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Hybrid thread-MPI parallelization for ADR equation

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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

First of all, we define the trial function space and test function space. For trial space, solution u belongs to the Sobolev space $H^1(\Omega)$ with Dirichlet boundary conditions incorporated:

$$V_g = \{u \in H^1(\Omega) : u = g \text{ on } \Gamma_D\}. \tag{1}$$

For test space, the test function v belongs to the Sobolev space $H^1(\Omega)$ with homogeneous Dirichlet boundary conditions:

$$V_0 = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D\}. \tag{2}$$

Multiply the governing equation by a test function $v \in V_0$ and integrate over the domain Ω:

$$\int_\Omega (-\nabla \cdot (\mu \nabla u) + \nabla \cdot (\boldsymbol{\beta} u) + \gamma u)\, v \, dx = \int_\Omega f v \, dx. \tag{3}$$

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

$$-\int_\Omega \nabla\cdot(\mu\nabla u)v\,dx + \int_\Omega \nabla\cdot(\boldsymbol{\beta}u)v\,dx + \int_\Omega \gamma uv\,dx = \int_\Omega fv\,dx. \tag{4}$$

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

$$-\int_\Omega \nabla\cdot(\mu\nabla u)v\,dx = \int_\Omega \mu\nabla u\cdot\nabla v\,dx - \int_{\partial\Omega} \mu(\nabla u\cdot\mathbf{n})v\,ds. \tag{5}$$

Substituting this back into the integral equation:

$$\int_\Omega \mu\nabla u\cdot\nabla v\,dx - \int_{\partial\Omega} \mu(\nabla u\cdot\mathbf{n})v\,ds + \int_\Omega \nabla\cdot(\boldsymbol{\beta}u)v\,dx + \int_\Omega \gamma uv\,dx = \int_\Omega fv\,dx. \tag{6}$$

Split the boundary integral into Dirichlet (Γ_D) and Neumann (Γ_N) parts:

$$\int_{\partial\Omega} \mu(\nabla u\cdot\mathbf{n})v\,ds = \int_{\Gamma_D} \mu(\nabla u\cdot\mathbf{n})v\,ds + \int_{\Gamma_N} \mu(\nabla u\cdot\mathbf{n})v\,ds. \tag{7}$$

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

$$\int_{\Gamma_N} \mu(\underbrace{\nabla u\cdot\mathbf{n}}_{h})v\,ds = \int_{\Gamma_N} \mu hv\,ds. \tag{8}$$

Find $u \in S_g$ such that for all $v \in V$:

$$\int_\Omega \mu\nabla u\cdot\nabla v\,dx + \int_\Omega \nabla\cdot(\boldsymbol{\beta}u)v\,dx + \int_\Omega \gamma uv\,dx = \int_\Omega fv\,dx + \int_{\Gamma_N} \mu hv\,ds \tag{9}$$

This can be written in the abstract form $a(u,v) = L(v)$ where:

$$a(u,v) = \int_\Omega (\mu\nabla u\cdot\nabla v + \nabla\cdot(\boldsymbol{\beta}u)v + \gamma uv)\,dx, \tag{10}$$

$$L(v) = \int_\Omega fv\,dx + \int_{\Gamma_N} \mu hv\,ds. \tag{11}$$

Since g may not be in the test space V_0, we introduce a lifting function $u_g \in V_g$ such that $u_g = g$ on Γ_D. We can express the solution as $u = u_0 + u_g$ where $u_0 \in V_0$. The weak formulation then becomes:

$$\text{Find } u_0 \in V_0 \text{ such that for all } v \in V_0\text{:}\quad a(u_0,v) = L(v) - a(u_g,v). \tag{12}$$

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:

$$u_{\text{ex}}(\mathbf{x}) = \prod_{i=1}^{d} \sin(\pi x_i). \tag{13}$$

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:

$$\boldsymbol{\beta}(\mathbf{x}) = \begin{cases} \begin{bmatrix} -x_2 \\ x_1 \end{bmatrix} & \text{if } d = 2, \\ \begin{bmatrix} -x_2 \\ x_1 \\ 0.1 \end{bmatrix} & \text{if } d = 3. \end{cases} \tag{14}$$

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:

$$\Delta u_{\text{ex}} = \sum_{i=1}^{d} \frac{\partial^2 u_{\text{ex}}}{\partial x_i^2} = \sum_{i=1}^{d} (-\pi^2 u_{\text{ex}}) = -d\pi^2 u_{\text{ex}}. \tag{15}$$

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:

$$f(\mathbf{x}) = \mu d\pi^2 u_{\text{ex}}(\mathbf{x}) + \boldsymbol{\beta}(\mathbf{x}) \cdot \nabla u_{\text{ex}}(\mathbf{x}) + \gamma u_{\text{ex}}(\mathbf{x}). \tag{16}$$

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:

$$h(\mathbf{x}) = \nabla u_{\text{ex}} \cdot \mathbf{n}\Big|_{x_1=1} = \frac{\partial u_{\text{ex}}}{\partial x_1}\Big|_{x_1=1}. \tag{17}$$

Computing the partial derivative:

$$\frac{\partial u_{\text{ex}}}{\partial x_1} = \pi \cos(\pi x_1) \prod_{j=2}^{d} \sin(\pi x_j). \tag{18}$$

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

$$h(\mathbf{x}) = -\pi \prod_{j=2}^{d} \sin(\pi x_j). \tag{19}$$

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

$$u = 0 \quad \text{on } \Gamma_D. \tag{20}$$

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:

$$V_{h,g} = \{u_h \in V_h^k : u_h|_{\Gamma_D} = I_h(g)\}, \tag{21}$$

$$V_{h,0} = \{v_h \in V_h^k : v_h|_{\Gamma_D} = 0\}, \tag{22}$$

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:

$$a(u_h, v_h) = L(v_h) \quad \forall v_h \in V_{h,0}. \tag{23}$$

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:

$$u_h(\mathbf{x}) = \sum_{j \in \mathcal{I}_{free}} U_j \varphi_j(\mathbf{x}) + \sum_{j \in \mathcal{I}_{dir}} g_j \varphi_j(\mathbf{x}), \tag{24}$$

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

$$\mathbf{A}\mathbf{U} = \mathbf{F}, \tag{25}$$

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 $a(\varphi_j, \varphi_i)$:

$$A_{ij} = \int\limits_{\Omega} \left(\mu \nabla \varphi_j \cdot \nabla \varphi_i + (\boldsymbol{\beta} \cdot \nabla \varphi_j) \varphi_i + \gamma \varphi_j \varphi_i \right) \, dx. \tag{26}$$

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:

$$A_{ij}^K = \sum_{q=1}^{N_q} \left(\mu \nabla \varphi_j(\mathbf{x}_q) \cdot \nabla \varphi_i(\mathbf{x}_q) + (\boldsymbol{\beta}(\mathbf{x}_q) \cdot \nabla \varphi_j(\mathbf{x}_q)) \varphi_i(\mathbf{x}_q) + \gamma \varphi_j(\mathbf{x}_q) \varphi_i(\mathbf{x}_q) \right) w_q |J_K(\mathbf{x}_q)|, \tag{27}$$

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:

$$F_i = \int\limits_{\Omega} f \varphi_i \, dx + \int\limits_{\Gamma_N} \mu h \varphi_i \, ds - \sum_{j \in \mathcal{I}_{dir}} g_j A_{ij}. \tag{28}$$

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.