

Parallel shared-memory open-source code for simulations of transient problems using isogeometric analysis, implicit direction splitting and residual minimization (IGA-ADS-RM)

Marcin Łoś Maciej Paszynski

AGH University of Krakow, Poland.

Abstract

We present an open-source parallel shared-memory C++ software for simulations of transient phenomena on tensor product grids, with the following features: (1) it supports isogeometric finite element method discretizations; (2) it employs alternating-directions (ADS) linear cost $\mathcal{O}(N)$ solver; (3) it uses implicit time-integration schemes suitable for ADS, including Peaceman-Reachford, Douglass-Gunn, Adams-Moulton, generalized alpha, and BDF; (4) it works for 2D/ 3D problems; (5) it enables residual minimization stabilization; (6) it supports scalar, vector fields, and systems of PDEs; (7) it provides a ParaView interface; (8) it supports an interface to parallel MUMPS direct solver for problems not suitable for ADS solver; (9) it also supports interface to Preconditioned Conjugate Gradients (PCG) solver; (10) it includes a large library of problems: (a) non-stationary heat transfer (2D/3D); (b) stationary advection-diffusion (2D); (c) non-stationary advection-diffusion (2D/3D); (d) laminar flow (Stokes equations) (2D/3D); (e) Navier-Stokes (2D); (f) pollution propagation (2D/3D); (g) pathogen propagation (3D).

Keywords: Residual minimization; Isogeometric analysis; Transient problems; Discontinuous Petrov-Galerkin method; Fast solvers

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43 1 Introduction

44 Simulations of transient problems require discretization in time and space. For space discretization, higher-order
 45 finite element method provides reliable and accurate solutions. The isogeometric analysis (IGA) employs higher-
 46 order and continuity B-spline basis functions for discretization with finite element method [21, 7]. The numerical
 47 problem is solved in every time step using either explicit or implicit methods. In the explicit method, the problem
 48 to solve in every time step is related to the inversion of the mass matrix, which is a simple task. The price to pay
 49 is the Courant-Friedrichs-Levy (CFL) condition [8], telling that the larger the spatial mesh, the smaller the time
 50 step size. Implicit time integration schemes can be employed to avoid these limitations. However, the implicit
 51 time integration schemes result in expensive matrices to be factorized. One way to avoid this problem is to use
 52 IGA on regular patches of elements. It can be solved efficiently using alternating direction solver [28, 13, 34, 4],
 53 rediscovered for isogeometric analysis with variational splitting. It requires splitting the differential operator
 54 and introducing a special time-integration scheme. Thus, for the time discretization, we introduce the time in-
 55 tegration schemes, such as Crank-Nicolson [9] or Peaceman-Reachford [29] with Strang [32] splitting, suitable
 56 for direction-splitting and fast linear cost $\mathcal{O}(N)$ spatial solver. Difficult computational problems, such as advec-
 57 tion-dominated diffusion [16] or Navier-Stokes with high Reynolds numbers [17], require special stabilization
 58 methods. We employ the residual minimization method [6], or Discontinuous-Galerkin [30, 24] for automatic
 59 stabilization of difficult computational problems. To support parallel shared-memory computations, we employ a
 60 GALOIS environment [31, 1, 19, 23, 22].

61 We present an open-source parallel shared-memory C++ software for simulations of time-dependent prob-
 62 lems with IGA discretizations on regular patches of elements. In this code, we combine the following unique
 63 features:

- 64 • we provide higher-order and continuity discretization with B-spline basis functions as provided by IGA;
- 65 • we implement alternating-directions (ADS) linear computational cost $\mathcal{O}(N)$ solver using variational split-
 66 ting;
- 67 • we use implicit time-integration schemes suitable for direction splitting, including Peaceman-Reachford,
 68 Douglas-Gunn, Adams-Moulton, generalized- α , and BDF;
- 69 • our code works for two- and three-dimensional problems;
- 70 • it supports scalar, vector fields, and systems of Partial Differential Equations (PDEs);
- 71 • it provides a ParaView interface for the generation of pictures and movies of simulations;
- 72 • it supports an interface to parallel MUMPS direct solver [14, 15] for problems not suitable for ADS solver;
- 73 • it supports Preconditioned Conjugate Gradient (PCG) solver;
- 74 • it incorporates residual minimization and Discontinuous Galerkin stabilization.

75 We call our method an isogeometric analysis implicit direction splitting residual minimization solver (IGA-ADS-
 76 RM).

77 The IGA-ADS-RM code has been built based on our explicit dynamics code IGA-ADS [25]. There are the
 78 following novelties of IGA-ADS-RM with respect to the IGA-ADS code. It supports implicit dynamics suitable
 79 for direction splitting using generalized- α , Adams-Moulton (AM), backward differentiation formulae (BDF),
 80 Strang splitting with Crank-Nicolson method, Peaceman-Reachford, Douglas-Gunn and Jean-Luc Guermond and

81 Petar Minev implicit time integration schemes. It provides a preconditioned conjugate gradient solver. It enables
 82 residual minimization with the direction-splitting method. It enables Discontinuous Galerkin stabilization. It also
 83 provides a library, with formulations and numerical results obtained with our IGA-RM-ADS code described in
 84 several papers:

- 85 • Simulations of pollution removal by artificially generated shock waves using -diffusion model and directions
 86 splitting solver [27];
- 87 • Residual minimization with preconditioned conjugate gradients (PCG) solver for stationary advection-
 88 dominated diffusion problems [5];
- 89 • Residual minimization with direction-splitting and higher-order time integration scheme for time-dependent
 90 Stokes and Navier-Stokes problems with implicit time integration scheme [35];
- 91 • Residual minimization with direction-splitting and higher-order time integration scheme for time-dependent
 92 advection-dominated diffusion problems using Strang splitting with Crank-Nicolson and Peaceman-Reachford
 93 implicit time integration scheme [36];
- 94 • Discontinuous Galerkin and residual minimization method with Preconditioner Conjugate Gradient (PCG)
 95 solver for stabilization of Stokes solver [37];
- 96 • Stabilized simulations of COVID-19 pathogen spread using direction-splitting solver with Douglas-Gunn
 97 implicit time integration scheme [38];
- 98 • 3D simulations of the hail cannon [26].

99 In this paper, we focus on the code structure and implementation of these new features in the IGA-ADS-RM code.

100 The structure of the paper is as follows. In Section 2, we compare RM-IGA-ADS with other IGA software
 101 available. Section 3 introduces the Residual Minimization IGA method in the context of non-stationary problems.
 102 Section 4 presents a high-level overview of the structure of the code. Multiple model problems are introduced
 103 in Section 5, together with annotated example implementations. Section 6 presents the numerical results of these
 104 example codes. Section 7 describes an automatic mesh refinement strategy based on the residual provided by
 105 the residual minimization method. Section 8 discusses various approaches to improving integration efficiency,
 106 and their applicability to the common use cases of our code. Finally, section 9 presents scalability results on
 107 shared-memory architecture machines.

108 2 Comparison of RM-IGA-ADS solver with alternative solvers

109 There are several high-quality numerical solvers for running simulations using B-spline discretizations. The list
 110 includes the PetIGA solver [10], GeoPDE solver [33], and IGA-ADS solver [25]. The main differences between
 111 PetIGA and the RM-IGA-ADS solver are the following

- 112 • PetIGA software is linked with PETSc, which provides several direct and iterative solvers
- 113 • RM-IGA-ADS relies on the linear computational cost alternating direction solver. The alternating direction
 114 solver is a fast implementation of the direct solver for tensor product geometries. It also supports an interface
 115 to a dedicated PCG iterative solver for residual minimization computations.
- 116 • Both RM-IGA-ADS and PETSc support an interface to the MUMPS solver.
- 117 • PetIGA supports arbitrary geometries of the computational domain, while RM-IGA-ADS works on tensor
 118 product geometries.
- 119 • RM-IGA-ADS contains the residual minimization method for automatic stabilization of difficult simula-
 120 tions, using Galerkin and DG discretizations, and it provided several build examples, including advection-
 121 dominated diffusion, Stokes, and Navier-Stokes problem. The implementation of the residual minimization
 122 method in PetIGA is possible, but it is not straightforward. Implementing the residual minimization and DG
 123 discretization methods in PetIGA is possible, but it is not straightforward.
- 124 • The RM-IGA-ADS is straightforward to install and use.
- 125 • RM-IGA-ADS supports parallelization on multi-core parallel machines using the Galois library, while the
 126 PetIGA supports parallel solvers available through the PETSc library.

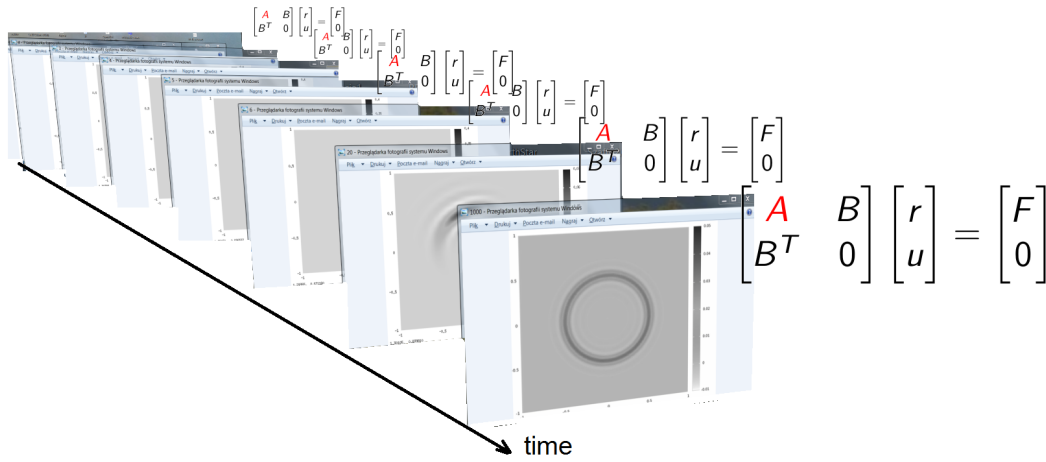


Figure 1: Stabilization of time-steps with residual minimization method

The differences between GeoPDE and RM-IGA-ADS are summarized below:

- GeoPDE is a MATLAB code that supports local adaptivity with hierarchical B-splines. The RM-IGA-ADS only supports global refinement on the tensor structure mesh.
- GeoPDE employs MATLAB direct and iterative solvers, while RM-IGA-ADS supports dedicated alternating directions and linear computational cost solvers. RM-IGA-ADS supports an interface to the MUMPS solver and a dedicated PCG iterative solver for residual minimization computations.
- RM-IGA-ADS is dedicated to residual minimization computations, while GeoPDE supports different formulations within the Galerkin method
- GeoPDE supports arbitrary geometries, while RM-IGA-ADS works on tensor product grids.

Finally, RM-IGA-ADS is an extension of IGA-ADS into residual minimization and Discontinuous Galerkin formulations.

3 Non-stationary residual minimization method

Our code employs unconditionally stable higher-order time integration schemes. It stabilizes time steps with the residual minimization method (see Figure 2). The spatial discretization is based on B-splines. Namely,

- It employs time-integration schemes suitable for direction-splitting (Strang scheme with Backward Euler method, Strang scheme with Crank-Nicolson method, generalized α method, Adams-Moulton (AM), Backward Differentiation Formulae (BDF), Peaceman Rachford, Douglass-Gun, as well as Jean-Luc Guermond scheme for Navier-Stokes equations).
- It employs unconditionally stable time integration schemes (Strang scheme with Crank-Nicolson method, generalized α method, Adams-Moulton (AM), Backward Differentiation Formulae (BDF), Peaceman Rachford, Douglass-Gun, as well as Jean-Luc Guermond scheme for Navier-Stokes equations).
- It employs higher-order time integration schemes (generalized α method, Adams-Moulton (AM), Backward Differentiation Formulae (BDF)).
- It solves the separate problems in each time step, using B-spline-based discretization.
- The stabilization in time is obtained using the residual minimization method (see Appendix A). In this method, we solve the saddle-point problem in every time step,

$$\underbrace{\text{test}} \{ \underbrace{\begin{bmatrix} G & B^T \\ B & 0 \end{bmatrix}}_{\text{trial}} \begin{bmatrix} r \\ u \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix}, \quad (1)$$

where G is the Gram matrix, and B is the problem matrix. There are different discretizations for the trial and test space.

155 The residual minimization method can be derived in the following way. For a general weak problem: Find
 156 $u \in U$ such that

$$b(u, v) = l(v), \quad \forall v \in V, \quad (2)$$

157 we define the operator $B : U \rightarrow V'$ such as

$$\langle Bu, v \rangle = b(u, v), \quad (3)$$

158 where $\langle \cdot, \cdot \rangle$ is the duality pairing between V and V' . Now (2) is

$$Bu - l = 0. \quad (4)$$

159 We wish to minimize the residual

$$u_h = \operatorname{argmin}_{w_h \in U_h} \frac{1}{2} \|Bw_h - l\|_{V'}^2. \quad (5)$$

160 We introduce the Riesz operator $R_V : V \ni v \rightarrow (v, \cdot) \in V'$ being the isometric isomorphism to project the problem
 161 back to V

$$u_h = \operatorname{argmin}_{w_h \in U_h} \frac{1}{2} \|R_V^{-1}(Bw_h - l)\|_V^2 \quad (6)$$

162 The minimum is attained at u_h when the Gâteaux derivative is equal to 0 in all directions

$$G(u_h) = \frac{1}{2} \|R_V^{-1}(Bu_h - l)\|_V^2 \quad (7)$$

$$dG(u_h; w_h) = \lim_{h \rightarrow 0} \frac{G(u_h + hw_h) - G(u_h)}{h}$$

163 since $\|a + b\|^2 = \|a\|^2 + 2(a, b) + \|b\|^2$ we have

$$\begin{aligned} 2G(u_h + hw_h) &= \|R_V^{-1}(B(u_h + hw_h) - l)\|_V^2 = \\ &= \|R_V^{-1}(Bu_h - l) + hR_V^{-1}Bw_h\|_V^2 = \\ &= \|R_V^{-1}(Bu_h - l)\|_V^2 + 2h(R_V^{-1}(Bu_h - l), R_V^{-1}Bw_h)_V + h^2\|R_V^{-1}Bw_h\|_V^2 \end{aligned}$$

164 so

$$\frac{G(u_h + hw_h) - G(u_h)}{h} = (R_V^{-1}(Bu_h - l), R_V^{-1}Bw_h)_V + \frac{1}{2}h\|R_V^{-1}Bw_h\|_V^2$$

165 In the limit $h \rightarrow 0$ we have

$$dG(u_h; w_h) = (R_V^{-1}(Bu_h - l), R_V^{-1}Bw_h)_V \quad (8)$$

166 If u_h is minimum, then for each w_h we have $G(u_h + hw_h)$ gets minimum for $h = 0$, so the Gâteaux derivative has
 167 to be zero

$$(R_V^{-1}(Bu_h - l), R_V^{-1}(Bw_h))_V = 0 \quad \forall w_h \in U_h \quad (9)$$

168 We define the residual $r = R_V^{-1}(Bu_h - l)$ and we get

$$(r, R_V^{-1}(Bw_h)) = 0 \quad \forall w_h \in U_h \quad (10)$$

169 From the definition of R_V for all functionals $f \in V'$

$$(v, R_V^{-1}f)_V = \langle f, v \rangle (= f(v) \text{ from definition of } \langle \cdot, \cdot \rangle) \quad (11)$$

170 so in particular for $f = Bw_h$ and $v = r$ we get

$$\langle Bw_h, r \rangle = 0 \quad \forall w_h \in U_h \quad (12)$$

171 From the definition of the residual we have

$$(r, v)_V = \langle Bu_h - l, v \rangle, \quad \forall v \in V. \quad (13)$$

172 Thus, from (12) and (13), our problem reduces to the following semi-infinite problem: Find $(r, u_h) \in V \times U_h$ such
 173 as

$$\begin{aligned} (r, v)_V - \langle Bu_h, v \rangle &= \langle l, v \rangle, & \forall v \in V, \\ \langle Bw_h, r \rangle &= 0, & \forall w_h \in U_h. \end{aligned} \quad (14)$$

174 We discretize the test space $V_h \in V$ to get the discrete problem: Find $(r_h, u_h) \in V_h \times U_h$ such as

$$\begin{aligned} (r_h, v_h)_{V_h} - \langle Bu_h, v_h \rangle &= \langle l, v_h \rangle, & \forall v \in V_h, \\ \langle Bw_h, r_h \rangle &= 0, & \forall w_h \in U_h, \end{aligned} \quad (15)$$

175 where $(\cdot, \cdot)_{V_h}$ is an inner product in V_h , $\langle Bu_h, v_h \rangle = b(u_h, v_h)$, and $\langle Bw_h, r_h \rangle = b(w_h, r_h)$.

4 Structure of the code

Running each simulation requires overwriting methods from the following class. The methods `before` and `after` are called once at the beginning and at the end of the simulation. The methods `before_step` and `after_step` are called before and after each time step of the simulation. The method `step` implements the time step of the simulation.

```

181 class simulation_base {
182     // executed once before the entire simulation
183     virtual void before() { }
184     // executed once after the entire simulation
185     virtual void after() { }
186     // executed before each time step
187     virtual void before_step(int iter, double t) { }
188     // timestep itself - put all the calculations here
189     virtual void step(int iter, double t) { }
190     // executed after each time step
191     virtual void after_step(int iter, double t) { }
192
193     // executes teh whole simulation (all the timesteps)
194     void run();
195 };
196
197 // dimension-specific base classes
198 class simulation_2d : public simulation_base { ... };
199 class simulation_3d : public simulation_base { ... };

```

We will explain the sketch of the simulation using the three-dimensional model heat transfer problem. We seek the temperature distribution $[0, 1]^3 \times [0, T] = \Omega \times I \ni (x, y, z, t) \rightarrow u(x, y, z, t) \in \mathcal{R}$ such that

$$\begin{cases} \partial_t u = \Delta u & \text{in } \Omega \times I, \\ \nabla u \cdot \hat{n} = 0 & \text{in } \partial\Omega \times I, \\ u(\cdot, 0) = u_0 & \text{in } \Omega. \end{cases}$$

We define our simulation class by deriving from one of the two base classes for 2D and 3D problems:

```

203 || class heat_3d : public simulation_3d { ... };

```

We introduce Forward Euler method where $\partial_t u^t = \frac{u^{t+1} - u^t}{\tau}$ with time step size τ . We derive the weak formulation from the integration by parts $(u_h^{n+1}, v_h) = (u_h^n, v_h) - \tau (\nabla u_h^n, \nabla v_h)$. The simulation is configured in `main` method with quadratic B-splines on $12 \times 12 \times 12$ mesh. We run 5000 times step with $\tau = 10^{-7}$. We will need the first derivatives to implement the weak formulation.

```

208 #include "heat_3d.hpp"
209
210 int main() {
211     // 12x12x12 mesh, quadratic B-spline basis functions
212     ads::dim_config dim{2, 12};
213     // 5,000 time steps, dt = 10^-7
214     ads::timesteps_config steps{5000, 1e-7};
215     // formulation uses values and first derivatives
216     int ders = 1;
217
218     ads::config_3d c{dim, dim, dim, steps, ders};
219     ads::problems::heat_3d sim{c};
220     sim.run();
221 }

```

The `heat_3d` class provides the pilot of the simulation. The `before` method for the explicit solver generates the mass matrices and computes the projection of the initial state. The `before_step` method stores the previous (or initial) time step solution. The `step` method generates the right-hand side and solves the L2 projection problem with mass matrix for the explicit solver. The problem formulation is implemented in the `compute_rhs` method. The term `u.val * v.val` corresponds to (u_h^n, v_h) , the `- steps.dt * gradient_prod` term corresponds to $-\tau (\nabla u_h^n, \nabla v_h)$, where `gradient_prod = grad_dot(u, v)`.

```

228 #include "ads/executor/galois.hpp"
229 #include "ads/output_manager.hpp"
230 #include "ads/simulation.hpp"
231
232 class heat_3d : public simulation_3d {

```

```

233 private:
234     using Base = simulation_2d;
235     vector_type u, u_prev; // current and previous solution
236
237     output_manager<3> output;
238     galois_executor executor{4};
239
240 public:
241     explicit heat_3d(const config_3d& config)
242         : Base{config}
243         , u{shape()}
244         , u_prev{shape()}
245         , output{x.B, y.B, 50} { }
246
247     // member functions
248     // ...
249 };

```

```

250 // called once at the beginning of the simulation
251 void before() override {
252     prepare_matrices();
253     auto init = [this](double x, double y, double z) {
254         /* initial state formula */
255     };
256     // L2 projection of initial state
257     projection(u, init);
258     solve(u);
259 }

```

```

260 // called before every step
261 void before_step(int /*iter*/, double /*t*/) override {
262     using std::swap;
263     swap(u, u_prev);
264 }

```

```

265 // time step implementation
266 void step(int /*iter*/, double /*t*/) override {
267     compute_rhs();
268     solve(u);
269 }

```

```

270
271
272 void compute_rhs() {
273     auto& rhs = u;
274     zero(rhs);
275
276     // parallel loop over mesh elements
277     executor.for_each(elements(), [&](index_type e) {
278         auto U = element_rhs(); // buffer for element DoF entries
279         double J = jacobian(e);
280         for (auto q : quad_points()) {
281             double w = weight(q);
282             for (auto a : dofs_on_element(e)) {
283                 auto aa = dof_global_to_local(e, a);
284                 // compute values and gradients at the quadrature point
285                 value_type v = eval_basis(e, q, a);
286                 value_type u = eval_fun(u_prev, e, q);
287
288                 double gradient_prod = grad_dot(u, v);
289                 double val = u.val * v.val - steps.dt * gradient_prod;
290                 U(aa[0], aa[1]) += val * w * J;
291             }
292         }
293         executor.synchronized([&]() { update_global_rhs(rhs, U, e); });
294     });
295     integration_timer.stop();
296 }

```

297 5 Collection of exemplary problems

298 In this section, we will present how to implement several exemplary problems in the RM-IGA-ADS code.

5.1 Time-dependent advection-dominated diffusion problem

We start with the unstable time-dependent advection-dominated diffusion problem. We seek the scalar concentration field $[0, 1]^2 \times [0, T] = \Omega \times I \ni (x, y, t) \rightarrow u(x, y, z, t) \in \mathcal{R}$ such that

$$\begin{cases} \partial_t u - \varepsilon \Delta u + \beta \cdot \nabla u = f & \text{in } \Omega \times I, \\ u|_{\partial\Omega} = 0 & \text{in } \partial\Omega \times I, \\ u(\cdot, 0) = u_0 & \text{in } \Omega. \end{cases}$$

Here ε is the diffusion constant, $\beta = (\beta_x, \beta_y)$ stands for the advection ‘‘wind’’, $f(x, y, t)$ is the source term. This problem is unstable when $\varepsilon \ll \|\beta\|$. We employ one of the time-integration schemes (Backward Euler, Crank-Nicolson, Peaceman-Rachford) using the splitting of the operator as $-\varepsilon \Delta u + \beta \cdot \nabla u = \underbrace{-\varepsilon \partial_{xx} u + \beta_x \partial_x u}_{\mathcal{L}_1}$

$\underbrace{-\varepsilon \partial_{yy} u + \beta_y \partial_y u}_{\mathcal{L}_2}$. For the Peaceman-Rachford time integration scheme we employ

$$\begin{cases} \frac{u^{n+1/2} - u^n}{\tau/2} + \mathcal{L}_1 u^{n+1/2} = f^{n+1/2} - \mathcal{L}_2 u^n, \\ \frac{u^{n+1} - u^{n+1/2}}{\tau/2} + \mathcal{L}_2 u^{n+1} = f^{n+1/2} - \mathcal{L}_1 u^{n+1/2}. \end{cases} \quad (16)$$

The variational formulation of the scheme (16) is

$$\begin{cases} (u^{n+1/2}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1/2}}{\partial x}, \frac{\partial v}{\partial x} \right) + \frac{\tau}{2} \left(\beta_x \frac{\partial u^{n+1/2}}{\partial x}, v \right) = \\ (u^n, v) - \frac{\tau}{2} \left(\alpha \frac{\partial u^n}{\partial y}, \frac{\partial v}{\partial y} \right) - \frac{\tau}{2} \left(\beta_y \frac{\partial u^n}{\partial y}, v \right) + \frac{\tau}{2} (f^{n+1/2}, v), \\ (u^{n+1}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1}}{\partial y}, \frac{\partial v}{\partial y} \right) + \frac{\tau}{2} \left(\beta_y \frac{\partial u^{n+1}}{\partial y}, v \right) = \\ (u^{n+1/2}, v) - \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1/2}}{\partial x}, \frac{\partial v}{\partial x} \right) - \frac{\tau}{2} \left(\beta_x \frac{\partial u^{n+1/2}}{\partial x}, v \right) + \frac{\tau}{2} (f^{n+1/2}, v), \end{cases} \quad (17)$$

Here (\cdot, \cdot) denotes the inner product of $L^2(\Omega)$. In the matrix form, this scheme translates into Kronecker product matrices

$$\begin{cases} \left[M^x + \frac{\tau}{2} (K^x + G^x) \right] \otimes M^y u^{n+1/2} = \\ M^x \otimes \left[M^y - \frac{\tau}{2} (K^y + G^y) \right] u^n + \frac{\tau}{2} F^{n+1/2}, \\ M^x \otimes \left[M^y + \frac{\tau}{2} (K^y + G^y) \right] u^{n+1} = \\ \left[M^x - \frac{\tau}{2} (K^x + G^x) \right] \otimes M^y u^{n+1/2} + \frac{\tau}{2} F^{n+1/2}, \end{cases} \quad (18)$$

where $M^{x,y}$, $K^{x,y}$ and $G^{x,y}$ are the 1D mass, stiffness and advection matrices, respectively.

Alternatively, in the Strang splitting scheme we divide the problem $u_t + \mathcal{L}u = f$ into s

$$\begin{cases} P_1 : u_t + \mathcal{L}_1 u = f, \\ P_2 : u_t + \mathcal{L}_2 u = 0, \end{cases} \quad (19)$$

the scheme integrates the solution from t_n to t_{n+1} into sub-steps (see Figure 2):

$$\begin{cases} \text{Solve } P_1 : u_t + \mathcal{L}_1 u = f, \text{ in } (t_n, t_{n+1/2}), \\ \text{Solve } P_2 : u_t + \mathcal{L}_2 u = 0, \text{ in } (t_n, t_{n+1}), \\ \text{Solve } P_1 : u_t + \mathcal{L}_1 u = f, \text{ in } (t_{n+1/2}, t_{n+1}), \end{cases} \quad (20)$$

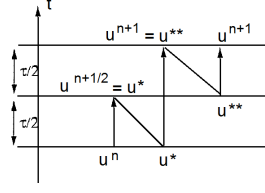


Figure 2: Strang splitting. In this method, we split the differential operator into two parts, we perform half step forward with the first part of the operator, followed by the full step forward with the second part of the operator, and finally, half step forward with the first part of the operator.

312 and we can employ different methods in each sub-step. The Strang splitting with Backward Euler method reads

$$\begin{cases} \frac{u^{n+1/2} - u^n}{\tau/2} + \mathcal{L}_1 u^{n+1/2} = f^{n+1/2}, \\ \frac{u^{n+1} - u^n}{\tau} + \mathcal{L}_2 u^{n+1} = 0, \\ \frac{u^{n+1} - u^{n+1/2}}{\tau/2} + \mathcal{L}_1 u^{n+1} = f^{n+1}. \end{cases} \quad (21)$$

313 and the weak form

$$\begin{cases} (u^{n+1/2}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1/2}}{\partial x}, \frac{\partial v}{\partial x} \right) + \frac{\tau}{2} \left(\beta_x \frac{\partial u^{n+1/2}}{\partial x}, v \right) \\ = (u^n, v) + \frac{\tau}{2} (f^{n+1/2}, v), \\ (u^{n+1}, v) + \tau \left(\alpha \frac{\partial u^{n+1}}{\partial y}, \frac{\partial v}{\partial y} \right) + \tau \left(\beta_y \frac{\partial u^{n+1}}{\partial y}, v \right) = (u^n, v), \\ (u^{n+1}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1}}{\partial x}, \frac{\partial v}{\partial x} \right) + \frac{\tau}{2} \left(\beta_x \frac{\partial u^{n+1}}{\partial x}, v \right) \\ = (u^{n+1/2}, v) + \frac{\tau}{2} (f^{n+1}, v), \end{cases} \quad (22)$$

314 In the matrix form, the Strang splitting scheme with Backward Euler method reads

$$\begin{cases} \left[M^x + \frac{\tau}{2} (K^x + G^x) \right] \otimes M^y u^* = M^x \otimes M^y u^n + \frac{\tau}{2} F^{n+1/2}, \\ M^x \otimes [M^y + \tau (K^y + G^y)] u^{**} = M^x \otimes M^y u^*, \\ \left[M^x + \frac{\tau}{2} (K^x + G^x) \right] \otimes M^y u^{n+1} = M^x \otimes M^y u^{**} + \frac{\tau}{2} F^{n+1}. \end{cases} \quad (23)$$

315 Finally, if we select the Crank-Nicolson method for Strang scheme we obtain

$$\begin{cases} \frac{u^{n+1/2} - u^n}{\tau/2} + \frac{1}{2} (\mathcal{L}_1 u^{n+1/2} + \mathcal{L}_1 u^n) = \frac{1}{2} (f^{n+1/2} + f^n), \\ \frac{u^{n+1} - u^n}{\tau} + \frac{1}{2} (\mathcal{L}_2 u^{n+1} + \mathcal{L}_2 u^n) = 0, \\ \frac{u^{n+1} - u^{n+1/2}}{\tau/2} + \frac{1}{2} (\mathcal{L}_1 u^{n+1} + \mathcal{L}_1 u^{n+1/2}) = \frac{1}{2} (f^{n+1} + f^{n+1/2}). \end{cases}$$

316 This Strang splitting scheme with Crank-Nicolson method in the weak form

$$\left\{ \begin{aligned}
 & \left(u^{n+1/2}, v \right) + \frac{\tau}{4} \left(\alpha \frac{\partial u^{n+1/2}}{\partial x}, \frac{\partial v}{\partial x} \right) + \frac{\tau}{4} \left(\beta_x \frac{\partial u^{n+1/2}}{\partial x}, v \right) = \\
 & = \left(u^n, v \right) - \frac{\tau}{4} \left(\alpha \frac{\partial u^n}{\partial x}, \frac{\partial v}{\partial x} \right) - \frac{\tau}{4} \left(\beta_x \frac{\partial u^n}{\partial x}, v \right) + \frac{\tau}{4} (f^{n+1/2} + f^n, v), \\
 & \left(u^{n+1}, v \right) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1}}{\partial y}, \frac{\partial v}{\partial y} \right) + \frac{\tau}{2} \left(\beta_y \frac{\partial u^{n+1}}{\partial y}, v \right) = \\
 & = \left(u^n, v \right) - \frac{\tau}{2} \left(\alpha \frac{\partial u^n}{\partial y}, \frac{\partial v}{\partial y} \right) - \frac{\tau}{2} \left(\beta_y \frac{\partial u^n}{\partial y}, v \right), \\
 & \left(u^{n+1}, v \right) + \frac{\tau}{4} \left(\alpha \frac{\partial u^{n+1}}{\partial x}, \frac{\partial v}{\partial x} \right) + \frac{\tau}{4} \left(\beta_x \frac{\partial u^{n+1}}{\partial x}, v \right) = \\
 & = \left(u^{n+1/2}, v \right) - \frac{\tau}{4} \left(\alpha \frac{\partial u^{n+1/2}}{\partial x}, \frac{\partial v}{\partial x} \right) - \frac{\tau}{4} \left(\beta_x \frac{\partial u^{n+1/2}}{\partial x}, v \right) + \frac{\tau}{4} (f^{n+1} + f^{n+1/2}, v).
 \end{aligned} \right. \quad (24)$$

317 and in the matrix form

$$\left\{ \begin{aligned}
 & \left[M^x + \frac{\tau}{4} (K^x + G^x) \right] \otimes M^y u^* = \\
 & \left[M^x - \frac{\tau}{4} (K^x + G^x) \right] \otimes M^y u^n + \frac{\tau}{4} (F^{n+1/2} + F^n), \\
 & M^x \otimes \left[M^y + \frac{\tau}{2} (K^y + G^y) \right] u^{**} = M^x \otimes \left[M^y - \frac{\tau}{2} (K^y + G^y) \right] u^*, \\
 & \left[M^x + \frac{\tau}{4} (K^x + G^x) \right] \otimes M^y u^{n+1} = \\
 & \left[M^x - \frac{\tau}{4} (K^x + G^x) \right] \otimes M^y u^{**} + \frac{\tau}{4} (F^{n+1} + F^{n+1/2}).
 \end{aligned} \right. \quad (25)$$

318 The implementation of different time marching schemes is available in the step routine. The system of
 319 linear equations generated in sub-step depends on the selected method that follows enum class scheme { BE,
 320 CN, peaceman_rachford, strang_BE, stranf_CN } corresponding to Backward Euler, Crank-Nicolson,
 321 Peaceman-Rachford, Strang (also called the leapfrog) with either Backward-Euler or Crank-Nicolson imple-
 322 mentation.

```

323 void step(int /*iter*/, double t) override {
324     // auxiliary definitions
325     auto dt = steps.dt;
326     auto f = [&](point_type x, double s) {
327         return forcing(x[0], x[1], epsilon, s);
328     };
329     auto F = [&](double s) {
330         return [&, s](point_type x) { return f(x, s); };
331     };
332     auto Favg = [&](double s1, double s2) {
333         return [=, &f](point_type x) {
334             return 0.5 * (f(x, s1) + f(x, s2));
335         };
336     };
337     auto zero = [&](point_type) { return 0; };

338     // system generation depends on the scheme
339     // schemes are defined as enumeration type
340     // enum class scheme { BE, CN, peaceman_rachford, strang_BE, strang_CN };
341     if (method == scheme::BE) {
342         substep(u, true, true, dt, dt, 0, 0, dt, F(t + dt));
343     }
344     if (method == scheme::CN) {
345         substep(u, true, true, dt/2, dt/2, -dt/2, -dt/2, dt, Favg(t, t + dt));
346     }
347     if (method == scheme::peaceman_rachford) {
348         substep(u, true, true, dt/2, 0, 0, -dt/2, dt/2, F(t + dt/2));

```

```

349     substep(u, true, true, 0, dt/2, -dt/2, 0, dt/2, F(t + dt/2));
350 }
351 // strang is a template for splitting schemes - substeps can be handled
352 // using any ordinary time marching scheme
353 if (method == scheme::strang_BE) {
354     substep(u, false, true, dt/2, 0, 0, 0, dt/2, F(t + dt/2));
355     substep(u, true, false, 0, dt, 0, 0, dt, zero);
356     substep(u, false, true, dt/2, 0, 0, 0, dt/2, F(t + dt));
357 }
358 if (method == scheme::strang_CN) {
359     substep(u, false, true, dt/4, 0, -dt/4, 0, dt/2, Favg(t, t +
360 dt/2));
361     substep(u, true, false, 0, dt/2, 0, -dt/2, dt, zero);
362     substep(u, false, true, dt/4, 0, -dt/4, 0, dt/2, Favg(t + dt
363 /2, t + dt));
364 }
365 }

```

The step method, depending on the selected scheme, calls the substep method several times, parameterized with the selected time integration scheme, to obtain a structure required for a sub-step of the scheme.

```

368 // Computes the next substep solution solving
369 // (1 + Lx_lhs Lx + Ly_lhs Ly) u_next = (1 + Lx_rhs Lx + Ly_rhs Ly) u_prev + F
370 // using iGRM with scalar product
371 // (u, v) + sx (Dx u, Dx v) + sy (Dy u, Dy v)
372 template <typename Fun>
373 void substep(vector_type& u, bool x_refine, bool y_refine,
374             double Lx_lhs, double Ly_lhs,
375             double Lx_rhs, double Ly_rhs, double dt, Fun&& f) {
376     // choose appropriate test space
377     // in iGRM we refine the space in one direction only
378     dimension& Vx = x_refine ? this->Vx : Ux;
379     dimension& Vy = y_refine ? this->Vy : Uy;
380
381     // buffer for solution and residual representation
382     vector_view r_rhs{full_rhs.data(), {Vx.dofs(), Vy.dofs()}};
383     vector_view u_rhs{full_rhs.data() + r_rhs.size(), {Ux.dofs(), Uy.dofs()}};
384
385     std::fill(begin(full_rhs), end(full_rhs), 0);
386     compute_rhs(Lx_rhs, Ly_rhs, Vx, Vy, r_rhs, u_rhs, dt, std::forward<Fun>(f));
387
388     zero_bc(r_rhs, Vx, Vy);
389     zero_bc(u_rhs, Ux, Uy);
390
391     // build the system matrix and solve using HUMPSS
392     int size = Vx.dofs() * Vy.dofs() + Ux.dofs() * Uy.dofs();
393     mumps::problem problem(full_rhs.data(), size);
394     double sx = x_refine ? 0 : 1;
395     double sy = y_refine ? 0 : 1;
396     assemble_problem(problem, Lx_lhs, Ly_lhs, sx, sy, Vx, Vy, matrices(x_refine,
397 y_refine));
398     solver.solve(problem);
399
400     copy_solution(u_rhs, r_rhs, u);
401 }

```

The substep method calls the assemble_problem to obtain a system of linear equations solved in a given sub-step. Namely, we build the system of linear equations resulting from the application of the residual minimization method. The Gram matrix A is built using the assumed inner product. The problem matrix B is constructed according to the selected time-integration method and is suitable for direction splitting. The problem matrix B for the residual minimization method is built using trial basis functions for rows and test basis functions for columns. The B^T matrix is constructed in a symmetric way, with test basis function in rows and trial basis functions in columns.

```

409 void assemble_problem(mumps::problem& problem, double cx, double cy,
410                     double sx, double sy, const dimension& Vx,
411                     const dimension& Vy, const matrix_set& M) {
412     auto N = Vx.dofs() * Vy.dofs();
413
414     // Gram matrix
415     for (auto i : internal_dofs(Vx, Vy)) {
416         for (auto j : overlapping_internal_dofs(i, Vx, Vy)) {
417             int ii = linear_index(i, Vx, Vy) + 1;

```

```

418         int jj = linear_index(j, Vx, Vy) + 1;
419
420         // explicit construction of the Kronecker product
421         double val = kron(M.MVx, M.MVy, i, j)
422             + sx * kron(M.KVx, M.MVy, i, j)
423             + sy * kron(M.MVx, M.KVy, i, j);
424         problem.add(ii, jj, val);
425     }
426 }
427
428 // Dirichlet BC - upper left
429 for_boundary_dofs(Vx, Vy, [&](index_type dof) {
430     int i = linear_index(dof, Vx, Vy) + 1;
431     problem.add(i, i, 1);
432 });
433
434 // B, B^T
435 for (auto i : dofs(Vx, Vy)) {
436     for (auto j : dofs(Ux, Uy)) {
437         double MM = kron(M.MUVx, M.MUVy, i, j);
438         double Lx =
439             c_diff[0] * kron(M.KUVx, M.MUVy, i, j) + beta[0] * kron(M.AUVx, M.
440                 MUVy, i, j);
441         double Ly =
442             c_diff[1] * kron(M.MUVx, M.KUVy, i, j) + beta[1] * kron(M.MUVx, M.
443                 AUVy, i, j);
444         double val = MM + cx * Lx + cy * Ly;
445
446         if (val != 0) {
447             if (!is_boundary(i, Vx, Vy) && !is_boundary(j, Ux, Uy)) {
448                 int ii = linear_index(i, Vx, Vy) + 1;
449                 int jj = linear_index(j, Ux, Uy) + 1;
450
451                 problem.add(ii, N + jj, -val);
452                 problem.add(N + jj, ii, val);
453             }
454         }
455     }
456 }
457
458 // Dirichlet BC - lower right
459 for_boundary_dofs(Ux, Uy, [&](index_type dof) {
460     int i = linear_index(dof, Ux, Uy) + 1;
461     problem.add(N + i, N + i, 1);
462 });
463 }
464
465 // B, B^T
466 for (auto i : dofs(Vx, Vy)) {
467     for (auto j : dofs(Ux, Uy)) {
468         double MM = kron(M.MUVx, M.MUVy, i, j);
469         double Lx = c_diff[0] * kron(M.KUVx, M.MUVy, i, j)
470             + beta[0] * kron(M.AUVx, M.MUVy, i, j);
471         double Ly = c_diff[1] * kron(M.MUVx, M.KUVy, i, j)
472             + beta[1] * kron(M.MUVx, M.AUVy, i, j);
473         double val = MM + cx * Lx + cy * Ly;
474
475         bool bd = is_boundary(i, Vx, Vy) || is_boundary(j, Ux, Uy);
476         if (val != 0 && !bd) {
477             int ii = linear_index(i, Vx, Vy) + 1;
478             int jj = linear_index(j, Ux, Uy) + 1;
479             problem.add(ii, N + jj, -val);
480             problem.add(N + jj, ii, val);
481         }
482     }
483 }
484 // Dirichlet BC - lower right
485 for_boundary_dofs(Ux, Uy, [&](index_type dof) {
486     int i = linear_index(dof, Ux, Uy) + 1;
487     problem.add(N + i, N + i, 1);
488 });
489 }

```

489 Finally, the right-hand side appropriate for a selected time integration scheme and sub-step structure is gen-
 490 erated within `compute_rhs` method.

```

491 // compute generic RHS of the iGRM system: [-L 0]
492 template <typename Fun>
493 void compute_rhs(double cx, double cy, const dimension& Vx, const dimension& Vy,
494                 vector_view& r_rhs, vector_view& u_rhs, double dt, Fun&& F) {
495     // parallel loop over the mesh elements
496     executor_for_each(elements(Vx, Vy), [&](index_type e) {
497         auto R = vector_type{{Vx.basis.dofs_per_element(), Vy.basis.dofs_per_element
498                               ()}};
499         auto U = vector_type{{Ux.basis.dofs_per_element(), Uy.basis.dofs_per_element
500                               ()}};
501
502         double J = jacobian(e);
503         for (auto q : quad_points(Vx, Vy)) {
504             double W = weight(q);
505             double WJ = W * J;
506             auto x = point(e, q);
507             value_type uu = eval(u, e, q, Ux, Uy);
508
509             for (auto a : dofs_on_element(e, Vx, Vy)) {
510                 auto aa = dof_global_to_local(e, a, Vx, Vy);
511                 value_type v = eval_basis(e, q, a, Vx, Vy);
512
513                 double M = uu.val * v.val;
514                 double Lx = c_diff[0] * uu.dx * v.dx + beta[0] * uu.dx * v.val;
515                 double Ly = c_diff[1] * uu.dy * v.dy + beta[1] * uu.dy * v.val;
516                 double lv = M + cx * Lx + cy * Ly + dt * F(x) * v.val;
517                 double val = -lv;
518                 R(aa[0], aa[1]) += val * WJ;
519             }
520         }
521         executor_synchronized([&]() {
522             update_global_rhs(r_rhs, R, e, Vx, Vy);
523             update_global_rhs(u_rhs, U, e, Ux, Uy); // U is always 0
524         });
525     });
526 }

```

527 5.2 Time-dependent Navier-Stokes problem

528 As the second example, we consider two-dimensional Navier-Stokes equations. We seek the vector velocity field
 529 $[0, 1]^2 \times [0, T] = \Omega \times I \ni (x, y, t) \rightarrow (u_1(x, y, t), u_2(x, y, t)) \in \mathcal{R}^2$ and the scalar pressure field $[0, 1]^2 \times [0, T] = \Omega \times I \ni$
 530 $(x, y, t) \rightarrow p(x, y, t) \in \mathcal{R}$ such that

$$\left\{ \begin{array}{ll} \partial_t v + v \cdot \nabla v - \frac{1}{Re} \Delta v + \nabla p = f & \text{in } \Omega \times I \\ \nabla \cdot v = 0 & \text{in } \Omega \times I \\ v|_{\partial\Omega} = g & \text{in } \partial\Omega \times I \\ v(\cdot, 0) = v^0 & \text{in } \Omega \\ p(\cdot, 0) = p^0 & \text{in } \Omega \end{array} \right.$$

531 The first equation is really a system of two equations, since $v = (v_1, v_2)$, so $f(x, y, t) = (f_1(x, y, t), f_2(x, y, t))$ is
 532 the vector forcing field, Re is the Reynolds number describing the properties of the fluid flow, g is the prescribed
 533 velocity on the boundary of the domain, and $v^0(x, y, t) = (v_1^0(x, y, t), v_2^0(x, y, t))$ and $p^0(x, y, t)$ are the initial velocity
 534 and pressure configurations. Following the ideas presented by Petar Minev and Jean Luc-Guermound [18], we

535 replace this original problem with the singularly perturbed problem

$$\left\{ \begin{array}{ll} \partial_t v_\varepsilon + v_\varepsilon \cdot \nabla v_\varepsilon - \frac{1}{Re} \Delta v_\varepsilon + \nabla p_\varepsilon = f & \text{in } \Omega \times I \\ \varepsilon A p_\varepsilon + \nabla \cdot v_\varepsilon = 0 & \text{in } \Omega \times I \\ \varepsilon \partial_t p_\varepsilon = p_\varepsilon - \chi \frac{1}{Re} \nabla \cdot v_\varepsilon & \text{in } \Omega \times I \\ v_\varepsilon|_{\partial\Omega} = g & \text{in } \partial\Omega \times I \\ v_\varepsilon(\cdot, 0) = v_0 & \text{in } \Omega \\ p_\varepsilon(\cdot, 0) = p_0 & \text{in } \Omega \end{array} \right.$$

536 where ε, A, χ are model parameters.

537 This perturbed problem allows introducing stable direction splitting scheme, with the following sub-steps:

538 • pressure predictor: $\tilde{p}^{n+\frac{1}{2}} = p^{n-\frac{1}{2}} + \phi^{n-\frac{1}{2}}$

539 • velocity update:

$$\begin{aligned} \left(1 - \frac{\tau \partial_x^2}{2Re}\right) v^{n+\frac{1}{2}} &= \left(1 + \frac{\tau \partial_y^2}{2Re} - v^n \cdot \nabla\right) v^n - \frac{\tau}{2} \nabla \tilde{p}^{n+\frac{1}{2}} + \frac{\tau}{2} f^{n+\frac{1}{2}} \\ \left(1 - \frac{\tau \partial_y^2}{2Re}\right) v^{n+1} &= \left(1 + \frac{\tau \partial_x^2}{2Re}\right) v^{n+\frac{1}{2}} - \frac{\tau}{2} \nabla \tilde{p}^{n+\frac{1}{2}} + \frac{\tau}{2} f^{n+\frac{1}{2}} \end{aligned}$$

540 • pressure update

$$(1 - \partial_x^2) \psi = -\frac{1}{\tau} \nabla \cdot v^{n+\frac{1}{2}}$$

$$(1 - \partial_y^2) \phi^{n+\frac{1}{2}} = \psi$$

541

$$p^{n+\frac{1}{2}} = p^{n-\frac{1}{2}} + \phi^{n+\frac{1}{2}} - \chi \frac{1}{Re} \nabla \cdot \frac{1}{2} (v^{n+1} + v^n)$$

542 These sub-steps are implemented in our step method

```
543 void step(int iter, double t) override {
544     // first step - simple summation
545     compute_pressure_predictor();
546
547     update_velocity_igrm(iter, t);
548     update_pressure_igrm();
549 }
```

550 The first comes the implementation of the velocity update

```
551 void update_velocity_igrm(int /*i*/, double t) {
552     // auxiliary definitions
553     auto dt = steps.dt;
554     auto f = [&](point_type x, double s) { return problem.forcing(x, s); };
555     auto F = [&](double s) { return [&, s](point_type x) { return f(x, s); }; };
556     auto Re = problem.Re;
557     auto conv = problem.navier_stokes ? dt / 2 : 0; // if false, nonlinear term
558     // omitted
559
560     auto dU1 = trial.U1x.dofs() * trial.U1y.dofs();
561     auto dU2 = trial.U2x.dofs() * trial.U2y.dofs();
562     auto dim_trial = dU1 + dU2;
563
564     auto DU1 = test.U1x.dofs() * test.U1y.dofs();
565     auto DU2 = test.U2x.dofs() * test.U2y.dofs();
566     auto dim_test = DU1 + DU2;
567
568     // Substep 1
569     // buffer for the whole right hand side
570     std::vector<double> rhs(dim_test + dim_trial);
571     // views on parts of the right-hand side
572     vector_view rhs_vx1{rhs.data(), {test.U1x.dofs(), test.U1y.dofs()}};
573     vector_view rhs_vy1{rhs.data() + DU1, {test.U2x.dofs(), test.U2y.dofs()}};
574     vector_view vx1{rhs.data() + dim_test, {trial.U1x.dofs(), trial.U1y.dofs()}};
```

```

574     vector_view vy1{vx1.data() + dU1, {trial.U2x.dofs(), trial.U2y.dofs()}};
575
576     compute_rhs(rhs_vx1, rhs_vy1, // right-hand sides
577               vx, vy, // v0 = v from previous step
578               vx, vy, // v from previous substep
579               p_star, // pressure predictor
580               F(t + dt / 2), // forcing
581               0, 0, // v0 coeffs
582               0, -dt / (2 * Re), // v coeffs
583               -conv, // u * |u| coeff (N-S term)
584               dt / 2, // pressure coeff
585               dt / 2 // forcing coeff
586     );
587
588     apply_velocity_bc(vx1, trial.U1x, trial.U1y, t + dt, 0);
589     apply_velocity_bc(vy1, trial.U2x, trial.U2y, t + dt, 1);
590
591     mumps::problem problem_vx1{rhs};
592     assemble_matrix_velocity(problem_vx1, dt / (2 * Re), 0);
593     solver.solve(problem_vx1);
594
595     // update the state
596     vx_prev = vx;
597     vy_prev = vy;
598     // (vx, vy) := (vx2, vy2);
599     for (auto i : dofs(trial.U1x, trial.U1y)) {
600         vx(i[0], i[1]) = vx2(i[0], i[1]);
601     }
602     for (auto i : dofs(trial.U2x, trial.U2y)) {
603         vy(i[0], i[1]) = vy2(i[0], i[1]);
604     }
605 }
606
607 // Substep 2
608 std::vector<double> rhs2(dim_test + dim_trial);
609 vector_view rhs_vx2{rhs2.data(), {test.U1x.dofs(), test.U1y.dofs()}};
610 vector_view rhs_vy2{rhs2.data() + DU1, {test.U2x.dofs(), test.U2y.dofs()}};
611 vector_view vx2{rhs2.data() + dim_test, {trial.U1x.dofs(), trial.U1y.dofs()}};
612 vector_view vy2{vx2.data() + dU1, {trial.U2x.dofs(), trial.U2y.dofs()}};
613
614 compute_rhs(rhs_vx2, rhs_vy2, // right-hand sides
615            vx, vy, // v0 = v from previous step
616            vx1, vy1, // v from previous substep
617            p_star, // pressure predictor
618            F(t + dt / 2), // forcing
619            0, 0, // v0 coeffs
620            -dt / (2 * Re), 0, // v coeffs
621            -conv, // u * |u| coeff (N-S term)
622            dt / 2, // pressure coeff
623            dt / 2 // forcing coeff
624    );
625
626    apply_velocity_bc(vx2, trial.U1x, trial.U1y, t + dt, 0);
627    apply_velocity_bc(vy2, trial.U2x, trial.U2y, t + dt, 1);
628
629    mumps::problem problem_vx2{rhs2};
630    assemble_matrix_velocity(problem_vx2, 0, dt / (2 * Re));
631    solver.solve(problem_vx2);

```

For each of the sub-steps we need to generate the right-hand side. This is done with the `compute_rhs` method

```

632 // Compute RHS as
633 // (v, w) + ax (dv0/dx, dw/dx) + ay (dv0/dy, dw/dy) +
634 //          bx (dv/dx, dw/dx) + by (dv/dy, dw/dy) +
635 //          conv * u * |u|
636 //          c (|p, w) + d (f, w)
637
638 template <typename RHS, typename S1, typename S2, typename S3, typename Fun>
639 void compute_rhs(RHS& rhsx, RHS& rhsy, const S1& vx0, const S1& vy0, const S2& vx,
640               const S2& vy,
641               const S3& p, Fun&& forcing, double ax, double ay, double bx,
642               double by,
643               double conv, double c, double d) const {
644     using shape = std::array<int, 2>;

```

```

645     auto u1_shape = shape{test.U1x.basis.dofs_per_element(), test.U1y.basis.
646         dofs_per_element()};
647     auto u2_shape = shape{test.U2x.basis.dofs_per_element(), test.U2y.basis.
648         dofs_per_element()};
649
650     // parallel loop over elements
651     executor.for_each(elements(trial.Px, trial.Py), [&](index_type e) {
652         auto vx_loc = vector_type{u1_shape};
653         auto vy_loc = vector_type{u2_shape};
654
655         double J = jacobian(e);
656         for (auto q : quad_points(trial.Px, trial.Py)) {
657             double W = weight(q);
658             auto x = point(e, q);
659             auto F = forcing(x);
660
661             // compute values and gradients of two previous stated
662             // (previous time step and possibly previous half-step)
663             value_type vvx0 = eval(vx0, e, q, trial.U1x, trial.U1y);
664             value_type vvy0 = eval(vy0, e, q, trial.U2x, trial.U2y);
665             value_type vvx = eval(vx, e, q, trial.U1x, trial.U1y);
666             value_type vvy = eval(vy, e, q, trial.U2x, trial.U2y);
667             value_type pp = eval(p, e, q, trial.Px, trial.Py);
668
669             for (auto a : dofs_on_element(e, test.U1x, test.U1y)) {
670                 auto aa = dof_global_to_local(e, a, test.U1x, test.U1y);
671                 value_type v = eval_basis(e, q, a, test.U1x, test.U1y);
672
673                 double val = vvx.val * v.val
674                     //
675                     + ax * vvx0.dx * v.dx
676                     //
677                     + ay * vvx0.dy * v.dy
678                     //
679                     + bx * vvx.dx * v.dx
680                     //
681                     + by * vvx.dy * v.dy
682                     //
683                     + c * pp.val * v.dx
684                     //
685                     + conv * (vvx.val * vvx.dx + vvy.val * vvx.dy) * v.val
686                     //
687                     + d * F[0] * v.val;
688                 vx_loc(aa[0], aa[1]) += val * W * J;
689             }
690             for (auto a : dofs_on_element(e, test.U2x, test.U2y)) {
691                 auto aa = dof_global_to_local(e, a, test.U2x, test.U2y);
692                 value_type v = eval_basis(e, q, a, test.U2x, test.U2y);
693
694                 double val = ... // same for the y velocity components
695                 vy_loc(aa[0], aa[1]) += val * W * J;
696             }
697         }
698         // update of the global RHS vector
699         executor.synchronized([&]() {
700             update_global_rhs(rhsx, vx_loc, e, test.U1x, test.U1y);
701             update_global_rhs(rhsy, vy_loc, e, test.U2x, test.U2y);
702         });
703     });
704 }
705 }

```

The next the pressure update sub-step is implemented in `update_pressure_igrm`

```

706
707 void update_pressure_igrm() {
708     auto dim_trial = trial.Px.dofs() * trial.Py.dofs();
709     auto dim_test = test.Px.dofs() * test.Py.dofs();
710
711     // Step 1 - computing psi
712     std::vector<double> rhs(dim_test + dim_trial);
713     vector_view rhs_p1{rhs.data(),
714         {test.Px.dofs(), test.Py.dofs()}};
715     vector_view p1{rhs.data() + dim_test,

```



```

716         {trial.Px.dofs(), trial.Py.dofs()}};
717
718     compute_rhs_pressure_1(rhs_p1, vx, vy,
719                          test.Px, test.Py, steps.dt);
720     mumps::problem problem_px{rhs};
721     assemble_matrix_pressure(problem_px, 1, 0);
722     solver.solve(problem_px);
723
724     // Step 2 - computing  $\phi^{n+1}$ 
725     std::vector<double> rhs2(dim_test + dim_trial);
726     vector_view rhs_p2{rhs2.data(),
727                      {test.Px.dofs(), test.Py.dofs()}};
728     vector_view p2{rhs2.data() + dim_test,
729                  {trial.Px.dofs(), trial.Py.dofs()}};
730
731     compute_rhs_pressure_2(rhs_p2, p1, test.Px, test.Py);
732     mumps::problem problem_py{rhs2};
733     assemble_matrix_pressure(problem_py, 0, 1);
734     solver.solve(problem_py);
735
736     // Put solution into phi
737     for (auto i : dofs(trial.Px, trial.Py)) {
738         phi(i[0], i[1]) = p2(i[0], i[1]);
739     }
740
741     // Update pressure
742     apply_pressure_corrector();
743 }

```

We also generate the right-hand sides for this sub-step in `compute_rhs_pressure_1` and `compute_rhs_pressure_2`.

```

744 template <typename RHS, typename Sol>
745 void compute_rhs_pressure_1(RHS& rhs, const Sol& vx, const Sol& vy, const dimension&
746                            Vx,
747                            const dimension& Vy, double dt) const {
748     using shape = std::array<int, 2>;
749     auto p_shape = shape{Vx.basis.dofs_per_element(), Vy.basis.dofs_per_element()};
750
751     // parallel loop over elements, quadrature points and basis functions
752     executor for_each(elements(trial.Px, trial.Py), [&](index_type e) {
753         auto loc = vector_type{p_shape};
754
755         double J = jacobian(e);
756         for (auto q : quad_points(trial.Px, trial.Py)) {
757             double W = weight(q);
758             value_type vvx = eval(vx, e, q, trial.U1x, trial.U1y);
759             value_type vvy = eval(vy, e, q, trial.U2x, trial.U2y);
760
761             for (auto a : dofs_on_element(e, Vx, Vy)) {
762                 auto aa = dof_global_to_local(e, a, Vx, Vy);
763                 value_type v = eval_basis(e, q, a, Vx, Vy);
764
765                 double val = -1 / dt * (vvx.dx + vvy.dy) * v.val;
766                 loc(aa[0], aa[1]) += val * W * J;
767             }
768         }
769         executor.synchronized([&]() { update_global_rhs(rhs, loc, e, Vx, Vy); });
770     });
771 }

```

The implementation of the `compute_rhs_pressure_2` is similar, except for `double val = pp.val * v.val;`. The Gram matrix A and the problem matrix B are generated in `assemble_matrix_pressure` routine.

```

774 void assemble_matrix_pressure(mumps::problem& problem, double cx, double cy) const {
775     // Here we build a matrix used to calculate psi and  $\phi^{n+1/2}$ 
776     // Stabilization using iGRM leads to the following structure:
777     //   G   B
778     //   B^T 0
779
780     // Assembling the Gram matrix - G
781     for (auto i : dofs(test.Px, test.Py)) {
782         for (auto j : overlapping_dofs(i, test.Px, test.Py)) {
783             int ii = linear_index(i, test.Px, test.Py) + 1;
784             int jj = linear_index(j, test.Px, test.Py) + 1;

```

```

785         if (!is_pressure_fixed(i) && !is_pressure_fixed(j)) {
786             auto eval = [&](auto form) {
787                 return integrate(i, j, test.Px, test.Py, test.Px, test.Py, form)
788                 ;
789             };
790             double val = eval([&](auto w, auto p) { return w.val * p.val; });
791             problem.add(ii, jj, val);
792         }
793     }
794 }
795
796 // Assembling B (and B^T at the same time)
797
798 // This auxiliary function makes sure the entries of B and B^T
799 // blocks are placed correctly inside the full matrix
800 auto DP = test.Px.dofs() * test.Py.dofs();
801 auto put = [&](int i, int j, int si, int sj, double val) {
802     int ii = i + si;
803     int jj = j + sj;
804     problem.add(ii, DP + jj, val);
805     problem.add(DP + jj, ii, val);
806 };
807
808 for (auto i : dofs(test.Px, test.Py)) {
809     for (auto j : overlapping_dofs(i, test.Px, test.Py, trial.Px, trial.Py)) {
810         if (!overlap(i, test.Px, test.Py, j, trial.Px, trial.Py))
811             continue;
812
813         int ii = linear_index(i, test.Px, test.Py) + 1;
814         int jj = linear_index(j, trial.Px, trial.Py) + 1;
815         auto eval = [&](auto form) {
816             return integrate(i, j, test.Px, test.Py, trial.Px, trial.Py, form);
817         };
818
819         double value = eval([cx, cy](auto u, auto v) {
820             return u.val * v.val + cx * u.dx * v.dx + cy * u.dy * v.dy;
821         });
822         put(ii, jj, 0, 0, value);
823     }
824 }
825 }
826
827 void apply_pressure_corrector() {
828     vector_type rhs{{trial.Px.dofs(), trial.Py.dofs()}};
829
830     double chi = 0;
831     compute_rhs_pressure_update(rhs, chi);
832     mumps::problem problem(rhs.data(), rhs.size());
833     assemble_matrix(problem, 0, 0, false, false, trial.Px, trial.Py);
834     solver.solve(problem);
835
836     p = rhs;
837 }
838
839 template <typename RHS>
840 void compute_rhs_pressure_update(RHS& rhs, double chi) const {
841     auto Re = problem.Re;
842     using shape = std::array<int, 2>;
843     auto p_shape = shape{trial.Px.basis.dofs_per_element(), trial.Py.basis.
844         dofs_per_element()};
845
846     // parallel loop over elements, quadratures points and basis functions
847     executor_for_each(elements(trial.Px, trial.Py), [&](index_type e) {
848         auto loc = vector_type{p_shape};
849
850         double J = jacobian(e);
851         for (auto q : quad_points(trial.Px, trial.Py)) {
852             double W = weight(q);
853             value_type pp = eval(p, e, q, trial.Px, trial.Py);
854             value_type pphi = eval(phi, e, q, trial.Px, trial.Py);
855             value_type vvx = eval(vx, e, q, trial.U1x, trial.U1y);
856             value_type vvy = eval(vy, e, q, trial.U2x, trial.U2y);

```

```

855         value_type vvx_prev = eval(vx_prev, e, q, trial.U1x, trial.U1y);
856         value_type vvy_prev = eval(vy_prev, e, q, trial.U2x, trial.U2y);
857
858         for (auto a : dofs_on_element(e, trial.Px, trial.Py)) {
859             auto aa = dof_global_to_local(e, a, trial.Px, trial.Py);
860             value_type v = eval_basis(e, q, a, trial.Px, trial.Py);
861
862             double vdiv = vvx.dx + vvy.dy;
863             double vdiv_prev = vvx_prev.dx + vvy_prev.dy;
864             double val = (pp.val + pphi.val - 0.5 * chi / Re * (vdiv + vdiv_prev
865                 )) * v.val;
866             loc(aa[0], aa[1]) += val * W * J;
867         }
868     }
869     executor.synchronized([&]() { update_global_rhs(rhs, loc, e, trial.Px, trial
870         .Py); });
871 });
872 }

```

```

873 void assemble_matrix(mumps::problem& problem, double cx, double cy, bool bcx, bool
874     bcy,
875         const dimension& Ux, const dimension& Uy) const {
876     // loop over pairs of overlapping DoFs
877     for (auto i : dofs(Ux, Uy)) {
878         for (auto j : overlapping_dofs(i, Ux, Uy)) {
879             int ii = linear_index(i, Ux, Uy) + 1;
880             int jj = linear_index(j, Ux, Uy) + 1;
881
882             bool at_bdx = is_boundary(i[0], Ux) || is_boundary(j[0], Ux);
883             bool at_bdy = is_boundary(i[1], Uy) || is_boundary(j[1], Uy);
884             bool fixed = (at_bdx && bcx) || (at_bdy && bcy);
885
886             if (!fixed) {
887                 auto form = [cx, cy](auto u, auto v) {
888                     return u.val * v.val + cx * u.dx * v.dx + cy * u.dy * v.dy;
889                 };
890                 auto product = integrate(i, j, Ux, Uy, Ux, Uy, form);
891                 problem.add(ii, jj, product);
892             }
893         }
894     }
895     // account for boundary conditions if necessary
896     for_boundary_dofs(Ux, Uy, [&](index_type dof) {
897         int i = linear_index(dof, Ux, Uy) + 1;
898         bool at_bdx = is_boundary(dof[0], Ux) || is_boundary(dof[0], Ux);
899         bool at_bdy = is_boundary(dof[1], Uy) || is_boundary(dof[1], Uy);
900         bool fixed = (at_bdx && bcx) || (at_bdy && bcy);
901         if (fixed) { problem.add(i, i, 1); }
902     });
903 }

```

5.3 Discontinuous Galerkin method

Similarly to the Galerkin method enhanced with the residual minimization, we also introduce the Discontinuous Galerkin method, and we enhance with residual minimization scheme. First, we illustrate the DG method on the example of the Poisson equation with Dirichlet boundary data. We seek the scalar field $[0, 1]^2 = \Omega \ni (x, y) \rightarrow u(x, y) \in \mathcal{R}$ such that

$$\begin{cases} -\Delta u = f \\ u|_{\partial\Omega} = g \end{cases} \quad (26)$$

with the Dirichlet boundary condition prescribed by $\partial\Omega \ni (x, y) \rightarrow u(x, y) \in \mathcal{R}$. Our DG formulation is based on standard Symmetric Interior Penalty (SIP) method:

$$a_h^{\text{SIP}}(u_h, v_h) = I_h(v_h) \quad (27)$$

911 where

$$\begin{aligned}
 a_h^{\text{sip}}(u_h, v_h) &= (\nabla_h u_h, \nabla_h v_h) \\
 &\quad - \sum_{F \in \mathcal{F}_h} \int_F (\{\nabla_h u_h\} \cdot n_F [v_h] + \{\nabla_h v_h\} \cdot n_F [u_h]) d\sigma \\
 &\quad + \sum_{F \in \mathcal{F}_h} \frac{\eta}{h_F} \int_F [u_h][v_h] d\sigma \\
 l_h(v_h) &= (f, v_h) + \sum_{F \in \mathcal{F}_h^{\partial}} \int_F \left(-\nabla g \cdot n_F v_h + \frac{\eta}{h_F} g v_h \right) d\sigma
 \end{aligned} \tag{28}$$

912 Here $[\psi(x)] = \psi|_{T_1}(x) - \psi|_{T_2}(x)$ denotes the jump across the shared edge between elements T_1 and T_2 , and
 913 $\{\psi\} = \frac{\psi|_{T_1}(x) + \psi|_{T_2}(x)}{2}$ defines an average. The n_F denotes the versor normal to the element edge. The setup of
 914 the DG formulation in the code is done in the following way. We define the number of elements in `elems`. We
 915 introduce equally spaced one-dimensional grids along x and y axis span between 0 and 1. We build regular 2d
 916 mesh from these grids. We define B-splines of order p and continuity c . We define the quadrature to integrate the
 917 B-splines exactly.

```

918 // Define the XY grid
919 int elems = 128;
920 auto xs = ads::evenly_spaced(0.0, 1.0, elems);
921 auto ys = ads::evenly_spaced(0.0, 1.0, elems);
922 auto mesh = ads::regular_mesh{xs, ys};
923
924 // p - spline order, c - spline continuity
925 auto bx = ads::make_bspline_basis(xs, p, c);
926 auto by = ads::make_bspline_basis(ys, p, c);
927
928 // Create representations of the discrete space
929 auto space = ads::space{&mesh, bx, by};
930
931 // Use quadrature with p+1 points to ensure accuracy
932 auto quad = ads::quadrature{&mesh, p + 1};

```

933 We will use the MUMPS solver [14, 15] to solve the DG problem.

```

934 // Allocate space for matrix and the right-hand side
935 auto F = std::vector<double>(n);
936 auto problem = ads::mumps::problem{F.data(), n};
937
938 // These functions instruct the integration code
939 // where to put the computed values
940 auto out = [&problem](int row, int col, double val) {
941     if (val != 0) {
942         problem.add(row + 1, col + 1, val);
943     }
944 };
945 auto rhs = [&F](int J, double val) { F[J] += val; };
946
947 // We are using MUMPS as our solver
948 auto solver = ads::mumps::solver{};

```

949 We assembly the system, component by component, following the formula 28.

```

950 // Assemble the first part of a^sip - elementwise gradient product
951 assemble(space, quad, out, [](auto u, auto v, auto /*x*/) {
952     return dot(grad(u), grad(v));
953 });
954
955 // Assemble the second part - edge integrals
956 auto form = [eta](auto u, auto v, auto /*x*/, const auto& edge) {
957     const auto& n = edge.normal;
958     const auto h = length(edge.span);
959     return - dot(grad(avg(v)), n) * jump(u).val
960            - dot(grad(avg(u)), n) * jump(v).val
961            + eta / h * jump(u).val * jump(v).val;
962 };
963 assemble_facets(mesh.facets(), space, quad, out, form);

```

964 The right-hand side for the DG code is formulated in `assemble_rhs` routine,

```

965 // As for the matrix - assemble first part of the linear form
966 // 'poisson' is an object representing the problem data
967 assemble_rhs(space, quad, rhs, [&poisson](auto v, auto x) {
968     return v.val * poisson.f(x); // f - part of problem data
969 });
970
971 // Second part - edge integrals
972 auto bd_form = [eta, &poisson](auto v, auto x, const auto& edge) {
973     const auto& n = edge.normal;
974     const auto h = length(edge.span);
975     const auto g = poisson.g(x); // g - part of problem data
976     return - dot(grad(v), n) * g
977            + eta/h * g * v.val;
978 };
979 // Here we only need the boundary edges, no the full skeleton
980 assemble_rhs(mesh.boundary_facets(), space, quad, rhs, bd_form);

```

The solution process and the postprocessing are invoked from the main routine in the following way

```

981
982 // Solve the assembled linear system
983 solver.solve(problem);
984
985 // Function object representing the solution
986 auto u = ads::bspline_function(&space, F.data());
987
988 // Compute error in L2 norm (assuming known exact solution)
989 auto err = error(mesh, quad, L2{ }, u, poisson.u());
990 fmt::print("error = {:.6}\n", err);
991
992 // Output
993 save_to_file("result.data", u);

```

5.4 Discontinuous Galerkin with residual minimization for Stokes problem

To illustrate the stabilization with the DG mixed with the residual minimization method, we focus now on the Stokes equation. We seek the vector velocity field $[0, 1]^3 = \Omega \ni (x, y, z) \rightarrow (u_1(x, y, z), u_2(x, y, z)) \in \mathcal{R}^3$ and the scalar pressure field $[0, 1]^3 = \Omega \ni (x, y, z) \rightarrow p(x, y, z) \in \mathcal{R}$ such that

$$\begin{cases} -\Delta u + \nabla p = f \\ \nabla \cdot u = 0 \\ u|_{\partial\Omega} = 0 \end{cases} \quad (29)$$

First, we write the standard DG formulation that will stand for the problem matrix B in the residual minimization setup

$$\begin{cases} a_h(u_h^{\text{DG}}, v_h) + b_h(v_h, p_h^{\text{DG}}) = (f, v_h) \\ -b_h(u_h^{\text{DG}}, q_h) + s_h(p_h^{\text{DG}}, q_h) = 0 \end{cases} \quad (30)$$

where

$$\begin{aligned} a_h(w_h, v_h) &= (\nabla_h w_h, \nabla_h v_h) + \sum_{F \in \mathcal{F}_h} \frac{\eta}{h_F} \int_F [u_h][v_h] d\sigma \\ &\quad - \sum_{F \in \mathcal{F}_h} \int_F (\{\nabla_h w_h\} \cdot n_F [v_h] + \{\nabla_h v_h\} \cdot n_F [w_h]) d\sigma \\ b_h(v_h, q_h) &= - \int_{\Omega} q_h \nabla \cdot v_h dx + \sum_{F \in \mathcal{F}_h^0} \int_F [v_h] \cdot n_F \{q_h\} d\sigma \\ s_h(p_h, q_h) &= \sum_{F \in \mathcal{F}_h^0} h_F \int_F [p_h][q_h] d\sigma \end{aligned} \quad (31)$$

Second, we denote the problem (31) in the following way: Find $\varphi \in V_h$ such that

$$C_h(\varphi_h, \psi_h) = (f, \psi_h) \quad \forall \psi_h \in V_h \quad (32)$$

and we construct the residual minimization stabilization on top of (31).

$$\varphi_h = \operatorname{argmin}_{w_h \in U_h} \|C_h(w_h, *) - (f, *)\|_{V_h^*} \quad (33)$$

1003 Namely, we solve

$$\begin{aligned} (r_h, \psi_h)_{V_h} + C_h(\phi_h, \psi_h) &= (f, \psi_h)_\Omega \quad \forall \psi_h \in V_h \\ C_h(w_h, r_h) &= 0 \quad \forall w_h \in U_h \end{aligned} \quad (34)$$

1004 In the residual minimization method, following [11], we introduce the following norm for building the Gram
1005 matrix

$$\begin{aligned} |||(v_h, q_h)|||_{Stokes}^2 &= \sum_{i=1, \dots, d} \left(\sum_{K \in T_h} \|\nabla v_{h,i}\|_{L^2(K)}^2 + \sum_{F \in F_h} \frac{1}{h_F} \| [v_{h,i}] \|_{L^2(F)}^2 \right) + \\ &\quad \|q_h\|_{L^2(\Omega)}^2 + \sum_{F \in F_h^{internal}} h_F \| [q_h] \|_{L^2(F)}^2 \end{aligned} \quad (35)$$

1006 The problem setup defines three one-dimensional grids with elements spanning between 0 and 1. It builds
1007 regular 3d mesh using these one-dimensional grids. It also constructs quadrature to integrate trial B-splines of
1008 order p_{trial} , and test B-splines of order p_{test} . It builds trial and test B-splines with given order and continuity
1009 along x , y , and z axes. It employs them for approximation of the velocity and pressure.

```

1010 // Mesh and quadrature rules
1011 auto xs = ads::evenly_spaced(0.0, 1.0, elems);
1012 auto ys = ads::evenly_spaced(0.0, 1.0, elems);
1013 auto zs = ads::evenly_spaced(0.0, 1.0, elems);
1014 auto mesh = ads::regular_mesh3{xs, ys, zs};
1015 auto quad = ads::quadrature3{&mesh, std::max(p_test, p_trial) + 1};
1016
1017 // Test space splines
1018 auto Bx = ads::make_bspline_basis(xs, p_test, c_test);
1019 auto By = ads::make_bspline_basis(ys, p_test, c_test);
1020 auto Bz = ads::make_bspline_basis(zs, p_test, c_test);
1021
1022 // Space factory ensures correct global DoF numbering
1023 auto tests = space_factory{};
1024 auto Wx = tests.next<ads::space3>(&mesh, Bx, By, Bz);
1025 auto Wy = tests.next<ads::space3>(&mesh, Bx, By, Bz);
1026 auto Wz = tests.next<ads::space3>(&mesh, Bx, By, Bz);
1027 auto Q = tests.next<ads::space3>(&mesh, Bx, By, Bz);
1028 auto N = Wx.dof_count() + Wy.dof_count() + Wz.dof_count()
1029         + Q.dof_count();
1030
1031 // Trial space splines
1032 auto bx = ads::make_bspline_basis(xs, p_trial, c_trial);
1033 auto by = ads::make_bspline_basis(ys, p_trial, c_trial);
1034 auto bz = ads::make_bspline_basis(zs, p_trial, c_trial);
1035
1036 // Trial space components
1037 auto trials = space_factory{};
1038 auto Vx = trials.next<ads::space3>(&mesh, bx, by, bz);
1039 auto Vy = trials.next<ads::space3>(&mesh, bx, by, bz);
1040 auto Vz = trials.next<ads::space3>(&mesh, bx, by, bz);
1041 auto P = trials.next<ads::space3>(&mesh, bx, by, bz);
1042 auto n = Vx.dof_count() + Vy.dof_count() + Vz.dof_count()
1043         + P.dof_count();

```

1043 We will employ the MUMPS solver in this example. We build the Gram matrix and the problem matrix to be
1044 solved.

```

1045 auto F = std::vector<double>(N + n);
1046 auto problem = ads::mumps::problem{F.data(), N + n};
1047 // G - Gram matrix, B - bilinear form matrix
1048 // Full matrix structure:
1049 //   G   B
1050 //   B^T 0
1051 auto G = [&problem](int row, int col, double val) {
1052     if (val != 0) {
1053         problem.add(row + 1, col + 1, val);
1054     }
1055 };
1056 auto B = [&problem, N](int row, int col, double val) {
1057     if (val != 0) {
1058         problem.add(row + 1, N + col + 1, val);

```

```

1059         problem.add(N + col + 1, row + 1, val);
1060     }
1061 };
1062 auto rhs = [&F](int row, double val) { F[row] += val; };
1063
1064 The Gram matrix and the problem matrices are assembled step by step according to formula 34 and 35
1065
1066 // Compute volume integrals of the test space product (Gram matrix)
1067 assemble(Wx, quad, G, [](auto ux, auto vx, auto /*x*/) { return dot(grad(ux), grad(
1068     vx)); });
1069 assemble(Wy, quad, G, [](auto uy, auto vy, auto /*x*/) { return dot(grad(uy), grad(
1070     vy)); });
1071 assemble(Wz, quad, G, [](auto uz, auto vz, auto /*x*/) { return dot(grad(uz), grad(
1072     vz)); });
1073 assemble(Q, quad, G, [](auto p, auto q, auto /*x*/) { return p.val * q.val;
1074     });
1075
1076 // Compute volume integrals of the problem bilinear form
1077 assemble(Vx, Wx, quad, B, [](auto ux, auto vx, auto /*x*/) { return dot(grad(ux),
1078     grad(vx)); });
1079 assemble(Vy, Wy, quad, B, [](auto uy, auto vy, auto /*x*/) { return dot(grad(uy),
1080     grad(vy)); });
1081 assemble(Vz, Wz, quad, B, [](auto uz, auto vz, auto /*x*/) { return dot(grad(uz),
1082     grad(vz)); });
1083 assemble(P, Wx, quad, B, [](auto p, auto vx, auto /*x*/) { return - p.val * vx.dx;
1084     });
1085 assemble(P, Wy, quad, B, [](auto p, auto vy, auto /*x*/) { return - p.val * vy.dy;
1086     });
1087 assemble(P, Wz, quad, B, [](auto p, auto vz, auto /*x*/) { return - p.val * vz.dz;
1088     });
1089 assemble(Vx, Q, quad, B, [](auto ux, auto q, auto /*x*/) { return ux.dx * q.val;
1090     });
1091 assemble(Vy, Q, quad, B, [](auto uy, auto q, auto /*x*/) { return uy.dy * q.val;
1092     });
1093 assemble(Vz, Q, quad, B, [](auto uz, auto q, auto /*x*/) { return uz.dz * q.val;
1094     });
1095
1096 // Compute edge integrals of the test space product (Gram matrix)
1097 assemble_facets(mesh.facets(), Wx, quad, G, [](auto ux, auto vx, auto /*x*/, const
1098     auto& face) {
1099     const auto h = face.diameter;
1100     return 1/h * jump(ux).val * jump(vx).val;
1101 });
1102 // ... same for Y and Z
1103 assemble_facets(mesh.interior_facets(), Q, quad, G, [](auto p, auto q, auto /*x*/,
1104     const auto& face) {
1105     const auto h = face.diameter;
1106     return h * jump(p).val * jump(q).val;
1107 });
1108
1109 // Compute edge integrals of the problem bilinear form
1110 assemble_facets(mesh.facets(), Vx, Wx, quad, B, [eta](auto ux, auto vx, auto /*x*/,
1111     const auto& face) {
1112     const auto& n = face.normal;
1113     const auto h = face.diameter;
1114     return - dot(grad(avg(vx)), n) * jump(ux).val
1115         - dot(grad(avg(ux)), n) * jump(vx).val
1116         + eta/h * jump(ux).val * jump(vx).val;
1117 });
1118 // ... same for (Vy, Wy) and (Vz, Wz)
1119 assemble_facets(mesh.facets(), P, Wx, quad, B, [](auto p, auto vx, auto /*x*/, const
1120     auto& face) {
1121     const auto& n = face.normal;
1122     const auto v = ads::point3_t{jump(vx).val, 0, 0};
1123     return avg(p).val * dot(v, n);
1124 });
1125 // ... same for Wy and Wz
1126 assemble_facets(mesh.facets(), Vx, Q, quad, B, [](auto ux, auto q, auto /*x*/, const
1127     auto& face) {
1128     const auto& n = face.normal;
1129     const auto u = ads::point3_t{jump(ux).val, 0, 0};
1130     return - dot(u, n) * avg(q).val;
1131 });
1132 // ... same for Vy and Vz

```

```

1130 We also assemble the right-hand side
1131 // Volume integral
1132 assemble_rhs(Wx, quad, rhs, [&stokes](auto vx, auto x) {
1133     return vx.val * stokes.fx(x); // fx - problem data
1134 });
1135 // ... same for Wy and Wz
1136
1137 // Boundary integral
1138 assemble_rhs(mesh.boundary_facets(), Wx, quad, rhs,
1139             [eta,&stokes](auto vx, auto x, const auto& face) {
1140     const auto& n = face.normal;
1141     const auto h = face.diameter;
1142     const auto g = stokes.vx(x); // vx - problem data
1143     return - dot(grad(vx), n) * g
1144            + eta/h * g * vx.val;
1145 });
1146 // ... same for Wy and Wz

```

1147 5.5 Stationary advection-diffusion stabilized with residual minimization using Conju- 1148 gate Gradients solver

1149 Finally, we focus on the stationary advection-diffusion problem with Dirichlet boundary conditions. We seek the
1150 scalar concentration field $[0, 1]^2 = \Omega \ni (x, y) \rightarrow u(x, y) \in \mathcal{R}$ such that

$$\begin{cases} -\varepsilon \Delta u + \beta \cdot \nabla u = f & \text{in } \Omega \\ v|_{\partial\Omega} = g & \text{in } \partial\Omega \end{cases} \quad (36)$$

1151 We derive a weak formulation with weak enforcement of the boundary conditions using Nitsche's method

$$\begin{aligned} b(u_h, v_h) &= \varepsilon (\nabla u_h, \nabla v_h) + (\beta \cdot \nabla u_h, v_h) \\ &\quad - \langle \varepsilon \nabla u_h \cdot \hat{\mathbf{n}}, v_h \rangle - \langle u_h, \varepsilon \nabla v_h \cdot \hat{\mathbf{n}} \rangle \\ &\quad + \langle u_h, \beta \cdot \hat{\mathbf{n}} v_h \rangle - \langle \gamma_h u_h, v_h \rangle \\ l(v_h) &= (f, v_h) - \langle g, \varepsilon \nabla v_h \cdot \hat{\mathbf{n}} \rangle \\ &\quad + \langle g, \beta \cdot \hat{\mathbf{n}} v_h \rangle - \langle \gamma_h g, v_h \rangle \end{aligned} \quad (37)$$

1152 On top of the problem formulation 37, we derive the residual minimization stabilization with the Gram matrix
1153 corresponding to the weighted H^1 norm, namely $G = M + \eta K$ where M, K corresponds to the mass and stiffness
1154 matrix, and η is the parameter.

$$\begin{bmatrix} G & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} r \\ u \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix} \quad (38)$$

1155 We employ an iterative procedure to solve the system 38. We replace the Gram matrix G by an easy-to-factorize
1156 approximation \tilde{G} that has a Kronecker product structure $\tilde{G} = (K_x + \eta M_x) \otimes (K_y + \eta M_y)$, and it is inexpensive to
1157 solve and only introduces an error of order η^2 . We use an iterative algorithm

$$\begin{bmatrix} r^{k+1} \\ u^{k+1} \end{bmatrix} = \begin{bmatrix} r^k \\ u^k \end{bmatrix} + \begin{bmatrix} d \\ c \end{bmatrix} \quad (39)$$

1158 where

$$\begin{bmatrix} \tilde{G} & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} d \\ c \end{bmatrix} = \begin{bmatrix} F - Gr^k - Bu^k \\ -B^T r^k \end{bmatrix} \quad (40)$$

1159 which is solved as

$$B^T \tilde{G}^{-1} Bc = B^T \tilde{G}^{-1} (F - (G - \tilde{G})r^k - Bu^k) \quad (41)$$

1160 using conjugate gradients solver. This time we setup the problem in the step routine, implementing the solver
1161 algorithm

```

1162 void step(int /*iter*/, double /*t*/) override {
1163     // buffers for auxiliary vectors
1164     auto dd = vector_type{{Vx.dofs(), Vy.dofs()}};
1165     auto dc = vector_type{{Ux.dofs(), Uy.dofs()}};
1166     auto Bc = vector_type{{Vx.dofs(), Vy.dofs()}};

```



```

1167
1168     int i = 0;
1169     for (; i < cfg.max_outer_iters; ++i) {
1170         // first we compute the RHS of the Shur complement system
1171         //  $dd = A^{-1} (F + Kr - Bu)$ 
1172         compute_dd(Vx, Vy, dd);
1173         zero_bc(dd, Vx, Vy);
1174         solve_A(dd);
1175
1176         //  $dc = B' dd$ 
1177         apply_Bt(dd, dc);
1178         zero_bc(dc, Ux, Uy);
1179
1180         // solve for c (this also updates u)
1181         auto c = cfg.use_cg ? substep_CG(dc) : substep_mumps();
1182
1183         // use computed c to update r
1184         //  $Bc = A^{-1} B c$ 
1185         apply_B(c, Bc);
1186         zero_bc(Bc, Vx, Vy);
1187         solve_A(Bc);
1188
1189         //  $r + d = dd - A^{-1} B c$ 
1190         update_residual(dd, Bc);
1191
1192         // check stopping condition
1193         auto dimU = Ux.dofs() * Uy.dofs();
1194         auto cc = norm(c, Ux, Uy) / dimU;
1195
1196         if (cc < cfg.tol_outer) {
1197             ++i;
1198             break;
1199         }
1200     }

```

The conjugate gradient solver is implemented in substep_CG routine

```

1201
1202     vector_view substep_CG(const vector_type& dc) {
1203         vector_type u_prev = u;
1204         auto p = dc;
1205         auto q = dc;
1206         auto theta = vector_type{{Vx.dofs(), Vy.dofs()}};
1207         auto delta = theta;
1208         auto Mp = vector_type{{Ux.dofs(), Uy.dofs()}};
1209
1210         for (int i = 0; i < cfg.max_inner_iters; ++i) {
1211             //  $\theta = Bp$ 
1212             apply_B(p, theta);
1213             zero_bc(theta, Vx, Vy);
1214             //  $\delta = A^{-1} \theta$ 
1215             delta = theta;
1216             solve_A(delta);
1217             //  $\alpha = (p, q) / (p, Mp)$ 
1218             double alpha = dot(p, q, Ux, Uy) / dot(theta, delta, Vx, Vy);
1219             //  $Mp = B' \delta$ 
1220             apply_Bt(delta, Mp);
1221             zero_bc(Mp, Ux, Uy);
1222
1223             double qnorm2_prev = norm_sq(q, Ux, Uy);
1224
1225             //  $u := u + \alpha p$ 
1226             //  $q := q - \alpha Mp$ 
1227             for (auto i : dofs(Ux, Uy)) {
1228                 u(i[0], i[1]) += alpha * p(i[0], i[1]);
1229                 q(i[0], i[1]) -= alpha * Mp(i[0], i[1]);
1230             }
1231             //  $\beta = |q_{prev}|^2 / |q|^2$ 
1232             double qnorm2 = norm_sq(q, Ux, Uy);
1233             double beta = qnorm2 / qnorm2_prev;
1234             //  $p := q + \beta p$ 
1235             for (auto i : dofs(Ux, Uy)) {
1236                 p(i[0], i[1]) = q(i[0], i[1]) + beta * p(i[0], i[1]);

```

```

1237     // check for convergence
1238     auto dimU = Ux.dofs() * Uy.dofs();
1239     double residuum = std::sqrt(qnorm2) / dimU;
1240     if (residuum < cfg.tol_inner)
1241         break;
1242     }
1243     vector_view du{full_rhs.data(), {Ux.dofs(), Uy.dofs()}};
1244     for (auto i : dofs(Ux, Uy)) {
1245         du(i[0], i[1]) = u(i[0], i[1]) - u_prev(i[0], i[1]);
1246     }
1247     return du;
1248 }

```

The matrices from the system of equations are formulated in the following routines

```

1250 // Interior part of the problem bilinear form
1251 double B(value_type u, value_type v, point_type x) const {
1252     auto diff = diffusion(x);
1253     return diff * grad_dot(u, v) + dot(beta(x), u) * v.val;
1254 }
1255
1256 // Boundary part of the problem bilinear form
1257 double bdB(value_type u, value_type v, point_type x, point_type n) const {
1258     return - epsilon * v.val * dot(u, n) // <eps \|u\|n, v> -- consistency
1259         - epsilon * u.val * dot(v, n) // <u, eps \|v\|n> -- symmetry
1260         - u.val * v.val * dot(beta(x), n) // <u, v beta*n> -- symmetry
1261         - u.val * v.val * gamma; // <u, gamma v> -- penalty
1262 }
1263
1264 // Boundary part of the problem RHS
1265 double bdL(value_type v, point_type x, point_type n) const {
1266     return - epsilon * g(x) * dot(v, n) // <g, eps \|v\|n>
1267         - g(x) * v.val * dot(beta(x), n) // <g, v beta*n>
1268         - g(x) * v.val * gamma; // <u, gamma v> -- penalty
1269 }
1270
1271 // Scalar product for iGRM stabilization
1272 double A(value_type u, value_type v) const {
1273     return u.val * v.val + h * h * grad_dot(u, v);
1274 }

```

Finally, the right-hand side vector is defined in the following routines

```

1275
1276 void compute_dd(const dimension& Vx, const dimension& Vy, vector_type& dd) {
1277     zero(dd);
1278     // parallel loop over mesh elements
1279     executor.for_each(elements(Vx, Vy), [&](index_type e) {
1280         auto R = vector_type{{Vx.basis.dofs_per_element(),
1281                               Vy.basis.dofs_per_element()}};
1282
1283         double J = jacobian(e);
1284         for (auto q : quad_points(Vx, Vy)) {
1285             double W = weight(q);
1286             double WJ = W * J;
1287             auto x = point(e, q);
1288             value_type uu = eval(u, e, q, Ux, Uy);
1289             // mixed xy derivative evaluation
1290             double rxy = eval_fun_dxy(r, e, q, Vx, Vy);
1291
1292             for (auto a : dofs_on_element(e, Vx, Vy)) {
1293                 auto aa = dof_global_to_local(e, a, Vx, Vy);
1294                 value_type v = eval_basis(e, q, a, Vx, Vy);
1295                 double vxy = eval_basis_dxy(e, q, a, Vx, Vy);
1296                 double Lv = F(x) * v.val;
1297
1298                 // F + Kr - Bu
1299                 double Kr = eta * eta * rxy * vxy;
1300                 // B is the bilinear form of the problem
1301                 double val = Lv + Kr - B(uu, v, x);
1302                 R(aa[0], aa[1]) += val * WJ;
1303             }
1304         }
1305     });
1306     executor.synchronized([&]() { update_global_rhs(dd, R, e, Vx, Vy); });

```

```

1307 // Boundary terms of -Bu
1308 for (auto i : dofs(Vx, Vy)) {
1309     double val = 0;
1310
1311     auto form = [&](auto v, auto u, auto x, auto n) {
1312         return this->bdB(u, v, x, n);
1313     };
1314     // loop over (subset) of boundary edges
1315     for_sides(~dirichlet, [&](auto side) {
1316         if (this->touches(i, side, Vx, Vy)) {
1317             val += integrate_boundary(side, i, Vx, Vy, u, Ux, Uy, form);
1318         }
1319     });
1320     dd(i[0], i[1]) -= val;
1321 }
1322
1323 // Boundary terms of RHS
1324 for (auto i : dofs(Vx, Vy)) {
1325     double val = 0;
1326
1327     auto form = [&](auto w, auto x, auto n) {
1328         return this->bdL(w, x, n);
1329     };
1330     // loop over (subset) of boundary edges
1331     for_sides(~dirichlet, [&](auto side) {
1332         if (this->touches(i, side, Vx, Vy)) {
1333             val += integrate_boundary(side, i, Vx, Vy, form);
1334         }
1335     });
1336     dd(i[0], i[1]) += val;
1337 }
1338 }

```

```

1339 template <typename U, typename Res>
1340 void apply_B(const U& u, Res& result) {
1341     zero(result);
1342     executor for_each(elements(Vx, Vy), [&](index_type e) {
1343         auto rhs = vector_type{{Vx.basis.dofs_per_element(), Vy.basis.
1344             dofs_per_element()}};
1345         double J = jacobian(e);
1346         for (auto q : quad_points(Vx, Vy)) {
1347             double W = weight(q);
1348             double WJ = W * J;
1349             auto x = point(e, q);
1350             value_type uu = eval(u, e, q, Ux, Uy);
1351
1352             for (auto a : dofs_on_element(e, Vx, Vy)) {
1353                 auto aa = dof_global_to_local(e, a, Vx, Vy);
1354                 value_type v = eval_basis(e, q, a, Vx, Vy);
1355                 double val = B(uu, v, x);
1356                 rhs(aa[0], aa[1]) += val * WJ;
1357             }
1358         }
1359         executor.synchronized([&]() { update_global_rhs(result, rhs, e, Vx, Vy); });
1360     });
1361     // Boundary terms of Bu
1362     for (auto i : dofs(Vx, Vy)) {
1363         double val = 0;
1364         auto form = [&](auto v, auto u, auto x, auto n) { return this->bdB(u, v, x,
1365             n); };
1366         for_sides(~dirichlet, [&](auto side) {
1367             if (this->touches(i, side, Vx, Vy)) {
1368                 val += integrate_boundary(side, i, Vx, Vy, u, Ux, Uy, form);
1369             }
1370         });
1371         result(i[0], i[1]) += val;
1372     }
1373 } // apply_Bt - analogous

```

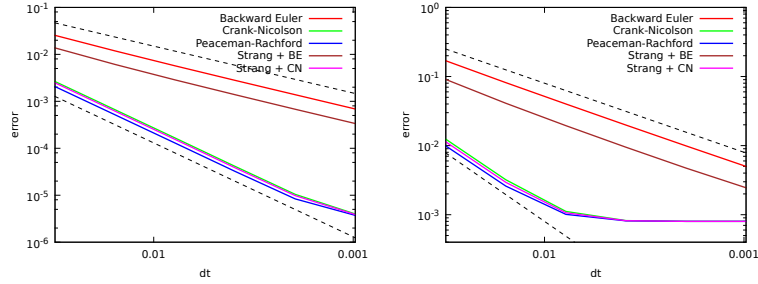


Figure 3: Horizontal axis denotes time step size. The vertical axis denotes the L2 and H1 norms of the solution for different time integration schemes on 32×32 mesh.

6 Numerical examples

The numerical examples section aims to illustrate the correctness of our code and show how it can be used to stabilize difficult computational problems. The first numerical result illustrates the application of different time-marching schemes for the non-stationary advection-dominated diffusion problem with a manufactured solution. The second numerical example concerns the stabilized simulations of the pollution propagation from a chimney with the Douglass-Gunn time integration scheme and residual minimization method. The third example concerns the cavity problem with Navier-Stokes equations. This example aims to show that the standard Galerkin formulation does not work, and thus, we can stabilize it by adding residual minimization on top of the time marching schemes. The fourth numerical example concerns the manufactured solution for the Stokes problem solved by using the Discontinuous Galerkin method with residual minimization. The goal of our simulation is to measure the numerical errors to show the high accuracy of our solutions. The fifth numerical example is the advection skew to the mesh, a stationary advection-dominated diffusion problem solved with residual minimization and conjugate gradient solver.

6.1 Manufactured solution for advection-dominated diffusion with different time marching schemes

We focus on time-dependent advection-diffusion problem

$$\frac{\partial u}{\partial t} - \varepsilon \nabla \cdot (\nabla u) + \beta \cdot \nabla u = f,$$

with $\varepsilon = 10^{-2}$, $\beta = (1, 0)$, solved on $[0, 1]^2$ domain. We set up the forcing $f(x, y, t)$ to deliver the manufactured solution $u(x, y, t) = \sin(\Pi x) \sin(\Pi y) \sin(\Pi t)$ for $t \in [0, 2]$. We investigate the error for different time step sizes dt varying from 0.1 to 0.001. We investigate the Backward-Euler, Crank-Nicolson, Peaceman-Rachford, and Strang method with Backward-Euler and Strang method with Crank-Nicolson schemes. The results are summarized in Figure 3.

From the numerical experiments, we can conclude that Peacemen-Rachford, together with Crank-Nicolson and Strang methods coupled with Crank-Nicolson schemes, are of the second order with respect to time. This means that decreasing the time step one in order of magnitude results in a two-order increase in numerical accuracy.

6.2 Three-dimensional advection-diffusion simulation with Douglass-Gunn time marching scheme and residual minimization method

We describe the numerical simulation of three-dimensional model advection-diffusion problem over a 3D cube shape domain with dimensions $5000 \times 5000 \times 5000$ meters.

$$\frac{du}{dt} - \nabla \cdot (K \nabla u) + \beta \cdot \nabla u = f \quad (42)$$

In our equation we have

$$K = \begin{bmatrix} 50 & 0 & \\ 0 & 50 & 0 \\ 0 & 0 & 0.5 \end{bmatrix}, \quad (43)$$

1404 the β is given by

$$\beta = (\beta^x(t), \beta^y(t), \beta^z(t)) = (\cos a(t), \sin a(t), v(t)), \quad (44)$$

1405 where

$$a(t) = \frac{\pi}{3} (\sin(s) + \frac{1}{2} \sin(2.3s)) + \frac{3}{8} \pi, \quad (45)$$

1406 and

$$v(t) = \frac{1}{3} \sin(s), \quad (46)$$

1407 with $s = \frac{t}{150}$. The source is given by

$$f(p) = (r-1)^2(r+1)^2, \quad (47)$$

1408 where $r = \min(1, (|p-p_0|/25)^2)$, and p represents the distance from the source, and p_0 is the location of the source
 1409 $p_0 = (3, 3, 2)$. The initial state is defined as the constant concentration of the order of 10^{-6} in the entire domain
 1410 (numerical zero). The physical meaning of this setup is the following. We model the propagation of the pollutant
 1411 generated by a chimney as modeled by the f function. The pollution is distributed by the wind as modeled by β
 1412 function and by the diffusion phenomena described by the diffusion matrix K . For this three-dimensional problem,
 1413 we need the Douglas-Gunn time integration scheme that is second-order accurate in time

$$\begin{cases} (1 + \frac{\tau}{2} \mathcal{L}_1) u^{n+1/3} = \tau f^{n+1/2} + (1 - \frac{\tau}{2} \mathcal{L}_1 - \tau \mathcal{L}_2 - \tau \mathcal{L}_3) u^n, \\ (1 + \frac{\tau}{2} \mathcal{L}_2) u^{n+2/3} = u^{n+1/3} + \frac{\tau}{2} \mathcal{L}_2 u^n, \\ (1 + \frac{\tau}{2} \mathcal{L}_3) u^{n+1} = u^{n+2/3} + \frac{\tau}{2} \mathcal{L}_3 u^n. \end{cases} \quad (48)$$

1414 which translates into

$$\begin{cases} (u^{n+1/3}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1/3}}{\partial x}, \frac{\partial v}{\partial x} \right) + \frac{\tau}{2} \left(\beta_x \frac{\partial u^{n+1/3}}{\partial x}, v \right) = \\ (u^n, v) - \frac{\tau}{2} \left(\alpha \frac{\partial u^n}{\partial x}, \frac{\partial v}{\partial x} \right) - \frac{\tau}{2} \left(\beta_x \frac{\partial u^n}{\partial x}, v \right) - \tau \left(\alpha \frac{\partial u^n}{\partial y}, \frac{\partial v}{\partial y} \right) \\ - \tau \left(\beta_y \frac{\partial u^n}{\partial y}, v \right) - \tau \left(\alpha \frac{\partial u^n}{\partial z}, \frac{\partial v}{\partial z} \right) - \tau \left(\beta_z \frac{\partial u^n}{\partial z}, v \right) + \tau (f^{n+1/2}, v), \\ (u^{n+2/3}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+2/3}}{\partial y}, \frac{\partial v}{\partial y} \right) + \frac{\tau}{2} \left(\beta_y \frac{\partial u^{n+2/3}}{\partial y}, v \right) = \\ (u^{n+1/3}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1/3}}{\partial y}, \frac{\partial v}{\partial y} \right) + \frac{\tau}{2} \left(\beta_y \frac{\partial u^{n+1/3}}{\partial y}, v \right), \\ (u^{n+1}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+1}}{\partial z}, \frac{\partial v}{\partial z} \right) + \frac{\tau}{2} \left(\beta_z \frac{\partial u^{n+1}}{\partial z}, v \right) = \\ (u^{n+2/3}, v) + \frac{\tau}{2} \left(\alpha \frac{\partial u^{n+2/3}}{\partial z}, \frac{\partial v}{\partial z} \right) + \frac{\tau}{2} \left(\beta_z \frac{\partial u^{n+2/3}}{\partial z}, v \right), \end{cases}$$

1415 where (\cdot, \cdot) denotes the inner product of $L^2(\Omega)$. The weak form is the following

$$\begin{cases} \left[M^x + \frac{\tau}{2} (K^x + G^x) \right] \otimes M^y \otimes M^z u^{n+1/3} \\ = \left[M^x - \frac{\tau}{2} (K^x + G^x) \right] \otimes M^y \otimes M^z u^n \\ - \tau M^x \otimes (K^y + G^y) \otimes M^z u^n - \tau M^x \otimes M^y \otimes (K^z + G^z) u^n + \tau F^{n+1/2} \\ M^x \otimes \left[M^y + \frac{\tau}{2} (K^y + G^y) \right] \otimes M^z u^{n+2/3} \\ = M^x \otimes M^y \otimes M^z u^{n+1/3} + M^x \otimes \frac{\tau}{2} (K^y + G^y) \otimes M^z u^n, \\ M^x \otimes M^y \otimes \left[M^z + \frac{\tau}{2} (K^z + G^z) \right] u^{n+1} \\ = M^x \otimes M^y \otimes M^z u^{n+2/3} + M^x \otimes M^y \otimes \frac{\tau}{2} (K^z + G^z) u^n, \end{cases}$$

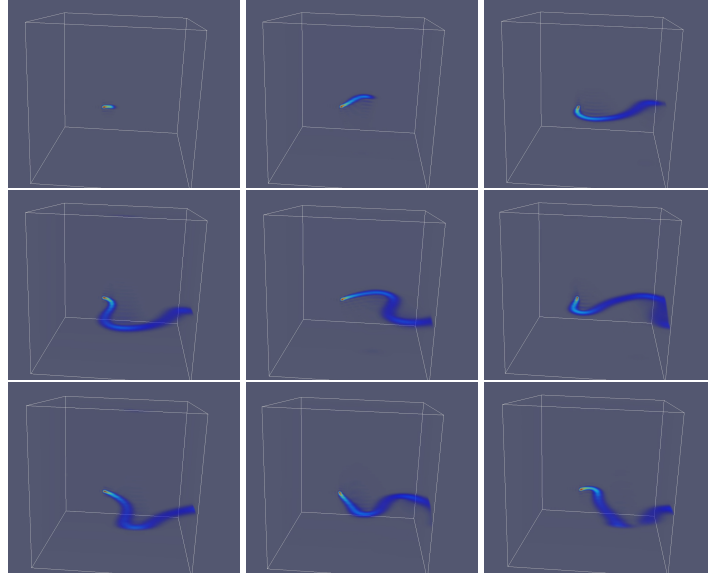


Figure 4: Simulation of pollution propagation from a chimney with Douglass-Gunn time integration scheme and residual minimization method. Snapshots for time steps 100, 200, 300, 400, 500, 600, 700, 800 and 900 with quadratic B-splines with C^1 continuity for trial and cubic B-splines with C^2 continuity for test over $50 \times 50 \times 50$ mesh.

1416 where $M^{x,y,z}$, $K^{x,y,z}$ and $G^{x,y,z}$ are the 1D mass, stiffness and advection matrices, respectively. The numerical results
 1417 from time steps 100,200,300,400,500,600,700,800, and 900 are presented in Figure 4.

1418 We can observe the propagation of the pollution generated from a single source, the central chimney, with
 1419 the non-constant wind varying in time. We do not have the exact solution for this problem, but we can observe
 1420 that the 900-time steps of the simulation are stable, do not oscillate, and do not explode.

1421 6.3 Navier-Stokes with residual minimization for cavity flow problem

1422 We consider the non-stationary cavity flow problem over a 2D domain $\Omega = [0, 1]^2$

$$\begin{cases} \partial_t v - (v \cdot \nabla)v - \frac{1}{Re} \Delta v + \nabla p = 0 \\ \nabla \cdot v = 0 \end{cases}$$

1423

$$\begin{aligned} v_x(1, y) &= 1 \text{ for } y \in (0, 1) & v_x(0, y) &= 0 \text{ for } y \in (0, 1) \\ v_x(x, 0) &= 0 \text{ for } x \in (0, 1) & v_x(x, 1) &= 0 \text{ for } x \in (0, 1) \\ v_y(x, y) &= 0 \text{ for } (x, y) \in \partial\Omega \end{aligned}$$

1424 This problem develops singularities of the pressure as illustrated in Figure 5. First, we employ the time integra-
 1425 tion scheme without the residual minimization. We show that for high Reynolds number $Re = 1000$ it implies an
 1426 unexpected oscillations of the solution. This is illustrated in Table 1. Next, we incorporate the residual minimiza-
 1427 tion stabilization, and we show numerical results for $Re = 100$ and $Re = 1000$ in Figure 6.

1428 The cavity flow problem can be naturally extended to three-dimensions, by defining the problem on a cube
 1429 $[0, 1]^3$, using zero Dirichlet boundary condition on bottom and side faces, and adding $v = (1, 0, 0)$ Dirichlet bound-
 1430 ary condition on the top face. The three-dimensional results are summarized in Figure 8.

1431 In the cavity flow problem, the fluid located inside the cavity starts rotating due to the flow on the upper
 1432 boundary. The velocity of the rotating fluid is directly related to the velocity of the flow on the boundary condition.
 1433 The Reynolds number grows when we increase the velocity. The location of the vortex moves to the right-hand
 1434 side corner of the domain when we increase the Reynolds number. For Reynolds number $Re=100$, both the
 1435 Galerkin and residual minimization method works. However, for $Re=1000$, the Galerkin method provides unstable
 1436 numerical results, while the residual minimization results in a correct solution.

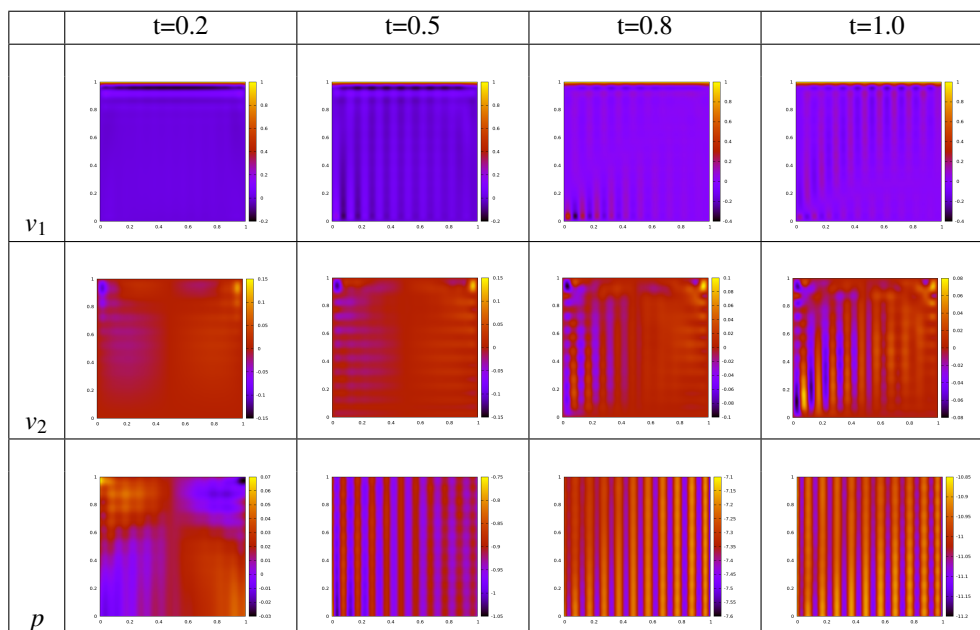


Table 1: Galerkin method for $Re = 1000$ for mesh 80×80 . Components v_1, v_2 of the velocity and p pressure scalar field at time steps 20, 50, 80, 100 of the solution of the non-stationary cavity flow problem.

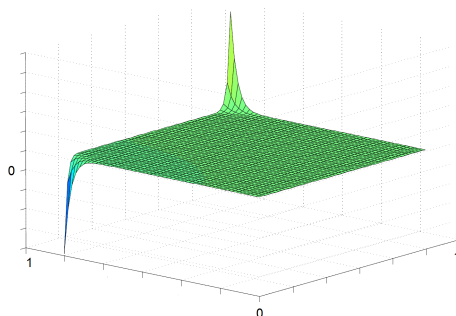


Figure 5: The singularities at the pressure solution.

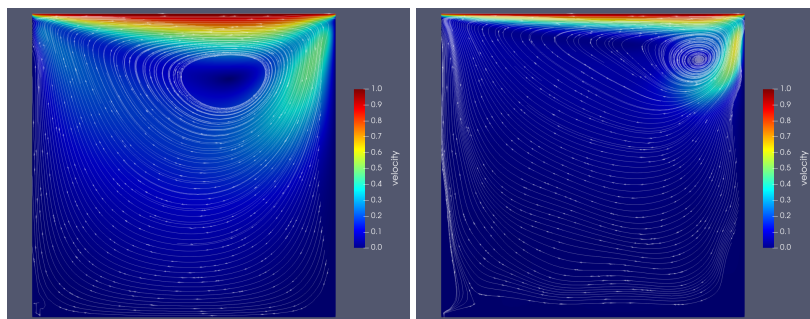


Figure 6: **Left panel:** Residual minimization method with cubic B-splines of C^1 continuity for trial and quartic B-splines of C^1 continuity for test. Mesh size of 40×40 elements with for $Re = 100$.

Middle panel: Residual minimization method with cubic B-splines of C^1 continuity for trial and quartic B-splines of C^1 continuity for test. Mesh size of 40×40 elements with for $Re = 1000$.

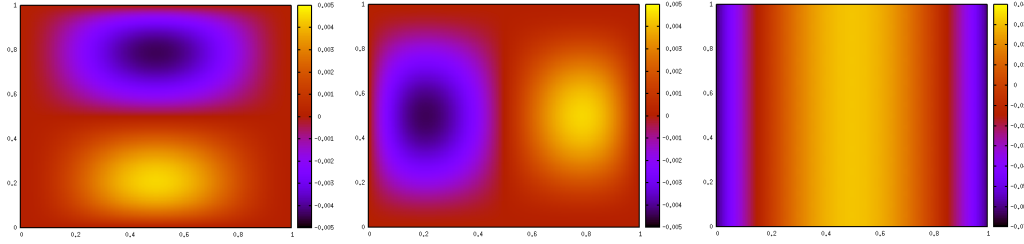


Figure 7: **Left panel:** Horizontal component v_x of the velocity scalar field of the solution of the model Stokes problem with isogeometric residual minimization method with trial = cubic B-splines of C^1 continuity, test = quartic B-splines of C^1 continuity, on a uniform mesh 20×20 elements. **Middle panel:** Vertical component v_y of the velocity of the solution of the model Stokes problem with isogeometric residual minimization method with trial = cubic B-splines of C^1 continuity, test = quartic B-splines of C^1 continuity on a uniform mesh 20×20 elements. **Right panel:** Pressure p scalar field of the solution of the model Stokes problem with isogeometric residual minimization method with trial = cubic B-splines, test = quartic B-splines on a uniform mesh 20×20 elements.

6.4 Discontinuous Galerkin with residual minimization for manufactured solution Stokes problem

We consider the Stokes equations a 2D domain $\Omega = [0, 1]^2$ with no-slip boundary conditions: find $v = (v_1, v_2)$ and p such that

$$\begin{cases} -\Delta v + \nabla p = F \\ \nabla \cdot v = 0 \\ v|_{\partial\Omega} = 0 \end{cases} \quad (49)$$

where $\mathbf{f} = (f_1, f_2)$ is given by

$$\begin{aligned} f_1(x, y) &= (12 - 24y)x^4 + (-24 + 48y)x^3 + (-48y + 72y^2 + 12)x^2 \\ &\quad + (-2 + 24y - 72y^2 + 48y^3)x + 1 - 4y + 12y^2 - 8y^3 \\ f_2(x, y) &= (8 - 48y + 48y^2)x^3 + (-12 + 72y - 72y^2)x^2 \\ &\quad + (4 - 24y + 48y^2 - 48y^3 + 24y^4)x - 12y^2 + 24y^3 - 12y^4 \end{aligned} \quad (50)$$

The resulting v_x , v_y , and p scalar fields are presented in Figure 7. We consider cubic B-splines of C^1 continuity as trial basis and quartic B-splines of C^1 continuity as test basis. We run the experiment on a uniform mesh 20×20 elements mesh. The numerical errors are summarized in Table 2.

Trial	Test	L2 v_x	L2 v_y	L2 p	L2 $\text{div}u$	H1 v_x	H1 v_y	H1 p	H1 $\text{div}u$
quadratic	cubic	0.0179	0.0179	0.0171	0.0127	0.31	0.31	0.31	1.95
cubic	quartic	0.00033	0.00033	0.0018	0.000328	0.0057	0.0057	0.0057	0.0444
quartic	quintic	3.76e-11	4.26e-11	1.21e-10	1.44e-11	3.46e-10	4.18e-10	2.94e-09	2.1e-09

Table 2: Convergence of the numerical errors while increasing the orders of both trial and test spaces with C^1 continuity for the Stokes model problem.

This problem has the manufactured exact solution, and our numerical experiments show that our solver can solve this problem with high numerical accuracy of the order of $10^{-9} - 10^{-11}$ as denoted in the last row of Table 2.

We also compare in Table 3 the residual minimization approach with the Galerkin method, including the computational costs expressed by the number of floating-point operations and the resulting numerical error.

6.5 Advection skew to the mesh solved with residual minimization and conjugate gradient solver

We focus on stationary advection-diffusion problem

$$-\varepsilon \nabla \cdot (\nabla u) + \beta \cdot \nabla u = 0,$$

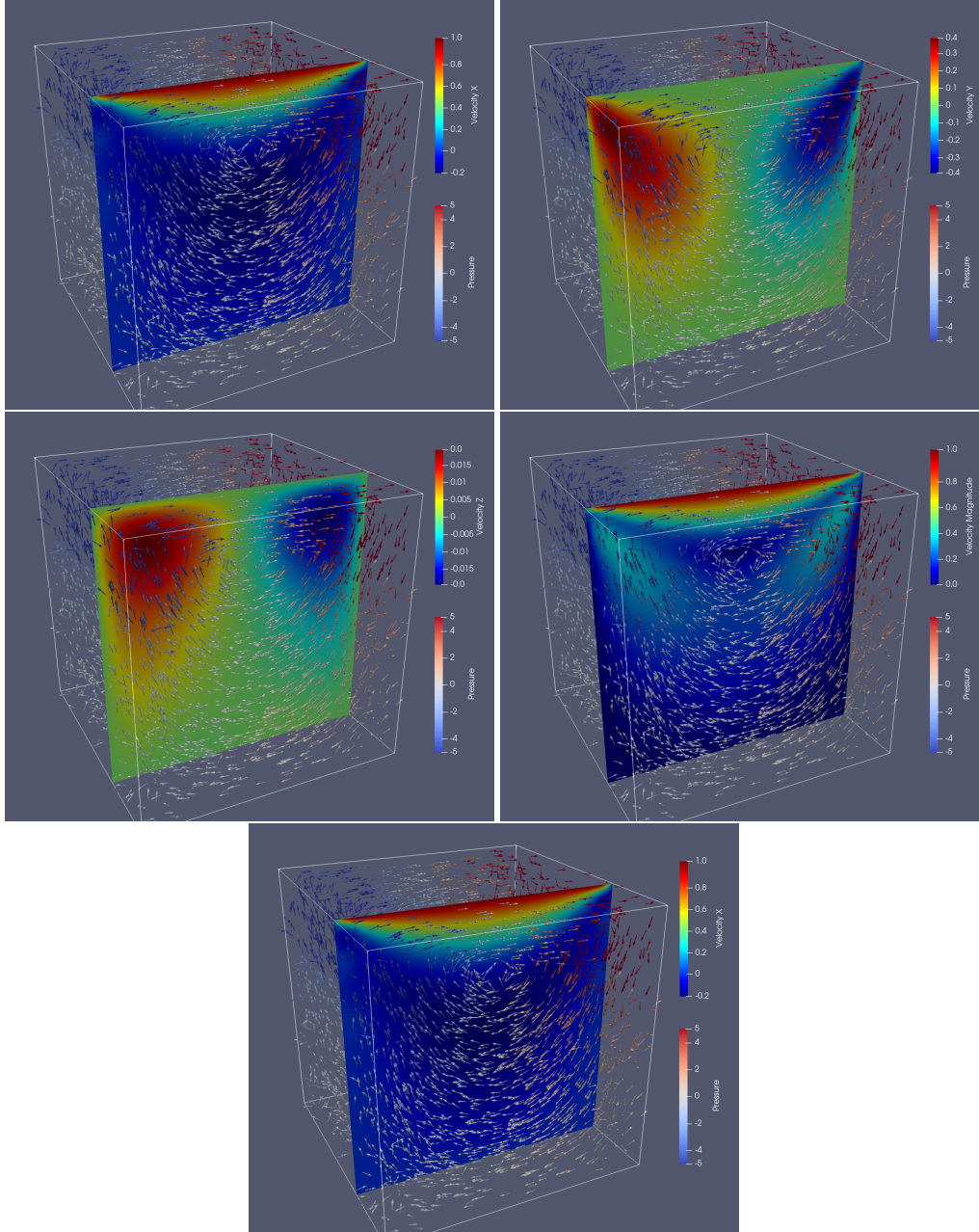


Figure 8: Cavity flow problem with isogeometric residual minimization method with trial = quartic B-splines of C^2 continuity, test = broken quartic B-splines, on a uniform mesh $8 \times 8 \times 8$ elements. **Left top panel:** Horizontal component v_x of the velocity field. **Right top panel:** Vertical component v_y of the velocity field. **Left middle panel:** Vertical component v_z of the velocity. **Right middle panel:** Magnitude of the vvelocity field. **Bottom panel:** Velocity vectors.

Trial	Test	L2 v_x	L2 v_y	L2 p	L2 $\text{div}u$	H1 v_x	H1 v_y	H1 p	H1 $\text{div}u$
quadratic	cubic	0.0179	0.0179	0.0171	0.0127	0.31	0.31	0.31	1.95
cubic	quartic	0.00033	0.00033	0.0018	0.000328	0.0057	0.0057	0.0057	0.0444
quartic	quintic	3.76e-11	4.26e-11	1.21e-10	1.44e-11	3.46e-10	4.18e-10	2.94e-09	2.1e-09

Table 3: Computational cost expressed as the number of floating-point operations and the numerical errors for the Galerkin method (trial space equal to test space) and residual minimization method (trial space different from the test space) applied for the Stokes model problem.

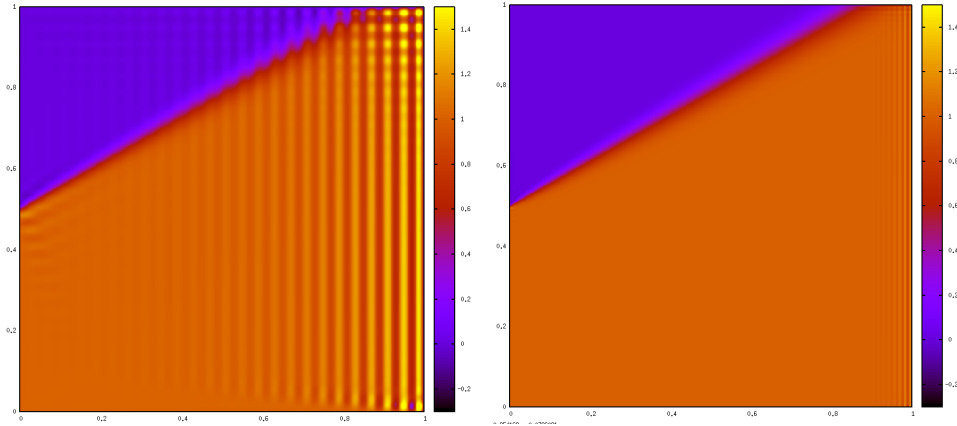


Figure 9: Advection skew to the mesh. **Left panel:** Unstable solution with Galerkin method. **Right panel:** Stabilized solution with residual minimization method.

Trial	Test	10×10	20×20	50×50	100×100	200×200
linear	cubic	3.88e+6	3.46e+6	1.75e+6	0.91e+6	0.46e+6
linear	quartic	22.5e+6	7.37e+6	2.97e+6	1.50e+6	0.74e+6
quadratic	cubic	15.6e+6	5.07e+6	1.20e+6	0.63e+6	0.32e+6
quadratic	quartic	15.6e+6	5.07e+6	2.04e+6	1.03e+6	0.51e+6

Table 4: Condition numbers of matrices in advection skew to the mesh problem.

1453 with $\varepsilon = 10^{-6}$, $\beta = (\sqrt{3}, 1)$, solved on $[0, 1]^2$ domain, with Dirichlet b.c.

$$\begin{aligned}
 v(x, 1) &= 0 \text{ for } x \in (0, 1) & v(x, 0) &= 1 \text{ for } x \in (0, 1) \\
 v(0, y) &= 0 \text{ for } y \in (0.5, 1) & v(0, y) &= 1 \text{ for } y \in (0, 0.5) \\
 v(1, y) &= 0 \text{ for } y \in (0, 1) \in \partial\Omega
 \end{aligned}$$

1454 Figure 9 presents the numerical results obtained with the Galerkin method (without stabilization) and with
 1455 residual minimization stabilization. We employ a high-fidelity mesh of 200×200 elements, with 100 elements
 1456 spread uniformly between $[0, 0.9]$ and 100 elements spread uniformly between $[0.9, 1.0]$. We use quadratic B-
 1457 splines with C^0 separators between elements as a trial basis and quartic B-splines with C^0 separators as a test
 1458 basis.

1459 The advection is the driving force to propagate the substance from the bottom half of the left side of the
 1460 domain, as well as from the bottom side of the domain, in the direction of the β vector. The exact solution exhibits
 1461 the boundary layer at the opposite sides of the domain. This problem cannot be solved with the Galerkin method,
 1462 as it is illustrated in the left panel in Figure 9. The residual minimization method can solve this problem well.

1463 Table 4 presents the impact of the discrete spaces choice and mesh size on the condition number of the
 1464 problem matrix. It seems that increasing the mesh size has a positive effect on the matrix conditioning. On the
 1465 other hand, a large gap between the polynomial order of trial and test space leads to a high condition number.

1466 Finally, we compare the computational costs of the Galerkin and residual minimization methods. We employ
 1467 uniform grids. For example, for the mesh 10×10 , for the Galerkin method we define

```

1468 knot_x = [0 0 0 1 2 3 4 5 6 7 8 9 10 10 10];
1469 points_x = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1];
1470 knot_y = [0 0 0 1 2 3 4 5 6 7 8 9 10 10 10];
1471 points_y = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1];

```

1472 For the residual minimization method, we employ the same trial space as for the Galerkin method, but for
 1473 the test space we reduce the continuity between the elements

```

1474 knot_trial_x = [0 0 0 1 2 3 4 5 6 7 8 9 10 10 10];
1475 knot_test_x = [0 0 0 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9 9 10 10 10];
1476 points_x = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1];
1477 knot_trial_y = [0 0 0 1 2 3 4 5 6 7 8 9 10 10 10];
1478 knot_test_y = [0 0 0 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9 9 10 10 10];

```

1479 `points_y = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1];`

1480 We compare the total computational costs, including the integration and generation of the right-hand side,
1481 and the cost of solving the system of linear equations.

	mesh size	Galerkin method	Residual minimization method
Execution time [s]	5×5	0.063	0.122
Execution time [s]	10×10	0.141	0.348
Execution time [s]	20×20	0.526	1.325
Execution time [s]	40×40	1.956	5.645
Execution time [s]	80×80	8.82	21.96

Table 5: Advection skew to the mesh. Computational cost of direct solver solution with the Galerkin and residual minimization method on uniform grids.

1482

1483 7 Automatic mesh refinements on tensor product grids

1484 In this section we present the algorithm for automatic refinements of tensor product grids with the residual min-
1485 imization method. The input to our algorithm are the know vectors along x and y axis, ξ_i^x , $i = 1, \dots, N_x$, and ξ_j^y ,
1486 $j = 1, \dots, N_y$.

1487

- 1488 1. We solve the residual minimization problem

$$\begin{bmatrix} G & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} r \\ u \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix} \quad (51)$$

1489 where B is the matrix related to the advection-skew to the mesh problem, and G is the corresponding Gram
1490 matrix.

- 1491 2. We loop through elements E and we compute $res_error(E) = \int_E r^2 + \varepsilon \nabla r \cdot \nabla r$ which represents the element
1492 local contribution to the weighted H^1 norm of the residuum
- 1493 3. We loop through pairs of two consecutive non-equal knot points $\xi_k < \xi_{k+1}$ from the knot vector along x axis,
1494 and we sum up all the $res_error(E)$ for elements E located between them. The sums represent contributions
1495 of the vertical strips of the mesh to the residual error.
- 1496 4. We refine the knot vector along x axis in the intervals fulfilling the Dörfler criterion [12].
- 1497 5. We repeat the last two steps along y axis.

1498 We tested the algorithm on the advection-skew to the mesh problem with $\varepsilon = 0.01$. The resulting sequence
1499 of meshes is presented in Figure 10. The sequence of obtained solutions is summarized in Figure 11. The
1500 convergence of the global residual error is illustrated in Figure 12. We have shown that this simple mesh refinement
1501 algorithm allows us to construct a computational mesh that provides a numerical solution with a residual error of
1502 less than 0.1.

1503 8 Quadrature improvements

1504 Some methods of speeding up the integration in FEM and IGA have been proposed [20]. Since when using an
1505 efficient linear solver, the integration time becomes a major portion of the total computational cost; these strategies
1506 seem to provide an attractive avenue to reduce it. That said since these approaches focus on evaluating integrals
1507 in the matrix, which in transient problems is typically only computed once, their applicability and usefulness in
1508 this context is limited. Below, we briefly comment on the applicability of three integration speedup strategies
1509 described in [20] in the context of integrating the right-hand side.

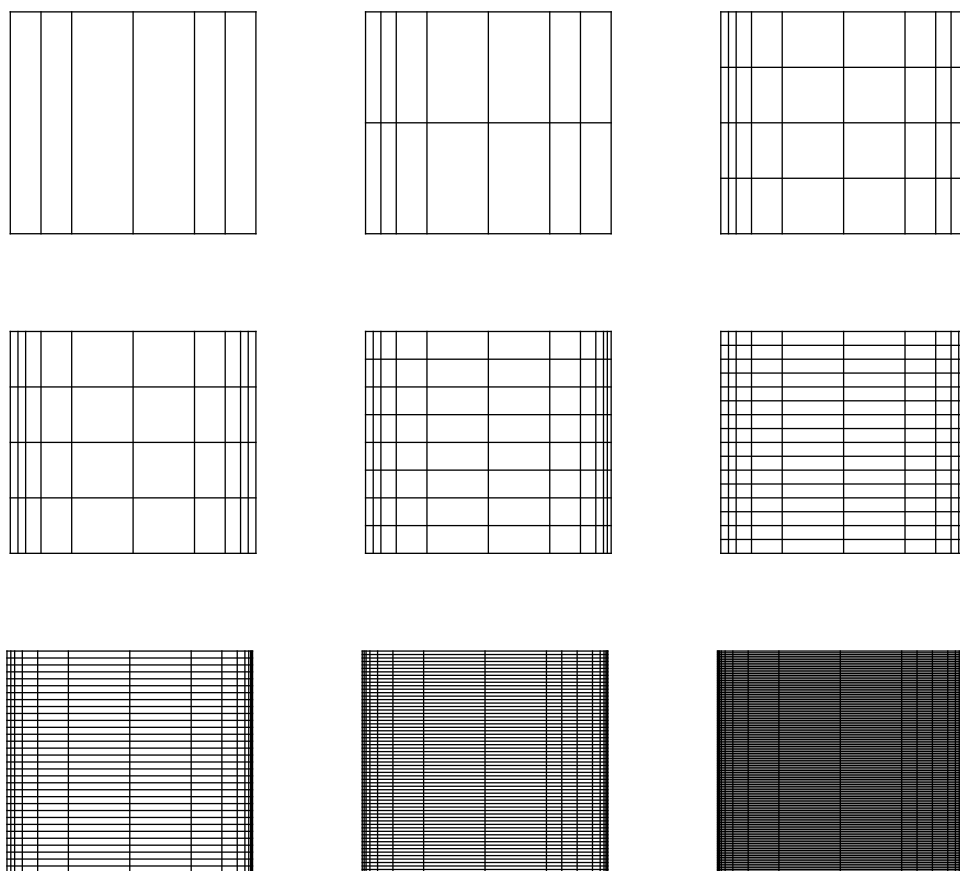


Figure 10: Advection skew to the mesh. A sequence of tensor product meshes refined using the adaptive algorithm with Dörfler criterion along the strips of the mesh using the weighted residual norm.

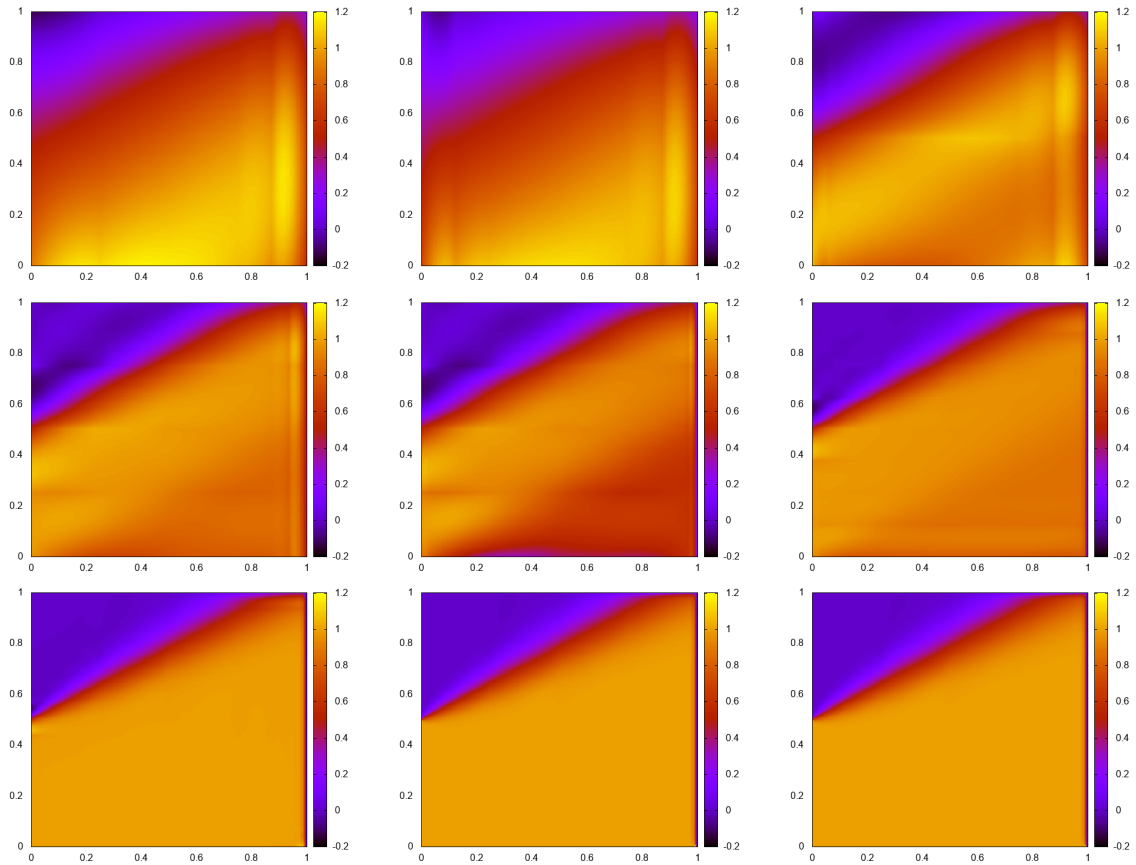


Figure 11: Advection skew to the mesh. A sequence of solution obtained on refined tensor product meshes using the adaptive algorithm.

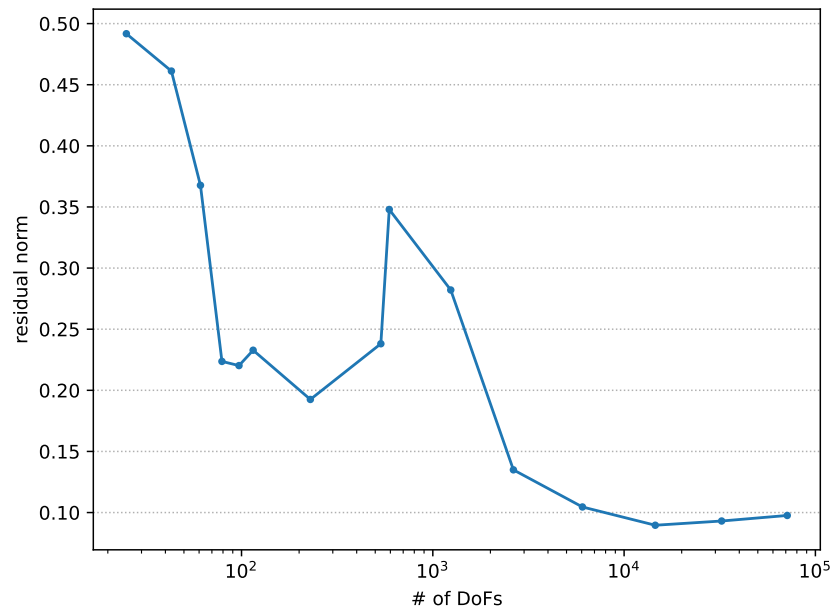


Figure 12: Advection skew to the mesh. Convergence of the residual error. The horizontal axis denotes degrees of freedom, the vertical axis denotes the norm of the residual error.

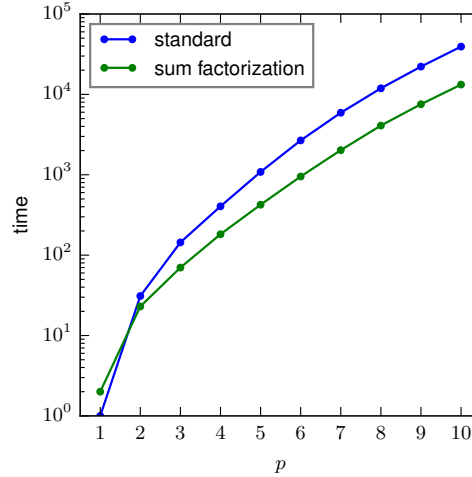


Figure 13: RHS integration time comparison

8.1 Sum factorization

Sum factorization is a technique for speeding up summations involving terms that have a tensor product structure, i.e., terms that can be represented as a product of quantities depending on a single summation index (or a subset of summation indices), by means of clever reuse of partial results. For a detailed description, we refer to [20]. This idea can be applied to integrating the right-hand side and reducing the computational cost per element from $\mathcal{O}(p^6)$ to $\mathcal{O}(p^4)$ for a 3D simulation, p being the discrete space polynomial order.

The big caveat is that this estimate assumes that the right-hand side consists of integrals of the form $\int_{\Omega} f e_i dx$, where e_i are the test functions, and f is a function with a constant evaluation cost. In practice, the right-hand side terms of the time discretization involve the solution at the previous time step. Computing its value at a single quadrature point requires evaluating a linear combination of $\mathcal{O}(p^3)$ terms since there are $(p+1)^3$ B-spline basis functions are supported on each mesh element. As a result, the asymptotic cost remains $\mathcal{O}(p^6)$ whether sum factorization is used or not, and while some efficiency gains are indeed possible to obtain (Figure 13), they are much less pronounced than in the case of computing the matrix entries.

8.2 Weighted quadratures

Replacing standard (say, Gauss-Legendre) quadrature rules with special, dedicated quadratures maintaining accuracy while using fewer quadrature points can improve efficiency of right-hand side integration of both the matrix and the right-hand side. That said, while general-purpose quadratures integrate simple functions (pure polynomials of a fixed order) exactly and offer well-understood error bounds for other functions. These special quadratures tend to be tailored to the specific form of the integrand [2, 3, 20], which makes it less suitable for integrating the right-hand side, which can often contain less regular and well-behaved terms.

Finally, we compare the computational costs of the Galerkin and residual minimization methods. We employ uniform grids, namely for the Galerkin method

```
knot_x = [0 0 0 1 2 3 4 5 6 7 8 9 10 10 10];
points_x = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1];
knot_y = [0 0 0 1 2 3 4 4 4];
points_y = [0 0.25 0.5 0.75 1];
```

For the residual minimization method, we employ

```
knot_x = [0 0 0 1 2 3 4 5 6 7 8 9 10 10 10];
points_x = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1];
knot_y = [0 0 0 1 2 3 4 4 4];
points_y = [0 0.25 0.5 0.75 1];
```

We compare the total computational costs, including the integration and generation of the right-hand side, and the cost of solving the system of linear equations.

	mesh size	Galerkin method	Residual minimization method
Execution time [s]	5×5	0.063	0.122
Execution time [s]	10×10	0.141	0.348
Execution time [s]	20×20	0.526	0.1325
Execution time [s]	40×40	1.956	0.5645

Table 6: Advection skew to the mesh. Computational cost of solution with the Galerkin and residual minimization method on uniform grids.

8.3 Assembly by row

The idea of assembly by row is to reorder the integration loop from the outer loop iterating over mesh elements, to the outer loop iterating over test functions. This change provides a benefit only in combination with sum factorization, effectively reducing the per-element cost of computing the matrix from $\mathcal{O}(p^6)$ (just sum factorization) to $\mathcal{O}(p^4)$ (sum factorization with assembly by row) for 3D simulation. As mentioned earlier, sum factorization for right-hand side matrix reduces the cost from $\mathcal{O}(p^6)$ to $\mathcal{O}(p^4)$, but a similar cost analysis reveals that assembling by row does not reduce it any further, which renders it not applicable to integrating right-hand side, even disregarding the fact that the cost is dominated by evaluating the previous time-step solution.

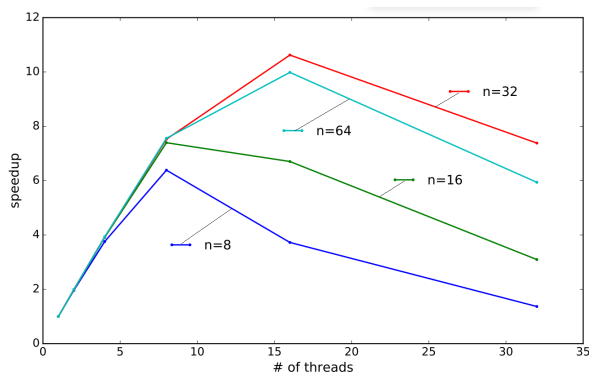
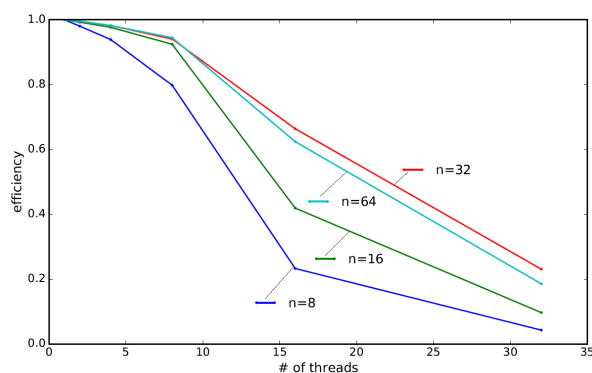
9 Parallel scalability

In this section we present the measurements of the parallel scalability for the three-dimensional simulations of the advection-diffusion problem. To measure the parallel scalability, we have moved to a shared memory machine with four Intel[®]Xeon[®] CPU E7-4860 processors, each possessing ten cores with hyperthreading (for a total of forty cores, while using more than twenty cores requires hyperthreading).

The speedup and efficiency of the code are presented in Figures 14-19. Different plots correspond to different mesh dimensions and different polynomial orders of approximation. Namely, by n we denote the mesh size in one dimension. We test our solver on a very small mesh of size $8 \times 8 \times 8$, through the mesh of size $16 \times 16 \times 16$, the mesh of size $32 \times 32 \times 32$ up to the large mesh of size $64 \times 64 \times 64$. We present the plots of the speedup and efficiency for quadratic and cubic B-splines. The speedup is defined as $S = \frac{T_1}{T_p}$, where T_1 stands for the execution time of the sequential algorithms and T_p stands for the execution time of the parallel algorithm using p cores. The perfect parallel algorithm delivers p speedup using p cores. The efficiency is defined as $E = \frac{T_1}{pT_p}$. The perfect parallel algorithm delivers efficiency equal to 1.0.

We can draw the following conclusions from the presented plots:

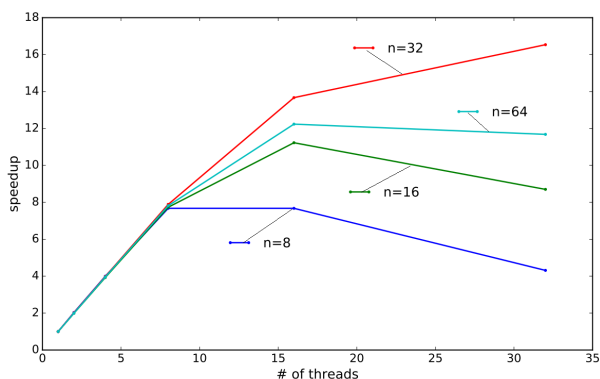
- For quadratic B-splines presented in Figures 14-15 and for small grids $8 \times 8 \times 8$ and $16 \times 16 \times 16$ the speedup grows up to 8 cores. The corresponding efficiency for 8 threads is of the order 0.9, and then it decreases rapidly.
- For quadratic B-splines and large grids $32 \times 32 \times 32$ and $64 \times 64 \times 64$ the speedup grows up to 16 cores. It is around 10-11 for 16 cores. The corresponding efficiency for 16 cores is around 0.7. Then, for 32 cores the speedup went down since for more than 20 cores used the hyperthreading is utilized.
- For cubic B-splines presented in Figures 16-17 and for small grid of $8 \times 8 \times 8$ the speedup grows up to 8 cores, and the corresponding efficiency is close to 1.0. Then both speedup and efficiency decrease.
- For cubic B-splines and large grids $32 \times 32 \times 32$ and $64 \times 64 \times 64$ the speedup grows up to 16 cores. It is around 12-14 for 16 cores. The corresponding efficiency for 16 cores is around 0.8-0.9. Then, for 32 cores and $32 \times 32 \times 32$ mesh the speedup grows up to 17, and for $64 \times 64 \times 64$ mesh is decreases slightly since for more than 20 cores the hyperthreading is used.
- For quartic B-splines presented in Figures 18-19 and for small grids of $8 \times 8 \times 8$ and $16 \times 16 \times 16$ the speedup grows up to 16 cores, and the corresponding efficiency is between 0.8-1.0. Then both speedup and efficiency decrease slightly.
- For quartic B-splines and large grids $32 \times 32 \times 32$ and $64 \times 64 \times 64$ the speedup grows up to 32 cores. It is around 15 for 16 cores (near perfect speedup) and around 20 for 32 cores, where we use the hyperthreading (more than 20 cores). The corresponding efficiency for 16 cores is around 0.9-1.0. Then, for 32 cores the efficiency decreases slightly down to 0.6-0.7.

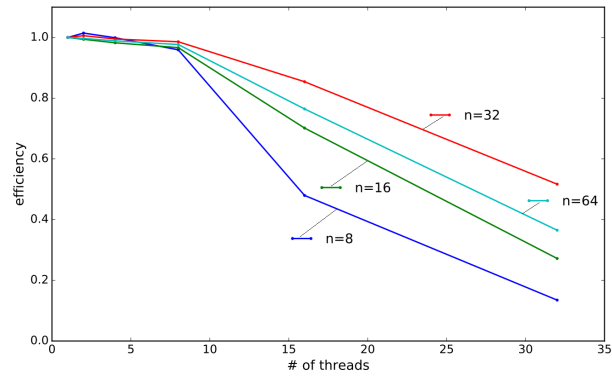
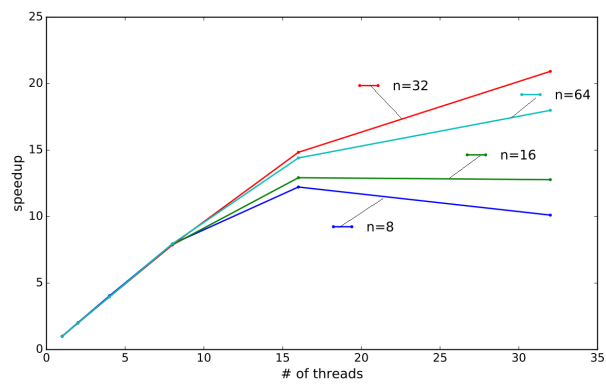
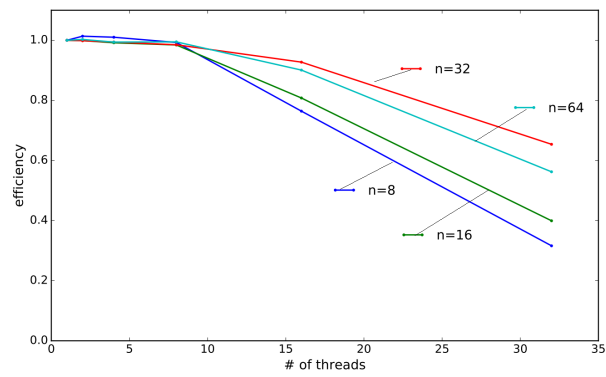
Figure 14: Speedup $p = 2$ Figure 15: Efficiency $p = 2$

- 1585 • Increasing the mesh size increases the parallel scalability up to $32 \times 32 \times 32$ mesh. Larger mesh, $64 \times 64 \times 64$
 1586 performs slightly worse than $32 \times 32 \times 32$ mesh.
- 1587 • The most interesting observation is that while increasing the B-splines order we observe improvement of
 1588 the parallel scalability.

1589 The plots depict the time of the integration, i.e. assembling of the system, which constitutes the vast majority
 1590 of the computational time. Cost of rest of each single time step – solving the system using ADS – was found to be
 1591 negligible in comparison, and preparatory steps (array allocation, etc.) become insignificant given a large number
 1592 of time steps computed in a full simulation.

1593 We measure the speedup for 8, 16, and 32 cores. The speedup of execution for a computational mesh of
 1594 $32 \times 32 \times 32$ elements is better than the speedup for a computational mesh of $64 \times 64 \times 64$ for the number of cores larger
 1595 than the number of physical cores. The computational nodes have 10 physical cores and a total of 40 cores using
 1596 the Hyper-threading (HT) technology. Hyper-threading allows a single physical core to execute multiple threads

Figure 16: Speedup $p = 3$

Figure 17: Efficiency $p = 3$ Figure 18: Speedup $p = 4$ Figure 19: Efficiency $p = 4$

1597 simultaneously. The physical core can only execute one instruction at a time. HT allows the CPU core to switch
 1598 between multiple threads quickly. This is highly beneficial when one thread waits for data from RAM or another
 1599 resource. The core can switch to another thread that is ready to execute. Please note that the speedup achieved by
 1600 Hyper-threading depends on the nature of the workload. Some applications and tasks benefit significantly from
 1601 HT, while others may see slight improvement or deterioration

1602 **10 Conclusions**

1603 We presented an open-source parallel shared-memory C++ software for simulations of time-dependent phenom-
 1604 ena. It supported IGA discretizations on tensor product grids and employs three solvers: the alternating-directions
 1605 (ADS) linear cost $O(\mathcal{N})$ solver for problems suitable for direction splitting of the differential operators, iterative
 1606 conjugate gradients solver, as well as an interface to the MUMPS direct solver. We implemented implicit time-
 1607 integration schemes suitable for direction splitting, including Peaceman-Reachford, Douglass-Gunn, and leapfrog
 1608 methods with Crank-Nicolson or explicit Euler. We provided support for scalar and vector fields and systems of
 1609 PDEs in two and three dimensions. We also supported the interface to ParaView and Gnuplot. The main novelty
 1610 of our software was the incorporation of the residual minimization and Discontinuous Galerkin stabilization meth-
 1611 ods. We presented several numerical examples, including two and three-dimensional advection-diffusion problems
 1612 with different time integration schemes using residual minimization stabilization, two-dimensional Navier-Stokes
 1613 problem with residual minimization stabilization, and two and three-dimensional Stokes problem with Discontin-
 1614 uous Galerkin stabilization. In our examples, we employed the alternating directions solver, direct solver, and the
 1615 conjugate gradients iterative solver.

1616 Several mature and high-quality numerical libraries exist for simulations with B-spline basis functions, in-
 1617 cluding PetIGA and GeoPDE. They support arbitrary geometries and provide interfaces to different direct and
 1618 iterative solvers. These libraries are generally dedicated to standard Galerkin method formulations. Our RM-
 1619 IGA-ADS software employs the residual minimization problem to automatically stabilize difficult problems for
 1620 which the Galerkin method results in unstable solutions. It also supports DG method discretization. RM-IGA-
 1621 ADS works on tensor product grids, and thus it often enables the use of an ultrafast alternating directions solver
 1622 for time-dependent problems. RM-IGA-ADS is an extension of IGA-ADS into residual minimization and DG
 1623 methods.

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 1626 of Krakow.

1627 **Appendix**

1628 **A Installation of the code**

1629 Installation of IGA-ADS solver on Linux server.

- 1630 1. Install cmake (version 3.13 or later)

```
1631     sudo apt install cmake
```

- 1632 2. Install gfortran

```
1633     sudo apt install gfortran
```

- 1634 3. Install LAPACK

```
1635     sudo apt install liblapack-doc
```

```
1636     sudo apt install liblapack-dev
```

- 1637 4. Install BLAS

```
1638     sudo apt install libblas-doc
```

```
1639     sudo apt install libblas-dev
```

```

1640 5. Install MUMPS
1641     sudo apt install libmumps-dev
1642 6. Install boost (version 1.58 or later)
1643     sudo apt install libboost-all-dev
1644 7. Install LLVM (necessary for Galois)
1645     sudo apt install llvm-12 llvm-12-dev
1646 8. Download IGA-ADS-RM code
1647     git clone https://github.com/marcinlos/iga-ads-rm
1648     cd iga-ads-rm
1649     git checkout develop
1650 9. Install other necessary libraries (including Galois)
1651     cd ..
1652     DEPS=$(realpath deps)
1653     iga-ads-rm/scripts/install-dependencies.sh $(realpath deps-build) "${DEPS}"
1654     As described in https://github.com/IntelligentSoftwareSystems/Galois/issues/401 Galois does not compile
1655     with GCC compiler version  $\geq 11$ . In order to fix this problem it is necessary to add to install-dependencies.sh
1656     the following line after line 82
1657     sed -i '36i #include <optional>' Galois/tools/graph-convert/graph-convert.cpp
1658     # Install Galois GALOIS_VER=6.0
1659     git clone -branch release-${GALOIS_VER} -depth=1 -quiet
1660         https://github.com/IntelligentSoftwareSystems/Galois
1661     sed -i '36i #include <optional>' Galois/tools/graph-convert/graph-convert.cpp
1662 10. Compile IGA-ADS-RM
1663     cd iga-ads-rm
1664     mkdir build
1665     cmake -S . -B build -D CMAKE_BUILD_TYPE=Release -D ADS_USE_GALOIS=ON -D USE_MUMPS=ON
1666     - D CMAKE_PREFIX_PATH="${DEPS}"
1667     cmake -build build -j $(nproc)
1668 11. Exemplary run
1669     cd build/examples
1670     ./heat_2d
1671 12. Generation of plots from out_* data files
1672     gnuplot
1673     gnuplot > plot "out_100.data" with imag

```

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- ```

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