Finite Difference and Finite Element Methods

Lars Ole Schwen
Fraunhofer Institute for Medical Image Computing MEVIS, Bremen

Based on a presentation by Tobias Preusser

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Practical Computer Modeling for Medical Device Development

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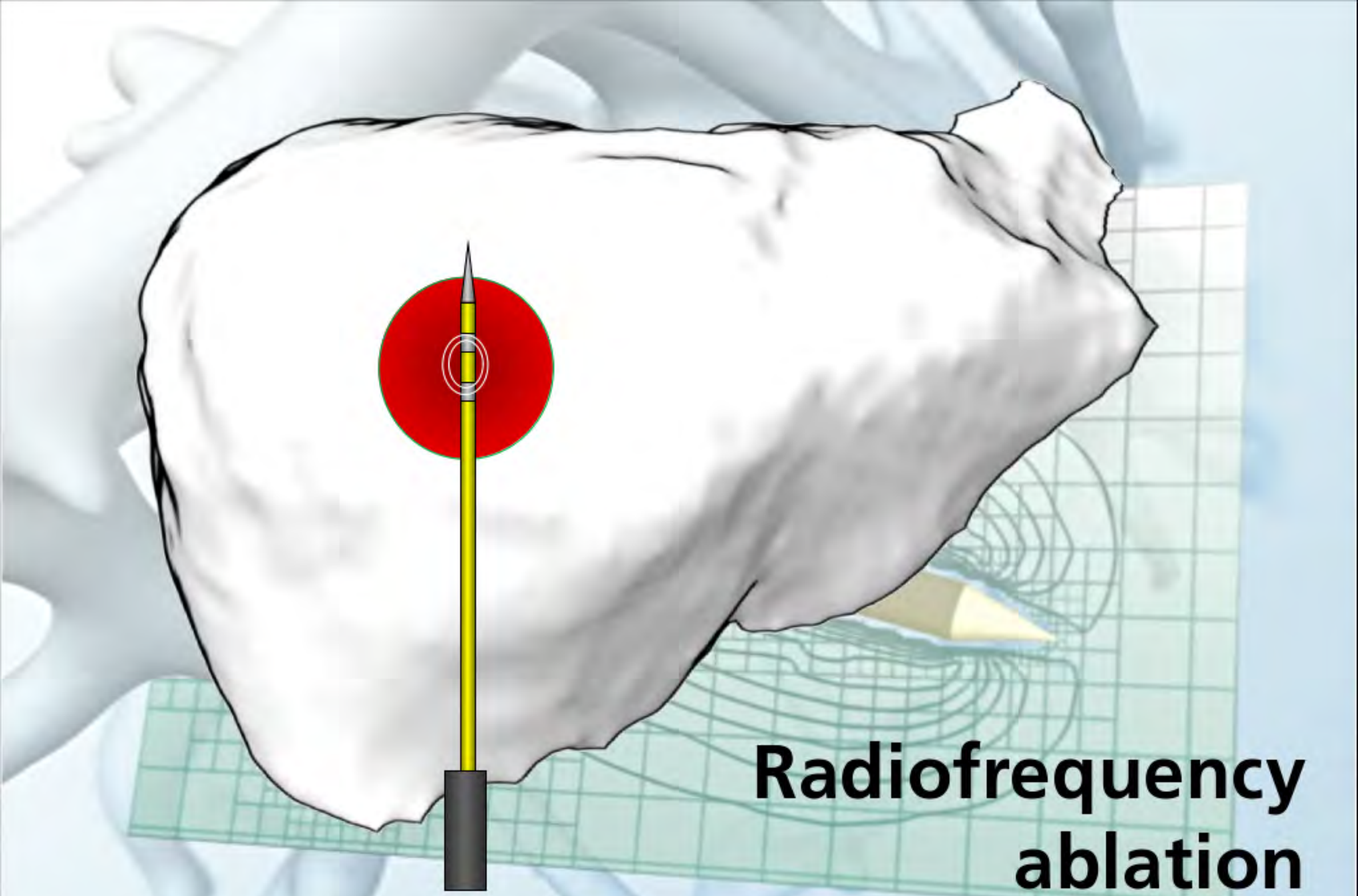
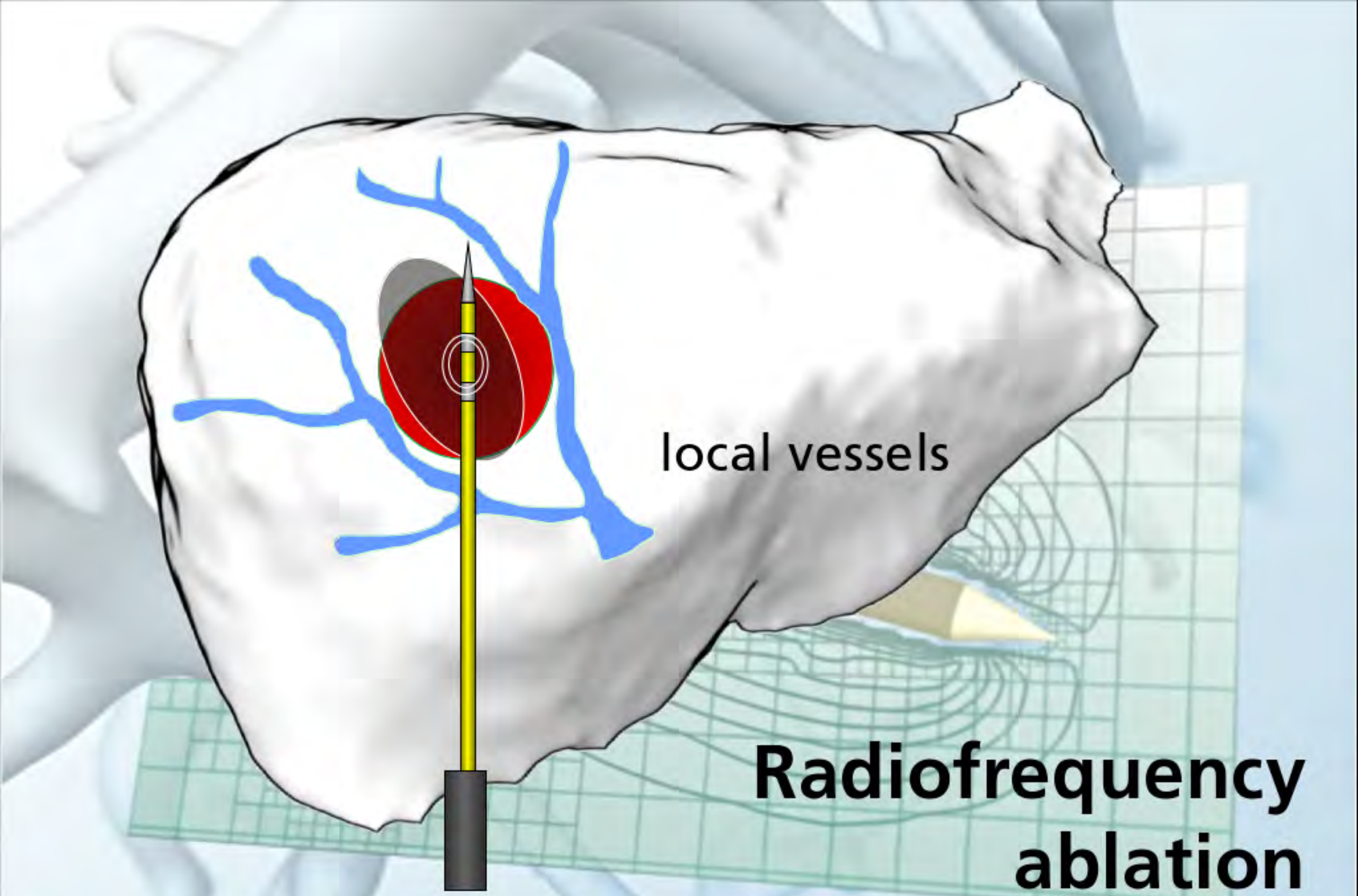
Modeling Thermal Ablation

Radiofrequency ablation

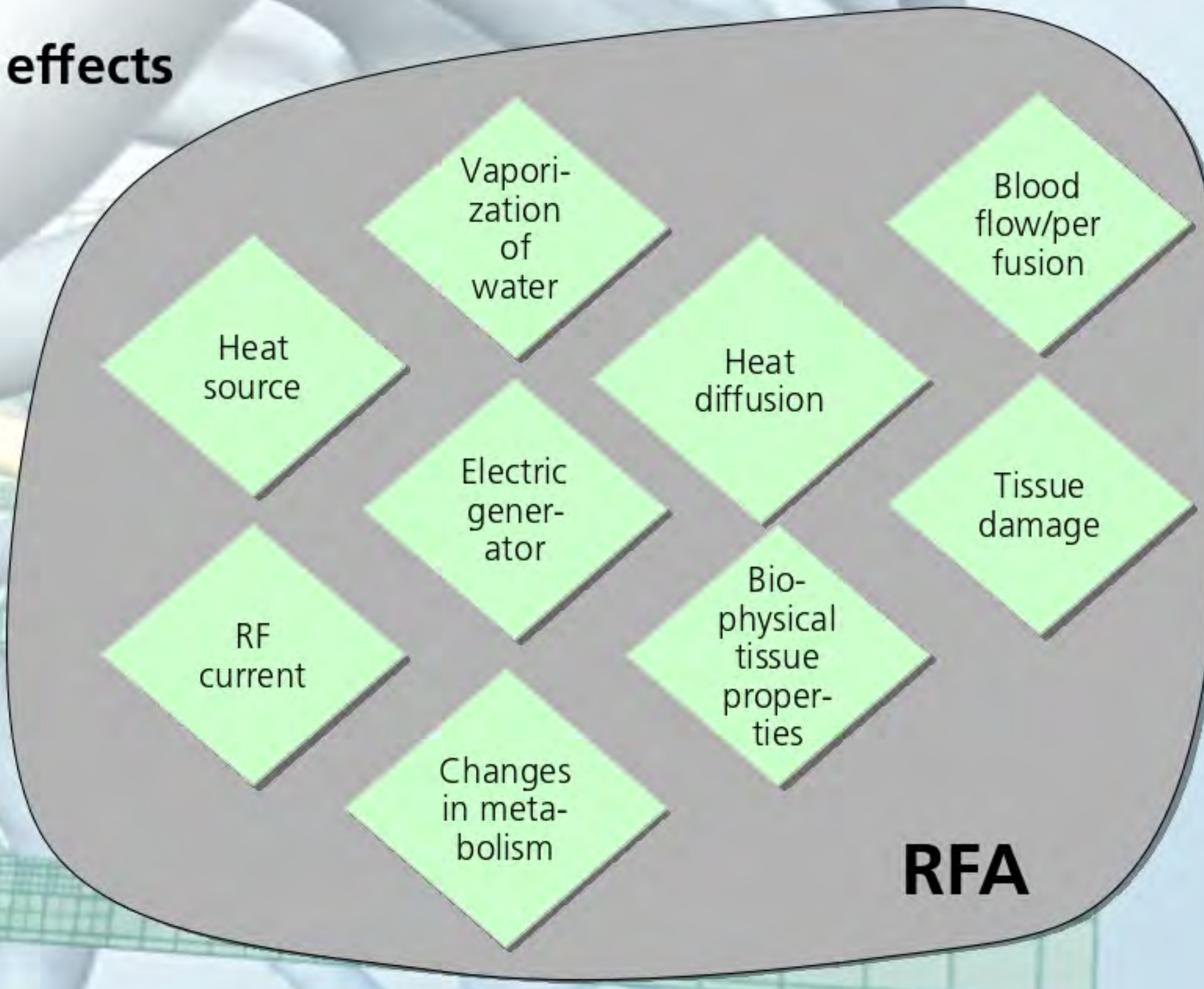


Radiofrequency ablation



Radiofrequency ablation

Bio-physical effects during RFA



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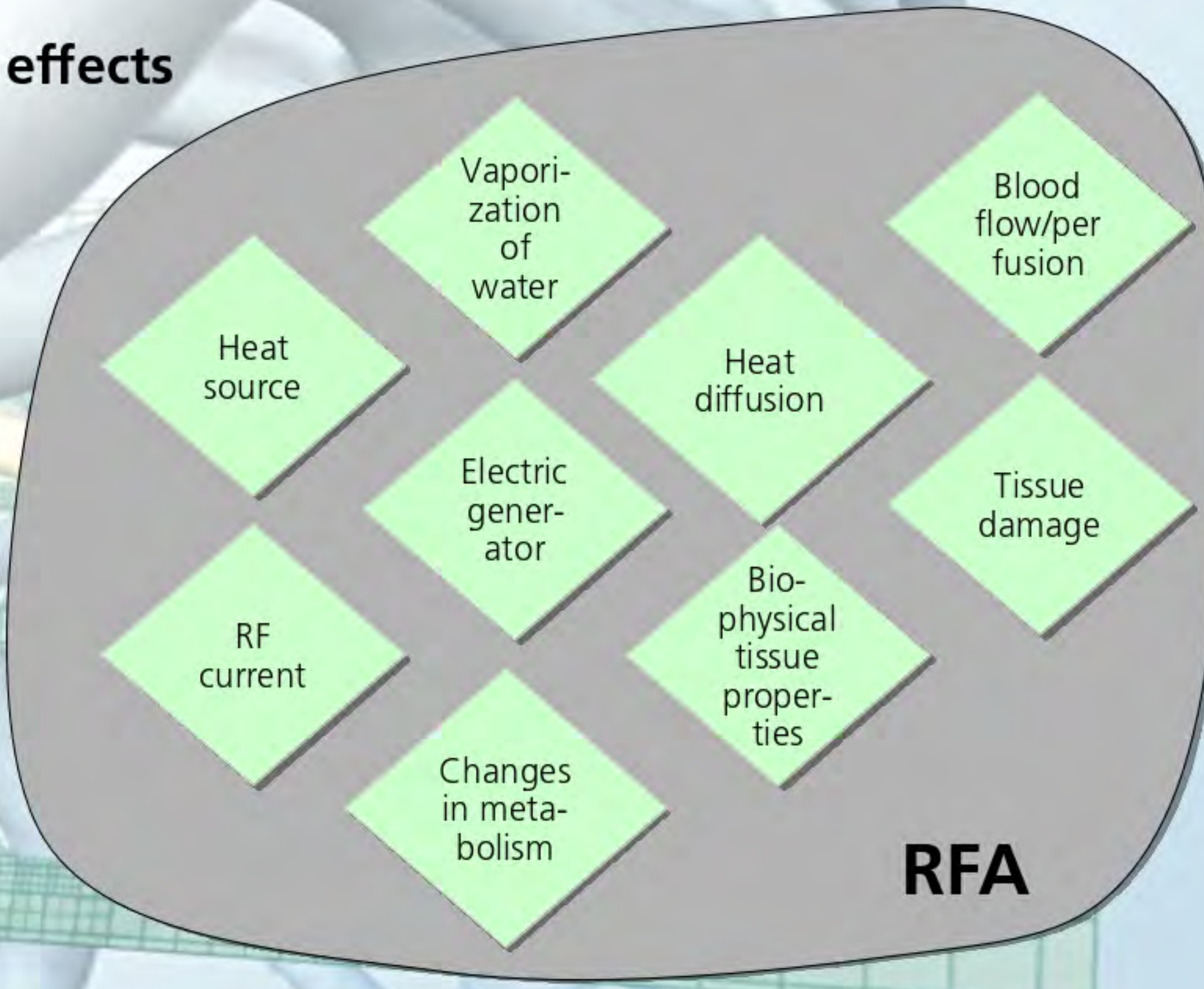

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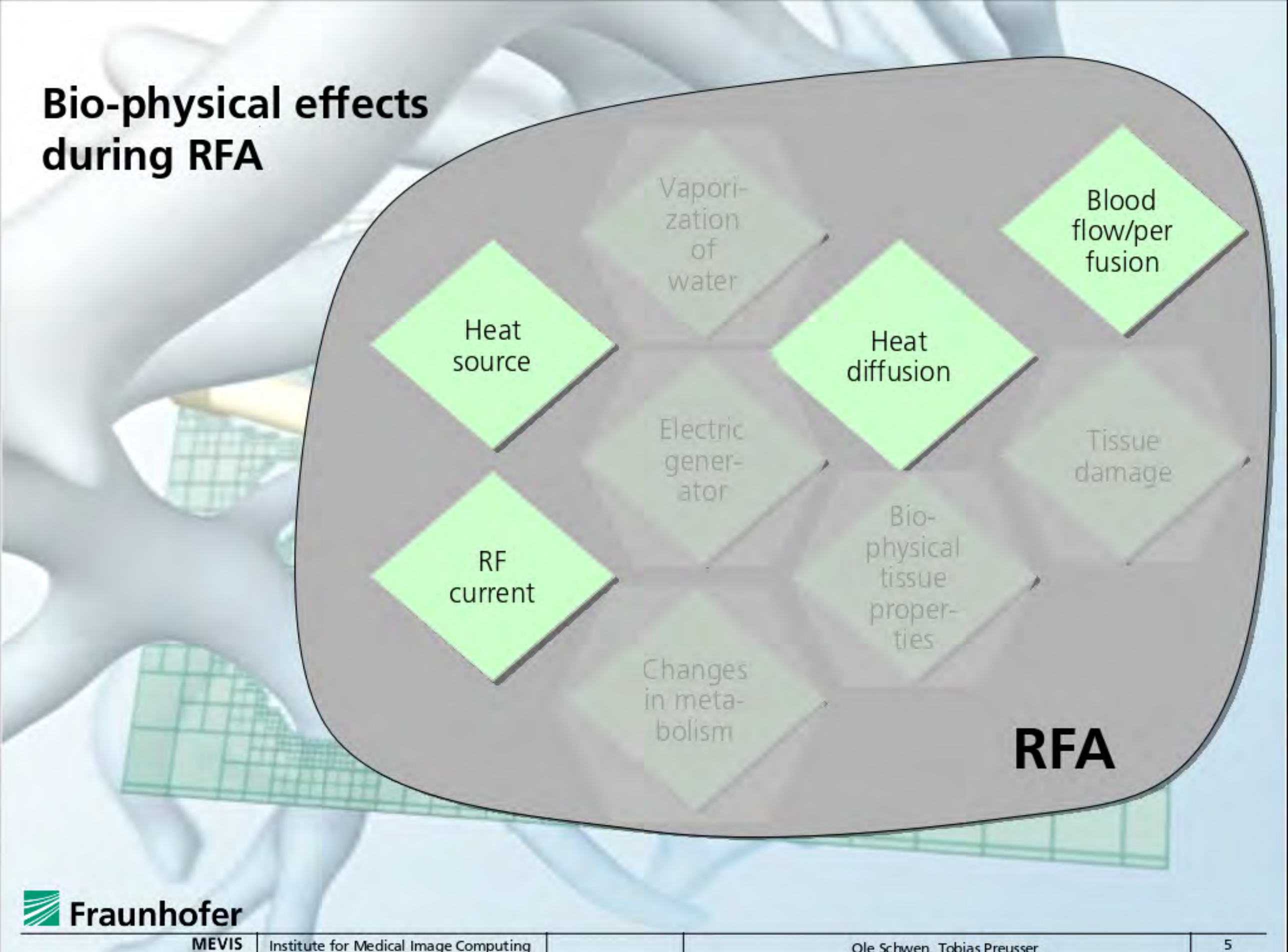
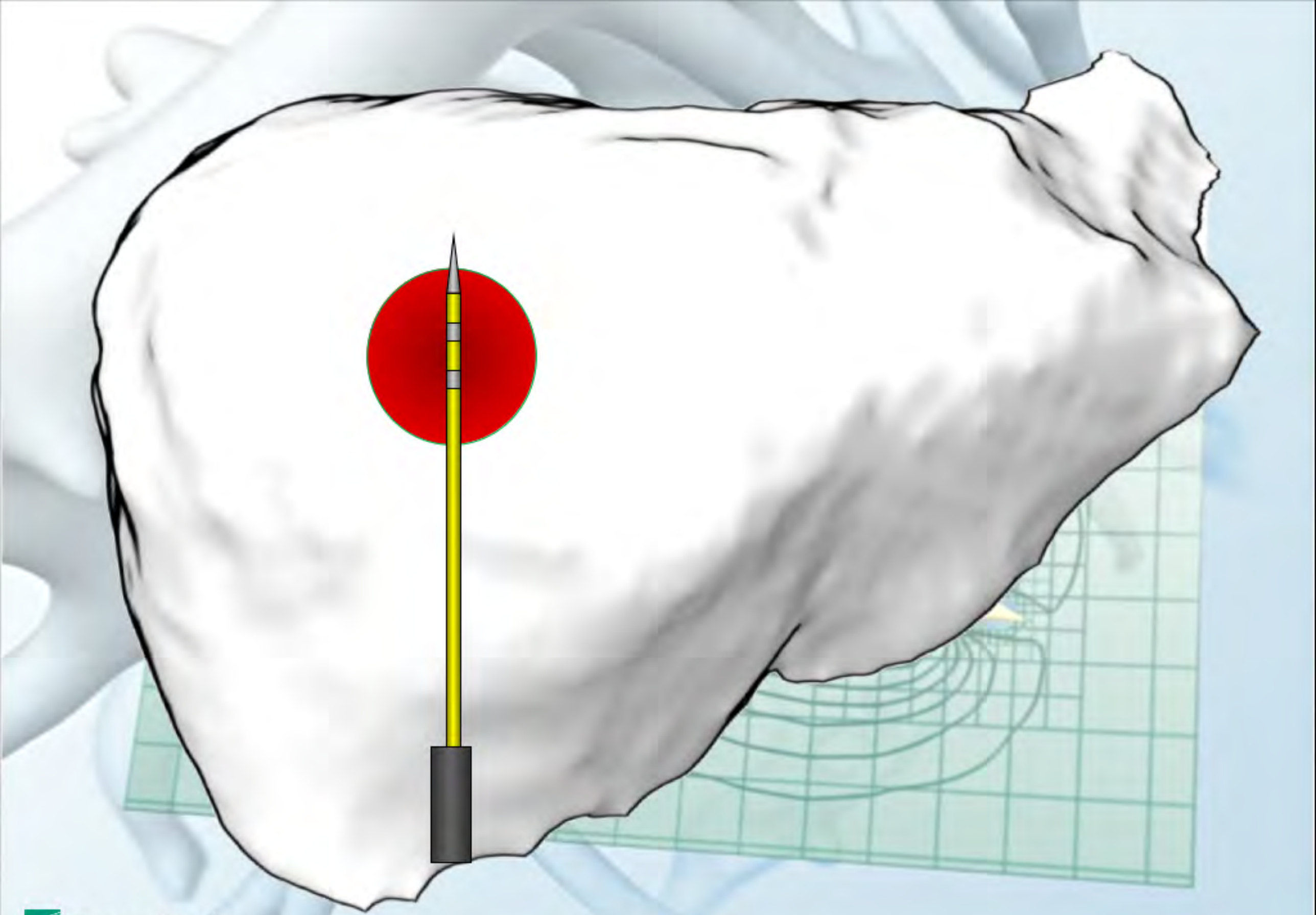
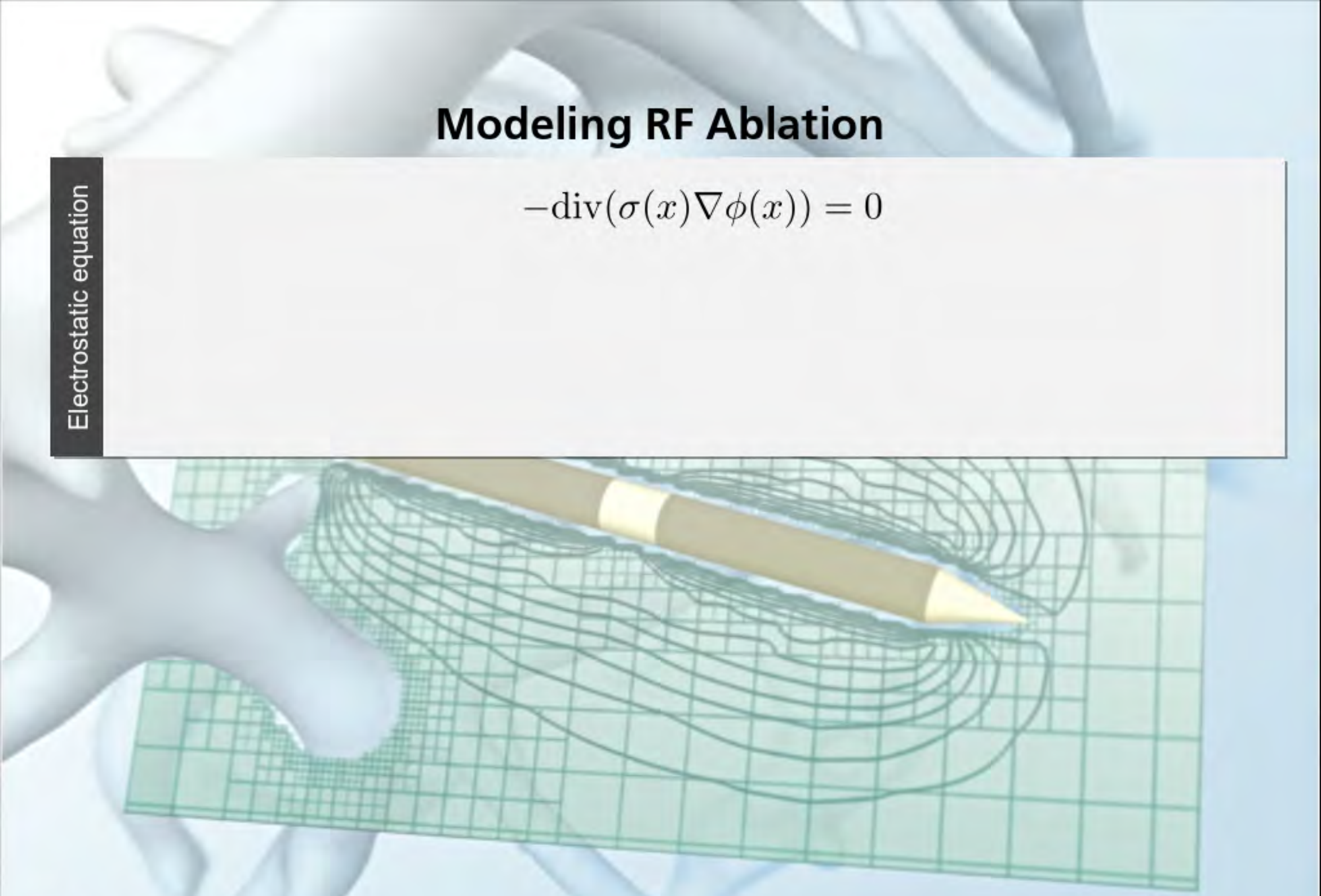




Modeling RF Ablation

Electrostatic equation

$$-\mathrm{div}(\sigma(x)\nabla\phi(x)) = 0$$



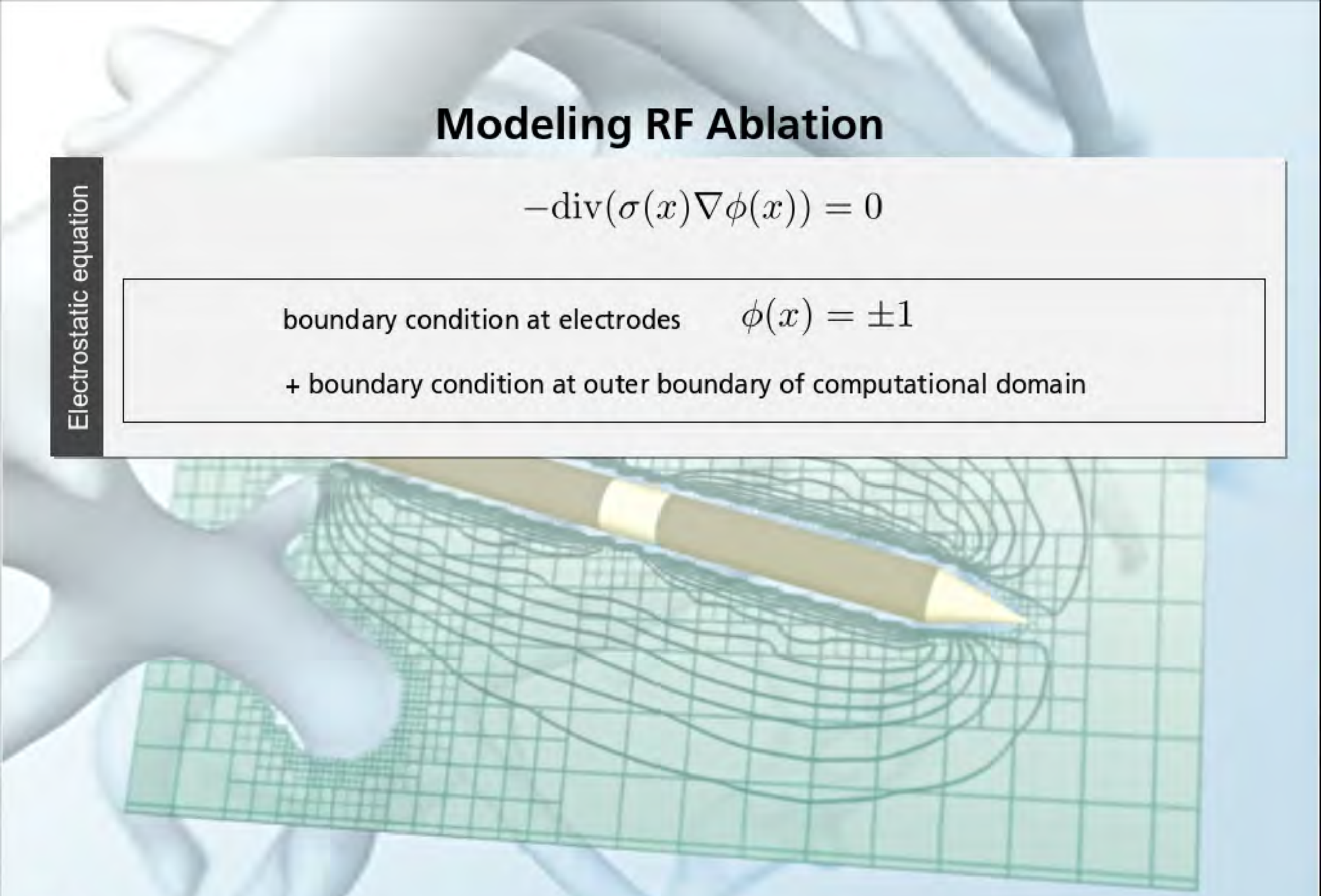
Modeling RF Ablation

Electrostatic equation

$$-\mathrm{div}(\sigma(x)\nabla\phi(x)) = 0$$

boundary condition at electrodes $\phi(x) = \pm 1$

+ boundary condition at outer boundary of computational domain



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Electric potential [V]

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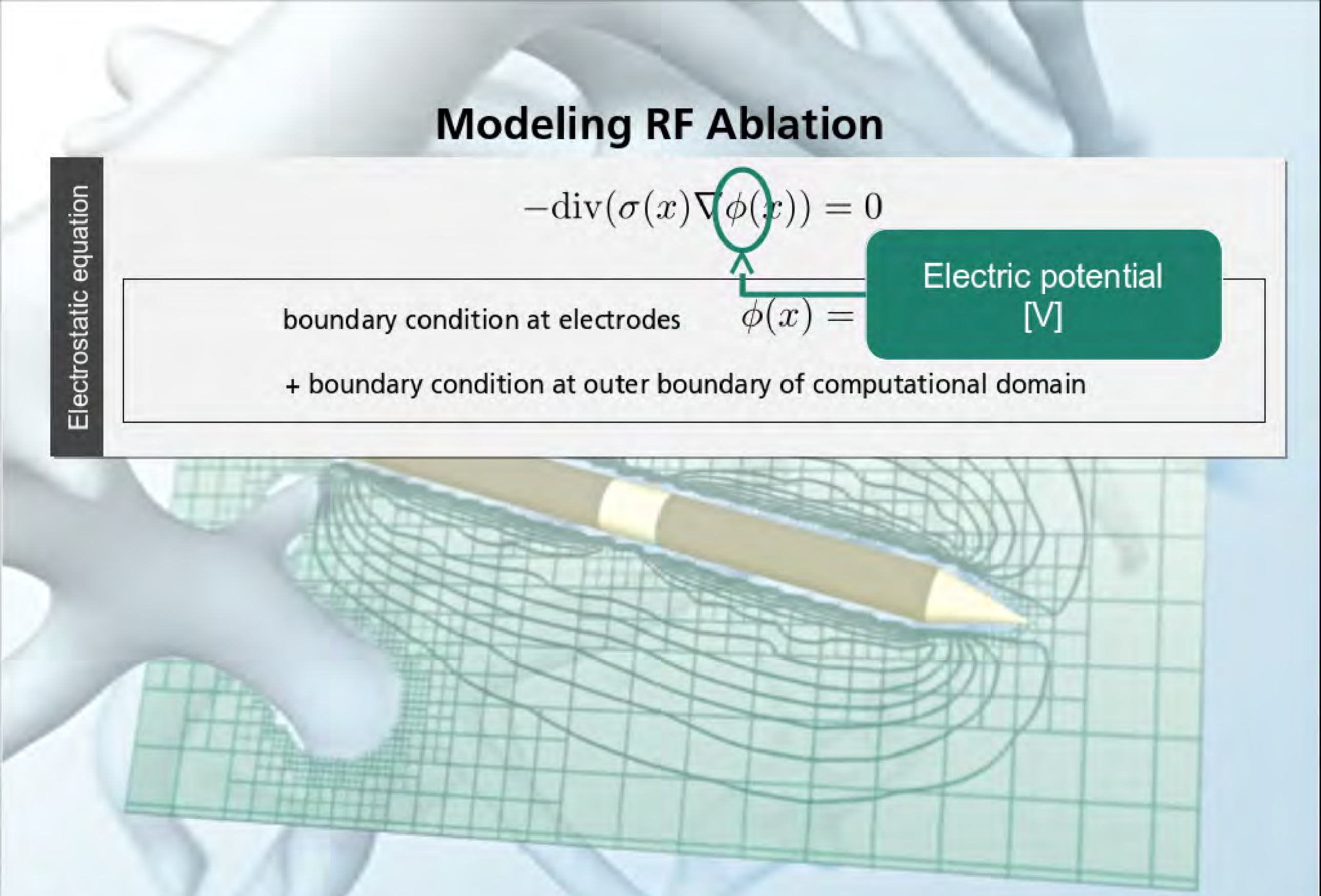

Modeling RF Ablation

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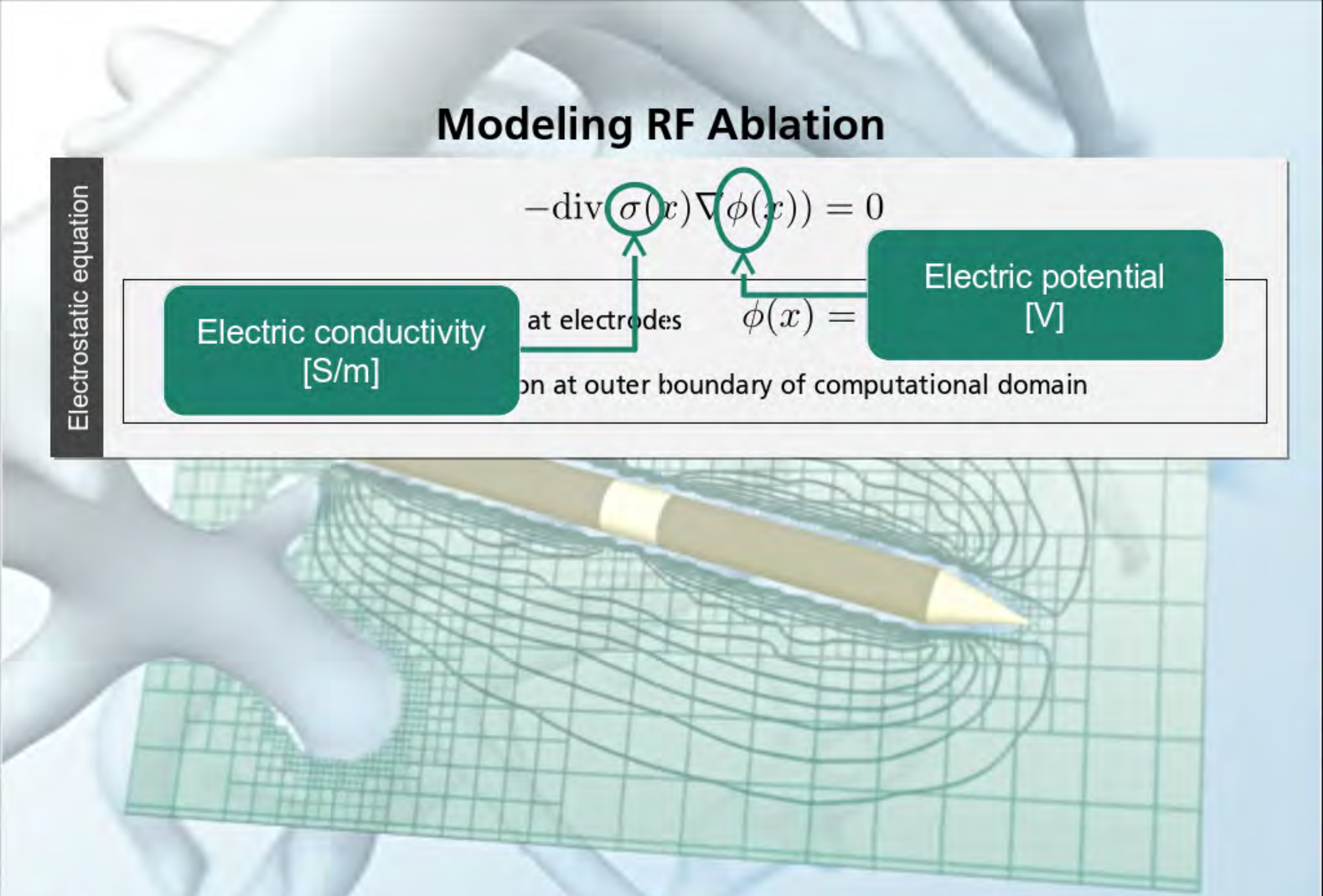
Electric conductivity [S/m]

at electrodes

$\phi(x) =$

Electric potential [V]

on at outer boundary of computational domain



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Bioheat transfer equation

$$\rho(x)c(x)\partial_t T(t,x) - \mathrm{div}(\lambda(x)\nabla T(t,x)) = \sigma(x)|\nabla\phi(x)|^2 - \nu(x)(T(t,x) - T_\mathrm{b})$$

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boundary condition at applicator $T(t,x) = T_\mathrm{b}$

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Relative perfusion rate [J/s m³ K]

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Electric conductivity [S/m]

Electric potential [V]

Body temperature [K]

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Heat capacity [J/kg K]

Temperature [K]

Relative perfusion rate [J/s m³ K]

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Electric potential [V]

Density [kg/m³]

Body temperature [K]

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Differential Operators

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Differential Operators

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Partial derivative = directional derivative in a coordinate direction

$$u(x_1, x_2, x_3) \qquad \frac{\partial u}{\partial x_1} = \partial_{x_1} u = \text{ slope of } u \text{ in direction } x_1$$

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Gradient = vector of all partial derivatives

$$\nabla u = (\partial_{x_1} u, \partial_{x_2} u, \partial_{x_3} u)^t$$

- Points in direction of steepest ascent
- Perpendicular to level lines

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Divergence = sum of partial derivatives of a vector field

$$\operatorname{div}(\nabla u) = \sum_{i=1}^{3} \partial_{x_i} (\nabla u)_i = \sum_{i=1}^{3} \partial_{x_i} (\partial_{x_i} u) = \sum_{i=1}^{3} \partial_{x_i}^2 u = \Delta u$$

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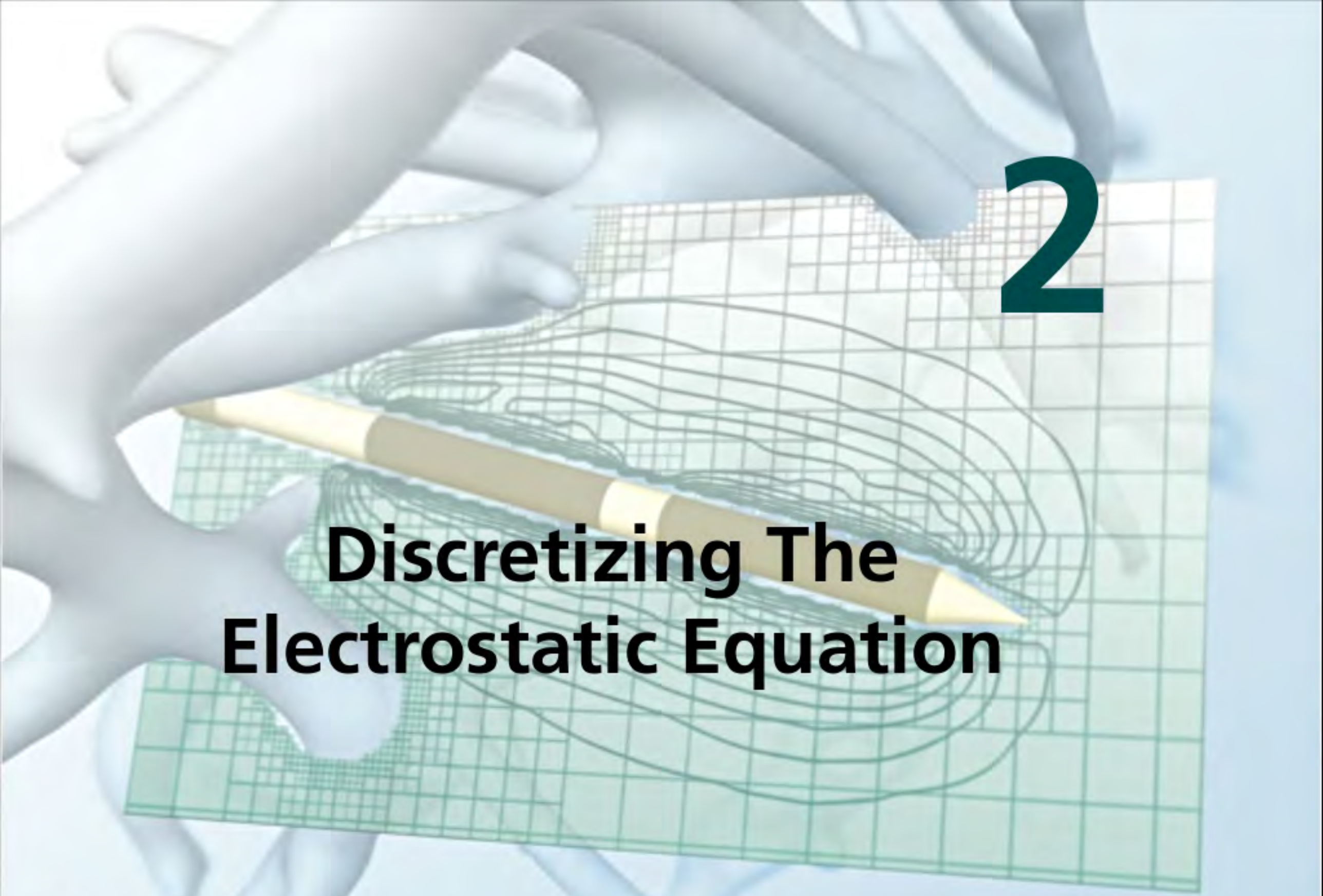
Electrostatic equation in 1D

$$-(\sigma\, \phi')' = 0$$

Electrostatic equation in 2D

$$-\partial_{x_1}(\sigma\, \partial_{x_1}\phi) - \partial_{x_2}(\sigma\, \partial_{x_2}\phi) = 0$$



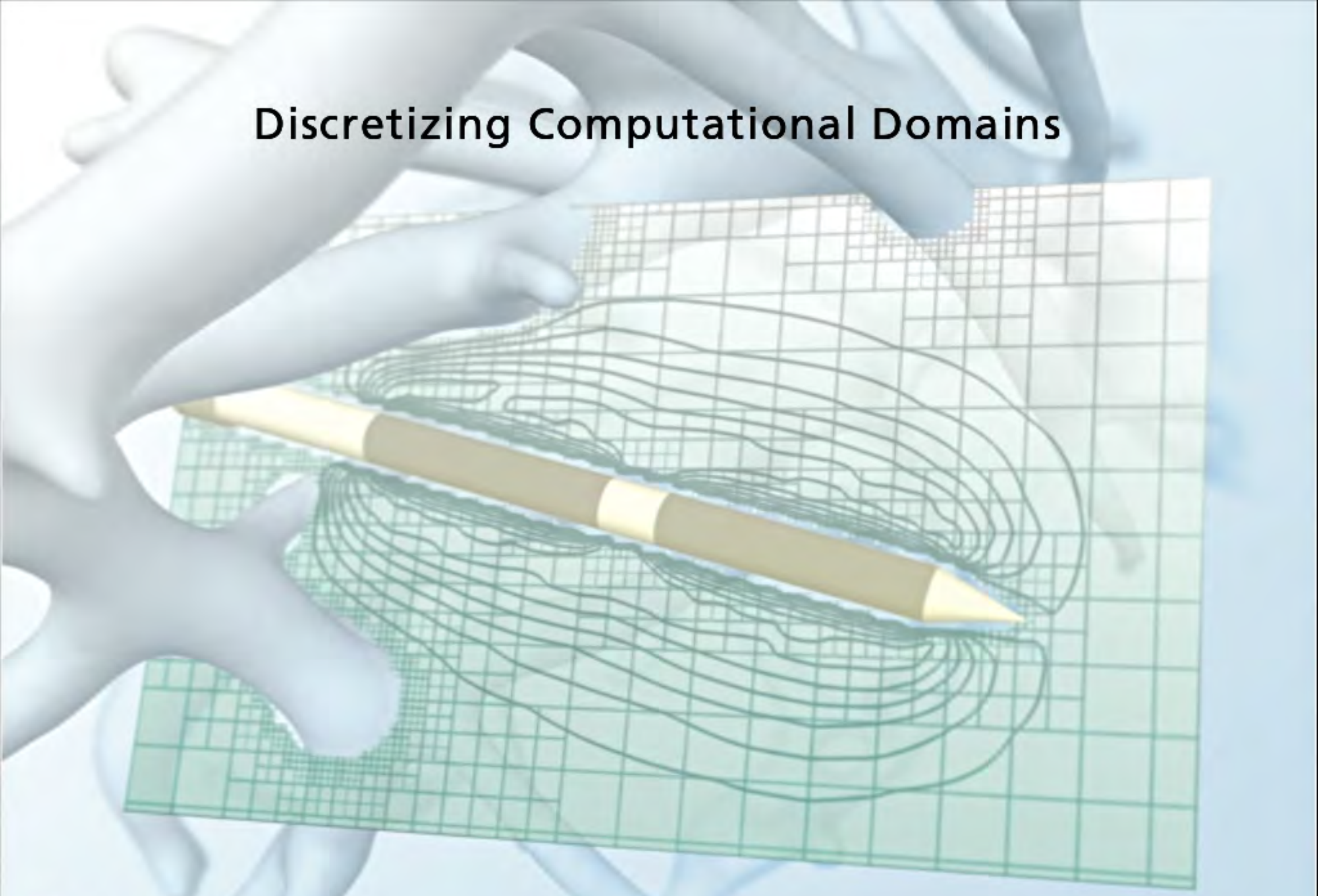
2

Discretizing The Electrostatic Equation

Solving Partial Differential Equations With a Computer

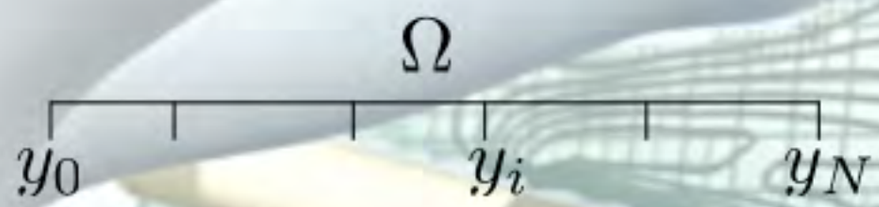
1. • **Discretize the computational domain**
2. • **Discretize the differential operators**
3. • **Solve a system of algebraic equations**

Discretizing Computational Domains



Discretizing Computational Domains

- One space dimension



Discretizing Computational Domains

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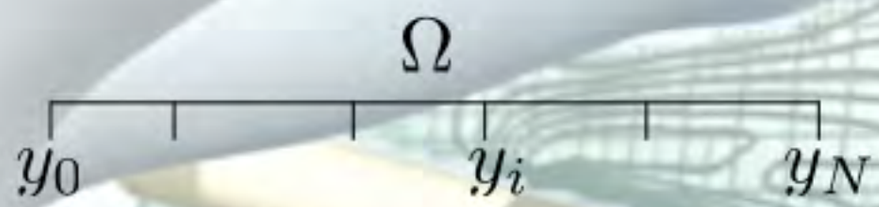
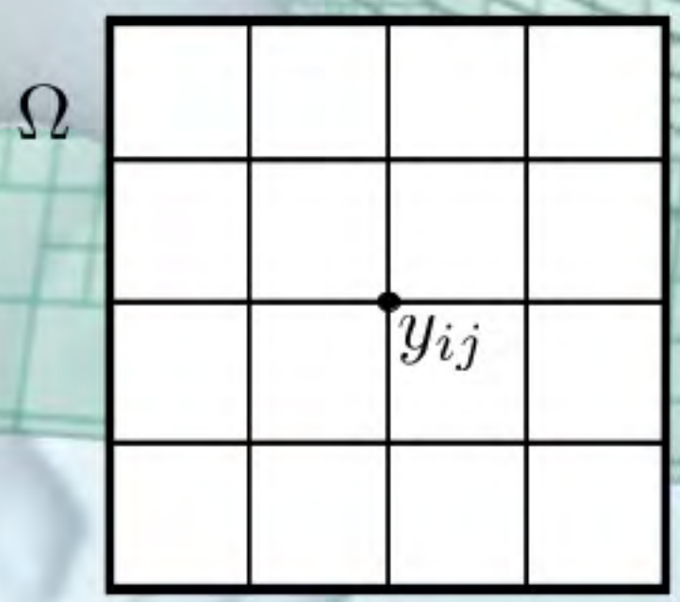


› Two space dimensions



Discretizing Computational Domains

› One space dimension

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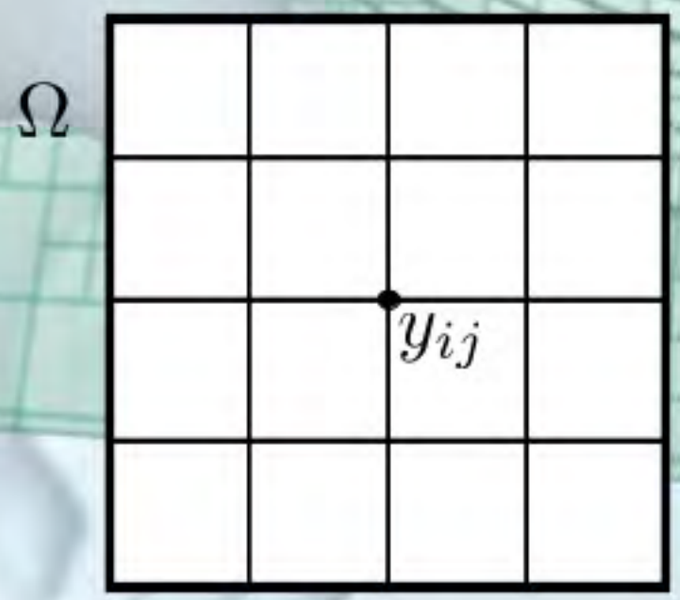
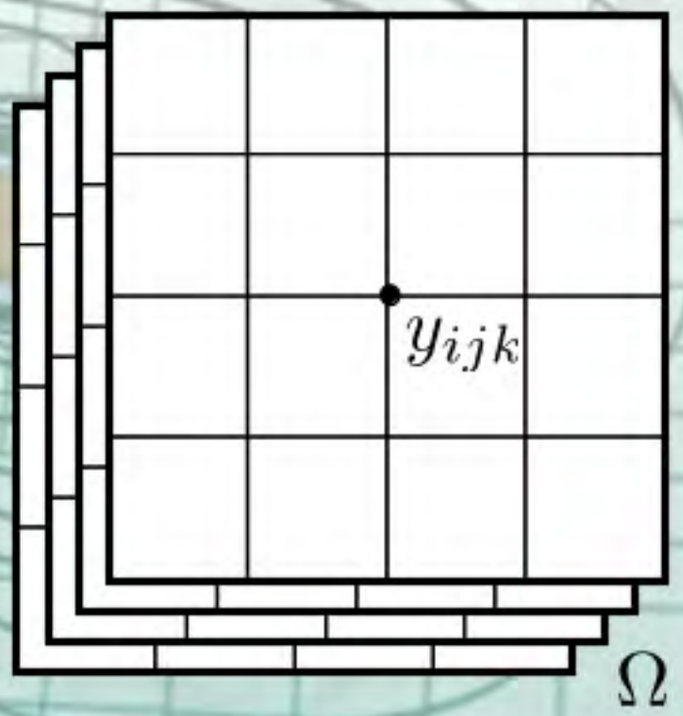


› Three space dimensions



Discretizing Differential Operators

Finite Difference Method (FDM)	Finite Element Method (FEM)

Discretizing Differential Operators

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› Difference quotients	

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Discretizing Differential Operators

Finite Difference Method (FDM)	Finite Element Method (FEM)
› Difference quotients › Easy to implement › Not very flexible w.r.t geometry of domain	› Shape functions of variable smoothness

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Finite Difference Method (FDM)	Finite Element Method (FEM)
› Difference quotients › Easy to implement › Not very flexible w.r.t geometry of domain	› Shape functions of variable smoothness › Difficult to implement

Discretizing Differential Operators

Finite Difference Method (FDM)	Finite Element Method (FEM)
› Difference quotients › Easy to implement › Not very flexible w.r.t geometry of domain	› Shape functions of variable smoothness › Difficult to implement › Very flexible w.r.t geometry of domain

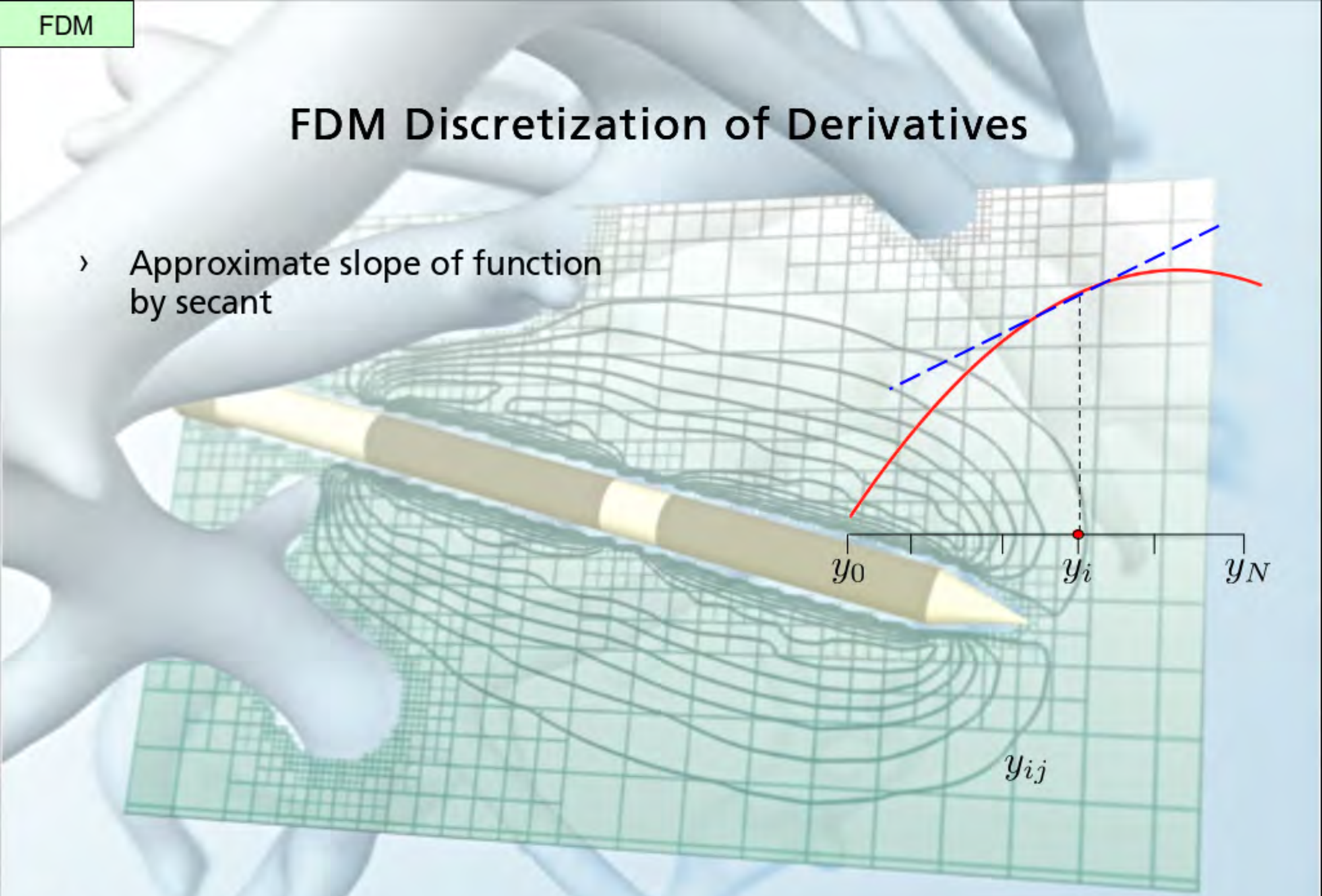
Discretizing Differential Operators

Finite Difference Method (FDM)	Finite Element Method (FEM)
› Difference quotients › Easy to implement › Not very flexible w.r.t geometry of domain	› Shape functions of variable smoothness › Difficult to implement › Very flexible w.r.t geometry of domain › Rich mathematical framework

The Finite Difference Method

FDM Discretization of Derivatives

- Approximate slope of function by secant



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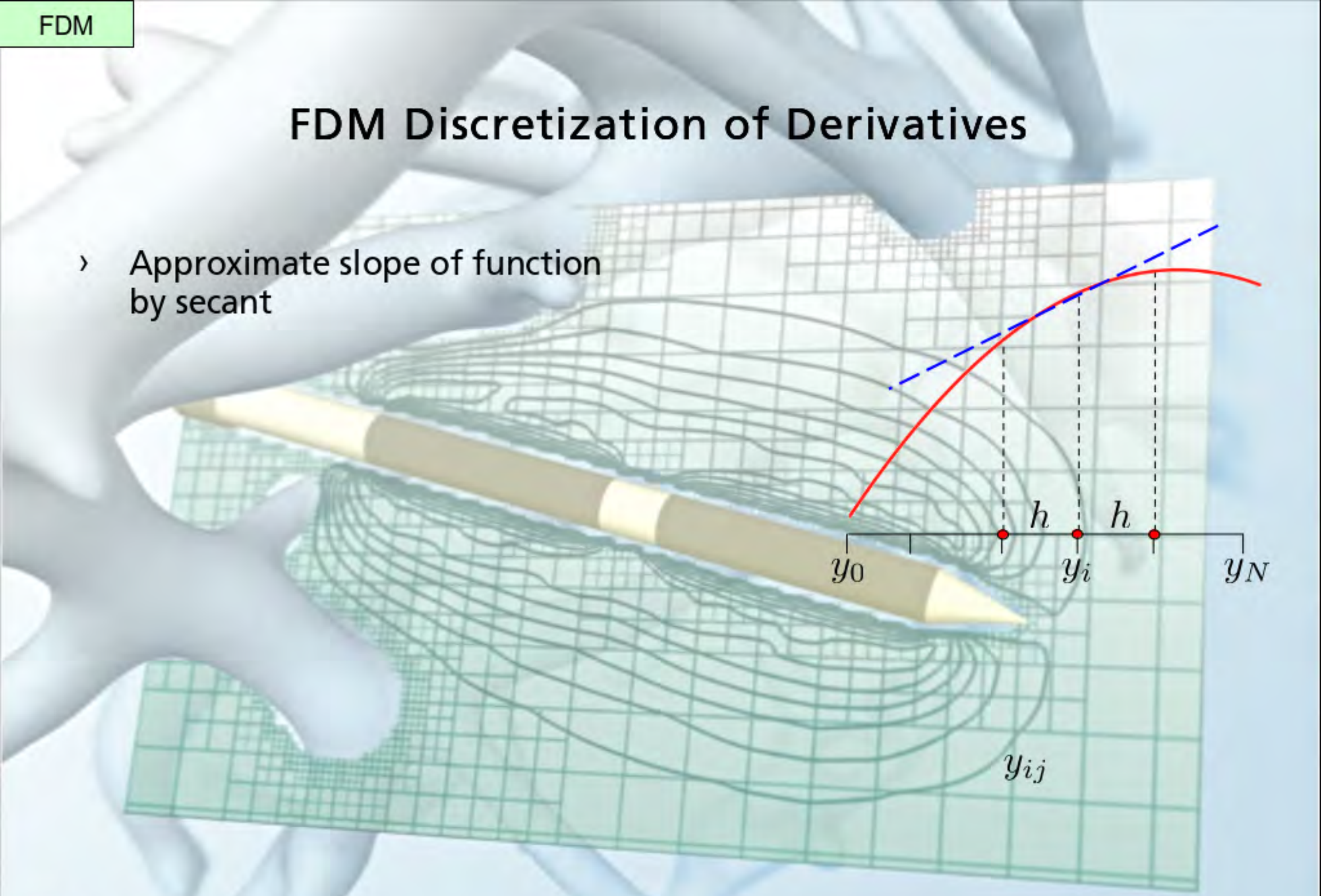
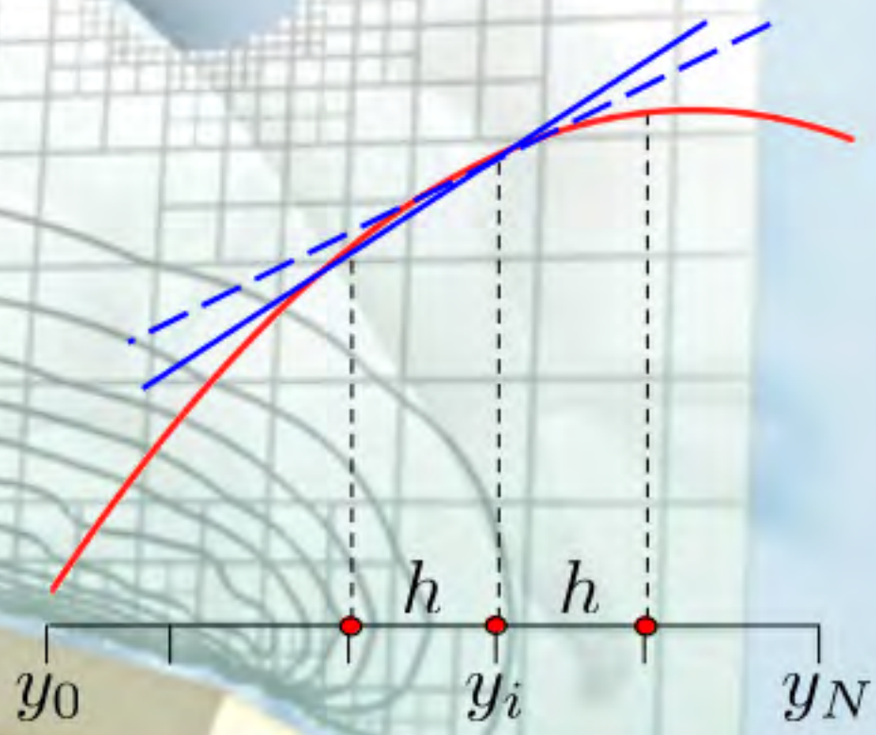


FDM Discretization of Derivatives

- Approximate slope of function by secant

Backward difference $$u'(y_i) \approx \frac{u_i - u_{i-1}}{h}$$

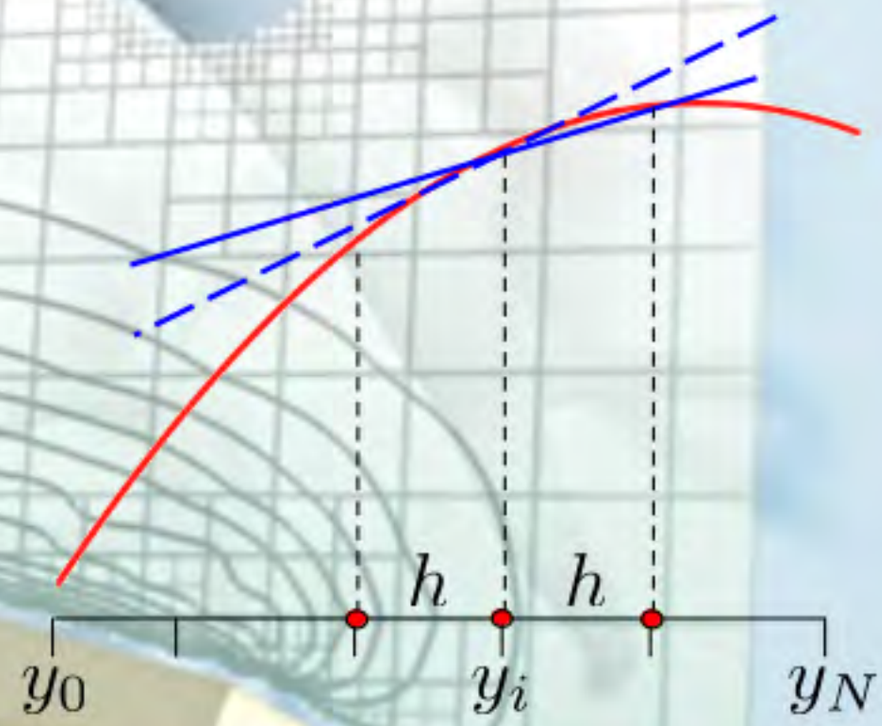


FDM Discretization of Derivatives

- Approximate slope of function by secant

Backward difference $u'(y_i) \approx \frac{u_i - u_{i-1}}{h}$

Forward difference $u'(y_i) \approx \frac{u_{i+1} - u_i}{h}$



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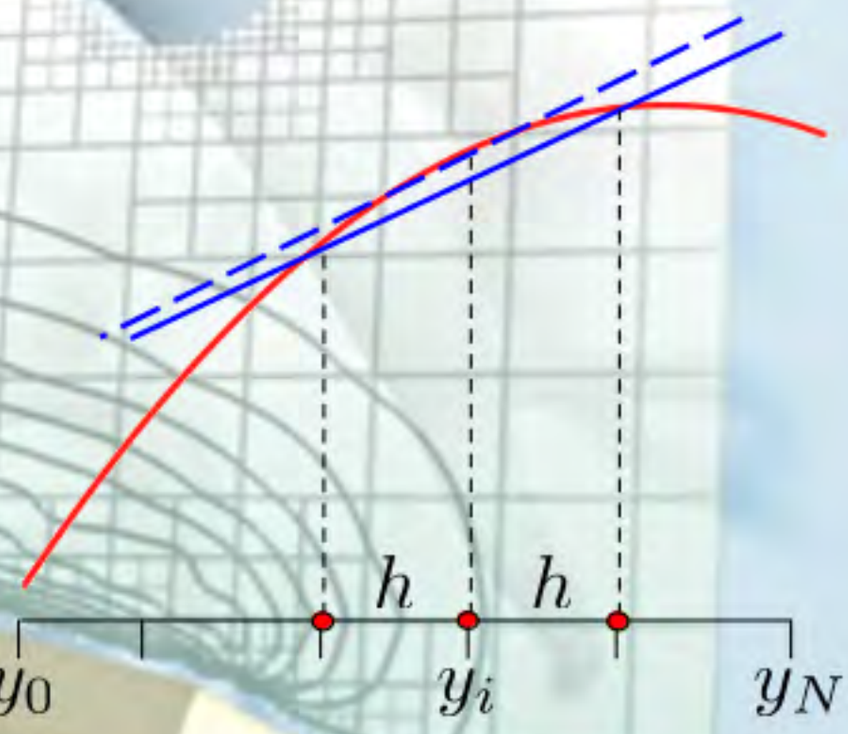
Central difference $u'(y_i) \approx \frac{u_{i+1} - u_{i-1}}{2h}$



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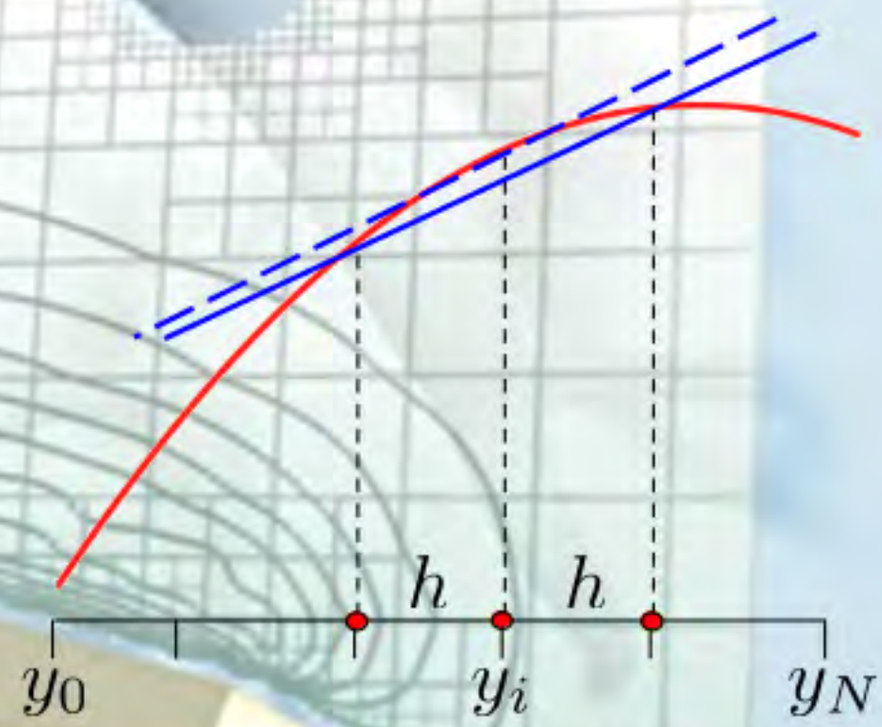
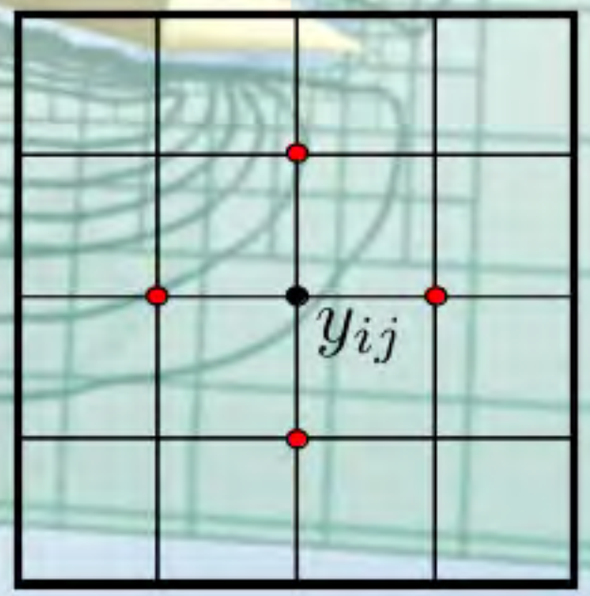


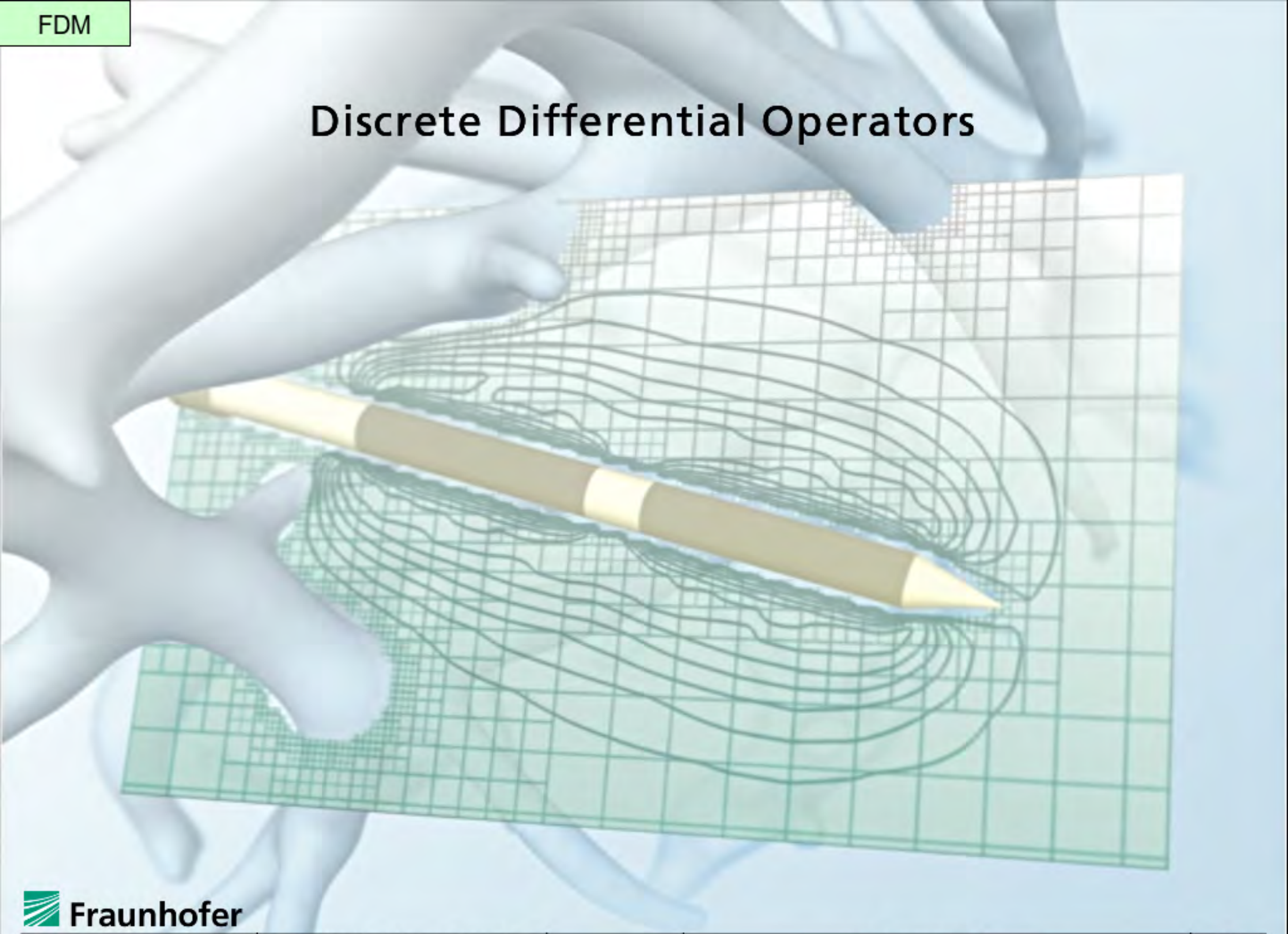
- Higher dimensions: partial derivatives

$$\partial_{x_1} u(y_{ij}) \approx \frac{u_{i,j} - u_{i-1,j}}{h}$$

$$\partial_{x_2} u(y_{ij}) \approx \frac{u_{i,j+1} - u_{i,j}}{h}$$



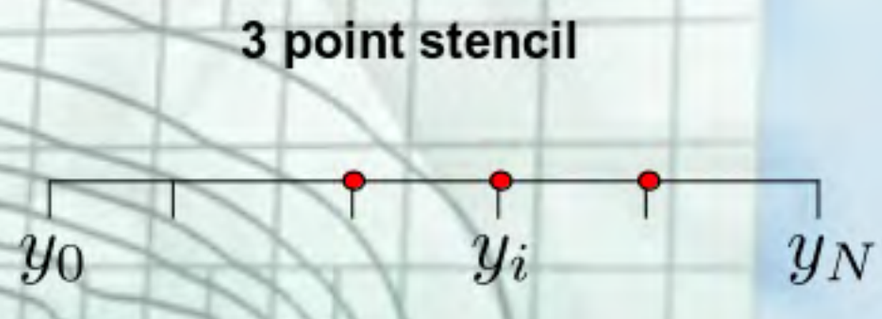
Discrete Differential Operators



Discrete Differential Operators

- Discrete Laplacian in 1D

$$\Delta u(y_i) = u''(y_i) \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}$$



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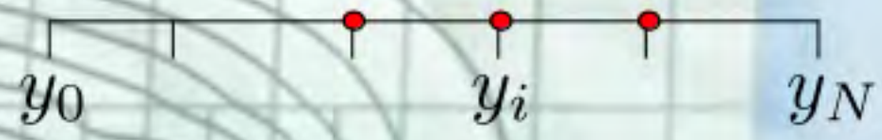
3 point stencil



- Discrete Laplacian in 2D

$$\Delta u(y_{ij}) = \partial_{x_1 x_1} u(y_{ij}) + \partial_{x_2 x_2} u(y_{ij})$$
$$\approx \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}}{h^2}$$

5 point stencil

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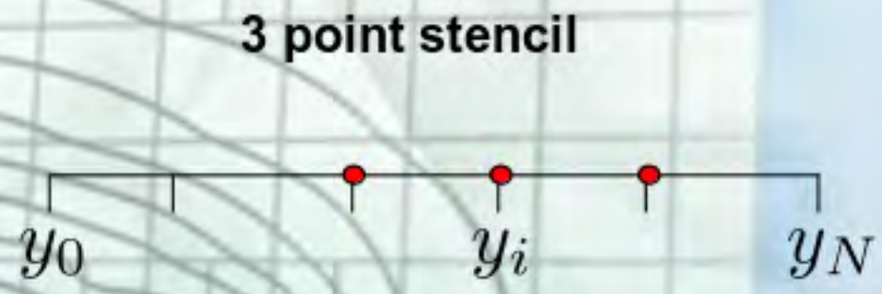


- Discrete Laplacian in 2D

$$\Delta u(y_{ij}) = \partial_{x_1 x_1} u(y_{ij}) + \partial_{x_2 x_2} u(y_{ij})$$
$$\approx \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}}{h^2}$$

5 point stencil

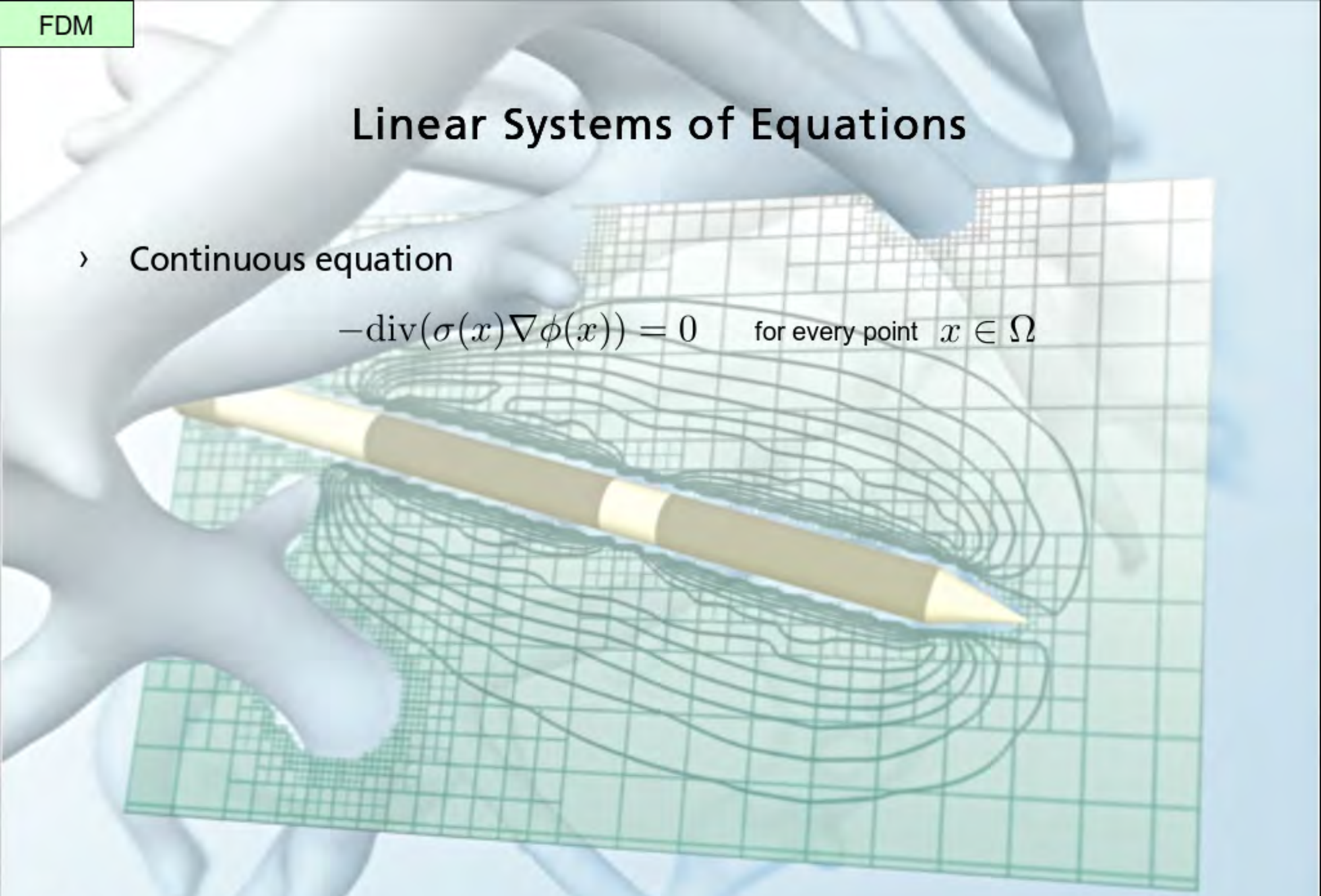
- Discrete Laplacian in 3D

7 point stencil

Linear Systems of Equations

- Continuous equation

$$-\mathrm{div}(\sigma(x)\nabla\phi(x)) = 0 \qquad \text{for every point } x \in \Omega$$



Linear Systems of Equations

- Continuous equation

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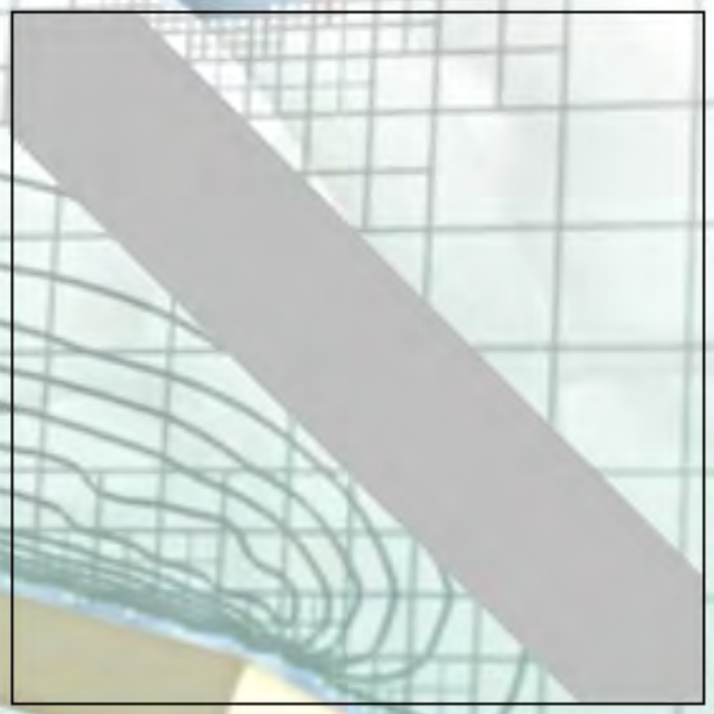
$$A\Phi = F$$

$$A \in I\!R^{(N+1)\times(N+1)}$$
$$\Phi, F \in I\!R^{(N+1)}$$

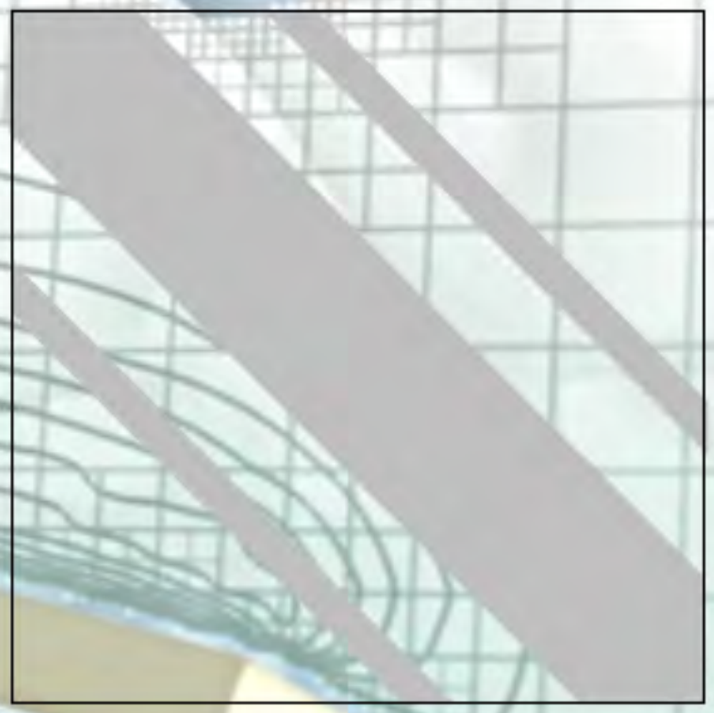
Solving Linear System of Equations

- 3-Band matrix in 1D



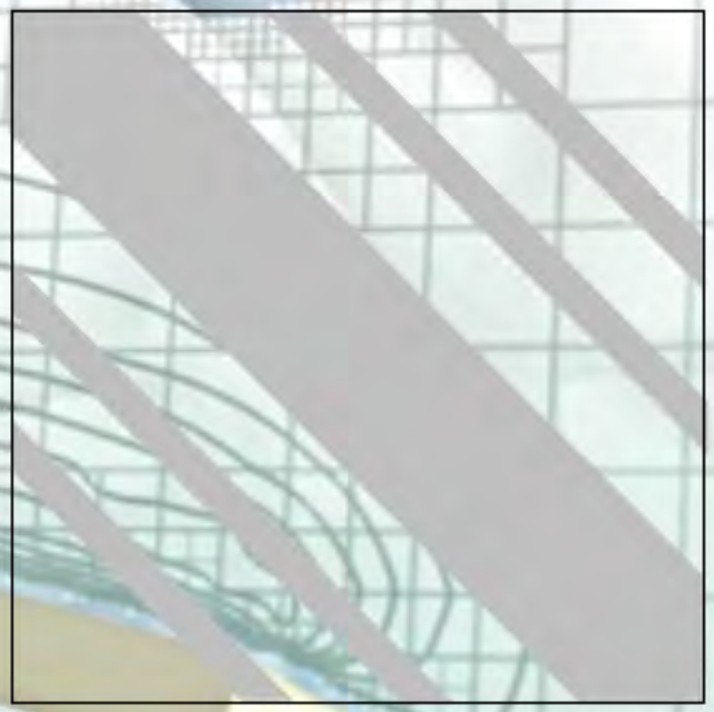
Solving Linear System of Equations

- 3-Band matrix in 1D
- 5-Band matrix in 2D



Solving Linear System of Equations

- 3-Band matrix in 1D
- 5-Band matrix in 2D
- 7-Band matrix in 3D



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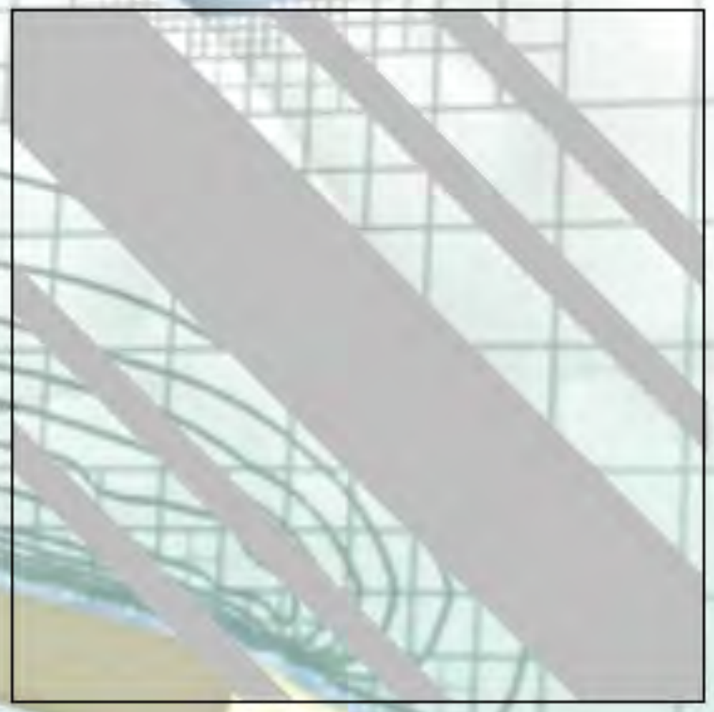
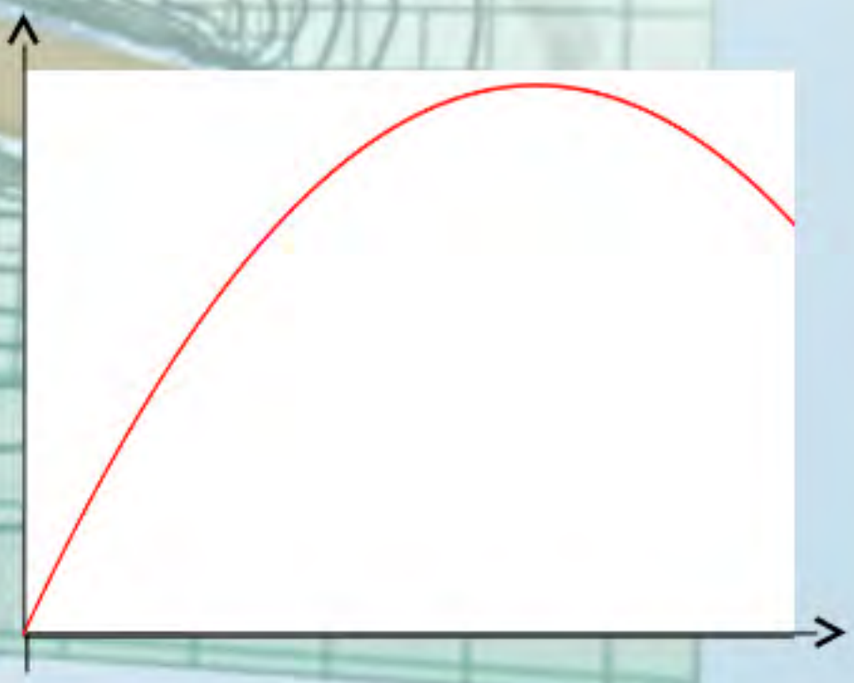


- Matrix inversion:
  - Direct method, e.g. Thomas algorithm
  - Iterative method: e.g. Gauss-Seidel method, conjugate gradients

Summary FDM

- Discretize the domain by a regular grid
- Approximate differential operators by difference quotients
- System of linear equations
- Solve by iterative or direct method
- Obtain a numerical solution ϕ_h of the PDE



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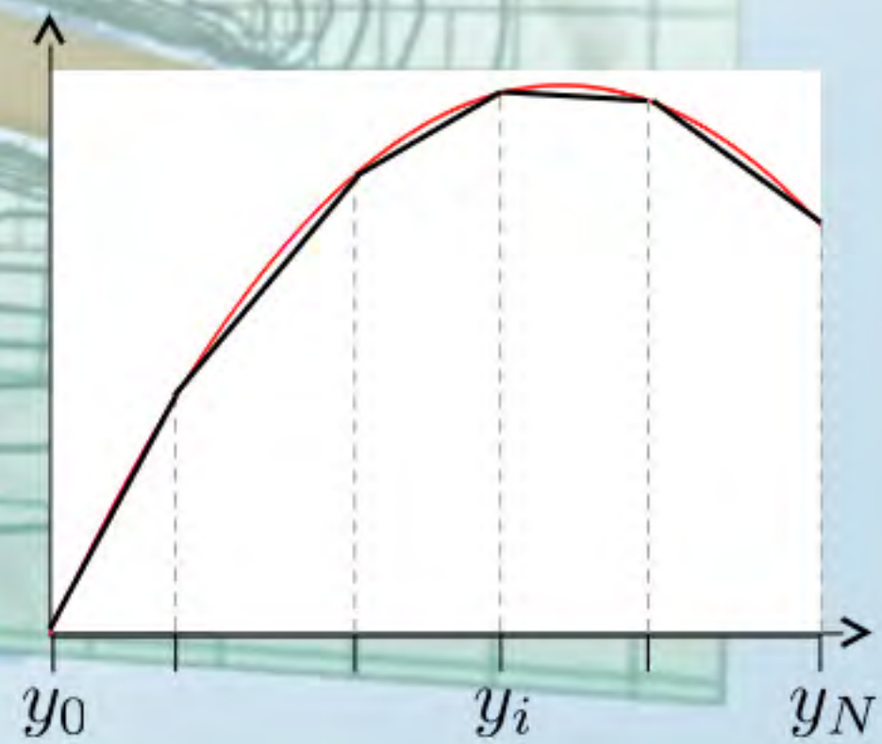

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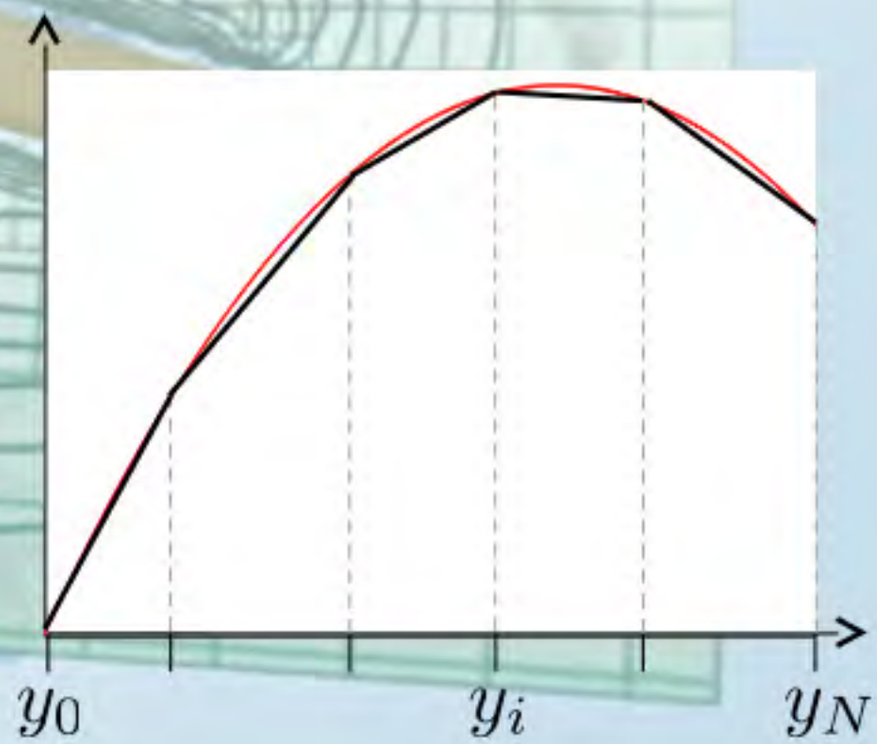
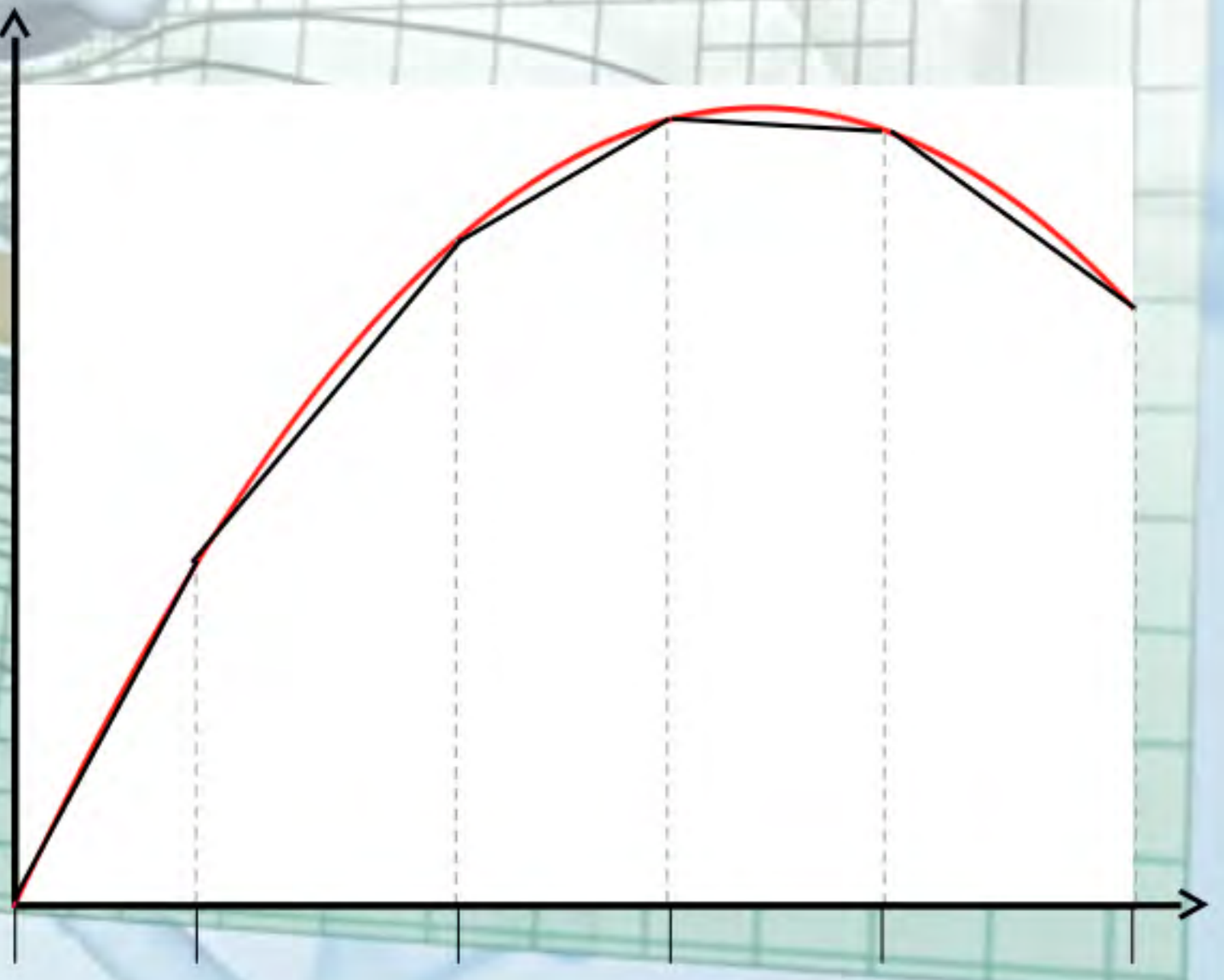
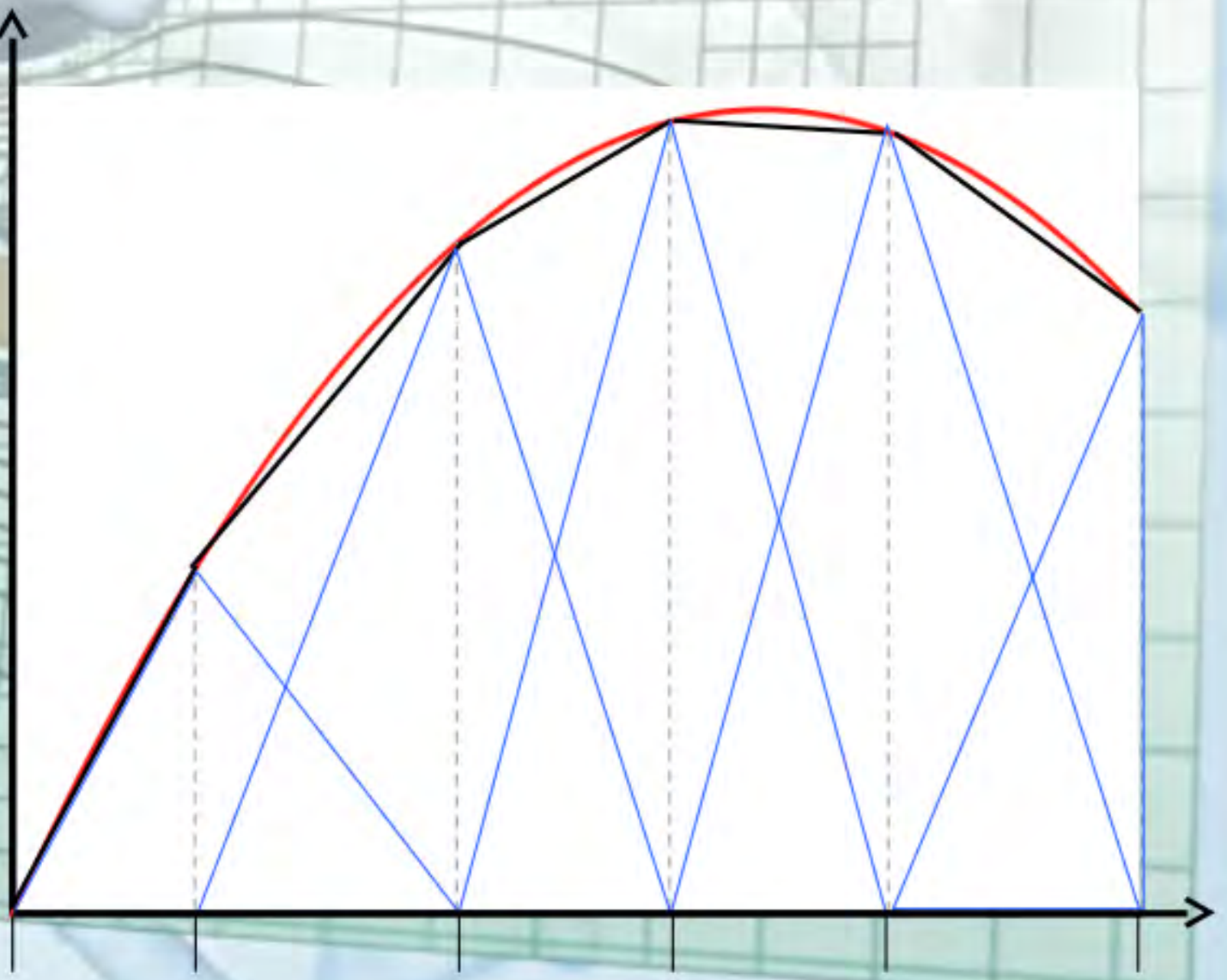


The Finite Element Method

Finite Element Shape Functions

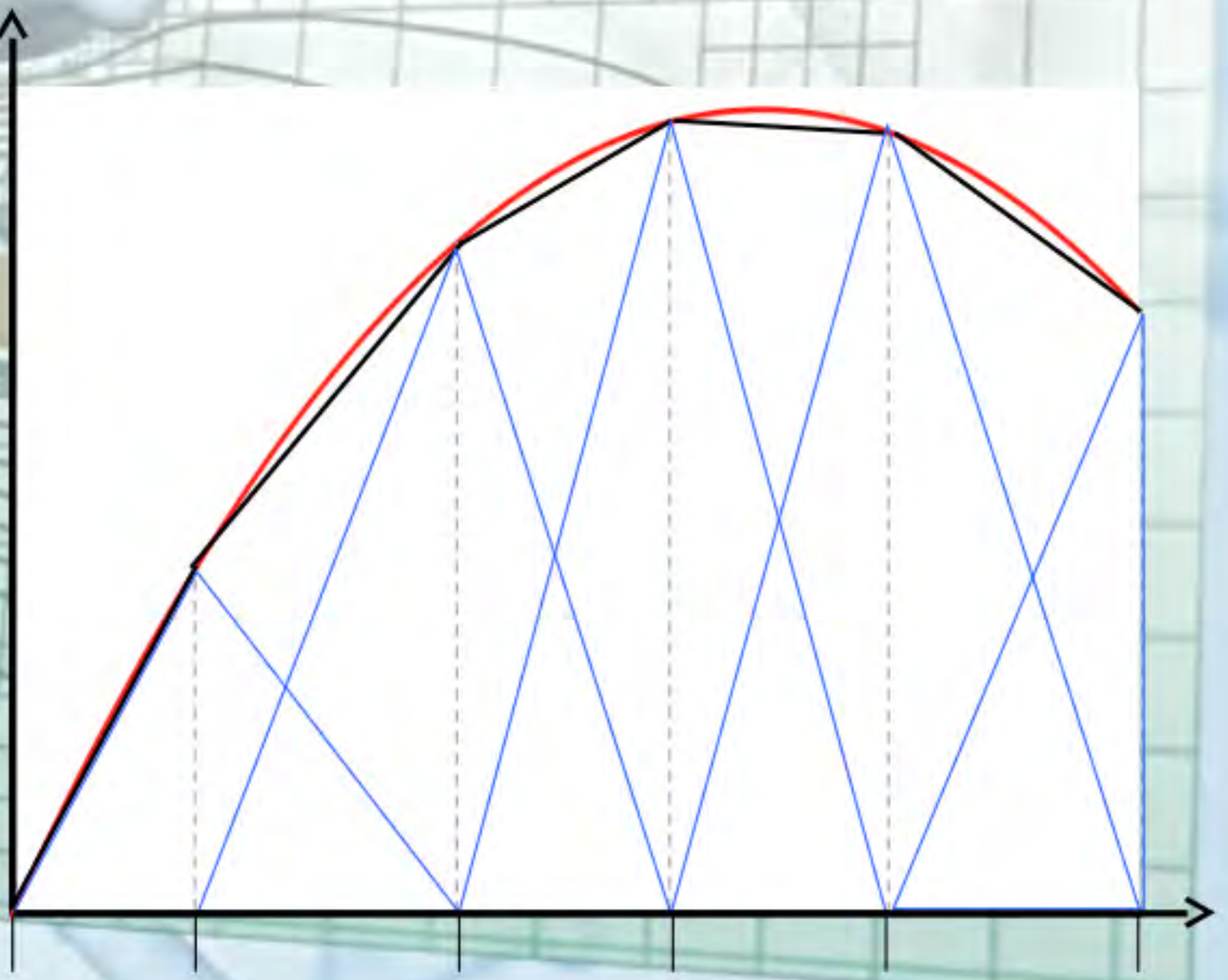


Finite Element Shape Functions



Finite Element Shape Functions

› Compose the solution from predefined shape functions



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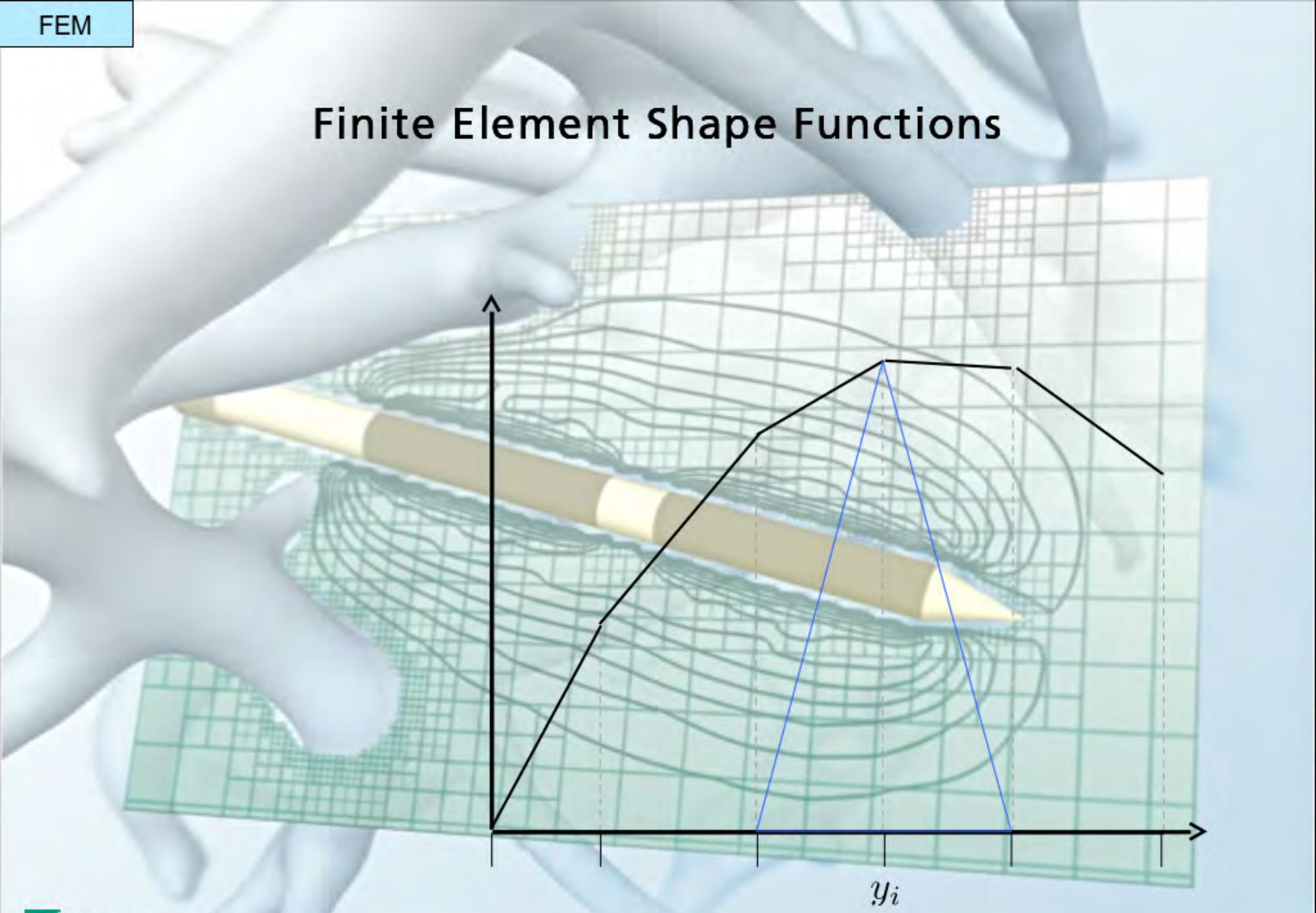

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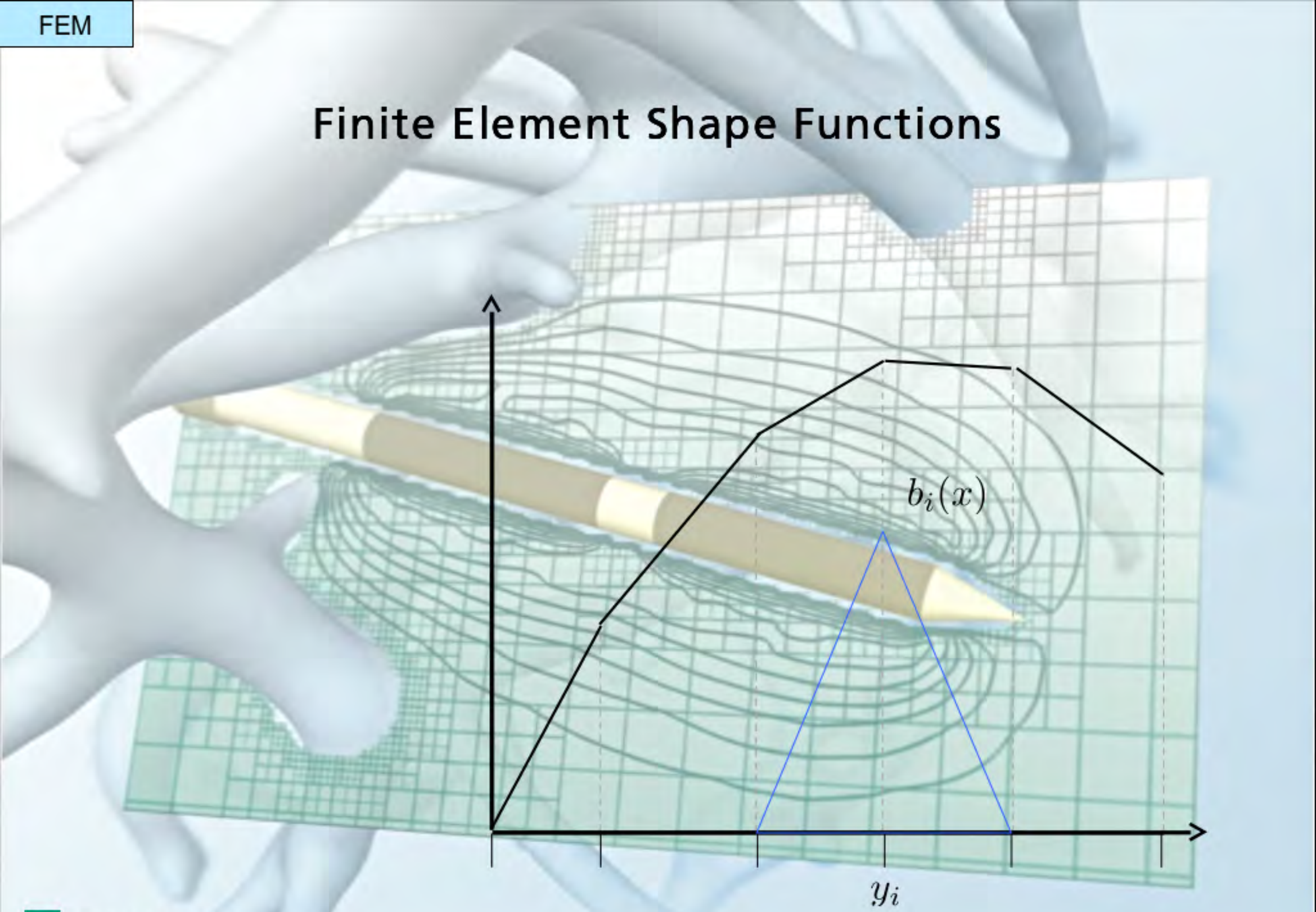

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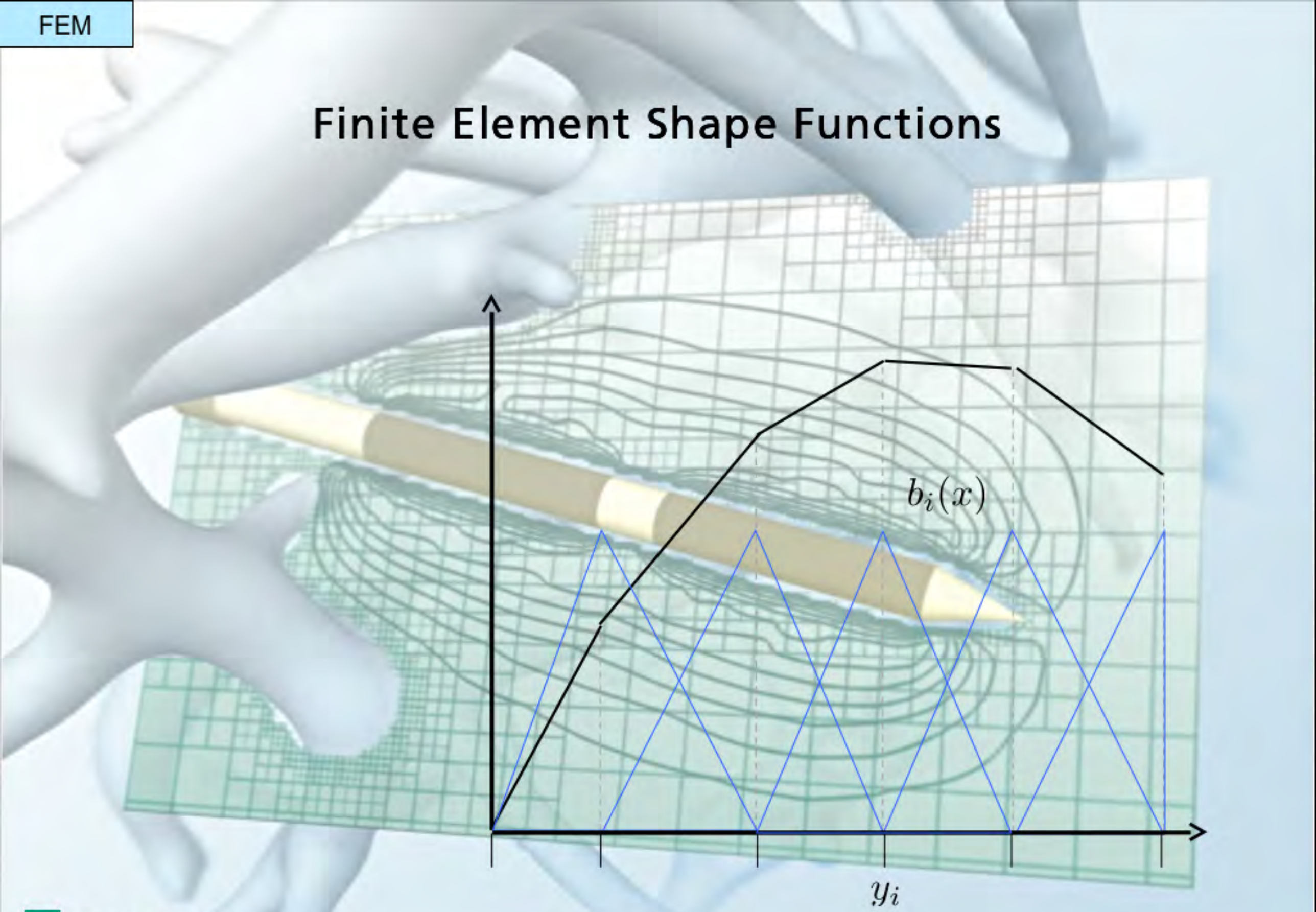

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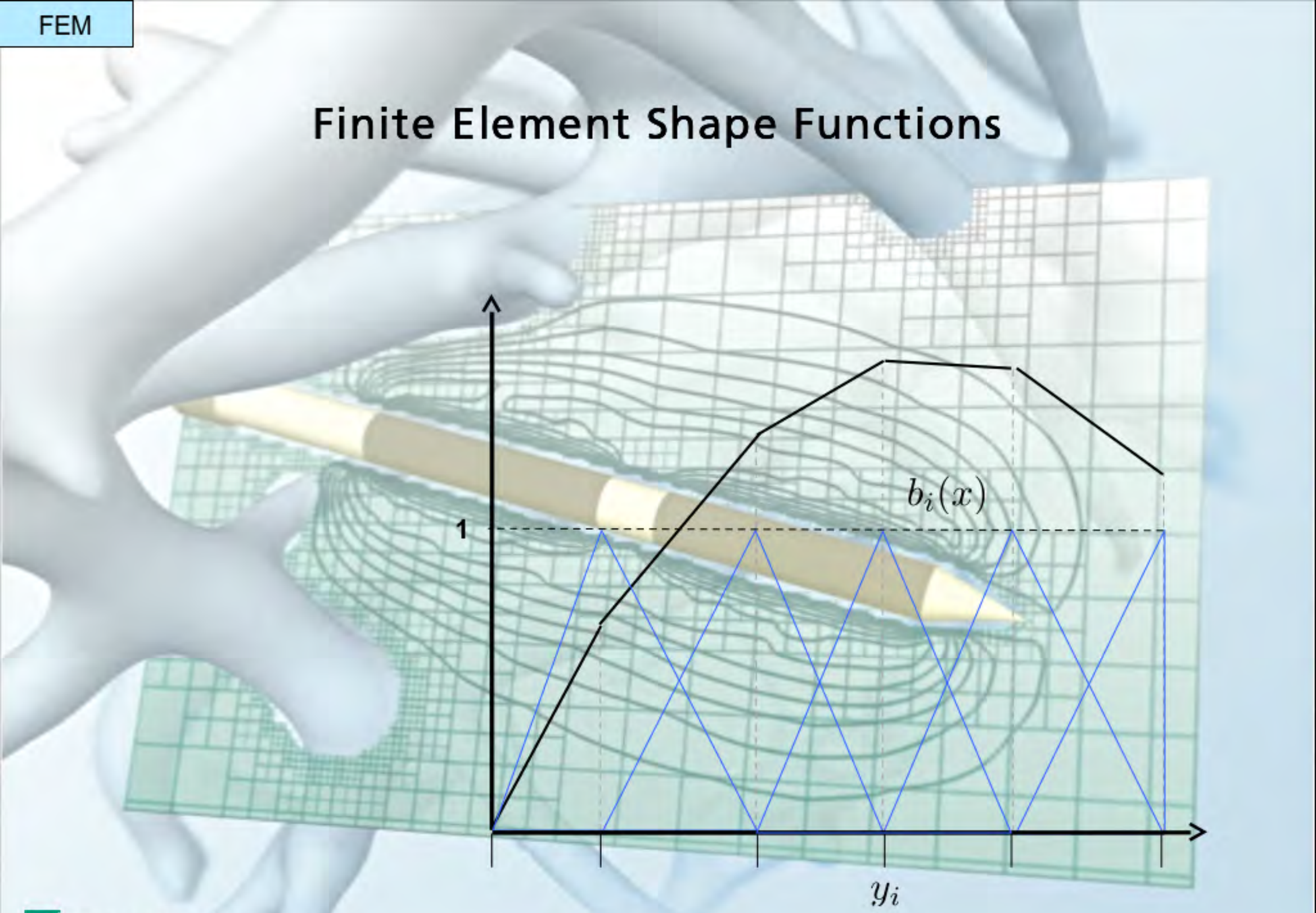
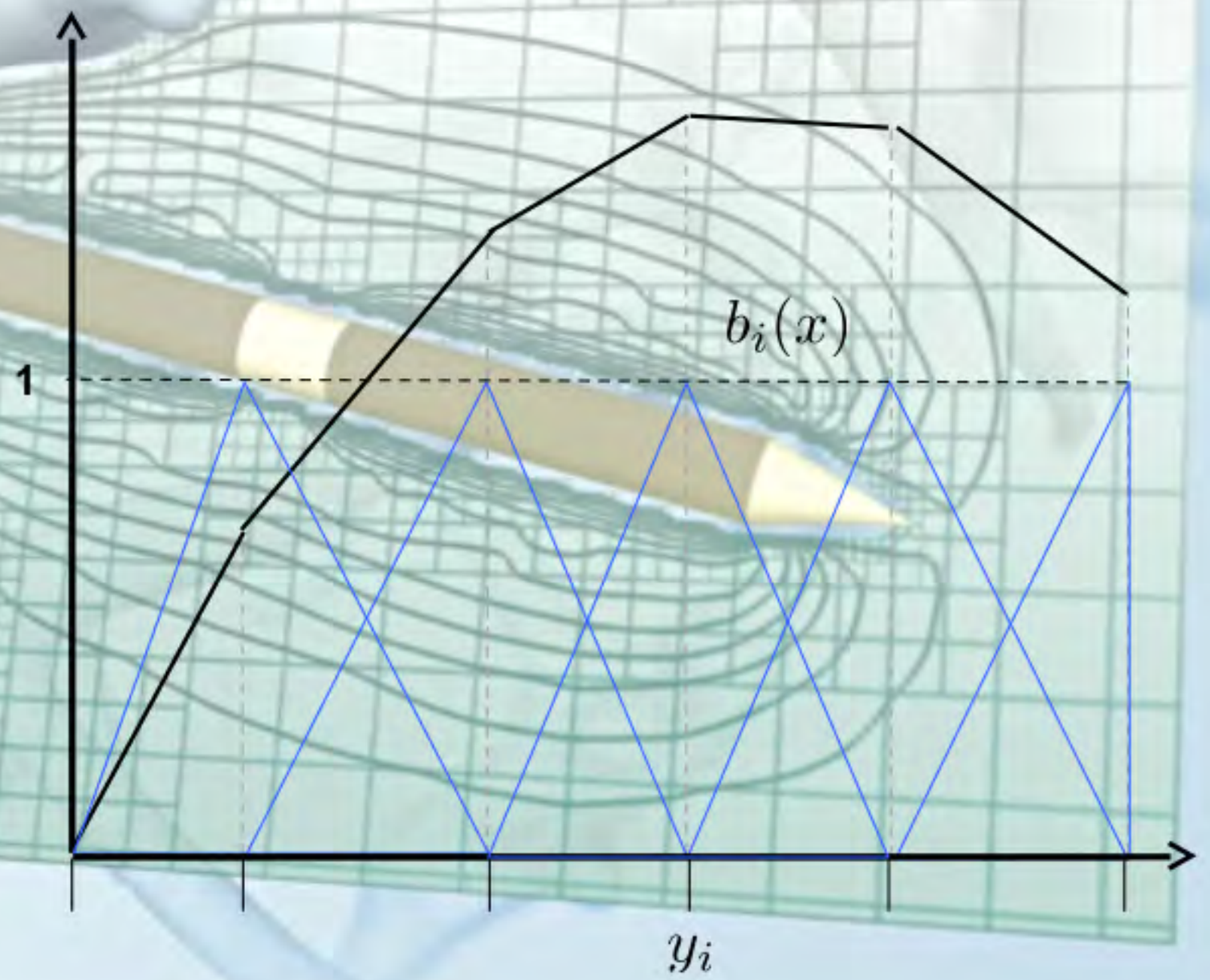


Finite Element Shape Functions

$$\phi(x) = \phi_0 b_0(x) + \phi_1 b_1(x) + \cdots + \phi_N b_N(x)$$

$$= \sum_{i=0}^{N} \phi_i b_i(x)$$



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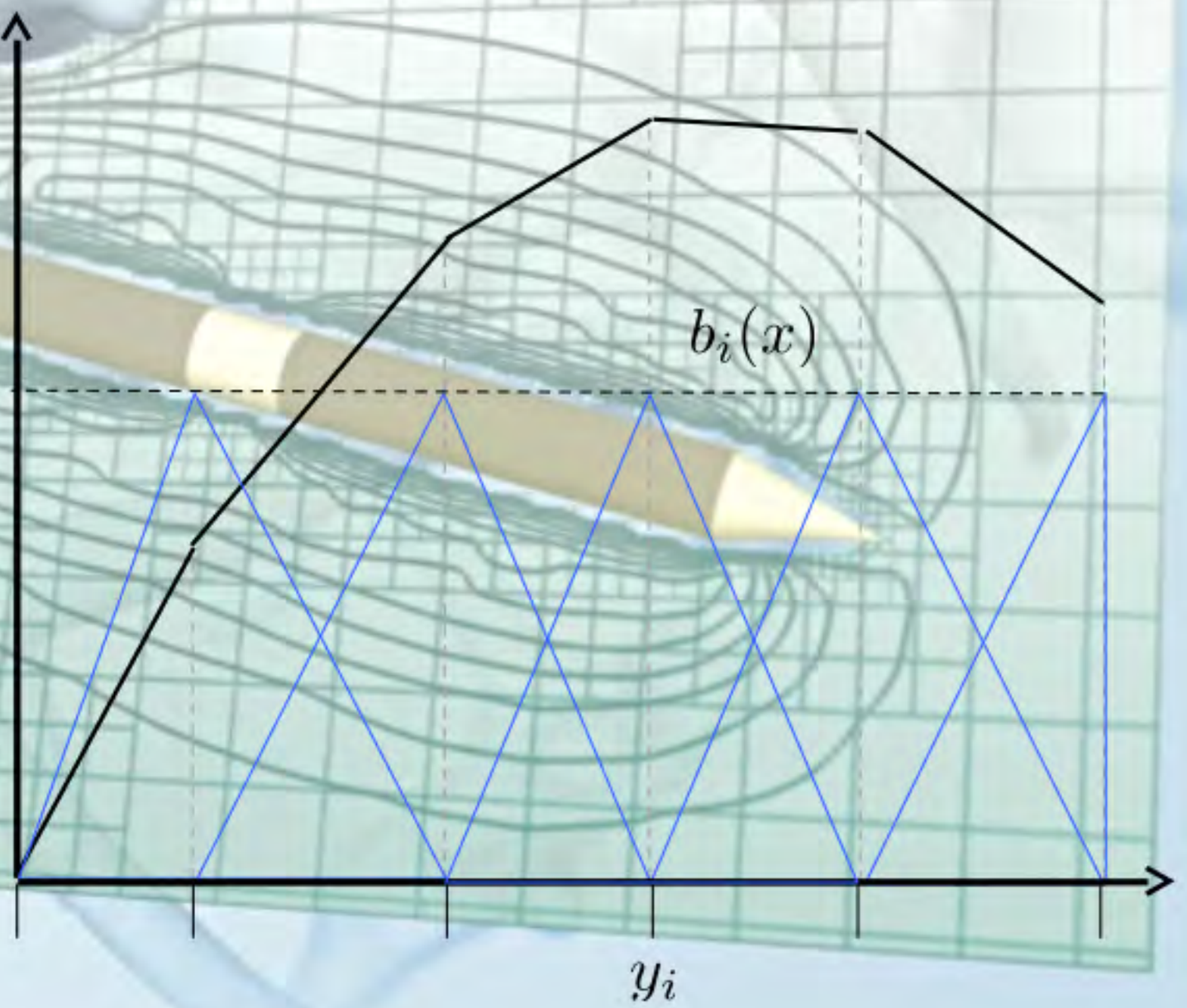
Piecewise linear function



Flexibility of Shape Functions

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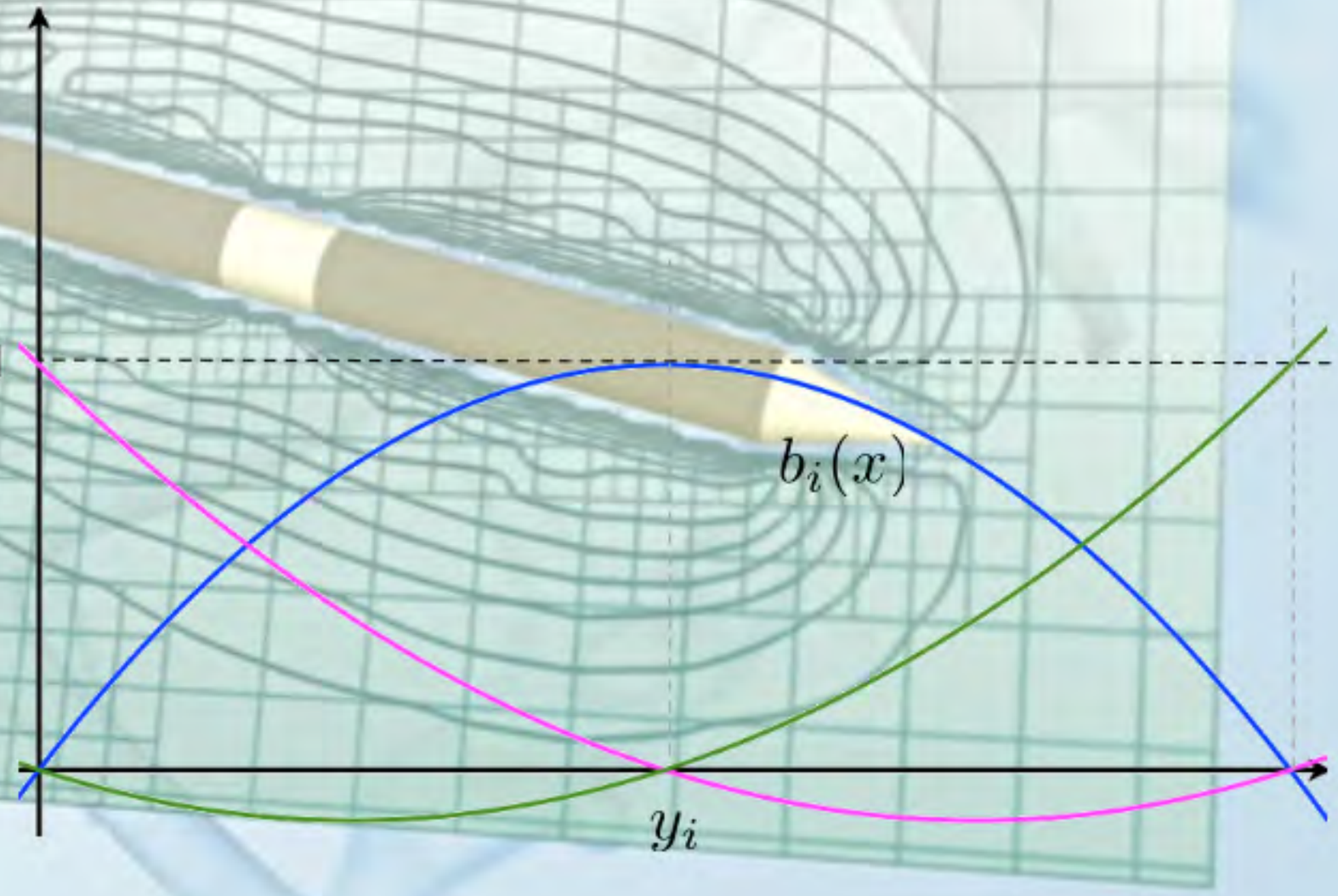
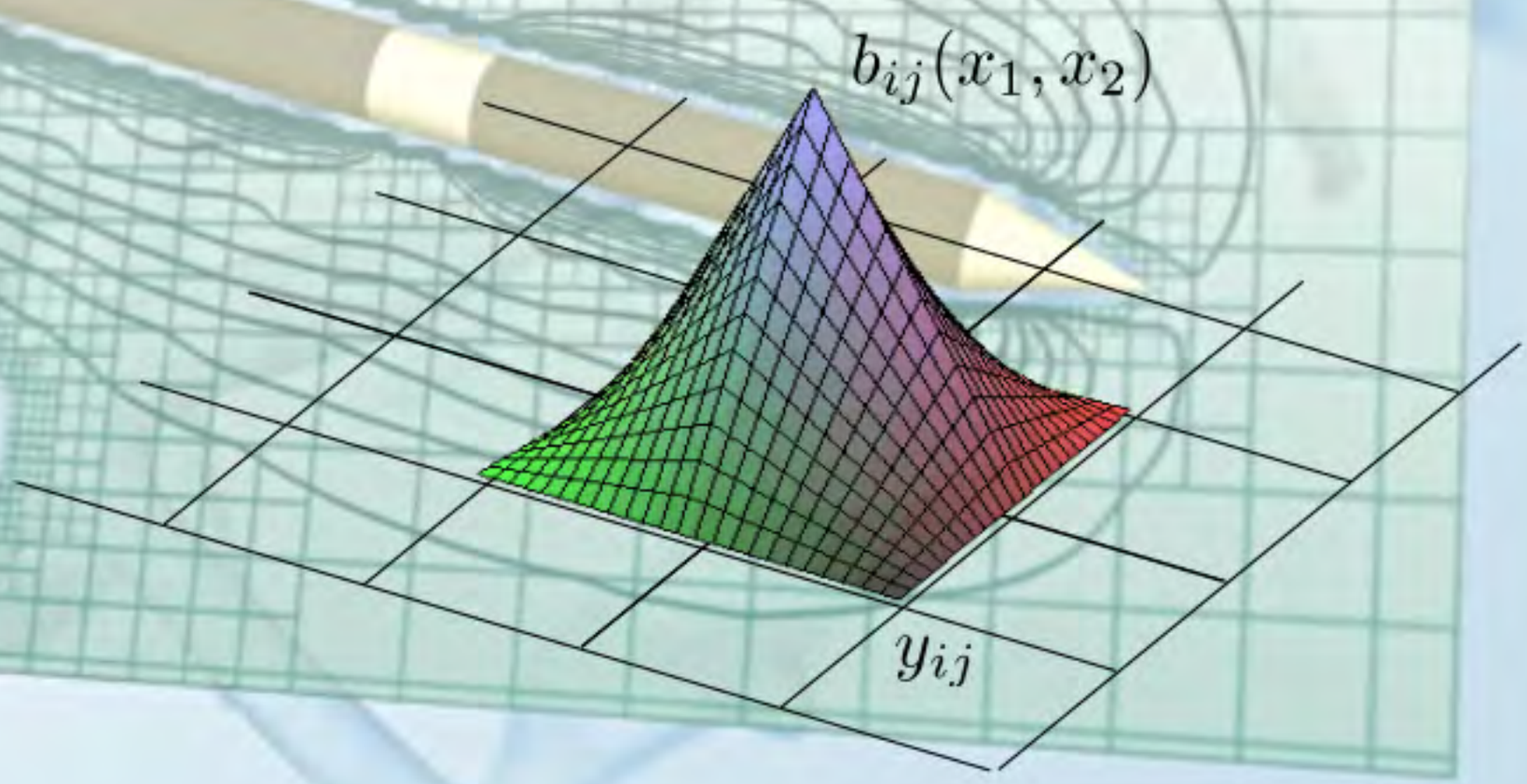


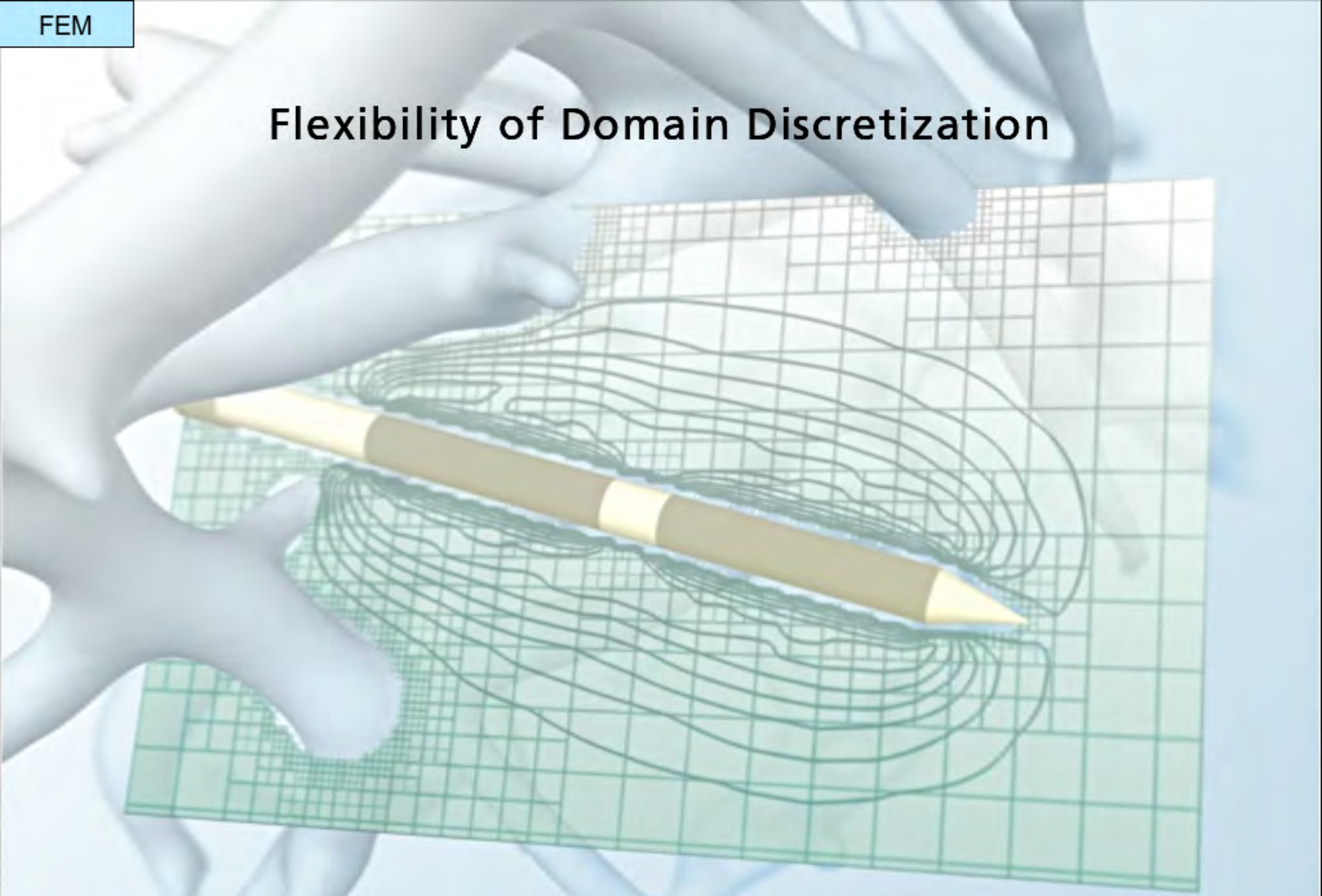
Shape Functions in 2D

$$\phi(x) = \phi(x_1, x_2) = \sum_{i,j} \phi_{ij} b_{ij}(x_1, x_2)$$

Piecewise bilinear function

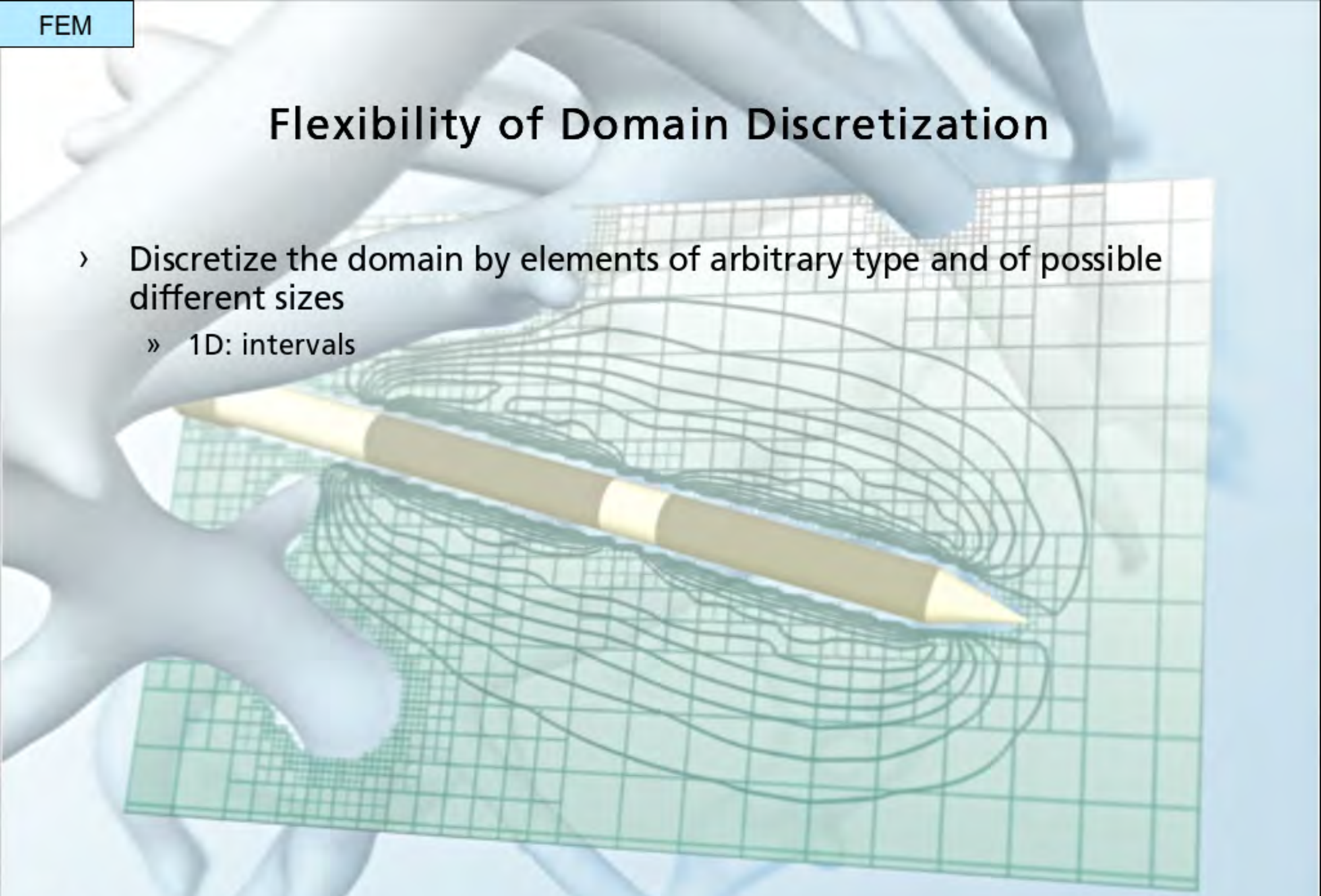


Flexibility of Domain Discretization



Flexibility of Domain Discretization

- Discretize the domain by elements of arbitrary type and of possible different sizes
  - 1D: intervals



Flexibility of Domain Discretization

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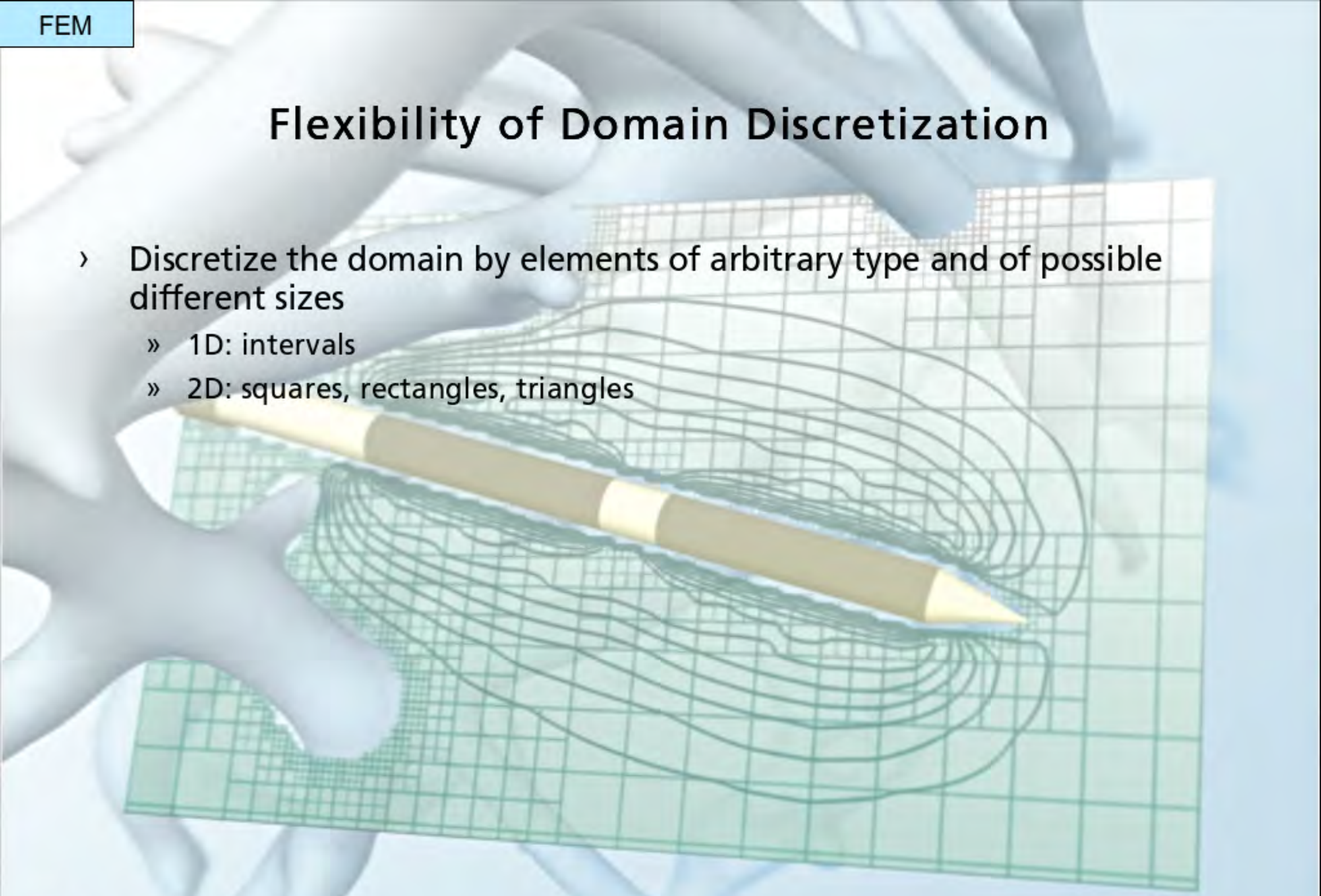
  - 1D: intervals
  - 2D: squares, rectangles, triangles



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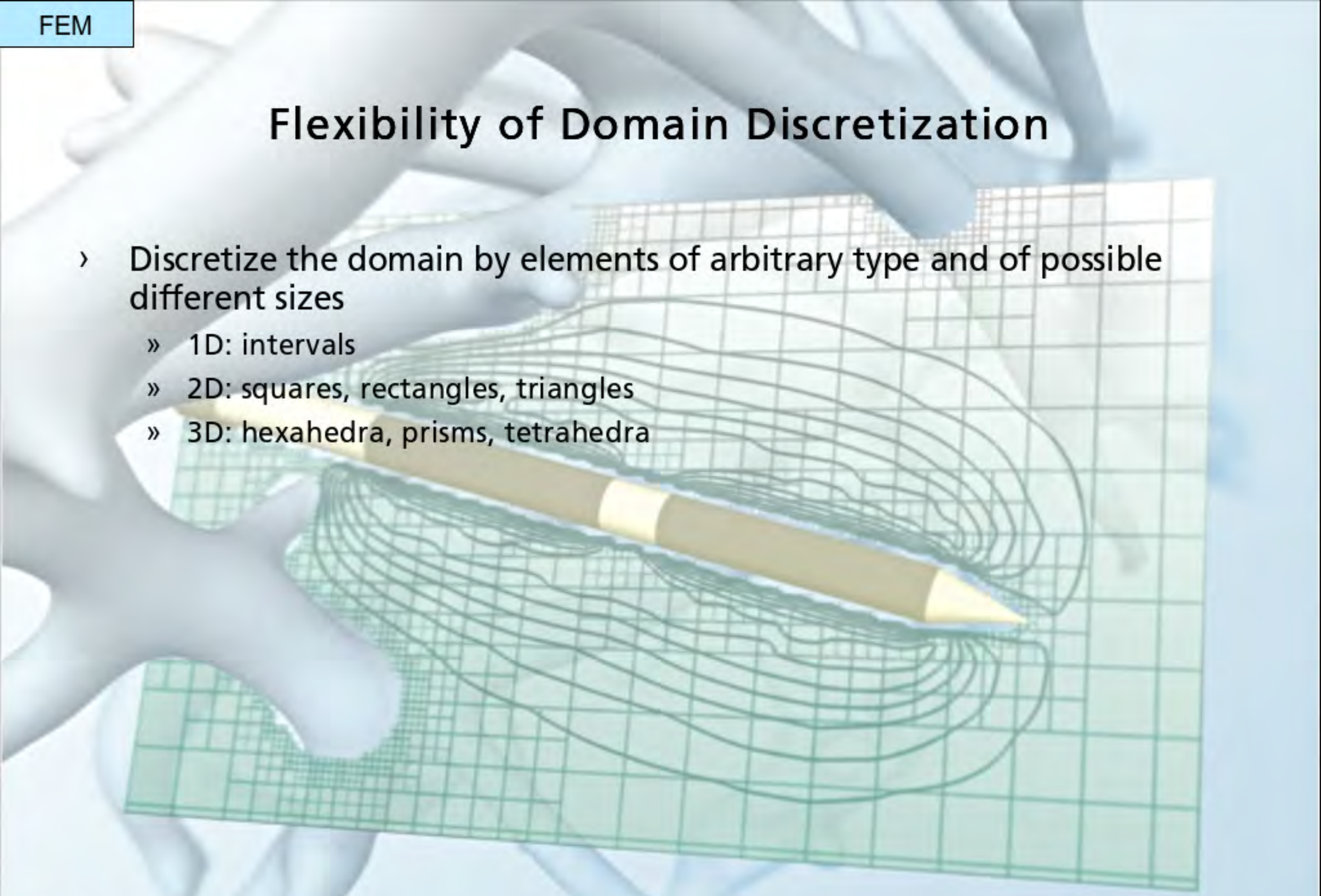

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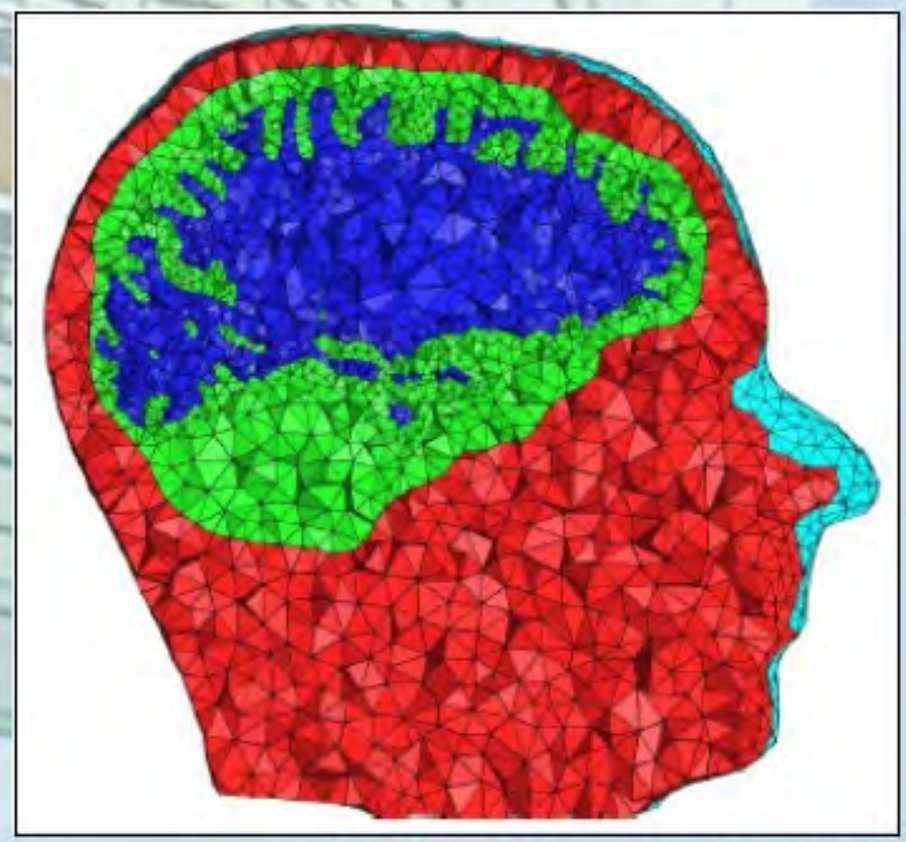

iso2mesh.sourceforge.net

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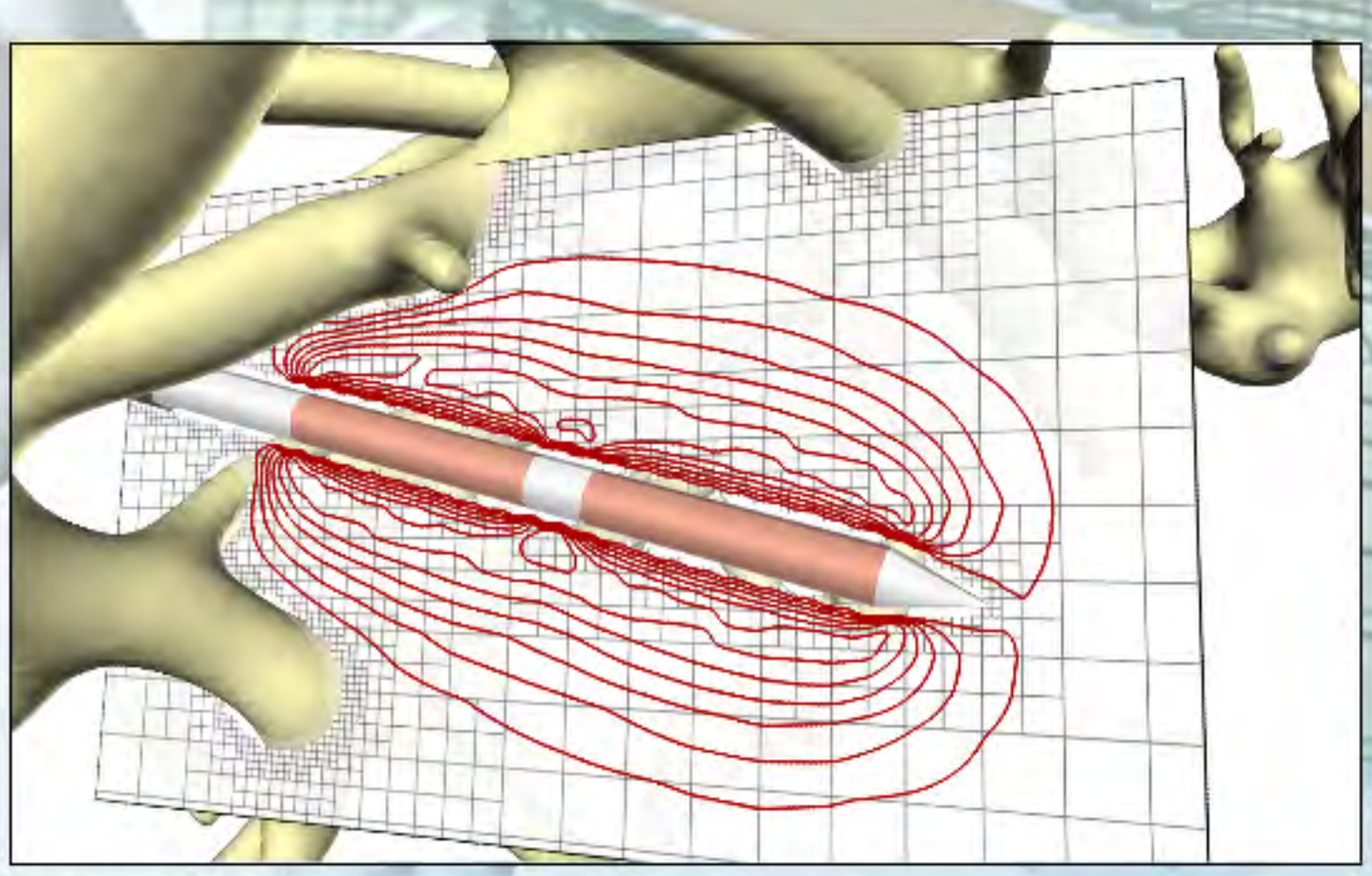

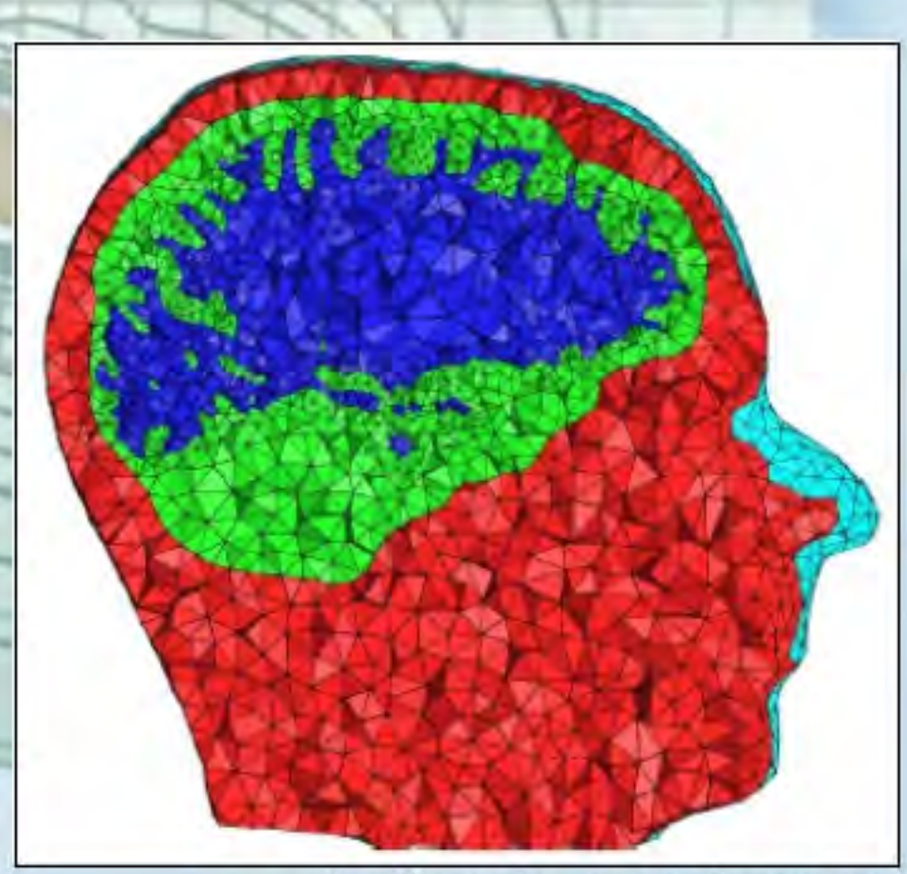

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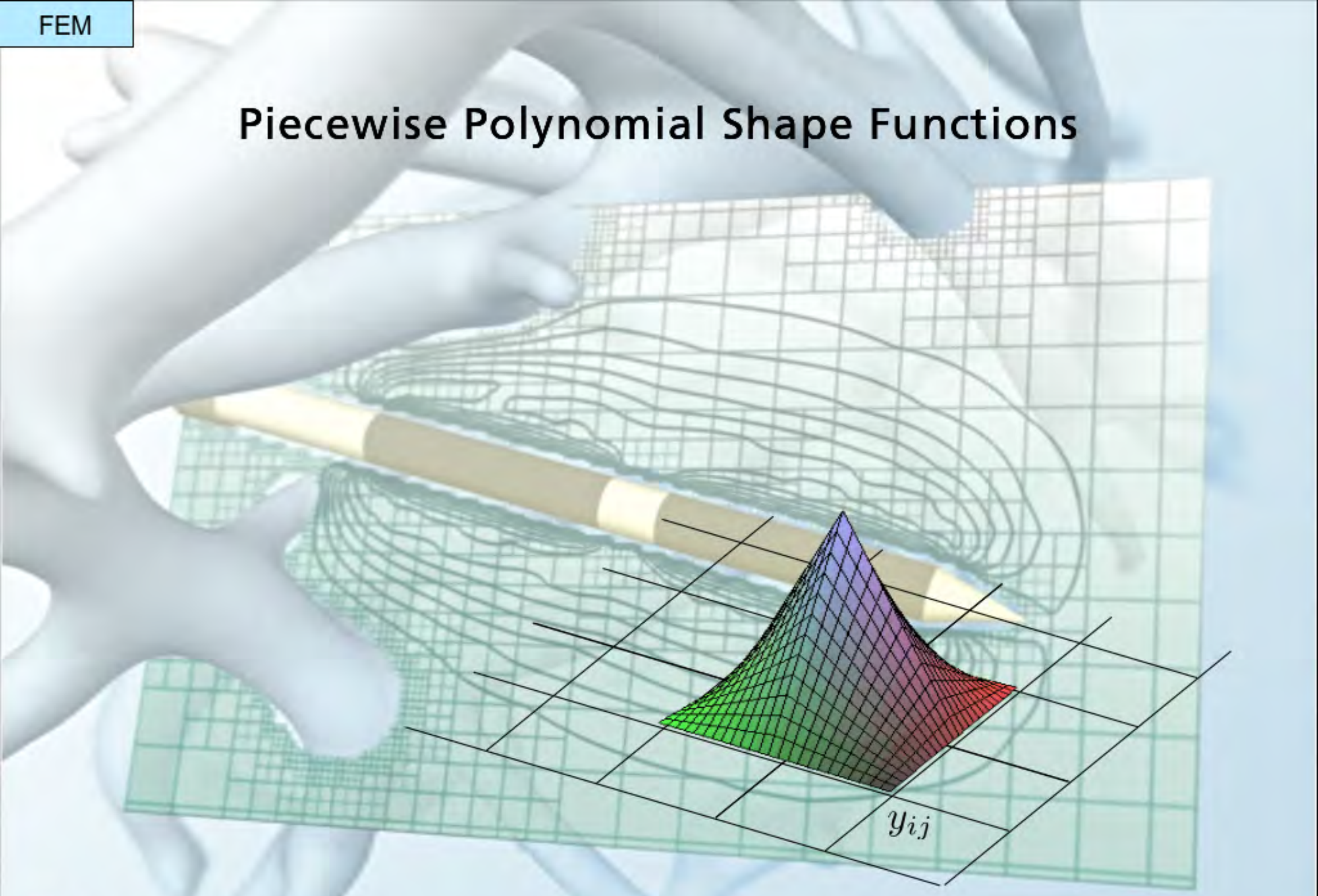
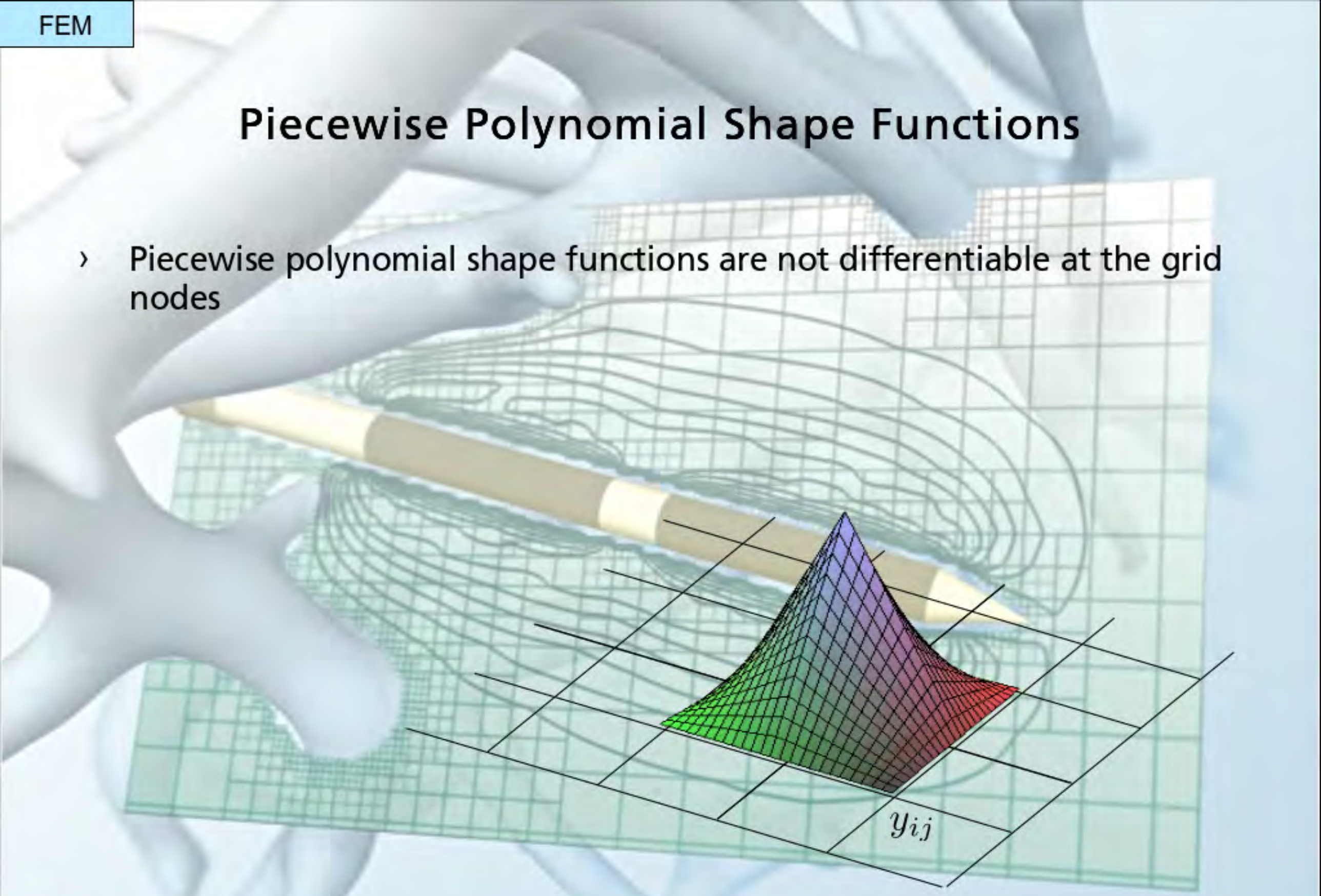
Piecewise Polynomial Shape Functions



Piecewise Polynomial Shape Functions

- Piecewise polynomial shape functions are not differentiable at the grid nodes



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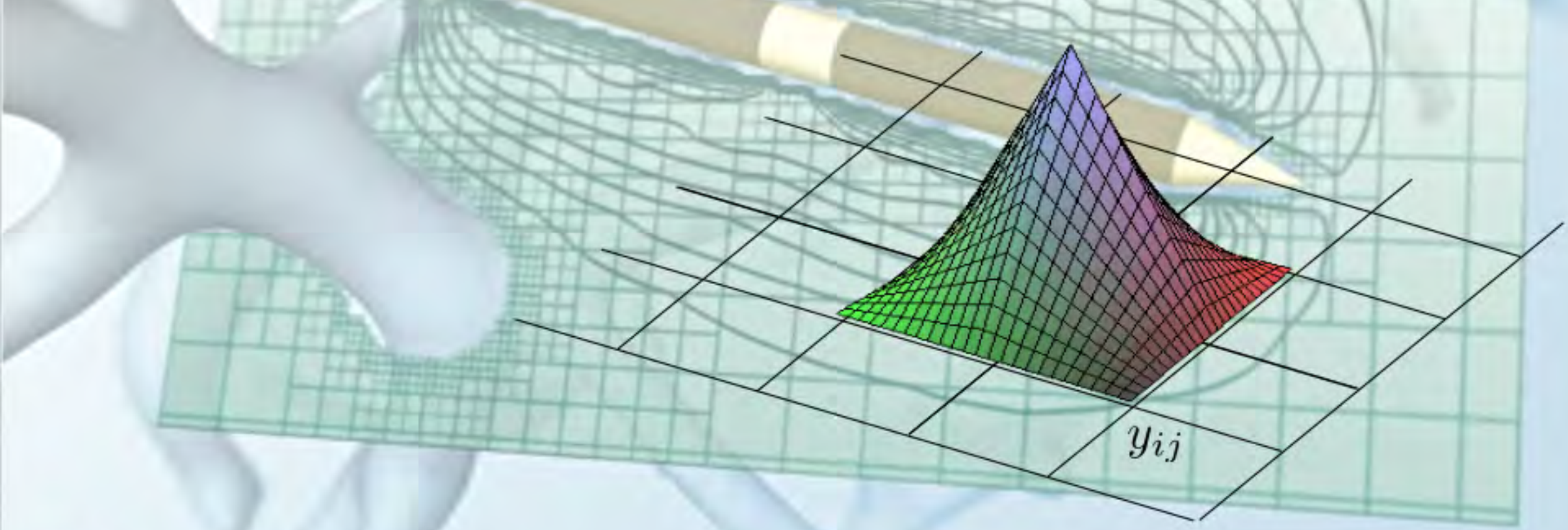
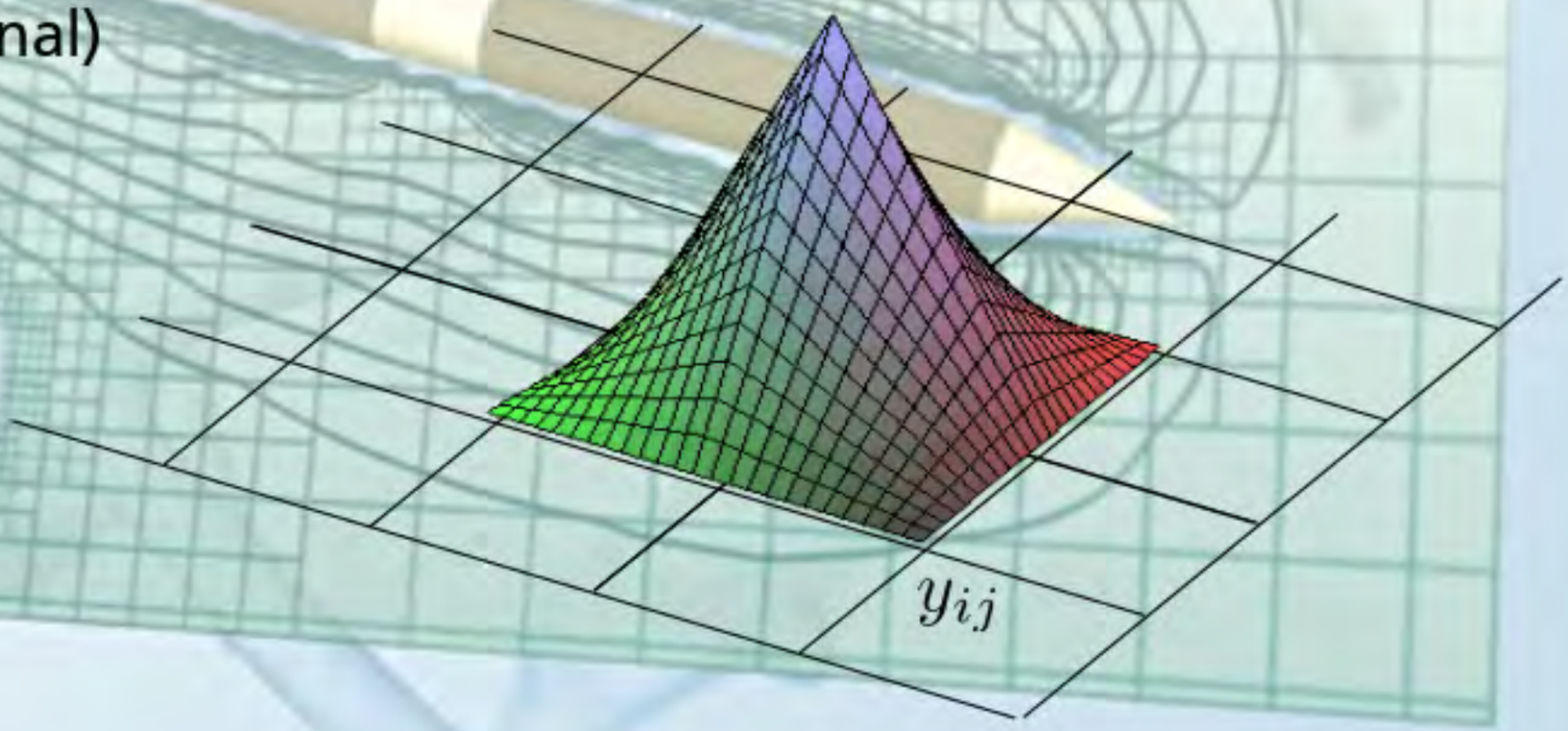


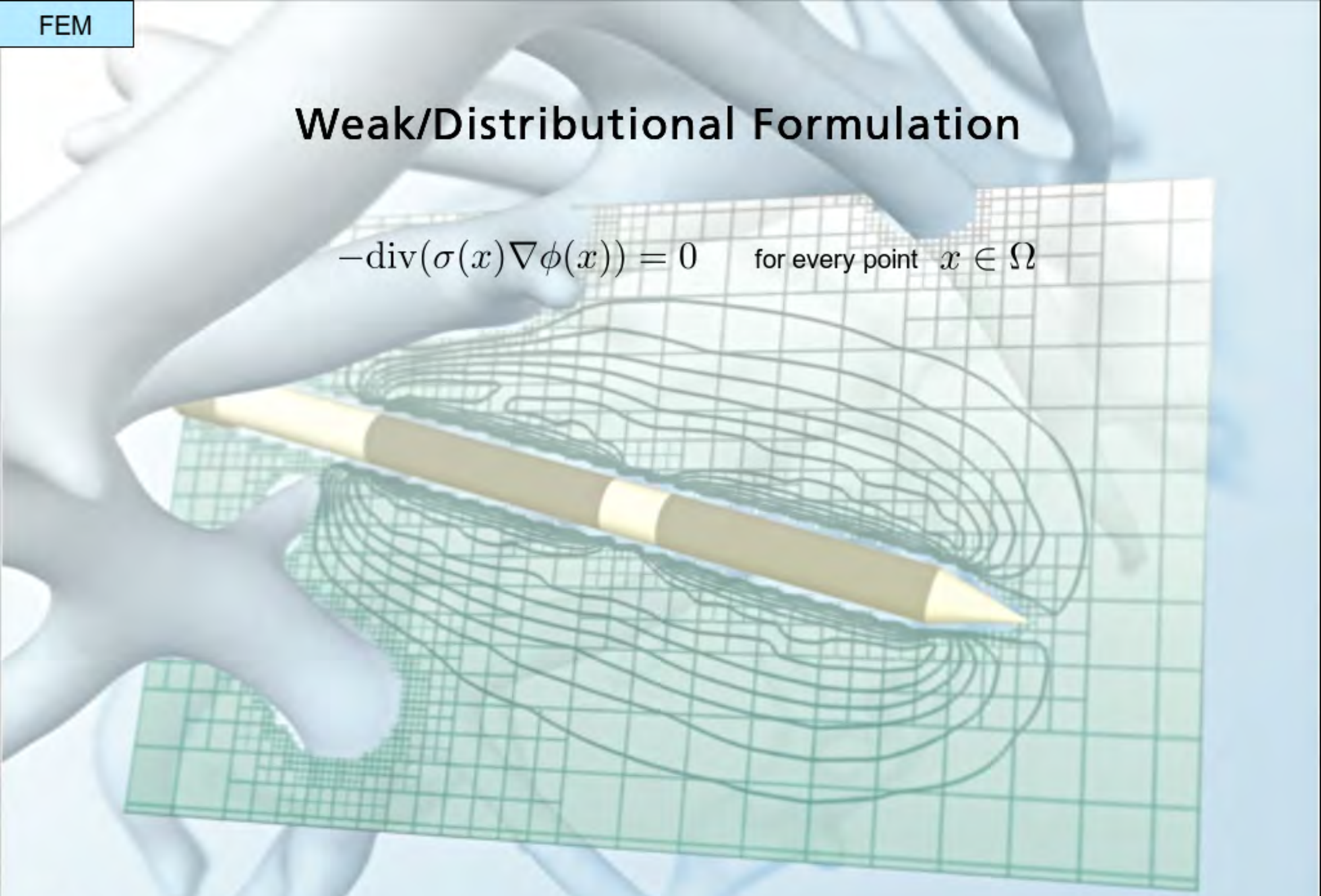
Piecewise Polynomial Shape Functions

- Piecewise polynomial shape functions are not differentiable at the grid nodes
- Need a different notion of differentiability
- Weak (distributional) derivative



Weak/Distributional Formulation

$$-\mathrm{div}(\sigma(x)\nabla\phi(x)) = 0 \qquad \text{for every point } x \in \Omega$$



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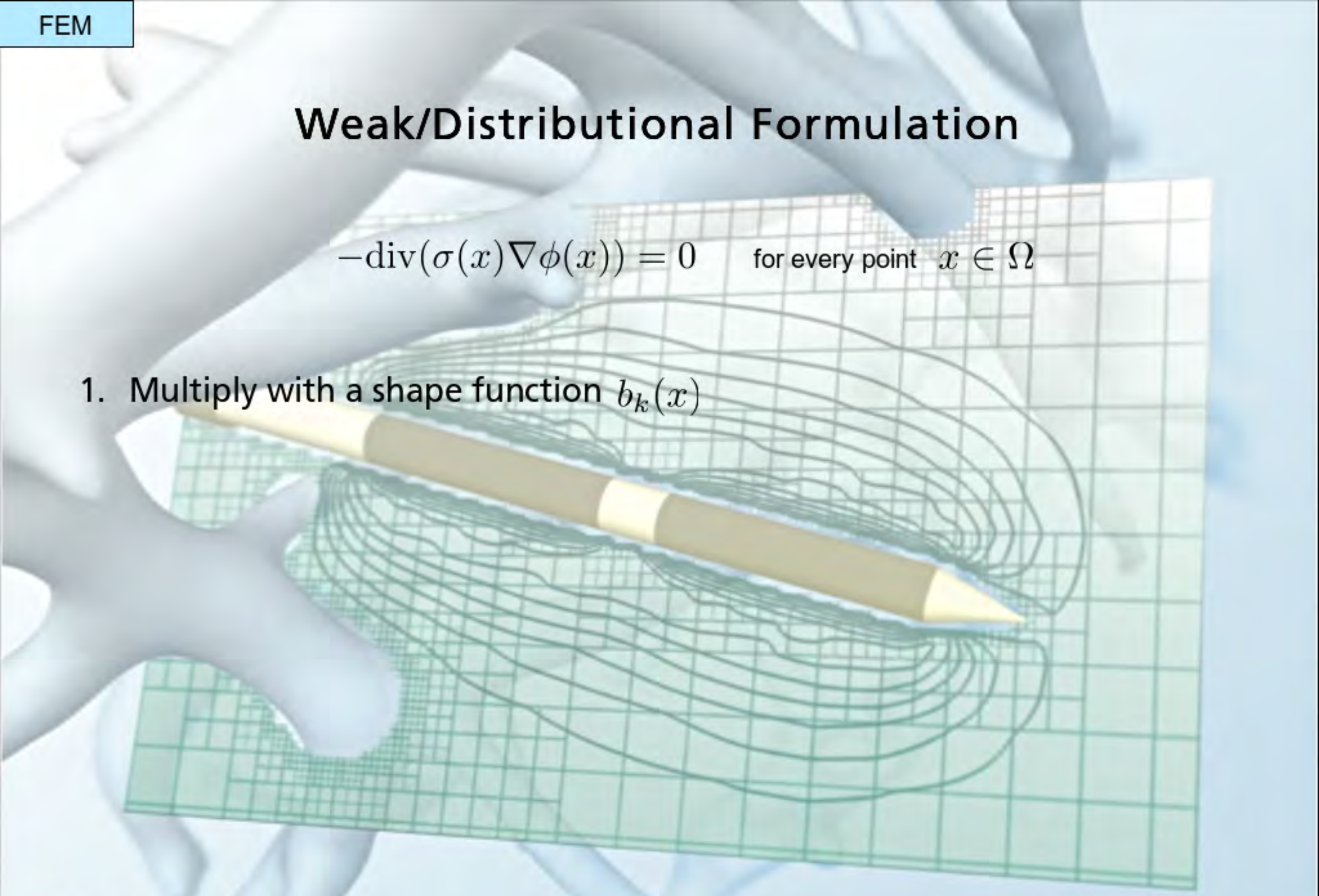

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Systems of Linear Equations

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for every shape function $b_k(x)$

› Matrix

$$A_{ik} = \int_\Omega \sigma \nabla \phi_i(x) \cdot \nabla \phi_j(x)\, dx$$

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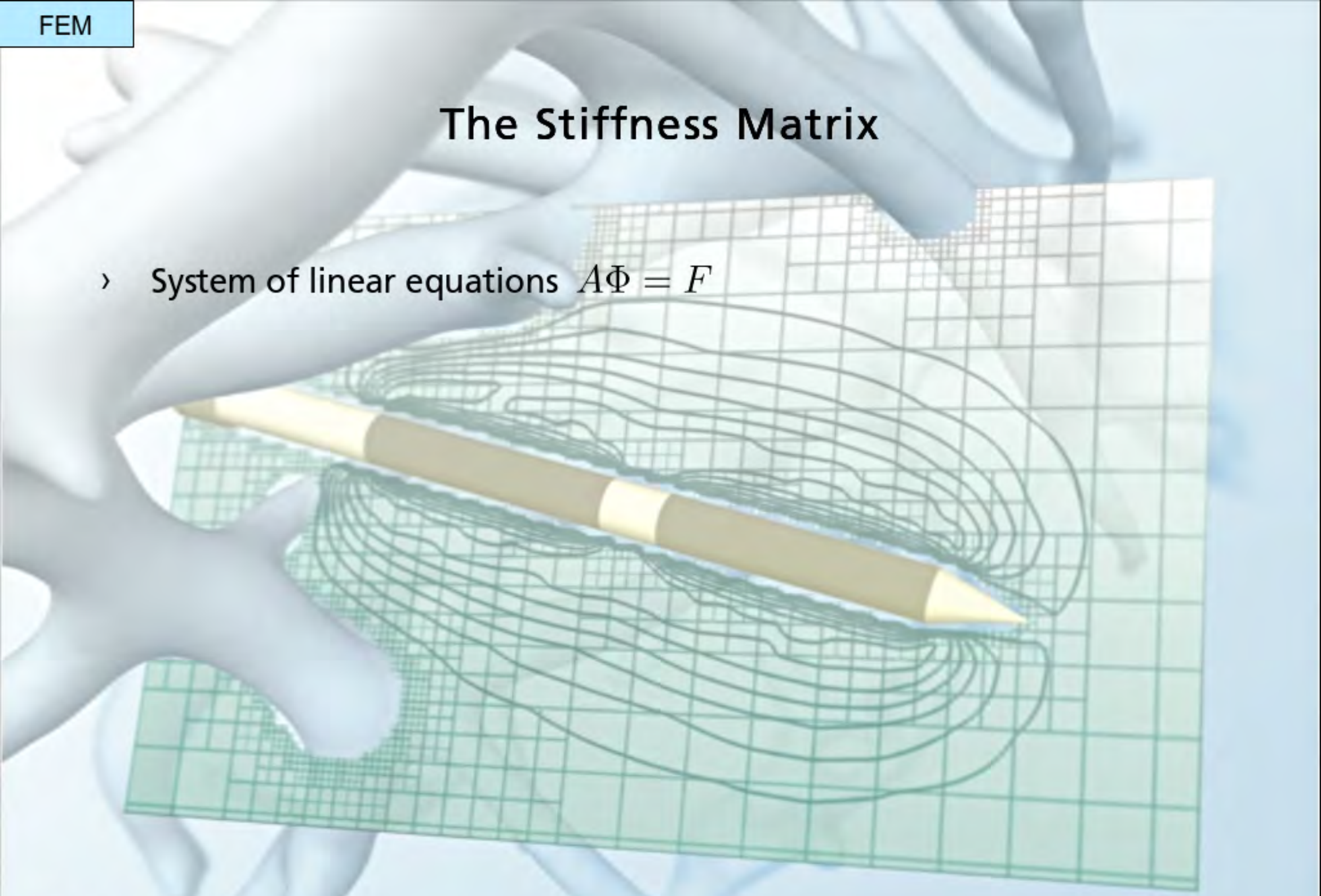
The Stiffness Matrix

- System of linear equations $A\Phi = F$



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compute these entries by traversing through the elements of the grid

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compute these entries by traversing through the elements of the grid

- Matrix inversion:
  - Iterative Method, e.g. Gauss–Seidel, conjugate gradient method
  - But also: Multigrid method

Summary FEM

- Compose functions by shape functions
- Shape functions = piecewise polynomial functions
- Discretization of domain by simplices of variable shape and size
- Weak formulation of differential equation
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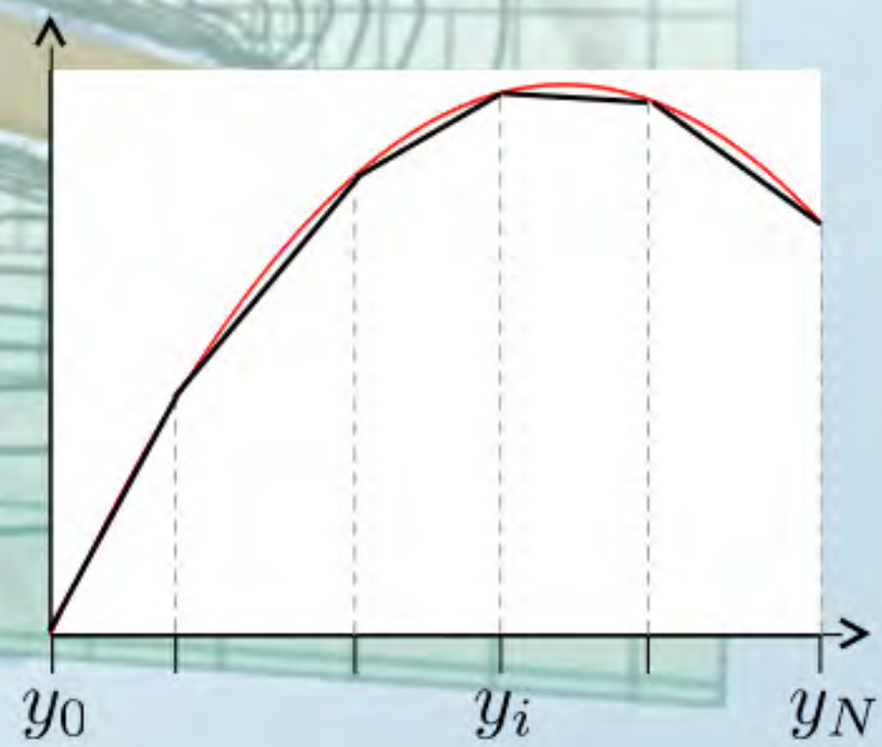

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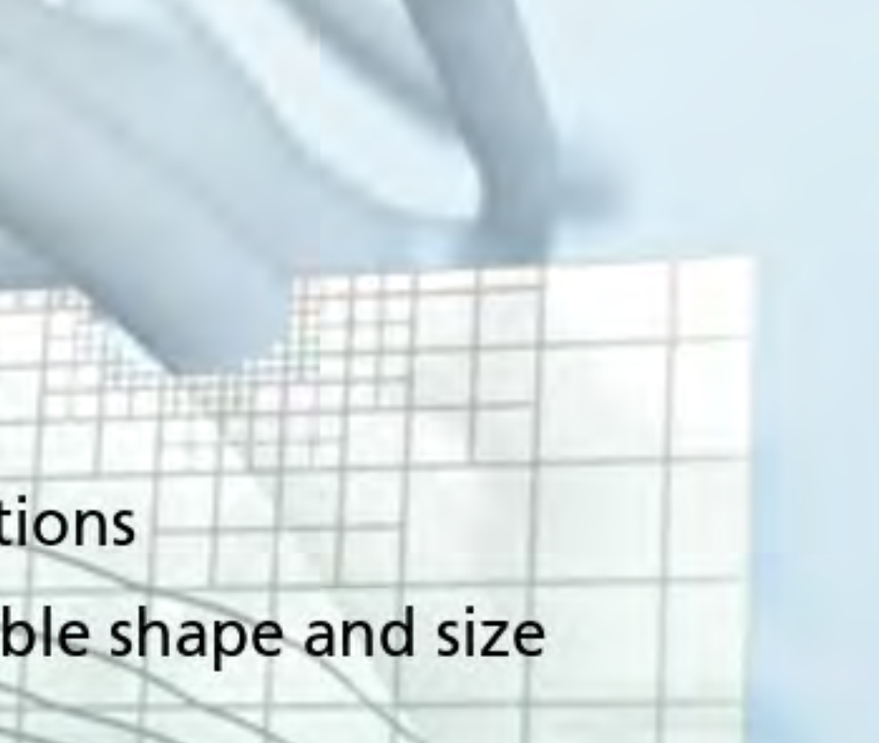
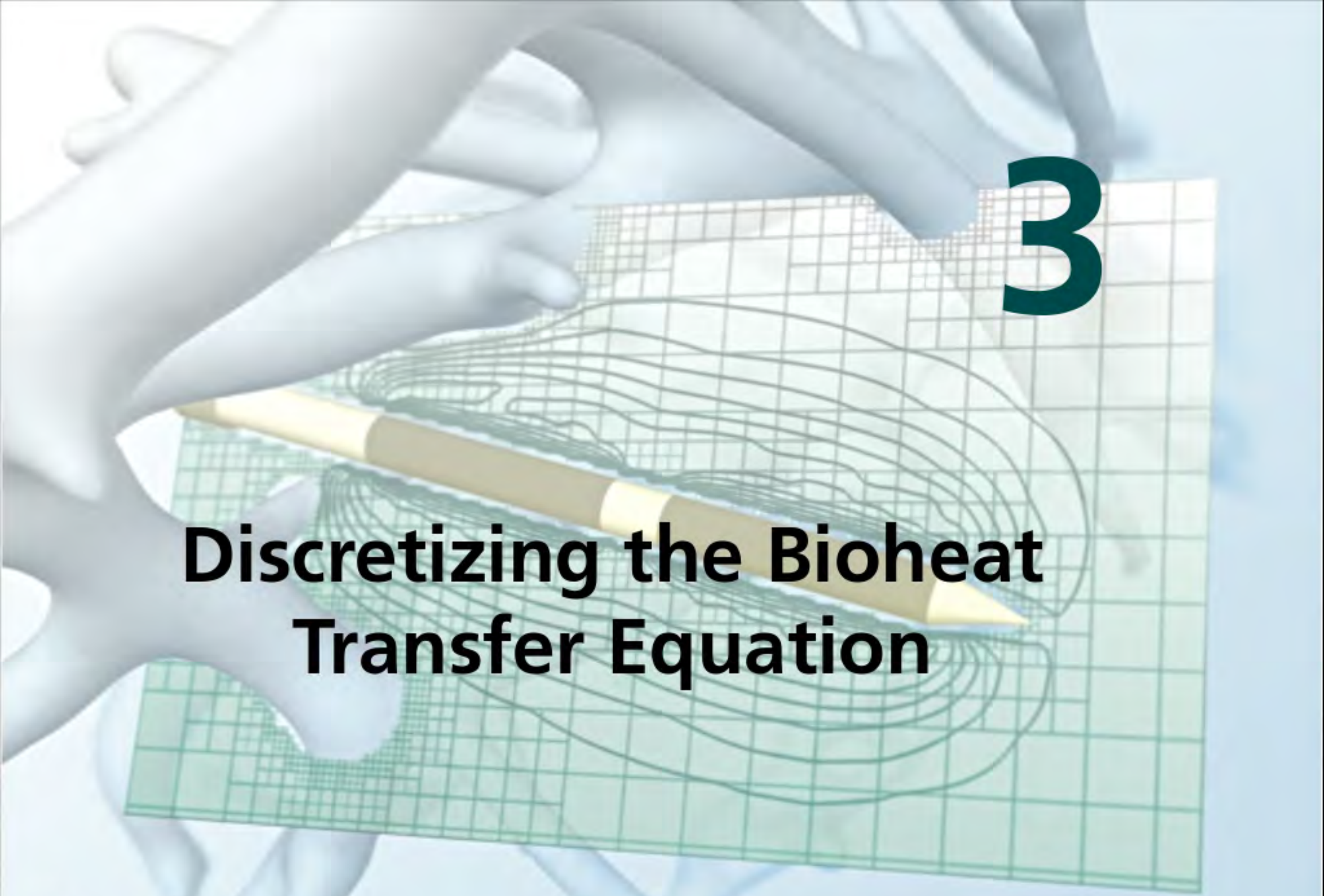


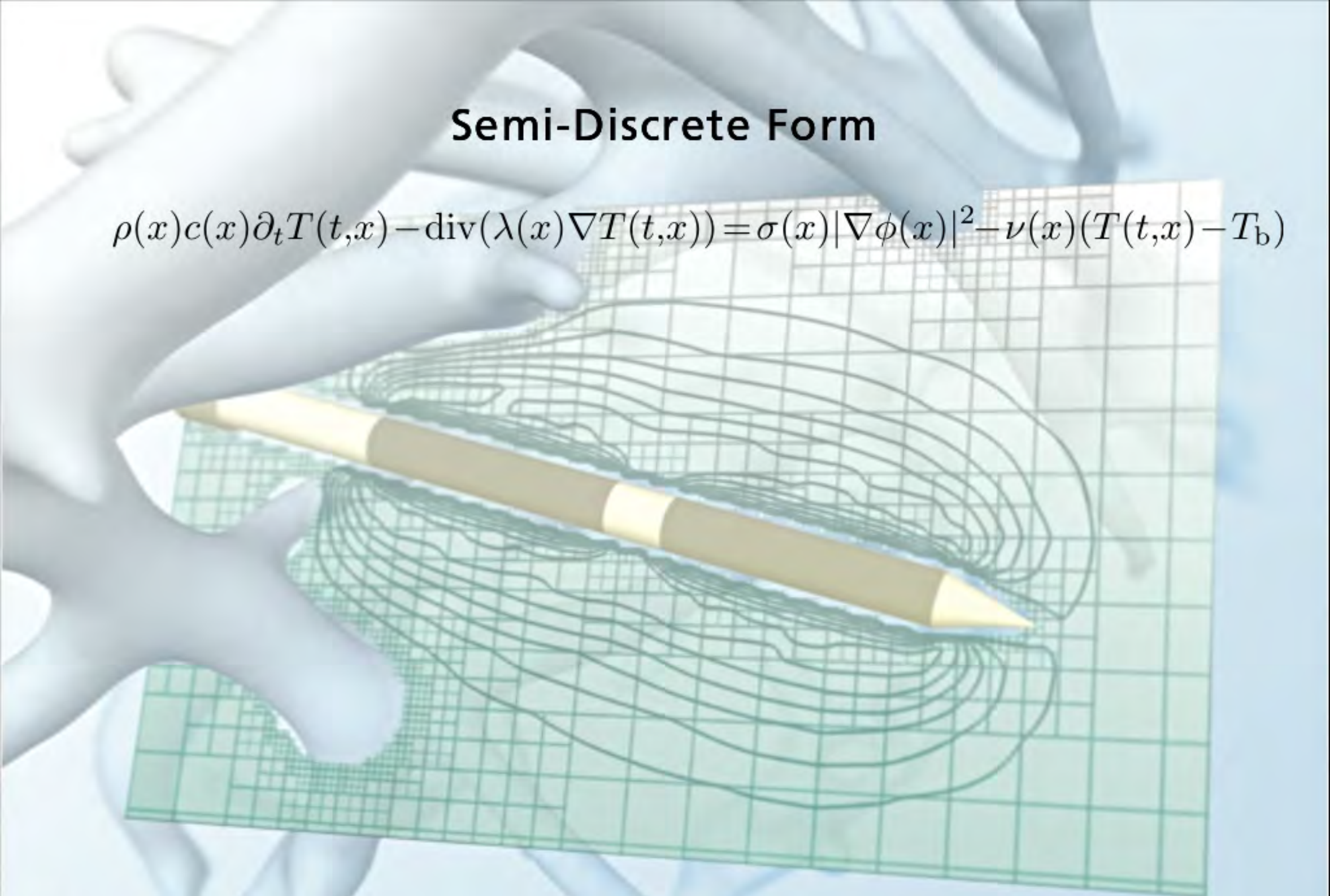


3

Discretizing the Bioheat Transfer Equation

Semi-Discrete Form

$$\rho(x)c(x)\partial_t T(t,x) - \mathrm{div}(\lambda(x)\nabla T(t,x)) = \sigma(x)|\nabla\phi(x)|^2 - \nu(x)(T(t,x) - T_\mathrm{b})$$



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Simplification

$$\partial_t T - \mathrm{div}(\lambda \nabla T) = 0$$

Semi-Discrete Form

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FDM or FEM discretization

$$\partial_t T - AT = 0$$

Semi-Discrete Form

$$\rho(x)c(x)\partial_t T(t,x) - \mathrm{div}(\lambda(x)\nabla T(t,x)) = \sigma(x)|\nabla\phi(x)|^2 - \nu(x)(T(t,x) - T_\mathrm{b})$$

Simplification

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FDM or FEM discretization

$$\partial_t T - AT = 0$$

$$\dot{T} - AT = 0$$

Matrix Exponentials

- Ordinary differential equation in the nodal values

$$\dot{T} - AT = 0$$

Matrix Exponentials

- Ordinary differential equation in the nodal values

$$\dot{T} - AT = 0$$

- Solution $T(t) = \exp(tA)\, T_0$

Note that this is the exponential function for matrices!

Matrix Exponentials

- Ordinary differential equation in the nodal values

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  Note that this is the exponential function for matrices!

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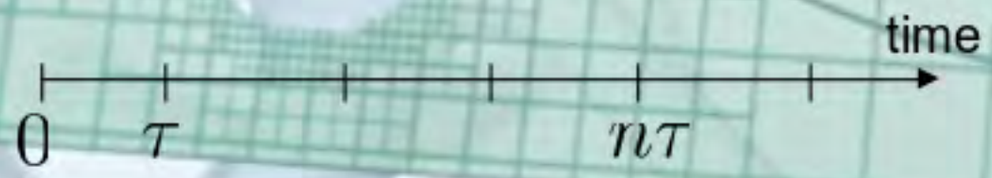

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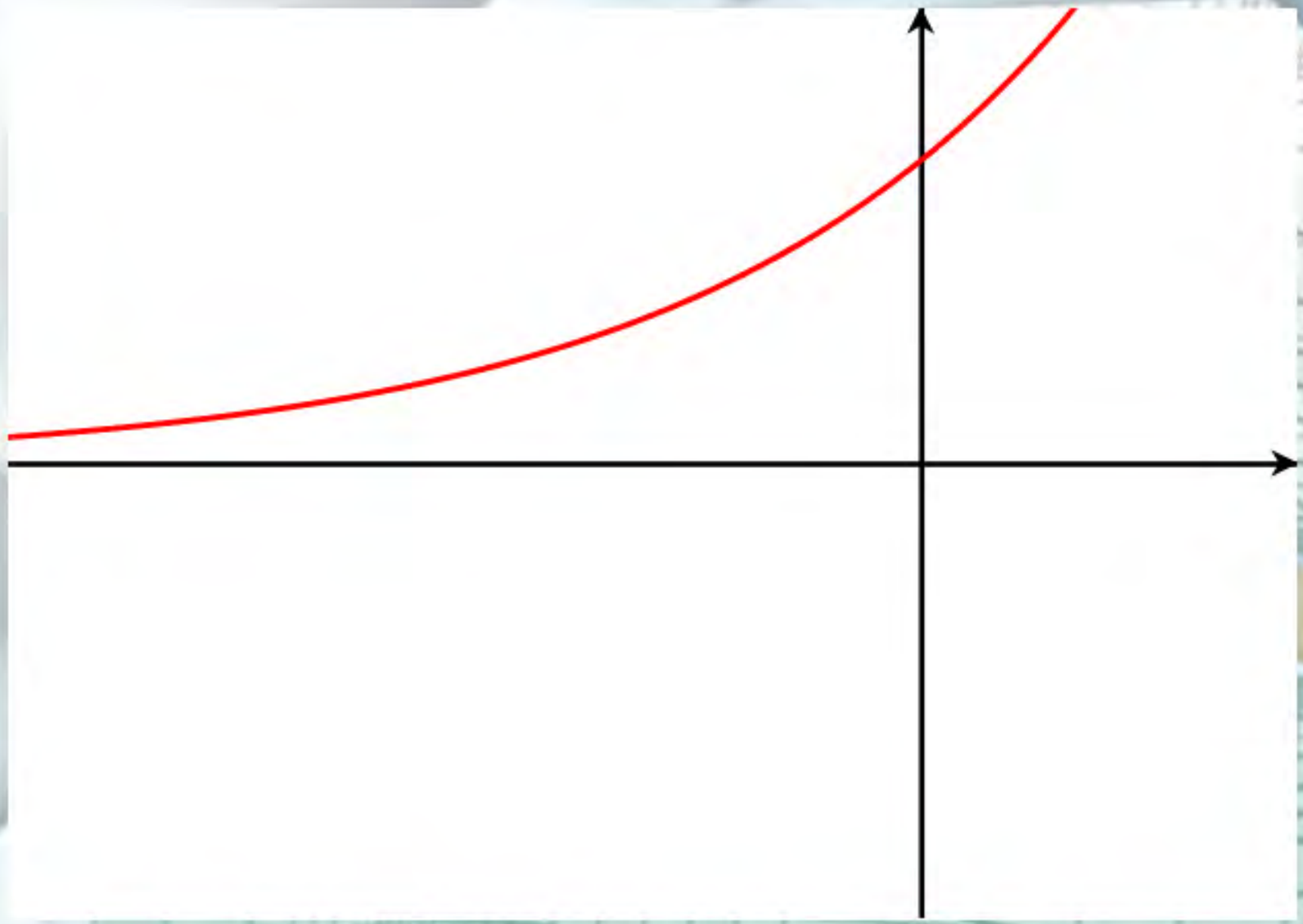

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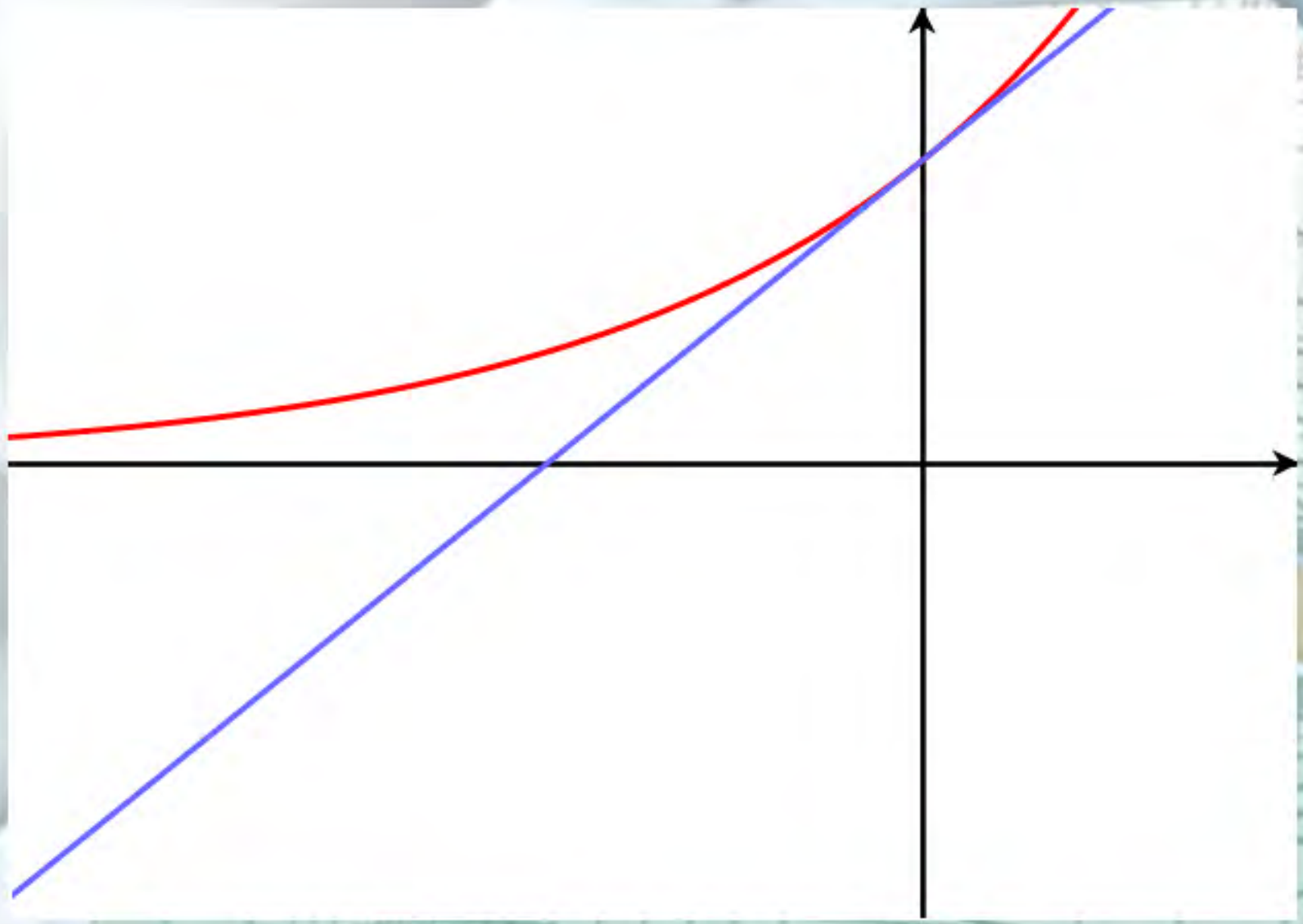

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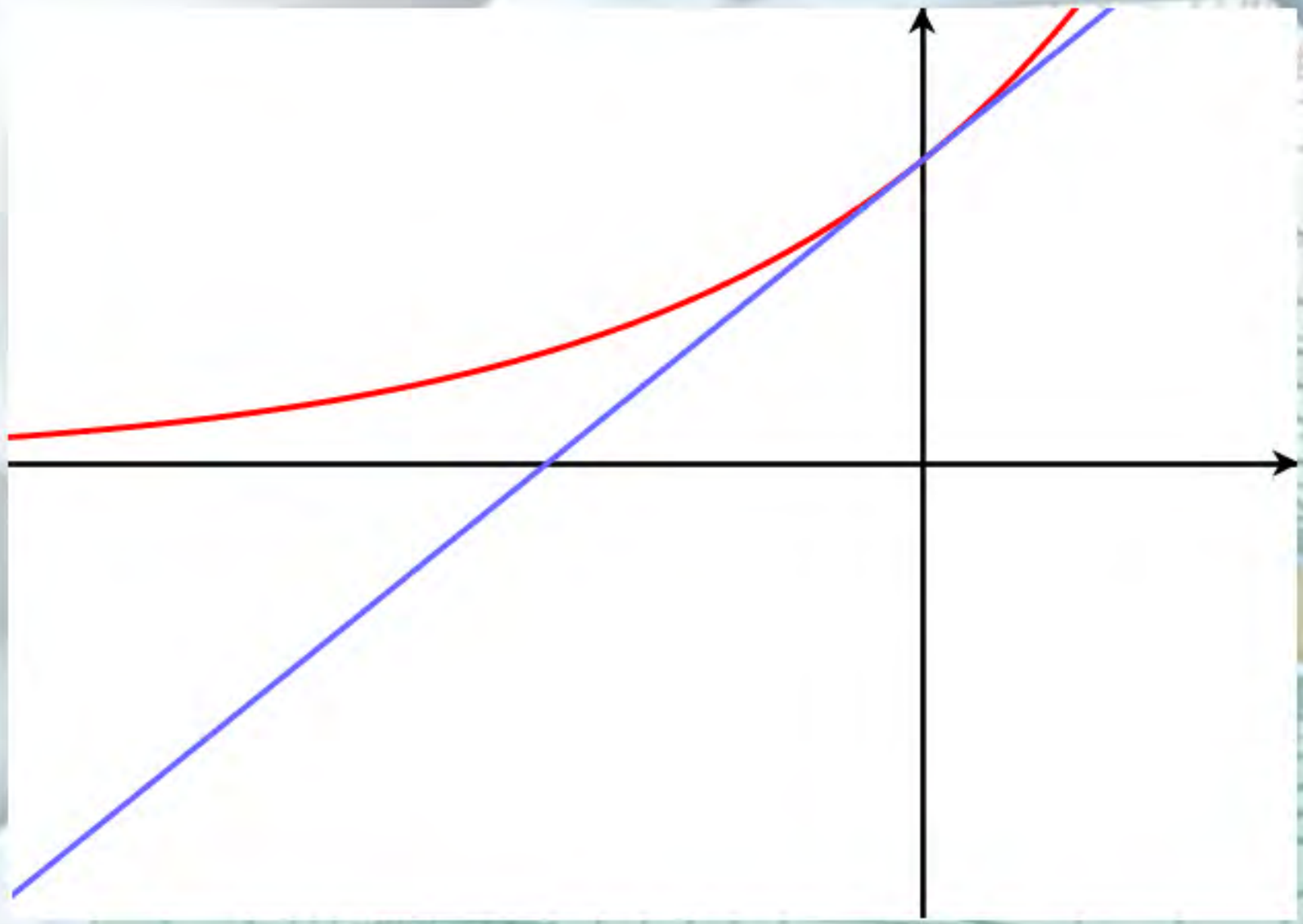

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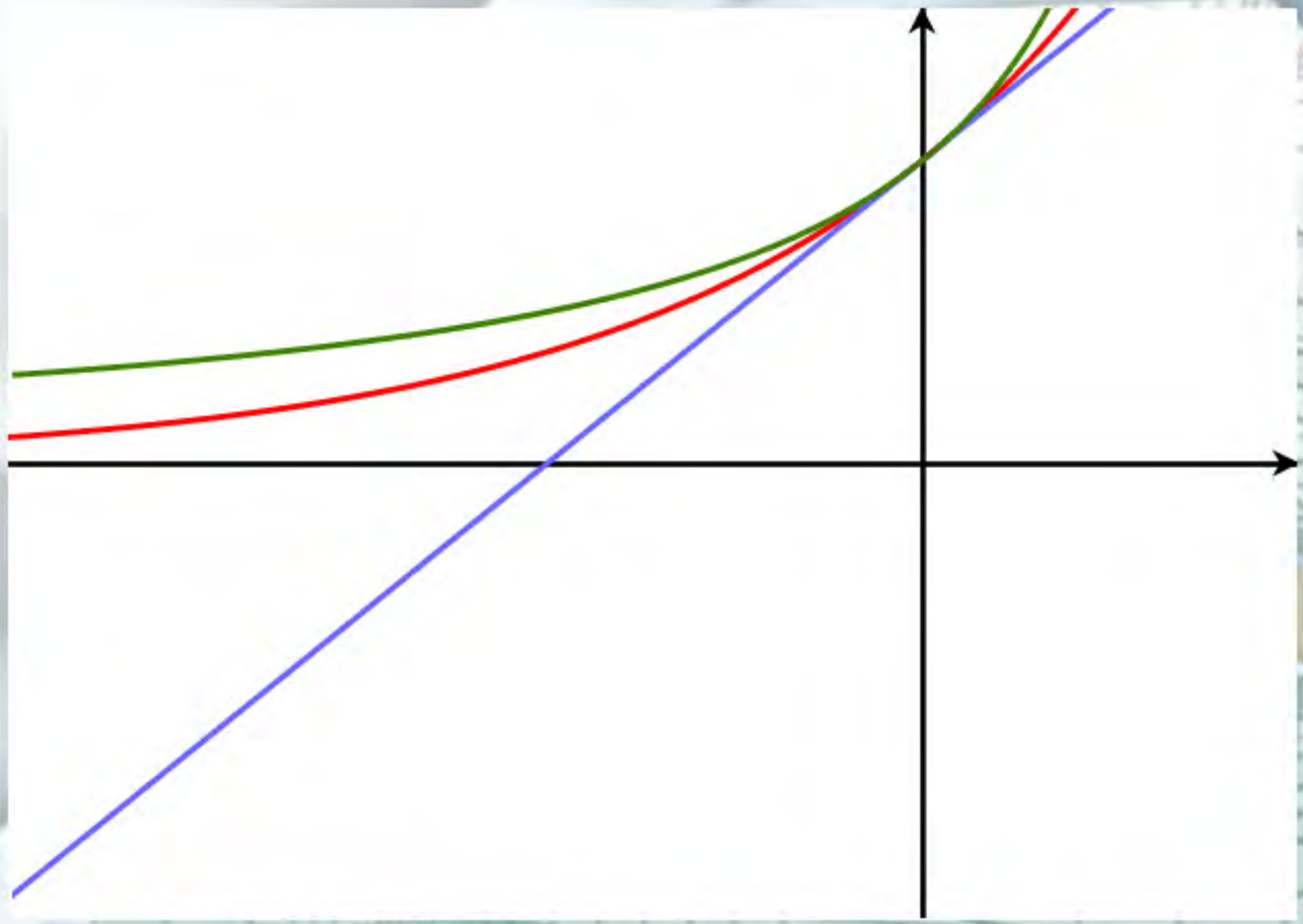

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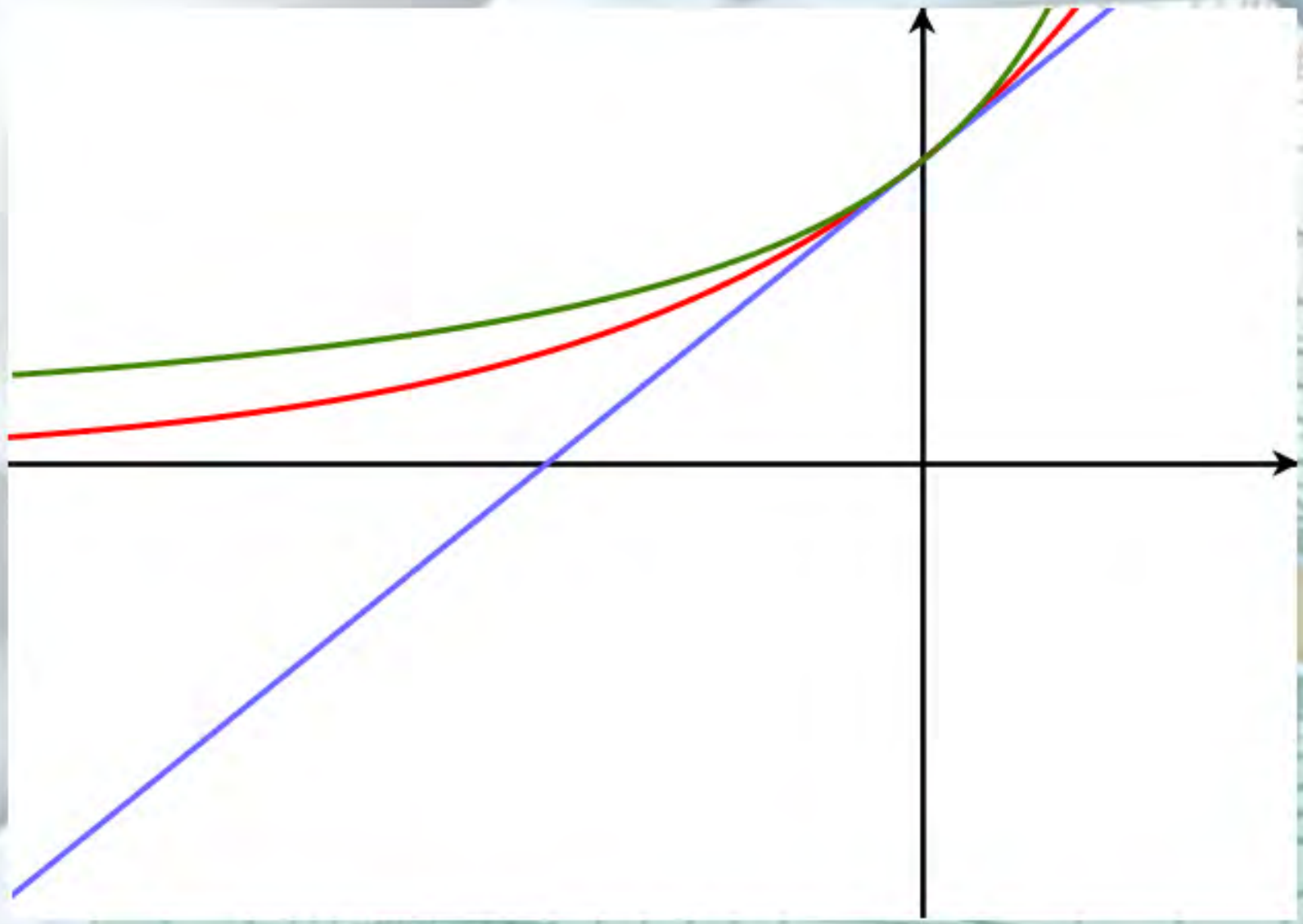

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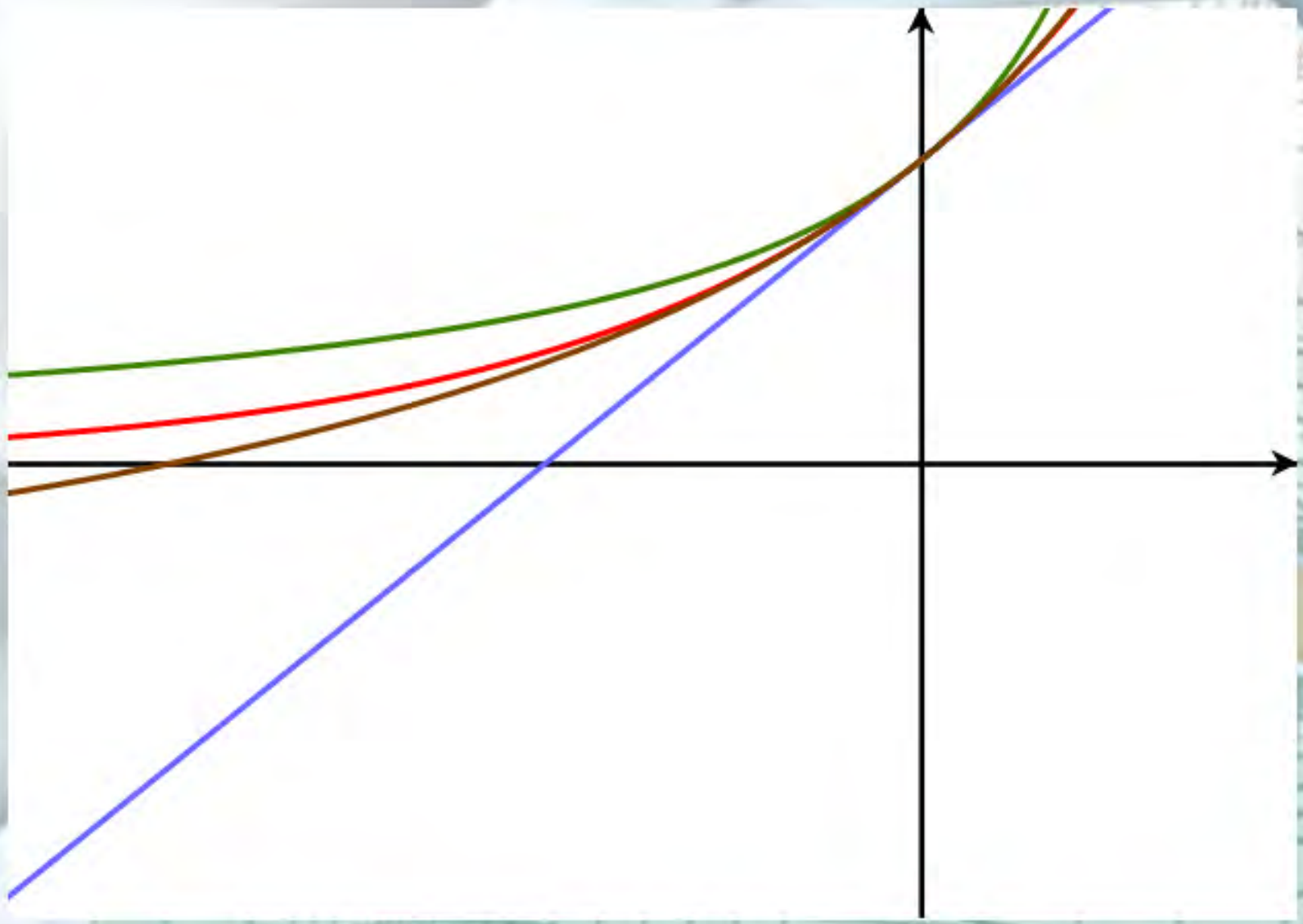

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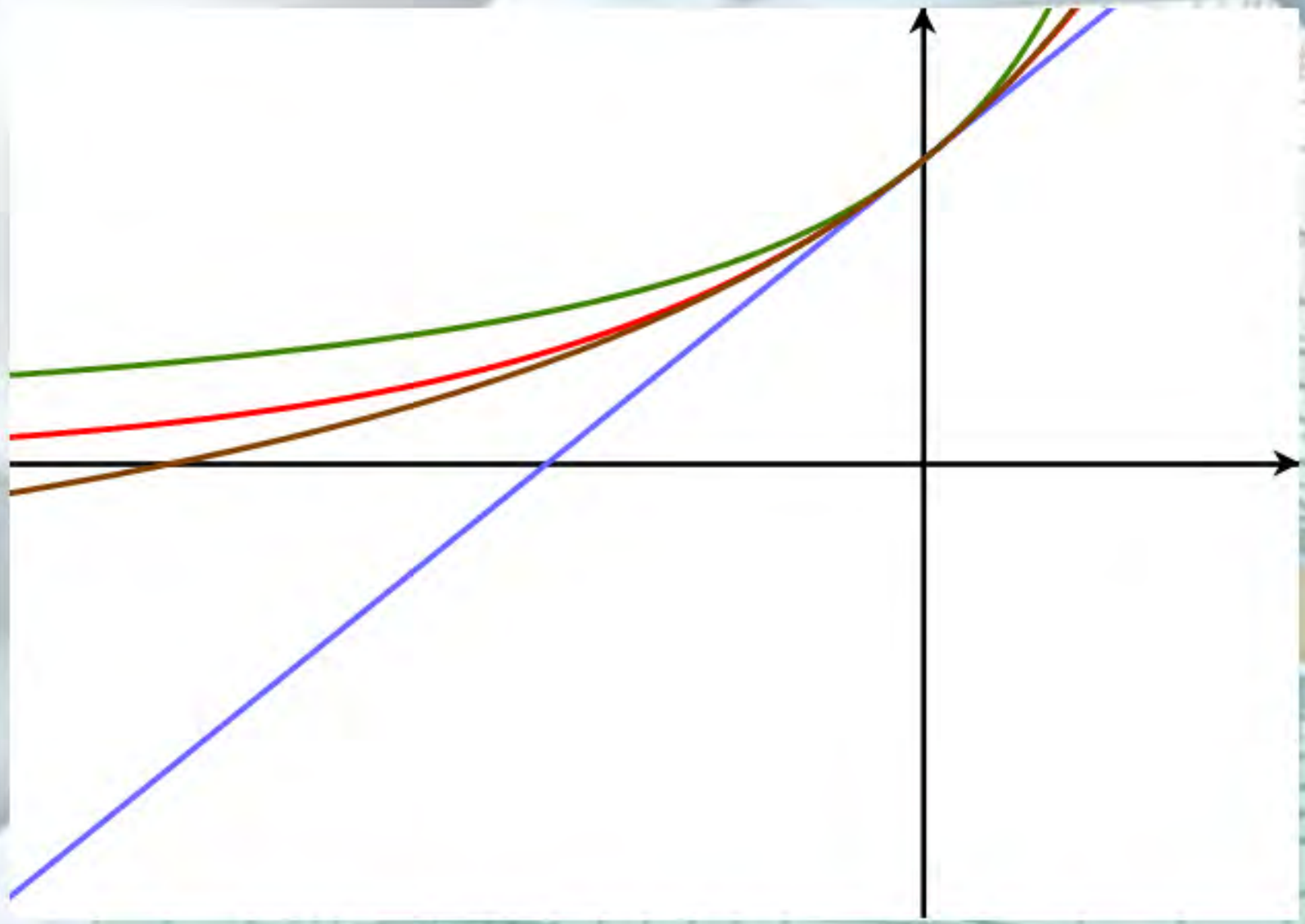

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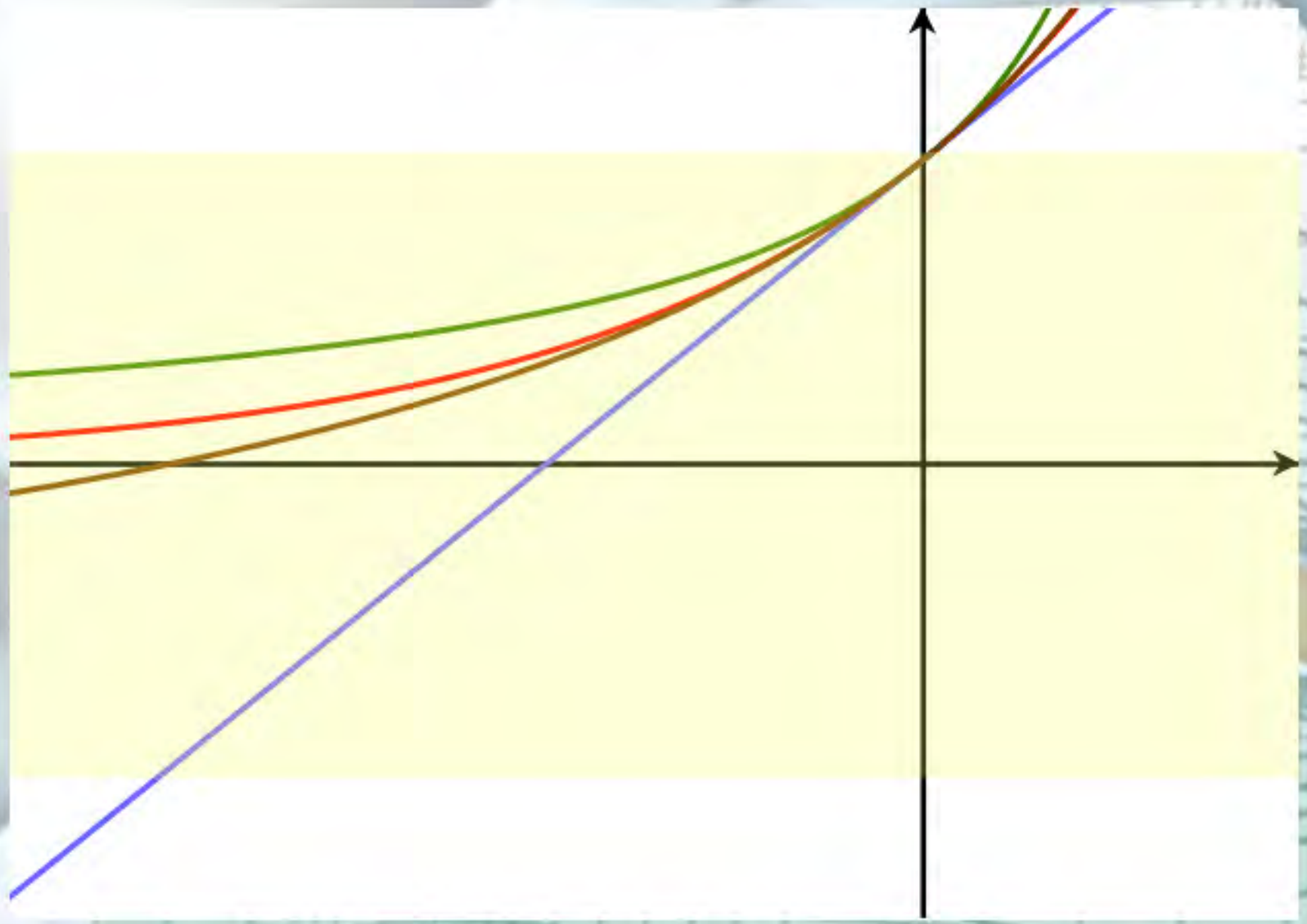

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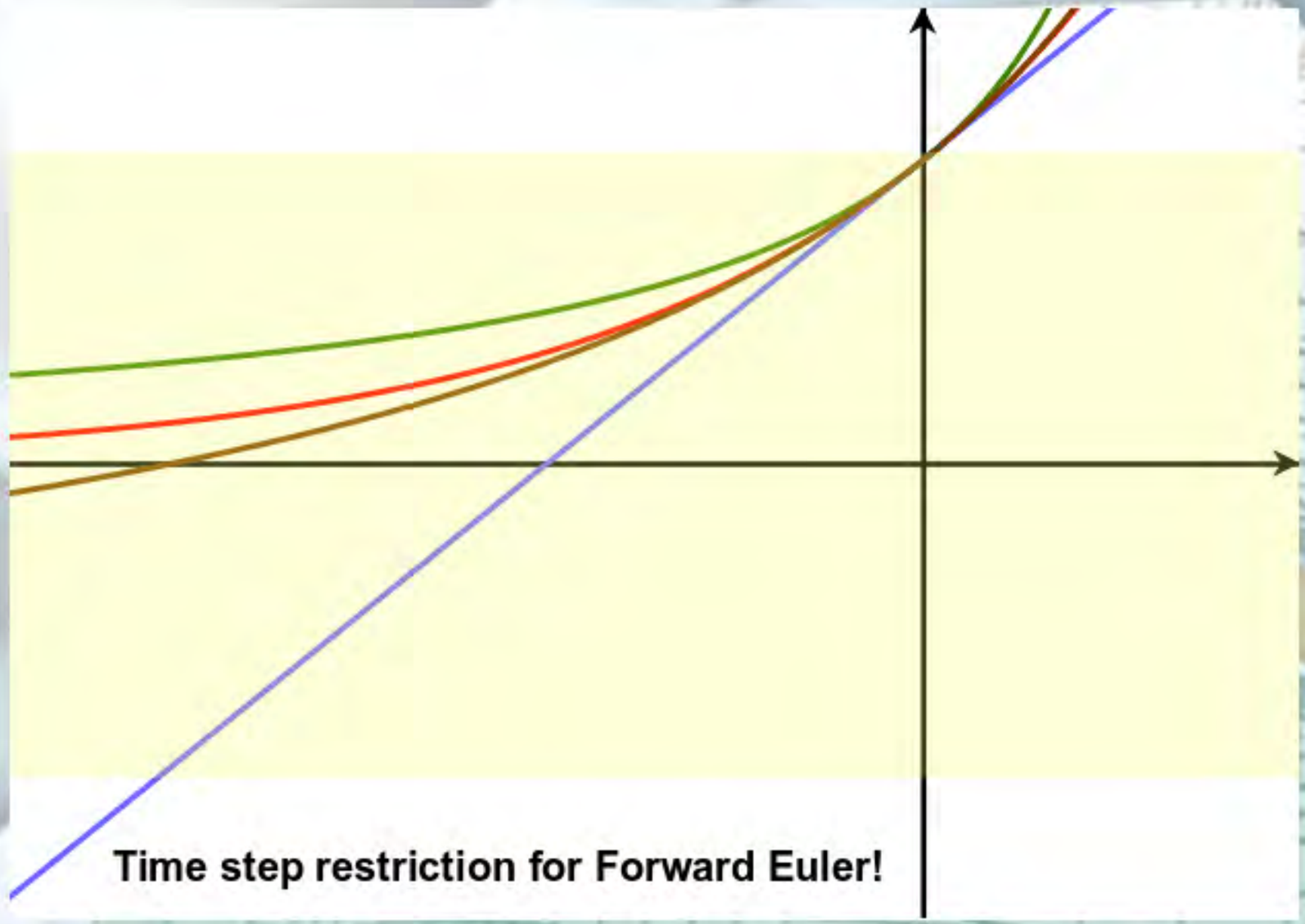

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4

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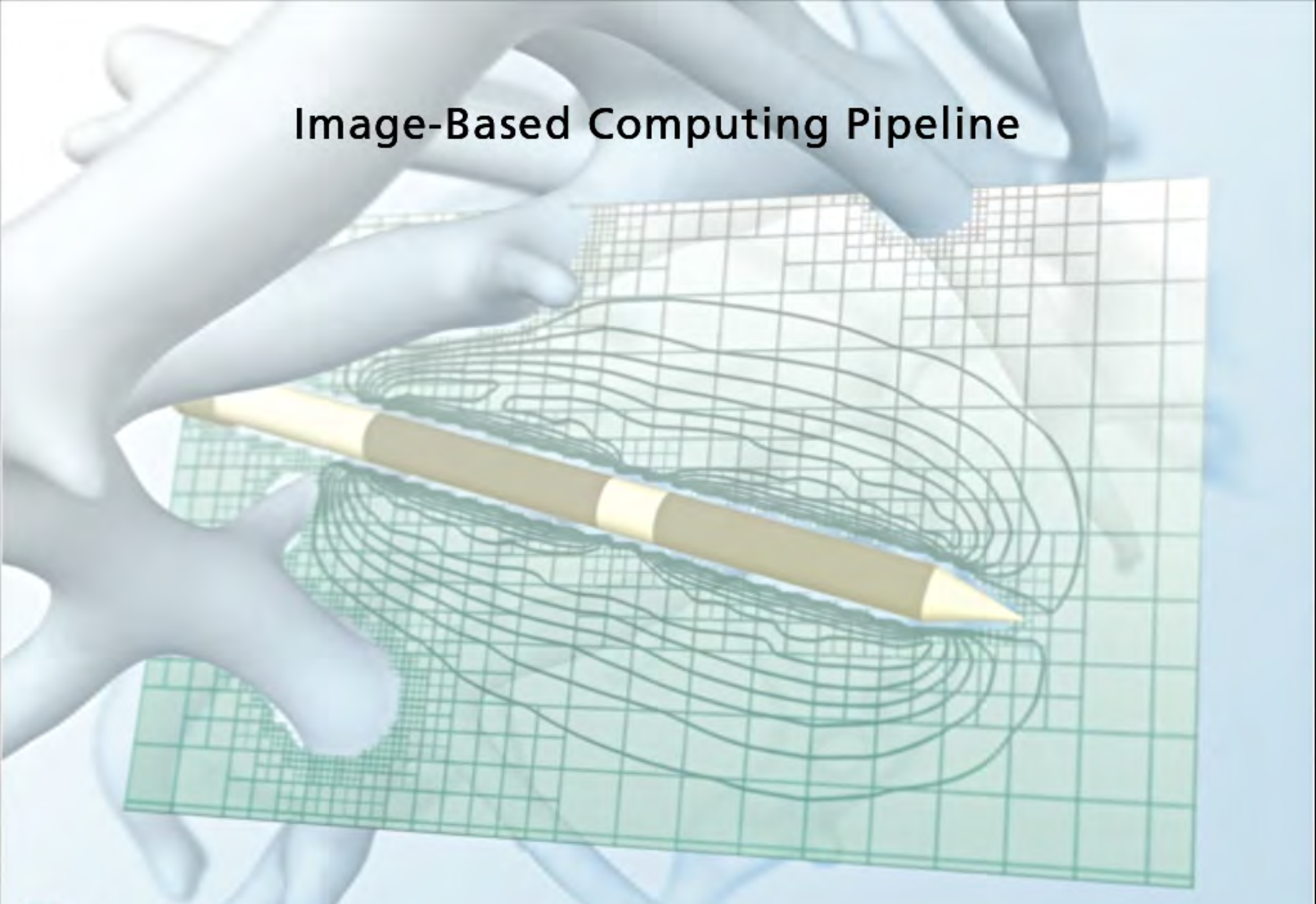
For 1D regular grids and piecewise linear shape functions: FDM = FEM

5

Examples

Image-Based Computing Pipeline



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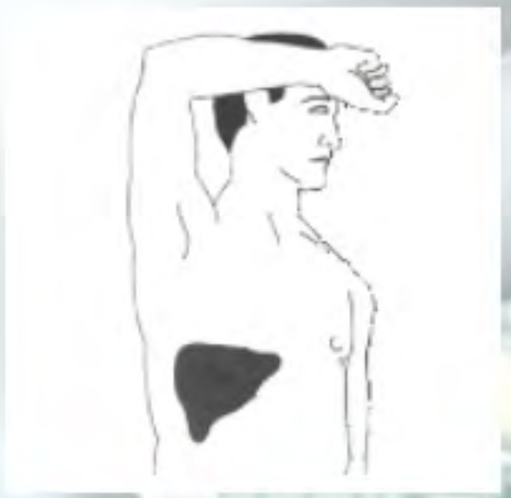

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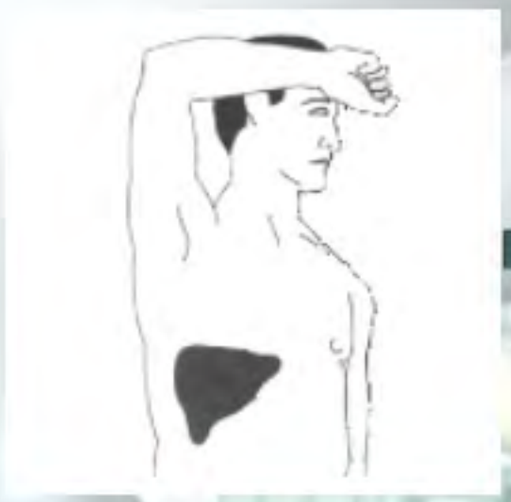

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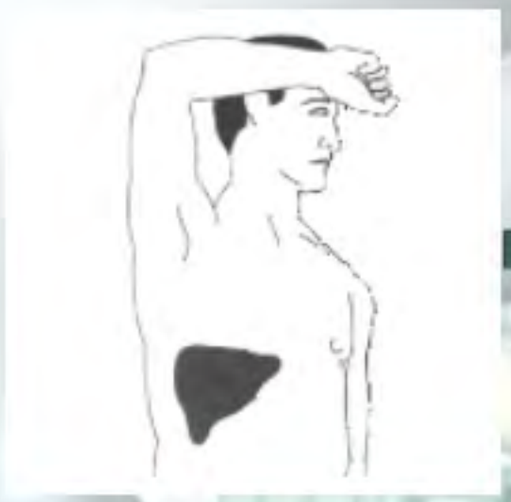

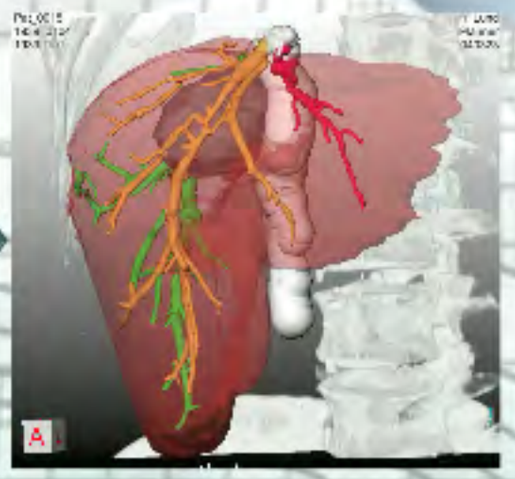

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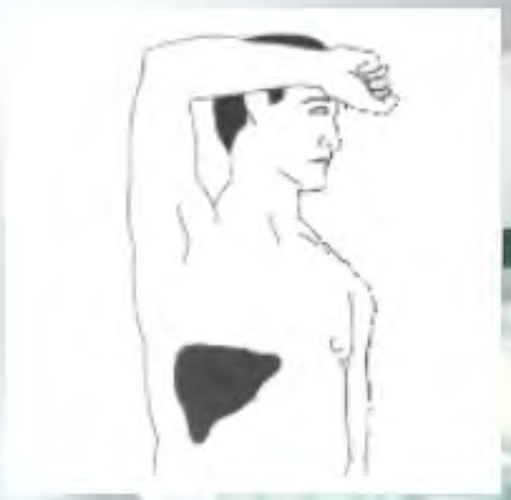

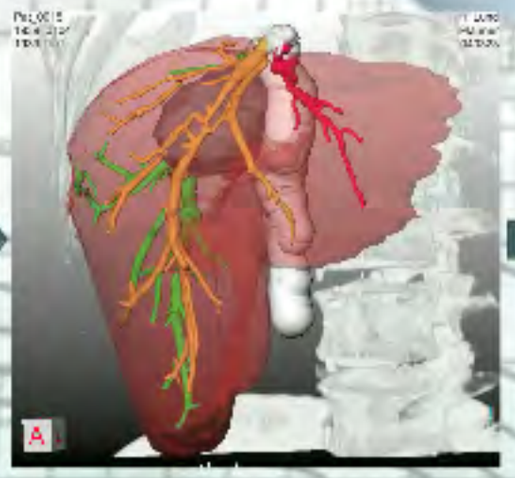

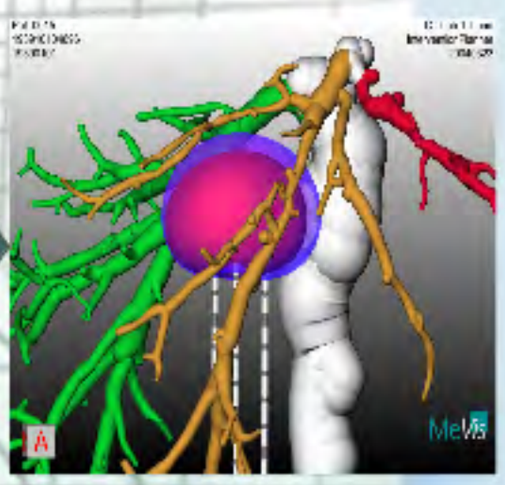

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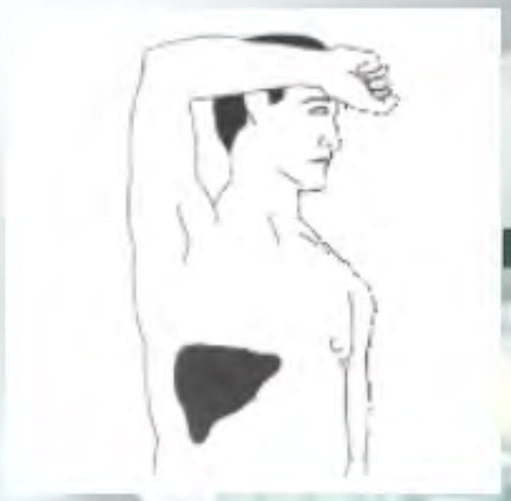

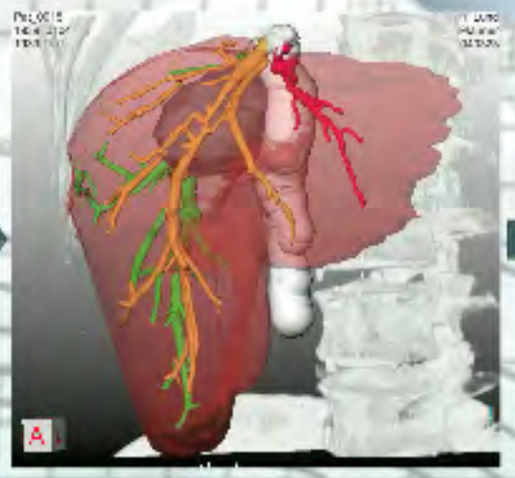

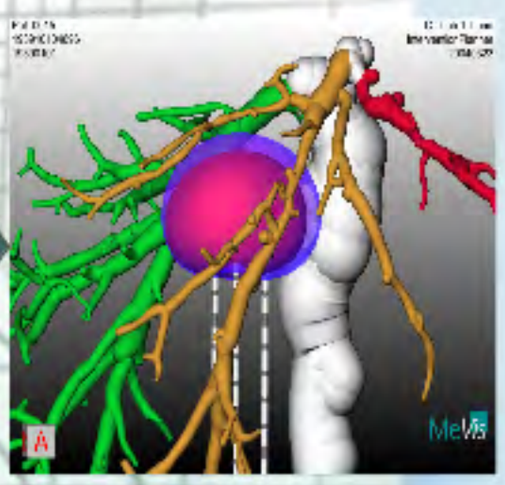

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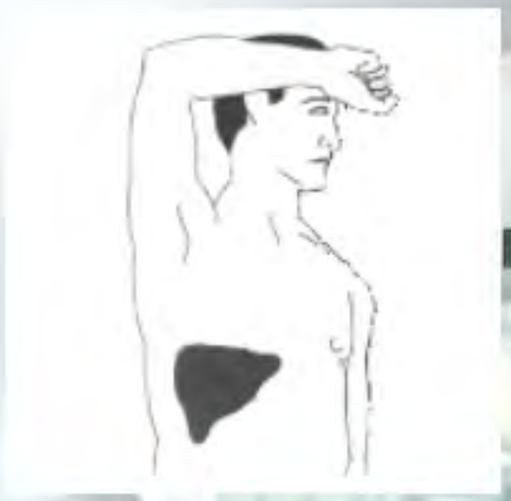

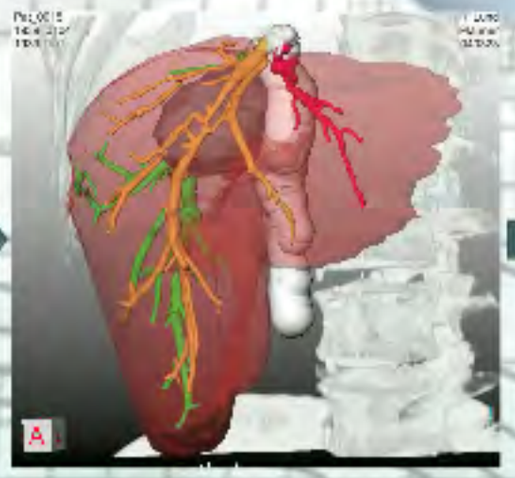

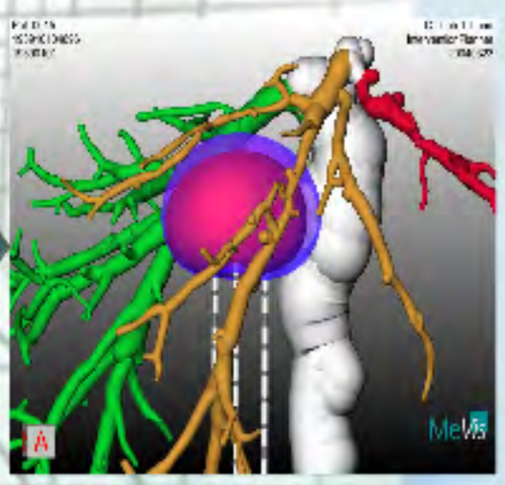

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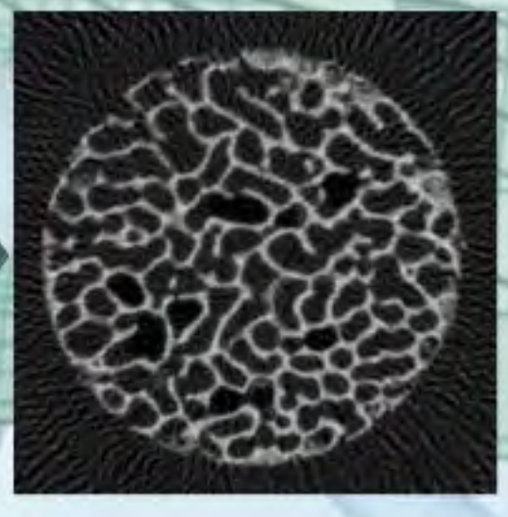

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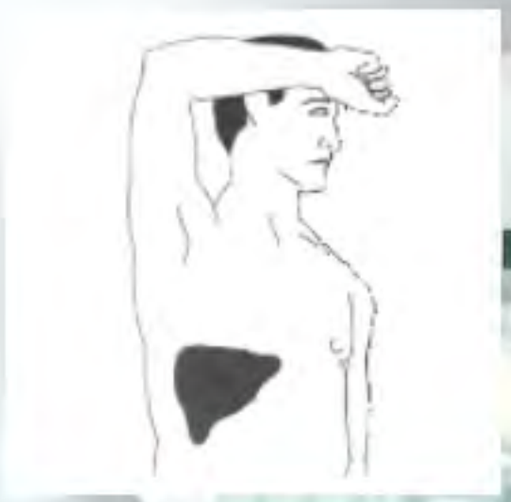

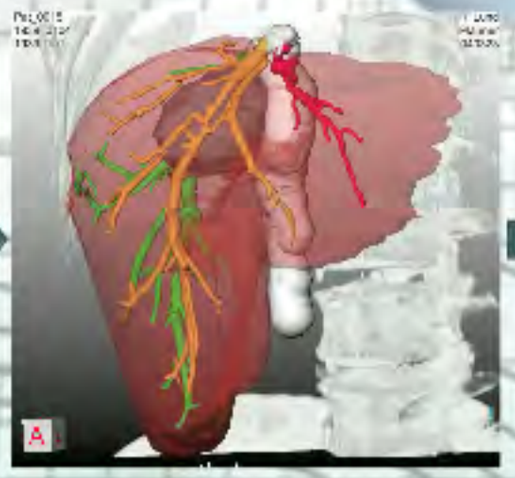

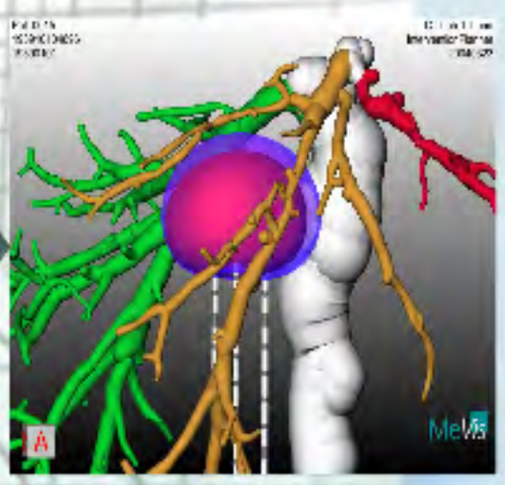

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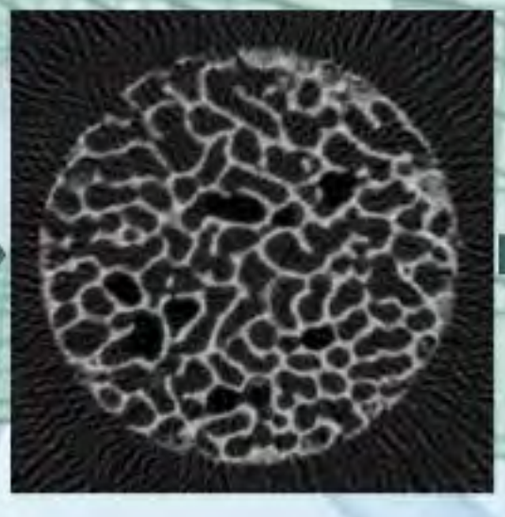

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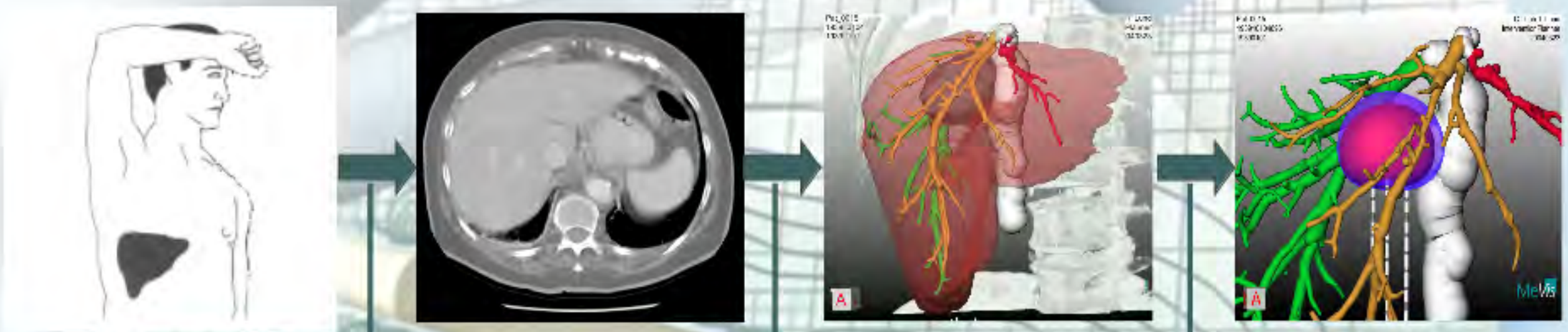

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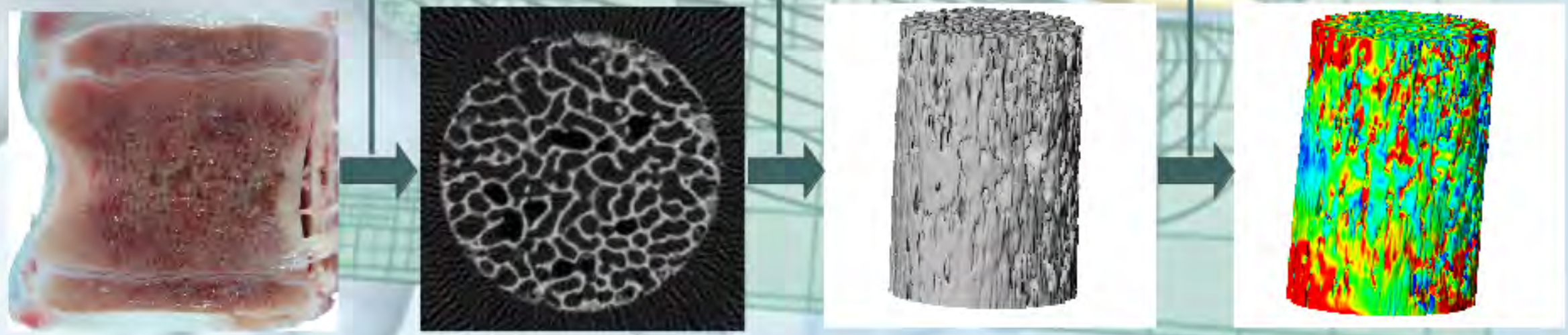

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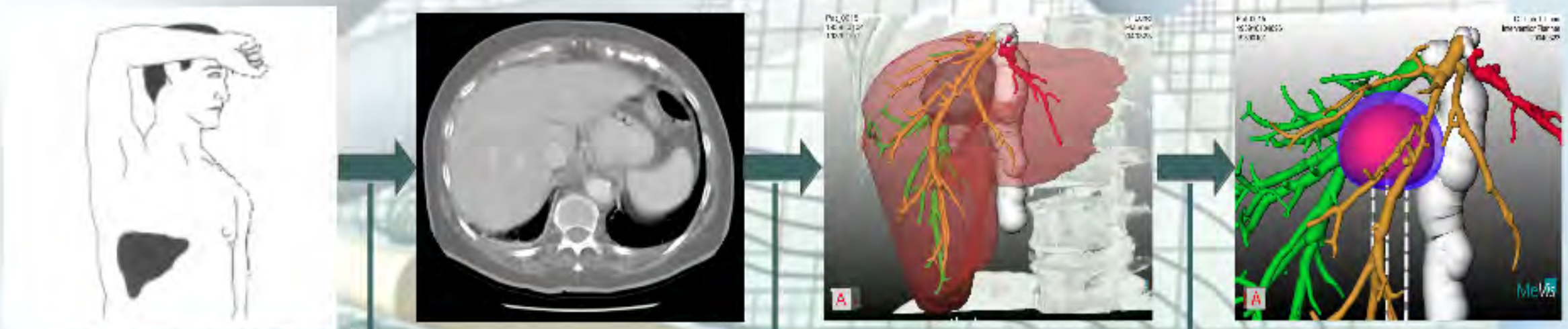

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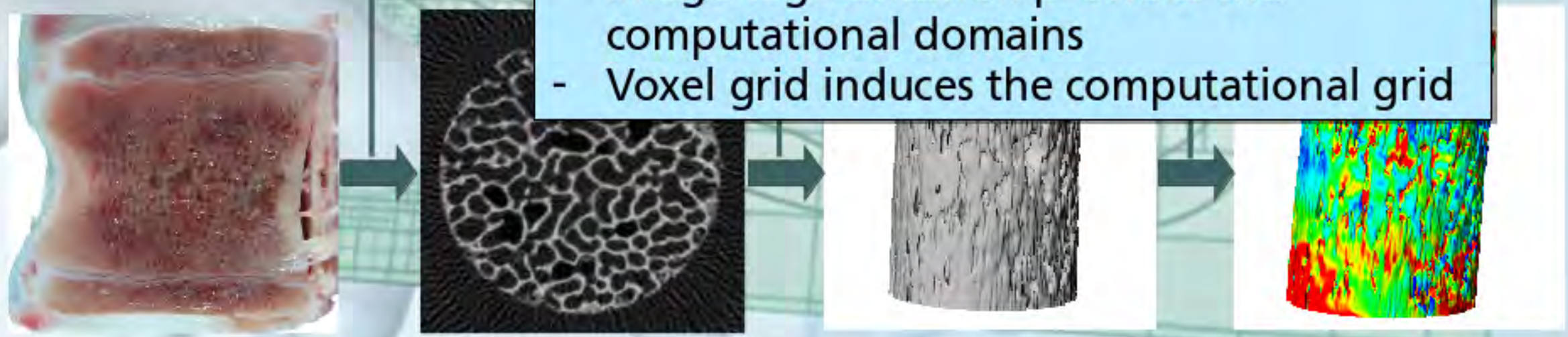

- Image segmentation provides the computational domains
- Voxel grid induces the computational grid

Simulation of RF Ablation

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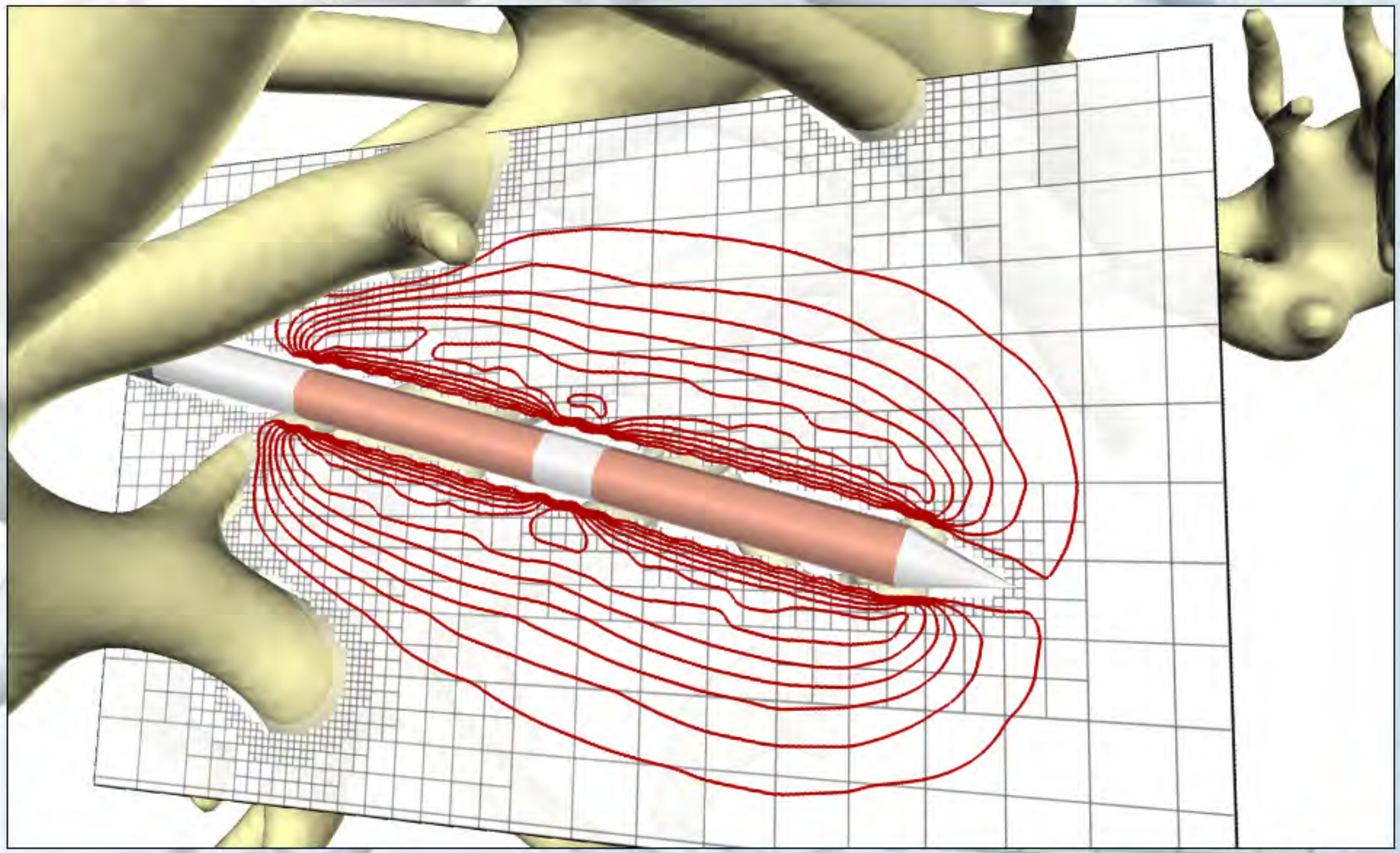
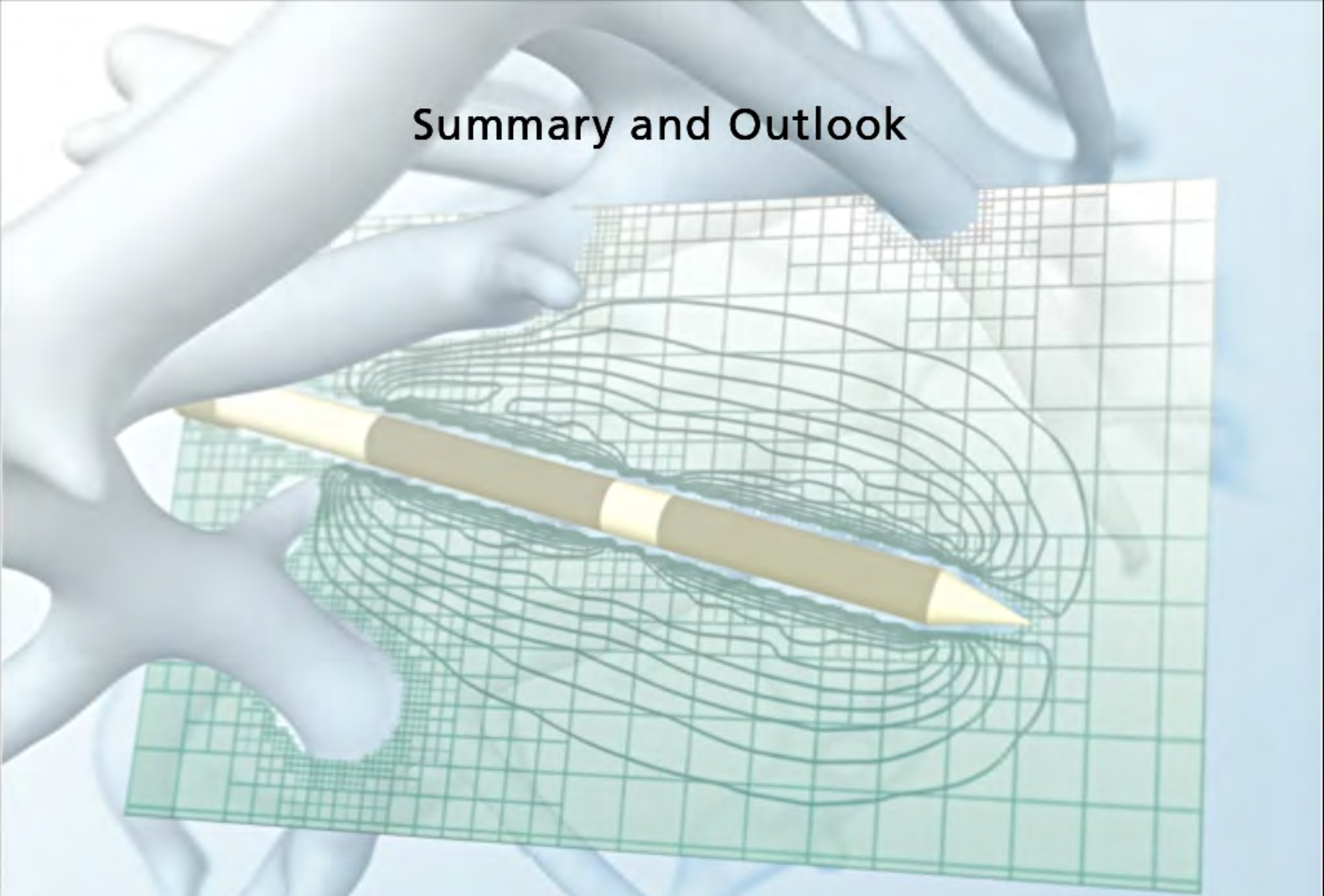


Summary and Outlook



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What happens under the hood of simulation software?

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Contact:

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