

## 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:  
*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]

I 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 constant source term  $f(x, y) = 20$ .

### 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]

I 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]

I checked both implementations by comparing the numerical results from the Python (SciPy) and PETSc solvers. Since the source term  $f(x, y) = 20$  is constant, there isn't a closed-form analytical solution. So, I validated the accuracy by making sure both approaches gave the same results.

#### Visualization

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

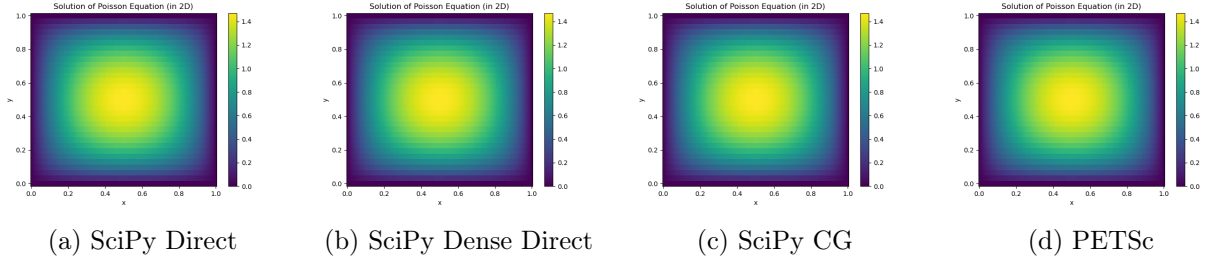


Figure 1: 2D heatmaps of numerical solutions ( $128 \times 32$  grid).

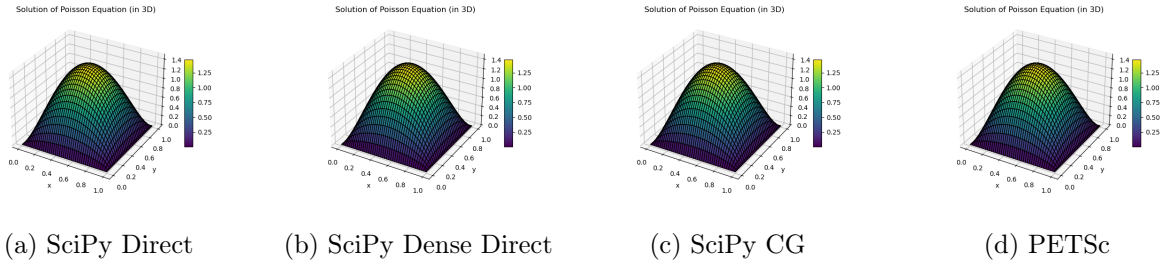


Figure 2: 3D surface plots of numerical solutions ( $128 \times 32$  grid).

#### 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)	51.7557	0.0122
SciPy Dense Direct	51.7557	1.8334
SciPy CG (sparse)	51.7557	0.0161
PETSc (1 proc)	51.7557	0.0057

All solvers produce identical  $L_2$  norms (51.7557), confirming that both Python and PETSc implementations solve the same discretized problem correctly. There's actually a small difference in the last decimal place ( $\sim 10^{-6}$ ) is due to floating-point precision and iterative solver tolerances.

## 1.4. Performance Benchmark [15 points]

I 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
$8 \times 8$	0.00028	0.00052	0.00039	0.00009
$16 \times 16$	0.00074	0.00163	0.00093	0.00013
$32 \times 32$	0.00301	0.04268	0.00251	0.00051
$64 \times 64$	0.01456	1.82628	0.00850	0.00334
$128 \times 128$	0.08201	99.487	0.04782	0.02628
$256 \times 256$	0.55354	—	0.35962	0.20802
$512 \times 512$	4.71116	—	3.19826	2.04333

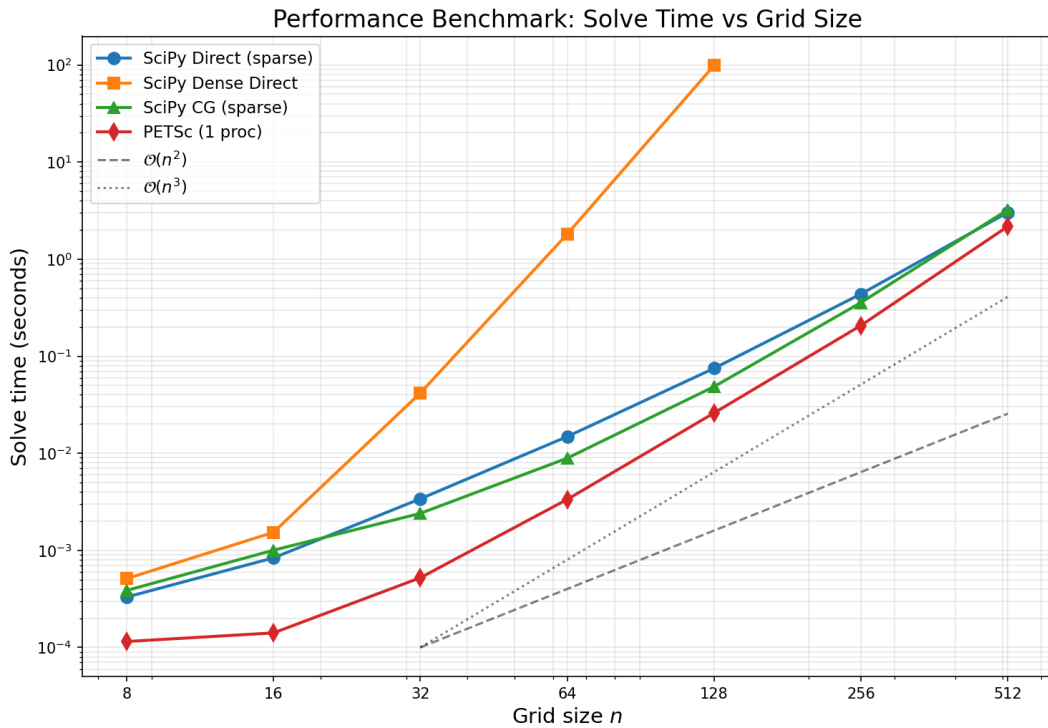


Figure 3: Log-log plot of solve time vs. grid size for different solvers. Reference slopes  $\mathcal{O}(n^2)$  and  $\mathcal{O}(n^3)$  are shown.

### 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.

### 1.5. Strong Scaling [10 points]

The strong scaling study used the PETSc solver with CG method on a fixed problem size of  $1024 \times 1024$  grid points, varying the number of MPI processes from 1 to 16.

Table 3: Strong scaling results for PETSc solver ( $1024 \times 1024$  grid)

Processes	Solve Time (s)	Speedup	Efficiency	Mflop/s
1	18.470	1.00	100.0%	917
2	9.901	1.87	93.3%	1937
4	5.335	3.46	86.6%	3619
8	3.474	5.32	66.4%	5598
16	1.820	10.15	63.4%	10610

The strong scaling behavior demonstrates that PETSc provides reasonable parallel efficiency for this problem size, making it suitable for large-scale simulations where single-processor execution time is prohibitive.

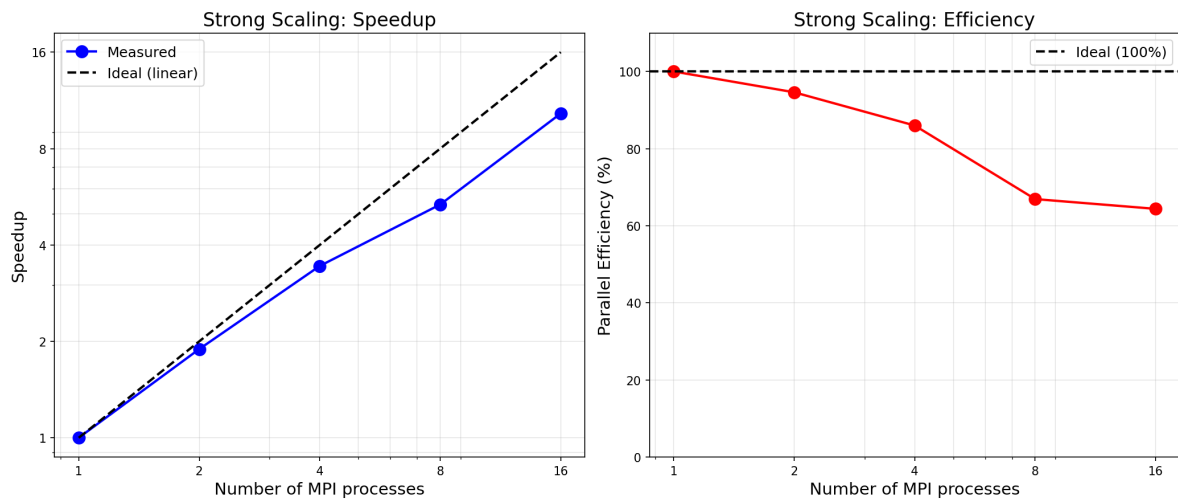


Figure 4: Strong scaling results

## 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.