A MESHLESS PARTICLE METHOD FOR POISSON AND DIFFUSION PROBLEMS WITH DISCONTINUOUS COEFFICIENTS AND INHOMOGENEOUS BOUNDARY CONDITIONS

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Abstract. We present a meshless particle method for Poisson and diffusion problems on domains with discontinuous coefficients and possibly inhomogeneous boundary conditions. The method is based on a domain-decomposition approach with suitable interface and boundary conditions between regions of different diffusivities, and on using discretization-corrected particle strength exchange operators [B. Schrader, S. Reboux, and I. F. Sbalzarini, J. Comput. Phys., 229 (2010), pp. 4159–4182]. We propose and compare two methods: The first one is based on an immersed interface approach, where interfaces are determined implicitly using a simplified phase-field equation. The second method uses a regularization technique to transform inhomogeneous interface or boundary conditions to homogeneous ones with an additional continuous volume contribution. After presenting the methods, we demonstrate their capabilities and limitations on several one-dimensional and three-dimensional test cases with Dirichlet and Neumann boundary conditions, and both regular and irregular particle distributions.

Key words. diffusion, particle method, discontinuity, interface condition, regularization, Poisson equation, PSE operators, DC-PSE

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1. Introduction. Poisson or diffusion equations with discontinuous coefficients occur in many practical applications from forward electroencephalography (EEG) and electrocardiography problems [12] to multiphase flows [3] and fluid-structure interaction [29].

A widespread approach to handling discontinuous coefficients in Poisson equations is the use of regularization techniques to smooth the singularities or discontinuities that appear in the governing equations as Dirac or Heaviside distributions. This usually entails replacing them with smooth(er) functions that can be discretized with standard numerical methods [8, 27, 48, 49]. In the same framework, it is also possible to use a continuum method to account for the singularity in the function to be evaluated at the interfaces. It is similar to what is done for multiphase flows when surface tension effects at the interfaces between different fluids are taken into account [3]. Using smooth(ed) functions eliminates the need for interface representation and tracking, simplifies the calculation of the corresponding function, and does not impose conceptual restrictions on the number and complexity of the interfaces. This smooth(ed)-interface approach has also recently been adapted to impose Neumann
and Robin interface conditions in advection-reaction-diffusion equations simulated using the smoothed particle hydrodynamics (SPH) method [31].

Several grid-based methods are available to treat immersed or embedded boundaries and discontinuities of the coefficients. This includes immersed boundary methods [29, 28, 40], immersed interface methods [20, 22], and the embedded interface method [39]. The interfaces are either represented implicitly using level sets [43, 44, 9, 15] or phase fields [42], or explicitly using, e.g., tracer particles [19, 50]. Although originally designed for flows with discontinuities, the ghost fluid method (GFM) can also be used to solve Poisson problems in the presence of interfaces where both the coefficients and the solution itself may be discontinuous [24]. In its original form, using linear extrapolation of the interface jump conditions in each Cartesian direction, the GFM is first-order accurate [24]. In the two-dimensional (2D) constant-coefficient case, the method has been improved by determining the correction function using a least-squares approximation. This allows calculating any point near interfaces using a bicubic formulation [25]. An extension to three dimensions, however, remains to be derived. The idea of using extended domains has also been used to solve Poisson problems on irregular domains with the help of an integral equation formulation [26]. Other popular methods for discontinuous-coefficient Poisson equations are boundary element methods [1, 18], finite-element methods [36, 53], and finite difference methods [13, 17].

Meshless methods bypass the need for mesh generation, which is particularly advantageous in complex geometries and in advection-dominated problems. A meshless finite-element method has been applied to problems with discontinuous diffusivity [23]. It only uses the boundary description and the node distribution, without explicitly meshing the geometry. A finite point mixed method (FPMM) based on a collocation scheme has been applied to discretize the diffusion equation with discontinuous coefficients associated with the EEG forward problem [52]. The electric potential is determined on a set of particles, regularly or irregularly located in the computational domain. The particle function approximation amounts to a local moving least squares approximation of the electric potential about the nodes in terms of a basis of simple functions. The method is called “mixed” since the solution does not exactly satisfy the differential equation and the boundary conditions, as only a weak, weighted-residual integral formulation of them is ensured. One of the main difficulties in this method is the correct consideration of the jump in the normal component of the gradient of the electric potential that occurs across interfaces. As the electric potential is as a linear combination of smooth shape functions, the interface condition cannot be enforced. The problem is usually circumvented by first considering each domain independently and then imposing the corresponding boundary conditions at the interfaces. This results in a linear system to be solved for the potential values on the particles. Another linear system of equations results from the discretization of the Laplace equation in each domain. This leads to a formulation where there are more equations than nodes. A solution is found by transforming the problem to a constrained optimization problem, finding the vector that minimizes the discretized Laplace equation under the constraints imposed by the boundary conditions. A similar approach, called the finite point-set method, has been proposed for solving the Poisson equation with a different functional to be minimized and additional boundary conditions [46, 47].

Here, we consider meshless particle methods based on discretization-corrected (DC) particle sterength exchange (DC-PSE) operators [37] for discretizing Poisson and diffusion equations with discontinuous coefficients and possibly inhomogeneous boundary conditions. Particle strength exchange (PSE) is a meshless discretization scheme for differential operators, first developed for diffusion operators [4, 5] and later
generalized to arbitrary differential operators [7]. PSE allows consistent approximation of differential operators on unconnected sets of particles that serve as collocation points. It has previously been used for simulations in complex geometries [34] and on complex-shaped curved surfaces [33]. Recently, a general discretization-correction framework for PSE operators has extended the method to remain constant also on irregular particle distributions and near boundaries where particles do not have a full set of neighbors [37]. In PSE-type methods, each particle carries a weight, which is called strength, representing the local function value. The effect of applying a differential operator on the function thus represented is approximated by particles exchanging strength with their neighbors within a certain, finite interaction range. This “flow of strength” between particles has to fulfill certain moment conditions to consistently approximate the desired differential operator [7]. Discretization correction accounts for the discrete nature of the numerical problem by imposing discrete moment conditions rather than continuous ones. This implicitly accounts for the specific spatial distribution of particles and hence remains consistent on almost any particle distribution [37], including distributions that self-organize as governed by a monitor function or error predictor [30].

The imposition of inhomogeneous boundary conditions on arbitrary, curved interfaces, however, has remained an open problem. Here we present two methods for imposing inhomogeneous interface and boundary conditions in PSE-type schemes: The first method amounts to an immersed interface method with implicitly determined interfaces using a simplified phase-field equation. The second method is based on a regularization technique that transforms inhomogeneous interface conditions to homogeneous ones with an additional continuous volume contribution to the Poisson equation. We show from the theoretical derivations in sections 4.1–4.3 and the implementation discussion in section 4.4 that our method leads to an overall simpler approach than FPMM [52]. We use DC-PSE since it provides more flexibility to place particles of various sizes close to interfaces between regions of different diffusivities. We implement the present methods using the parallel particle mesh (PPM) library [35, 2]. The PPM library provides a parallelization middleware for hybrid particle-mesh methods with automatic domain decomposition, load balancing, and communication scheduling. The library actualizes a set of abstract parallel data structures and abstract operators for particle methods [32].

The remainder of this paper is structured as follows: In sections 2 and 3, we introduce the discontinuous-coefficient Poisson problem and the benchmark test cases used to validate our approach, respectively. The computational method and the imposition of inhomogeneous interface and boundary conditions using either an immersed-interface/phase-field method or a continuous surface-reaction method are presented in section 4. In section 5, we discuss and compare the benchmark results using test cases for which either analytical solutions or solutions obtained with other numerical methods are available. Section 6 concludes the paper and outlines future work.

2. Discontinuous-coefficient Poisson problems. We consider Poisson problems that can be modeled with the following general Poisson equation for the scalar field \( \Phi(\vec{x}) \):

\[
\nabla \cdot (\sigma(\vec{x}) \nabla \Phi(\vec{x})) = S(\vec{x})
\]

on a \( d \)-dimensional domain \( \Omega \subset \mathbb{R}^d \) with Neumann or Dirichlet conditions on its boundary \( \Gamma \). The term \( S(\vec{x}) \) is a given scalar function. The diffusion coefficient \( \sigma(\vec{x}) \) is a piecewise constant scalar function of the position \( \vec{x} \), such
that the domain $\Omega$ is composed of $N$ disjoint subdomains $\Omega_i$ ($i = 1, \ldots, N$), each with a different, but constant $\sigma_i$ within. The interface between subdomains $\Omega_i$ and $\Omega_{i+1}$ is denoted $\Gamma_i$, as shown in Figure 2.1. In subdomain $\Omega_i$, we hence consider the Poisson problem

$$\sigma_i \nabla^2 \Phi(\vec{x}) = S(\vec{x}), \quad \vec{x} \in \Omega_i,$$

with associated interface conditions

$$\Phi(\vec{x})|_{\Gamma_i^-} = \Phi(\vec{x})|_{\Gamma_i^+}$$

and

$$[\sigma_i \nabla \Phi(\vec{x}) \cdot \vec{n}(\vec{x})]|_{\Gamma_i^-} = [\sigma_{i+1} \nabla \Phi(\vec{x}) \cdot \vec{n}(\vec{x})]|_{\Gamma_i^+} + [S_i(\vec{x})]|_{\Gamma_i}.$$

Here, $\Gamma_i^+$ denotes the $\Omega_{i+1}$-side of the interface $\Gamma_i$ and $\Gamma_i^-$ the $\Omega_i$-side; $\vec{n}$ is the unit normal onto the interface. The continuous field $S_i(\vec{x})$ in the last term is a specified flux density difference at that interface. Subdomains need not be connected, and multiple inclusions are possible. However, there must be no triple points, i.e., no points where three (or more) subdomains meet.

3. Test cases. For our convergence studies, we consider two benchmark problems for which analytical solutions are available: a discontinuous one-dimensional (1D) Poisson problem with three subdomains, each of them with a different diffusion constant, and a three-dimensional (3D) Poisson problem in a three-region spherical geometry with local Dirichlet and Neumann conditions. In addition, we consider a more complex multi-inclusion case where no analytical solution is available. In all cases, we consider both regular and irregular particle distributions.

3.1. 1D dipole in a two-region domain. The 1D test case considers the problem of determining the electric potential generated by a dipole located at $x = 0$
inside the first subdomain of conductivity $\sigma_1$ extending from $-R_1$ to $R_1$. A second subdomain of conductivity $\sigma_2$ is located in the intervals $[-R_2, -R_1]$ and $[R_1, R_2]$, where $R_2 > R_1 > 0$. To make the solution of the problem easier by removing the source singularity induced by the dipole, it is convenient to consider the potential $\phi$ induced by the dipole as the sum of two terms $\phi = \phi_d + \Phi$ [36, 52], where $\phi_d$ is the potential induced by the dipole in an infinite homogeneous medium, and $\Phi$ is a correction potential. The potential induced by a dipole at $x = 0$ with moment $q_d$ in an infinite medium of conductivity $\sigma_1$ is

\[(3.1)\]

$$\phi_d(x) = \frac{q_d}{4\pi\sigma_1|x|}$$

with its gradient

\[(3.2)\]

$$\frac{d\phi_d}{dx} = -\frac{q_d}{2\pi\sigma_1x^3}.$$ 

The correction potential $\Phi$ satisfies Laplace’s equation on the interval $[-R_2, R_2]$, i.e.,

\[(3.3)\]

$$\frac{d^2\Phi}{dx^2} = 0,$$

which means that it is a linear function of the form $\Phi(x) = a_1 x + b_1$ in each subdomain $\Omega$. By imposing the interface conditions (2.3) and (2.4) on $\Phi$ and its derivative at $x = -R_2$, $x = -R_1$, $x = R_1$, $x = R_2$, the correction potential is uniquely determined on the whole domain $[-R_2, R_2]$ as

\[(3.4)\]

$$\Phi(x) = \begin{cases} 
F_2 x + R_1 (F_2 - F_1) + \phi_0, & x \in [-R_2, -R_1], \\
F_1 x + \phi_0, & x \in [-R_1, R_1], \\
F_2 x - R_1 (F_2 - F_1) + \phi_0, & x \in [R_1, R_2], 
\end{cases}$$

where $\phi_0$ is an arbitrary constant and the constants $F_1$ and $F_2$ are given by

\[(3.5)\]

$$F_1 = \left(\frac{\sigma_2}{\sigma_1} - 1\right) R_1 \left.\frac{d\phi_d}{dx}\right|_{R_1} - \left(\frac{\sigma_2}{\sigma_1}\right) R_2 \left.\frac{d\phi_d}{dx}\right|_{R_2},$$

\[(3.6)\]

$$F_2 = -R_2 \left.\frac{d\phi_d}{dx}\right|_{R_2}.$$ 

Due to the symmetry of the problem, it is $\frac{d\phi_d}{dx}|_{R_2} = \frac{d\phi_d}{dx}|_{-R_2}.$

### 3.2. 3D multilayered spherical domain.

The second test case considers a 3D sphere consisting of three concentric shells of radii $R_1$, $R_2$, and $R_3$ (0 < $R_1 < R_2 < R_3$) with diffusivities $\sigma_1$, $\sigma_2$, and $\sigma_3$, respectively. Furthermore, we suppose that the solution $\Phi$ is known and constant in a small sphere of radius $R_0 < R_1$ with the same center, and an inhomogeneous Neumann condition $\nabla \Phi \cdot \vec{n} = g$ is imposed on the surface of the largest sphere $r = R_3$, where $g$ is a given constant. We assume in addition that all functions $\nabla \Phi$ in (2.4) vanish. Due to the spherical symmetry of the problem, Laplace’s equation can be expressed in spherical coordinates as

\[(3.7)\]

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial \Phi}{\partial r}\right) = 0,$$
which means that $\Phi$ has the following form on each subdomain $\Omega_i$, $i = 1, 2, 3$:

\begin{align}
\Phi(r) &= -\frac{A_i}{r} + B_i, \quad x \in [R_{i-1}, R_i].
\end{align}  

(3.8)

Applying the interface conditions (2.3) and (2.4) to $\Phi$ and its derivative at the interfaces $r = R_1$, $r = R_2$, and $r = R_3$, as well as the Dirichlet condition $\Phi(r) = \Phi_0$ on the sphere $r = R_0$, allows determination of the solution in the whole domain $R_0 < r < R_3$. The constants $A_i$ and $B_i$ are given by

\begin{align}
A_1 &= \frac{\sigma_3}{\sigma_1} g R_3^2, \\
A_2 &= \frac{\sigma_3}{\sigma_2} g R_3^2, \\
A_3 &= g R_3^2, \\
B_1 &= \Phi_0 + \frac{\sigma_3}{\sigma_1} g R_0^2 R_1^2, \\
B_2 &= \left(1 - \frac{\sigma_2}{\sigma_1}\right) \frac{\sigma_3}{\sigma_2} g R_1^2 R_2^2 + \phi_0 + \frac{\sigma_3}{\sigma_1} g R_0^2 R_2^2, \\
B_3 &= \left(1 - \frac{\sigma_3}{\sigma_2}\right) g R_2^3 + \left(1 - \frac{\sigma_2}{\sigma_1}\right) \frac{\sigma_3}{\sigma_2} g R_1^2 R_3^2 + \phi_0 + \frac{\sigma_3}{\sigma_1} g R_0^2 R_3^2.
\end{align}  

(3.9) (3.10) (3.11) (3.12) (3.13) (3.14)

The one- and two-region cases can be obtained in a straightforward manner by setting the corresponding diffusivities to be identical.

**4. Methods.** After briefly reviewing the DC-PSE discretization scheme, we derive and detail two methods for imposing inhomogeneous interface and boundary conditions in meshless DC-PSE discretizations. We also provide some implementation notes.

**4.1. Discretization using DC-PSE operators.** The PSE scheme is well suited for solving elliptic problems [5]. It is based on replacing the differential operator in the governing equation by an integral operator involving a kernel function used to approximate the Laplacian. The integral is then discretized by a quadrature over the particle positions. The method has been extended to approximate arbitrary differential operators with arbitrary order of convergence [7]. The integration kernels are determined by moment conditions up to the desired order of accuracy [7]. The method induces two types of errors, the first due to approximating the differential operator by an integral one (mollification) and the second due to the quadrature (discretization) of the integral. To guarantee consistency of the discretized operator, the ratio $h/\epsilon$ between the interparticle spacing $h$ (defined as the $d$th root of the average particle volume in $\mathbb{R}^d$) and the width $\epsilon$ of the operator kernel has to tend to zero as both parameters do. In addition, the sampling condition of the quadrature requires that $h/\epsilon < 1$.

Both constraints can be alleviated by replacing the continuous moment conditions for the integration kernel by discrete ones [37]. It has been demonstrated that such DC PSE kernels ensure that the quadrature error cannot dominate the overall order of accuracy. DC-PSE operators are hence always consistent, independent of the value of the ratio $h/\epsilon$, leading to the desired rate of convergence for any resolution, both on uniform Cartesian and irregular particle distributions, as well as near boundaries. DC-PSE operators also do not require the first condition, allowing the kernel width $\epsilon$ to become arbitrarily small for a constant interparticle spacing $h$. In the limit,
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this includes finite-difference stencils as a special case [37]. We briefly recall the formulation of DC-PSE operators, including the determination of the corresponding kernel parameters.

In the PSE formulation, partial derivatives of order $\vec{\beta}$, evaluated at location $\vec{x}$,

$$D^{\vec{\beta}} \Phi(\vec{x}) = \frac{\partial^{\vec{\beta}} \Phi(\vec{x})}{\partial x_1^{\beta_1} \ldots \partial x_d^{\beta_d}},$$

are approximated by discrete operators of the type

$$D_h^{\vec{\beta}} \Phi(\vec{x}) = \frac{1}{e^{||\vec{\beta}||}} \sum_{p \in V(\vec{x}, h, r_c)} h^d(\Phi(\vec{x}_p) + (-1)^{||\vec{\beta}||+1} \Phi(\vec{x})) \eta^{\vec{\beta}}(\vec{x}, \vec{x}_p, \epsilon),$$

where $|\vec{\beta}| = \sum_{j=1}^d \beta_j$. The interparticle spacing (i.e., the resolution of the method) is $h$, and $d$ is the dimension of the space (here: $d = 1$ or 3). This formulation results from the approximation of the differential operator by an integral one involving the kernel function $\eta^{\vec{\beta}}$, followed by discretizing the integral by a quadrature over the particle positions $\vec{x}_p$ [37]. Efficient computation of this operator involves defining a cut-off radius $r_c$, such that the sphere $S(\vec{x}, r_c)$ with radius $r_c$ approximates the support of $\eta^{\vec{\beta}}$.

The index $p$ runs over particles and $V(\vec{x}, h, r_c)$ is the set of particles that are located inside $S(\vec{x}, r_c)$. The kernel $\eta^{\vec{\beta}}(\vec{x}, \vec{x}_p, \epsilon)$ is chosen according to the template [37]

$$\eta^{\vec{\beta}}(\vec{x}, \vec{x}_p, \epsilon) = \left( \sum_{|\gamma|=\alpha_{\text{min}}}^{\beta_1+m-1} a_{\gamma}(\vec{x}) \left( \frac{\vec{x} - \vec{x}_p}{\epsilon} \right)^|\gamma| e^{-|\vec{x} - \vec{x}_p|^2} \right)^{\vec{\beta}}.$$

where $m$ is the convergence order of the approximation, $\alpha_{\text{min}}$ is equal to 1 if $|\vec{\beta}|$ is even and 0 otherwise, and the coefficients $a_{\gamma}(\vec{x})$ are determined by solving the following linear system of equations, resulting from the discrete moment conditions up to order $m-1$:

$$\sum_{|\gamma|=\alpha_{\text{min}}}^{\beta_1+m-1} a_{\gamma}(\vec{x}) w_{\vec{\alpha}+\vec{\gamma}}(\vec{x}) = (-1)^{|\vec{\beta}|} \beta_1^{\vec{\beta}} \delta_{\vec{\alpha} \vec{\beta}}$$

for any vector $\vec{\alpha}$ such that $\alpha_{\text{min}} \leq |\vec{\alpha}| \leq |\vec{\beta}|+m-1$. The Kronecker symbol $\delta_{\vec{\alpha} \vec{\beta}}$ is equal to 1 if the two vectors $\vec{\alpha}$ and $\vec{\beta}$ are identical, 0 otherwise. The symbol $\beta_1^{\vec{\beta}} = \prod_{j=1}^d \beta_j!$ denotes the product of the factorials of each component of $\vec{\beta}$. The weights $w_{\vec{\alpha}+\vec{\gamma}}(\vec{x})$ are

$$w_{\vec{\alpha}+\vec{\gamma}}(\vec{x}) = \frac{1}{\epsilon^{\vec{\alpha}+\vec{\gamma}+d}} \sum_{p \in V(\vec{x})} h^d(\vec{x} - \vec{x}_p)^{\vec{\alpha}+\vec{\gamma}} e^{-|\vec{x} - \vec{x}_p|^2}.$$

We solve (2.2) by iterating the equivalent unsteady formulation

$$\frac{\partial \Phi(\vec{x}, t)}{\partial t} = \sigma_1 \nabla^2 \Phi(\vec{x}, t) - S(\vec{x}), \quad \vec{x} \in \Omega_1,$$

to steady state [6]. This amounts to solving the corresponding diffusion equation. We do this separately for each subdomain $\Omega_i$, considering the corresponding boundary and interface conditions (2.3) and (2.4). An arbitrary initial condition $\Phi(\vec{x}, 0)$ can be used. Alternatively, iterative solvers can be used. Successive overrelaxation or preconditioning can be used to accelerate convergence.
Imposing the continuity conditions (2.3) is trivial, since the method (by construction) adjusts the $\Phi$ values of particles located on either side of the interface to ensure continuity. No special treatment is hence required. The interface conditions related to the gradients (2.4) are less obvious. We present two methods for handling these inhomogeneous boundary conditions: the first is based on a combined immersed method with implicit determination of the interface location using a phase-field-like equation; the second uses a continuum smoothing approach of the discontinuities at the interface.

4.2. The immersed interface (II) method. Enforcing boundary or interface conditions amounts to imposing values of $\Phi$ on specific particles. We first consider a variant of the immersed interface method, where these particles are called immersed ghost particles (IGPs). For the interface $\Gamma_i$, they are located inside subdomain $\Omega_{i+1}$ within a tube/band of width $r_c$, the cut-off radius of the PSE operator. It is possible to find the interface intercept point (IIP) corresponding to the projection of the IGP onto the interface as shown in Figure 4.1. Mirroring the IGP about this point yields the image point (IP) in subdomain $\Omega_i$. The IP does not need to coincide with any “regular” particle in $\Omega_i$. The solution at the IP position is hence computed by interpolation from the neighboring particles. For second-order accuracy, linear interpolation from the nearest neighbors is sufficient, but higher-order methods are also available [40, 30].

For simplicity, we restrict ourselves to the second-order case. We first discuss the enforcement of the normal derivative condition (2.4) at interfaces and then explain how inhomogeneous Dirichlet and Neumann conditions can be imposed at boundaries.

The normal derivative of $\Phi$ at the IIP can be approximated using a (in this case) first-order Taylor expansion:

\[
\Phi_{\text{IGP}} = \Delta l \left. \frac{\partial \Phi}{\partial n} \right|_{\text{IIP}} + \Phi_{\text{IP}}.
\]
This approximation results in a total error of order $O(\Delta t^2) + O(\frac{h^2}{\Delta t})$, where $h$ is the interparticle spacing and $\Delta t$ the distance between the IGP and the IP (see Figure 4.1). $\Phi$ can expressed as a second-order expansion in terms of the coordinates $x_j$. In three dimensions, e.g., this expansion reads

$$\Phi(x_1, x_2, x_3) = C_1 x_1 x_2 x_3 + C_2 x_1 x_2 + C_3 x_2 x_3 + C_4 x_1 x_3 + C_5 x_1 + C_6 x_2 + C_7 x_3 + C_8.$$  

The coefficients $C_i$ are computed as

$$C = X^{-1} \Phi,$$

where in three dimensions, $C = (C_1, \ldots, C_8)$, and $\Phi = (\Phi_1, \ldots, \Phi_8)$ is the vector of solution values at the neighboring particles. The matrix $X$ is given by

$$
\begin{bmatrix}
  x_1 x_2 x_3 |_1 & x_1 x_2 |_1 & \ldots & x_3 |_1 \\
  \vdots & \vdots & \ddots & \vdots \\
  x_1 x_2 x_3 |_8 & x_1 x_2 |_8 & \ldots & x_3 |_8 
\end{bmatrix},
$$

where the monomials are evaluated at the positions of the 8 nearest-neighbor particles 1, \ldots, 8. To enforce condition (2.4), $\frac{\partial \Phi}{\partial n} |_{\text{IP}}$ is evaluated from (2.4) with the right-hand side evaluated using $\Phi$ on $\Omega_{i+1}$.

The same procedure is used to impose boundary conditions at the internal boundary of $\Omega$ (if it exists) and the external boundary of $\Omega_N$. In particular, an (inhomogeneous) Dirichlet condition can be imposed on the former by approximating $\Phi$ at the IGP using a first-order Taylor expansion

$$\Phi_{\text{IGP}} = 2\Phi_{\text{IP}} - \Phi_{\text{IP}}.$$  

This approximation results in a total error of order $O(\Delta t^2) + O(h^2)$. Using the prescribed value at IIP and the interpolated value at IP enables one to impose a consistent solution value at the IGP. An (inhomogeneous) Neumann condition at the external boundary of $\Omega_N$ is treated as an interface condition with a fictitious subdomain $\Omega_{N+1}$ with zero diffusivity.

Prescribing boundary or interface conditions requires determining the location of the corresponding interface. This can, e.g., be done using a phase-field method [42], which is a level-set method with an additional partial differential equation describing the evolution of the phase field $\psi$. The zero level set of $\psi$ represents the interface. The function $\psi$ is represented on the same set of particles as $\Phi$ [14]. The phase-field evolution equation is derived from an interface advection equation by expressing the interface normal and curvature in terms of a hyperbolic tangent profile across the interface, as shown in Figure 4.2. Since we are not considering curvature-driven interface motion, a correction term is used in the phase-field equation to cancel such motion [10]. Also, since the interfaces between the subdomains are stationary, no interface advection occurs. The phase-field partial differential equation hence simplifies to

$$\frac{\partial \psi}{\partial t} = \nabla^2 \psi + \frac{\psi}{w^2}(1 - \psi^2) - |\nabla \psi| \nabla \left( \frac{\nabla \psi}{|\nabla \psi|} \right).$$  

The parameter $w$ controls the width of the transition region. Away from the interface $\psi$ asymptotically converges to $\pm 1$ in $\Omega_i$ and $\Omega_{i+1}$, respectively. A simple step function can be used as initial condition for $\psi$ in the above equation, which is then solved using DC-PSE operators as described in section 4.1.
In practice, interfaces between $N$ subdomains are considered. This can, e.g., be done by shifting the initial $\psi$ in each subdomain by a predefined value (e.g., the integer $i$), such that each interface corresponds to phase-field contours of a given level. As there is no interface physics involved in the present phase field, the interface is no longer considered diffuse and the method shares some similarities with level-set methods. The use of the evolution equation (4.10), however, renders level-set reinitialization unnecessary and better generalizes to arbitrary, non-Cartesian particle distributions. Interface normals and curvatures can be calculated from the phase field in a straightforward way and used to compute the IP locations. The present phase field is related to a signed distance function to the interface $D$ by

$$
\psi(\vec{x}) = -\tanh\left(\frac{D(\vec{x})}{\sqrt{2w}}\right)
$$

and the interface location corresponds to $D = 0$.

For each $\Omega_i$, bounded by $\Gamma_{i-1}$ and $\Gamma_i$, the IGP are determined by selecting all neighbors of particles inside $\Omega_i$ within $D < r_c$ to either $\Gamma_{i-1}$ or $\Gamma_i$. An example is shown in Figure 5.7.

4.3. The continuum surface reaction (CSR) method. As an alternative to determining a sharp interface, one can use a smoothing technique to impose the related conditions. This has been described in the literature under various names, including regularization techniques [8, 27, 48, 49], continuum surface methods [3, 31], diffuse interfaces [16], and continuous immersed boundary methods [29]. Compared to the method described in the previous section, this approach alleviates interface topology constraints by not requiring any explicit or implicit determination of the interface location.

Here we consider the possibility of transforming the original Poisson equation (2.2) with inhomogeneous normal-derivative conditions (2.4) into an equivalent Poisson
problem with homogeneous Neumann boundary conditions by including an additional nonzero source term near interfaces. This is inspired by a related approach used for modeling surface tension in multiphase flows [3], which has recently been adapted to Neumann and Robin boundary conditions for advection-diffusion problems discretized using SPH [31]. The approach uses a smoothing kernel to produce a diffuse interface.

The discontinuous indicator function $\chi_i$ of a closed subdomain $\Omega_i$ is defined as

$$
\chi_i(\vec{x}) = \begin{cases} 
1, & \vec{x} \in \Omega_i \setminus \Gamma_i, \\
0, & \vec{x} \in \Omega_{i+1} \setminus \Gamma_i, \\
1/2, & \vec{x} \in \Gamma_i \cap \Omega_{i+1}.
\end{cases}
$$

(4.12)

In the CSR approach, we apply a smoothing functional $S$, such that $S(\chi_i)$ smoothly varies from 1 to 0 over a distance of order $O(w)$. The smoothing length $w$ is chosen to be comparable to the resolution of the spatial discretization near the interface. This replaces the boundary-value problem at the interface by an approximate continuous problem across the interface. The interface where the diffusion coefficient discontinuously changes from $\sigma_i$ to $\sigma_{i+1}$ is hence replaced by a continuous transition, and condition (2.4) is no longer needed at the interface. In the general case of more than two subdomains with different coefficients, the indicator function takes a different integer value in each subdomain. For the following derivation, however, we restrict ourselves to the case of two subdomains. A three-subdomain case is shown in the benchmarks section.

We start by considering the flux density difference $S_s^i$ across interface $\Gamma_i$:

$$
S_s^i(\vec{x}_s) = \sigma_i \nabla \Phi(\vec{x}_s^-) \cdot \vec{n}(\vec{x}_s) - \sigma_{i+1} \nabla \Phi(\vec{x}_s^+) \cdot \vec{n}(\vec{x}_s)
$$

(4.13)

with

$$
\vec{x}_s^- \in \Gamma_i^-, \; \vec{x}_s^+ \in \Gamma_i^+ 
$$

(4.14)

for $i = 1, \ldots, N - 1$ and

$$
S_s^N(\vec{x}_s) = \sigma_N \nabla \Phi(\vec{x}_s^-) \cdot \vec{n}(\vec{x}_s). 
$$

The subscript $s$ in the previous equation means that the subscripted quantity is evaluated on a surface.

The original unsteady Poisson problem

$$
\frac{\partial \Phi(\vec{x}, t)}{\partial t} = \sigma_i \nabla^2 \Phi(\vec{x}, t) - S(\vec{x}), \; \vec{x} \in \Omega_i,
$$

(4.15)

$$
\Phi(\vec{x}, 0) = \Phi_0(\vec{x}),
$$

(4.16)

$$
\Phi(\vec{x}_s^-, t) = \Phi(\vec{x}_s^+, t), \; \vec{x}_s^- \in \Gamma_i^-, \; \vec{x}_s^+ \in \Gamma_i^+,
$$

(4.17)

$$
S_s^i(\vec{x}_s) = \sigma_i \nabla \Phi(\vec{x}_s^-) \cdot \vec{n}(\vec{x}_s) - \sigma_{i+1} \nabla \Phi(\vec{x}_s^+, t) \cdot \vec{n}(\vec{x}_s), \; \vec{x}_s \in \Gamma_i,
$$

(4.18)

can then be reformulated as:

$$
\frac{\partial \Phi(\vec{x}, t)}{\partial t} = \sigma_i \nabla^2 \Phi(\vec{x}, t) - S(\vec{x}) - S_s^i(\vec{x}), \; \vec{x} \in \Omega_i,
$$

(4.19)

$$
\Phi(\vec{x}, 0) = \Phi_0(\vec{x}),
$$

(4.20)

$$
\Phi(\vec{x}_s^-, t) = \Phi(\vec{x}_s^+, t), \; \vec{x}_s^- \in \Gamma_i^-, \; \vec{x}_s^+ \in \Gamma_i^+,
$$

(4.21)

$$
S_s^i(\vec{x}_s) = 0, \; \vec{x}_s \in \Gamma_i.
$$

(4.22)
The additional source term \( S^i_v(x) \) in (4.19) can be expressed in terms of \( S_i^v(x_s) \), as we will show hereafter. In practice, condition (4.21) is automatically satisfied, so there is no need to take it into account. The problem can be formulated for the entire domain \( \Omega \) as

\[
\frac{\partial \Phi(x, t)}{\partial t} = \sigma(x) \nabla^2 \Phi(x, t) - S(x) - S_v(x), \quad x \in \Omega = \bigcup_{i=1}^{N} \Omega_i,
\]

with boundary condition

\[
S_v(x_s) = 0, \quad x_s \in \Gamma = \Gamma_N,
\]

and

\[
\sigma(x) = \sigma_i, \quad x \in \Omega_i.
\]

This boundary condition can also be automatically satisfied by treating \( S^N_v \) as presented below. The function \( S_v \) in (4.23) is the prolongation of the \( S^i_v \) over \( \Omega \), i.e., \( S^i_v \) is the restriction of \( S_v \) on \( \Omega_i \cup \Omega_i+1 \). All \( S^i_v \) vanish everywhere except near the corresponding interfaces.

Smoothing of the indicator function \( \chi_i \) of each subdomain \( \Omega_i \) can be achieved by the convolution

\[
S(\chi_i)(x) = \int_{\Omega_i \cup \Omega_i+1} \chi_i(y) G(x - y, T_w) \, dy, \quad x \in \Omega_i \cup \Omega_i+1,
\]

where the kernel \( G \) can be taken, e.g., as a Green’s function of the Poisson problem:

\[
G(z, t) = \frac{1}{(4\pi t)^{\frac{d}{2}}} e^{-\frac{z^2}{4t}}.
\]

The parameter \( T_w \) tunes the interface width \( w \), but there is no simple explicit relation between \( T_w \) and \( w \). The smoothing function \( S(\chi_i) \) is efficiently found as the solution at time \( t = T_w \) of the diffusion problem

\[
\frac{\partial u(x, t)}{\partial t} = \Delta u(x, t), \quad x \in \Omega_i \cup \Omega_i+1, \quad t \in [0, T_w],
\]

with initial condition

\[
u(x, 0) = \chi_i(x), \quad x \in \Omega_i \cup \Omega_i+1,
\]

so that

\[
S(\chi_i)(x) = u(x, T_w).
\]

The gradient of \( S(\chi_i) \) can be expressed as

\[
\nabla S(\chi_i)(x) = \int_{\Omega_i \cup \Omega_i+1} \chi_i(y) \nabla_x G(x - y, T_w) \, dy.
\]

Decomposing the integral as a sum of two integrals over the subdomains, using the definition of \( \chi_i(x) \), and applying the divergence theorem leads to

\[
\nabla S(\chi_i)(x) = \int_{\Omega_i} \nabla_x G(x - y, T_w) \, dy
\]

\[
= \int_{\Gamma_i} n(x_s) G(x - y_s, T_w) \, dy_s
\]

\[
= \int_{\Gamma_i} \hat{n}(x_s) \int G(x - y_s, T_w) \, dy_s + O\left(\frac{w^{d-1}}{\rho^{d-1}}\right).
\]
In the last equation, which results from a Taylor expansion, \( x_s \) denotes the closest point to \( x \) on \( \Gamma_i \), and \( \rho \) is the radius of normal curvature at \( x_s \). If the kernel \( G \) has bounded support, the part of the interface contributing to the integral is of order \( O(w^{d-1}) \). Assuming that the point \( x \) lies within a distance \( w \) of \( \Gamma_i \), letting \( w \) tend to zero implies that

\[
(4.35) \quad \lim_{w \to 0} n(x) \cdot \nabla S(\chi_i)(x) = \lim_{w \to 0} \int_{\Gamma_i} \delta(x - y, T_w) \, dy = 1 \quad \forall \Gamma_i \leq w.
\]

This results from letting both \( x \) and \( G \) tend toward \( x_s \) and from the Dirac function \( \delta \) as \( w \) vanishes. This also implies that

\[
(4.36) \quad \lim_{w \to 0} n(x) \cdot \nabla S(\chi_i)(x) S_s(x) = S_s(x) \quad \forall \Gamma_i \leq w.
\]

Therefore, if the function \( S_s^i \) is defined as

\[
(4.37) \quad S_s^i(x) = S_s^i(x) n(x) \cdot \nabla S(\chi_i)(x), \quad x \in \Omega_i \cup \Omega_{i+1},
\]

it tends to \( S_s^i \) as the interface width \( w \) tends to zero. The regularization is hence consistent.

Using (4.27) and (4.31), the gradient of the smoothed indicator function can be expressed as

\[
\nabla S(\chi_i)(x) = \frac{1}{2T_w} \int_{\Omega_i \cup \Omega_{i+1}} \chi_i(y) (x - y) G(x - y, T_w) \, dy
\]

\[
= \frac{1}{2T_w} \left( x \int_{\Omega_i \cup \Omega_{i+1}} \chi_i(y) G(x - y, T_w) \, dy - \int_{\Omega_i \cup \Omega_{i+1}} \chi_i(y) G(x - y, T_w) \, dy \right)
\]

\[
(4.38) \quad = \frac{1}{2T_w} \left( x \nabla S(\chi_i)(x) - S(I \times \chi_i)(x) \right),
\]

where \( I \) is the identity function and the function \( I \times \chi_i \) is defined as \( I \times \chi_i(x) = \chi_i(x) \).

Therefore, the source term \( S_s(x) \) can be expressed as

\[
(4.39) \quad S_s^i(x) = \frac{S_s^i(x)}{2T_w} n(x) \cdot \left( x \nabla S(\chi_i)(x) - S(I \times \chi_i)(x) \right), \quad x \in \Omega_i \cup \Omega_{i+1}.
\]

### 4.4. Implementation and additional remarks.

The main steps of the algorithmic implementations of the above methods are given in Tables 4.1 and 4.2. After initializing the particle positions (Step 2), some preliminary calculations are performed before solving the Poisson problem. Verlet lists [51] are used to efficiently find the neighbors of each particle (Step 3). They are needed in Steps 4, 6, 8, and 9 for operator evaluations and field updates at the IGPs. According to the method variant—II or CSR—the interfaces are either implicitly determined by solving a phase-field equation for signed-distance functions \( D_i \), or smoothed fields are generated using a few diffusion steps to compute the boundary reaction term \( S_s \) (Step 6). Normal vectors are computed at particles near the interfaces (Step 7) to determine the IGPs or the reaction term (Step 8). Finally, the Poisson problem is solved iteratively to steady state (Step 9 and Table 4.2).

The continuity equation (2.3) is implicitly satisfied by both methods. Homogeneous Neumann conditions are automatically imposed by the DC-PSE scheme, since
either somehow compensate for the drift or stop the solver before a wave develops. This causes the isocontour defining the interface to drift. Although predicted that a traveling wave develops if

\[ f \]

from the transition region. From the theory of reaction-diffusion systems, it can be predicted that a traveling wave develops in the solution \( \Phi \) after a certain number of solver iterations. This causes the isocontour defining the interface to drift. Although this issue has not been mentioned before [42], it is important to be aware of it, as the interface location is used to impose the interface conditions. In practice, one should either somehow compensate for the drift or stop the solver before a wave develops.

The two integral terms \( S(\chi_1)(\vec{x}) \) and \( S(I \times \chi_1)(\vec{x}) \) in (4.39) are computed by solving a heat equation that is equivalent to convolving with Green’s function, as outlined in section 4.3. In practice, a few pseudo-time-steps of the diffusion problem discretized with an explicit time-stepping scheme are sufficient, rendering evaluation of the reaction term \( S^0_\beta \) efficient. Alternatively, one could use fast Gauss transforms [11, 45, 41] or fast Fourier transforms [21].
Due to interface smoothing, the value of $\nabla \Phi$ in the CSR method is incorrect in a small region close to the external boundary $\Gamma_N$. The extent of that region is controlled by the parameter $w$. If one needs to compute the solution gradient close to the external boundary, it can be extrapolated from $\Phi$ values outside the smoothed region. Alternatively, the II method can be used to enforce the corresponding Neumann condition.

5. Results. We present results from numerical experiments confirming the expected order of accuracy of the proposed methods. We further compare the two methods with respect to their accuracy and computational cost. The accuracy of the methods is evaluated using the $\ell^2$ and $\ell^\infty$ norms of the relative errors at the particle locations with respect to the analytical solution (see section 3). We consider both regular Cartesian particle distributions and irregular (random) particle distributions.

5.1. 1D dipole in a two-region domain. This simple test case as introduced in section 3.1 enables verification of the correct imposition of the interface conditions. Here, the source term $S$ in (4.6) vanishes. The analytical solution for $\Phi$ is a piecewise linear function. We only report results using the CSR method, as the imposition of interface and boundary conditions with the II method is trivial in one dimension. Figure 5.1 visualizes the solution for regular particle distributions of different resolutions $h$. As expected, the computed solution approaches the analytical one as the number of particles is increased. In the smoothed regions around the interfaces and boundaries, the solution deviates due to the imposition of the homogeneous Neumann conditions. The width of these regions decreases with decreasing interparticle spacing.

The surface reaction function $S_v$ is plotted for the same case in Figure 5.2 for different $h$. As expected, $S_v$ tends toward a one-sided Dirac function as $h$ decreases. The relative errors as a function of the number of particles are shown in Figure 5.3. The convergence is second order, as expected from the use of second-order DC-PSE.

**Fig. 5.1. Solution of the 1D test case with $\Phi_0 = 4000$, $F_1 = 20$, and $F_2 = 80$ for four different interparticle spacings $h = 2$ (crosses), 1 (circles), 0.5 (dotted line), and 0.25 (dashed line) with regular Cartesian particle distributions. The solid line corresponds to the analytical solution. The dashed line corresponding to $h = 0.25$ is visually indiscernible from the analytical solution.**
The CSR surface reaction term \( S_v(x) \) in the 1D test case with regular particle distributions for four different interparticle spacings \( h = 2 \) (dotted line with stars), 1 (dashed line with urchins), 0.5 (dashed line), and 0.25 (dotted line with squares).

As required by (4.35), as the diffuse interface width \( w \) is decreased, the dot product \( \vec{n}(\vec{x}) \cdot (\vec{E}_S(\chi_i)(\vec{x}) - S(\vec{I} \times \chi_i)(\vec{x})) \) numerically tends to 1.

We also repeat the same test case for irregularly distributed particles. We generate random irregular particle distributions by initially placing particles on a regular Cartesian lattice of resolution \( h \) and then perturbing the particle positions by adding uniformly distributed random numbers in \([-h/2, h/2]\). We then plot errors with respect to the average spacing \( h \). The resulting convergence plot for the irregular case is shown in Figure 5.4. As expected, the error magnitudes are larger in the irregular case. However, the method still converges with the desired rate, indicating its consistency also on irregularly distributed sets of particles. The solution profiles for the irregular case are shown in Figure 5.5. The plot of the CSR surface reaction term for the irregular case is not shown, since it is visually indistinguishable from Figure 5.2.

5.2. 3D multilayered spherical domain. We consider the test case introduced in section 3.2 with radii \( R_1 = 32, R_2 = 56, \) and \( R_3 = 80 \). For both the CSR and II methods, a Dirichlet boundary condition is imposed on an additional internal sphere of radius \( R_0 = 16 \) using the II method. The source term \( S \) in (4.6) is not present.

Figure 5.6 shows an example solution plotted along the line \( y = z = 0 \) and obtained with the II method with \( h = 2 \). For all smaller values of \( h \) tested, the numerical and analytical solution profiles are visually indistinguishable and hence not shown in the plot. The IGPs for the imposition of the interface conditions are shown in Figure 5.7. The relative errors in the solution \( \Phi \) are shown in Figure 5.8 as a function of the interparticle spacing \( h \). Convergence is of order two, as expected from the use of second-order DC-PSE kernels.
Fig. 5.3. Relative errors versus total number of particles in the 1D test case for regular Cartesian particle distributions. We show the $\ell^2$ (triangles) and $\ell^\infty$ (squares) norms of the errors at the particle locations. The dotted line with plus symbols corresponds to the theoretical second-order convergence.

Fig. 5.4. Relative errors versus total number of particles in the 1D test case for an irregular particle distribution (see text for details). We show the $\ell^2$ (triangles) and $\ell^\infty$ (squares) norms of the errors at the particle locations. The dotted line with plus symbols corresponds to the theoretical second-order convergence.
Fig. 5.5. Solution of the 1D test case with \( \Phi_0 = 4000, F_1 = 20, \) and \( F_2 = 80 \) for four different average interparticle spacings \( h = 2 \, \text{(crosses)}, 1 \, \text{(circles)}, 0.5 \, \text{(dotted line), and 0.25 (dashed line)} \) with irregular particle distributions. The solid line corresponds to the analytical solution.

Fig. 5.6. Solution profile for the II method in the 3D benchmark, plotted along the \( x \)-axis. The circles show the solution at the particle locations for \( h = 2 \). The parameters of the test case are \( R_0 = 16, R_1 = 32, R_2 = 56, R_3 = 80, \Phi_0 = 5000, \frac{A_1}{R_1} = -20, \frac{A_2}{R_2} = -40, \) and \( \frac{A_3}{R_3} = -60 \). The solid line shows the analytical solution.

The influence of the particle spacing \( h \) on the solution computed using the CSR method is shown in Figure 5.9 along the \( y = z = 0 \) line. As in the 1D case, increasing the number of particles improves the solution quality. The corresponding relative errors are shown in Figure 5.10. The order of convergence is again two, as expected.
Fig. 5.7. Immersed ghost particles (IGPs, filled circles) near the interfaces and the external boundary in the 3D test case for $h = 2$ and regularly distributed particles. The solid lines show the true interface locations. IGPs from different subdomains are shown in different shades of gray.

Fig. 5.8. Relative errors versus interparticle spacing $h$ in the 3D test case for the II method with regularly distributed particles. We show the $\ell^2$ (squares) and $\ell^\infty$ (diamonds) norms of the errors at the particle locations. The solid lines correspond to second-order convergence.

Compared to the errors obtained with the II method, however, the errors of the CSR method are about one order of magnitude larger. This is caused by the larger local absolute error. This is the price one pays for CSR's better ability to handle complex interface geometries, as interface detection is an implicit part of computing.
Fig. 5.9. Solution profile for the CSR method in the 3D benchmark, plotted along the x-axis. The circles show the solution at the particle locations for $h = 1$ (filled circles) and $h = 4$ (open circles). The parameters of the test case are $R_0 = 16$, $R_1 = 32$, $R_2 = 56$, $R_3 = 80$, $\Phi_0 = 5000$, $\frac{A_1}{R_2} = -20$, $\frac{A_2}{R_2} = -40$, and $\frac{A_3}{R_2} = -60$. The solid line shows the analytical solution.

Fig. 5.10. Relative errors versus interparticle spacing $h$ in the 3D test case for the CSR method with regularly distributed particles. We show the $\ell^2$ (squares) and $\ell^\infty$ (diamonds) norms of the errors at the particle locations. The solid lines correspond to second-order convergence.

The smoothed functions involved in the source term $S_v$ (cf. Step 6 in Table 4.1 and (4.39)).

The error plots when using random irregular particle distributions (obtained as described above) are shown in Figure 5.11) for the II method and in Figure 5.12 for the CSR method. Global second-order convergence with the average particle spacing is observed in all cases.
5.3. 3D domain with two inclusions. As an additional test case we consider a spherical domain with two inclusions of different diffusivity, as shown in Figure 5.13. The main sphere is of radius 80 and centered at the origin of the coordinate system. The inclusions have radii 24 and 16, respectively, and their centers are at $(-32, 0, 0)$ and $(48, 0, 0)$. As no analytical solution is available for this case, we compare our results with results obtained by a finite-element method with refined mesh. Figure 5.13
Inhomogeneous Dirichlet boundary conditions are used for both inner spheres (left: $\Phi = 5000$, right: $\Phi = 10000$). The potential normal gradient on the outer surface is imposed to be $-50$.

shows a 2D view of the solution in the plane $z = 0$ with contours corresponding to iso-values on a regular scale. The corresponding solution profile along the line $y = z = 0$ is shown in Figure 5.14 in comparison with the finite-element solution. We only show results for the II method, as those for the CSR method look indistinguishable.
6. Conclusions. We have presented a meshless particle method for solving discontinuous-coefficient Poisson and diffusion problems in domains with arbitrary boundary conditions. The method is based on using discretization-corrected PSE operators (DC-PSE) and a domain-decomposition approach. The main contribution is the imposition of inhomogeneous conditions at interfaces between subdomains and at internal and external boundaries. Two variants of the method have been proposed and compared. The first is based on an II approach, which explicitly determines the interface location. To do so, we proposed a simplified phase-field equation to locate the interfaces. The second variant is based on a regularization technique that transforms the inhomogeneous interface conditions to homogeneous ones with an additional continuous volume contribution to the Poisson equation. We have tested the methods in 1D and 3D benchmarks for which analytical solutions can be derived. Both methods show the proper order of convergence, both for regular and irregular particle distributions. The error levels of the CSR method are generally higher than those of the II method. The CSR method, however, is better suited for complex interface geometries, and it is easier to implement to integrate into existing solvers.

Both presented methods are particle extensions of well-known approaches [28, 31]. We have used DC-PSE operators in the presented work, but the II and CSR methods are more generally applicable, provided the discretization remains consistent on irregular particle distributions. The focus here was on imposing interface and boundary conditions in a domain-decomposition setting, and on transforming inhomogeneous interface conditions to homogeneous ones using the CSR framework. This possibly outlines a generic strategy that could also be adapted to other numerical schemes. The method could also be extended to reaction-diffusion problems with discontinuously varying diffusion coefficients and to more general problems involving convection, reaction, and diffusion where specific conditions must be imposed at interfaces. For the sake of simplicity, we have considered the case where \( \sigma \) is constant within a subdomain. Extensions to smoothly varying coefficients inside each subdomain, and to anisotropic diffusion, are straightforward using the corresponding inhomogeneous or anisotropic DC-PSE operators. The presented methods, however, are limited to domain geometries without triple points. If three or more subdomains of different coefficients meet in a single point, the present method is not applicable.

The errors of the CSR method decrease with diminishing smoothing length \( w \) of the interface. Since \( w \) is related to the particle spacing \( h \), the CSR method would benefit from locally increasing the particle density near interfaces. This could be achieved, e.g., using adaptive-resolution or self-organizing particle methods [30]. In complex geometries, the II method would also benefit from adaptive spatial resolution, as the phase fields could resolve geometric detail where needed. It also remains to be seen how the present methods affect theoretical performance models for such operators in particle methods [38].

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