Practical realization of boundary conditions

- Robin boundary value problem

\[- \nabla \cdot \delta \tilde{\nabla} u = f \quad \text{in } \Omega\]

\[\delta \tilde{\nabla} u + \alpha (u - g) = 0 \quad \text{on } \partial \Omega\]

- Weak formulation: search $u \in H^1(\Omega)$ such that

\[
\int_{\Omega} \delta \tilde{\nabla} u \tilde{\nabla} v \, d\vec{x} + \int_{\partial \Omega} \alpha uv \, ds = \int_{\Omega} fv \, d\vec{x} + \int_{\partial \Omega} \alpha gv \, ds \quad \forall v \in H^1(\Omega)
\]

- In 2D, for $P^1$ FEM, boundary integrals can be calculated by trapezoidal rule without sacrificing approximation order

- Use Dirichlet penalty method to handle Dirichlet boundary conditions
More complicated integrals

- Assume non-constant right hand side $f$, space dependent heat conduction coefficient $\delta$.

- Right hand side integrals

  $$f_i = \int_K f(x) \lambda_i(x) \, d\vec{x}$$

- $P^1$ stiffness matrix elements

  $$a_{ij} = \int_K \delta(x) \vec{\nabla} \lambda_i \cdot \vec{\nabla} \lambda_j \, d\vec{x}$$

- $P^k$ stiffness matrix elements created from higher order ansatz functions
Quadrature rules

- **Quadrature rule:**
  \[
  \int_K g(x) \, d\vec{x} \approx |K| \sum_{l=1}^{l_q} \omega_l g(\xi_l)
  \]

- \(\xi_l\): nodes, Gauss points
- \(\omega_l\): weights
- The largest number \(k\) such that the quadrature is exact for polynomials of order \(k\) is called *order* \(k_q\) of the quadrature rule, i.e.
  \[
  \forall k \leq k_q, \forall p \in \mathbb{P}^k, \int_K p(x) \, d\vec{x} = |K| \sum_{l=1}^{l_q} \omega_l p(\xi_l)
  \]

- Error estimate:
  \[
  \forall \phi \in C^{k_q+1}(K), \left| \frac{1}{|K|} \int_K \phi(x) \, d\vec{x} - \sum_{l=1}^{l_q} \omega_l \phi(\xi_l) \right| 
  \leq c h_K^{k_q+1} \sup_{x \in K, |\alpha|=k_q+1} |\partial^\alpha \phi(x)|
  \]
Some common quadrature rules

Nodes are characterized by the barycentric coordinates

<table>
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<tr>
<th>$d$</th>
<th>$k_q$</th>
<th>$l_q$</th>
<th>Nodes</th>
<th>Weights</th>
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Matching of approximation order and quadrature order

“Variational crime”: instead of

\[ a(u_h, v_h) = f(v_h) \quad \forall v_h \in V_h \]

we solve

\[ a_h(u_h, v_h) = f_h(v_h) \quad \forall v_h \in V_h \]

where \( a_h, f_h \) are derived from their exact counterparts by quadrature.

For \( P^1 \) finite elements, zero order quadrature for volume integrals and first order quadrature for surface integrals is sufficient to keep the convergence order estimates stated before.

The rule of thumb for the volume quadrature is that the highest order terms must be evaluated exactly if the coefficients of the PDE are constant.
Practical realization of integrals

- Integral over barycentric coordinate function
  \[ \int_K \lambda_i(x) \, d\vec{x} = \frac{1}{3} |K| \]

- Right hand side integrals. Assume \( f(x) \) is given as a piecewise linear function with given values in the nodes of the triangulation
  \[ f_i = \int_K f(x) \lambda_i(x) \, d\vec{x} \approx \frac{1}{3} |K| (f(a_0) + f(a_1) + f(a_2)) \]

- Integral over space dependent heat conduction coefficient: Assume \( \delta(x) \) is given as a piecewise linear function with given values in the nodes of the triangulation
  \[ a_{ij} = \int_K \delta(x) \, \vec{\nabla} \lambda_i \, \vec{\nabla} \lambda_j \, d\vec{x} = \frac{1}{3} (\delta(a_0) + \delta(a_1) + \delta(a_2)) \int_K \vec{\nabla} \lambda_i \, \vec{\nabla} \lambda_j \, d\vec{x} \]
P1 FEM stiffness matrix condition number

• Homogeneous dirichlet boundary value problem

\[-\nabla \cdot \delta \nabla u = f \quad \text{in } \Omega\]

\[u|_{\partial \Omega} = 0\]

• Lagrange degrees of freedom $a_1 \ldots a_N$ corresponding to global basis functions $\phi_1 \ldots \phi_N$ such that $\phi_i|_{\partial \Omega} = 0$ aka $\phi_i \in V_h \subset H^1_0(\Omega)$

• Stiffness matrix $A = (a_{ij})$:

\[a_{ij} = a(\phi_i, \phi_j) = \int_{\Omega} \delta \nabla \phi_i \nabla \phi_j \, d\vec{x} \]

• Bilinear form $a(\cdot, \cdot)$ is self-adjoint, therefore $A$ is symmetric, positive definite

• Condition number estimate for $P^1$ finite elements on quasi-uniform triangulation:

\[\kappa(A) \leq ch^{-2} \]
Row sums:

\[ \sum_{j=1}^{N} a_{ij} = \sum_{j=1}^{N} \int_{\Omega} \nabla \phi_i \nabla \phi_j \, dx = \int_{\Omega} \nabla \phi_i \nabla \left( \sum_{j=1}^{N} \phi_j \right) \, dx \]

\[ = \int_{\Omega} \nabla \phi_i \nabla (1) \, dx \]

\[ = 0 \]
Local stiffness matrix \( S_K \)

\[
s_{ij} = \int_K \vec{\nabla} \lambda_i \vec{\nabla} \lambda_j \, dx = \frac{|K|}{2|K|^2} \left( y_{i+1} - y_{i+2}, x_{i+2} - x_{i+1} \right) \left( y_{j+1} - y_{j+2}, x_{j+2} - x_{j+1} \right)
\]

- Main diagonal entries positive
- Local contributions from element stiffness matrices: Scalar products of vectors orthogonal to edges. These are nonpositive if the angle between the edges are \( \leq 90^\circ \)
- \textit{weakly acute triangulation}: all triangle angles are less than \( \leq 90^\circ \)
- In fact, for constant coefficients, in 2D, Delaunay is sufficient, as contributions from opposite angles compensate each other
- All row sums are zero \( \Rightarrow A \) is singular
- Matrix becomes irreducibly diagonally dominant if we add at least one positive value to the main diagonal, e.g. from Dirichlet BC
Assume additional process in each REV which produces or destroys species depending on the amount of species present with given rate $r$.

Search function $u : \Omega \rightarrow \mathbb{R}$ such that

$$-\nabla \cdot \delta \vec{\nabla} u + ru = f \quad \text{in} \Omega$$

$$\delta \vec{\nabla} u \cdot \vec{n} + \alpha (u - g) = 0 \quad \text{on} \partial \Omega$$

Coercivity guaranteed e.g. for $\alpha \geq 0$, $r > 0$ which means species destruction FEM formulation: search $u_h \in V_h = \text{span}\{\phi_1 \ldots \phi_N\}$ such that

$$\int_{\Omega} \delta \vec{\nabla} u_h \vec{\nabla} v_h \, d\vec{x} + \int_{\Omega} ru_h v_h \, d\vec{x} + \int_{\partial \Omega} \alpha u_h v_h \, ds$$

"stiffness matrix"  
"mass matrix"  
"boundary mass matrix"

$$= \int_{\Omega} f v_h \, d\vec{x} + \int_{\partial \Omega} \alpha g v_h \, ds \quad \forall v_h \in V_h$$

Coercivity + symmetry $\Rightarrow$ positive definiteness
Mass matrix properties

- Mass matrix (for $r = 1$): $M = (m_{ij})$:
  \[
  m_{ij} = \int_{\Omega} \phi_i \phi_j \, dx
  \]

- Self-adjoint, coercive bilinear form $\Rightarrow M$ is symmetric, positive definite

- For a family of quasi-uniform, shape-regular triangulations, for every eigenvalue $\mu$ one has the estimate
  \[
  c_1 h^d \leq \mu \leq c_2 h^d
  \]
  $T \Rightarrow$ condition number $\kappa(M)$ bounded by constant independent of $h$:
  \[
  \kappa(M) \leq c
  \]

- How to see this? Let $u_h = \sum_{i=1}^{N} U_i \phi_i$, and $\mu$ an eigenvalue (positive, real!) Then
  \[
  \|u_h\|_0^2 = (U, MU)_{\mathbb{R}^N} = \mu (U, U)_{\mathbb{R}^N} = \mu \|U\|_{\mathbb{R}^N}^2
  \]
  From quasi-uniformity we obtain
  \[
  c_1 h^d \|U\|_{\mathbb{R}^N}^2 \leq \|u_h\|_0^2 \leq c_2 h^d \|U\|_{\mathbb{R}^N}^2
  \]
For $P^1$-finite elements, all integrals $m_{ij} = \int_{\Omega} \phi_i \phi_j \, dx$ are zero or positive, so we get positive off diagonal elements.

No $M$-Property!
Local mass matrix for P1 FEM on element $K$
(calculated by 2nd order exact edge midpoint quadrature rule):

\[ M_K = |K| \begin{pmatrix}
\frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\
\frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\
\frac{1}{12} & \frac{1}{12} & \frac{1}{6}
\end{pmatrix} \]

Lumping: sum up off diagonal elements to main diagonal, set off diagonal entries to zero

\[ \tilde{M}_K = |K| \begin{pmatrix}
\frac{1}{3} & 0 & 0 \\
0 & \frac{1}{3} & 0 \\
0 & 0 & \frac{1}{3}
\end{pmatrix} \]

Interpretation as change of quadrature rule to first order exact vertex based quadrature rule

Loss of accuracy, gain of stability
Effect of mass matrix lumping

- For P1 FEM on weakly acute or Delaunay triangulations, mass matrix lumping can guarantee M-Property of system matrix.

- Adding a mass matrix which is not lumped yields a positive definite matrix (due to coercivity) and thus nonsingularity, but destroys $M$-property unless the absolute values of its off diagonal entries are less than those of $A$, i.e. for small $r$.

- Same situation with Robin boundary conditions and boundary mass matrix.

- Introducing the Dirichlet Penalty trick at continuous level without mass lumping would be disastrous.