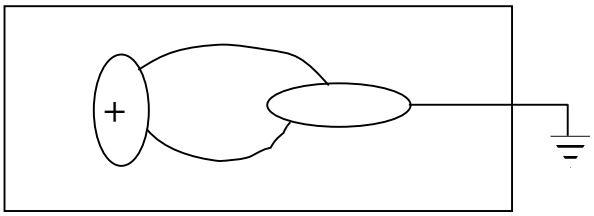
Introduction to PDE with Comsol

School-science project: Ion movement

A blotting paper is wetted by brine, and heavy electrodes are placed on it and connected to DC electric power. $KMnO_4$-crystals placed on the wet paper are dissolved and violet streaks show the paths traced by the ions as they move under the influence of the electric field.



We model this experiment by COMSOL, and first formulate the differential equation.

Let the electric field be $\mathbf{E} = -\operatorname{grad} V$ where V is the electric potential. A charge q experiences the force $q\mathbf{E}$, so it moves with velocity $\mathbf{v} = mq\mathbf{E}$. The phenomenological coefficient m is called *mobility*. When the ion concentration is n ions/m^2 the current density (the flux of electric charge) is

$$\mathbf{F} = -\sigma \operatorname{grad} V,$$

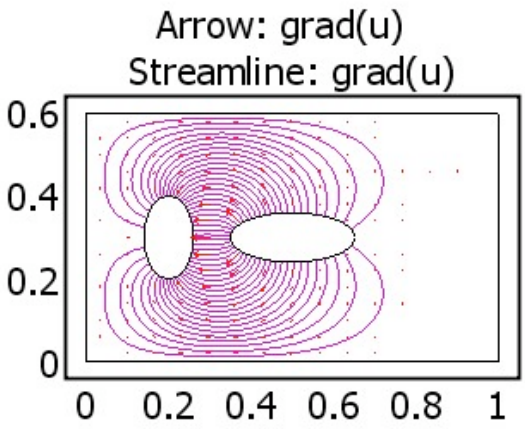
where $\sigma = nmq^2$ is the electric conductivity. The conservation of (ionic) charge becomes

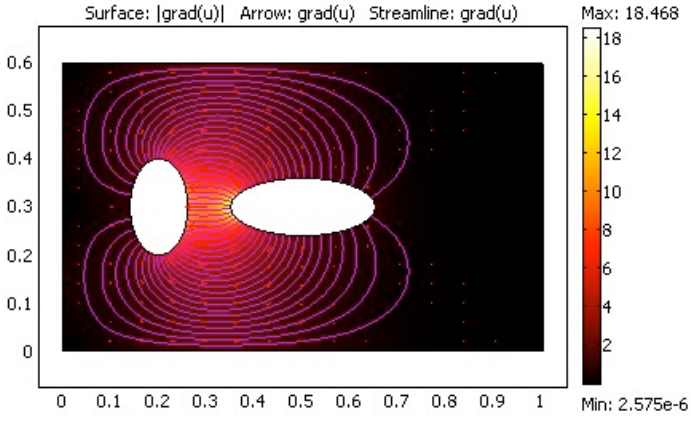
$$0 = \nabla \cdot (\sigma \nabla V) \Leftrightarrow \Delta V = 0$$

since we assume σ constant. $V = 1$ V on the left electrode (the anode), and 0 on the right (the cathode). No current passes through the paper's edge, so $\mathbf{F}.\mathbf{n} = 0$ or $\sigma \operatorname{grad} V \, \mathbf{n} = 0$ where $\mathbf{n}$ is the normal to the edge.

This is the *Laplace* equation with *Dirichlet*-conditions on the electrode edges and homogeneous *Neumann*-conditions on the outer boundary, a standard problem.

1. When the problem has been solved we can draw the ion-trajectories $\mathbf{r}(t)$.
We have $d\mathbf{r}/dt = \mathbf{v} = -mq\nabla V$ and use the `streamline`-plot. The field is shown by arrows (left)





2. We visualize also the field strength $|\nabla V|$ by colored surfaces (right).

3. The resistance between the electrodes is $\Delta V/I$ where I is the total current and ΔV the electric potential difference. We can compute that by a line integral (`boundary integration`) over the boundary Γ of an electrode, $I = \int_\Gamma \sigma \nabla V \cdot \mathbf{n} dl$.

Formulation of PDE and models

Models – conservation laws and constitutive relations.

Example: $N(\mathbf{r},t)$ yellow molecules per m^3 in a flowing continuum, in $\boldsymbol{R}^n$, $n = 3$

Def. *Flux*: $|\mathbf{F}|$ = # yellow molecules per second through 1 m^2 orthogonal to $\mathbf{F}$.

The total flow across a stationary surface S becomes

$$Q = \int_S \mathbf{F} \cdot \hat{\mathbf{n}} dS \quad \text{st/sek.}$$

If yellow molecules are created at a net rate $f(\mathbf{r},t)$ [st/sec/m^3], it is obvious that, if S contains a volume V, that

$$\underbrace{\frac{d}{dt}\int_V N(\mathbf{r},t)dV}_{\substack{\text{Net change rate} \\ \text{in } V}} = \underbrace{\int_V f(\mathbf{r},t)dV}_{\text{Net production in } V} - \underbrace{\int_S \mathbf{F}\cdot\hat{\mathbf{n}}dS}_{\text{Net flow out of } V \text{ through } S} \quad \text{st/sek.}$$

which becomes, by the Gauss theorem,

$$\int_V \{\frac{\partial}{\partial t} N(\mathbf{r},t) - f(\mathbf{r},t) + \nabla \cdot \mathbf{F}(\mathbf{r},t)\} dV = 0$$

Since this holds for any volume V we get

$$\frac{\partial}{\partial t} N(\mathbf{r},t) + \nabla \cdot \mathbf{F}(\mathbf{r},t) = f(\mathbf{r},t),$$

the conservation law for yellow molecules. But that is only one equation for the $2 + n$ unknowns N, f, and $\mathbf{F}$. The system becomes closed if we manage to formulate models for $\mathbf{F}$ and f expressed in N.

Example.

1. For molecules which passively follow a given velocity field $\mathbf{u}(\mathbf{r},t)$,

$$\mathbf{F} = N\mathbf{u}$$

In the absence of sources (and sinks) we get

$$\frac{\partial N}{\partial t} + \nabla \cdot (N\mathbf{u}) = 0$$

$$\underbrace{\frac{\partial N}{\partial t} + \mathbf{u}\cdot\nabla N}_{\substack{\text{The material derivative,} \\ \frac{DN}{Dt}}} = -N \underbrace{\nabla \cdot \mathbf{u}}_{-\text{"volume source density"}}$$

If we count *all* molecules, i.e. the mass density $\rho(\mathbf{r},t)$ [kg/m^3], we obtain the *equation of continuity* of continuum mechanics,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

2. The heat flux in a solid body is, according to the Fourier (phenomenological and empirical) law, proportional to the negative temperature gradient,

$$\mathbf{F}(\mathbf{r},t) = -k(...)\nabla T(\mathbf{r},t) \text{ [W/m}^2\text{]}$$

The rate of change of thermal energy per m^3 is $\rho(\mathbf{r})C(\mathbf{r})\frac{\partial T}{\partial t}$ where C is the specific heat J/kg/^{o}K.
The conservation law for thermal energy becomes the *Heat equation*

$$\rho(\mathbf{r})C(\mathbf{r})\frac{\partial T}{\partial t} - \nabla \cdot (k(...)\nabla T) = f$$

where we also assumed a heat source f W/m^3. There is a multitude of similar models for other processes (see below). The *Comsol model–equation* for them reads

$$e\frac{\partial^2 u}{\partial t^2} + d\frac{\partial u}{\partial t} - \nabla \cdot (c\nabla u) = f \qquad \text{i } \Omega$$

$$\text{On the boundary : } \begin{cases} h \cdot u = r & \text{Dirichlet - conditions} \\ c\mathbf{n} \cdot \nabla u = q \cdot u + g & \text{Neumann - conditions} \end{cases} \qquad (*)$$

where the second time derivative is included to cover also Newton's equation.

Note: The latter type of boundary condition with non-zero q is called a mixed or radiation condition or Robin-condition, and the term Neumann-condition is then reserved for the case q = 0.

Other processes modeled by the Comsol equation

Transversal deflection of membrane:
u = displacement, c = membrane (tensile) stress, f = normal load, d = damping coefficient, e = mass density
Heat conduction (**Fourier's** law):
u = temperature, c = heat conductivity, f = heat source, e = 0, d = heat capacity;
q = heat transfer coefficient
Diffusion (**Fick's** law):
u = concentration, c = coefficient of diffusion, f = source; e = 0, d = 1;
q = (mass) transfer coefficient
Stationary DC current in resistive medium (**Ohm's** law) – the ion movement example:
u = potential, c = conductivity (= 1/resistivity), f = charge source, e = d = 0;
q = resistance to ground (at edge)
Elektrostatics in charge-free dielectric
u = potential, c = dielectrical coefficient (permittivity), f = 0, d = e = 0

r = potential on conductors, q = g = 0 mean insulation

Steady flow in porous medium (**Darcy's** law):

u = "hydraulic head" (pressure), c = Darcy-coefficient, f = volume source, e = d = 0;

Irrotational ($\nabla \times \mathbf{u} = 0$) incompressible ($\frac{D\rho}{Dt} = 0 \Rightarrow \nabla \cdot \mathbf{u} = 0$) flow:

u = velocity potential, c = 1, f = 0; d = e = 0

q = g = 0 along impermeable fixed walls; u = 1on inflow boundary, u = 0 on outflow.

Variational formulation

This section shows a means to solve the equation approximately. As example we take a linear problem,

$$\begin{aligned} &Lu = f : au - \nabla \cdot (c\nabla u) = f \text{ i } \Omega \\ &c\nabla u \cdot \mathbf{n} = qu + g \text{ on the boundary} \end{aligned} \qquad \text{(S)}$$

This may look a very small problem class, but:

1. Non–linear equations can be linearized (the Newton method) to produce a sequence of problems of type (S).
2. Transient processes are discretized in time to give a problem (S) to be solved in every time-step.

If u satisfies the differential equation for every x it is called a *strong* or classical solution. For a strong solution $\int_\Omega (Lu - f) \cdot v(x) d\Omega = 0$ for every function v for which the integral can be evaluated. Conversely, if u has two continuous derivatives and $\int_\Omega (Lu - f) \cdot v(x) d\Omega = 0$ for all v then $Lu = f(x)$ in every x in Ω.

So far nothing new; but the simple trick of re-writing the integral by the Gauss theorem brings in the boundary conditions and gives a wider class of solutions:

$$\begin{aligned} &\int_\Omega (au - \nabla \cdot (c\nabla u) - f) \cdot v(x) d\Omega = \int_\Omega (auv + c\nabla u \cdot \nabla v - fv) d\Omega - \int_{\partial\Omega} c\nabla u \cdot \mathbf{n} v dS = \\ &\int_\Omega (auv + c\nabla u \cdot \nabla v - fv) d\Omega - \int_{\partial\Omega} (qu + g) v dS = 0 \end{aligned} \qquad \text{(V)}$$

A function u which satisfies the last relation for every v for which the integral exists is a *weak* solution. The integral formulation is the *variational formulation*. A strong solution also weak, but the reverse is not necessarily true. This is because weak solutions need only square-integrable first derivatives, whereas strong solutions must have two pointwise derivatives. So it is easier to construct approximative solutions for the variational formulation than for the differential equation.

Ex. 1 Let V be the volume in the derivation of the differential equation above. Take

$v(x) = 1$ for x i V, 0 outside

The variational formulation is just the integral–form which is the starting point for the derivation..

Ex. 2 Equations in R^n.
If $\mathbf{Ax} = \mathbf{b}$ (the differential equation) then $\mathbf{v}^T(\mathbf{Ax} - \mathbf{b}) = 0$ (variational formulation) for all $\mathbf{v}$ in R^n. Conversely, if $\mathbf{v}^T(\mathbf{Ax} - \mathbf{b}) = 0$ for n linearly independent **v,** then the weak solution **x** is also an exact (strong) solution to $\mathbf{Ax} = \mathbf{b}$.

Ex. 3
Many models for equilibrium problems are formulated as minimization problems for a potential energy. For the deflection of the membrane,

$$E = \underbrace{\frac{1}{2}\int_\Omega c|\nabla u|^2 d\Omega}_{\text{Elastic energy}} + \underbrace{\int_\Omega fud\Omega}_{\text{"virtual" work}}$$

Variational calculus shows that a minimizer of E must satisfy

$$0 = \int_\Omega (c\nabla u \cdot \nabla v + fv)d\Omega, \text{ for all } v \text{ that vanish on the boundary}$$
$$u = 0 \text{ on the boundary}$$

and that a sufficiently smooth such weak solution must satisfy the *Euler-Lagrange* differential equation

$$\nabla \cdot (c\nabla u) = f \text{ i } \Omega$$
$$u = 0 \text{ on the boundary}$$

The Galerkin method

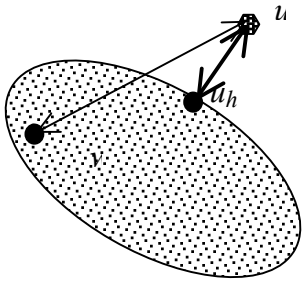
Look for an approximative *weak* solution u_h in an N–dimensional function space V_h, with a basis $\varphi_k(x), k = 1,...,N$. So we wish to determine the coefficients c_k in the ansatz (or trial) function $u_h = \sum_{k=1}^{N} c_k \varphi_k$ so that

$$\int_\Omega (au_h v_k + c\nabla u_h \cdot \nabla v_k - fv_k)d\Omega - \int_{\partial\Omega} (qu_h + g)v_k dS = 0$$

for a number of suitable test functions v_k. In the Galerkin method the choice is $v_k = \varphi_k$ and it always produces exactly N linear equations $\mathbf{Ac} = \mathbf{f}$ for the N unknowns c_k. The properties of the coefficient matrix **A** depend on the differential equation and the basis functions. If, e.g., a and $c > 0$, **A** becomes symmetric positive definite, and there is a unique solution which can be calculated stably both by elimination and by iterative schemes.

Notes.

1. For differential equation problems whose solutions give minimum for an energy (e.g. a and $c > 0$), the Galerkin method minimizes the energy over the sub-space V_h. That means also



that u_h is the best possible function in V_h since it minimizes the error in the sense

$$u_h = \arg\min_{w \in V_h} \int_\Omega (ae^2 + c|\nabla e|^2) d\Omega$$

2. The corresponding for linear systems of equations is the following: Let $\mathbf{Ax} = \mathbf{b}$ have symmetric, positive definite matrix $\mathbf{A}$. Then the solution gives min. to

$$E(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{Ax} - \mathbf{b}^T\mathbf{x}$$

If we look for an approximation in a sub-space $W^N \subset R^n$ spanned by $\mathbf{w}_k$, $k = 1,...,N$, $(N < n)$

$$\mathbf{x}_h = \sum_{k=1}^{N} c_k \mathbf{w}_k = \mathbf{Wc}, \mathbf{W} = \begin{pmatrix} \mathbf{w}_1 & \mathbf{w}_2 & ... & \mathbf{w}_N \end{pmatrix}, \text{a } n \times N \text{ - matrix}$$

we must minimize

$$E(\mathbf{Wc}) = \frac{1}{2}\mathbf{c}^T\mathbf{Bc} - \mathbf{d}^T\mathbf{c}, \mathbf{B} = \mathbf{W}^T\mathbf{AW}, \text{an } NxN \text{ matris}, \mathbf{d} = \mathbf{W}^T\mathbf{b}$$

where $\mathbf{B}$ is also positive definite, i.e., solve $\mathbf{Bc} = \mathbf{d}$. Then, $\mathbf{Wc}$ is the best approximation to $\mathbf{x}$ in the sense

$$\mathbf{Wc} = \arg\min_{\mathbf{w} \in W^N} (\mathbf{x} - \mathbf{w})^T \mathbf{A}(\mathbf{x} - \mathbf{w}) \qquad (* \text{ - proof as addendum})$$

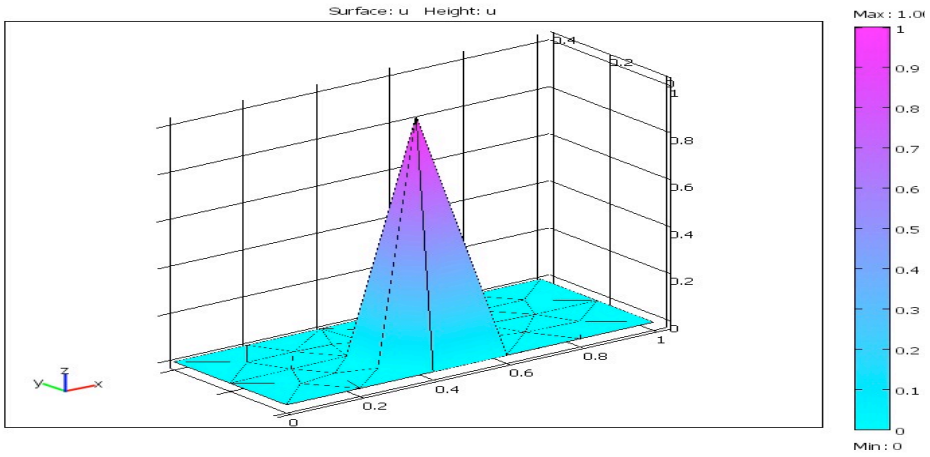
3. The Galerkin method is used also for problems without minimization properties, such as the convection-diffusion equation for the concentration $u(x,t)$

$$\mathbf{v} \cdot \nabla u = \nabla \cdot (c \nabla u) + f(x)$$

where $\mathbf{v}(x,t)$ is the velocity field. One often chooses other test-functions than φ_k, and the approximation properties of u_h are more difficult to discover for such equations.

Finite Elements

In the Finite Element method one chooses basis functions which are non-zero only over small subdomains, the *elements*. In 2D, the computational domain Ω is cut up into e.g. triangles (in 3D tetrahedra). For the variational equations above, basis functions with square-integrable first derivatives are smooth enough, $\int_\Omega |\nabla \varphi|^2 d\Omega < \infty$. The simplest construction is provided by piecewise first degree polynomials, one per triangle vertex. Such a basis function is shown in a triangulation of a rectangle, below:



Computation of A and b: the assembly process.

One computes **A** by summing the contributions from every triangle T_k; the integrals over triangles are calculated by numerical quadrature

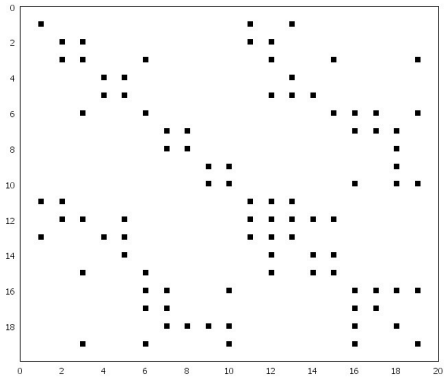
$$\Omega = \bigcup T_k, \int_{\Omega} f(x)d\Omega = \sum_k \int_{T_k} f(x)d\Omega \approx \sum_k |T_k| (\sum_j \underbrace{w_j}_{\text{weights}} \quad f(\underbrace{x_{kj}}_{\text{quadrature points}}))$$

Integrals of the types

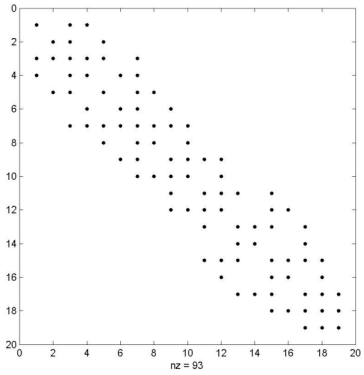
$$\int_T c\nabla\varphi_k \cdot \nabla\varphi_j d\Omega, \int_T a\varphi_k\varphi_j d\Omega, \int_T f\varphi_k d\Omega, \int_{\partial T} q\varphi_k\varphi_j d\partial\Omega, \text{ och } \int_{\partial T} h\varphi_k d\partial\Omega,$$

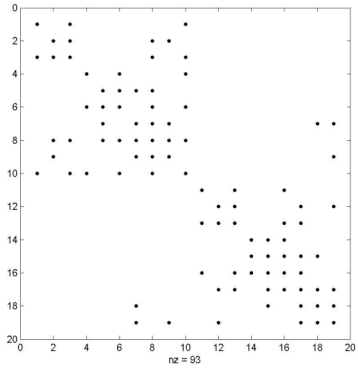
are computed and summed to coefficient matrix **A** and right hand side **b**. The contributions come both from Ω and the boundary.

All details are left out here, both theoretical and implementational, but you can find them in advanced courses on numerical analysis and courses in finite elements. The point is to show how the whole process is automated. The user specifies the geometry, (there are automatic triangulators), the differential equation (integration by parts is done by the program) and boundary conditions (should be explained more, but will have to wait) . The system of equations is then solved by e.g. Gaussian elimination. The solution is post-processed by visualization of arrows, color surfaces, by computation of interesting quantities like the line integral in the ion movement example, etc.
The choice of basis functions makes the matrix sparse: $a_{kj} = 0$ unless the supports of the basis functions involved overlap, i.e., unless nodes k and j are in the same same triangle. The matrix for the rectangle above with 19 nodes has only 93 non-zeros, i.e, in the mean, less than six per row:



The pattern is symmetric: neighborship is a reflexive relation. Also the values are the same if the differential equation is self-adjoint. The pattern will change if the nodes are re-numbered. It is important to number such that the elimination process creates not too many new non-zeros.
The RCM-algorithm gives the left plot and AMD the right. Elisabeth Cuthill & Sean McKee's method numbers neighbor nodes after one another and gives a "band" structure,– Approx. Minimal Degree chooses pivot elements to give minimal fill-in in each step.





An efficient numbering solves problems like the above with half a million unknowns in seconds on a modern PC. So one may solve problems with one node per pixel!
But for three-dimensional problems the matrices are less sparse, there are many more unknowns, and iterative methods are competitive. For a and $c > 0$ there are multi-grid methods with computational complexity O(N). $a < 0$, which appears e.g. for frequency-domain description of time-harmonic wave propagation, the Helmholtz equation, is much more difficult.

Addendum: Proof of optimality in energy norm - $\mathbf{R}^n$ model

Let $\mathbf{Ax} = \mathbf{b}$ have symmetric, positive definite matrix $\mathbf{A}$. Then the solution gives min. to

$$E(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{Ax} - \mathbf{b}^T\mathbf{x}$$

for $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} = \mathbf{x}^*$. We look for an approximation in a sub-space $W^N \subset R^n$ spanned by $\mathbf{w}_k$, $k = 1,...,N$, $(N < n)$

$$\mathbf{x}_h = \sum_{k=1}^{N} c_k \mathbf{w}_k = \mathbf{Wc}, \mathbf{W} = \begin{pmatrix}\mathbf{w}_1 & \mathbf{w}_2 & ... & \mathbf{w}_N\end{pmatrix}, \text{a } n \times N \text{ - matrix}$$

by minimizing

$$E(\mathbf{Wc}) = \frac{1}{2}\mathbf{c}^T\mathbf{Bc} - \mathbf{d}^T\mathbf{c}, \mathbf{B} = \mathbf{W}^T\mathbf{AW}, \text{an } NxN \text{ matris}, \mathbf{d} = \mathbf{W}^T\mathbf{b}$$

where $\mathbf{B}$ is also positive definite, i.e., solve $\mathbf{Bc}^* = \mathbf{d}$.

Then, $\mathbf{Wc}^*$ is the best approximation to $\mathbf{x}$ in the sense

$$\mathbf{Wc}^* = \arg\min_{\mathbf{w}\in W^N}(\mathbf{x}^* - \mathbf{w})^T\mathbf{A}(\mathbf{x}^* - \mathbf{w})$$

Preliminaries:

The formula $\langle \mathbf{x},\mathbf{y} \rangle = \mathbf{x}^T\mathbf{Ay}$ defines an inner product on $\boldsymbol{R}^n$. The symmetry and linearity axioms for this are easy to check. Then, the formula

$$\|\mathbf{x}\|_E = \langle \mathbf{x},\mathbf{x} \rangle^{(1/2)}$$

defines the energy norm. (*Exercise.* Prove the triangle inequality for $\| \cdot \|_E$)

Proof:

The equation for $\mathbf{c}$ says

$$\mathbf{W}^T\mathbf{AWc}^* = \mathbf{W}^T\mathbf{b}:$$

$$\mathbf{W}^T(\underbrace{\mathbf{AWc}^* - \mathbf{b}}_{-residual}) = 0 \Leftrightarrow \mathbf{W}^T\mathbf{A}(\underbrace{\mathbf{Wc}^* - \mathbf{x}^*}_{error\ \mathbf{e}^*})$$

These statements are referred to as "Galerkin orthogonality":

$\mathbf{W}$ is orthogonal

in the Euclidean sense ($\mathbf{x}^T\mathbf{y}$) to the *residual* $\mathbf{AWc}^*\text{-}\mathbf{b}$

in the energy sense ($\mathbf{x}^T\mathbf{Ay}$) to the *error vector* $\mathbf{Wc}^*\text{-}\mathbf{x}^*$

There follows

$$\|\mathbf{Wc}^* - \mathbf{x}^*\|_E \le \|\mathbf{Wc} - \mathbf{x}^*\|_E \ \forall \mathbf{c} \in R^N$$

For:

$$\|\mathbf{Wc} - \mathbf{x}^*\|_E^2 = \left\|\underbrace{\mathbf{Wc}^* - \mathbf{x}^*}_{\mathbf{e}^*} + \underbrace{\mathbf{W}(\mathbf{c} - \mathbf{c}^*)}_{\mathbf{w}}\right\|_E^2 = \langle \mathbf{e}^* + \mathbf{w}, \mathbf{e}^* + \mathbf{w} \rangle =$$

$$= \langle \mathbf{e}^*,\mathbf{e}^* \rangle + \underbrace{\langle \mathbf{w},\mathbf{w} \rangle}_{\ge 0} + 2\underbrace{\langle \mathbf{e}^*,\mathbf{w} \rangle}_{=0} \ge \langle \mathbf{e}^*,\mathbf{e}^* \rangle = \|\mathbf{Wc}^* - \mathbf{x}^*\|_E^2$$

QED