Politecnico di Milano
School of Industrial and Information Engineering
M.Sc. in High Performance Computing

Hybrid thread-MPI parallelization for ADR equation

Peng Rao, **Jiali Claudio Huang**, **Ruiying Jiao**

Contents

1 Problem statement **1**
1.1 Strong formulation . . . 1
1.2 Weak formulation . . . 1
1.3 Manufactured solution . . . 3

2 Finite Element Discretization **5**
2.1 Triangulation and Finite Element Space . . . 5
2.2 Galerkin Approximation . . . 5
2.3 Algebraic System . . . 5
2.4 Treatment of Advection Dominance . . . 6

1 Problem statement

1.1 Strong formulation

Consider the following **Advection-Diffusion-Reaction** equation with mixed Dirichlet-Neumann boundary conditions:

$$\begin{cases} -\nabla \cdot (\mu \nabla u) + \nabla \cdot (\boldsymbol{\beta} u) + \gamma u = f & \text{in } \Omega, \\ u = g & \text{on } \Gamma_D \subset \partial\Omega, \\ \nabla u \cdot \boldsymbol{n} = h & \text{on } \Gamma_N = \partial\Omega \setminus \Gamma_D. \end{cases}$$

where:

- $\Omega \subset \mathbb{R}^d$ (with $d = 1, 2, 3$) is an open bounded domain with boundary $\partial\Omega$;
- $\mu > 0$ is the diffusion coefficient;
- $\boldsymbol{\beta} \in [L^\infty(\Omega)]^d$ is the advection velocity field;
- $\gamma \geq 0$ is the reaction coefficient;
- $f \in L^2(\Omega)$ is a source term;
- $g \in H^{1/2}(\Gamma_D)$ is the Dirichlet boundary data;
- $h \in L^2(\Gamma_N)$ is the Neumann boundary data;
- $\boldsymbol{n}$ is the outward unit normal vector on the boundary $\partial\Omega$.
- u is the unknown scalar function to be solved for.
- Γ_D and Γ_N are the Dirichlet and Neumann parts of the boundary, respectively.

It models how a scalar quantity u (such as concentration, temperature, or chemical potential) is distributed within a domain due to three competing physical processes: diffusion, advection, and reaction.

1.2 Weak formulation

We begin by defining the trial and test function spaces. To accommodate the non-homogeneous Dirichlet boundary condition, we introduce a *lifting function* $u_g \in H^1(\Omega)$ such that $u_g = g$ on Γ_D:

$$V_g := \{v \in H^1(\Omega) : v = g \quad \text{on } \Gamma_D\}$$

The test space is the linear subspace of $H^1(\Omega)$ with homogeneous Dirichlet boundary conditions:

$$V_0 := \{v \in H^1(\Omega) : v = 0 \quad \text{on } \Gamma_D\}$$

Consequently, we decompose the solution as $u = u_0 + u_g$, where the unknown $u_0 \in V_0$. Multiply the equation by a test function $v \in V_0$ and integrate over the domain Ω:

$$\int_{\Omega} \left(-\nabla \cdot (\mu \nabla u) + \nabla \cdot (\boldsymbol{\beta} u) + \gamma u\right) v \, d\Omega = \int_{\Omega} f v \, d\Omega$$

Using the linearity of the integral, we separate the terms:

$$-\int_{\Omega} \nabla \cdot (\mu \nabla u) v \, d\Omega + \int_{\Omega} \nabla \cdot (\boldsymbol{\beta} u) v \, d\Omega + \int_{\Omega} \gamma u v \, d\Omega = \int_{\Omega} f v \, d\Omega$$

We apply Green's first identity to the diffusion term to reduce the order of differentiation:

$$-\int_{\Omega} \nabla \cdot (\mu \nabla u) v \, d\Omega = \int_{\Omega} \mu \nabla u \cdot \nabla v \, d\Omega - \int_{\partial\Omega} (\mu \nabla u \cdot \mathbf{n}) v \, d\Gamma$$

Substituting this back into the integral equation:

$$\int_{\Omega} \mu \nabla u \cdot \nabla v \, d\Omega - \int_{\partial\Omega} (\mu \nabla u \cdot \mathbf{n}) v \, d\Gamma + \int_{\Omega} \nabla \cdot (\boldsymbol{\beta} u) v \, d\Omega + \int_{\Omega} \gamma u v \, d\Omega = \int_{\Omega} f v \, d\Omega$$

Split the boundary integral into contributions from Γ_D and Γ_N:

$$\int_{\partial\Omega} (\mu \nabla u \cdot \mathbf{n}) v \, d\Gamma = \int_{\Gamma_D} (\mu \nabla u \cdot \mathbf{n}) v \, d\Gamma + \int_{\Gamma_N} (\mu \nabla u \cdot \mathbf{n}) v \, d\Gamma$$

Since $v = 0$ on Γ_D, the first term vanishes. On Γ_N, we use the Neumann condition $\nabla u \cdot \mathbf{n} = h$:

$$\int_{\Gamma_N} (\mu \nabla u \cdot \mathbf{n}) v \, d\Gamma = \int_{\Gamma_N} \mu h v \, d\Gamma$$

Substituting back, we have:

$$\int_{\Omega} \mu \nabla u \cdot \nabla v \, d\Omega + \int_{\Omega} \nabla \cdot (\boldsymbol{\beta} u) v \, d\Omega + \int_{\Omega} \gamma u v \, d\Omega = \int_{\Omega} f v \, d\Omega + \int_{\Gamma_N} \mu h v \, d\Gamma$$

Substituting $u = u_0 + u_g$ into the equation, we get:
Find $u_0 \in V_0$ such that

$$a(u_0, v) = F(v), \quad \forall v \in V_0$$

where the *bilinear form* $a : V_0 \times V_0 \to \mathbb{R}$ is defined as:

$$a(u, v) = \int_{\Omega} \mu \nabla u \cdot \nabla v \, d\Omega + \int_{\Omega} \nabla \cdot (\boldsymbol{\beta} u) v \, d\Omega + \int_{\Omega} \gamma u v \, d\Omega$$

and the *linear functional* $F : V_0 \to \mathbb{R}$ is given by:

$$F(v) = \int_{\Omega} f v \, d\Omega + \int_{\Gamma_N} \mu h v \, d\Gamma - a(u_g, v)$$

1.3 Manufactured solution

We define the exact solution $u_{\text{ex}} : \Omega \to \mathbb{R}$ on the unit hypercube domain $\Omega = [0,1]^d$ (where $d = 2, 3$) as the product of sine functions:

$$u_{\text{ex}}(\mathbf{x}) = \prod_{i=1}^{d} \sin(\pi x_i). \tag{1}$$

This function vanishes on the boundary hyperplanes where $x_i = 0$ or $x_i = 1$, making it naturally suitable for homogeneous Dirichlet boundary conditions.

The physical coefficients for the benchmark problem are chosen as follows:

- **Diffusion:** A constant isotropic diffusion coefficient $\mu = 1.0$.
- **Reaction:** A constant reaction coefficient $\gamma = 0.1$.
- **Advection:** A rotational velocity field $\boldsymbol{\beta}(\mathbf{x})$, defined to make the problem non-symmetric:

$$\boldsymbol{\beta}(\mathbf{x}) = \begin{cases} \begin{bmatrix} -x_2 \\ x_1 \end{bmatrix} & \text{if } d = 2, \\ \begin{bmatrix} -x_2 \\ x_1 \\ 0.1 \end{bmatrix} & \text{if } d = 3. \end{cases} \tag{2}$$

Substituting u_{ex} into the governing equation $-\nabla \cdot (\mu \nabla u) + \nabla \cdot (\boldsymbol{\beta} u) + \gamma u = f$, we compute the source term f.

First, we observe that the Laplacian of the chosen exact solution is:

$$\Delta u_{\text{ex}} = \sum_{i=1}^{d} \frac{\partial^2 u_{\text{ex}}}{\partial x_i^2} = \sum_{i=1}^{d} (-\pi^2 u_{\text{ex}}) = -d\pi^2 u_{\text{ex}}. \tag{3}$$

Assuming $\boldsymbol{\beta}$ is divergence-free ($\nabla \cdot \boldsymbol{\beta} = 0$, which holds for the rotational field defined above), the advection term simplifies to $\boldsymbol{\beta} \cdot \nabla u_{\text{ex}}$. The source term f is therefore implemented as:

$$f(\mathbf{x}) = \mu d \pi^2 u_{\text{ex}}(\mathbf{x}) + \boldsymbol{\beta}(\mathbf{x}) \cdot \nabla u_{\text{ex}}(\mathbf{x}) + \gamma u_{\text{ex}}(\mathbf{x}). \tag{4}$$

The problem domain boundary $\partial\Omega$ is split into Dirichlet (Γ_D) and Neumann (Γ_N) portions to test mixed boundary conditions.

Neumann Boundary (Γ_N) We apply a Neumann condition on the "Right" face of the hypercube, defined as the plane $x_1 = 1$. The outward unit normal is $\mathbf{n} = (1, 0, \dots)^T$. The required flux h is derived from the exact solution:

$$h(\mathbf{x}) = \nabla u_{\text{ex}} \cdot \mathbf{n} \Big|_{x_1=1} = \frac{\partial u_{\text{ex}}}{\partial x_1} \Big|_{x_1=1}. \tag{5}$$

Computing the partial derivative:

$$\frac{\partial u_{\text{ex}}}{\partial x_1} = \pi \cos(\pi x_1) \prod_{j=2}^{d} \sin(\pi x_j). \tag{6}$$

Evaluated at $x_1 = 1$, where $\cos(\pi) = -1$, the Neumann data imposed is:

$$h(\mathbf{x}) = -\pi \prod_{j=2}^{d} \sin(\pi x_j). \tag{7}$$

Dirichlet Boundary (Γ_D) On all other boundaries ($\partial\Omega \backslash \Gamma_N$), we enforce a homogeneous Dirichlet condition:

$$u = 0 \quad \text{on } \Gamma_D. \tag{8}$$

This is consistent with the exact solution, as $\sin(\pi x_i) = 0$ when $x_i \in \{0, 1\}$.

2 Finite Element Discretization

To solve the weak formulation (section 1) numerically, we employ the Finite Element Method (FEM). This involves approximating the infinite-dimensional function spaces V_g and V_0 with finite-dimensional subspaces defined on a computational mesh.

2.1 Triangulation and Finite Element Space

We consider a triangulation $\mathcal{T}_h = \{K\}$ of the domain Ω, consisting of non-overlapping hexahedral (or quadrilateral in 2D) cells K such that $\overline{\Omega} = \bigcup_{K\in\mathcal{T}_h} \overline{K}$. The parameter h denotes the characteristic mesh size, $h = \max_{K\in\mathcal{T}_h} \operatorname{diam}(K)$.

We introduce the finite-dimensional space $V_h^k \subset H^1(\Omega)$ consisting of continuous piecewise polynomial functions of degree k. In the context of the `deal.II` library, we utilize Lagrangian finite elements (tensor product polynomials of degree k, denoted as Q_k). The discrete trial and test spaces are defined as:

$$V_{h,g} = \{u_h \in V_h^k : u_h|_{\Gamma_D} = I_h(g)\}, \tag{9}$$

$$V_{h,0} = \{v_h \in V_h^k : v_h|_{\Gamma_D} = 0\}, \tag{10}$$

where $I_h(g)$ is the nodal interpolation of the Dirichlet boundary data onto the mesh nodes on Γ_D.

2.2 Galerkin Approximation

The discrete problem is obtained by restricting the weak form to these subspaces. We seek $u_h \in V_{h,g}$ such that:

$$a(u_h, v_h) = L(v_h) \quad \forall v_h \in V_{h,0}. \tag{11}$$

We expand the approximate solution u_h in terms of the standard nodal basis functions $\{\varphi_j\}_{j=1}^{N_{dof}}$. Let u_h be decomposed into a part satisfying the homogeneous boundary conditions and a lifting of the Dirichlet data:

$$u_h(\mathbf{x}) = \sum_{j\in\mathcal{I}_{free}} U_j\varphi_j(\mathbf{x}) + \sum_{j\in\mathcal{I}_{dir}} g_j\varphi_j(\mathbf{x}), \tag{12}$$

where U_j are the unknown coefficients (degrees of freedom), $\mathcal{I}_{free}$ is the set of indices for nodes not on Γ_D, and $\mathcal{I}_{dir}$ contains indices for nodes on the Dirichlet boundary with known values g_j.

2.3 Algebraic System

Substituting the basis expansion into Eq. (11) and testing with each basis function φ_i (for $i \in \mathcal{I}_{free}$), we obtain the linear system of equations:

$$\mathbf{AU} = \mathbf{F}, \tag{13}$$

where $\mathbf{U}$ is the vector of unknown coefficients. The entries of the global stiffness matrix $\mathbf{A}$ and the right-hand side vector $\mathbf{F}$ are computed by assembling contributions from each cell $K \in \mathcal{T}_h$.

The matrix entries A_{ij} correspond to the bilinear form $a(\varphi_j, \varphi_i)$:

$$A_{ij} = \int_{\Omega} (\mu \nabla \varphi_j \cdot \nabla \varphi_i + (\boldsymbol{\beta} \cdot \nabla \varphi_j)\varphi_i + \gamma \varphi_j \varphi_i) \, dx. \tag{14}$$

Using numerical quadrature, the integral over Ω is computed as the sum of integrals over cells K. For a specific cell K, the local matrix contributions are:

$$A_{ij}^K = \sum_{q=1}^{N_q} (\mu \nabla \varphi_j(\mathbf{x}_q) \cdot \nabla \varphi_i(\mathbf{x}_q) + (\boldsymbol{\beta}(\mathbf{x}_q) \cdot \nabla \varphi_j(\mathbf{x}_q))\varphi_i(\mathbf{x}_q) + \gamma \varphi_j(\mathbf{x}_q)\varphi_i(\mathbf{x}_q)) \, w_q |J_K(\mathbf{x}_q)|, \tag{15}$$

where $\{\mathbf{x}_q\}$ and $\{w_q\}$ are the quadrature points and weights defined on the reference element, mapped to physical space via the Jacobian determinant $|J_K|$.

The right-hand side vector $\mathbf{F}$ includes the source term, the Neumann boundary contributions, and the modifications due to the Dirichlet lifting:

$$F_i = \int_{\Omega} f \varphi_i \, dx + \int_{\Gamma_N} \mu h \varphi_i \, ds - \sum_{j \in \mathcal{I}_{dir}} g_j A_{ij}. \tag{16}$$

The Neumann term is only non-zero if the support of φ_i intersects with Γ_N.

2.4 Treatment of Advection Dominance

It is well known that for convection-dominated problems (where the Péclet number $Pe = \frac{|\boldsymbol{\beta}|h}{2\mu} > 1$), the standard Galerkin formulation described above may produce spurious non-physical oscillations. While the manufactured solution chosen in **??** allows for convergence testing, typical industrial applications often require stabilization techniques such as Streamline-Upwind Petrov-Galerkin (SUPG) to ensure robust solutions. For this verification benchmark, we utilize a sufficiently refined mesh to maintain stability within the standard Galerkin framework.