Master/Diploma Thesis Project

(Mathematics, Computational Science & Engineering)

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Simulation of Non-Local Electrostatic Effects

Prerequisites. Knowledge about the finite element method for the numerical solution of elliptic boundary value problems [1], cf. course of numerical solution of elliptic and parabolic partial differential equations.

Problem description. Given a domain $\Omega \subset \mathbb{R}^3$ and a charge distribution $\rho \in L^2(\Omega)$, the electrostatic energy in the presence of a polar solution, e.g., ions in water, can be modelled by

$$\begin{aligned} E(u) =& \tfrac{1}{2}\int_\Omega |\,\mathbf{grad}\, u|^2 \,\mathrm{d}\mathbf{x} + \tfrac{1}{2}\int_\Omega\int_\Omega k(\mathbf{x},\mathbf{y})\ \mathbf{grad}\, u(\mathbf{x}) \cdot \mathbf{grad}\, v(\mathbf{x})\,\mathrm{d}(\mathbf{x},\mathbf{y}) \\ & - \int_\Omega \rho\, u \,\mathrm{d}\mathbf{x}\ , \quad u \in H_0^1(\Omega)\ . \end{aligned} \tag{1}$$

Here, the asymptotically smooth and exponentially decaying kernel is

$$k(\mathbf{x},\mathbf{y}) = \frac{e^{-\alpha|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}\ , \quad \alpha > 0\ .$$

In a 2D model, a similar kernel would involve certain special functions. The actual potential is obtained by solving the minimization problem for the quadratic functional E.

We aim at a direct Galerkin discretization of the minimization problem (1) on a hierarchy of nested triangular meshes using prewavelet basis functions [3, 4] and clustering techniques [2] for the evaluation of the non-local part of the energy functional.

Task. The focus of this project is on efficient implementation of the wavelet Galerkin scheme in MATLAB. Conditioning of the resulting discrete linear system and the convergence of the discretization should be studied experimentally.

References

[1] D. Braess, *Finite Elements*, Cambridge University Press, 2nd ed., 2001.

[2] W. Hackbusch and S. Börm, *$\mathcal{H}^2$-matrix approximation of integral operators by interpolation*, Appl. Numer. Math., 43 (2002), pp. 129–143.

[3] R. Stevenson, *Stable three-point wavelet bases on general meshes*, Numer. Math., 80 (1998), pp. 131–158.

[4] T. von Petersdorff and C. Schwab, *Wavelet-discretizations of parabolic integro-differential equations*, Research Report 2001-07, SAM, ETH Zürich, Zürich Switzerland, 2001.