Laplace-Example with MPI and PETSc

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Laplace Example

- Compute steady temperature distribution for given temperatures on a boundary
- i.e., solve Laplace partial differential equation (PDE)

$$-\Delta u(x,y) = -[\frac{\partial^2}{\partial x^2}u(x,y) + \frac{\partial^2}{\partial y^2}u(x,y)] = 0 \quad \text{on } \Omega \subset R^2$$

- with boundary condition

$$u(x,y) = \phi(x,y) \text{ on } \partial\Omega$$

- area $\Omega = [x_{min},x_{max}]x[y_{min},y_{max}]$
- Compare:
  - Chap. [6] A Heat-Transfer Example with MPI
  - Explicit time-step integration of the the unsteady heat conduction

$$\partial u/\partial t = \Delta u$$

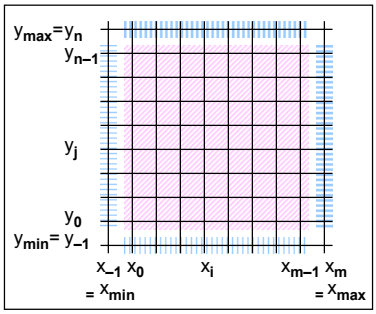
Discretization

- $x_i = (i+1)h + x_{min}$ $\quad i = -1, 0, \ldots, m-1, m$
- $y_i = (j+1)h + y_{min}$ $\quad j = -1, 0, \ldots, n-1, n$
- same discretization in x and y: $h = (x_{max} - x_{min})/(m+1)$
  $= (y_{max} - y_{min})/(n+1)$
- $u_{i,j} = u(x_i, y_j)$
- Boundaries ($\partial\Omega$)

$i = -1,$	$j = 0,\ldots,n-1$
$i = m,$	$j = 0,\ldots,n-1$
$i = 0,\ldots,m-1,$	$j = -1$
$i = 0,\ldots,m-1,$	$j = n$ *)

- Area to be solved ($\Omega - \partial\Omega$)

$i = 0,\ldots,m-1,$	$j = 0,\ldots,n-1$



*) corners are unused

From PDE to the linear difference equations system

- Differentiation:

$$\frac{\partial}{\partial x} u(x_{i+½}, y_j) = (u_{i+1,j} - u_{i,j}) / h$$

$$\frac{\partial^2}{\partial x^2} u_{i,j} = \left(\frac{\partial}{\partial x} u_{i+½,j} - \frac{\partial}{\partial x} u_{i-½,j}\right) / h$$

$$\frac{\partial^2}{\partial x^2} u_{i,j} = (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) / h^2$$

$$\frac{\partial^2}{\partial y^2} u_{i,j} = (u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) / h^2$$

- $-\Delta u(x,y) = 0$

$$\Rightarrow \boxed{-u_{i-1,j} - u_{i,j-1} + 4u_{i,j} - u_{i,j+1} - u_{i+1,j} = 0 \qquad \text{for } i=0,\ldots,m-1,\ j=0,\ldots,n-1}$$

Boundary conditions in the linear difference equations system

- $\boxed{-u_{i-1,j} - u_{i,j-1} + 4u_{i,j} - u_{i,j+1} - u_{i+1,j} = 0 \qquad \text{for } i=0,\ldots,m-1,\ j=0,\ldots,n-1}$

⇒ **Boundary condition** are used in the equations with i=0, i=m-1, j=0, j=n-1:

i=0, j=0	→		$+4u_{i,j}$	$-u_{i,j+1}$	$-u_{i+1,j}$	$= u_{-1,0}$	$+ u_{0,-1}$
i=0, 0<j<n–1	→	$-u_{i,j-1}$	$+4u_{i,j}$	$-u_{i,j+1}$	$-u_{i+1,j}$	$= u_{-1,j}$	
i=0, j=n–1	→	$-u_{i,j-1}$	$+4u_{i,j}$		$-u_{i+1,j}$	$= u_{-1,n-1}$	$+ u_{0,n}$
0<i<m–1, j=0	→	$-u_{i-1,j}$	$+4u_{i,j}$	$-u_{i,j+1}$	$-u_{i+1,j}$	$=$	$u_{i,-1}$
0<i<m–1, 0<j<n–1	→	$-u_{i-1,j}$ $-u_{i,j-1}$	$+4u_{i,j}$	$-u_{i,j+1}$	$-u_{i+1,j}$	$= 0$	
0<i<m–1, j=n–1	→	$-u_{i-1,j}$ $-u_{i,j-1}$	$+4u_{i,j}$		$-u_{i+1,j}$	$=$	$u_{i,n}$
i=m–1, j=0	→	$-u_{i-1,j}$	$+4u_{i,j}$	$-u_{i,j+1}$		$= u_{m,0}$	$+ u_{m-1,-1}$
i=m–1, 0<j<n–1	→	$-u_{i-1,j}$ $-u_{i,j-1}$	$+4u_{i,j}$	$-u_{i,j+1}$		$= u_{m,j}$	
i=m–1, j=n–1	→	$-u_{i-1,j}$ $-u_{i,j-1}$	$+4u_{i,j}$			$= u_{m,n-1}$	$+ u_{m-1,n}$

Matrix notation

- Ordering – lexicographical mapping (i,j) → **I**

  i,j= 0,0; 0,1; … 0,n-1; 1,0; 1,1; … 1,n-1; … m-1,0; … m-1,n-1

  → **I**= 0; 1; … n-1; n; n+1; … 2n-1; … (m-1)n; … mn-1

- Matrix equation: Au=**b**

$$A = (A_{IJ})_{\substack{I=0,\,mn-1\\ J=0,\,mn-1}} = \begin{pmatrix} B & -\mathbf{I} & & & \\ -\mathbf{I} & B & -\mathbf{I} & & \\ & -\mathbf{I} & B & \ldots & \\ & & \ldots & \ldots & -\mathbf{I} \\ & & & -\mathbf{I} & B \end{pmatrix} \in R^{mn\times mn}$$

"Laplace Matrix"

$$\text{with } B = \begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & -1 & 4 & \ldots & \\ & & \ldots & \ldots & -1 \\ & & & -1 & 4 \end{pmatrix} \in R^{n\times n}, \qquad \mathbf{I} = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ldots & \\ & & & & 1 \end{pmatrix} \in R^{n\times n}$$

Matrix notation, continued

- $-\Delta u(x,y) = 0 \quad \Leftrightarrow \quad Au=\mathbf{b}$ with

$i=0,$	$j=0$	➔		$u_{0,0}$	$\mathbf{u}_{-1,0} + \mathbf{u}_{0,-1}$	
$i=0,$	$0<j<n-1$	➔		$\dots$	$\dots$	
$i=0,$	$j=n-1$	➔		$u_{0,j}$	$\mathbf{u}_{-1,j}$	
				$\dots$	$\dots$	
				$u_{0,n-1}$	$\mathbf{u}_{-1,n-1} + \mathbf{u}_{0,n}$	
$0<i<m-1,$	$j=0$	➔	$u =$	$\dots$	$\dots$	
$0<i<m-1,$	$0<j<n-1$	➔		$u_{i,0}$	$\mathbf{u}_{i,-1}$	
$0<i<m-1,$	$j=n-1$	➔		$\dots$	$\dots$	
				$u_{i,j}$	$\mathbf{0}$	
				$\dots$	$\dots$	
				$u_{i,n-1}$	$\mathbf{u}_{i,n}$	
$i=m-1,$	$j=0$	➔		$\dots$	$\dots$	
$i=m-1,$	$0<j<n-1$	➔		$u_{m-1,0}$	$\mathbf{u}_{m,0} + \mathbf{u}_{m-1,-1}$	
$i=m-1,$	$j=n-1$	➔		$u_{m-1,j}$	$\mathbf{u}_{m,j}$	
				$\dots$	$\dots$	
				$u_{m-1,n-1}$	$\mathbf{u}_{m,n-1} + \mathbf{u}_{m-1,n}$	

$\mathbf{b} =$ (repeated for $0 < i < m-1$)

Laplace example: boundary and solution

- Boundary & Solution: $\mathbf{u(x,y) = x}$ on $[0,1]\times[0,1]$
- $(u_{ij})_{i=-1,\dots,m,\ j=-1,\dots,n} =$

$$\begin{array}{c} \\ x \end{array}\overset{y}{\begin{pmatrix} u_{-1,-1} & u_{-1,0} & \dots & u_{-1,n-1} & u_{-1,n} \\ u_{0,-1} & u_{0,0} & \dots & u_{0,n-1} & u_{0,n} \\ \dots & \dots & \dots & \dots & \dots \\ u_{m-1,-1} & u_{m-1,0} & \dots & u_{m-1,n-1} & u_{m-1,n} \\ u_{m,-1} & u_{m,0} & \dots & u_{m,n-1} & u_{m,n} \end{pmatrix}} := h\cdot \begin{pmatrix} 0 & 0 & \dots & 0 & 0 \\ 1 & 1 & \dots & 1 & 1 \\ \dots & \dots & \dots & \dots & \dots \\ m & m & \dots & m & m \\ m+1 & m+1 & \dots & m+1 & m+1 \end{pmatrix}$$

with $h = \dfrac{1}{m+1} = \dfrac{1}{n+1}$

Example with n=m=4, general boundary

$$
\begin{pmatrix}
4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4
\end{pmatrix}
\cdot
\begin{pmatrix}
u_{0,0} \\ u_{0,1} \\ u_{0,2} \\ u_{0,3} \\ u_{1,0} \\ u_{1,1} \\ u_{1,2} \\ u_{1,3} \\ u_{2,0} \\ u_{2,1} \\ u_{2,2} \\ u_{2,3} \\ u_{3,0} \\ u_{3,1} \\ u_{3,2} \\ u_{3,3}
\end{pmatrix}
=
\begin{pmatrix}
u_{-1,0} + u_{0,-1} \\ u_{-1,1} \\ u_{-1,2} \\ u_{-1,3} + u_{0,4} \\ u_{1,-1} \\ 0 \\ 0 \\ u_{1,4} \\ u_{2,-1} \\ 0 \\ 0 \\ u_{2,4} \\ u_{4,0} + u_{3,-1} \\ u_{4,1} \\ u_{4,2} \\ u_{4,3} + u_{3,4}
\end{pmatrix}
$$

Example with n=m=4, with solution & boundary u(x,y) := x

$$
\begin{pmatrix}
4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4
\end{pmatrix}
\cdot
\begin{pmatrix}
0.2 \\ 0.2 \\ 0.2 \\ 0.2 \\ 0.4 \\ 0.4 \\ 0.4 \\ 0.4 \\ 0.6 \\ 0.6 \\ 0.6 \\ 0.6 \\ 0.8 \\ 0.8 \\ 0.8 \\ 0.8
\end{pmatrix}
=
\begin{pmatrix}
0.0 + 0.2 \\ 0.0 \\ 0.0 \\ 0.0 + 0.2 \\ 0.4 \\ 0 \\ 0 \\ 0.4 \\ 0.6 \\ 0 \\ 0 \\ 0.6 \\ 1.0 + 0.8 \\ 1.0 \\ 1.0 \\ 1.0 + 0.8
\end{pmatrix}
$$

Laplace-Example with MPI and PETSc

1st practical: Writing a parallel MPI program with a CG-solver

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(program code)

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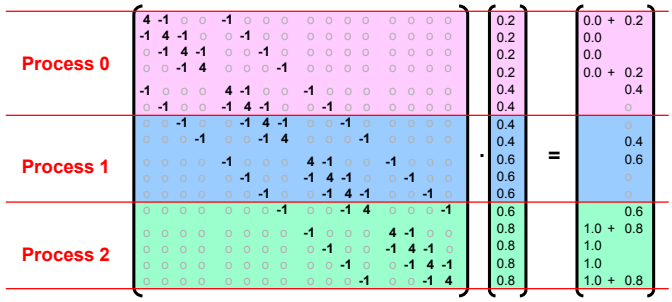
Solving Laplace equation with CG Solver

```
Initialize matrix A;            Initialize boundary condition vector b;
Initialize i_max (≤ size of A); Initialize ε (>0);     Initialize solution vector x;
/* p = b – Ax ;     */   { p = x;          /* Reason: */
/* substituted by */     { v = Ap;         /* Parallelization halo needed */
                         { p = b – v;      /* for same vector (p) as in loop */
r = p;
α = (|| r ||_2)^2 ;
for ( i=0; (i < i_max)  &&  (α > ε); i++)
{    v = Ap;
     λ = α / (v,p)_2 ;
     x = x + λp;
     r = r – λv;
     α_new = (|| r ||_2)^2 ;
     p = r + (α_new/α)p;
     α = α_new;
}
Print x, √α, ||b–Ax||_2;
```

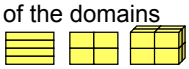
See, e.g.,
Andreas Meister: Numerik linearer Gleichungssysteme.
Vieweg, 1999, p. 124.

The parallelization

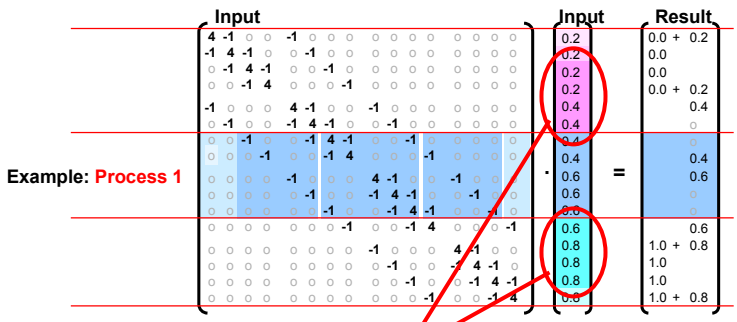
- Distribute Laplace matrix and vectors in slices (chunks)



- 2- and 3-dimensional distribution — depends on form of the domains
  - choose global indexing:
    - first lines of the matrix = elements of 1st domain,
    - next lines … = … 2nd domain, …

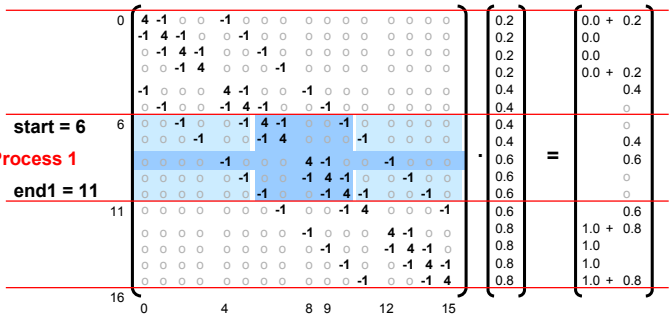


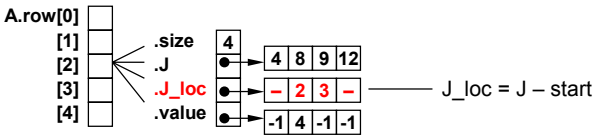
Matrix-Vector-Multiply



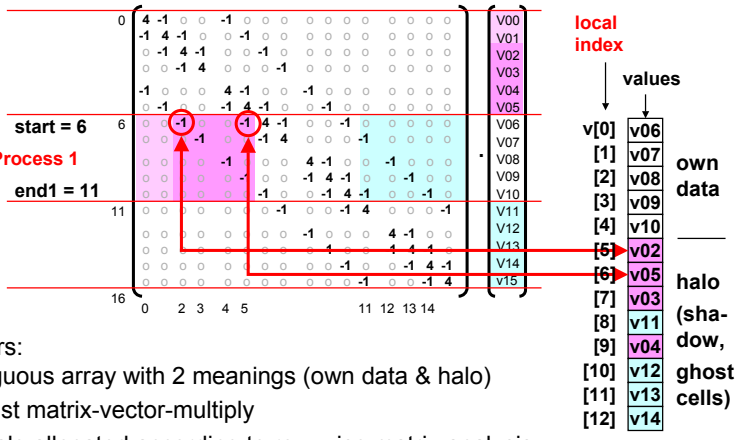
- Data needed from other processes → Halo information
- Halo need not to be contiguous!!!
  - Depends on entries of the matrix

Data-structures — Sparse Matrix



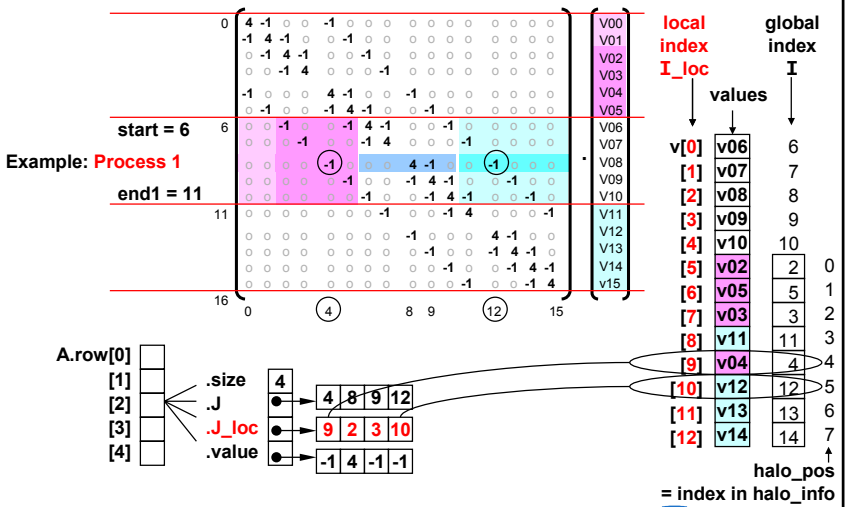


Data-structures — Vector & Halo

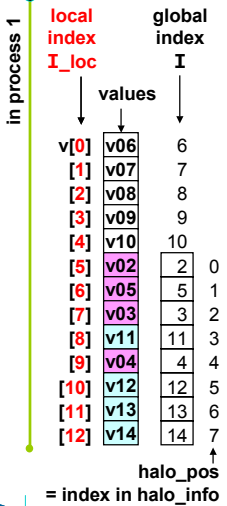


- vectors:
  contiguous array with 2 meanings (own data & halo)
  - fast matrix-vector-multiply
  - halo allocated according to row-wise matrix analysis

Data-structures — Vector & Halo

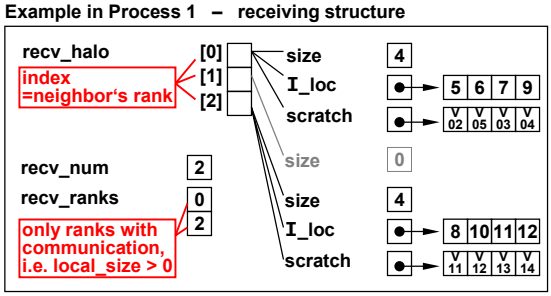


Data-structures — Updating the halos

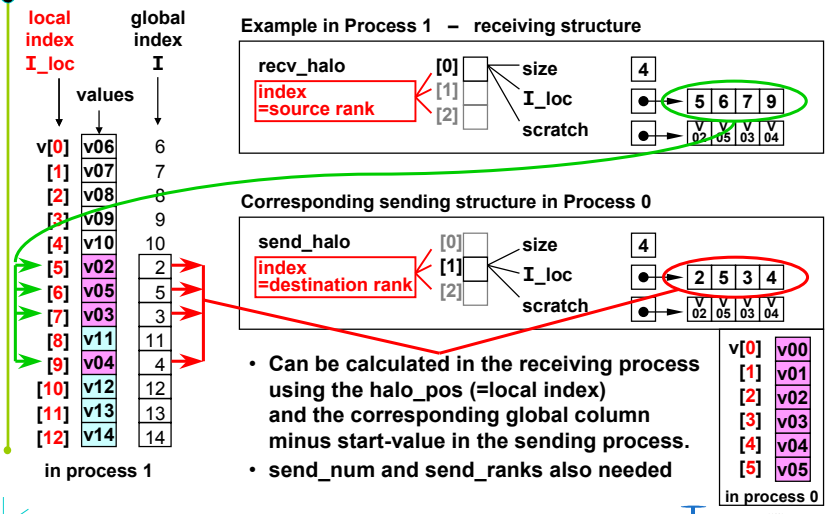


- Needed:
  - receiving structure for each neighbor
    - **Given by left diagram**
    - **Global index → rank**
  - sending structure for each neighbor
    - **Must be constructed from the receiving structure of the neighbor**

Example in Process 1 – receiving structure

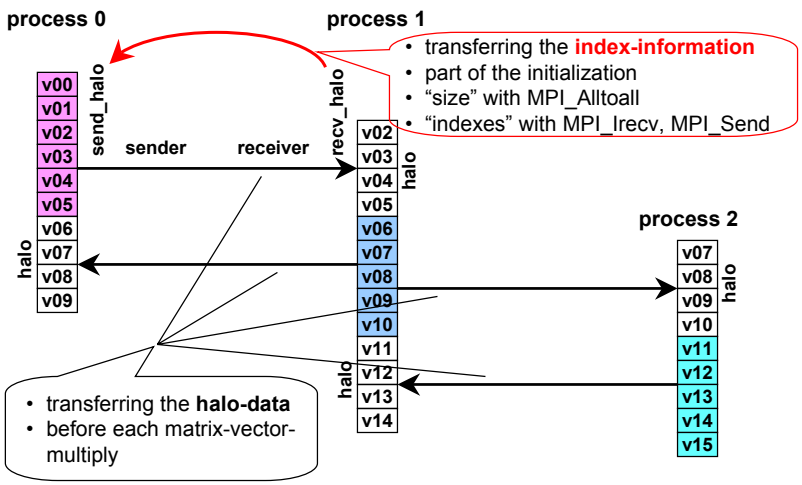


Data-structures — Corresponding sending structure



- Can be calculated in the receiving process using the halo_pos (=local index) and the corresponding global column minus start-value in the sending process.
- send_num and send_ranks also needed

Halo communication



Vector Routines

2a • Allocate vector and initialize with 0

b • Store vector-value in row j (global index)

• Vector calculation routines:

c – duplicate ($v_2 = v_1$)

d – add ($v_3 = v_1 + \beta v_2$)

e – dot product ($\beta = (v_1, v_2)_2$)

  • **with MPI_Allreduce(…MPI_SUM…)**

f – sqr_norm ($\beta = (||v_1||_2)^2$)

  • **with MPI_Allreduce(…MPI_SUM…)**

g – max_norm ($\beta = ||v_1||_\infty$)

  • **with MPI_Allreduce(…MPI_MAX…)**

```
Initialize matrix A;
Initialize boundary condition vector b;
Initialize i_max (≤ size of A);  Initialize ε (>0);
Initialize solution vector x;
p = x;
v = Ap;
p = b – v;
r = p;
α = (|| r ||_2)^2 ;
for ( i=0; (i < i_max)  &&  (α > ε); i++)
{     v  = Ap;
      λ  = α / (v,p)_2 ;
      x  = x + λp;
      r  = r – λv;
      α_new = (|| r ||_2)^2 ;
      p  = r + (α_new/α)p;
      α = α_new ;
}
Print x, √α, ||b–Ax||_2;
```


Matrix Routines, I.

3a • Allocate matrix and initialize as empty

b • Allocate storage for one row

b • Store matrix-values in row I (global index)

• Matrix-vector-multiply ($v_2 = Av_1$)

4 – initializing vector halo structure

  • **analyzing the matrix entries in columns outside of [start .. end1–1]**

5 – initializing vector halo receiver info

  • **analyzing the vector halo structure**

```
Initialize matrix A;
Initialize boundary condition vector b;
Initialize i_max (≤ size of A);  Initialize ε (>0);
Initialize solution vector x;
p = x;
v = Ap;
p = b – v;
r = p;
α = (|| r ||_2)^2 ;
for ( i=0; (i < i_max)  &&  (α > ε); i++)
{     v  = Ap;
      λ  = α / (v,p)_2 ;
      x  = x + λp;
      r  = r – λv;
      α_new = (|| r ||_2)^2 ;
      p  = r + (α_new/α)p;
      α = α_new;
}
Print x, √α, ||b–Ax||_2;
```

Matrix Routines, II.

⑥ – initializing vector halo sender info, part 1
- **analyzing the receiver info**
- **receiver must inform the sender: The local_size can be transferred with MPI_Alltoall** (MPI-1) **or MPI_Put** (MPI-2).

⑦ – initializing vector halo sender info, part 2
- **The send_neighbor.local_index values can be transferred with MPI_Irecv, MPI_Send, MPI_Waitall.**

⑧ – updating the halo of v_1
- **with MPI_Irecv, MPI_Isend, MPI_Waitall**

⑨ – the multiplication ($v_2 = Av_1$)
- **using the halo information of v_1**

```
Initialize matrix A;
Initialize boundary condition vector b;
Initialize i_max (≤ size of A);  Initialize ε (>0);
Initialize solution vector x;
p = x;
v = Ap;
p = b – v;
r = p;
α = (|| r ||₂)² ;
for ( i=0; (i < i_max)  &&  (α > ε); i++)
{     v  = Ap;
      λ  = α / (v,p)₂ ;
      x  = x + λp;
      r  = r – λv;
      α_new = (|| r ||₂)² ;
      p  = r + (α_new/α)p;
      α = α_new;
}
Print x, √α, ||b–Ax||₂;
```


Distribution, Printing, CG-solver, and Application program

① • Distribution:

ⓐ – init(mat_size, num_procs)
- **internal module data: mat_size, chunk_size = (mat_size–1) / num_procs + 1**

ⓑ – start(rank), end1(rank)

ⓒ – rank(row)

⑩ • Domain Decomposition

• Application:

⑪ – Initialize matrix A
- **only rows [start .. end1–1]**

⑫ – Initialize boundary vector b
- **only rows [start .. end1–1]**

• Printing:

⑬ – Print matrix A

⑭ – Print solution vector x

⑮ • CG-solver

⑯ • main

```
Initialize matrix A;
Initialize boundary condition vector b;
Initialize i_max (≤ size of A);  Initialize ε (>0);
Initialize solution vector x;
p = x;
v = Ap;
p = b – v;
r = p;
α = (|| r ||₂)² ;
for ( i=0; (i < i_max)  &&  (α > ε); i++)
{     v  = Ap;
      λ  = α / (v,p)₂ ;
      x  = x + λp;
      r  = r – λv;
      α_new = (|| r ||₂)² ;
      p  = r + (α_new/α)p;
      α = α_new;
}
Print x, √α, ||b–Ax||₂;
```

Naming scheme — Indexes

- m,n — dimensions of the physical problem
- i,j — index in physics (0..m–1, 0..n–1 – without boundary)
- **I** — global row index in Laplace matrix and vector (0 .. nm–1)
- J — global column index in the Laplace matrix (0 .. nm–1)
  - process-local data: start .. end1–1
- **I**_loc — local row index in Laplace matrix and vector (and in halo)
- J_loc — local column in Laplace matrix
  - process-local data: 0 .. end1–start–1
  - **I**_loc = **I** – start
- halo_pos — index in the halo (0 .. halo_info.size–1)
  - halo_pos = **I**_loc – (end1–start)

Domain Decomposition & Data Distribution

- load-balanced distribution of the physical data matrix
  - each physical data entry = one row in the Laplace matrix
  - same amount of physical entries on each process

1-dimensional

	j=0	1	2	3	4	5	6	7	8
i=0	I = 0	1	2	3	4	5	6	7	8
1	9	10	11	12	13	14	15	16	17
2	18	19	20	21	22	23	24	25	26
3	27	28	29	30	31	32	33	34	35
4	36	37	38	39	40	41	42	43	44
5	45	46	47	48	49	50	51	52	53
6	54	55	56	57	58	59	60	61	62

2-dimensional domain decomposition

	j=0	1	2	3	4	5	6	7	8
i=0	I = 0	1	2	3	4	20	21	22	23
1	5	6	7	8	9	24	25	26	27
2	10	11	12	13	14	28	29	30	31
3	15	16	17	18	19	32	33	34	35
4	36	37	38	39	40	51	52	53	54
5	41	42	43	44	45	55	56	57	58
6	46	47	48	49	50	59	60	61	62

Domain Decomposition & Data Distribution

- communication-optimized distribution of the physical data matrix
  - full horizontal set of physical entries on each process

if
m is multiple of m_procs
and
n is multiple of n_procs
then
load-opt. == comm.-opt.

1-dimensional

		j=0	1	2	3	4	5	6	7	8
i=0	I =	0	1	2	3	4	5	6	7	8
1		9	10	11	12	13	14	15	16	17
2		18	19	20	21	22	23	24	25	26
3		27	28	29	30	31	32	33	34	35
4		36	37	38	39	40	41	42	43	44
5		45	46	47	48	49	50	51	52	53
6		54	55	56	57	58	59	60	61	62

- full domain on each process

2-dimensional domain decomposition

		j=0	1	2	3	4	5	6	7	8
i=0	I =	0	1	2	3	4	20	21	22	23
1		5	6	7	8	9	24	25	26	27
2		10	11	12	13	14	28	29	30	31
3		15	16	17	18	19	32	33	34	35
4		36	37	38	39	40	51	52	53	54
5		41	42	43	44	45	55	56	57	58
6		46	47	48	49	50	59	60	61	62

The Laplace-Equation with arbitrary domain decomposition

- arbitrary mapping
  - physical 2-dim indexes (i,j) → I = global row index of the Laplace matrix
  - (i,j) → J = global column index of the Laplace matrix and global row index of the vectors
- choosing identical mappings: I(i,j) = J(i,j) := functions ij2I_1dim(i,j) and ij2I_2dim(i,j)
- $-u_{i-1,j} - u_{i,j-1} + 4u_{i,j} - u_{i,j+1} - u_{i+1,j} = 0$ for i=0,…,m-1, j=0,…,n-1
- at matrix row I(i,j):

at column J(i-1,j), J(i,j-1), J(i,j), J(i,,j+1), J(i+1,j)

$$\begin{pmatrix} -1 & -1 & 4 & -1 & -1 \end{pmatrix} \begin{pmatrix} u_{i-1,j} \\ u_{i,j-1} \\ u_{i,j} \\ u_{i,j+1} \\ u_{i+1,j} \end{pmatrix}$$

only if i>0 | only if j>0 | only if j<n-1 | only if i<m-1

at solution vector column J(i,j)

at boundary vector row I(i,j):

$$= 0 + u_{i-1,j} + u_{i,j-1} + u_{i,j+1} + u_{i+1,j}$$

only if i=0 | only if j=0 | only if j=n-1 | only if i=m-1

Practical

- Tasks – each group works on **one** task only!!!!

– no./ difficulty (1=simple .. 5=hard)	lines of real code
00 / – / global decl. & memory	
01 / 1 / distribution: global index range → ranks	7
02 / 3 / vector routines	25
03 / 2 / matrix allocation & store	14
04 / 3 / build halo vector info	22
05 / 4 / build halo recv info	38
06 / 4 / build halo send info, part 1 (communicate "size" with MPI_Alltoall)	11
07 / 5 / build halo send info, part 2 (communicate "indexes" with Irecv & Send)	44
08 / 5 / communicate vector data from "own data" to "halo"	40
09 / 2 / matrix-vector-multiply	9
10 / 1 / 1-dim domain decomposition, and / 4 / 2-dim domain decomp.	2+26
11 / 4 / initialization of Laplace matrix A	9
12 / 3 / initialization of boundary vector b and exact solution vector u	15
13 / – / printing application data	
14 / – / printing vectors, matrices, halo information, …	
15 / 2 / the CG solver	19
16 / – / main and options reading and distributing	
Sum: 13 tasks as practical, 3 tasks and all declarations are given, to do:	281

- MPI routines needed
- part of domain decomposition or distribution, but without communication

Practical — Working environment

- Your working directory: ~/CG/**<nr>**
- Choose your task: **<task>**
- Fetch your skeleton: cp ~/CG/skel/cg_**<task>**.c **.**
- **Add your code**, compile, run and test it (correct result?, same as serial result?)

Do not modify any lines outside of your task segment

- If your task works:
  - **extract your part (from** ***/*== task_ii begin ==*/*** **to** ***/*== task_ii end ==*/*** **) into cgp<task>.c**
- Advanced exercise: Implement the communication-optimized distribution
  - **in a copy of your cg_<task>.c**
  - **compare execution time: 1-dim decomposition / 2-dim load optimal / 2-dim comm.-opt.**
- When all groups have finished, everyone can check the total result with:
  - **ls –l ../*/cgp*.c**
  - **cat ../00/cgp00.c ../*/cgp01.c ../*/cgp02.c ../*/cgp03.c ../*/cgp04.c ../*/cgp05.c ../*/cgp06.c ../*/cgp07.c ../*/cgp08.c ../*/cgp09.c ../*/cgp10.c ../*/cgp11.c ../*/cgp12.c ../00/cgp13.c ../00/cgp14.c ../*/cgp15.c ../00/cgp16.c > cg_all.c**
  - **duplicate parts must be selected by hand (<nr> instead of *)**
  - **missing parts may be fetched also from ../source/parts/cgp<task>.c**
  - **Compile and run cg_all.c**

Practical — Options

- Compile-time options [default]:
  - –Dserial — compile without MPI and without distribution [parallel]
- Run-time options [default]:
  - –m <m> — vertical dimension of physical heat area [4]
  - –n <n> — horizontal dimension … [4]
  - –imax <iter_max> — maximum number of iterations in the CG solver [500]
  - –eps <epsilon> — abort criterion of the solver for residual vector [1e-6]
  - –twodims — choose 2-dimensional domain decomposition [1-dim]
  - –mprocs <m_procs> — choose number of processors, vertical, (–twodims needed)
  - –nprocs <n_procs> — … and horizontal [given by MPI_Dims_create]
  - –prtlev 0|1|2|3|4|5 — printing and debug level [1]:

    1 = only || result – exact solution || and partial result matrix
    2 = and residual norm after each iteration
    3 = and result of physical heat matrix
    4 = and all vector and matrix information in 1st iteration
    5 = and in all iterations

Goals of the practical

- Major goal:
  - You get time to understand the parallelization of solvers
- Minor goals:
  - You get additional experience with MPI
  - You are involved with domain decomposition
  - You are involved in programming iterative solvers
- Nice, but not necessary
  - All groups together write this parallel program
- → tasks

Laplace-Example with MPI and PETSc

2nd practical: PETSc

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Solving Laplace equation with PETSc *)

- Initialization of PETSc
- Initialization of Laplace matrix **A**
- Initialization of the boundary condition **b**
  - Data: Vector **u** := predefined exact solution
    Vector **b** := boundary condition (RHS)
    Vector **x** := approximate solution computed
  - Initialization of **b**, **u**: b, u – see previous slides [heat, u(*x*,*y*)=*x*]
    or with **–random_exact_sol**: u = random values, b := Au
- Solving **Ax=b**
- Checking the solution error_norm = $\| x - u \|_2$

*) based on **petsc/src/sles/examples/tutorials/ex2.c**

Initialization of PETSc

```
21: /* Include "petscsles.h" so that we can use SLES solvers. Note that this file
       automatically includes:
         petsc.h        - base PETSc routines     petscvec.h   - vectors
         petscsys.h     - system routines         petscmat.h   - matrices
         petscis.h      - index sets              petscksp.h   - Krylov subspace methods
         petscviewer.h  - viewers                 petscpc.h    - preconditioners          */

28: #include petscsles.h

33: int main(int argc,char **args)
34: {
35:     Vec          x, b, u;     /* approx solution, RHS, exact solution */
36:     Mat          A;           /* linear system matrix */
37:     SLES         sles;        /* linear solver context */
38:     PetscRandom  rctx;        /* random number generator context */
39:     PetscReal    norm;        /* norm of solution error */
40:     int          i,j, I,J, Istart, Iend, ierr, m = 4, n = 4, its;
41:     PetscTruth   flg;
42:     PetscScalar  v, h, one = 1.0, neg_one = –1.0;
43:     KSP          ksp;         KSPType ksptype;   PC pc;   PCType pctype;

45:     PetscInitialize(&argc, &args, (char *)0, help);
46:     PetscOptionsGetInt(PETSC_NULL,"–m",&m,PETSC_NULL);
47:     PetscOptionsGetInt(PETSC_NULL,"–n", &n, PETSC_NULL);
```


Initialization of matrix A

```
55:  /*  When using MatCreate(), the matrix format can be specified at runtime.
         Also, the parallel partitioning of the matrix is determined by PETSc at runtime.
         Performance tuning note: For problems of substantial size, preallocation of matrix memory is crucial for
         attaining good performance. Since preallocation is not possible via the generic matrix creation routine
         MatCreate(), we recommend for practical problems instead to use the creation routine for a particular
         matrix format, e.g.,   MatCreateMPIAIJ() – parallel AIJ (compressed sparse row)
                                MatCreateMPIBAIJ() – parallel block AIJ
         See the matrix chapter of the users manual for details. */
69:  MatCreate(PETSC_COMM_WORLD,PETSC_DECIDE,PETSC_DECIDE,m*n,m*n,&A);
70:  MatSetFromOptions(A);

73:  /*  Currently, all PETSc parallel matrix formats are partitioned by contiguous chunks of rows
         across the processors. Determine which rows of the matrix are locally owned.  */

77:  MatGetOwnershipRange(A,&Istart,&Iend);

92:  for (I=Istart; I<Iend; I++) {

93:      v = –1.0;  i = I/n;  j = I – i*n;
94:      if (i>0)      {J = I – n;  MatSetValues(A, 1,&I, 1,&J, &v, INSERT_VALUES);}
95:      if (i<m–1)  {J = I + n;  MatSetValues(A, 1,&I, 1,&J, &v, INSERT_VALUES);}
96:      if (j>0)      {J = I – 1;  MatSetValues(A, 1,&I, 1,&J, &v, INSERT_VALUES);}
97:      if (j<n–1)  {J = I + 1;  MatSetValues(A, 1,&I, 1,&J, &v, INSERT_VALUES);}
98:      v = 4.0;  MatSetValues(A,1,&I,1,&I,&v,INSERT_VALUES);
     }
107: MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
108: MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);
```

Initialization of u, b, x

```
110:  /*
      Create parallel vectors.
        – We form 1 vector from scratch and then duplicate as needed.
        – When using VecCreate(), VecSetSizes and VecSetFromOptions()
          in this example, we specify only the
          vector's global dimension; the parallel partitioning is determined at runtime.
        – When solving a linear system, the vectors and matrices MUST
          be partitioned accordingly. PETSc automatically generates
          appropriately partitioned matrices and vectors when MatCreate()
          and VecCreate() are used with the same communicator.
        – The user can alternatively specify the local vector and matrix
          dimensions when more sophisticated partitioning is needed
          (replacing the PETSC_DECIDE argument in the VecSetSizes() statement
          below).
      */
126:  VecCreate(PETSC_COMM_WORLD,&u);
127:  VecSetSizes(u,PETSC_DECIDE,m*n);
128:  VecSetFromOptions(u);
129:  VecDuplicate(u,&b);
130:  VecDuplicate(b,&x);
```


Initializing the values of b (and u)

```
145:  PetscOptionsHasName(PETSC_NULL,"–random_exact_sol",&flg);
146:  if ( ! flg) {
          VecGetOwnershipRange(b,&Istart,&Iend);
          h = 1.0 / (m+1);
          for (I=Istart; I<Iend; I++) {
              v = 0;  i = I/n;  j = I – i*n;  h = 1/(m+1);
              if (i==0)      v = v +   /* u(-1,j): */  h * 0;
              if (i==m-1)  v = v +   /* u(m,j): */  h * (m+1);
              if (j==0)      v = v +   /* u(i,-1): */  h * (i+1);
              if (j==n-1)   v = v +   /* u(i, n): */  h * (i+1);
              if (v != 0) ; VecSetValues(b,1,&I,&v,INSERT_VALUES);
              v =  /* u(i, j): */  h * (i+1); VecSetValues(u,1,&I,&v,INSERT_VALUES);
          }
          VecAssemblyBegin(b); VecAssemblyEnd(b);
          VecAssemblyBegin(u); VecAssemblyEnd(u);
160:  } else {
          PetscRandomCreate(PETSC_COMM_WORLD,RANDOM_DEFAULT,&rctx);
          VecSetRandom(rctx,u);  PetscRandomDestroy(rctx);
          MatMult(A,u,b);
164:  }
167:  /* View the exact solution vector if desired */
169:  PetscOptionsHasName(PETSC_NULL,"–view_exact_sol",&flg);
170:  if (flg) {VecView(u,PETSC_VIEWER_STDOUT_WORLD);}
```

Solving Ax=b

```
173:  /* - - - - - - Create the linear solver and set various options - - - - - - - */
177:  /* Create linear solver context */
179:  SLESCreate(PETSC_COMM_WORLD,&sles);

182:  /* Set operators. Here the matrix that defines the linear system
          also serves as the preconditioning matrix. */
185:  SLESSetOperators(sles,A,A,DIFFERENT_NONZERO_PATTERN);

188:  /* Set linear solver defaults for this problem (optional).
          – By extracting the KSP (Krylov subspace methods) and PC (Preconditioner) contexts from
            the SLES context, we can then directly call any KSP and PC routines to set various options.
          – The following two statements are optional; all of these parameters could
            alternatively be specified at runtime via SLESSetFromOptions().
            All of these defaults can be overridden at runtime, as indicated below. */
198:  SLESGetKSP(sles,&ksp);
199:  KSPSetTolerances(ksp,1.e-2/((m+1)*(n+1)),1.e-50,PETSC_DEFAULT,PETSC_DEFAULT);

202:  /* Set runtime options, e.g., -ksp_type <type> -pc_type <type> -ksp_monitor -ksp_rtol <rtol>
          These options will override those specified above as long as SLESSetFromOptions()
          is called _after_ any other customization routines. */
208:  SLESSetFromOptions(sles);

211:  /* - - - - - - Solve the linear system - - - - - - - */
214:  SLESSolve(sles,b,x,&its);
```


Printing the solution

```
229:  /*  Draw solution grid  */

233:  PetscOptionsHasName(PETSC_NULL,"–view_sol_serial",&flg);
234:  if (flg) {VecView( x, PETSC_VIEWER_STDOUT_WORLD); }

236:  PetscOptionsHasName(PETSC_NULL,"–view_sol",&flg);
237:  if (flg) {
238:      PetscScalar  *xx;
239:      VecGetArray( x, &xx );
240:      VecGetOwnershipRange(x,&Istart,&Iend);
241:      PetscPrintf( PETSC_COMM_WORLD,
                       "Solution Grid (without boundary conditions):\n" );
242:      for (I=Istart; I<Iend; I++) {
243:         i = I/n;  j = I – i*n;
244:            PetscSynchronizedPrintf( PETSC_COMM_WORLD, "%8.6f  ", xx[I–Istart] );
245:            if (j == (n–1) ) PetscSynchronizedPrintf( PETSC_COMM_WORLD, "\n");
246:      }
247:      PetscSynchronizedFlush( PETSC_COMM_WORLD );
248:      VecRestoreArray( x, &xx );
249:  }
```

Printing the solution via X Window

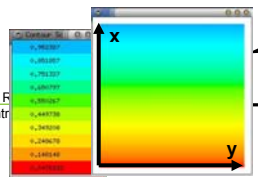
```
29: #include petscda.h

251:  PetscOptionsHasName(PETSC_NULL,"–view_sol_x",&flg);
252:  if (flg) { /* view solution grid in an X window */
253:      PetscScalar *xx;        DA  da;
          AO          ao;         Vec x_da;
257:      DACreate2d(PETSC_COMM_WORLD,DA_NONPERIODIC,DA_STENCIL_STAR,
258:         n,m,PETSC_DECIDE,PETSC_DECIDE,1,0,PETSC_NULL,PETSC_NULL,&da);
259:      DACreateGlobalVector(da, &x_da);
260:      DAGetAO(da, &ao);
261:      VecGetOwnershipRange(x, &Istart, &Iend);
262:      VecGetArray(x, &xx);
263:      for (I=Istart; I<Iend; I++)  {
264:         i = I; AOApplicationToPetsc(ao,1,&i);
265:         VecSetValues(x_da, 1, &i, &xx[I-Istart], INSERT_VALUES);
266:      }
267:      VecRestoreArray(x, &xx);
268:      VecAssemblyBegin(x_da); VecAssemblyEnd(x_da);
269:      PetscOptionsHasName(PETSC_NULL,"-view_sol_x_da",&flg);
270:      if (flg) VecView(x_da,PETSC_VIEWER_STDOUT_WORLD);
271:      VecView(x_da, PETSC_VIEWER_DRAW_(PETSC_COMM_WORLD));
272:      DADestroy(da);
          VecDestroy(x_da);
273:  }
```

Create a 2-dimensional vector x_da

Copy values of x into x_da

Controling the distribution of x_da

View the solution as a 2-dimensional plot



Check solution and clean up

```
283:  /* Check the error */
285:  VecAXPY(&neg_one,u,x);
286:  VecNorm(x,NORM_2,&norm);
287:  /* Optional: Scale the norm:    norm *= sqrt(1.0/((m+1)*(n+1))); */

290:  /* Print convergence information. PetscPrintf() produces a single
         print statement from all processes that share a communicator.
         An alternative is PetscFPrintf(), which prints to a file.  */
294:  PetscPrintf(PETSC_COMM_WORLD,"Norm of error %A iterations %d\n",norm,its);

297:  /* Free work space.
          All PETSc objects should be destroyed when they are no longer needed. */
300:  SLESDestroy(sles);
301:  VecDestroy(u); VecDestroy(x);
302:  VecDestroy(b); MatDestroy(A);

305:  /* Always call PetscFinalize() before exiting a program. This routine
         – finalizes the PETSc libraries as well as MPI
         – provides summary and diagnostic information if certain runtime
           options are chosen (e.g., –log_summary). */
310:  PetscFinalize();
```

Program start

```
1: /* Program usage: mpirun –np <procs> ./heat_petsc [–help] [all PETSc options] */

3: static char help[ ] = "Solves a linear system in parallel with SLES: Compute steady   \n
4:                        temperature distribution for given temperatures on a boundary.\n
5:                        Input parameters include:                                     \n
6:                          –random_exact_sol : use a random exact solution vector      \n
7:                          –view_exact_sol   : write exact solution vector to stdout   \n
8:                          –view_sol_serial  : write solution grid to stdout (1 item/line) \n
9:                          –view_sol         : write solution grid to stdout (as matrix) \n
10:                         –view_sol_x –draw_pause 3 : view solution x on a X window   \n
11:                         –view_mat_x –draw_pause 3 : view matrix A on a X window     \n
12:                         –m <mesh_x>       : number of mesh points in x-direction    \n
13:                         –n <mesh_y>       : number of mesh points in y-direction    \n";
...
46:     PetscInitialize(&argc, &args, (char *)0, help);
```


Other Options

–help	prints **all** options
–ksp_type <type>	e.g., cg (**Conjugate Gradient**), cr (**Conjugate Residual**), bcgs (**BiCGSTAB**), cgs (**Conjugate Gradient Squared**), tfqmr (**Transpose-Free Quasi-Minimal Residual**), bicg (**BiConjugate Gradient**), qmres (**Generalized Minimal Residual**)
–ksp_rtol <rtol>	convergence criterion set by the program to **1.e-2/((m+1)*(n+1))**
–pc_type <type>	e.g., bjacobi (**BlockJacobi**), asm (**Additive Schwarz**)
–sub_pc_type <type>	e.g., jacobi (**Block Jacobi**), sor (**SOR**), ilu (**Incomplete LU**)
–ksp_monitor	prints an estimate of the l_2 -norm of the residual at each iteration
–sles_view	prints information on chosen KSP (solver) and PC (preconditioner)
–log_summary	prints statistical data
–options_table	prints all used options
–options_left	prints options table and unused options

Runtime Script Example, I.

```
1  #! /bin/csh
2  #
3  # Sample script: Experimenting with linear solver options.
4  # Can be used with, e.g., petsc/src/sles/examples/tutorials/ex2.c
5  # or heat_petsc.c
6  #
7  set appl='./heat_petsc'                          # path of binary
8  set options='–ksp_monitor –sles_view –log_summary –options_table –options_left
                –m 10 –n 10'
9  set num='0'
10 foreach np (1 2 4 8)                             # number of processors
11   foreach ksptype (gmres bcgs tfqmr)             # Krylov solver
12     set pctypes_parallel='bjacobi asm'           # parallel preconditioners
13     set pctypes_serial='ilu'                     # non-parallel preconditioners
14     if ($np == 1) then
15       set pctype_list="$pctypes_serial $pctypes_parallel"
16     else
17       set pctype_list="$pctypes_parallel"
18     endif
19     foreach pctype ($pctype_list)
20–49  ...          (see next slide)
50     end #for pctype
51   end #for ksptype
52 end #for np
```


Runtime Script Example, II.

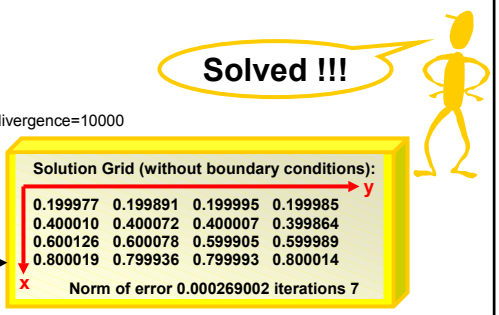
```
10 foreach np (1 2 4 8)                             # number of processors
11   foreach ksptype (gmres bcgs tfqmr)             # Krylov solver
12     set pctypes_parallel='bjacobi asm'           # parallel preconditioners
13     set pctypes_serial='ilu' # non-parallel preconditioners
14     if ($np == 1) then ; set pctype_list="$pctypes_serial $pctypes_parallel"
16     else               ; set pctype_list="$pctypes_parallel"
18     endif
19     foreach pctype ($pctype_list)
20       if ($pctype == ilu) then                   # non-parallel preconditioner
21         foreach level (0 1 2)                    # level of fill for ILU(k)
22           echo ' '
23           echo '********************** Beginning new run **********************'
24           echo ' '
25           set cmd="mpirun –np $np $appl –ksp_type $ksptype –pc_type $pctype
                        –pc_ilu_levels $level $options"
26           set num=`expr $num + 1`; echo "$num : $cmd"
27           eval $cmd
28         end #for level
29       else                                       # parallel preconditioner
30–48  ...          (see next slide)
49       endif #pctype
50     end #for pctype
51   end #for ksptype
52 end #for np
```

Runtime Script Example, III.

```
20      if ($pctype == ilu) then                    #  non-parallel preconditioner
21–28 ...
29      else                                        #  parallel preconditioner
30        foreach  subpctype (jacobi  sor  ilu)  #  subdomain solver
31          if ($subpctype == ilu) then
32            foreach level (0 1 2)  #  level of fill for ILU(k)
34              echo '************************ Beginning new run ************************'
36              set  cmd="mpirun   –np $np   $appl   –ksp_type $ksptype   –pc_type  $pctype
                                   –sub_ksp_type  preonly   –sub_pc_type  $subpctype
                                   –sub_pc_ilu_levels  $level   $options"
37              set  num=`expr  $num + 1`;  echo "$num :  $cmd"
38              eval  $cmd
39            end #for level
40          else
42              echo '************************ Beginning new run ************************'
44              set  cmd="mpirun   –np $np   $appl   –ksp_type $ksptype   –pc_type  $pctype
                                   –sub_ksp_type  preonly   –sub_pc_type  $subpctype
                                   $options"
45              set  num=`expr  $num + 1`;  echo "$num :  $cmd"
46              eval  $cmd
47          endif #subpctype
48        end #for subpctype
49      endif #pctype
```


Output Example

```
t3e> setenv  PETSC_DIR  /usr/local/lib/PETSC  ;  setenv PETSC_ARCH t3e
t3e> make  BOPT=O  heat_petsc
t3e> mpirun  –np 3  ./heat_petsc  –ksp_type cg  –m 4  –n 4  –ksp_monitor
                                  –sles_view  –view_sol  –log_summary  –options_table  –options_left
 0 KSP Residual norm 1.242025913946e+00
...
 6 KSP Residual norm 8.610435306905e–04
 7 KSP Residual norm 2.704366376622e–04
KSP Object:
 type: cg
 maximum iterations=10000, initial guess is zero
 tolerances:  relative=0.0004, absolute=1e–50, divergence=10000
 left preconditioning
PC Object:
 type: bjacobi
   block Jacobi: number of blocks = 3
KSP Object:(sub_)
   type: preonly
   tolerances:  relative=1e–05, absolute=1e–50,
   left preconditioning
 PC Object:(sub_)
   type: ilu
     ILU: 0 levels of fill
     ILU: max fill ratio allocated 1
     ILU: tolerance for zero pivot 1e–12
...
```



	Max	Max/Min	Avg	Total
Time (sec):	**7.033e–02**	1.01369	6.971e–02	
Objects:	4.100e+01	1.00000	4.100e+01	
Flops:	1.071e+03	1.28571	9.370e+02	**2.811e+03**
Flops/sec:	1.523e+04	1.26883	1.343e+04	**4.030e+04**

Makefile

```
ALL: heat_petsc

CFLAGS     =
FFLAGS     =
CPPFLAGS   =
FPPFLAGS   =

include ${PETSC_DIR}/bmake/common/base

heat_petsc: heat_petsc.o  chkopts
<TAB>  –${CLINKER} –o heat_petsc heat_petsc.o ${PETSC_SNES_LIB}
<TAB>  ${RM} heat_petsc.o
```


Installation

- Set the environmental variable PETSC_DIR to the full path of the PETSc home directory, for example:
  setenv PETSC_DIR /home/username/petsc-2.1.3
- Set the environmental variable PETSC_ARCH, which indicates the architecture on which PETSc will be configured. For example, use
  setenv PETSC_ARCH solaris_gnu
  setenv PETSC_ARCH `$PETSC_DIR/bin/petscarch`
- In the PETSc home directory, type
  make BOPT=g all >& make_log
  to build a debugging version of the PETSc or
  make BOPT=O all >& make_log
  to build optimized version of the PETSc libraries.

Customized installation

Under the following circumstances it might be necessary to customize your installation of PETSc:

- packages like BLAS or Lapack are not installed in the default directories
- you want to use additional packages like Matlab or BlockSolve
- you want to use special compiler or linker options

Customized installation

The PETSc Makefile System is located in ${PETSC_DIR}/bmake.
This directory has subdirectories for each supported platform.
If you want to customize your installation you have to edit the following files:

- ${PETSC_DIR}/bmake/${PETSC_ARCH}/packages
  - locations of all needed packages
- ${PETSC_DIR}/bmake/${PETSC_ARCH}/variables
  - definitions of compilers, linkers, etc.

Example - /bmake/linux/packages

```
# $Id: packages,v 1.63 2001/10/10 18:50:03 balay Exp $
# This file contains site-specific information.  The definitions below
# should be changed to match the locations of libraries at your site.
# The following naming convention is used:
#     XXX_LIB - location of library XXX
#     XXX_INCLUDE - directory for include files needed for library XXX
# Location of BLAS and LAPACK.
# See ${PETSC_DIR}/docs/intallation.html for information on
# retrieving them.
# BLASLAPACK_LIB      = -L/home/petsc/software/blaslapack/linux
                        -lflapack -lfblas
BLASLAPACK_LIB        = -L/home/petsc/software/mkl_linux/LIB
                        -lmkl32_lapack -lmkl32_def -lpthread
#
# Location of MPI (Message Passing Interface) software
#
MPI_HOME              = /home/petsc/software/mpich-1.2.0/linux
MPI_LIB               = -L${MPI_HOME}/lib -lmpich
MPI_INCLUDE           = -I${MPI_HOME}/include
MPIRUN                = ${MPI_HOME}/bin/mpirun -machinefile
                        ${PETSC_DIR}/maint/hosts.local
```


Example - /bmake/linux/packages

```
# ----------------------------------------------------------------------------
#  Locations of OPTIONAL packages. Comment out those
#  you do not have.
# ----------------------------------------------------------------------------
# Location of X-windows software
X11_INCLUDE           =
X11_LIB               = -L/usr/X11R6/lib -lX11
PETSC_HAVE_X11        = -DPETSC_HAVE_X11
# Location of MPE
# If using MPICH version 1.1.2 or higher use the flag
#DPETSC_HAVE_MPE_INITIALIZED_LOGGING
#MPE_INCLUDE          = -I/home/petsc/mpich-1.1.1/mpe
#MPE_LIB              = -L/home/petsc/mpich-1.1.1/lib/LINUX/ch_p4
                        -lmpe -lpmpich
#MPE_INCLUDE          =
#MPE_LIB              = -L${MPI_HOME}/lib -lmpe
#PETSC_HAVE_MPE       = -DPETSC_HAVE_MPE
```

Summary

- **Laplace equation**: $-\Delta u(x,y) = 0$ on $\Omega \subset R^2$ with $\Omega = [x_{min},x_{max}]\times[y_{min},y_{max}]$
- **Boundary condition**: $u(x,y)$ given on $\partial\Omega$
- **Discretization**: $-u_{i-1,j} - u_{i,j-1} + 4u_{i,j} - u_{i,j+1} - u_{i+1,j} = 0$ for $i=0\ldots m-1$, $j=0\ldots n-1$
- **4 Boundaries**: $i=-1$, $i=m$, $j=-1$, $j=m$
- **New ordering**: $(i,j)_{i=0..m-1,\ j=0..n-1}$ ➔ $I = 0..mn-1$
- **Matrix equation**: **Au = b**, **A**=sparse matrix, **b**=based on u on $\partial\Omega$, **u**=solution on $\Omega-\partial\Omega$
- **Example** with n=m=4, with solution & boundary **u(x,y) := x**
- **Linear Equation Solver (SLES) with PETSc**
  - MatSetValues(**A**, 1,&I, 1,&J, &v, INSERT_VALUES);
  - VecSetValues(**b**,1,&I,&v,INSERT_VALUES);
  - SLESSetOperators(sles,**A**,A,DIFFERENT_NONZERO_PATTERN);
  - SLESSolve(sles,**b**,**x**,&its); ➔ **x** is the solution vector, ordered with $I = 0..mn-1$
  - printing **x** in ordering $(i,j)_{i=0..m-1,\ j=0..n-1}$ (transposed)
- **mpirun** –np 3 ./heat_petsc –ksp_type cg –m 4 –n 4 –ksp_monitor –sles_view –view_sol –log_summary –options_table –options_left
- **Solved !!!**

Solution Grid (without boundary conditions):

y →, x ↓

0.199977	0.199891	0.199995	0.199985
0.400010	0.400072	0.400007	0.399864
0.600126	0.600078	0.599905	0.599989
0.800019	0.799936	0.799993	0.800014

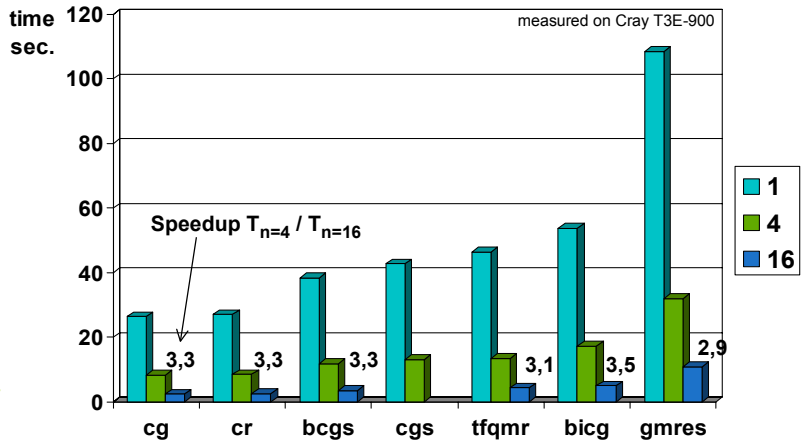
Norm of error 0.000269002 iterations 7

Practical

- **Test the heat_petsc example:**
  - cd ~/PETSC/#nr
  - mpirun –np 4 **./**heat_petsc
  - mpirun –np 4 **./**heat_petsc **–wrong_option –options_left**
  - mpirun –np 4 **./**heat_petsc **–ksp_monitor –view_mat_x –draw_pause 3** –op...
  - mpirun –np 4 **./**heat_petsc **–sles_view –view_sol –view_sol_x –draw_pause 3**
- **Which is default KSP? / Compare the execution time:**
  - mpirun –np 4 **./**heat_petsc **–m 300 –n 300** –log_summary –options_left
  - mpirun –np 4 **./**heat_petsc –m 300 –n 300 **–ksp_type cg** –log_summary –op...
  - mpirun –np 4 **./**heat_petsc –m 300 –n 300 **–ksp_type cr** –log_summary ...
  - mpirun –np 4 **./**heat_petsc –m 300 –n 300 **–ksp_type bcgs** –log_summary ...
- **Calculate Speedup of CG:**
  - mpirun **–np 1 ./**heat_petsc –m 300 –n 300 **–ksp_type cg** –log_summary ...
  - mpirun **–np 16 ./**heat_petsc –m 300 –n 300 **–ksp_type cg** –log_summary ...
- **If you want to compile:**
  - cp **../**source/heat_petsc.c **../**source/Makefile **./**
  - setenv PETSC_DIR ... or export PETSC_DIR=...
  - setenv PETSC_ARCH ... or export PETSC_ARCH=...
  - make BOPT=O heat_petsc

Results for heat_petsc (300x300) – time

for n = 1 PC is ilu
for n > 1 PC is bjacobi (sub=ilu)



Results for heat_petsc (300x300) – iterations

for n = 1 PC is ilu
for n > 1 PC is bjacobi (sub=ilu)