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New integral equation approach to solution of diffusion equation[1]

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The paper concerns the theoretical derivation of a new formulation for solution of the initial-boundary value problems for the diffusion equation. The global and local integral equations are derived by using the fundamental solution for the Laplace differential operator. Assuming certain approximations with respect to spatial variable, we obtain a set of the ordinary differential equations (ODE) with continuous time variable. Standard methods for the time integration can be applied to these ODEs. Besides a review of the one step θ-method we propose a new integral equation method for solution of a set of linear ODEs. The paper deals also with the numerical implementation of the global and local integral equations yielding the ODEs.

1. Introduction

A large amount of physical processes is governed by the diffusion equation that is the partial differential equation (PDE) of the parabolic type. Because of the first order derivative with respect to time and the second order with respect to spatial coordinates one has to solve an initial/boundary-value problem with a prescribed initial value of the sought solution throughout the whole domain Ω and prescribed boundary values of certain physical quantities on the boundary Γ. Owing to the complexity of the geometrical shape as well as the prescribed initial and boundary conditions in engineering practice, one is confined to numerical computational methods almost exclusively.

Before the great expansion of the Finite Element Method (FEM) the Finite Difference Method (FDM) was employed frequently. Application of the discretization and approximation to spatial variation of the sought solution leads to the semidiscrete diffusion equation which is given by a set of the ordinary differential equations (ODE) for the spatial nodal values with leaving the time variable to be continuous [4]. The initial problems for the ordinary differential equations are often solved numerically by using the so-called one step θ-method including the forward (explicit) and backward (implicit) Euler methods as well as the Crank–Nicolson (midpoint) method. Rather an oposite order of the treatment of the time and spatial variations is assumed in the formulation for solution by boundary integral equations [1, 3]. Sometimes the time variable is eliminated by using the Laplace (and/or Fourier) transform or assuming the finite difference approximation for the time variation. Then, the PDE of the parabolic type is converted to that of elliptic type with the initial condition playing the role of an additional domain source. Standard BEM approaches are applicable to solution of the relevant boundary value problems. Another Boundary Integral

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Equation (BIE) formulation is available when the time dependent fundamental solution is used together with approximating the time variation polynomially within finite time steps. Then, two approaches can be distinguished according to the choice of the origin of the time integration [3]. The advantages of the BIE formulations consist in the localization of unknowns on the boundary (in each time step at least), in better conditioning of the set of algebraic equations and higher accuracy possibility. On the other hand, one can name also certain disadvantages such as the necessity of inverse transformations to time variable, or integration of matrix coefficients at different time instants or alternatively evaluation of "initial" values (throughout the whole domain) at different time instants.

In this paper, we present the integral equation formulation leading to a set of ODEs with respect to time and preserving the better conditioning as compared with the FEM formulation. On the other hand, the method is as general as the FEM. The nodal unknowns are spread throughout the whole domain including the boundary with the spatial approximation either by interpolation polynomials within finite size boundary elements and domain cells or by the Moving Least Square (MLS)-approximation within the meshless implementation. A special attention is devoted to the treatment of singularities. Finally, a new method is developed for solution of the set of the ordinary differential equations.

2. Governing equation, integral representations

Let us consider the time-dependent boundary value problem for diffusion equation

$$\nabla^2 u(x,t) - \frac{1}{k}\frac{\partial u}{\partial t}(x,t) = f(x,t) \qquad \text{in } \Omega \tag{1}$$

with the prescribed boundary conditions (on $\Gamma = \Gamma_D \cup \Gamma_N$ with $\Gamma_D \cap \Gamma_N = \emptyset$)

$$\begin{aligned} u(\eta,t) &= \tilde{u}(\eta,t) && \text{on } \Gamma_D\,, \\ \frac{\partial u}{\partial n}(\eta,t) &= \frac{\partial \tilde{u}}{\partial n}(\eta,t) && \text{on } \Gamma_N\,, \end{aligned} \tag{2}$$

and the initial condition

$$u(x,0) = u_0(x) \qquad \text{in } \Omega. \tag{3}$$

Obviously, one can recast Eq. (1) into the integral identity

$$\int_{\Omega'} \left(\nabla^2 u(x,t) - \frac{1}{k}\frac{\partial u}{\partial t}(x,t) \right) v^*(x-y)\, \mathrm{d}\Omega(x) = \int_{\Omega'} f(x,t) v^*(x-y)\, \mathrm{d}\Omega(x), \tag{4}$$

in which $\Omega' \subseteq \Omega$. Assuming $v^*(r)$ to be the fundamental solution of the Laplace operator and making use of the Gauss divergence theorem, one obtains from Eq. (4)

$$\begin{aligned} \Delta(y) u(y,t) + \int_{\Gamma'} \left[\frac{\partial u}{\partial n}(\eta,t)\, v^*(\eta - y) - u(\eta,t) \frac{\partial v^*(\eta - y)}{\partial n(\eta)} \right] \mathrm{d}\Gamma(\eta) \\ - \frac{1}{k}\int_{\Omega'} \frac{\partial u}{\partial t}(x,t)\, v^*(x-y)\, \mathrm{d}\Omega(x) = \int_{\Omega'} f(x,t)\, v^*(x-y)\, \mathrm{d}\Omega(x), \end{aligned} \tag{5}$$

where $y \notin \Gamma'$ and $\Delta(y)$ is defined as

$$\Delta(y) = \begin{cases} 1 & y \in \Omega', \\ 0 & y \notin \Omega' \cup \Gamma'. \end{cases}$$

Note that in this concept, the potential field $u(y,t)$ is represented integrally not only in terms of the boundary densities $u(\eta,t)$ and $\partial u(\eta,t)/\partial n$ but also in terms of the domain density of the potential velocity $\dot{u}(x,t)$.

3. Polynomial interpolation of the spatial variation of the potential within finite size elements

In a numerical treatment, it is reasonable to divide the domains of unknowns into finite size elements with assuming a polynomial interpolation within such elements. Then, the number of degrees of freedom is reduced from infinite to a finite number N, because the unknowns are localized at nodal points employed in the definition of the approximation over the elements. Thus, the problem of the evolution of the potential field is converted to the problem of the time-evolution of the nodal values of the potential field, because the spatial distribution of the potential field at any time instant is approximated within the boundary and domain element, respectively, by

$$\begin{aligned} u(\eta,t)|_{\Gamma_p\subset\Gamma_N} &= \sum_{a=1}^{3} u(\eta^{ap},t)\,N^a(\xi), \\ u(x,t)|_{\Omega_e} &= \sum_{a=1}^{8} u(x^{ae},t)\,N^a(\xi_1,\xi_2). \end{aligned} \tag{6}$$

Since the unknowns are spread throughout the whole domain Ω (they are not localized on the boundary alone), the unknown normal derivative of the potential along $\Gamma_p \subset \Gamma_D$ and/or L_e^c(where L_e^c is an arbitrary contour in Ω_e) can be expressed by using gradients of the approximated potential on Ω_e as

$$\begin{aligned} \frac{\partial u}{\partial n}(\eta,t)\bigg|_{\Gamma_p\subset\Omega_e} &= \sum_{a=1}^{8} u(x^{ae},t)\,M^{aep}(\xi), \\ \frac{\partial u}{\partial n}(x,t)\bigg|_{L_e^c} &= \frac{1}{h^e(\varphi)}\sum_{a=1}^{8} u(x^{ae},t)\,K^{aec}(\varphi). \end{aligned} \tag{7}$$

Note that $M^{aep}(\xi)$, $K^{aec}(\varphi)$ and $h^e(\varphi)$ are geometry dependent polynomials, and their expressions given in Appendix A are obtained by using the isoparametric elements for approximation of both the geometry and physical fields.

Recall that boundary conditions prescribe certain nodal values in Eq. (7) as long as $x^{ae} \in \Gamma_D$. In other words, having known the time-evolution of the potential at the nodal points on Γ_D as well as at interior of Ω, we can use the integral representation (5) supplemented with the approximation of the spatial variation of the boundary and/or domain densities by Eqs. (6) and (7).

In order to get a relevant set of equations for computation of the time-evolution of unknown nodal values, one can use the global as well as local integral equations (IE) resulting from Eq. (5). Assuming $\Omega' = \Omega$, $\Gamma' = \Gamma = \Gamma_D \cup \Gamma_N$ and collocating Eq. (5) at the boundary nodes $\zeta^b \in \Gamma - \Gamma_D$, with $b = 1, 2, \ldots, m$, we obtain the global integral equation (GIE)

$$\begin{aligned} &u(\zeta^b,t)\int_{\Gamma_D}\frac{\partial v^*(\eta-\zeta^b)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta) + \int_{\Gamma_N}\Big[u(\zeta^b,t)-u(\eta,t)\Big]\frac{\partial v^*(\eta-\zeta^b)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta) \\ &\quad + \int_{\Gamma_D}\frac{\partial u}{\partial n}(\eta,t)\,v^*(\eta-\zeta^b)\,\mathrm{d}\Gamma(\eta) - \frac{1}{k}\int_{\Omega}\frac{\partial u}{\partial t}(x,t)\,v^*(x-\zeta^b)\,\mathrm{d}\Omega(x) \\ &\qquad = \int_{\Omega} f(x,t)\,v^*(x-\zeta^b)\,\mathrm{d}\Omega(x) + \int_{\Gamma_D}\tilde{u}(\eta,t)\frac{\partial v^*(\eta-\zeta^b)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta) \\ &\qquad\quad - \int_{\Gamma_N}\frac{\partial \tilde{u}}{\partial n}(\eta,t)\,v^*(\eta-\zeta^b)\,\mathrm{d}\Gamma(\eta). \end{aligned} \tag{8}$$

Subtraction and addition technique [7] has been utilized for regularization of the strongly singular integral over Γ_N.

Surrounding each interior point y^c $(c = 1, 2, \ldots, N-m)$ by a finite domain $\Omega^c \subset \Omega$, we may write the local integral equation (LIE) as

$$u(y^c,t) + \int_{L^c} \left[\frac{\partial u}{\partial n}(\eta,t)\, w^*(\eta - y^c) - u(\eta,t)\, \frac{\partial w^*(\eta - y^c)}{\partial n(\eta)} \right] \mathrm{d}\Gamma(\eta)$$

$$- \frac{1}{k} \int_{\Omega^c} \frac{\partial u}{\partial t}(x,t)\, w^*(x - y^c)\, \mathrm{d}\Omega(x) = \int_{\Omega^c} f(x,t)\, w^*(x - y^c)\, \mathrm{d}\Omega(x), \tag{9}$$

where $L^c$is the boundary of the sub-domain Ω^c, and $w^*(r)$ is the fundamental solution differing form $v^*(r)$ by an additional constant. This LIE is non-singular in contrast to the GIE. Note that it is inappropriate to select L^c as a circle in the global coordinate space as long as the potential is approximated by interpolation within finite size elements. Then, it is more appropriate to consider L^c as a closed contour given as the union of the curved lines corresponding to circular arcs considered at the intrinsic spaces of the domain elements adjacent to y^c. The circular arcs are centred at y^c with the radius ξ_0. Modelling of geometry for Ω^c and L^c is given in Appendix A.

Applying the discretization procedure to Eq. (8), we obtain the set of the ordinary differential equations,

$$u(\zeta^b,t) \sum_{\substack{p \\ \zeta^b \notin \Gamma_p}} \tilde{W}^{pb} - \sum_{\substack{p \\ \Gamma_p \subset \Gamma_N}} \sum_{a=1}^{3} u(\eta^{ap},t)\, W^{apb} + \sum_{\substack{p \\ \Gamma_p \subset \Gamma_D}} \sum_{\substack{e \\ \Gamma_p \subset \Omega_e}} \sum_{\substack{a=1 \\ x^{ae} \notin \Gamma_p}}^{8} u(x^{ae},t)\, V^{aepb}$$

$$- \sum_{e} \sum_{\substack{a=1 \\ x^{ae} \notin \Gamma_D}}^{8} \frac{\partial u}{\partial t}(x^{ae},t)\, Y^{aeb} = \bar{F}^b(t), \tag{10}$$

with

$$\tilde{W}^{pb} = \sum_{a=1}^{3} W^{apb} \qquad \text{(note that } \zeta^b \notin \Gamma_p\text{)},$$

$$W^{apb} = \begin{cases} \displaystyle\int_{-1}^{1} N^a(\xi)\, \frac{1}{2\pi}\, \frac{\eta_i^p(\xi) - \zeta_i^b}{|\eta^p(\xi) - \zeta^b|^2}\, \varepsilon_{ik3} h_k^p(\xi)\, \mathrm{d}\xi, & \zeta^b \notin \Gamma_p, \\ \displaystyle\int_{-1}^{1} \left[N^a(\xi) - N^a(\xi^{bp}) \right] \frac{1}{2\pi}\, \frac{\eta_i^p(\xi) - \zeta_i^b}{|\eta^p(\xi) - \zeta^b|^2}\, \varepsilon_{ik3} h_k^p(\xi)\, \mathrm{d}\xi, & \zeta^b \in \Gamma_p, \end{cases}$$

$\eta_i^p(\xi) = \eta_i|_{\Gamma_p}$, ξ^{bp} – intrinsic coordinate of ζ^b on Γ_p,

$$V^{aepb} = \int_{-1}^{1} M^{aep}(\xi)\, \frac{1}{2\pi} \ln|\eta^p(\xi) - \zeta^b|\, h^p(\xi)\, \mathrm{d}\xi,$$

$$Y^{aeb} = \frac{1}{2\pi k} \int_{-1}^{1} \int_{-1}^{1} N^a(\xi_1, \xi_2) \ln|x^e(\xi_1, \xi_2) - \zeta^b|\, J^e(\xi_1, \xi_2)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2, \tag{11}$$

$$\bar{F}^b(t) = \sum_{e} \frac{1}{2\pi} \int_{-1}^{1} \int_{-1}^{1} f(x^e(\xi_1, \xi_2), t) \ln|x^e(\xi_1, \xi_2) - \zeta^b|\, J^e(\xi_1, \xi_2)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2$$

$$+ \sum_{\substack{p \\ \Gamma_p \subset \Gamma_D}} \frac{1}{2\pi} \int_{-1}^{1} \tilde{u}(\eta^p(\xi), t)\, \frac{\eta_i^p(\xi) - \zeta_i^b}{|\eta^p(\xi) - \zeta^b|^2}\, \varepsilon_{ik3} h_k^p(\xi)\, \mathrm{d}\xi$$

$$- \sum_{\substack{p \\ \Gamma_p \subset \Gamma_N}} \frac{1}{2\pi} \int_{-1}^{1} \frac{\partial \tilde{u}}{\partial n}(\eta^p(\xi), t) \ln|\eta^p(\xi) - \zeta^b|\, h^p(\xi)\, \mathrm{d}\xi$$

$$- \sum_{\substack{p \\ \Gamma_p \subset \Gamma_D}} \sum_{\substack{e \\ \Gamma_p \subset \Omega_e}} \sum_{\substack{a=1 \\ x^{ae} \in \Gamma_p}}^{8} \tilde{u}(x^{ae},t)\, V^{aepb} + \sum_{e} \sum_{\substack{a=1 \\ x^{ae} \in \Gamma_D}}^{8} \frac{\partial \tilde{u}}{\partial t}(x^{ae},t)\, Y^{aeb}.$$

Similarly, one can discretize also the LIE given by Eq. (9) with the result

$$u(y^c,t)+\sum_{\substack{e\\ y^c\in\Omega_e}}\sum_{\substack{a=1\\ x^{ae}\notin\Gamma_D}}^{8}\left(u(x^{ae},t)Z^{aec}-\frac{\partial u}{\partial t}(x^{ae},t)\,T^{aec}\right)=\tilde{F}^c(t), \tag{12}$$

where

$$Z^{aec} = \frac{1}{2\pi}\int_{\varphi_1^{ce}}^{\varphi_2^{ce}}\left[K^{aec}(\varphi)\,\ln\left(\frac{R^e}{r_0}\right)-N^a\left(\vec{\xi}^{ce}(\xi_0\,,\,\varphi)\right)\varepsilon_{ik3}h_k^e(\varphi)\,\frac{R_i^e}{(R^e)^2}\right]\mathrm{d}\varphi\,,$$

$$R_j^e = x_j|_{L_e^c}-y_j^c=\sum_{a=1}^{8}x_j^{ae}\left[N\left(\vec{\xi}^{ce}(\xi_0\,,\,\varphi)\right)-N^a(\xi_1^{ce},\xi_2^{ce})\right],\qquad (R^e)^2=R_k^eR_k^e\,,$$

$$T^{aec} = \frac{1}{2\pi k}\int_0^{\xi_0}\int_{\varphi_1^{ce}}^{\varphi_2^{ce}}N^a\left(\vec{\xi}^{ce}(\rho,\varphi)\right)\ln\left(\frac{r^e}{r_0}\right)J^{ce}(\rho,\varphi)\,\rho\,\mathrm{d}\varphi\mathrm{d}\rho\,, \tag{13}$$

$$\tilde{F}^c(t) = \sum_{\substack{e\\ y^c\in\Omega_e}}\frac{1}{2\pi}\int_0^{\xi_0}\int_{\varphi_1^{ce}}^{\varphi_2^{ce}}f(\tilde{x}^{ec},t)\,\ln\left(\frac{r^e}{r_0}\right)J^{ce}(\rho,\varphi)\,\rho\,\mathrm{d}\varphi\mathrm{d}\rho$$

$$-\sum_{\substack{e\\ y^c\in\Omega_e}}\sum_{\substack{a=1\\ x^{ae}\in\Gamma_D}}^{8}\left(\tilde{u}(x^{ae},t)\,Z^{aec}-\frac{\partial\tilde{u}}{\partial t}(x^{ae},t)\,T^{aec}\right).$$

Now, the discretized GIE and LIE can be written in matrix form as

$$\sum_{n=1}^{N}\left[u(x^n,t)\,K^{bn}-\frac{\partial u}{\partial t}(x^n,t)\,M^{bn}\right]=F^b(t)\qquad(b=1,2,\ldots,N) \tag{14}$$

with the conductivity (stiffness) and capacity (mass) matrices

$$K^{bn} = \delta_{bn}\sum_{\substack{p\\ \zeta^b\notin\Gamma_p}}\tilde{W}^{pb}-\sum_{\substack{p\\ \Gamma_p\subset\Gamma_N}}\sum_{\substack{a=1\\ (ap)=n}}^{3}W^{apb}+\sum_{\substack{p\\ \Gamma_p\subset\Gamma_D}}\sum_{\substack{e\\ \Gamma_p\subset\Omega_e}}\sum_{\substack{a=1\\ x^{ae}\notin\Gamma_p\\ (ae)=n}}^{8}V^{aepb}\qquad(b=1,2,\ldots,m),$$

$$M^{bn} = \sum_{e}\sum_{\substack{a=1\\ x^{ae}\notin\Gamma_D\\ (ae)=n}}^{8}Y^{aeb}\qquad(b=1,2,\ldots,m),$$

$$K^{bn} = \delta_{n(m+c)}+\sum_{\substack{e\\ y^c\in\Omega_e}}\sum_{\substack{a=1\\ x^{ae}\notin\Gamma_D\\ (ae)=n}}^{8}Z^{aec}\qquad(b=m+c\ \wedge\ c=1,2,\ldots,N-m), \tag{15}$$

$$M^{bn} = \sum_{\substack{e\\ y^c\in\Omega_e}}\sum_{\substack{a=1\\ x^{ae}\notin\Gamma_D\\ (ae)=n}}^{8}T^{aec}\qquad(b=m+c\ \wedge\ c=1,2,\ldots,N-m),$$

in which (ap) and (ae) stand for the global numbers of the nodal points $\eta^{ap}\in\Gamma_p$ and $x^{ae}\in\Omega_e$, respectively. The r.h.s. in Eq. (15) is given as

$$F^b(t)=\begin{cases}\bar{F}^b(t)\,, & b=1,2,\ldots,m,\\ \tilde{F}^c(t)\,, & b=m+c\ \wedge\ c=1,2,\ldots,N-m.\end{cases} \tag{16}$$

The final step in computation of the time-evolution of nodal values of the potential is the solution of the system of linear ordinary differential equations given by Eq. (14) with the inital condition $u(x^n,0)=u_o(x^n)$.

4. MLS-APPROXIMATION OF THE SPATIAL VARIATION OF THE POTENTIAL

Without going into details, we present some basic formulae employed in the MLS-approximations. For more details we refer the reader to [2]. Assuming the MLS-approximation of the spatial variation of the time-dependent potential field at any time instant (separation of the time and spatial variables), we may write the approximated field as

$$u(x,t) \approx u^h(x,t) = \sum_{a=1}^{N} H(w_a(x))\, \hat{u}^a(t)\, \phi^a(x), \tag{17}$$

where N is the total number of nodal points and $H(z)$ is the Heaviside unit step function. The Gaussian distribution around x^a is employed most frequently for weight functions $w_a(x)$. The other possibility is to use spline weights [2] for instance. Recall that

$$u(x^a) \neq \hat{u}^a, \qquad u^h(x^a) \neq \hat{u}^a,$$

and the number of nodal points n_x which are effective for approximation at the point$x$ is less or equal to the total number of nodal points, since

$$n_x = \sum_{a=1}^{N} H(w_a(x)).$$

The domain of the definition of the MLS-approximation at the point x is defined as

$$\Omega_x = \left\{ \forall x' \in \Omega;\ \ H(w_a(x')) = H(w_a(x)),\ \ a = 1,2,\ldots,N \right\}.$$

The shape function $\phi^a(x)$ is given by

$$\phi^a(x) = \sum_{\beta=1}^{\mu} p_\beta(x) \left[A^{-1}(x)B(x)\right]_{\beta a} = \sum_{\alpha,\beta=1}^{\mu} p_\beta(x)\, A^{-1}_{\beta\alpha}(x)\, B_{\alpha a}(x), \tag{18}$$

where $\{p_\alpha(x)\}_{\alpha=1}^{\mu}$ is a complete monomial basis of order μ and the matrices $\mathbf{A}$ and $\mathbf{B}$ are given as

$$A_{\alpha\beta}(x) = \sum_{a=1}^{N} w_a(x)\, p_\alpha(x^a)\, p_\beta(x^a),$$

$$B_{\beta a}(x) = p_\beta(x^a)\, w_a(x), \qquad \alpha,\beta = 1,2,\ldots,\mu; \quad a = 1,2,\ldots,N.$$

The gradients of the approximated field within Ω_x can be replaced by

$$u^h_{,k}(x) = \sum_{a=1}^{N} H(w_a(x))\, \hat{u}^a\, \phi^a_{,k}(x), \tag{19}$$

where the gradients of the shape functions within Ω_x are given as

$$\phi^a_{,k}(x) = \sum_{\alpha,\beta=1}^{\mu} \left[p_{\beta,k}(x)\, A^{-1}_{\beta\alpha}(x)\, B_{\alpha a}(x) + p_\beta(x) \left(A^{-1}_{\beta\alpha,k}(x)\, B_{\alpha a}(x) + A^{-1}_{\beta\alpha}(x)\, B_{\alpha a,k}(x) \right) \right],$$

with $A^{-1}_{\beta\lambda,k}(x) = -A^{-1}_{\beta\alpha}(x)\, A_{\alpha\gamma,k}(x)\, A^{-1}_{\gamma\lambda}(x)$.

It can be seen that this approximation is in the global coordinate system. The geometry of the whole domain and its boundary, however, is approximated usually in terms of intrinsic coordinates defined on finite size elements as considered in the Appendix A. Then, the global coordinates of any point on Γ and/or in Ω are given by Eqs. (A1) and (A4). The time-evolution of the potential field

is transferred to the time-evolution of the nodal unknowns $\hat{u}^a$, which are non-physical quantities. Therefore $\hat{u}^a$ is not prescribed at any nodal point and Eq. (5) should be collocated at each nodal point. In the case of the GIE collocated at boundary nodal points, one should be careful in the treatment of the boundary integrals involving strongly singular kernels. Note that the subtraction technique is not effective in the case of MLS-approximation and we have to use the limit form of the integral equations [6]. The GIE collocated at $\zeta^b \in \Gamma - \Gamma_D$ can be written as

$$
\begin{aligned}
&u(\zeta^b,t) + \int_{\Gamma_D} \frac{\partial u}{\partial n}(\eta,t)\, v^*(\eta-\zeta^b)\,\mathrm{d}\Gamma(\eta) - \lim_{z\to\zeta^b}\int_{\Gamma_N} u(\eta,t)\,\frac{\partial v^*(\eta-z)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta)\\
&\quad - \frac{1}{k}\int_\Omega \frac{\partial u}{\partial t}(x,t)\, v^*(x-\zeta^b)\,\mathrm{d}\Omega(x) = \int_\Omega f(x,t)\, v^*(x-\zeta^b)\,\mathrm{d}\Omega(x)\\
&\quad + \int_{\Gamma_D} \tilde{u}(\eta,t)\,\frac{\partial v^*(\eta-\zeta^b)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta) - \int_{\Gamma_N} \frac{\partial \tilde{u}}{\partial n}(\eta,t)\, v^*(\eta-\zeta^b)\,\mathrm{d}\Gamma(\eta),
\end{aligned}
\tag{20}
$$

while for $\zeta^b \in \Gamma_D$, the GIE becomes

$$
\begin{aligned}
&\int_{\Gamma_D} \frac{\partial u}{\partial n}(\eta,t)\, v^*(\eta-\zeta^b)\,\mathrm{d}\Gamma(\eta) - \int_{\Gamma_N-\Gamma_{N_s}} u(\eta,t)\,\frac{\partial v^*(\eta-\zeta^b)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta)\\
&\quad - \lim_{z\to\zeta^b}\int_{\Gamma_{N_s}} u(\eta,t)\frac{\partial v^*(\eta-z)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta) - \frac{1}{k}\int_\Omega \frac{\partial u}{\partial t}(x,t)\, v^*(x-\zeta^b)\,\mathrm{d}\Omega(x)\\
&\quad = -u(\zeta^b,t) + \int_\Omega f(x,t)\, v^*(x-\zeta^b)\,\mathrm{d}\Omega(x) + \lim_{z\to\zeta^b}\int_{\Gamma_D} \tilde{u}(\eta,t)\,\frac{\partial v^*(\eta-z)}{\partial n(\eta)}\,\mathrm{d}\Gamma(\eta)\\
&\quad - \int_{\Gamma_N} \frac{\partial \tilde{u}}{\partial n}(\eta,t)\, v^*(\eta-\zeta^b)\,\mathrm{d}\Gamma(\eta).
\end{aligned}
\tag{21}
$$

Recall that $\Gamma_{N_s} = \{\emptyset\}$ if $\zeta^b \notin \Gamma_N$, and Γ_{N_s} is a finite part of Γ_N with $\zeta^b \in \Gamma_{N_s}$, if $\zeta^b = \Gamma_D \cap \Gamma_N$. In order to perform the integrations in Eqs. (20) and (21), the geometry can be modelled by quadratic approximation over finite size elements as shown in Appendix A.

On the other hand, in the case of the LIE there is no problem with singularities and its form by Eq. (9) is appropriate also for implementation by using the MLS-approximation of the spatial variation of the potential. Now, in contrast to the implementation based on the approximation of the potential by interpolation within finite size elements, the spatial integration is performed in the global coordinate space, since the approximation of the spatial variation as well as geometry modelling are considered in the global space. Bearing in mind Section A.4, the discretization of the LIE results in the system of ordinary differential equations

$$
\sum_{a=1}^{N}\left[\hat{u}^a(t)\hat{K}^{ba} - \frac{\mathrm{d}\hat{u}^a(t)}{\mathrm{d}t}\,\hat{M}^{ba}\right] = \hat{F}^b(t),
\tag{22}
$$

in which $b = m+1,\ldots,N$, and

$$
\begin{aligned}
\hat{K}^{ba} &= H(w_a(y^c))\phi^a(y^c) - \frac{1}{2\pi}\int_0^{2\pi} H\left(w_a(x|_{L^c})\right)\phi^a\left(x|_{L^c}\right)\mathrm{d}\varphi,\\
\hat{M}^{ba} &= \frac{1}{2\pi k}\int_0^{r_0} \rho\ln\left(\frac{\rho}{r_0}\right)\int_0^{2\pi} H\left(w_a(x|_{\Omega^c})\right)\phi^a\left(x|_{\Omega^c}\right)\mathrm{d}\varphi\mathrm{d}\rho, \qquad c = b-m,\\
\hat{F}^b(t) &= \frac{1}{2\pi}\int_0^{r_0} \rho\ln\left(\frac{\rho}{r_0}\right)\int_0^{2\pi} f\left(x|_{\Omega^c},\, t\right)\mathrm{d}\varphi\mathrm{d}\rho.
\end{aligned}
\tag{23}
$$

In case of the GIE, the situation is rather more complicated, owing to singularities occurring in the limit forms of nearly-singular integrals. This problem can be solved successfully as shown

in Appendix B. The discretized GIE take the form given by Eq. (22) with $b = 1, 2, \ldots, m$ and the matrix coefficients are given as

$$\begin{aligned}
\hat{K}^{ba} &= \frac{\theta^b}{2\pi} H(w_a(\zeta^b))\phi^a(\zeta^b) + \frac{\varepsilon_{ik3}}{2\pi} \sum_{\substack{p \\ \Gamma_p \subset \Gamma_D}} \int_{-1}^{1} \ln|\eta^p(\xi) - \zeta^b|\, h_k^p(\xi)\, H(w_a(\eta^p(\xi)))\, \phi^a_{,i}(\eta^p(\xi))\, \mathrm{d}\xi \\
&\quad - \frac{1}{2\pi} \sum_{\substack{p \\ \zeta^b \in \Gamma_p \subset \Gamma_N}} E^p \int_{\xi_-^p}^{\xi_+^p} \frac{H\left(w_a(\eta^p(\xi_o^p + \rho))\right)}{d^p(\rho)}\, \phi^a(\eta^p(\xi_o^p + \rho))\, \mathrm{d}\rho \\
&\quad - \frac{\varepsilon_{ik3}}{2\pi} \sum_{\substack{p \\ \zeta^b \notin \Gamma_p \subset \Gamma_N}} \int_{-1}^{1} H\left(w_a(\eta^p(\xi))\right) \phi^a(\eta^p(\xi))\, \frac{\eta_i^p(\xi) - \zeta_i^b}{|\eta^p(\xi) - \zeta^b|^2}\, h_k^p(\xi)\, \mathrm{d}\xi, \\
\hat{M}^{ba} &= \frac{1}{2\pi k} \sum_e \int_{-1}^{1} \int_{-1}^{1} \ln\left|x^e(\xi_1, \xi_2) - \zeta^b\right| H\left(w_a\left(x^e(\xi_1, \xi_2)\right)\right) \phi^a(x^e(\xi_1, \xi_2))\, J^e(\xi_1, \xi_2)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2, \\
\hat{F}^b(t) &= \frac{1}{2\pi} \sum_e \int_{-1}^{1} \int_{-1}^{1} f(x^e(\xi_1, \xi_2), t)\, \ln\left|x^e(\xi_1, \xi_2) - \zeta^b\right| J^e(\xi_1, \xi_2)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \qquad (24) \\
&\quad + \frac{\varepsilon_{ik3}}{2\pi} \sum_{\substack{p \\ \Gamma_p \subset \Gamma_D}} \int_{-1}^{1} \tilde{u}(\eta^p(\xi), t)\, \frac{\eta_i^p(\xi) - \zeta_i^b}{|\eta^p(\xi) - \zeta^b|^2}\, h_k^p(\xi)\, \mathrm{d}\xi \\
&\quad - \frac{1}{2\pi} \sum_{\substack{p \\ \Gamma_p \subset \Gamma_N}} \int_{-1}^{1} \frac{\partial \tilde{u}}{\partial n}(\eta^p(\xi), t)\, \ln\left|\eta^p(\xi) - \zeta^b\right| h^p(\xi)\, \mathrm{d}\xi,
\end{aligned}$$

as long as $\zeta^b \in \Gamma - \Gamma_D$, while for $\zeta^b \in \Gamma_D$ we have

$$\begin{aligned}
\hat{K}^{ba} &= \frac{\varepsilon_{ik3}}{2\pi} \sum_{\substack{p \\ \Gamma_p \subset \Gamma_D}} \int_{-1}^{1} \ln\left|\eta^p(\xi) - \zeta^b\right| h_k^p(\xi)\, H(w_a(\eta^p(\xi)))\, \phi^a_{,i}(\eta^p(\xi))\, \mathrm{d}\xi \\
&\quad - \frac{\varepsilon_{ik3}}{2\pi} \sum_{\substack{p \\ \zeta^b \notin \Gamma_p \subset \Gamma_N}} \int_{-1}^{1} H\left(w_a(\eta^p(\xi))\right) \phi^a(\eta^p(\xi))\, \frac{\eta_i^p(\xi) - \zeta_i^b}{|\eta^p(\xi) - \zeta^b|^2}\, h_k^p(\xi)\, \mathrm{d}\xi \\
&\quad - \frac{1}{2\pi} \sum_{\substack{p \\ \zeta^b \in \Gamma_p \subset \Gamma_N}} E^p \int_{\xi_-^p}^{\xi_+^p} \frac{H\left(w_a(\eta^p(\xi_o^p + \rho))\right)}{d^p(\rho)}\, \phi^a(\eta^p(\xi_o^p + \rho))\, \mathrm{d}\rho, \\
\hat{M}^{ba} &= \frac{1}{2\pi k} \sum_e \int_{-1}^{1} \int_{-1}^{1} \ln\left|x^e(\xi_1, \xi_2) - \zeta^b\right| H\left(w_a(x^e(\xi_1, \xi_2))\right) \phi^a(x^e(\xi_1, \xi_2))\, J^e(\xi_1, \xi_2)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2, \\
\hat{F}^b(t) &= -\frac{\theta^b}{2\pi} \tilde{u}(\zeta^b, t) + \frac{1}{2\pi} \sum_e \int_{-1}^{1} \int_{-1}^{1} f\left(x^e(\xi_1, \xi_2), t\right) \ln\left|x^e(\xi_1, \xi_2) - \zeta^b\right| J^e(\xi_1, \xi_2)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2 \\
&\quad + \frac{1}{2\pi} \sum_{\substack{p \\ \zeta^b \in \Gamma_p \subset \Gamma_D}} E^p \int_{\xi_-^p}^{\xi_+^p} \frac{\tilde{u}(\eta^p(\xi_o^p + \rho), t)}{d^p(\rho)}\, \mathrm{d}\rho \qquad (25) \\
&\quad + \frac{\varepsilon_{ik3}}{2\pi} \sum_{\substack{p \\ \zeta^b \notin \Gamma_p \subset \Gamma_D}} \int_{-1}^{1} \tilde{u}(\eta^p(\xi), t)\, \frac{\eta_i^p(\xi) - \zeta_i^b}{|\eta^p(\xi) - \zeta^b|^2}\, h_k^p(\xi)\, \mathrm{d}\xi \\
&\quad - \frac{1}{2\pi} \sum_{\substack{p \\ \Gamma_p \subset \Gamma_N}} \int_{-1}^{1} \frac{\partial \tilde{u}}{\partial n}(\eta^p(\xi), t)\, \ln\left|\eta^p(\xi) - \zeta^b\right| h^p(\xi)\, \mathrm{d}\xi.
\end{aligned}$$

The initial conditions $\hat{u}^a(0) = \hat{u}_0^a$ can be deduced from the set of algebraic equations

$$\sum_{a=1}^{N} H^{ba}\hat{u}_0^a = u_0(x^b) \qquad (b = 1, 2, \ldots, N) \tag{26}$$

with $H^{ba} = H(w_a(x^b))\,\phi^a(x^b)$. Making use of the matrix notations, we may write Eq. (26) as

$$[H]\,[\hat{u}_0] = [u_0].$$

Hence, the initial values can be computed by

$$[\hat{u}_0] = [H]^{-1}[u_0].$$

The final task is to find the time-evolution of the nodal values of the potential and/or nodal values $\hat{u}^a(t)$ governed by the system of the ordinary differential equations given by Eq. (14) or (22), respectively.

5. Time evolution of nodal values

The analysis of the governing equations for both kinds of the nodal unknowns considered in the previous section is reduced to the investigation of a set of ordinary differential equations that can be written in matrix form as

$$[\mathbf{K}][\mathbf{v}(t)] - [\mathbf{M}]\frac{\mathrm{d}[\mathbf{v}(t)]}{\mathrm{d}t} = [\mathbf{F}(t)]. \tag{27}$$

The most familiar method for solving Eq. (27) with the initial condition $[\mathbf{v}(0)] = [\mathbf{v}_0]$ is the one-step θ (theta) method. Assuming

$$[\mathbf{v}^n] = [\mathbf{v}(n\Delta t)],$$

$$[\mathbf{v}^{n+\theta}] = (1-\theta)[\mathbf{v}^n] + \theta[\mathbf{v}^{n+1}],$$

$$\frac{\mathrm{d}[\mathbf{v}(t)]}{\mathrm{d}t} \approx \frac{[\mathbf{v}^{n+1}] - [\mathbf{v}^n]}{\Delta t}, \text{for } t = (n+\theta)\Delta t,$$

we may write Eq. (27) for the instant $t = (n+\theta)\Delta t$ as

$$\left(\theta[\mathbf{K}] - \frac{1}{\Delta t}[\mathbf{M}]\right)[\mathbf{v}^{n+1}] = [\mathbf{F}^{n+\theta}] - \left((1-\theta)[\mathbf{K}] + \frac{1}{\Delta t}[\mathbf{M}]\right)[\mathbf{v}^n] \tag{28}$$

with the initial condition given as $[\mathbf{v}^0] = [\mathbf{v}_0]$. The θ-method is absolutely stable for $1/2 < \theta < 1$. For $\theta = 1/2$, the accuracy is of second order (in time), while for $\theta \neq 1/2$ the order of accuracy is one. According to values of θ, the θ-methods are classified as

$\theta = 0$ – explicit Euler's method

$\theta = 1/2$ – Crank–Nicolson's method

$\theta = 2/3$ – Galerkin's implicit scheme

$\theta = 1$ – implicit Euler's method.

Now, we present an analytical integral formulation for a solution of the system of equations given by (27). For this purpose, we rewrite the system (27) as

$$S_{ab}v_b(t) = g_a(t), \tag{29}$$

in which the summation is assumed over the repeated Latin subscripts (within the range from 1 to N) and

$$S_{ab} = \delta_{ab}\frac{\mathrm{d}}{\mathrm{d}t} + Q_{ab}\,, \qquad g_a(t) = -M_{ac}^{-1}F_c(t), \qquad Q_{ab} = -M_{ac}^{-1}K_{cb}\,. \tag{30}$$

Let the matrix $G_{ac}(t)$be the fundamental solution for the differential operator $S_{..}^T$, i.e.,

$$S_{ba}^T G_{ac}(t) = \delta_{bc}\delta(t), \tag{31}$$

with $G_{ac}(t) = 0$ for $t \leq 0$. Note that the superscript T denotes the transpose matrix and $\delta(t)$ is the Dirac δ-function. It can be seen that the matrix exponential function

$$G_{ac}(t) = H(t)\left(e^{-t[\mathbf{Q}^T]}\right)_{ac} \tag{32}$$

obeys Eq. (31).

Bearing in mind Eq. (29), one can write the integral identity

$$\int_0^\infty G_{ac}(t-\tau)\,S_{ab}\,v_b(\tau)\,\mathrm{d}\tau = \int_0^\infty G_{ac}(t-\tau)\,g_a(\tau)\,\mathrm{d}\tau. \tag{33}$$

Hence, in view of Eq. (30) and the integration by parts, we have

$$G_{ac}(t-\tau)\,v_a(\tau)|_{\tau=0}^{\tau=\infty} + \int_0^\infty v_b(\tau)\,S_{ab}\,G_{ac}(t-\tau)\,\mathrm{d}\tau = \int_0^\infty G_{ac}(t-\tau)\,g_a(\tau)\,\mathrm{d}\tau.$$

Finally, taking into account Eq. (31) and the initial condition for $G_{ac}(t)$, one obtains the sought solution in the integral form

$$v_c(t) = v_a(0)\,G_{ac}(t) + \int_0^t g_a(\tau)\,G_{ac}(t-\tau)\,\mathrm{d}\tau. \tag{34}$$

Although we have a formal expression (32) for the Green function, the main problem in the formulation based on Eq. (34) is to find an effective method for determining the matrix exponential function.

Having solved the eigenproblem for the matrix $[\mathbf{Q}]$ (i.e., $([\mathbf{Q}]-\lambda[\mathbf{E}])[\mathbf{w}]) = \mathbf{0}$; $[\mathbf{E}]$ is unit matrix), one can find the canonical form expression of this matrix. An interesting case occurs when each eigenvalue $\lambda^{(\alpha)}$ $(\alpha = 1, 2, \ldots, N)$ is single (i.e., $\det(\mathbf{Q}-\lambda\mathbf{E}) = \prod_{\alpha=1}^N (\lambda - \lambda^{(\alpha)})$), because $[\mathbf{Q}]$ can be expressed in terms of the diagonal matrix $D_{\alpha\beta} = \lambda^{(\alpha)}\delta_{\alpha\beta}$ as $[\mathbf{Q}] = [\mathbf{S}][\mathbf{D}][\mathbf{S}^{-1}]$ with the matrix $[\mathbf{S}]$ being given by eigenvectors as $S_{a\alpha} = w_a^{(\alpha)}$. Then,

$$[\mathbf{Q}^T]_{ab} = Q_{ba} = \sum_{\alpha,\beta=1}^N S_{b\alpha}\,D_{\alpha\beta}\,S_{\beta a}^{-1} = \sum_{\alpha=1}^N S_{b\alpha}\,S_{\alpha a}^{-1}\,\lambda^{(\alpha)}$$

and hence,

$$\begin{aligned}\left(e^{-t[\mathbf{Q}^T]}\right)_{ab} &= \delta_{ab} - t[\mathbf{Q}^T]_{ab} + \frac{t^2}{2}\left([\mathbf{Q}^T][\mathbf{Q}^T]\right)_{ab} + \cdots \\ &= \sum_{\alpha=1}^N S_{b\alpha}\,S_{\alpha a}^{-1}\left(1 - t\lambda^{(\alpha)} + \frac{1}{2}\left(t\lambda^{(\alpha)}\right)^2 + \cdots\right) = \sum_{\alpha=1}^N S_{b\alpha}\,S_{\alpha a}^{-1}\,e^{-t\lambda^{(\alpha)}}.\end{aligned} \tag{35}$$

Inserting Eq. (35) into (32), we obtain the expression

$$G_{ab}(t) = H(t)\sum_{\mu=1}^N S_{b\alpha}\,S_{\alpha a}^{-1}\,e^{-t\lambda^{(\mu)}} \tag{36}$$

that can be used successfully in Eq. (34).

Unfortunately, the matrix exponential function in $G_{ac}(t)$ cannot be eliminated, if multiple eigenvalues are occurring ($\det(Q-\lambda E)=\prod_{\alpha=1}^{r}(\lambda-\lambda^{(\alpha)})^{k_\alpha}$, $\sum_{\alpha=1}^{r}k_\alpha=N$), in general. Moreover, the algorithm for getting the canonical form expression of $[\mathbf{Q}]$ in terms of a quasi-diagonal matrix is much more complicated. On the other hand, a symmetric real matrix $[\mathbf{Q}]$ can be transformed to a diagonal matrix by a similarity transformation even in case of multiple eigenvalues. In the present formulation, however, the matrix $[\mathbf{Q}]$ might be non-symmetric even if the matrices $[\mathbf{M}]$ and $[\mathbf{K}]$ (or $[\mathbf{K}^{-1}]$) were symmetric.

6. Conclusions

The paper presents a new formulation for solution of the initial/boundary-value problems for diffusion equation by using both the Global and Local Integral Equations. The GIE are sufficient to incorporate the relevant physical interaction in the model of continuum or in other words the coupling among all nodal values (prescribed by boundary conditions as well as nodal unknowns) in the discretized form of the governing equations. Hence, the system of discretized GIE can be supplemented by the LIE in order to get a sufficient number of independent algebraic equations for computation of nodal unknowns. Consequently, the resulting stiffness matrix is sparse like in a FEM formulation. Moreover, the algebraic equations are good conditioned like in a formulation based on the singular integral equations. Two concepts of the spatial variation are employed in approximation of physical fields. Finally, an analytical approach is presented for a numerical solution of the system of ordinary differential equations governing the time-evolution of unknowns located at nodal points in the analysed domain.

Appendix A

In this Appendix, we present several important formulas resulting from modelling of geometry. Although the potential field is approximated by using either the polynomial interpolation within finite size elements (approximation in terms of intrinsic coordinates) or the meshless approximation (in terms of the global coordinates), we need to discretize both the whole domain and its boundary in order to model the geometry and finally to perform the integration over both the domain and the boundary contour at least in case of the global integral equations.

A.1. Modelling of the global geometry (in terms of intrinsic coordinates)

Owing to a more faithful modelling of curved boundary contours, we adopt the quadratic approximation of Cartesian coordinates of the interior points along boundary elements. Then, it is appropriate to use quadratic approximation also over the domain cells, in order to meet compatibility. Thus, we assume

$$\Gamma=\bigcup_p \Gamma_p\,, \qquad \eta_k|_{\Gamma_p}=\sum_{a=1}^{3}\eta_k^{ap}N^a(\xi)\,, \qquad \xi\in[-1,1] \tag{A1}$$

where η_k^{ap} are Cartesian coordinates of the a-th nodal point on Γ_p and $N^a(\xi)$ are the quadratic Lagrange interpolation polynomials. Then, the unit tangent and outward normal vectors are given as

$$t_i(\eta)|_{\Gamma_p}=\frac{h_i^p(\xi)}{h^p(\xi)}\,, \qquad h_i^p(\xi)=\sum_{a=1}^{3}\eta_k^{ap}\frac{\mathrm{d}N^a(\xi)}{\mathrm{d}\xi}\,, \qquad h^p(\xi)=\sqrt{h_i^p(\xi)\,h_i^p(\xi)}\,,$$
$$n_i(\eta)|_{\Gamma_p}=\varepsilon_{ik3}t_k(\eta)|_{\Gamma_p}\,, \tag{A2}$$

with $h^p(\xi)$ being the Jacobian of the transformation from the global Cartesian coordinates to the local intrinsic coordinate ξ and ε_{ij3} being the permutation symbol. Thus,

$$\int_\Gamma (\cdot)\, \mathrm{d}\Gamma(\eta) = \sum_p \int_{\Gamma_p} (\cdot)\, \mathrm{d}\Gamma(\eta) = \sum_p \int_{-1}^{1} (\cdot)|_{\Gamma_p} h^p(\xi)\, \mathrm{d}\xi, \tag{A3}$$

Similar approximation we use within domain cells, assuming

$$\Omega = \bigcup_e \Omega_e\,, \qquad x_k|_{\Omega_e} = \sum_{a=1}^{8} x_k^{ae}\, N^a(\xi_1\,,\, \xi_2), \qquad \xi_1\,,\, \xi_2 \in [-1,1], \tag{A4}$$

where $N^a(\xi_1\,,\, \xi_2)$ are the quadratic Lagrange interpolation polynomials of two variables and x_k^{ae} are the Cartesian coordinates of the a-th nodal point on the domain elementΩ_e.

The Jacobian of the transformation from the global Cartesian coordinates to the local intrinsic ones is given by

$$J^e(\xi_1\,,\, \xi_2) = \left|\varepsilon_{3ij}\, h^e_{1i}(\xi_1\,,\, \xi_2)\, h^e_{2j}(\xi_1\,,\, \xi_2)\right|, \qquad \text{with} \qquad h^e_{ki}(\xi_1\,,\, \xi_2) = \sum_{a=1}^{8} x_k^{ae}\, N^a_{,k}(\xi_1\,,\, \xi_2). \tag{A5}$$

Finally,

$$\int_\Omega (\cdot)\, \mathrm{d}\Omega(x) = \sum_e \int_{\Omega_e} (\cdot)\, \mathrm{d}\Omega(x) = \sum_e \int_{-1}^{1}\int_{-1}^{1} (\cdot)|_{\Omega_e}\, J^e(\xi_1\,,\, \xi_2)\, \mathrm{d}\xi_1 \mathrm{d}\xi_2\,. \tag{A6}$$

A.2. Potential gradients by using polynomial interpolation for potential

Bearing in mind the approximations by Eq. (6) and the geometry modelling, the gradients of any approximated field over Ω_e are expressed in terms of the derivatives with respect to the intrinsic coordinates by

$$\left.\frac{\partial(\cdot)}{\partial x_i}\right|_{\Omega_e} = \frac{\partial \xi_j}{\partial x_i}\left.\frac{\partial(\cdot)}{\partial \xi_j}\right|_{\Omega_e} = (h^e)^{-1}_{ij}\left.\frac{\partial(\cdot)}{\partial \xi_j}\right|_{\Omega_e}, \tag{A7}$$

where $(h^e)^{-1}$ is the inverse matrix to $h^e_{..}$ defined in Eq. (A5). Since

$$(h^e)^{-1}_{ij} = \frac{\varepsilon_{3il}\, \varepsilon_{3jk}\, h^e_{kl}(\xi_1\,,\, \xi_2)}{\varepsilon_{3mn}\, h^e_{1m}(\xi_1\,,\, \xi_2)\, h^e_{2n}(\xi_1\,,\, \xi_2)}, \tag{A8}$$

we may write

$$\left.\frac{\partial u(x)}{\partial x_i}\right|_{\Omega_e} = \frac{\varepsilon_{3il}\, \varepsilon_{3jk}\, h^e_{kl}(\xi_1\,,\, \xi_2)}{\varepsilon_{3mn}\, h^e_{1m}(\xi_1\,,\, \xi_2)\, h^e_{2n}(\xi_1\,,\, \xi_2)} \sum_{a=1}^{8} u(x^{ae})\, N^a_{,j}(\xi_1\,,\, \xi_2). \tag{A9}$$

Furthermore, we need to know the normal derivative of the potential over $\Gamma_p \subset \Gamma_D$. Apparently, the distribution of the potential over Γ_D is not sufficient for the computation of this normal derivative. Therefore it is necessary to identify Ω_e to which Γ_p belong by finding z and e from the coincidence $\eta^{2p} = x^{ze}$. Note that $z \in \{5,6,7,8\}$. Denoting the values of the intrinsic coordinates $(\xi_1\,,\, \xi_2)$ on Γ_p as $(\xi_1^z\,,\, \xi_2^z)$, we have

$$(\xi_1^z\,,\, \xi_2^z) = \begin{cases} (\xi, -1)\,, & z = 5 \\ (1, \xi)\,, & z = 6 \\ (-\xi, 1)\,, & z = 7 \\ (-1, -\xi)\,, & z = 8 \end{cases} \qquad \text{with} \quad \xi \in [-1,1]. \tag{A10}$$

One can easily verify that the normal vector on Γ_p is given by

$$n_i(\eta)|_{\Gamma_p} = (1 - 2H(z - 6.1))\, \varepsilon_{ik3} \frac{h^e_{\mu k}(\xi^z_1, \xi^z_2)}{h^e_{\mu}(\xi^z_1, \xi^z_2)}, \qquad h^e_{\mu}(\xi^z_1, \xi^z_2) = \sqrt{h^e_{\mu k}(\xi^z_1, \xi^z_2)\, h^e_{\mu k}(\xi^z_1, \xi^z_2)}, \tag{A11}$$

where $H(x)$ is the Heaviside unite step function

$$H(x) = \begin{cases} 1, & x > 0 \\ 0, & x \leq 0 \end{cases}$$

and the parameter μ is defined as

$$\mu = \begin{cases} 1, & z = 5 \text{ or } 7, \\ 2, & z = 6 \text{ or } 8. \end{cases}$$

Thus, the normal derivative of the potential is given by

$$\frac{\partial u}{\partial n}(\eta)\bigg|_{\Gamma_p \subset \Omega_e} = \sum_{a=1}^{8} u(x^{ae})\, M^{aep}(\xi), \tag{A12}$$

where

$$M^{aep}(\xi) = (1 - 2H(z - 6.1))\, \varepsilon_{ik3} \frac{h^e_{\mu k}(\xi^z_1, \xi^z_2)}{h^e_{\mu}(\xi^z_1, \xi^z_2)} \frac{\varepsilon_{3il}\, \varepsilon_{3jn}\, h^e_{nl}(\xi^z_1, \xi^z_2)}{\varepsilon_{3sq}\, h^e_{1s}(\xi^z_1, \xi^z_2)\, h^e_{2q}(\xi^z_1, \xi^z_2)} N^a_{,j}(\xi^z_1, \xi^z_2).$$

A.3. Modelling the local geometry using intrinsic coordinates

If the physical fields are approximated by polynomial interpolation in terms of intrinsic coordinates, it is necessary to employ the same coordinates also for modelling of geometry. If L^c were selected as a circle in global coordinate system, it would not be a trivial task to determine the shape of the corresponding curve in the intrinsic spaces associated with the cells $\Omega_e y^c$. Therefore it is more appropriate to assume $L^c = \bigcup_e{}' L^c_e$ where the superposed prime stands for consideration of those domain cells Ω_e which contain the nodal point y^c and L^c_e is the imagination of the circular arc of the radius ξ_0 and centred at (ξ^{ce}_1, ξ^{ce}_2) in the intrinsic space associated with Ω_e. Because of the circular geometry, it is appropriate to use polar coordinates in the intrinsic coordinate space. According to the position of the global nodal point y^c within the element $\Omega_e y^c$, we can define the local intrinsic coordinates of this node and the bounds for the angular variable on the circular arc as

$y^c = x^{ae}$	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$	$a=7$	$a=8$
φ^{ce}_1	0	$\pi/2$	π	$3\pi/2$	0	$\pi/2$	π	$-\pi/2$
φ^{ce}_2	$\pi/2$	π	$3\pi/2$	2π	π	$3\pi/2$	2π	$\pi/2$
ξ^{ce}_1	-1	1	1	-1	0	1	0	-1
ξ^{ce}_2	-1	-1	1	1	-1	0	1	0

Now,

$$\int_{L^c} (\cdot)\, \mathrm{d}\Gamma = \sum_{\substack{e \\ y^c \in \Omega_e}} \int_{L^c_e} (\cdot)\, \mathrm{d}\Gamma = \sum_{\substack{e \\ y^c \in \Omega_e}} \int_{\varphi^{ce}_1}^{\varphi^{ce}_2} (\cdot)\, h^e(\varphi)\, \mathrm{d}\varphi, \tag{A13}$$

where the curved arc L_e^c is parametrized as

$$L_e^c = \left\{ \forall \mathbf{x} \in \mathcal{R}^3 ; \quad x_k = \sum_{a=1}^{8} x_k^{ae} N^a\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right), \quad \vec{\xi}^{ce}(\xi_0, \varphi) = (\xi_1^{ce} + \xi_0 \cos\varphi, \xi_2^{ce} + \xi_0 \sin\varphi), \right.$$
$$\left. \varphi \in \lfloor \varphi_1^{ce}, \varphi_2^{ce} \rfloor \right\}, \tag{A14}$$

and the Jacobian of the transformation from $x \in L_e^c$ to the angular variable of polar coordinates in the corresponding intrinsic space is given by

$$h^e(\varphi) = \sqrt{h_k^e(\varphi)\, h_k^e(\varphi)},$$
$$h_k^e(\varphi) = \left.\frac{\mathrm{d}x_k}{\mathrm{d}\varphi}\right|_{L_e^c} = \xi_0 \sum_{a=1}^{8} x_k^{ae} \left[-\sin\varphi\, N_{,1}^a\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right) + \cos\varphi\, N_{,2}^a\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right)\right]. \tag{A15}$$

The unit tangent and outward normal vectors on L_e^c are defined by

$$t_k(x)|_{L_e^c} = \frac{h_k^e(\varphi)}{h^e(\varphi)}, \qquad n_i(x)|_{L_e^c} = \varepsilon_{ik3}\, t_k(x)|_{L_e^c}. \tag{A16}$$

Thus, the normal derivative on L_e^c can be written as

$$\left.\frac{\partial u}{\partial n}(x)\right|_{L_e^c} = \frac{1}{h^e(\varphi)} \sum_{a=1}^{8} u(x^{ae})\, K^{aec}(\varphi), \tag{A17}$$

with

$$K^{aec}(\xi) = \varepsilon_{ik3}\, h_k^e(\varphi) \frac{\varepsilon_{3il}\, \varepsilon_{3jn}\, h_{nl}^e\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right)}{\varepsilon_{3sq}\, h_{1s}^e\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right)\, h_{2q}^e\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right)} N_{,j}^a\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right). \tag{A18}$$

Note that $h_{nl}^e\left(\vec{\xi}^{ce}(\xi_0, \varphi)\right)$ is obtained from $h_{nl}^e(\xi_1, \xi_2)$ replacing (ξ_1, ξ_2) by $\xi_1^{ce}(\xi_0, \varphi) = \xi_1^{ce} + \xi_0 \cos\varphi$ and $\xi_2^{ce}(\xi_0, \varphi) = \xi_2^{ce} + \xi_0 \sin\varphi$.

Since the domain bounded by L^c is $\Omega^c = \bigcup_{\substack{e \\ y^c \in \Omega_e}} \Omega_e^c$ with

$$\Omega_e^c = \left\{ \forall \mathbf{x} \in \mathcal{R}^3 ; \quad x_k = \sum_{a=1}^{8} x_k^{ae} N^a\left(\vec{\xi}^{ce}(\rho, \varphi)\right), \quad \vec{\xi}^{ce}(\rho, \varphi) = (\xi_1^{ce} + \rho\cos\varphi, \xi_2^{ce} + \rho\sin\varphi), \right.$$
$$\left. \rho \in [0, \xi_0], \quad \varphi \in \lfloor \varphi_1^{ce}, \varphi_2^{ce} \rfloor \right\}, \tag{A19}$$

we may write

$$\int_{\Omega^c} (\cdot)\, \mathrm{d}\Omega = \sum_{\substack{e \\ y^c \in \Omega_e}} \int_{\Omega_e^c} (\cdot)\, \mathrm{d}\Omega = \sum_{\substack{e \\ y^c \in \Omega_e}} \int_0^{\xi_0} \int_{\varphi_1^{ce}}^{\varphi_2^{ce}} (\cdot)\, J^{ce}(\rho, \varphi)\, \rho\, \mathrm{d}\rho\mathrm{d}\varphi,$$

where $J^{ce}(\rho, \varphi)$ is obtained from $J^e(\xi_1, \xi_2)$ by taking $(\xi_1, \xi_2) = (\xi_1^{ce}(\rho, \varphi), \xi_2^{ce}(\rho, \varphi))$.

In view of Eq. (A9), the gradients of the potential within Ω_e^c are approximated as

$$\left.\frac{\partial u(x)}{\partial x_i}\right|_{\Omega_e^c} = \sum_{a=1}^{8} u(x^{ae})\, P_i^{aec}(\rho, \varphi)$$

with

$$P_i^{aec}(\rho, \varphi) = \frac{\varepsilon_{3il}\, \varepsilon_{3jk}\, h_{kl}^e\left(\vec{\xi}^{ce}(\rho, \varphi)\right)}{\varepsilon_{3mn}\, h_{1m}^e\left(\vec{\xi}^{ce}(\rho, \varphi)\right)\, h_{2n}^e\left(\vec{\xi}^{ce}(\rho, \varphi)\right)} N_{,j}^a\left(\vec{\xi}^{ce}(\rho, \varphi)\right).$$

A.4. Modelling the local geometry in the global coordinate system

This modelling is applicable when the LIE are implemented by using the MLS-approximation for physical fields (Eqs. (17) and (19)). Since the shape of Ω^c and L^c are arbitrary, it is appropriate to select the circular form

$$L^c = \{\forall(x_1, x_2) \in \Omega;\ x_k = y_k^c + r_0(\delta_{k1}\cos\varphi + \delta_{k2}\sin\varphi),\ \varphi \in [0, 2\pi]\},$$
$$\Omega^c = \{\forall(x_1, x_2) \in \Omega;\ x_k = y_k^c + \rho(\delta_{k1}\cos\varphi + \delta_{k2}\sin\varphi),\ \rho \in [0, r_0],\ \varphi \in [0, 2\pi]\}.$$

Then, one can consider the fundamental solution in the form

$$w^*(x - y^c)|_{L^c} = 0, \qquad \frac{\partial w^*}{\partial n}(x - y^c)\bigg|_{L^c} = \frac{1}{2\pi r_0}, \qquad w^*(x - y^c)|_{\Omega^c} = \frac{1}{2\pi}\ln\left(\frac{\rho}{r_0}\right).$$

APPENDIX B

In this appendix, we present an algorithm for numerical computation of the strongly singular integral given as a limit of the nearly singular integral

$$I^p = \lim_{z \to \zeta^b} \int_{-1}^{1} f(\eta^p(\xi))\, \varepsilon_{ik3}\, h_k^p(\xi)\, \frac{\eta_i^p(\xi) - z_i}{|\eta^p(\xi) - z|^2}\, \mathrm{d}\xi \tag{B1}$$

in which the integration is performed in the intrinsic space of a singular boundary element $\Gamma_p \ni \zeta^b$ and z is a point from the interior of domain Ω bounded by $\Gamma \supset \Gamma_p$. The approach is based on the extraction of peak-like factors and optimal transformations of the integration variables [5]. Without methodological restrictions we shall assume the quadratic interpolation for geometry modelling within Γ_p.

Let ξ_0^p be the intrinsic coordinate of the singular point ζ^b on Γ_p. Then

$$r_i^p = \eta_i^p(\xi) - \zeta_i = \sum_{a=1}^{3} \eta_i^{ap}[N^a(\xi) - N^a(\xi_0^p)] = \tilde{\xi}(\tilde{\xi}\alpha_i^p + \beta_i^p),$$
$$\tilde{r}_i^p = \eta_i^p(\xi) - z_i = r_i^p + \Delta_i,$$

where

$$\alpha_i^p = \frac{1}{2}\left(\eta_i^{1p} + \eta_i^{3p}\right) - \eta_i^{2p}, \qquad \beta_i^p = 2\xi_0^p\alpha_i^p + \tilde{\beta}_i^p, \qquad \tilde{\beta}_i^p = \frac{1}{2}\left(\eta_i^{3p} - \eta_i^{1p}\right), \qquad \Delta_i = \zeta_i - z_i,$$

and

$$\tilde{\xi} = \xi - \xi_0^p \in \lfloor \xi_-^p, \xi_+^p \rfloor \qquad \text{with} \qquad \xi_-^p = -(1 + \xi_0^p), \quad \xi_+^p = 2 + \xi_-^p.$$

Making use of the notations

$$e_i = \frac{\Delta_i}{\Delta}, \qquad a = \frac{\beta_i^p}{\beta^p}e_i, \qquad b = \frac{\Delta}{\beta^p}, \qquad c^2 = b^2(1 - a^2), \qquad \beta^p = \sqrt{\beta_i^p\,\beta_i^p},$$

we may write

$$\tilde{r}_i^p = \rho\beta_i^p + \Delta\gamma_i^p(\rho) + (\rho^2 + c^2)\alpha_i^p, \qquad (\tilde{r}^p)^2 = (\rho^2 + c^2)/B^p(\rho),$$
$$h_i^p = 2\alpha_i^p(\rho - ab) + \beta_i^p, \tag{B2}$$

where

$$\rho = \tilde{\xi} + ab \in [ab + \xi_-^p\,,\ ab + \xi_+^p],$$

$$\gamma_i^p(\rho) = e_i - \frac{a}{\beta^p} h_i^p - \frac{\alpha_i^p b}{\beta^p}\,,$$

$$B^p(\rho) = \frac{1}{(\beta^p)^2 \left(1 + \frac{A(\rho)}{\rho^2 + c^2}\right)}\,,$$

with

$$A(\rho) = \left(\frac{1}{\beta^p}\right)^2 (\rho - ab)^2 \left[(\rho - ab)^2 (\alpha^p)^2 + 2(\rho - ab)\,\alpha_i^p \beta_i^p + 2\alpha_i^p \Delta_i\right].$$

Now, the integral (B1) can be rewritten as

$$I^p = \lim_{\Delta \to 0} \int_{ab+\xi_-^p}^{ab+\xi_+^p} \tilde{f}^p(\xi_0^p - ab + \rho) \left[E^p + \frac{\Delta}{\rho^2 + c^2}\,\Omega^p(\rho)\right] B^p(\rho)\,\mathrm{d}\rho, \tag{B3}$$

where we have used the notations

$$\tilde{f}^p(\xi) = f(\eta^p(\xi)), \qquad E^p = \varepsilon_{ik3}\,\beta_i^p\,\alpha_k^p\,, \qquad \Omega^p(\rho) = \varepsilon_{ik3}\left[e_i h_k^p + \frac{\alpha_i^p \beta_k^p}{\beta^p}\,(2a(\rho - ab) + b)\right].$$

Now, it is important to know the asymptotic behaviour of the integrand in Eq. (B3) as $\Delta \to 0$. Since

$$\hat{B}^p(\rho) \equiv \lim_{\Delta \to 0} B^p(\rho) = \frac{1}{d^p(\rho)}\,, \qquad d^p(\rho) = (\beta_i^p + \rho\alpha_i^p)(\beta_i^p + \rho\alpha_i^p),$$

and

$$\hat{\Omega}^p(\rho) \equiv \lim_{\Delta \to 0} \Omega^p(\rho) = \varepsilon_{ik3}\left[e_i(2\rho\alpha_k^p + \beta_k^p) + \frac{\alpha_i^p \beta_k^p}{\beta^p}\,2a\rho\right]$$

are bounded within the integration limits, the only singularity is the strong singularity contained in the peak-like factor $\Delta/(\rho^2 + c^2)$ at $\rho = 0$ as $\Delta \to 0$. Thus, the considered integral becomes

$$I^p = E^p \int_{\xi_-^p}^{\xi_+^p} \frac{\tilde{f}^p(\xi_0 + \rho)}{d^p(\rho)}\,\mathrm{d}\rho + \lim_{\Delta \to 0} \int_{ab+\xi_-^p}^{ab+\xi_+^p} \frac{\Delta}{\rho^2 + c^2}\,F^p(\rho)\,\mathrm{d}\rho \tag{B4}$$

in which

$$F^p(\rho) = \tilde{f}^p(\xi_0^p - ab + \rho)\,\Omega^p(\rho)\,B^p(\rho).$$

Assuming $\tilde{f}^p(\xi_0^p - ab + \rho)$ to be Hölder continuous at $\rho = 0$, one can asses the limit of the integral

$$\lim_{\Delta \to 0} \int_{ab+\xi_-^p}^{ab+\xi_+^p} \frac{\Delta}{\rho^2 + c^2}[F^p(\rho) - F^p(0)]\,d\rho = 0. \tag{B5}$$

Hence, and from Eq. (B4), we have

$$I^p = E^p \int_{\xi_-^p}^{\xi_+^p} \frac{\tilde{f}^p(\xi_0^p + \rho)}{d^p(\rho)}\,\mathrm{d}\rho + \hat{F}^p(0) \lim_{\Delta \to 0} \int_{ab+\xi_-^p}^{ab+\xi_+^P} \frac{\Delta}{\rho^2 + c^2}\,\mathrm{d}\rho, \tag{B6}$$

where

$$\hat{F}^p(0) = \tilde{f}^p(\xi_0^p)\,\hat{\Omega}^p(0)\,\hat{B}^p(0) = \frac{e_i n_i^p(\zeta^b)}{\beta^p}\,\tilde{f}^p(\xi_0^p).$$

In the last equation, we have utilized the fact that the tangent vector to Γ_p at ζ^b is given by $\tau_i^p(\zeta^b) = \beta_i^p/\beta^p$. Bearing in mind that

$$\lim_{\Delta\to 0}\int_{ab+\xi_-^p}^{ab+\xi_+^p}\frac{\Delta}{\rho^2+c^2}\,\mathrm{d}\rho = \lim_{\Delta\to 0}\frac{\Delta}{c}\left[\arctan\left(\frac{ab+\xi_+^p}{c}\right) - \arctan\left(\frac{ab+\xi_-^p}{c}\right)\right] = \frac{\beta^p}{\sqrt{1-a^2}}\,\varphi^p, \tag{B7}$$

where

$$\varphi^p = \begin{cases} \left[\dfrac{\pi}{2} - \arctan\left(\dfrac{a}{\sqrt{1-a^2}}\right)\right], & \text{if } \xi_0 = -1, \\ \pi, & \text{if } \xi_0 \in (-1,1), \\ \left[\arctan\left(\dfrac{a}{\sqrt{1-a^2}}\right) + \dfrac{\pi}{2}\right], & \text{if } \xi_0 = 1. \end{cases}$$

In performing the limit $\Delta \to 0$ in Eq. (B7), we have utilized the fact that

$$\begin{aligned} &\xi_-^p = 0, && \xi_+^p = 2 && \text{if } \xi_0^p = -1, \\ &\xi_-^p \in (-2,0), && \xi_+^p \in (0,2) && \text{if } \xi_0^p \in (-1,1), \\ &\xi_-^p = -2, && \xi_+^p = 0 && \text{if } \xi_0^p = 1. \end{aligned}$$

Since $a = e_i\tau_i^p(\zeta^b)$, we have $1 - a^2 = (e_i\, n_i^p(\zeta^b))^2$ and hence

$$\frac{e_i\, n_i^p(\zeta^b)}{\beta^p}\,\frac{\beta^p}{\sqrt{1-a^2}} = 1.$$

Expressing a as $\cos\omega^p$, we have $a = \sin\left(\frac{\pi}{2} - \omega^p\right)$, $\sqrt{1-a^2} = \sin\omega^p = \cos\left(\frac{\pi}{2} - \omega^p\right)$ and $\arctan\left(\frac{a}{\sqrt{1-a^2}}\right) = \frac{\pi}{2} - \omega^p$. Thus,

$$\varphi^p = \begin{cases} \omega^p, & \text{if } \xi_0^p = -1, \\ \pi, & \text{if } \xi_0^p \in (-1,1) \\ \pi - \omega^p, & \text{if } \xi_0^p = 1. \end{cases} \tag{B8}$$

where ω^p is clearly defined as the angle within two unit vectors $\vec{e}$ and $\vec{\tau}^p(\zeta^b)$.

Now, in view of (B7), Eq. (B6) becomes

$$I^p = E^p\int_{\xi_-^p}^{\xi_+^p}\frac{\tilde{f}^p(\xi_0^p+\rho)}{d^p(\rho)}\,\mathrm{d}\rho + \tilde{f}^p(\xi_0^p)\,\varphi^p, \tag{B9}$$

where φ^p is given by (B8) and $\tilde{f}^p(\xi_0^p) = f(\eta^p(\xi_0^p)) = f(\zeta^b)$.

Note that the singular segment is represented by Γ_p if $\zeta^b \in \Gamma_p$ with $\xi_0^p \in (-1,1)$, but it is given by $\Gamma_p \cup \Gamma_{p-1}$ if $\xi_0^p = -1$ ($\xi_0^{p-1} = 1$) and/or by $\Gamma_p \cup \Gamma_{p+1}$ if $\xi_0^p = 1$ ($\xi_0^{p+1} = -1$). It can be seen that

$$\sum_{\substack{p \\ \zeta^b\in\Gamma_p}} \tilde{f}^p(\xi_0^p)\,\varphi^p = f(\zeta^b)\,(2\pi - \theta^b), \tag{B10}$$

where θ^b is the angle within two tangent lines to Γ at ζ^b. The proof is trivial in the case when $\xi_0^p \in (-1,1)$, while for $\xi_0^p = -1$ and $\xi_0^p = 1$ we have, respectively,

$$\varphi^p + \varphi^{p-1} = \omega^p + (\pi - \omega^{p-1}) = 2\pi - (\pi + \omega^{p-1} - \omega^p) = 2\pi - \theta^b$$

or

$$\varphi^p + \varphi^{p+1} = (\pi - \omega^p) + \omega^{p+1} = 2\pi - (\pi + \omega^p - \omega^{p+1}) = 2\pi - \theta^b.$$

Finally, the sum of the considered strongly singular integrals is given by

$$\sum_{\substack{p \\ \zeta^b \in \Gamma_p}} I^p = (2\pi - \theta^b)\, f(\zeta^b) + \sum_{\substack{p \\ \zeta^b \in \Gamma_p}} E^p \int_{\xi_-^p}^{\xi_+^p} \frac{\tilde{f}^p(\xi_0^p + \rho)}{d^p(\rho)}\, \mathrm{d}\rho. \tag{B11}$$

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