Syllabus of the course
Partial Differential Equations in Biology - Part 2

- Partial differential equations (PDEs)

Classification for linear second order PDEs in two variables [Greenspan–Casulli, pp. 182–185]:

$$au_{xx} + 2bu_{xy} + cu_{yy} + \text{lower order terms} = \dots \quad \begin{cases} ac - b^2 > 0 & \text{elliptic} \\ ac - b^2 = 0 & \text{parabolic} \\ ac - b^2 < 0 & \text{hyperbolic} \end{cases}$$

Linear second order elliptic PDEs, parabolic PDEs, hyperbolic PDEs in space dimension $d \geq 2$ [Quarteroni–Valli, pp. 159, 363–364, 497–498]

$$\text{elliptic} \quad Lu := -\sum_{i,j=1}^{d} D_i(a_{ij} D_j u) + \sum_{i=1}^{d} b_i D_i u + qu = f \text{ with } \sum_{i,j=1}^{d} a_{ij}\xi_j\xi_i \geq \alpha_0 |\boldsymbol{\xi}|^2$$

$$\text{parabolic} \quad D_t u + Lu = f \quad , \quad L \text{ elliptic}$$

$$\text{hyperbolic} \quad D_t^2 u + Lu = f \quad , \quad L \text{ elliptic}$$

- Boundary value problems and initial–boundary value problems for linear second order PDEs [Quarteroni–Valli pp. 161–163; 364; 497–498]

  elliptic

$$\text{Dirichlet} \quad u \text{ given on } \partial D$$

$$\text{Neumann} \quad \sum_{i,j=1}^{d} a_{ij} D_j u \, n_i \text{ given on } \partial D$$

$$\text{mixed} \quad u \text{ given on } \Gamma_D \text{ and } \sum_{i,j=1}^{d} a_{ij} D_j u \, n_i \text{ given on } \Gamma_N \quad (\partial D = \overline{\Gamma_D} \cup \overline{\Gamma_N},\, \Gamma_D \cap \Gamma_N = \emptyset)$$

$$\text{Robin} \quad \sum_{i,j=1}^{d} a_{ij} D_j u \, n_i + \kappa \, u \text{ given on } \partial D$$

  parabolic

  Dirichlet or Neumann or mixed or Robin on the boundary, and $u_{|t=0}$ given in D

  hyperbolic

  Dirichlet or Neumann or mixed or Robin on the boundary, and $u_{|t=0}$ and $(D_t u)_{|t=0}$ given in D

- Weak form for linear second order elliptic PDEs [Quarteroni–Valli, pp. 159–163]

$$b(\varphi, \psi) := \sum_{i,j=1}^{d} \int_D a_{ij} D_j \varphi D_i \psi + \sum_{i=1}^{d} \int_D b_i (D_i \varphi) \, \psi + \int_D q\varphi \, \psi = \begin{cases} \int_D f\psi & \text{Dirichlet (homogeneous)} \\ \int_D f\psi + \int_{\partial D} g\psi & \text{Neumann} \\ \int_D f\psi + \int_{\Gamma_N} g\psi & \text{mixed} \end{cases}$$

$$b(\varphi, \psi) := \sum_{i,j=1}^{d} \int_D a_{ij} D_j \varphi D_i \psi + \sum_{i=1}^{d} \int_D b_i (D_i \varphi) \, \psi + \int_D q\varphi \, \psi + \int_{\partial D} \kappa \, \varphi \, \psi = \int_D f\psi + \int_{\partial D} g\psi \quad \text{Robin}$$

- Calculus of variations and minimization problems [Quarteroni–Valli pp. 163–164]:

$$\min_{\psi}\Big(\frac{1}{2}\sum_{i,j=1}^{d}\int_D a_{ij}D_j\psi D_i\psi+\frac{1}{2}\int_D q\psi^2-\int_D f\,\psi\Big)\quad\text{Dirichlet (homogeneous)}$$

  [Note: no first order terms in the operator L...]
  Similarly for the other boundary value problems

- Existence and uniqueness

Minimization problem: direct method of calculus of variations (selection of a convergent subsequence from a minimization sequence)

Weak problem: Riesz representation theorem ($b(\varphi,\psi)$ is a scalar product in a Hilbert space V, equivalent to the scalar product of V) or Lax-Milgram lemma ($b(\varphi,\psi)$ is continuous and coercive bilinear form in a Hilbert space V) [Quarteroni–Valli pp. 133–135]:

$$\begin{aligned}&|b(\varphi,\psi)|\le\gamma||\varphi||_V||\psi||_V\quad\text{continuous}\\&b(\psi,\psi)\ge\alpha||\psi||_V^2\quad\text{coercive}\end{aligned}$$

Space of functions:

$$V=\begin{cases}H^1_0(D):=\{\psi:D\to\mathbf{R}\,|\,\int_D\psi^2<\infty\ ,\ \int_D|\nabla\psi|^2<\infty\ ,\ \psi_{|\partial D}=0\} & \text{Dirichlet (homogeneous)}\\ H^1(D):=\{\psi:D\to\mathbf{R}\,|\,\int_D\psi^2<\infty\ ,\ \int_D|\nabla\psi|^2<\infty\} & \text{Neumann}\\ H^1_{\Gamma_N}(D):=\{\psi:D\to\mathbf{R}\,|\,\int_D\psi^2<\infty\ ,\ \int_D|\nabla\psi|^2<\infty\ ,\ \psi_{|\Gamma_N}=0\} & \text{mixed}\\ H^1(D):=\{\psi:D\to\mathbf{R}\,|\,\int_D\psi^2<\infty\ ,\ \int_D|\nabla\psi|^2<\infty\} & \text{Robin}\end{cases}$$

Sufficient conditions for continuity:

$$\begin{cases}a_{ij},b_i,q\text{ bounded in }D & \text{Dirichlet (homogeneous)}\\ a_{ij},b_i,q\text{ bounded in }D & \text{Neumann}\\ a_{ij},b_i,q\text{ bounded in }D & \text{mixed}\\ a_{ij},b_i,q\text{ bounded in }D\ ,\ \kappa\text{ bounded on }\partial D & \text{Robin}\end{cases}$$

Sufficient conditions for coerciveness [Quarteroni–Valli pp. 164–167]:

$$\begin{cases}q-\frac{1}{2}\text{div}\mathbf{b}\ge0\text{ in }D & \text{Dirichlet (homogeneous)}\\ q-\frac{1}{2}\text{div}\mathbf{b}\ge\mu_0>0\text{ in }D\ ,\ \mathbf{b}\cdot\mathbf{n}\ge0\text{ on }\partial D & \text{Neumann}\\ q-\frac{1}{2}\text{div}\mathbf{b}\ge0\text{ in }D\ ,\ \mathbf{b}\cdot\mathbf{n}\ge0\text{ on }\Gamma_N & \text{mixed}\\ q-\frac{1}{2}\text{div}\mathbf{b}\ge\mu_0>0\text{ in }D\ ,\ \frac{1}{2}\mathbf{b}\cdot\mathbf{n}+\kappa\ge0\text{ on }\partial D & \text{Robin}\end{cases}$$

An alternative for Neumann: choose $V=\{\psi\in H^1(D)\,|\,\int_D\psi=0\}$ and assume $q-\frac{1}{2}\text{div}\mathbf{b}\ge0$ in D, $\mathbf{b}\cdot\mathbf{n}\ge0$ on ∂D [but pay attention to the correct interpretation of the weak problem!].
An alternative for Robin: assume $q-\frac{1}{2}\text{div}\mathbf{b}\ge0$ in D, $\frac{1}{2}\mathbf{b}\cdot\mathbf{n}+\kappa\ge0$ on ∂D and $\int_{\partial D}(\frac{1}{2}\mathbf{b}\cdot\mathbf{n}+\kappa)>0$.
Assumptions on the data: $f\in L^2(D)$, $g\in L^2(\partial D)$ (Neumann and Robin) or $g\in L^2(\Gamma_N)$ (mixed), where

$$L^2(D):=\{\psi:D\to\mathbf{R}\,|\int_D\psi^2<\infty\}$$

and similarly for $L^2(\partial D)$ and $L^2(\Gamma_N)$.
For Neumann, if $q=0$ and $\mathbf{b}=\mathbf{0}$: assume also the (necessary) compatibility condition $\int_D f+\int_{\partial D}g=0$.

- Galerkin approximation method [Quarteroni–Valli, pp. 136–144]

Choice of a finite dimensional subspace V_h of V, and minimization in V_h (or solution of the weak problem in V_h).

Examples:

trigonometric polynomials in $D = [a, b]^d$ (Fourier methods for periodic problems);
global polynomials in $D = [a, b]^d$ (spectral methods) [Quarteroni–Valli, pp. 176–179];
global polynomials in $D = [a, b]^d$ with Gaussian quadrature formulas (spectral collocation methods) [Quarteroni–Valli, pp. 179–186];
piecewise polynomials in a polygonal domain (finite element methods) [Quarteroni–Valli, pp. 170–176]

- The finite element method [Quarteroni–Valli, pp. 73–91, 170–174, 190, 192–193]

Family of triangulations:

$$\overline{D} = \cup_{K \in \mathcal{T}_h} K \quad , \quad K \text{ polyhedron}$$

Piecewise-polynomials finite dimensional subspaces:

i.

$$X_h^r := \{\psi_h : D \to \mathbf{R} \,|\, \psi_{h|K} \in \mathbf{P}_r \ , \ \psi_h \in C^0(\overline{D})\}$$

$\mathbf{P}_r$ polynomials of degree less than or equal to r, K triangle/tetrahderon.

ii.

$$X_h^r := \{\psi_h : D \to \mathbf{R} \,|\, \psi_{h|K} \circ T_K \in \mathbf{Q}_r \ , \ \psi_h \in C^0(\overline{D})\}$$

$\mathbf{Q}_r$ polynomials of degree less than or equal to r with respect to each variable, K parallelogram/parallepiped, T_K affine map from $[0, 1]^d$ onto K.

Degrees of freedom: values of functions in the nodes $\mathbf{P}_i$

Shape functions (basis functions): "hat" functions η_i, such that $\eta_i(\mathbf{P}_i) = 1$ and $\eta_i(\mathbf{P}_j) = 0$ for each $j \neq i$. Consequently: η_i has "small" support.

Interpolation operator and interpolation error

Error estimates for the approximate solution via Céa lemma

Algebraic form: stiffness matrix A,

$$A_{ij} := b(\eta_j, \eta_i)$$

A is symmetric if $b(\varphi, \psi)$ is symmetric (namely, $b(\varphi, \psi) = b(\psi, \varphi)$: this is never true if the first order terms are present)
A is positive definite if $b(\varphi, \psi)$ is coercive
A is sparse as the basis functions have small support.

- The mixed finite element method

Elliptic equations (without first and zero order terms) [Quarteroni–Valli, pp. 217–218, 222–227, 230-231].

Example: Laplace operator

$$\begin{cases} \mathbf{p} - \nabla\varphi = \mathbf{0} \\ \text{div } \mathbf{p} + f = 0 \end{cases}$$

Weak form (homogeneous Dirichlet): $\mathbf{p} \in V$, $\varphi \in Q$ such that

$$\begin{cases} \int_D (\mathbf{p} \cdot \mathbf{q} + \varphi \text{ div } \mathbf{q}) = 0 \\ \int_D (\text{div } \mathbf{p})\, \psi = -\int_D f\, \psi \end{cases}$$

with

$$V = H(\text{div }; D) := \{\mathbf{q} : D \to \mathbf{R}^d \,|\, \int_D |\mathbf{q}|^2 < \infty \ , \ \int_D (\text{div } \mathbf{q})^2 < \infty\}$$

$$Q = L^2(D)$$

Raviart–Thomas finite elements

Stokes problem [Quarteroni–Valli, pp. 297–302, 304–311]

$$\begin{cases} -\Delta\mathbf{u} + \nabla p = \mathbf{f} \\ \text{div } \mathbf{u} = 0 \end{cases}$$

Weak form (homogeneous Dirichlet): $\mathbf{u} \in (H_0^1(D))^d$, $p \in L^2(D)$ such that

$$\begin{cases} \int_D (\nabla\mathbf{u} \cdot \nabla\mathbf{v} - p \text{ div}\mathbf{v}) = \int_D \mathbf{f} \cdot \mathbf{v} \\ -\int_D (\text{div } \mathbf{u})\, q = 0 \end{cases}$$

Discontinuous pressure finite elements (Crouzeix–Raviart)

Continuous pressure finite elements (Taylor–Hood, Arnold–Brezzi–Fortin mini element)

The algebraic structure [Quarteroni–Valli, pp. 241–242, 303–304]

$$S := \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix}$$

where A is a $N \times N$ matrix and B is a $K \times N$ matrix

S is non-singular if and only if $\Pi A_{|\ker B}$ is non-singular and $\ker B^T = \{0\}$
(Π orthogonal projection from $\mathbf{R}^N$ onto $\ker B$)

$\ker B^T = \{0\}$ is equivalent to the inf–sup condition:

$$\exists\, \beta > 0 \;:\; \forall\, \mathbf{p} \in \mathbf{R}^K \;\exists\, \mathbf{v} \in \mathbf{R}^N \setminus \mathbf{0} \;:\; B^T\mathbf{p} \cdot \mathbf{v} \geq \beta ||\mathbf{p}||\, ||\mathbf{v}||$$

Good finite element approximations: the inf–sup condition holds with β independent of the mesh size h

References

D. Greenspan, V. Casulli, *Numerical Analysis for Applied Mathematics, Science and Engineering*, Addison-Wesley, Redwood City, 1988

A. Quarteroni, A. Valli, *Numerical Approximation of Partial Differential Equations*, Springer, Berlin, 2nd printing, 1997