Mathematisches Forschungsinstitut Oberwolfach

Report No. 5/2020

DOI: 10.4171/OWR/2020/5

# Boundary Element Methods

Organized by
Stéphanie Chaillat-Loseille, Palaiseau
Ralf Hiptmair, Zürich
Olaf Steinbach, Graz

2 February – 8 February 2020

Abstract. **Instructions for contributors**:

(1) Only the file `Talk_XX.tex` should be edited.
(2) Run LaTeXon `OWR-2006a_XX.tex` and and create a final PDF file. Seek assistance from TeXperts in case of problems.
(3) **All graphics have to be included in EPS format** using the `\includegraphics` command.
(4) Insert your extended abstract in the `talk` environment in `Talk_XX.tex`:
   - Minimum two full pages, standard three pages, maximum four pages.
   - Also give references to review and survey works.
(5) Run LaTeXon `OWR-2006a_XX.tex` again, create a PDF, and make sure that everything is all right.
(6) Rename the file `Talk_XX.tex` to `Talk_<your last name>.tex`
(7) If no other files are required, please send `Talk_<your last name>.tex` to Stephanie: `stephanie.chaillat@ensta-paris.fr`.
(8) If your extended abstract incorporates other (graphics) files, please create a zip-archive and send that to Stephanie: `stephanie.chaillat@ensta-paris.fr`.

*Mathematics Subject Classification (2010):* 65N38, 65M38, 74S15, 78M15, 80M15.

## Introduction by the Organizers

The workshop *Boundary element methods* organised by Stéphanie Chaillat-Loseille, Ralf Hiptmair, and Olaf Steinbach

*Acknowledgement:* The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1641185, "US Junior Oberwolfach Fellows".

Moreover, the MFO and the workshop organizers would like to thank the Simons Foundation for supporting NAME(S) in the "Simons Visiting Professors" program at the MFO.

## Workshop: Boundary Element Methods

## Table of Contents

# Abstracts

## Quadrature for Parabolic Space-Time Galerkin BEM

Johannes Tausch

Boundary integral formulations of parabolic PDEs involve layer operators on the lateral boundary $\Sigma$ of the space-time domain $Q$. For instance, the single layer operator of the heat equation is given by

$$\mathcal{V}q(\mathbf{x},t) = \int\limits_{\Sigma} E(\mathbf{x}-\mathbf{y},t-\tau)q(\mathbf{y},\tau)\,d\Sigma_{y,\tau}, \quad (\mathbf{x},t) \in \Sigma,$$

where the heat kernel is

$$E(\mathbf{x}-\mathbf{y},t-\tau) = \begin{cases} \frac{1}{(4\pi(t-\tau))^{d/2}} \exp\left(-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}\right), & t > \tau, \\ 0, & t \leq \tau. \end{cases}$$

There are two choices for the construction of finite element spaces for the Galerkin discretization

(1) A tensor product of a finite element space on the boundary surface and a finite element space on the time interval.
(2) A space of piecewise polynomials on a triangulation of $\Sigma$. Since a parabolic PDE has a time and space variables, the triangulation consists of triangles in two, and tetrahedra in three spatial dimensions.

The first choice is easier to implement and has been analyzed in [1]. The second choice has received some recent interest [2] and enables space-time adaptivity and moving geometries with changes of topology. In either case, the numerical realization of Galerkin method involves computing possibly singular integrals. In the context of layer potentials for elliptic operators it is well known how to obtain singularity removing transformations which lead to efficient quadrature rules [4]. For parabolic operators discretized with tensor product meshes a similar methodology was developed in [3].

The goal of this work is to introduce these transformations for the case of a triangulation of $\Sigma$. If $\Sigma_x, \Sigma_y$ are two patches on the space-time boundary, then the task is to compute integrals of the form

$$I = \int_{\Sigma_x} \int_{\Sigma_y} E(\mathbf{x}-\mathbf{y},t-\tau)\psi(\mathbf{x},\mathbf{y},t,\tau)\,d\Sigma_{y,\tau}\,d\Sigma_{x,t}\,. \tag{1}$$

Here $\psi(\mathbf{x},\mathbf{y},t,\tau)$ is a smooth function that incorporates contributions of the shape functions and the kernel has singularities if $\Sigma_x$ and $\Sigma_y$ coincide, have a common vertex, edge or, in the case of three spatial dimensions, have a common face.

The patches $\Sigma_x$ and $\Sigma_y$ can be parametrized by the standard simplex

$$\sigma^{(n)} = \{\,\widehat{\mathbf{x}} : 0 \leq \widehat{x}_n \leq \cdots \leq \widehat{x}_1 \leq 1\}$$

using an affine transformation. Thus integral (1) becomes

$$I = \int_{\sigma^{(n)}} \int_{\sigma^{(n)}} k(\widehat{\mathbf{x}}, \widehat{\mathbf{y}})\, d\widehat{\mathbf{y}}\, d\widehat{\mathbf{x}}. \tag{2}$$

The integration domain $\sigma^{(n)} \times \sigma^{(n)}$ is a complex polytope in $2n$ dimension which is the convex hull of the vertices

$$\mathbf{e}_{i,j} = \begin{bmatrix} \mathbf{e}_i \\ \mathbf{e}_j \end{bmatrix}, \quad i, j \in \{0, \dots, n\},$$

where the $\mathbf{e}_i$'s denote the vertices of the standard simplex $\sigma^{(n)}$

$$\mathbf{e}_0 = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \mathbf{e}_2 = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 0 \end{bmatrix} \dots \mathbf{e}_n = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}.$$

The polytope $\sigma^{(n)} \times \sigma^{(n)}$ is then divided into simplices in $\mathbb{R}^{2n}$ using the planes $x_1 = y_1, \dots, x_n = y_n$

$$\sigma^{(n)} \times \sigma^{(n)} = \bigcup_{k=1}^{N_n} S_k\,.$$

We obtain $N_2 = 6$ and $N_3 = 20$. The next step is to introduce the singular and non-singular variables. For two spatial dimensions ($n = 2$) we set

$$\begin{array}{lll} s = 2: & s = 3: & s = 4: \\ z_1' = y_1 - x_1, & z_1' = y_1 - x_1, & z_1' = x_1, \\ z_2' = y_2 - x_2, & z_2' = x_2, & z_2' = x_2, \\ \breve{z}_1 = x_1, & z_3' = y_2, & z_3' = x_1, \\ \breve{z}_2 = x_2, & \breve{z}_1 = x_1, & z_4' = x_2, \end{array}$$

depending on whether $\Sigma_x$ and $\Sigma_y$ are identical (s=2), have a common edge (s=3) or a common vertex (s=4). Here, $s$ is the number of singular variables. Proceeding analogously for three spatial dimensions implies that the number of singular variables is $s \in \{3, 4, 5, 6\}$.

The simplices $S_k$ are again images of simplices in $\mathbf{z}$-coordinates, the latter simplices can be mapped by a second linear transformation to the standard simplex $\sigma^{(2n)}$. By construction, the singular variables are mapped on the $s$-dimensional standard simplex $\sigma^{(s)}$. The domain for the remaining variables is a simplex in $\mathbb{R}^{2n-s}$ whose vertices depend linearly on the singular variables. Since the latter variables do not enter the kernel, they only appear as polynomials and can be integrated analytically. Thus integral (2) appears as

$$I_k = \int_{\sigma^{(s)}} \frac{1}{\mathbf{b} \cdot \mathbf{w}'^{\frac{n}{2}}}\, E\left( \frac{|B\mathbf{w}'|}{\mathbf{b} \cdot \mathbf{w}'^{\frac{1}{2}}} \right) \psi(\mathbf{w}')\, d\mathbf{w}'. \tag{3}$$

where $\psi(\cdot)$ is a polynomial, and $B$ and $\mathbf{b}$ represent the coefficients of the transformation that maps $\mathbf{w}'$ to $\mathbf{x}-\mathbf{y}$ and $t-\tau$. This integral is singular at $\mathbf{w}'=0$ which suggests to use the Duffy-like transform

$$\mathbf{w}' = \begin{bmatrix} \xi^2 \\ \xi^2 \mathbf{w} \end{bmatrix} \quad \text{where } \mathbf{w} \in \sigma^{(s-1)},$$

which has Jacobian $\xi^{2s-1}$. Then

$$t-\tau = \mathbf{b}' \cdot \mathbf{w} = \xi^2 \left(b_0 + b_1 w_1 + \cdots + b_{s-1} w_{s-1}\right) := \xi^2 \beta(\mathbf{w}),$$

and integral (3) becomes

$$I_k = \int_0^1 \int_{\sigma^{(s-1)}} \frac{\xi^{2s-1-n}}{\beta(\mathbf{w})^{\frac{n}{2}}} E\left(\xi \frac{c(\mathbf{w})}{\beta(\mathbf{w})^{\frac{1}{2}}}\right) \psi(\xi^2 \mathbf{w})\, d\mathbf{w}\, d\xi. \tag{4}$$

Note that the smallest power of $\xi$ in the numerator occurs when $n=2$ and $s=2$. In this case $2s-1-n=1$, so the singularity at $\xi=0$ gets canceled by this power. However, this does not prove that the integrand will always be a smooth function. In particular, the integrand is singular when the quantity $t-\tau$ (and hence $\beta(\mathbf{w})$) changes signs when $\Sigma_x$ and $\Sigma_y$ overlap in the time variable.

Recall that the function $E(\cdot)$ is continued by zero when $\beta(\mathbf{w}) \le 0$, thus we have to integrate integral (4) only over the intersection of $\sigma^{(s-1)}$ with the half-space $H^+ = \{\mathbf{w} : \beta(\mathbf{w}) \ge 0\}$, i.e., the domain

$$T := \sigma^{(s-1)} \cap H^+.$$

We will now describe the geometry of $T$ in more detail. We set $d = s-1$ and re-name the vertices of $\sigma^{(d)}$ to $\mathbf{v}_i$ such that

$$\mathbf{v}_i \in H^+, \quad i \in \{0, \ldots, \widehat{d}\},$$
$$\mathbf{v}_{\widehat{d}+j} \in H^-, \quad j \in \{1, \ldots, \widetilde{d}\}.$$

Here, $H^-$ defines the complementary half-space. Since a simplex has an edge between any pair of vertices, there are intersection points $\mathbf{v}_{i,j}$ with the plane $H^0$ on the edges between $\mathbf{v}_i$ and $\mathbf{v}_{\widehat{d}+j}$. For convenience, we also denote the vertices $\mathbf{v}_i$ by $\mathbf{v}_{i,0}$. It is then easy to verify that the vertices of $T$ are the convex hull of the points $\mathbf{v}_{i,j}$, $i = 0 \ldots \widehat{d}$, $j = 0 \ldots \widetilde{d}$, which motivates us to define the transform

$$\mathbf{w} = \phi(\widehat{\mathbf{w}}, \widetilde{\mathbf{w}}) = \sum_{i,j} \mathbf{v}_{i,j}\, \phi_i(\widehat{\mathbf{w}}) \phi_j(\widetilde{\mathbf{w}}). \tag{5}$$

Here $\phi_i$ denote the linear Lagrange polynomials of the standard simplex, i.e., $\phi_i(\mathbf{e}_j) = \delta_{i,j}$. Since $0 \le \phi_i \le 1$ and $\sum_i \phi_i = 1$ it follows that $\phi$ maps $\sigma^{(\widehat{d})} \times \sigma^{(\widetilde{d})}$ into $T$. The following result states that the map $\phi$ is also onto.

**Theorem 1.** *If the plane $H^0$ does not contain any of the vertices of $\sigma^{(d)}$ then $T$ is combinatorially equivalent to $\sigma^{(\widehat{d})} \times \sigma^{(\widetilde{d})}$ and equation* (5) *defines a bijective map between $\sigma^{(\widehat{d})} \times \sigma^{(\widetilde{d})}$ and $T$.*

We do not give a careful proof of this result here. We only mention that the idea is to arrange the vertices $\mathbf{e}_{i,j}$ in and $\mathbf{v}_{i,j}$ into two rectangular arrays. The faces of each polytope are obtained by canceling rows and columns from the array. Thus there is a one-to-one correspondence of all faces. Further, beginning with the lowest-dimension, we see that $\phi$ in (5) maps bijectively between the corresponding faces.

Returning to the affine function $\beta(\mathbf{w})$, we see that

$$\beta(\mathbf{w}) = \sum_{i,j} \beta(\mathbf{v}_{i,j})\phi_i(\widehat{\mathbf{w}})\phi_j(\widetilde{\mathbf{w}}) = \sum_i \beta(\mathbf{v}_{i,0})\phi_i(\widehat{\mathbf{w}})(1-\widetilde{w}_1)$$

Here, the last step follows from the fact that $\beta$ vanishes on the vertices on $H^0$ and that $\phi_0(\widetilde{\mathbf{w}}) = 1 - \widetilde{w}_1$. Now introduce another Duffy transform

$$\widetilde{\mathbf{w}} = \begin{bmatrix} 1-\zeta \\ (1-\zeta)\breve{\mathbf{w}} \end{bmatrix} \quad \text{where } \breve{\mathbf{w}} \in \sigma^{(\tilde{d}-1)}.$$

Thus $\zeta = 1 - \widetilde{w}_1$ and integral(4) becomes

$$I_k = \int_0^1 \int_0^1 \int_{\sigma^{(\hat{d})}} \int_{\sigma^{(\tilde{d}-1)}} \frac{\xi}{\zeta} E\left(\frac{\xi}{\zeta}\psi_1(\zeta, \widehat{\mathbf{w}}, \breve{\mathbf{w}})\right) \psi_2\left(\xi, \zeta, \widehat{\mathbf{w}}, \breve{\mathbf{w}}\right)\, d\widehat{\mathbf{w}} d\breve{\mathbf{w}}\, d\zeta d\xi$$

where $\psi_1 > 0$ is smooth and $\psi_2$ is a polynomial. To handle the ratio $\xi/\zeta$ we introduce the following two transform which map $(\lambda, \mu) \in [0,1]^2$ to two triangles in the $(\xi, \zeta)$ plane which add up to $[0,1]^2$,

$$(a) \begin{bmatrix} \xi \\ \zeta \end{bmatrix} = \begin{bmatrix} \lambda\mu \\ \lambda \end{bmatrix}, \quad \text{and} \quad (b) \begin{bmatrix} \xi \\ \zeta \end{bmatrix} = \begin{bmatrix} \lambda \\ \lambda\mu \end{bmatrix}$$

Since the Jacobian contributes an additional factor of $\lambda$ we find that $I_k$ is the sum of

$$I_k^{(a)} = \int_0^1 \int_0^1 \int_{\sigma^{(\hat{d})}} \int_{\sigma^{(\tilde{d}-1)}} E\Big(\mu\psi_1\left(\lambda, \mu, \widehat{\mathbf{w}}, \breve{\mathbf{w}}\right)\Big)\psi_2\left(\lambda, \mu, \widehat{\mathbf{w}}, \breve{\mathbf{w}}\right)\, d\widehat{\mathbf{w}} d\breve{\mathbf{w}}\, d\lambda d\mu$$

$$I_k^{(b)} = \int_0^1 \int_0^1 \int_{\sigma^{(\hat{d})}} \int_{\sigma^{(\tilde{d}-1)}} \frac{1}{\mu} E\left(\frac{1}{\mu}\psi_1\left(\lambda, \mu, \widehat{\mathbf{w}}, \breve{\mathbf{w}}\right)\right) \psi_2\left(\lambda, \mu, \widehat{\mathbf{w}}, \breve{\mathbf{w}}\right)\, d\widehat{\mathbf{w}} d\breve{\mathbf{w}}\, d\lambda d\mu$$

These integrands are smooth and can be treated using standard quadrature rules.

## References

[1] M. Costabel, *Boundary integral operators for the heat equation* Integral Equations Operator Theory, **13**, (1990) 498-552

[2] S. Dohr, J. Zapletal, G. Of, M. Merta and M. Kravenko, *A parallel space time boundary element method for the heat equation* Comput. Math. Appl., **77** (2019), 2852-2866

[3] N. Mason and J. Tausch, *Quadrature for parabolic Galerkin BEM with moving surfaces* Comput. Math. Appl., **78** (2019), 1-14

[4] S. Sauter and C. Schwab, *Randelementmethoden: Analyse, Numerik und Implementierung schneller Algorithmen*, Teubner, Stuttgart, 2004

*Reporter: Ralf Hiptmair*