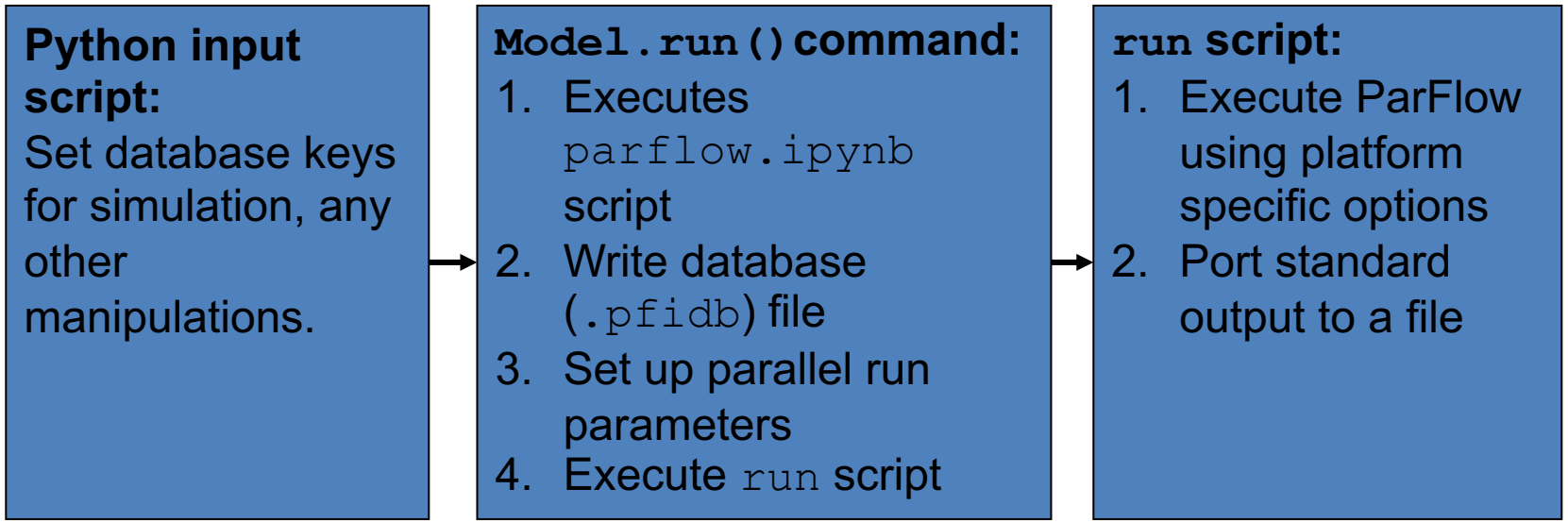
Overview: Interacting with ParFlow

ParFlow Short Course

1. *How do I tell it what I want it to do?*
2. *How do I get my inputs into the model?*
3. *How do I press go?*
4. *What comes out and how do I look at it?*

1. Model input file:
(How you tell ParFlow what to do)



Input Scripts

- TCL/TK scripting language with python interface
- All parameters input as keys using `pfset` command (tcl) or `model.”key_name”` (python)
- Keys used to build a database that ParFlow uses
- ParFlow executed by `pfrun` command (for tcl) and `model.run()` for python
- Since input file is a script may be run like a program

Example: Setting up the input grid

```
#---------------------------------------------------------
# Computational Grid
#---------------------------------------------------------
#Locate the origin in the domain.
model.ComputationalGrid.Lower.X = 0.0
model.ComputationalGrid.Lower.Y = 0.0
model.ComputationalGrid.Lower.Z = 0.0

# Define the size of each grid cell. The length units are
the same as those on hydraulic conductivity, here that is
meters.
model.ComputationalGrid.DX = 1000.0
model.ComputationalGrid.DY = 1000.0
model.ComputationalGrid.DZ = 200.0

# Define the number of grid blocks in the domain.
model.ComputationalGrid.NX = 64
model.ComputationalGrid.NY = 32
model.ComputationalGrid.NZ = 10
```

Coordinates (length units)

Cell size (length units)

Grid dimensions (integer)

Example: Setting up the timing

```
#-----------------------------------------------------------
# Setup timing info
#-----------------------------------------------------------

model.TimingInfo.BaseUnit = 1.0

model.TimingInfo.StartCount = 0

model.TimingInfo.StartTime = 0
model.TimingInfo.StopTime = 72.0

model.TimingInfo.DumpInterval = 1.0

model.TimeStep.Type = "Constant"

model.TimeStep.Value = 1.0
```

Sets time units for time cycles (T)

Initial output file number

Start and finish time for simulation (T)

Interval to write output (T)
-1 outputs at every timestep

Timestep type

ΔT (T)

Best practices for building an input file:

- Start from an existing script:
  - Look at the annotated input scripts in the manual
  - Look at the test problems that come with ParFlow (See list in section 3.5)
  - Use scripts for test problems presented in this course
- Get the details on every input key from the manual (Section 6)

2. Reading gridded files
(How you get your inputs into ParFlow)

- Some keys allow you to specify a file as your input. Like this:

```
model.GeomInput.indi_input.InputType = "IndicatorField"
model.GeomInput.indi_input.GeomNames = "s1 s2 s3 g1 g2 g3"
model.Geom.indi_input.FileName = "Indicator_LW_USGS_Bedrock.pfb"
```

- After getting correct gridded inputs you will need to convert to PFB before they can be read into the model

ParFlow File Types

- PFB: **P**ar**F**low **B**inary. ParFlow's native file type, can be written, read into ParFlow, read into and written by PFTools.
- SILO. VisIt's native file type, can be written by ParFlow, read into and written by PFTools

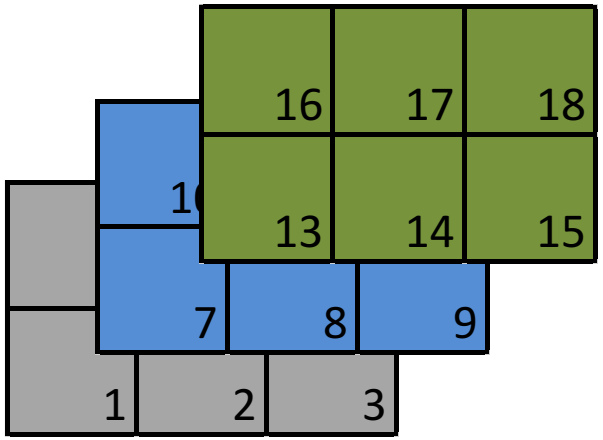
Getting from raster files to ParFlow

Start with a raster which will be formatted as a matrix and convert to a vector in the correct ParFlow order with the grid dimensions at the top

9	10	11	12
5	6	7	8
1	2	3	4

4 3 1
1
2
3
4
5
6
7
8
9
10
11
12

3D ParFlow Inputs



3 2 3
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18

Getting from raster files to ParFlow

- Refer to *Manual 6.37* for details on conversion with NetCDF4
- Start in the lower left corner of the bottom layer and work your way to the upper right corner of the top layer looping over x, y and z in that order
- Header is nx ny nz

```
<integer : NX> <integer : NY> <integer : NZ>
FOR k=0 TO  <nz>-1
BEGIN
    FOR j=0  TO   <ny>-1
    BEGIN
        FOR i= 0 TO  <nx>-1
        BEGIN
            <double : data_ijk>
        END
    END
END
```

Getting from raster files to ParFlow

- If you generate your ParFLow inputs as text files you will need to convert to PFB before they can be read into the model

- You can do this using PFTools. For example:

```
set       input          [pfload -sa input.sa]
pfsetgrid {nz ny nz} {x0 y0 z0} {dx dy dz} $input
pfsave $input -silo input.silo
pfsave $input -pfb  input.pfb
```

Getting from nparray to pfb

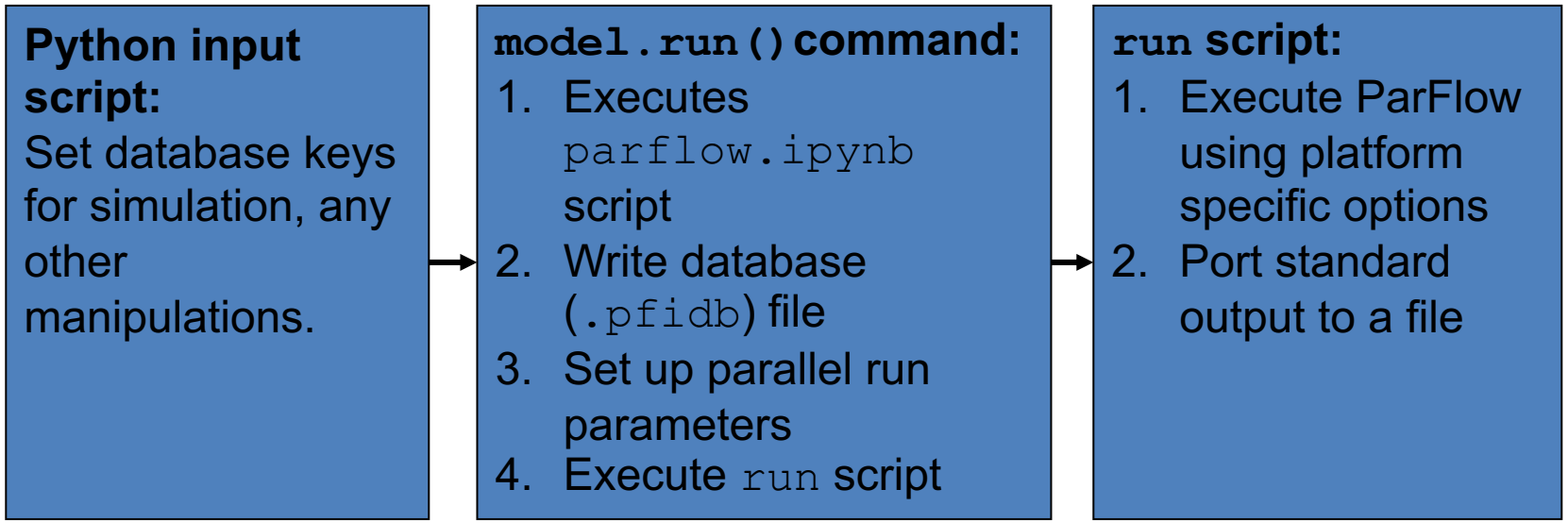
- Refer to *Manual 9.3.3* for details
- This creates a 3D numpy array that covers the entire domain and changes the values of X = 9 to 0.001.
  - Note numpy array translation to PFB reads dimensions as (Z, Y, X).
- write_pfb(get_absolute_path('Flow_Barrier_X.pfb'), FBx_data) writes the data from the FBx_data numpy array to a file called 'Flow_Barrier_X.pfb'

```
from parflow import Run
from parflow.tools.fs import get_absolute_path
from parflow.tools.io import write_pfb, read_pfb
import numpy as np

# Create numpy array
FBx_data = np.ones((20, 20, 20))

# Reduction of 1E-3
 FBx_data[:, :, 9] = 0.001

# Write flow boundary file as PFB with write_pfb() function
write_pfb(get_absolute_path('Flow_Barrier_X.pfb'), FBx_data)
```

PFTools Commands (Manual 7.1)

- Many commands load and write files
- `pf.read_pfb()` reads files that are parflow binary, simple binary and ascii
- `pf.write_pfb()` writes files that are parflow binary, simple binary and ascii
- One a dataset is loaded (from a file) it may be manipulated with many different tools commands (e.g. convert pressure head to head potential)

3. Running ParFlow simulations (*How to press go*)



Running ParFlow

- `model.run()` command
  - Builds database of keys
  - Executes program
- Some error checking of keys
- Actual command line runs executable or mpirun's executable
- May run parflow code more than once in single script
- Need parflow package/header information

Running ParFlow (input file)

Mandatory Content at the top of your python script:

```
# Import required packages

import os
import numpy as np
from parflow import Run
import shutil from parflow.tools.fs
import mkdir, cp, get_absolute_path, exists from
parflow.tools.settings
import set_working_directory
…
model.run()
```

Load the recommended packages to run parflow in python

Run parflow, execute run command on model object

To run the model:

model.run()

Parallelization: splitting your problem up across multiple processors

- Domain parallelized by specifying number of processor divisions in x,y,z
- Parallelization done on computational domain
- Done using P,Q,R values
  - Total processors=P*Q*R
  - Domain divided by nx/P, ny/Q, nz/R
- Load balancing issues
- Usually keep R as 1 and split in the x and y directions only

Parallelization (input file)

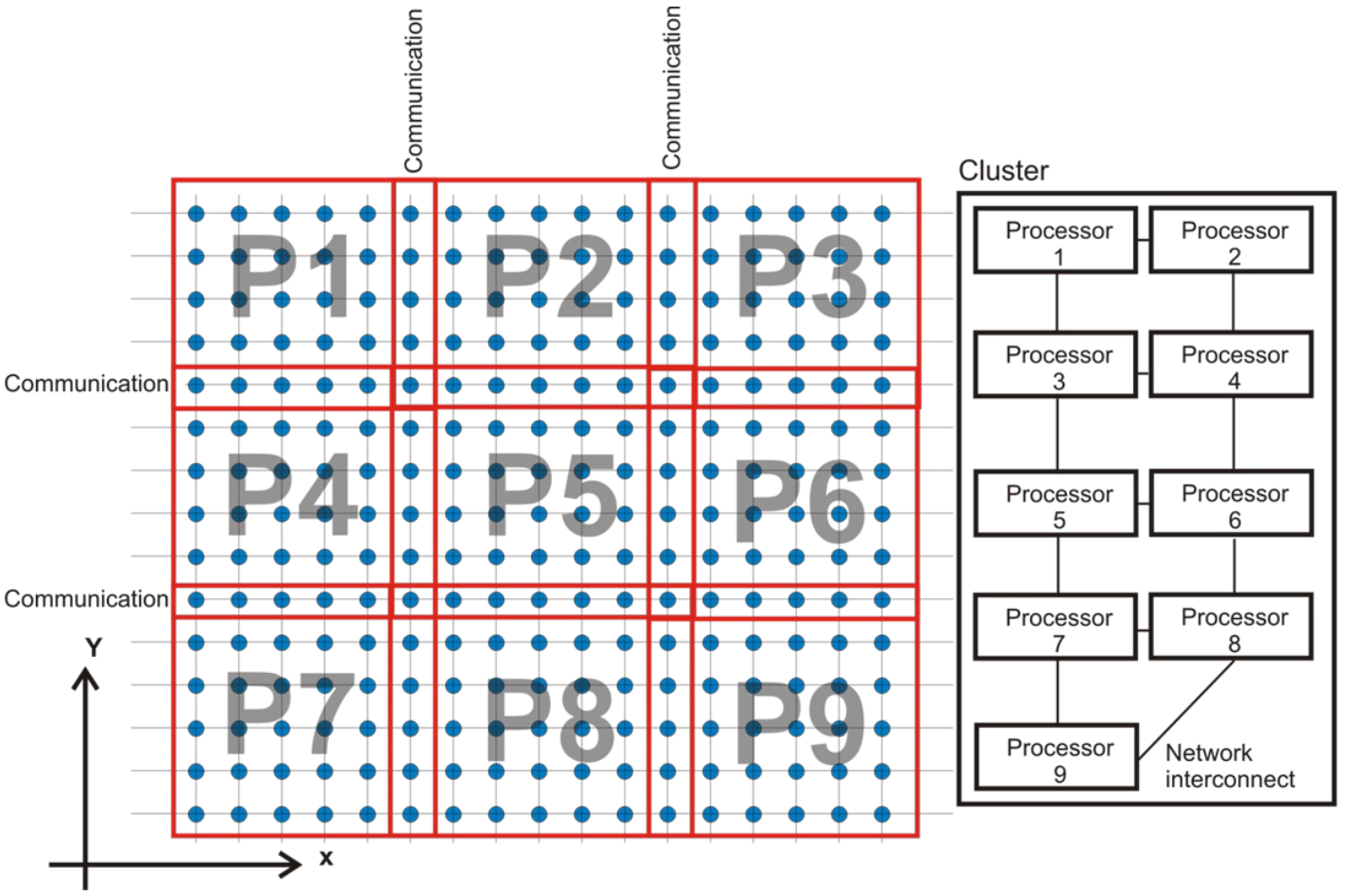
```
model.Process.Topology.P = 1
model.Process.Topology.Q = 1
model.Process.Topology.R = 1
```

Single processor simulation,
P,Q,R are integer values

```
model.Process.Topology.P = 4
model.Process.Topology.Q = 2
model.Process.Topology.R = 1
```

Eight processor simulation,
P*Q*R=4*2*1=8

Domain decomposition



- Lateral transport processes
- Inter-processor communication required
- “Perfect” parallel scaling can not be obtained
- I/O and load balance still constitute bottlenecks

Distributing Files (8.3/9.3.2)

- ParFlow reads and writes parallel files
- One portion of the file per processor (except for sequential/shared memory build)
- ParFlow binary files (.pfb) must be distributed (split up) before being read in
- ParFlow binary files (.pfb) must be undistributed at the end of the simulation
- Two tools to do this, `model.dist()` and `pfundist`, may be run directly in the python input script.

File Parallelism

- ParFlow has several options for parallel io
  - PFB may be distributed as *n* files or as a single file with companion file (.dist)
  - SILO has two options, PMPIO where *n* processors write to *m* files and regular where *n* files are written
- The best file type depends upon application

Distributing Files (input file)

```
model.dist("my.input.file.pfb")
```

Distribute an input file
Must have specified processor topology, can happen anywhere in script before model.run() command

```
pfundist default_over

pfundist my.input.file.pfb
```

First line undistributes an entire run

Second line undistributes a particular file

*** You can dist and undist files using separate scripts outside your main model run or you can do it all in one step**

4. Handling outputs
(*What comes out and how to look at it*)

Running ParFlow (file structure)

- Project name is the base for all output
- Most output is *project*.out.*var*.*time*.ext

For a project called ‘myrun’

Log files:

```
myrun.out.log
myrun.out.kinsol.log
```

Pressure/Saturation files:

```
myrun.out.press.00001.pfb
myrun.out.satur.00001.pfb
```

Output time step, 00000 is initial, integer values depending on output times

Mask file:

```
myrun.out.mask.00000.pfb
```

The mask is a file of zero’s and ones, 0=inactive cell, 1=active cell

Perm/porosity files:

```
myrun.out.perm_x.pfb
myrun.out.porosity.pfb
```

Other/diagnostic files:

```
myrun.pfidb
```
Parflow database

```
myrun.out.pftcl
myrun.out.txt
```
Line output

Visualizing Outputs

ParaView:

- Free, developed by Kitware Inc
- https://paraview.org
- VTK and pfb formats supported

Visit:

- Free, developed at LLNL
- (http://www.llnl.gov/visit/)
- VTK and SILO format, which has many options within ParFlow (converting or IO), fully-supported

PFTools

- TCL keys that you can use to manipulate ParFLow inputs and outputs:
  - Extract parts of your domain to look at
  - Calculate water balance components (hydrology module)
  - Convert pfb outputs to other file types

Example: adding Solid File geometry

```
#---------------------------------------------------------
# Geometries (Solid File Geometry)
#---------------------------------------------------------
#Declare the geometries that you will use for the problem
model.GeomInput.Names = "solid_input indi_input"

#Define the solid_input geometry.
#Note the naming convention here GeomInput.{GeomName}.key
model.GeomInput.solid_input.InputType = "SolidFile"
model.GeomInput.solid_input.GeomNames = "domain"
model.GeomInput.solid_input.FileName = "LW.pfsol"

#First set the name for your `Domain` and setup the patches
for this domain model.Domain.GeomName = "domain"
model.Geom.domain.Patches = "top bottom side"
```