Hands-On I
The Heat Conduction Example – Overview

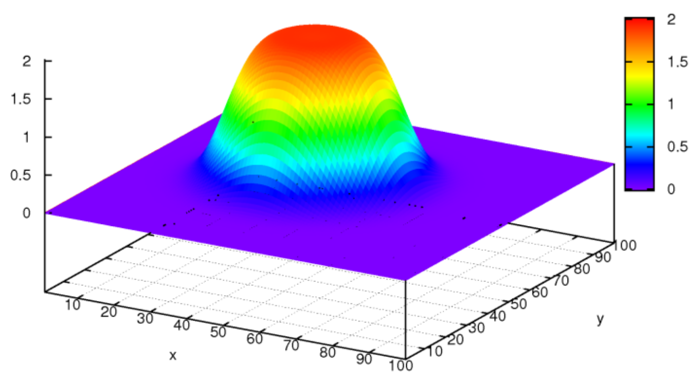
- Heat equation solver as debugging example
- Heat equation describes heat distribution in a region over time
- Equation (2D):

$$\frac{\partial u}{\partial t} = k\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

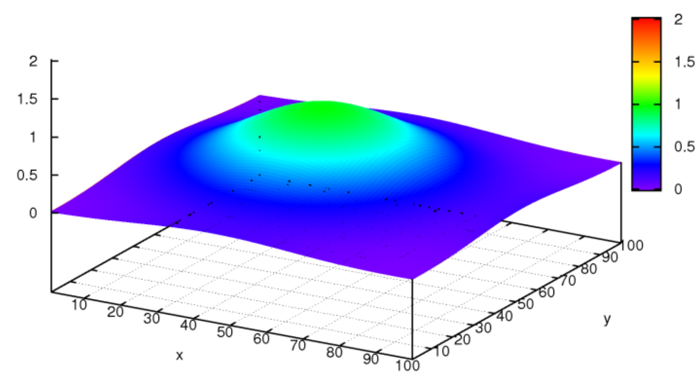
- Example implements solution on a 2D grid
- Time step for a grid cell (x,y):

$$\frac{\Delta u[x,y]}{\Delta t} = k\left(\frac{u[x-1,y]+u[x+1,y]-2u[x,y]}{\Delta x^2} + \frac{u[x,y-1]+u[x,y+1]-2u[x,y]}{\Delta y^2}\right)$$

- Visualization as 3D chart:



Time Steps

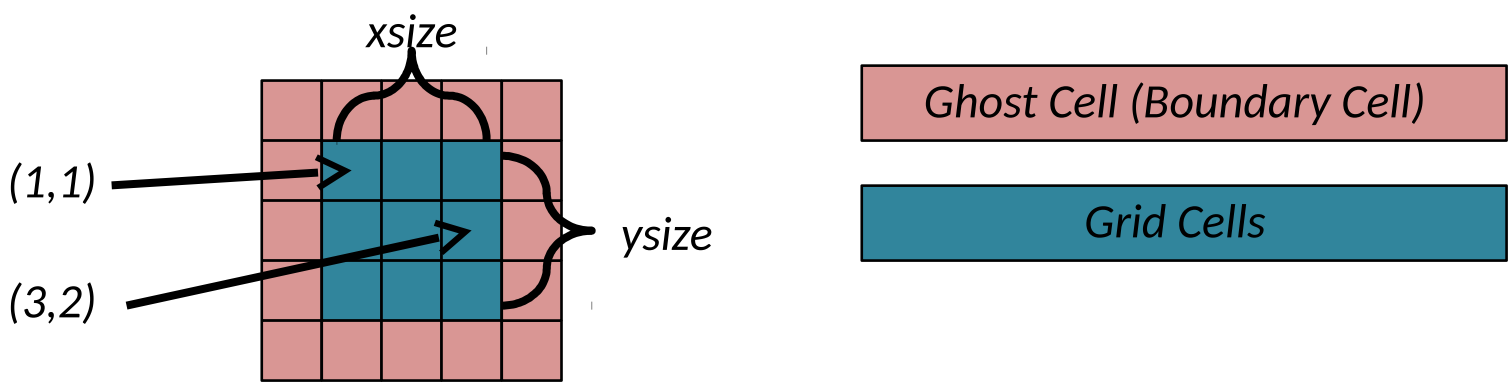


Hands-On I
The Heat Conduction Example – Source Code

- Available in C + Fortran90
- Parallel versions with MPI + OpenMP
- Key object is the structure for the 2D grid
- Functions:
  - heatAllocate & heatDeallocate – Creates/Frees the grid
  - heatInitialize & heatInitFunc – Sets the initial heat distribution
  - heatPrint – Prints the grid to stdout
  - heatTimestep – Calculates one timestep for the full grid
  - heatBoundary – Exchanges boundary data
  - heatTotalEnergy – Calculates overall energy amount
  - Main function – Contains main loop

Hands-On I
The Heat Conduction Example – 2D Grid

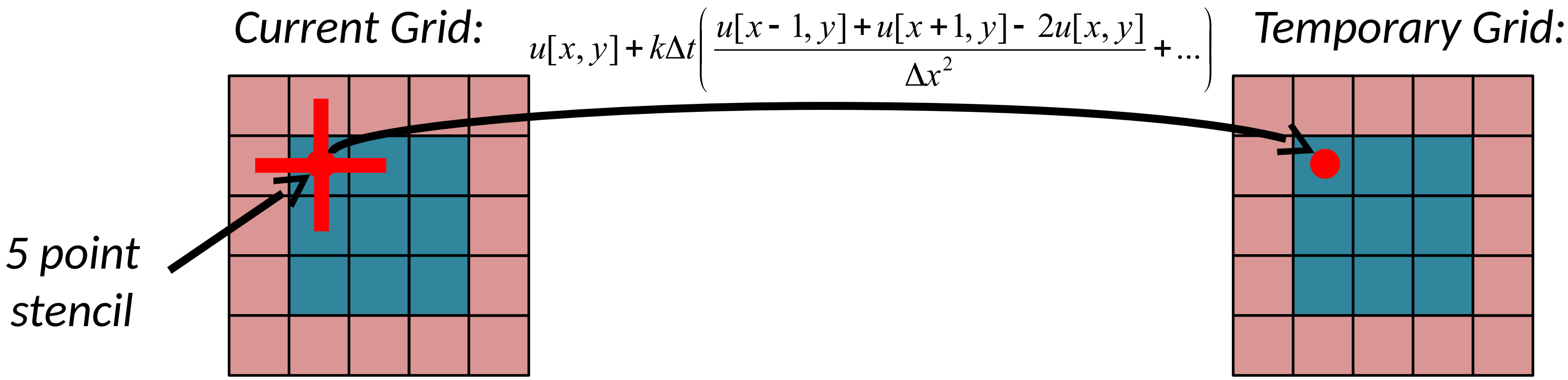
- Grid Structure contains 2 grids and the grid size
- Grid:



- Ghost cells used as neighbors, needed for border cells of actual grid

Hands-On I
The Heat Conduction Example – Time Steps

- Time steps are calculated for all actual grid cells, results stored in second grid:



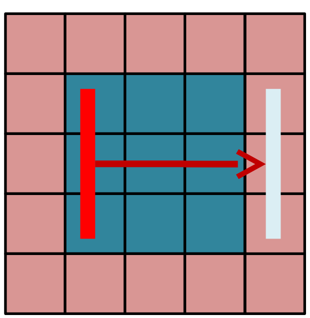
- Application switches grid after calculation for all grid cells

Hands-On I
The Heat Conduction Example – Boundary

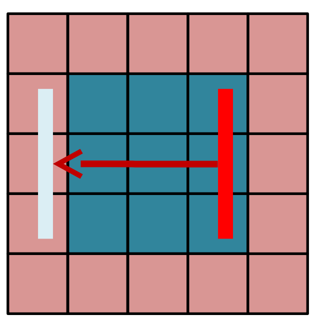
- 5 point stencil needs left, right, up, down neighbor for each grid point
- Ghost cells serve as neighbors
- Code uses periodic ghost cells
- After time step: copy operation to update ghost cells (=> “heatBoundary”)
- Update:

Grid:

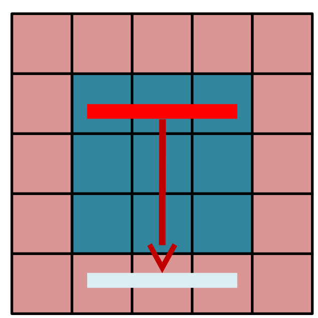
(1) Left border



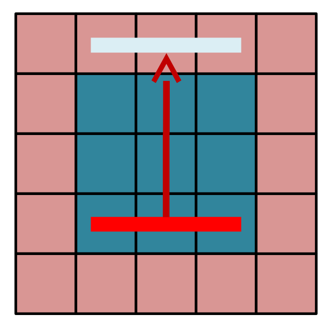
(2) Right border



(3) Top border



(4) Bottom border



Hands-On I
The Heat Conduction Example – Main Function

- Starts initialization
- Iterates time steps and boundary exchange (heatTimestep, heatBoundary)
- Uses 20 iterations
- Prints initial and final grid to standard output
- Calculates total energy at beginning and end (simple basic verification)

Hands-On I
The Heat Conduction Example – OpenMP Version

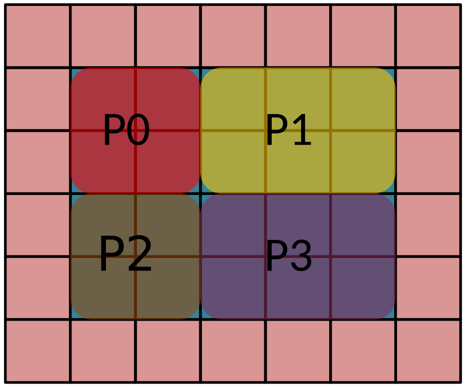
- Parallel for loop around the timestep function:

```
void heatTimestep(heatGrid* grid, double dt, double* dthetamax)
{
...
#pragma omp parallel  private(dtheta, x, y)
  {
#pragma omp for
      for (x=1; x <= grid->xsize;x++)
      {
        for (y=1; y <= grid->ysize; y++)
        {
          dtheta =...;
          grid->thetanew[x][y] = ...;
        }
      }
```

- Each thread covers part of the 2D grid

Hands-On I
The Heat Conduction Example – MPI Version

- Each process has a copy of both grids
- Initialization and set-up done by all processes
- Each process calculates on a part of the overall grid:

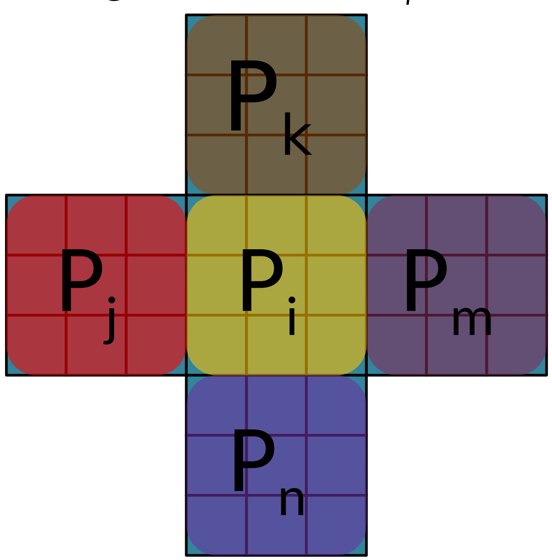


- Exchange with neighbors uses 2D Cartesian communicator
- Communications of a data columns uses a derived datatype
- Consequences:
  - New border exchange
  - Gathering of data necessary for output

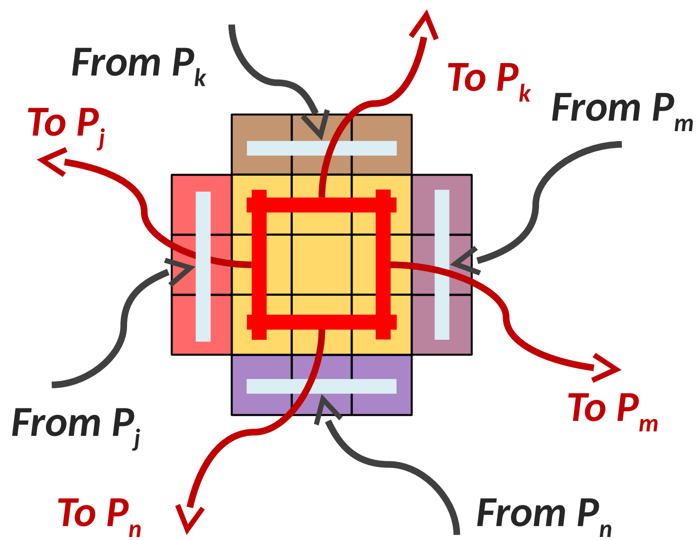
Hands-On I
The Heat Conduction Example – MPI Boundary

- MPI processes exchange borders with neighbors
- Cartesian grid provides up, down, left, right neighbors
- Periodic boundaries => grid is a donut
- Boundary exchange for process “P_i”:

Neighborhood of P_i



Exchange for P_i



Hands-On I
The Heat Conduction Example – MPI Gather

- Data distributed between processes
- Printing requires I/O or gathering data on one process
- Implementation gathers data on process 0: