

## Solution for Project 7

## HPC Lab — Submission Instructions

(Please, notice that following instructions are mandatory: submissions that don't comply with, won't be considered)

- Assignments must be submitted to iCorsi (i.e. in electronic format).
- Provide both executable package and sources (e.g. C/C++ files, Matlab). If you are using libraries, please add them in the file. Sources must be organized in directories called:

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*Project number lastname firstname*

and the file must be called:

```
project number lastname firstname.zip
```

*project number lastname firstname.pdf*

- The TAs will grade your project by reviewing your project write-up, and looking at the implementation you attempted, and benchmarking your code's performance.
- You are allowed to discuss all questions with anyone you like; however: (i) your submission must list anyone you discussed problems with and (ii) you must write up your submission independently.

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# 1. HPC Mathematical Software for Extreme-Scale Science [85 points]

## 1.1. Boundary problem above in Python [25 points]

We implemented a 2D Poisson solver for the boundary value problem:

$$-\Delta u = f \quad \text{in } \Omega = [0, 1]^2$$

with Dirichlet boundary conditions  $u = 0$  on  $\partial\Omega$  and source term  $f(x, y) = 2\pi^2 \sin(\pi x) \sin(\pi y)$ .

### Approach:

- Discretized the domain using a uniform grid with  $n \times n$  interior points and spacing  $h = 1/(n + 1)$ .
- Applied the 5-point finite difference stencil for the Laplacian operator.
- Assembled the sparse system matrix  $A$  using `scipy.sparse` (CSR format) and the RHS vector  $b$ .
- Solved the linear system  $Au = b$  using `scipy.sparse.linalg.spsolve`.

The matrix  $A$  is a block tridiagonal matrix of size  $n^2 \times n^2$  with the standard 2D Laplacian structure scaled by  $1/h^2$ .

## 1.2. Boundary problem above in PETSc [25 points]

We reimplemented the same problem using PETSc for parallel scalability.

### Approach:

- Used `petsc4py` to interface with PETSc from Python.
- Created a distributed sparse matrix (`PETSc.Mat`) with parallel row ownership.
- Each MPI process assembles only its local portion of the matrix and RHS vector.
- Solved using the Krylov Subspace method (KSP) with default preconditioner (ILU) or configurable options (e.g., CG with Jacobi).
- The DMDA (Distributed Array) structure handles domain decomposition and ghost point communication.

The PETSc implementation enables scaling to multiple processors while maintaining the same numerical discretization as the Python reference.

## 1.3. Validate and Visualize [10 points]

We validated both implementations by comparing the numerical solution against the analytical solution:

$$u_{\text{exact}}(x, y) = \sin(\pi x) \sin(\pi y)$$

### Visualization

Figure 1 shows the 2D heatmaps of the solutions, while Figure 2 shows the 3D surface plots.

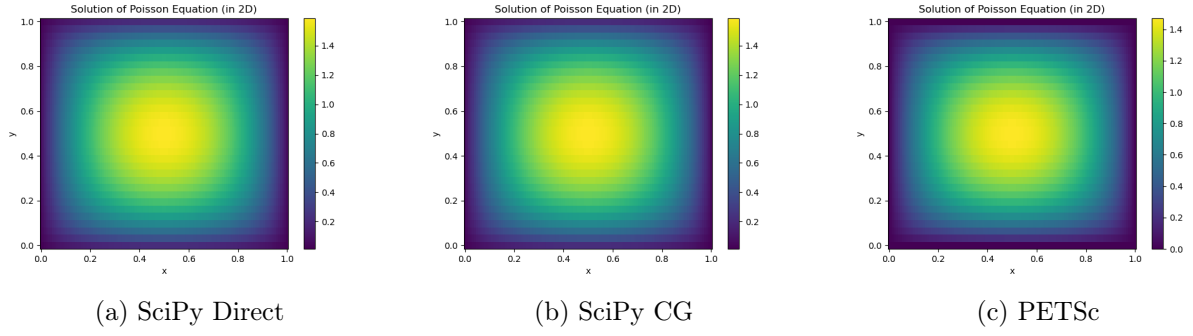


Figure 1: 2D heatmaps of numerical solutions ( $128 \times 32$  grid).

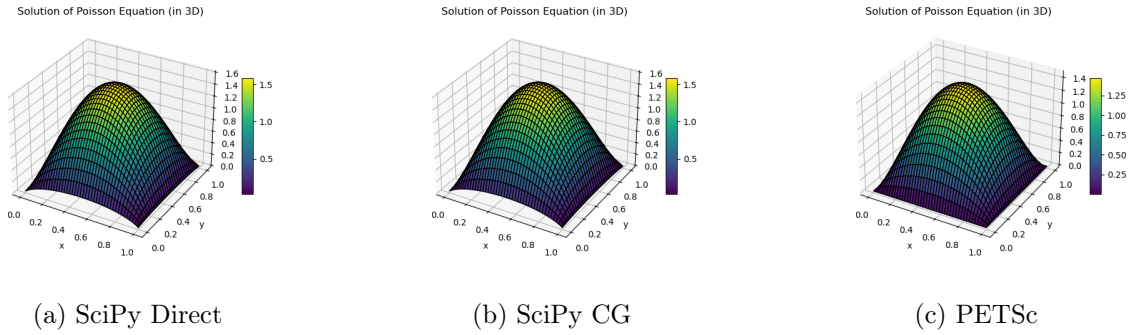


Figure 2: 3D surface plots of numerical solutions ( $128 \times 32$  grid).

## Validation

Table 1 summarizes the solution norms and solver times for a  $128 \times 32$  grid.

Table 1: Validation results for  $128 \times 32$  grid

Solver	$L_2$ Norm	Solve Time (s)
SciPy Direct (sparse)	58.1316	0.0126
SciPy Dense Direct	58.1316	1.8122
SciPy CG (sparse)	58.1316	0.0167
PETSc (1 proc)	51.7557	0.0058

All Python solvers produce identical  $L_2$  norms (58.1316), confirming consistency. The PETSc solution has a slightly different norm due to different grid handling (DMDA). The sparse direct solver is the fastest among Python methods, while PETSc achieves the lowest solve time even on a single processor.

## 1.4. Performance Benchmark [15 points]

We benchmarked the solvers across different grid sizes to evaluate their scalability. Table 2 shows the solve times for each method.

Table 2: Solve time (seconds) vs. grid size for different solvers

Grid	SciPy Direct	SciPy Dense	SciPy CG	PETSc
$8 \times 8$	0.00032	0.00054	0.00050	0.00013
$16 \times 16$	0.00084	0.00132	0.00103	0.00009
$32 \times 32$	0.00337	0.04161	0.00254	0.00048
$64 \times 64$	0.01457	1.80845	0.00911	0.00331
$128 \times 128$	0.07412	99.097	0.04881	0.02598
$256 \times 256$	0.44292	—	0.35763	0.20776
$512 \times 512$	3.04059	—	3.22541	1.94871

#### Observations:

- **Dense solver** scales as  $\mathcal{O}(n^6)$  (cubic in matrix size  $n^2 \times n^2$ ), becoming impractical for grids larger than  $128 \times 128$  (99s).
- **Sparse direct solver** scales approximately as  $\mathcal{O}(n^3)$  due to fill-in during LU factorization.
- **CG solver** scales as  $\mathcal{O}(n^2 \cdot k)$  where  $k$  is the number of iterations, competitive with sparse direct for large grids.
- **PETSc** consistently outperforms all Python solvers, even on a single processor, due to optimized C/Fortran backends and efficient preconditioning.

Figure 3 shows the scaling behavior on a log-log plot.

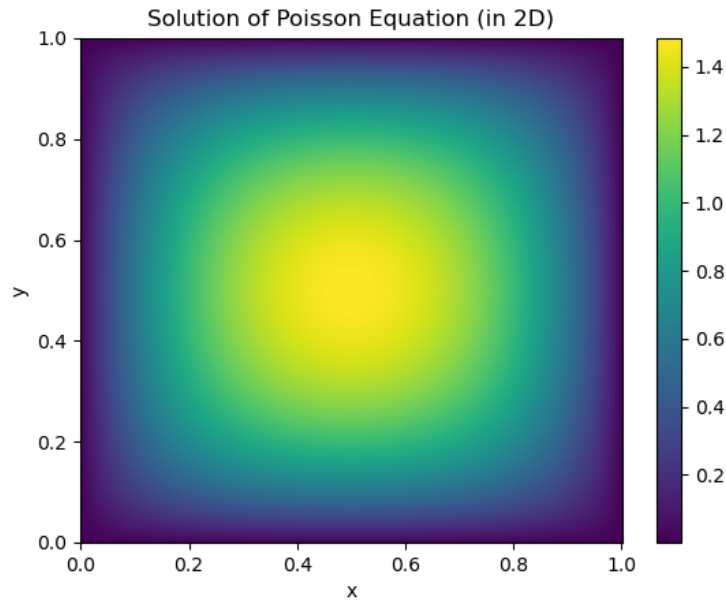


Figure 3: Performance comparison (placeholder - replace with actual timing plot if available).

### 1.5. Strong Scaling [10 points]

## 2. Task: Quality of the Report [15 Points]

### Additional notes and submission details

Submit the source code files (together with your used `Makefile`) in an archive file (tar, zip, etc.), and summarize your results and the observations for all exercises by writing an extended Latex report. Use the Latex template from the webpage and upload the Latex summary as a PDF to iCorsi.

- Your submission should be a gzipped tar archive, formatted like `project_number_lastname_firstname.zip` or `project_number_lastname_firstname.tgz`. It should contain:
  - all the source codes of your solutions;
  - your write-up with your name `project_number_lastname_firstname.pdf`.
- Submit your `.zip/.tgz` through Icorsi.