A direct method for modeling and simulations of elliptic and parabolic interface problems

Kumudu Gamage(kgamage@odu.edu) And Yan Peng(ypeng@odu.edu)
Department of Mathematics and Statistics, Old Dominion University, Norfolk, VA

Abstract

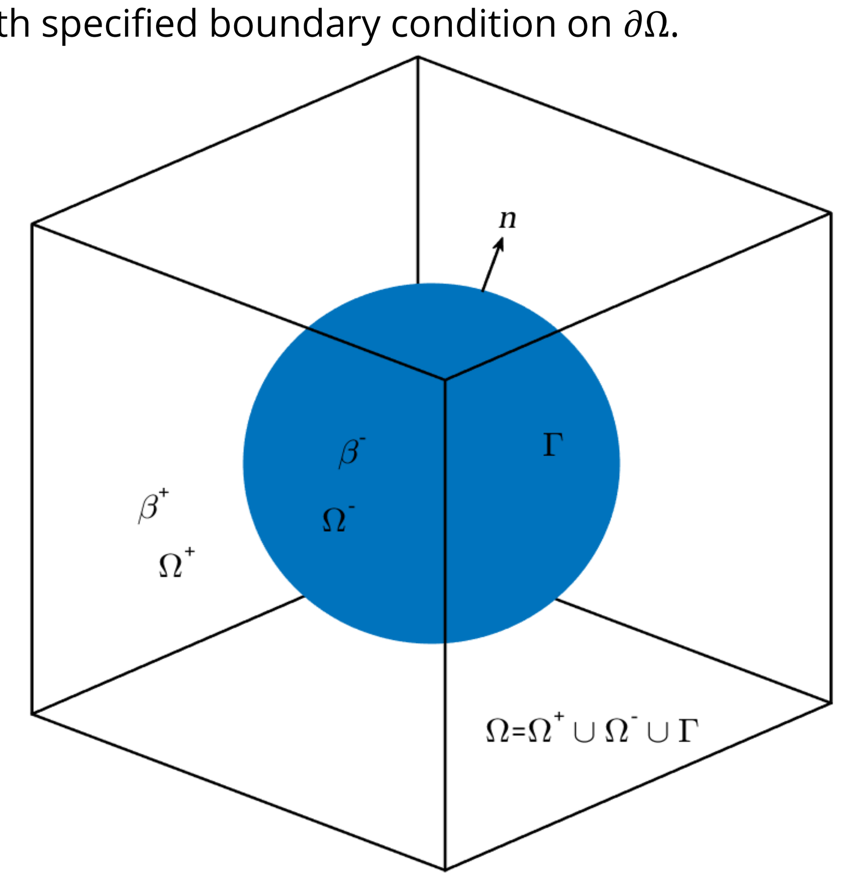
Interface problems have many applications in fluid dynamics, molecular biology, electromagnetism, material science, heat distribution in engines, and hyperthermia treatment of cancer. Mathematically, interface problems commonly lead to partial differential equations (PDE) whose input data are discontinuous or singular across the interfaces in the solution domain. Many standard numerical methods designed for smooth solutions poorly work for interface problems as solutions of the interface problems are mostly non-smoothness or discontinuous. Moving interface problems depends on the accuracy of the gradient of the solution at the interface. Therefore, it became essential to derive a method for interface problems that gives second-order accuracy for both the solution and its gradients. As most applications in the real world are in 3D settings, the development of three-dimensional elliptic interface solvers and the study of their convergence is significant. We have developed a novel Direct Method for solving three-dimensional elliptic interface problems that preserve the discontinues in solution and gradient across the interface. The method uses a standard seven-point central difference scheme at regular grid points and a compact twenty-seven-point scheme only at irregular grid points by incorporating the interface's jump conditions. The model was implemented using both MATLAB and FORTRAN routines and showed that the computed solution and gradient of the solution near the interface are second-order accurate in infinity norm. We also have modified the developed direct method to solve the 3D heat equation with fixed interfaces. Numerical results showed that the proposed method is unconditionally stable and is second-order accurate in both time and space.

Three-Dimensional elliptic Interface problem

Consider the following three-dimensional elliptic interface problem with piecewise constant coefficients.

$$\nabla.(\beta(x,y,z)\nabla u) = f(x,y,z), \quad (x,y,z) \in \Omega \backslash \Gamma$$
$$[u](\mathbf{x}) = u^+(\mathbf{x}) - u^-(\mathbf{x}) = w, \quad \mathbf{x} \in \Gamma$$
$$[\beta u_{\mathbf{n}}](\mathbf{x}) = \beta^+(\mathbf{x})u^+_{\mathbf{n}}(\mathbf{x}) - \beta^-(\mathbf{x})u^-_{\mathbf{n}}(\mathbf{x}) = v, \quad \mathbf{x} \in \Gamma$$

with specified boundary condition on $\partial\Omega$.



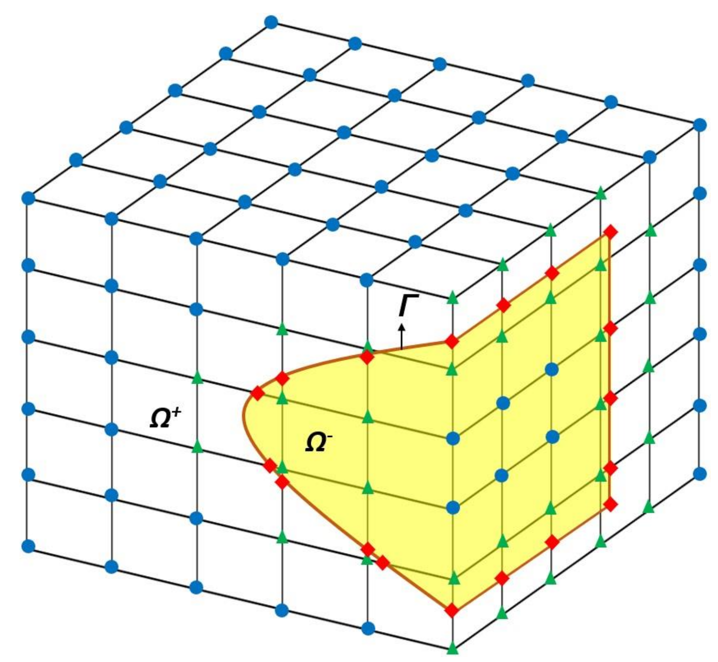
Domain Ω with a smooth interface Γ

Interface representation for computational framework

$$\Gamma = \{(x,y,z), \quad \phi(x,y,z) = 0, \quad (x,y,z) \in \Omega\}$$

Position of the interface relative to level set function ϕ is given by,

$$\phi(x,y,z) < 0 \quad \text{for} \quad (x,y,z) \in \Omega^-$$
$$\phi(x,y,z) = 0 \quad \text{for} \quad (x,y,z) \in \Gamma$$
$$\phi(x,y,z) > 0 \quad \text{for} \quad (x,y,z) \in \Omega^+$$



A cross-section of domain Ω with an interface Γ. where Solid dots are regular grid points, solid triangles are irregular grid points, solid diamonds are the control points

Finite Difference scheme for elliptic interface problem

FD scheme for a regular grid point (x_i, y_j, z_l) is the standard 7-point Laplacian. FD scheme for irregular grid point is given by,

$$\frac{U_{i-1,j,l} - 2U_{i,j,l} + U_{i+1,j,l}}{h^2} + C^x_{i,j,l} +$$
$$\frac{U_{i,j-1,l} - 2U_{i,j,l} + U_{i,j+1,l}}{h^2} + C^y_{i,j,l} +$$
$$\frac{U_{i,j,l-1} - 2U_{i,j,l} + U_{i,j,l+1}}{h^2} + C^z_{i,j,l} = \frac{f_{i,j,l}}{\beta_{i,j,l}}$$

- Correction terms $C^x_{i,j,l}, C^y_{i,j,l}$ and $C^z_{i,j,l}$, are calculated using jump conditions.

$$C^x_{i,j,l} = \sum_m^{n_s} \gamma_m U_{i+i_m, j+j_m, l+l_m} + \gamma_c$$

- n_s is the number of grid points involves in the FD scheme
- γ_m depends on β and the position of the interface relative to the grid.
- γ_c depends on jumps in the solutions, flux, and their derivatives.
- Linear system for FD scheme is $A_h U = F$

Outline of the algorithm for elliptic interface problems

Step 1: Immersed the interface into a cubic Domain and represent the interface using zero level set function
Step 2: Find regular, irregular grid points and control points
Step 3: Use standard 7-point scheme at the regular grid points
Step 4: Calculate correction terms at irregular grid points
Step 5: Find a 27-point compact scheme at irregular points
Step 6: Solve linear system $A_h U = F$
Step 7: Recover the gradients of the solution

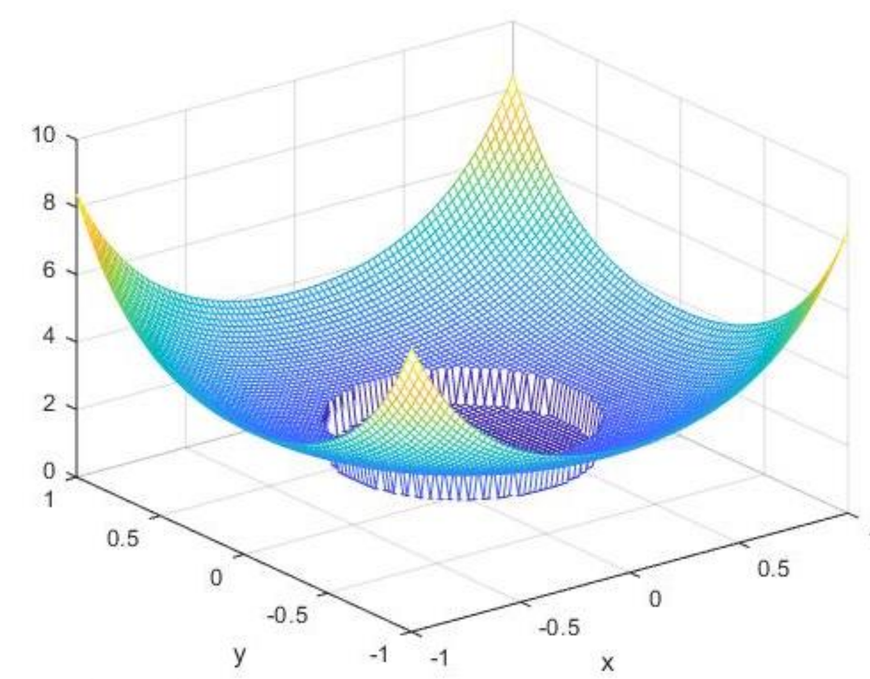
Results

Example:

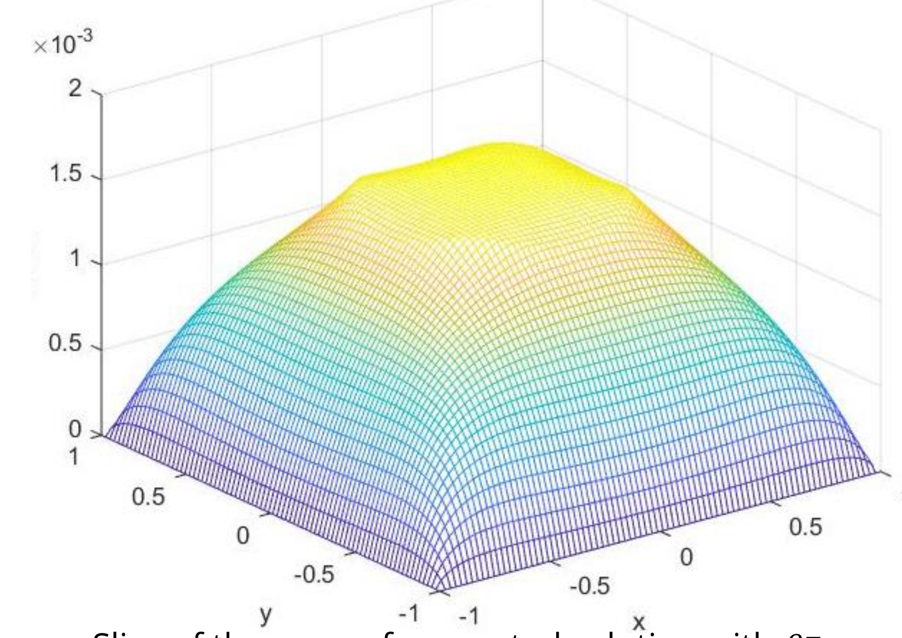
$$(\beta u_x)_x + (\beta u_y)_y + (\beta u_z)_z = f,$$
$$\Omega = [-1,1] \times [-1,1] \times [-1,1], \ \Gamma = x^2 + y^2 + z^2 - 0.25$$
$$\beta(x,y,z) = \begin{cases} \beta^- & \text{if} \quad (x,y,z) \in \Omega^- \\ \beta^+ & \text{if} \quad (x,y,z) \in \Omega^+ \end{cases}$$
$$f(x,y,z) = \begin{cases} 2\beta^- e^{r^2}(3+2r^2) & \text{if} \quad (x,y,z) \in \Omega^- \\ 2\beta^+ e^{r^2}(3+2r^2) & \text{if} \quad (x,y,z) \in \Omega^+ \end{cases}$$
$$[u] = 1, [\beta u_n] = (\beta^+ - \beta^-)e^{0.25}$$

Boundary conditions are taken from the exact solution,

$$u(x,y,z) = \begin{cases} e^{r^2} & \text{if} \quad (x,y,z) \in \Omega^- \\ e^{r^2} + 1 & \text{if} \quad (x,y,z) \in \Omega^+ \end{cases}$$



Slice of the computed solution with $\beta^- = 1$ and $\beta^+ = 10$



Slice of the error of computed solution with $\beta^- = 1$ and $\beta^+ = 10$

Grid refinement analysis with $\beta^- = 1$ and $\beta^+ = 10$

N	$E(u)$	order	$E(u_n)$	order
10	8.28E-02		1.17E-01	
20	2.34E-02	1.82	3.51E-02	1.74
40	6.20E-03	1.92	8.44E-03	2.06
80	1.58E-03	1.97	3.07E-03	1.46
160	4.01E-04	1.98	8.48E-04	1.86

Three-Dimensional parabolic Interface problem

Consider the following parabolic interface problem with piecewise constant coefficients,

$$u_t = \nabla.(\beta(x,y,z)\nabla u) - f(x,y,z), \quad (x,y,z) \in \Omega \backslash \Gamma$$
$$[u](\mathbf{x}) = u^+(\mathbf{x}) - u^-(\mathbf{x}) = w(:,t), \quad \mathbf{x} \in \Gamma$$
$$[\beta u_n](\mathbf{x}) = \beta^+(\mathbf{x})u^+_n(\mathbf{x}) - \beta^-(\mathbf{x})u^-_n(\mathbf{x}) = v(:,t), \quad \mathbf{x} \in \Gamma$$

with specified boundary and initial conditions.

Crank-Nicolson scheme for parabolic interface problem

$$\frac{U^{n+1}_{ijl} - U^n_{ijl}}{\beta \Delta t} = \frac{1}{2}(\delta_{xx}u^{n+1}_{ijl} + (C^x_{ijl})^{n+1} + \delta_{yy}u^{n+1}_{ijl} + (C^y_{ijl})^{n+1} + \delta_{zz}u^{n+1}_{ijl} + (C^z_{ijl})^{n+1} + \delta_{xx}u^n_{ijl} + (C^x_{ijl})^n + \delta_{yy}u^n_{ijl} + (C^y_{ijl})^n + \delta_{zz}u^n_{ijl} + (C^z_{ijl})^n) - \frac{f^{n+1}_{ijl} + f^n_{ijl}}{2\beta_{ijl}}$$

where, $\delta_{xx}u^n_{ijl} = \dfrac{U^n_{i-1,j,l} - 2U^n_{i,j,l} + U^n_{i+1,j,l}}{h^2}$

$$(C^x_{ijl})^n = \sum \gamma^x_m U^n_{i+i_m, j+j_m, l+l_m} + (\gamma^x_c)^n$$

- γ^x_m does not depend on time
- γ^x_c depend on time

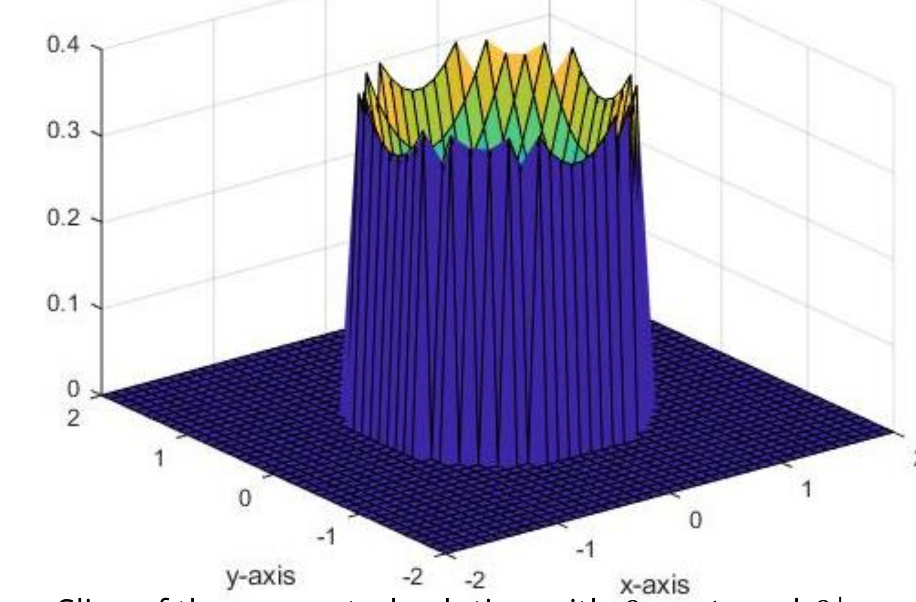
Results

Example: $u_t = (\beta u_x)_x + (\beta u_y)_y + (\beta u_z)_z - f$

$$\Omega = [-2,2] \times [-2,2] \times [-2,2], \Gamma = x^2 + y^2 + z^2 - r_0^2$$
$$\beta(x,y,z) = \begin{cases} \beta^- & \text{if} \quad (x,y,z) \in \Omega^- \\ \beta^+ & \text{if} \quad (x,y,z) \in \Omega^+ \end{cases}$$
$$f(x,y,z) = \begin{cases} 6\beta^- cos(t) + sin(t)(x^2+y^2+z^2) & \text{if} \quad (x,y,z) \in \Omega^- \\ 0 & \text{if} \quad (x,y,z) \in \Omega^+ \end{cases}$$
$$[u] = -r_0^2 cos(t), [\beta u_n] = -2\beta^- r_0 cos(t) \text{ and } r_0 = 1$$

Boundary and initial conditions were taken from the exact solution,

$$u(x,y,z) = \begin{cases} cos(t)(x^2+y^2+z^2) & \text{if} \quad (x,y,z) \in \Omega^- \\ 0 & \text{if} \quad (x,y,z) \in \Omega^+ \end{cases}$$



Slice of the computed solution with $\beta^- = 1$ and $\beta^+ = 10000$ at $T = 1$

Grid refinement analysis

N	Error	order
10	1.22E-06	
20	3.84E-07	1.67
40	9.83E-08	1.97
80	2.47E-08	1.99