-15}	10^{-15}	cm^2
σ_p	10^{-17}	10^{-17}	cm^2
v_{th}	10^7	10^7	cm s^{-1}
ρ	2.2	3.98	g cm^{-3}
E_i	28	28	eV
N_t	3×10^{19}	3×10^{19}	cm^{-3}
v_e	0.8×10^5	1.35×10^5 unpolished 2×10^5 polished	cm/s

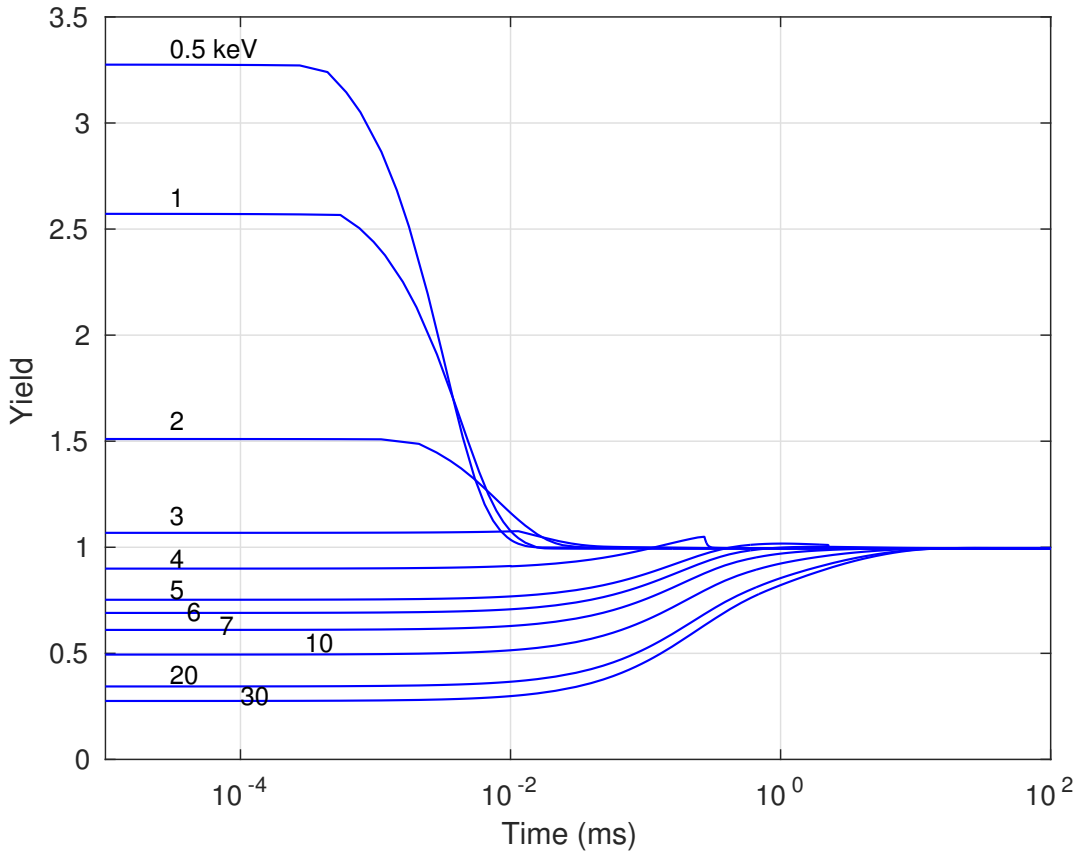
Calibration: tune unknown/uncertain parameters against experimental data



Calibrated results: standard yield, sapphire

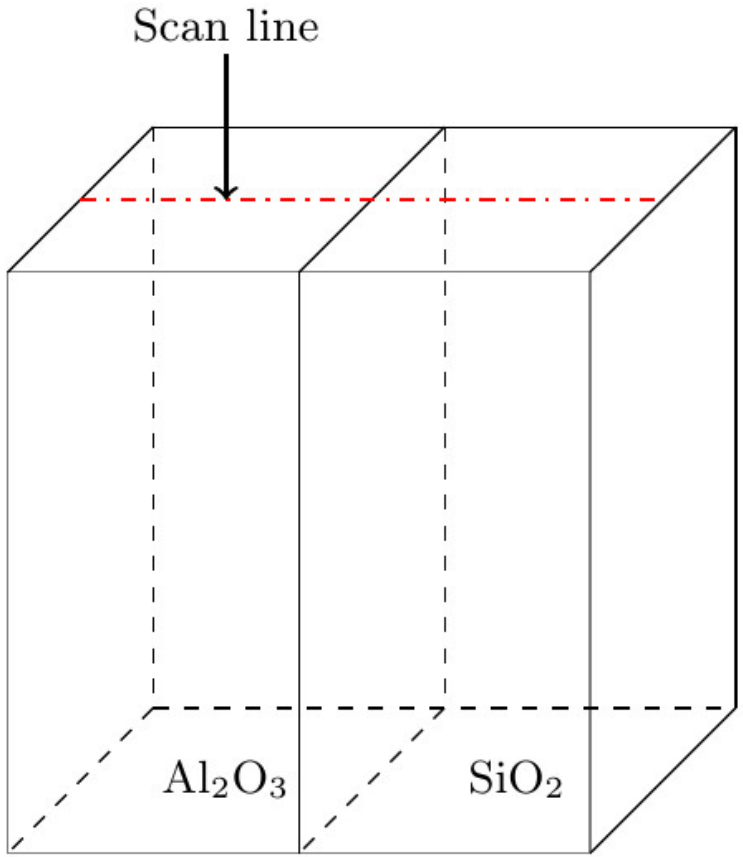


Compare with others: yield evolution for amorphous alumina

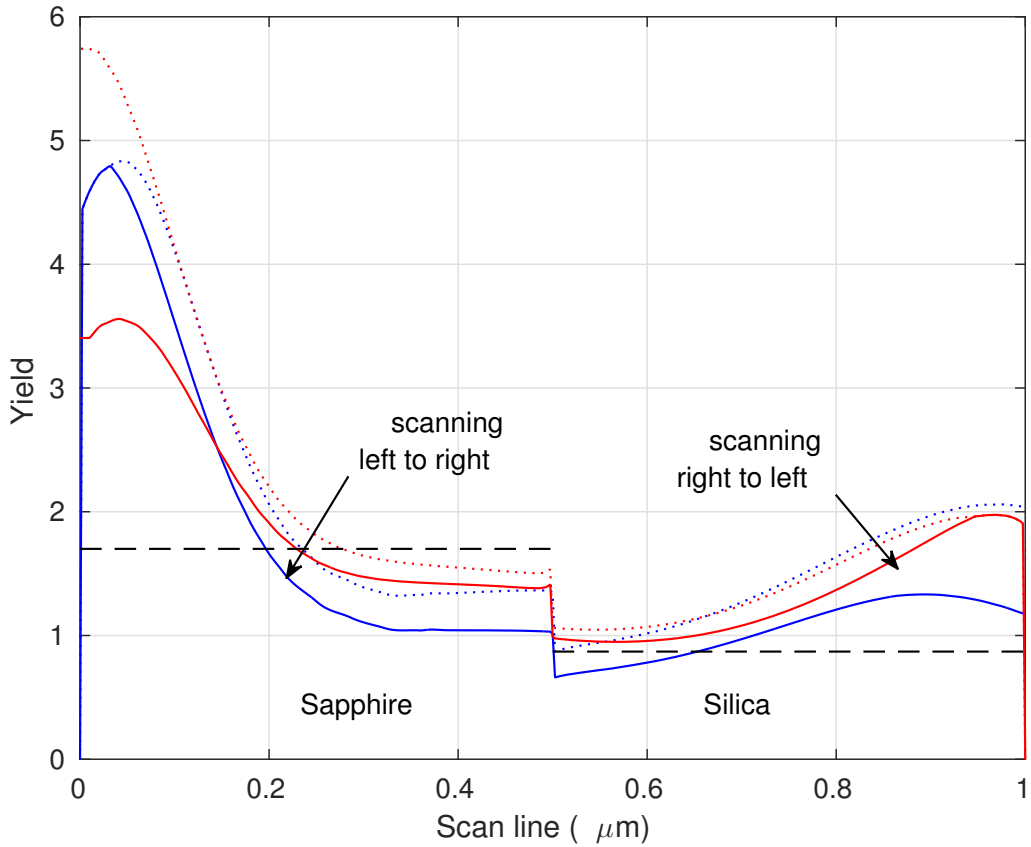


Agrees with 1D Flight-Drift model of Touzin et al 2006 (beam current 10^{-5} A/cm^2)

Studying a new configuration: scanning of inhomogeneous samples

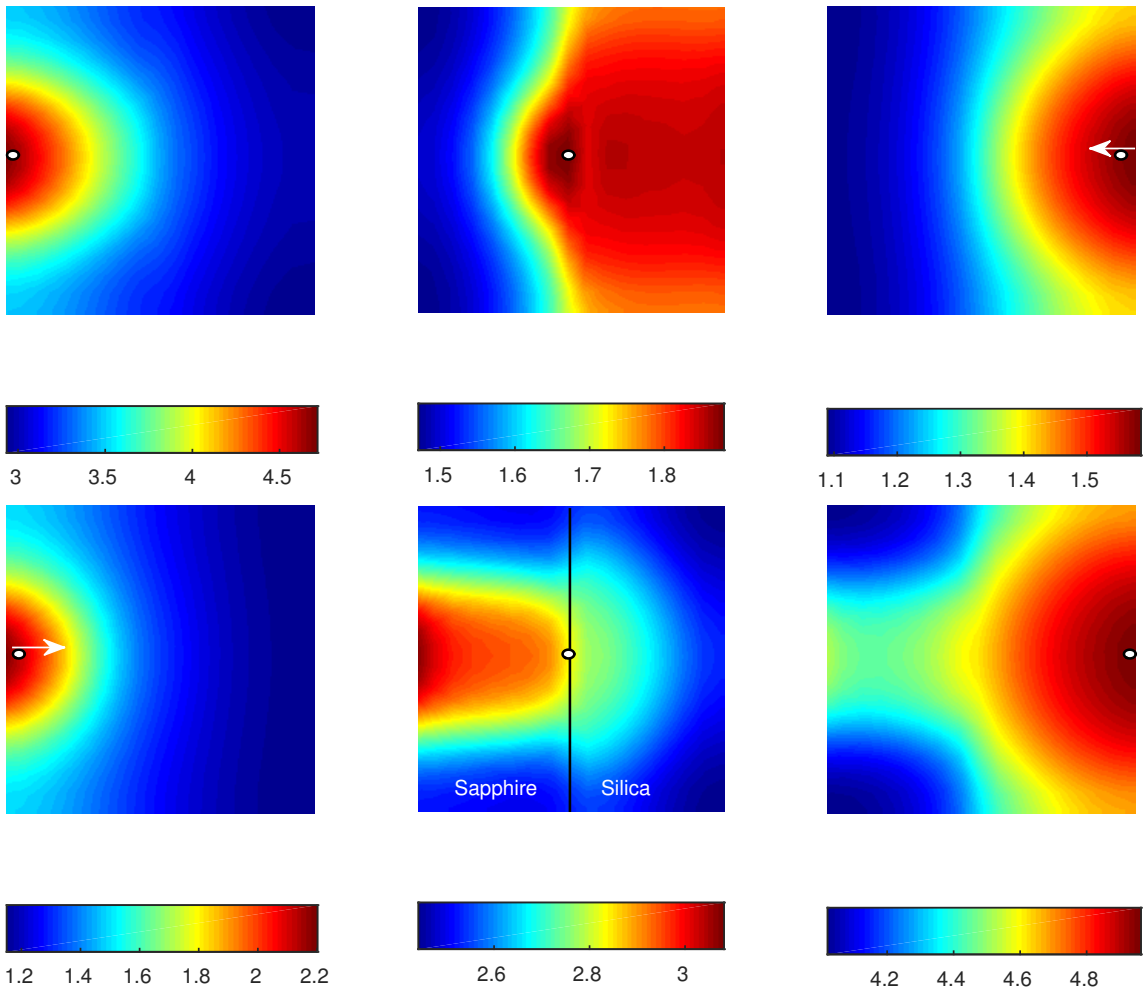


Making conclusions: image depends on the beam current, scanning speed and direction, etc.



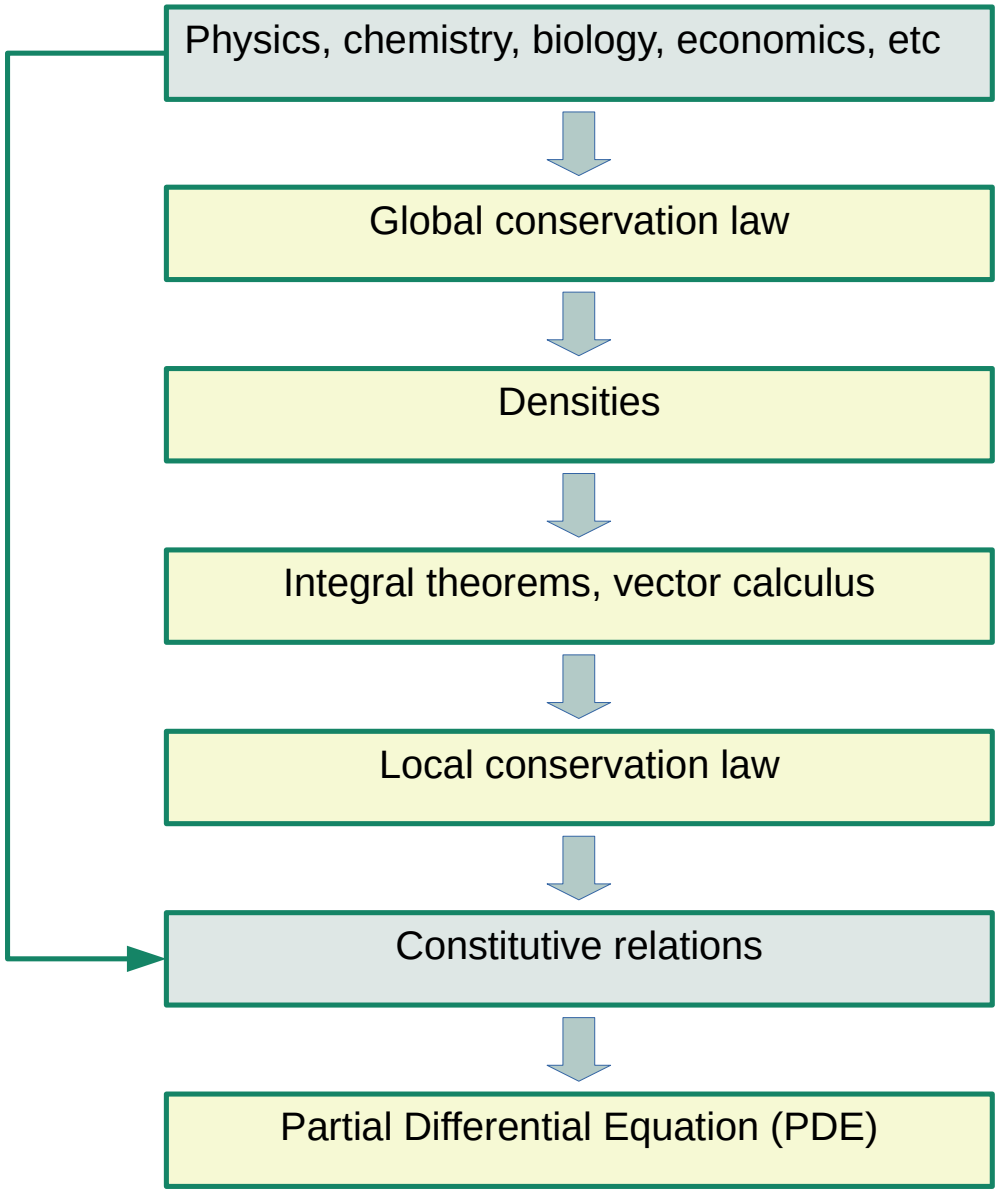
Yield evolution during dynamic scanning at 5 keV, 10 pA

Demonstrating/explaining a new/strange effect: charging depends on the direction of scanning



Mathematical Preliminaries

Derivation of PDE's



Gradient

Given a scalar function $u(x, y, z)$ of three variables, the *gradient* of u is the vector:

$$\operatorname{grad} u = \frac{\partial u}{\partial x}\,\vec{i} + \frac{\partial u}{\partial y}\,\vec{j} + \frac{\partial u}{\partial z}\,\vec{k} = \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \\ \frac{\partial u}{\partial z} \end{bmatrix}$$

Alternatively, using the *nabla* operator ∇ the gradient of u is:

$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix}, \quad \operatorname{grad} u = \nabla u$$

Directional Derivative and Gradient

Directional derivative $D_{\vec{v}}u$ of the function u in the direction of the unit vector $\vec{v} = v_x\,\vec{i} + v_y\,\vec{j} + v_z\,\vec{k}$, $|\vec{v}| = 1$ is defined as:

$$D_{\vec{v}}u = v_x\,\frac{\partial u}{\partial x} + v_y\,\frac{\partial u}{\partial y} + v_z\,\frac{\partial u}{\partial z} = \nabla u \cdot \vec{v} = |\nabla u|\,|\vec{v}|\,\cos\theta = |\nabla u|\,\cos\theta$$

Hence, the maximum value of the directional derivative $D_{\vec{v}}u$ is $|\nabla u|$ and it occurs when $\vec{v}$ has the same direction as ∇u.

Thus, the gradient vector ∇u gives both the direction of the maximum rate of growth of $u(x, y, z)$ at the point (x, y, z) and the magnitude of this rate.

Applications of gradient: heat flow

Fourier's law: Heat flows from warm to cold, the stronger is the temperature difference, the faster is the flow. Mathematically: Heat flux density $\vec{q}$ is proportional to the negative temperature gradient:

$$\vec{q} = -k\nabla T$$

$\vec{q}$ is the local heat flux density [W m^{-2}],
k is material's thermal conductivity [W m^{-1}K^{-1}],
∇T is the temperature gradient [K m^{-1}],
$T(x, y, z)$ is the local temperature [K]

Gradient in electrostatics, hydrostatics and diffusion

Electrostatic field: The electrostatic field $\vec{E}$ is defined as the negative of the gradient of the electrostatic potential ϕ, i.e., $\vec{E} = -\nabla\phi$. If ϕ is in Volts, what are the units of $\vec{E}$? The electric displacement field (electric flux density) $\vec{D}$ is defined as $\varepsilon\vec{E}$, where ε, [F m^{-1}] is the dielectric permittivity of the material. What is the expression of $\vec{D}$ in terms of ϕ?

Darcy's law: the (slow) flow of water through porous medium is driven by the hydrostatic pressure and depends linearly on the height of the ground water level h. What is the mathematical expression for the water flow density $\vec{q}$ in terms of h?

Fick's law: a substance diffuses from higher to lower concentrations at a rate proportional to the concentration difference. Write diffusion flow density $\vec{q}$ in terms of the local substance concentration c? What are the dimensions of all quantities in SI units?

Divergence

Given a vector field $\vec{U}(x, y, z) = U_x(x, y, z)\,\vec{i} + U_y(x, y, z)\,\vec{j} + U_z(x, y, z)\,\vec{k}$, the *divergence* of $\vec{U}$ is the scalar:

$$\operatorname{div} \vec{U} = \frac{\partial U_x}{\partial x} + \frac{\partial U_y}{\partial y} + \frac{\partial U_z}{\partial z} = \nabla \cdot \vec{U}$$

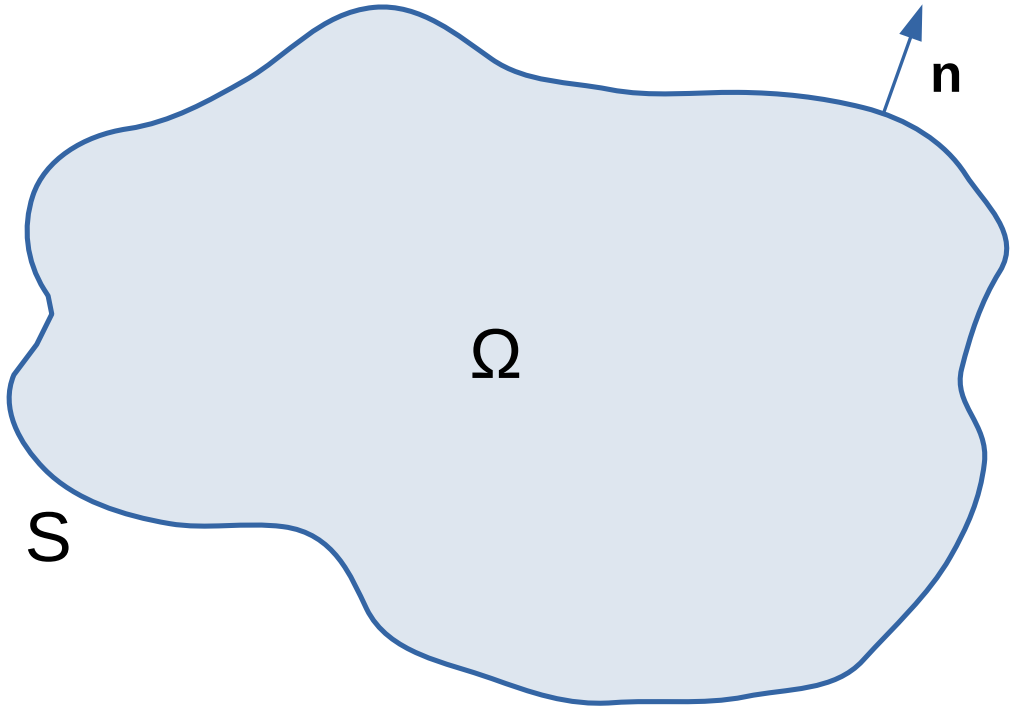
Scalar functions U_x, U_y, and U_z are called *components* of the vector field $\vec{U}$. Sometimes denoted as U_1, U_2, and U_3.

In books and papers vectors and vector fields are denoted with bold font:

$$\vec{U} = \boldsymbol{u}, \quad \text{or} \quad \boldsymbol{q} = -k\nabla T$$

This notation will be used from now on.

Domain Ω, boundary surface S, normal vector $\boldsymbol{n}$



Flux of a vector field

- We exclude nonorientable surfaces such as the Möbius strip and consider only two-sided surfaces
- If it is possible to define a normal vector $\boldsymbol{n}$ at every point of S so that $\boldsymbol{n}$ varies continuously over S, then S is called **oriented surface** and the given choice of $\boldsymbol{n}$ provides S with an **orientation**

Definition. If $\boldsymbol{F}$ is a continuous vector field defined on an oriented surface S with unit normal vector $\boldsymbol{n}$, then the **surface integral of $\boldsymbol{F}$ over** S is

$$\Phi = \iint_S \boldsymbol{F} \cdot d\boldsymbol{S} = \iint_S (\boldsymbol{F} \cdot \boldsymbol{n})\, dS$$

Φ is called the **flux of $\boldsymbol{F}$ across** S, and $\boldsymbol{F}$ is often called the **flux density**.

Applications of fluxes: Gauss's law, heat flow

Gauss's law: the net charge Q enclosed by a closed surface S is given by

$$Q = \varepsilon_0 \iint_S \boldsymbol{E} \cdot d\boldsymbol{S}$$

Heat flow: From the Fourier law $\boldsymbol{q} = -k\nabla T$. The rate of heat flow Q across the surface S is

$$\Phi = \iint_S \boldsymbol{q} \cdot d\boldsymbol{S} = -\iint_S k\nabla T \cdot d\boldsymbol{S}$$

Global form of conservation laws

Let $Q(t)$ be the total amount of some quantity inside the domain Ω at time t. There are two reasons for Q to change with time: the outward flux Φ across the boundary S of Ω and the creation or destruction of this quantity at the rate $R(t)$ inside Ω.

Then, the rate of change of Q inside Ω can be written as:

$$\frac{dQ}{dt} = -\Phi + R$$

This is the general **global** form of the **conservation law**.

Divergence Theorem

Divergence Theorem. Let Ω be a simple solid region and let S be a boundary surface of Ω with positive (outward) orientation. Let $\boldsymbol{F}$ be a vector field whose component functions have continuous partial derivatives on an open region that contains Ω. Then

$$\iint_S \boldsymbol{F} \cdot d\boldsymbol{S} = \iiint_\Omega (\nabla \cdot \boldsymbol{F})\, dV$$

In words: the flux of $\boldsymbol{F}$ across the boundary surface of Ω is equal to the triple integral of the divergence of $\boldsymbol{F}$ over Ω.

Local form of conservation laws

Let $\rho(x, y, z, t)$ be the **density** of some quantity and $f(x, y, z, t)$ be the local rate of its creation/destruction. Then,

$$Q(t) = \iiint_{\Omega} \rho \, dV, \quad R(t) = \iiint_{\Omega} f \, dV$$

If $\boldsymbol{J}$ is the flux (current) density, then the conservation law is

$$\begin{aligned} \frac{d}{dt} \iiint_{\Omega} \rho \, dV &= - \iint_{S} \boldsymbol{J} \cdot d\boldsymbol{S} + \iiint_{\Omega} f \, dV \\ &= - \iiint_{\Omega} (\nabla \cdot \boldsymbol{J}) dV + \iiint_{\Omega} f \, dV \end{aligned}$$

If this holds for any Ω, then the **local conservation law** (continuity law) is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{J} = f$$

Diffusion equation

As we know, there is a **constitutive relation** $\boldsymbol{J}_{\text{diffusion}} = -k\nabla\rho$, which connects $\boldsymbol{J}$ and ρ via a constitutive parameter of the medium k. Then, the conservation law becomes a PDE:

$$\frac{\partial\rho}{\partial t} - \nabla\cdot(k\nabla\rho) = f$$

which is called the **diffusion equation**.

Advection equation

Convection (advection) current density has the form:

$$\boldsymbol{J}_{\text{convection}} = \rho \boldsymbol{v}$$

where $\boldsymbol{v}$ is a given velocity field. Then, the local conservation law yields the PDE:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = f$$

which is called the **advection equation**. Since $\nabla \cdot (\rho \boldsymbol{v}) = \boldsymbol{v} \cdot \nabla \rho + \rho \nabla \cdot \boldsymbol{v}$, in the case where $\nabla \cdot \boldsymbol{v} = 0$ (incompressible flow, solenodial $\boldsymbol{v}$) we get a simpler advection equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{v} \cdot \nabla \rho = f$$

Convection-Diffusion equation

If current density contains both the advection (convection) and the diffusion contributions:

$$\boldsymbol{J} = \boldsymbol{J}_{\text{diffusion}} + \boldsymbol{J}_{\text{convection}}$$

Then, the conservation law becomes

$$\frac{\partial \rho}{\partial t} - \nabla \cdot (k \nabla \rho) + \nabla \cdot (\rho \boldsymbol{v}) = f$$

which is called the advection-diffusion or **convection-diffusion equation**. In the incompressible case:

$$\frac{\partial \rho}{\partial t} - \nabla \cdot (k \nabla \rho) + \boldsymbol{v} \cdot \nabla \rho = f$$

Poisson equation, Laplace's operator

In the steady state

$$\frac{\partial \rho}{\partial t} = 0$$

and the diffusion equation reduces to the **Poisson equation**:

$$-\nabla \cdot (k \nabla \rho) = f$$

If also $k \neq 0$ is a constant (uniform in space), then

$$-\Delta \rho = \frac{1}{k} f$$

where

$$\Delta \rho = \nabla \cdot \nabla \rho = \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} + \frac{\partial^2 \rho}{\partial z^2}$$

$\Delta = \nabla \cdot \nabla$ is called the **Laplace operator**.

Electrostatic potential

By definition $\boldsymbol{E} = -\nabla\phi$, where ϕ is the electrostatic potential. The Gauss law and the Divergence Theorem give

$$Q = \iiint_\Omega \rho \, dV = \varepsilon_0 \iint_S \boldsymbol{E} \cdot d\boldsymbol{S} = \varepsilon_0 \iiint_\Omega \nabla \cdot \boldsymbol{E} \, dV = -\varepsilon_0 \iiint_\Omega \nabla \cdot \nabla\phi \, dV$$

where ρ is the charge density. Hence, ϕ satisfies the Poisson equation

$$-\Delta\phi = \frac{1}{\varepsilon_0}\rho$$

Gradient of a vector

In some equations we meet:

$$\nabla \boldsymbol{u} = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix} \begin{bmatrix} u_x & u_y & u_z \end{bmatrix} = \begin{bmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_y}{\partial x} & \frac{\partial u_z}{\partial x} \\ \frac{\partial u_x}{\partial y} & \frac{\partial u_y}{\partial y} & \frac{\partial u_z}{\partial y} \\ \frac{\partial u_x}{\partial z} & \frac{\partial u_y}{\partial z} & \frac{\partial u_z}{\partial z} \end{bmatrix}$$

Or the nonlinear term:

$$\begin{aligned} \boldsymbol{u} \cdot \nabla \boldsymbol{u} &= \begin{bmatrix} u_x & u_y & u_z \end{bmatrix} \begin{bmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_y}{\partial x} & \frac{\partial u_z}{\partial x} \\ \frac{\partial u_x}{\partial y} & \frac{\partial u_y}{\partial y} & \frac{\partial u_z}{\partial y} \\ \frac{\partial u_x}{\partial z} & \frac{\partial u_y}{\partial z} & \frac{\partial u_z}{\partial z} \end{bmatrix} \\ &= \begin{bmatrix} u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z}, & u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z}, \\ u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \end{bmatrix} \end{aligned}$$

Divergence of a tensor

In elasticity the stress $\mathbb{T}$ is a tensor:

$$\mathbb{T} = \begin{bmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{yx} & T_{yy} & T_{yz} \\ T_{zx} & T_{zy} & T_{zz} \end{bmatrix}$$

The divergence of a tensor is defined as

$$\begin{aligned} \nabla \cdot \mathbb{T} &= \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{bmatrix} \begin{bmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{yx} & T_{yy} & T_{yz} \\ T_{zx} & T_{zy} & T_{zz} \end{bmatrix} \\ &= \left[\frac{\partial T_{xx}}{\partial x} + \frac{\partial T_{yx}}{\partial y} + \frac{\partial T_{zx}}{\partial z}, \quad \frac{\partial T_{xy}}{\partial x} + \frac{\partial T_{yy}}{\partial y} + \frac{\partial T_{zy}}{\partial z}, \right. \\ &\quad \left. \frac{\partial T_{xz}}{\partial x} + \frac{\partial T_{yz}}{\partial y} + \frac{\partial T_{zz}}{\partial z} \right] \end{aligned}$$