Using R on HPC Clusters Part 1

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Oak Ridge National Laboratory

August 17, 2022

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Get this presentation:

```
git clone https://github.com/RBigData/R4HPC.git
```

- Open

  ```
  R4HPC_Part1.html
  ```

  in your web browser
- Navigation help is the question mark: ?

Many thanks to my colleagues and former colleagues who contributed to the software and ideas presented here and who are listed in the RBigData Organization on Github: https://github.com/RBigData. Also, many thanks to all R developers of packages used in this presentation.

Any errors are mine alone.

Using R on HPC Clusters Webinar

- A basic workflow for how to use R on an HPC cluster
- Speed up R scripts with parallel computing concepts
- Many packages in R offer parallel computing abstractions, yet they use a much smaller set of underlying approaches:
  - multithreading in compiled code, the unix fork, and MPI
- We take a narrow path to focus on the direct approaches
- Targeted for current users of OLCF, CADES, ALCF and NERSC
- Others are welcome to the lecture portions but will not be able to participate in all of the hands-on activities

Objectives

- Learn a workflow to edit R code on your laptop and run it on an HPC cluster

- Learn how to use multicore and distributed parallel concepts in R on an HPC cluster system

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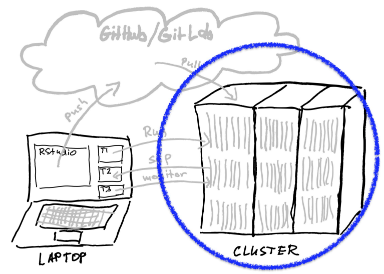


The Clusters

ORNL OLCF Andes

- 704 nodes, each with two 16-core 3.0 GHz AMD EPYC processors

ORNL CADES SHPC Condos

- ~650 nodes, a mix of x86_64 processors with 32 to 128 cores
- New LMOD software stack (see https://docs.cades.ornl.gov/#condos/software/bash-env/#new-software-stack)

LBL NERSC Cori

- 9,688 nodes, each an Intel Xeon Phi with 64 cores
- 2,388 nodes, Intel Xeon "Haswell" processor with 32 cores

ANL ACLF Theta KNL- Intel-Cray XC40

- 4,392 nodes, each with a 64-core, 1.3-GHz Intel Xeon Phi 7230

Access to HPC Clusters

- DOE OLCF https://docs.olcf.ornl.gov/accounts/accounts_and_projects.html
- DOE ORNL CADES https://cades.ornl.gov/
- DOE ALCF https://www.alcf.anl.gov/support-center/account-and-project-management/allocations
- DOE NERSC https://www.nersc.gov/users/accounts/allocations/
- NSF XSEDE to ACCESS https://www.xsede.org/
- EU PRACE https://prace-ri.eu/hpc-access/ (for example IT4I.cz https://www.it4i.cz/en/for-users/computing-resources-allocation)
- Institutional Clusters

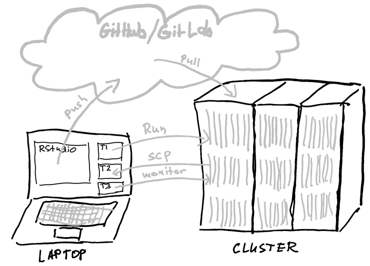
Section I: Environment and Workflow

Section II: Parallel Hardware and Software Overview

Section III: Shared Memory Tools

Section IV: Distributed Memory Tools

Working with a remote cluster using R



Laptop RStudio (Posit in October, 2022)

- Familiar custom editing environment (Windows, Mac, Unix)
- Interactive Syntax checking

GitHub/GitLab

- Portability to remote computing
- Version control
- Collaboration

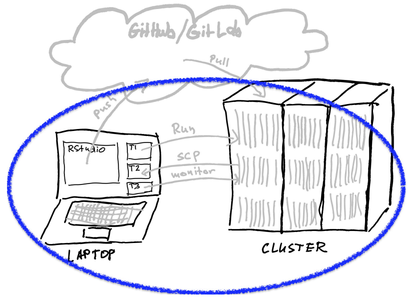
Cluster unix

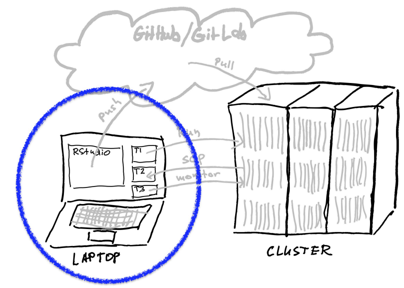
- Same environment for all
- Batch job submission

Advanced: interactive multinode development and debugging

- Available now (packages: launchr, pbdCS, pbdRPC, remoter)

Running Distributed on a Cluster

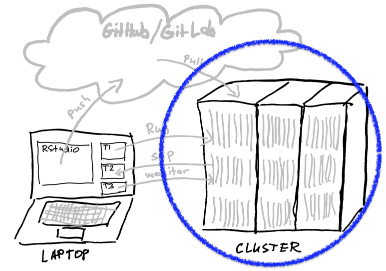




Software Needed on Laptop

- Mac
  - R, RStudio
  - terminal, git (in Xcode)
- Windows
  - R, RStudio
  - putty
  - git
  - WinSCP

Software on Cluster

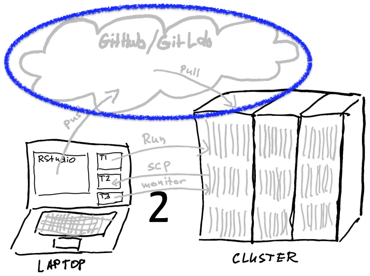


- OpenBLAS
- FlexiBLAS
- OpenMPI
- HDF5 (for parallel I/O)
- R (>= 4.0)

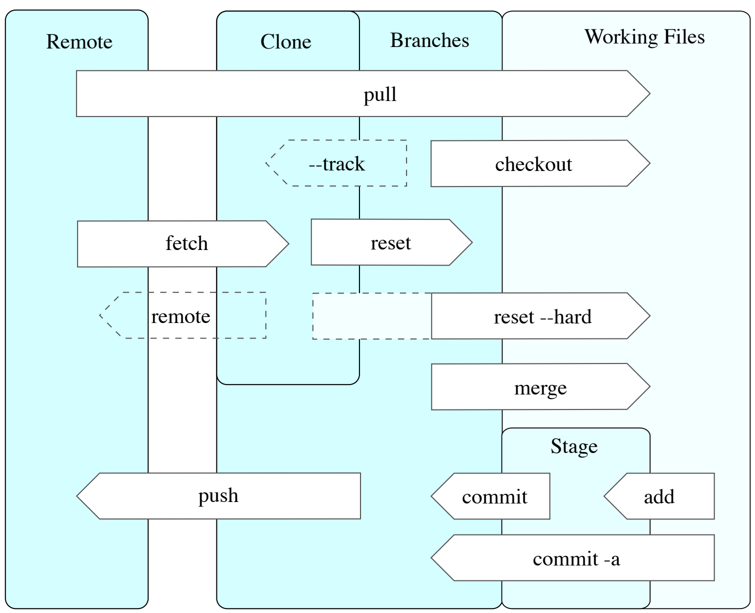
Packages:
Day 1: `flexiblas`, `remotes`, `RBigData/pbdMPI`, `randomForest`, `mlbench`
Day 2: `RBigData/kazaam`, `RBigData/pbdDMAT`

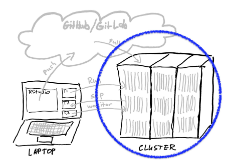
R vs conda-R Deployment

- Direct R is preferred
- CRAN and Anaconda differ in package management philosophy
- Can end up with conflicts if mixing
- Conda adds a layer of complexity
- If already used to Conda, you may find it useful



GitHub and git (laptop to cluster)





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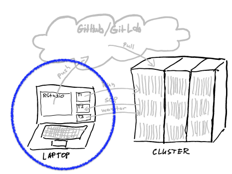

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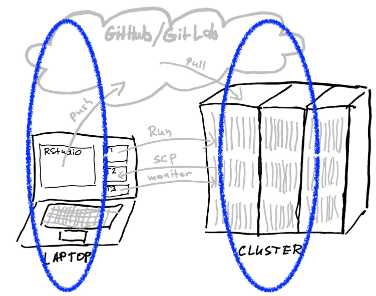
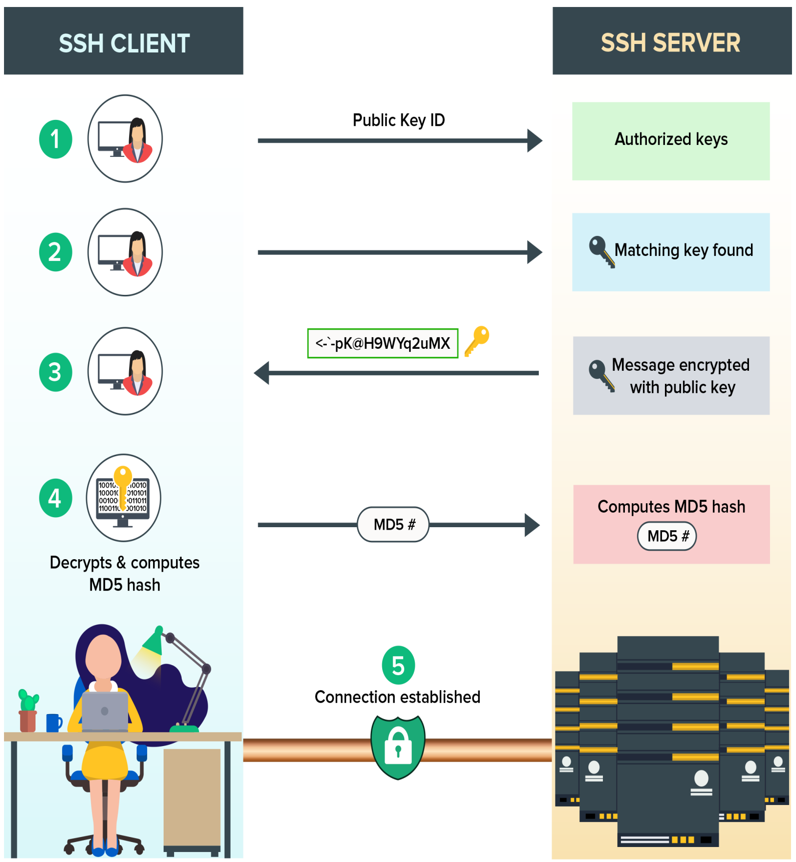


Making git easy: set ssh keys



A message encrypted by public key is decrypted by private key

Works like a single-use password generator and authenticator

Your private keys are protected in your account (laptop and cluster)

Put your public key on GitHub to enable easy access

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Graphic from https://www.manageengine.com/key-manager/information-center/what-is-ssh-key-management.html

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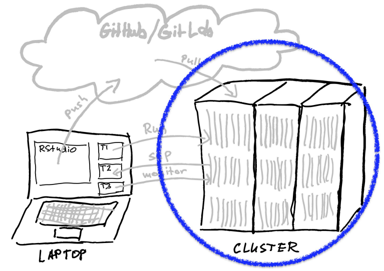

Clusters are Linux systems

- Linux is one of many descendants of original Unix. MacOS is another.
- Like all file systems, Linux files are organized as a tree.
- When in a terminal, you are talking to a *shell* program (*bash* is most common)
  - Each command can have a list of *options* and a list of *arguments*
  - *Standard input* and *standard output* of a command is the terminal but can be redirected
  - <, <<, >, >> redirect standard input and output
  - *command1* | *command2* pipes standard output1 to standard input2
  - Commands are looked up in directories listed in your PATH variable (try "echo $PATH")
  - $ means substitute variable value
  - *export* lists (or sets) shell variables and their values
- There are many resources on the web to learn Linux basics

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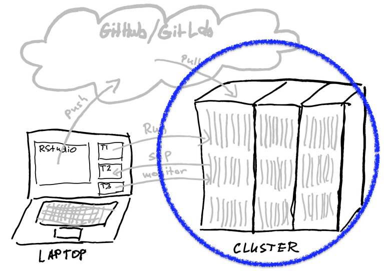

Job Submission on Cluster

- Command line submission
- Shell script submission (preferred)

Slurm (Andes, CADES,)

sbatch *your-shell-script.sh*

squeue -u *uid*

scancel *jobnumber*

PBS (Theta,)

qsub *your-shell-script.sh*

qstat -u *uid*

qdel *jobname*

- **module** to set software environment (PATH)
  - *module list* - list what is loaded
  - *module avail* - list what is available
  - *module load r*

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Hands-on Session 1 - Fork and clone your R4HPC

- Fork R4HPC to your GitHub account
  - Login to GitHub
  - Navigate to RBigData/R4HPC repository
  - Click Fork button near top-right
  - Copy forked repo green Code url
- Clone to New Project in RStudio
- Open Terminal window (ssh or putty)
- Login to cluster
- clone your R4HPC (git clone ...)
- You are ready for the development loop:
  - edit -> commit -> push -> pull -> run -> examine output

Hands-on Session 1 - On Login Node

- Go to `R4HPC/code_1` directory
- `cat hello_MACHINE_slurm.sh` to see what modules to load and do so
- Start R and install needed packages:
  - `install.pacages("remotes")`
  - `install.packages("flexiblas")`
  - `remotes::install_github("RBigData/pbdMPI")`
- Submit the hello_MACHINE_slurm.sh
- Examine output in `hello.e` and `hello.o` and notice that:
  - 4 nodes are involved
  - 4 R sessions were running on each node
  - Each R session ran `mclapply` on several cores
  - All `mclapply` process id's are reported
  - The code figured out how many cores in total
  - Only one R session wrote the output

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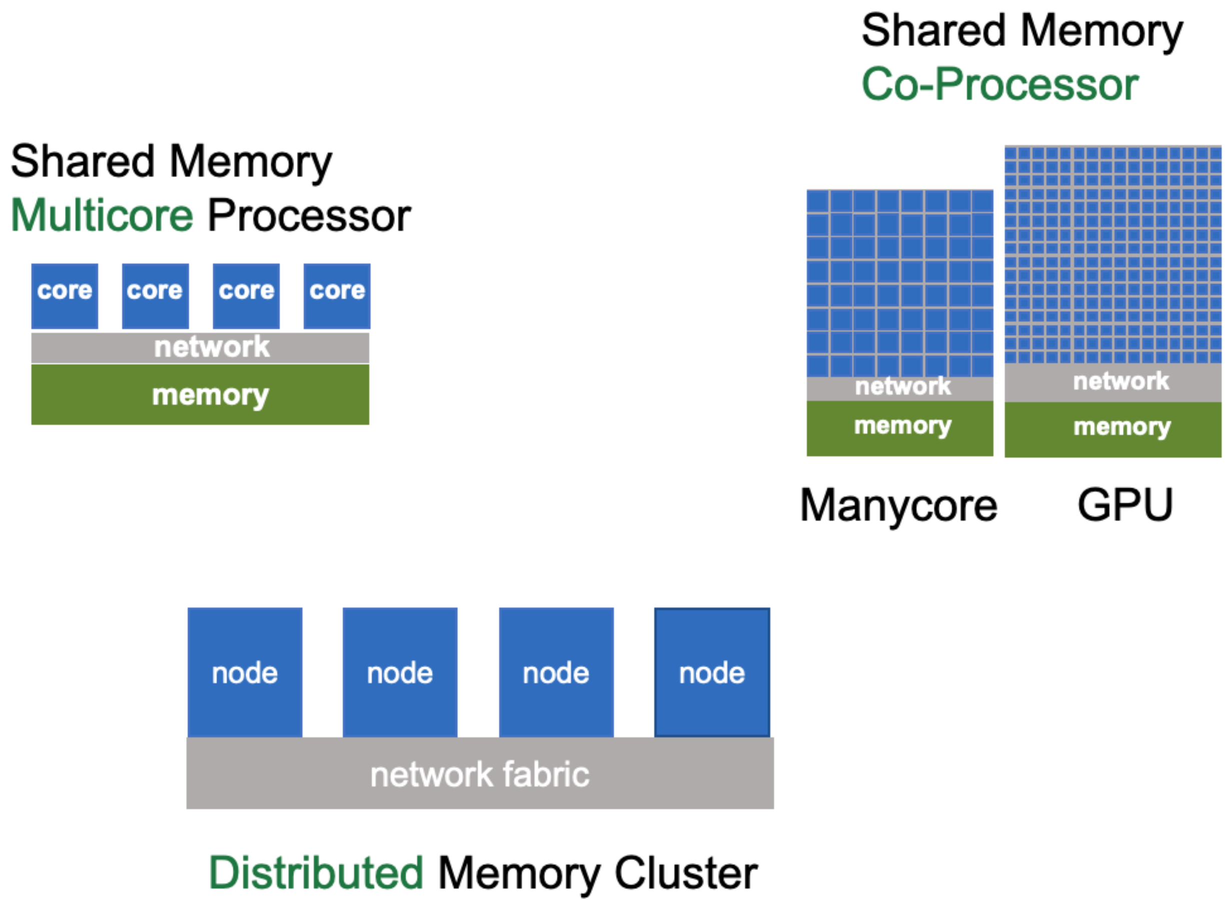
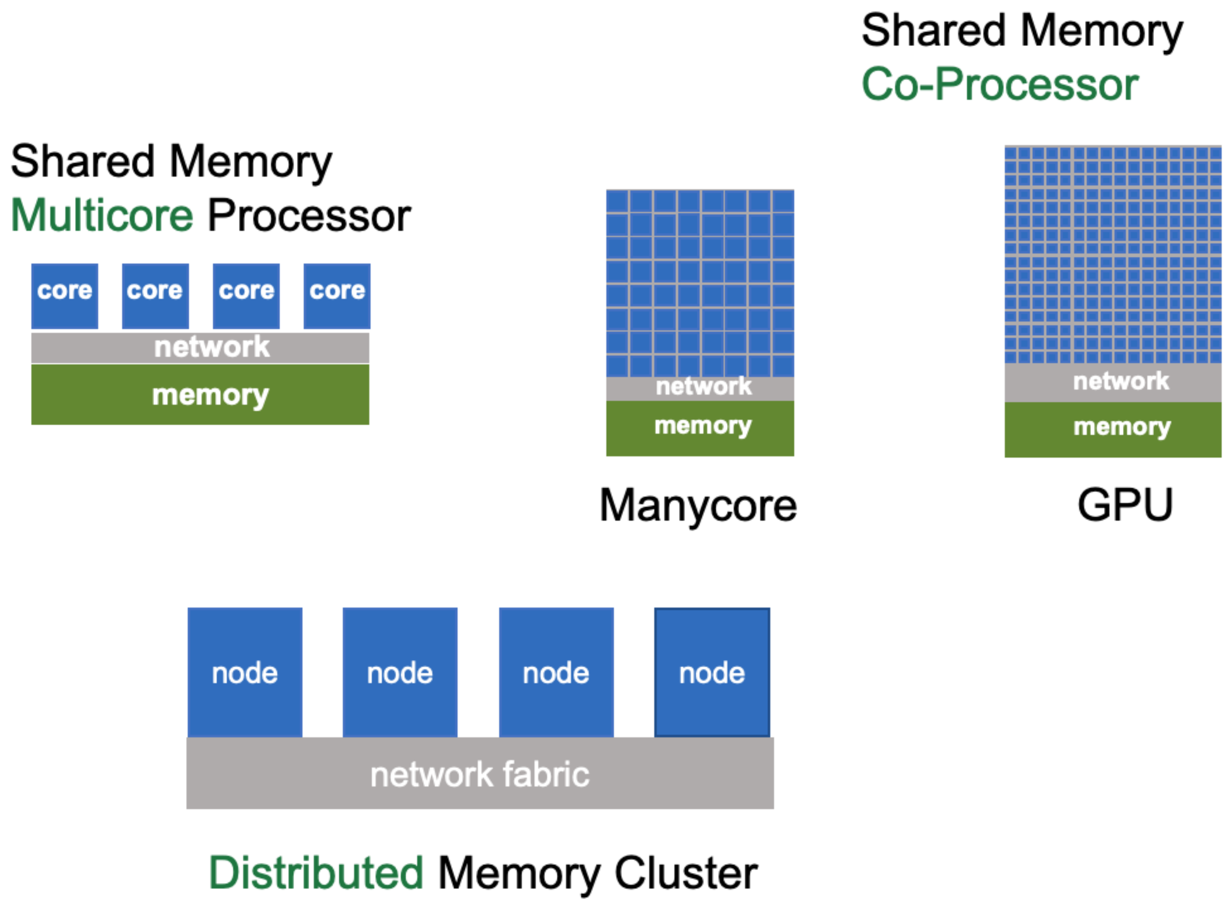
Section II:

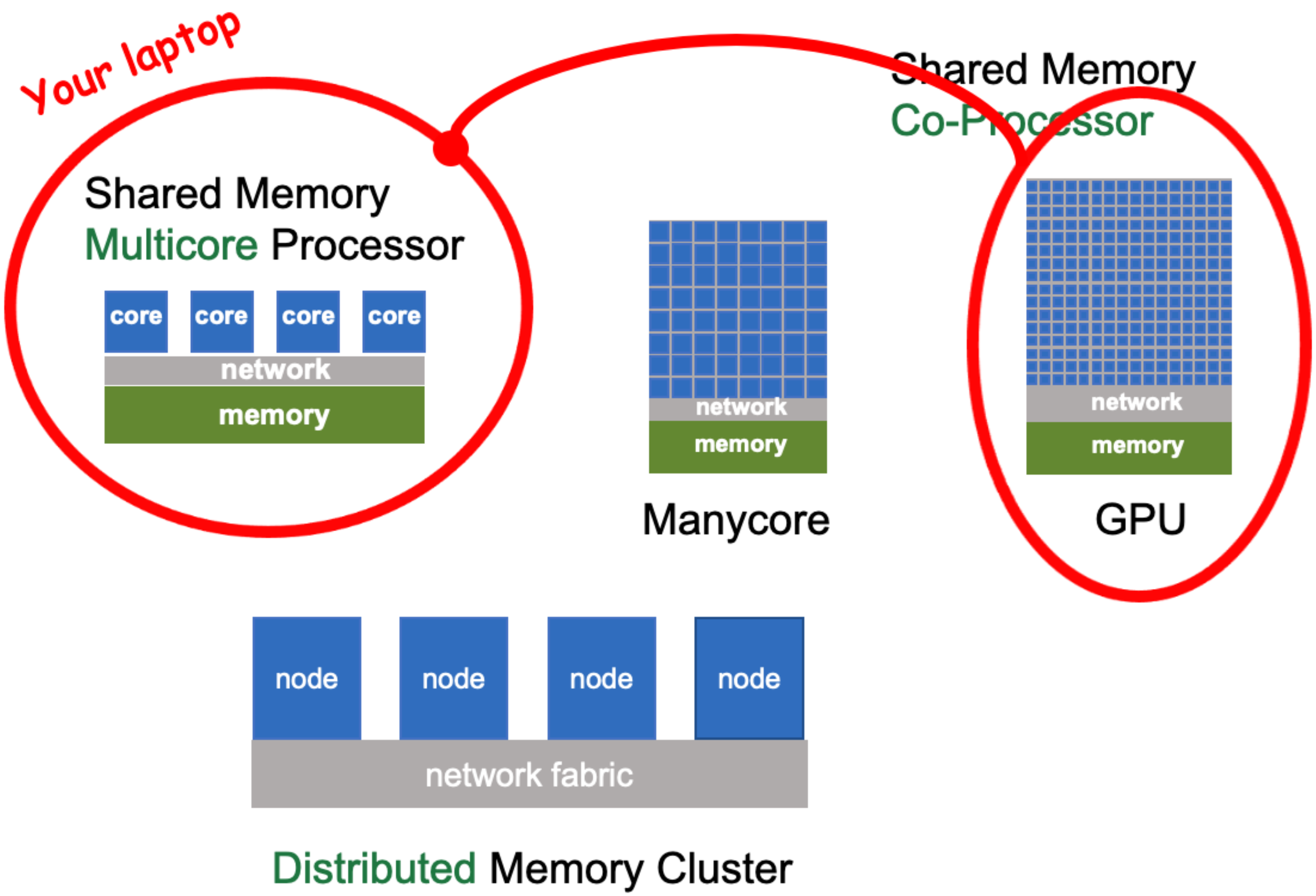
Parallel Hardware

Three Basic Concepts in Hardware



Three Basic Concepts in Hardware





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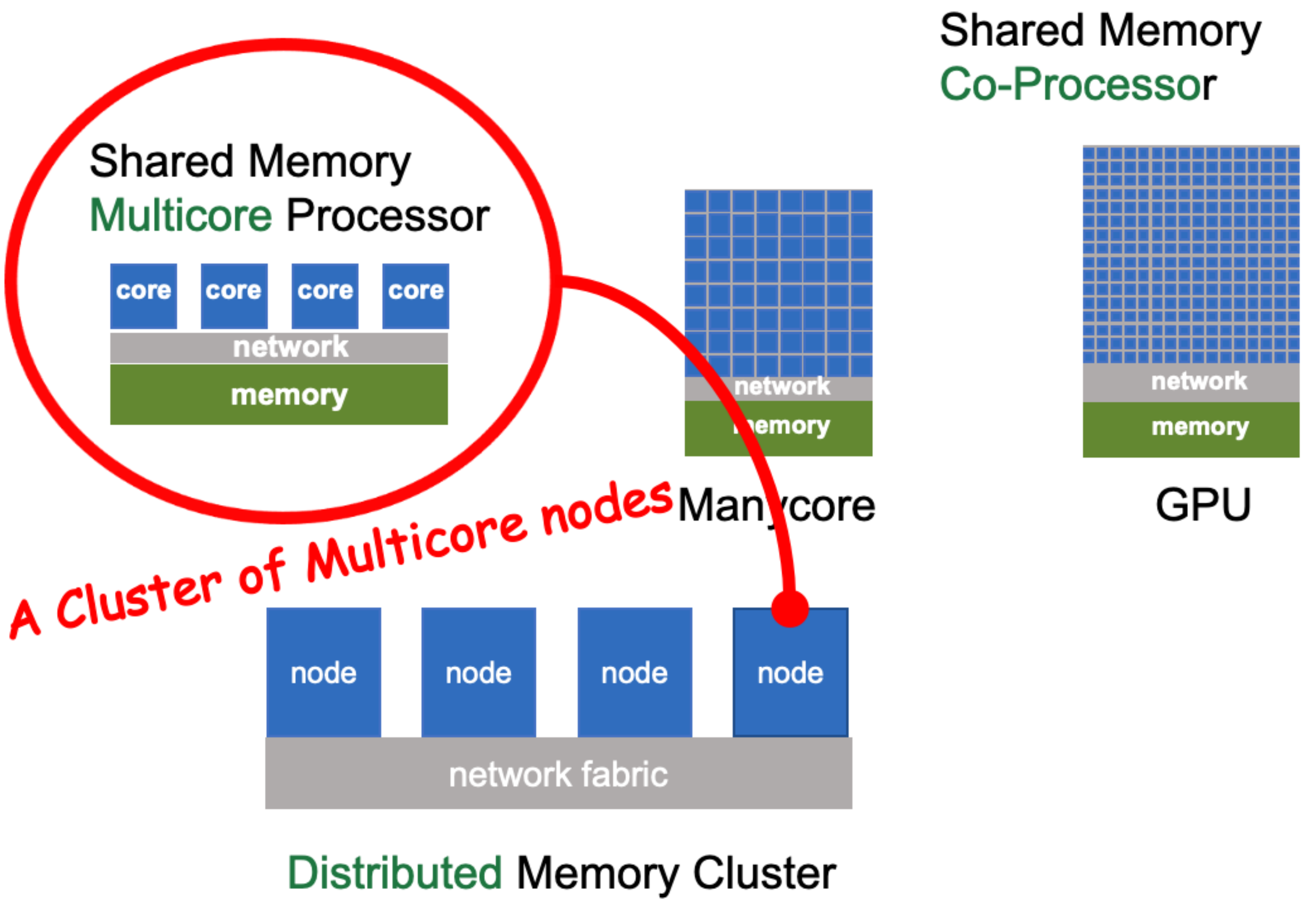
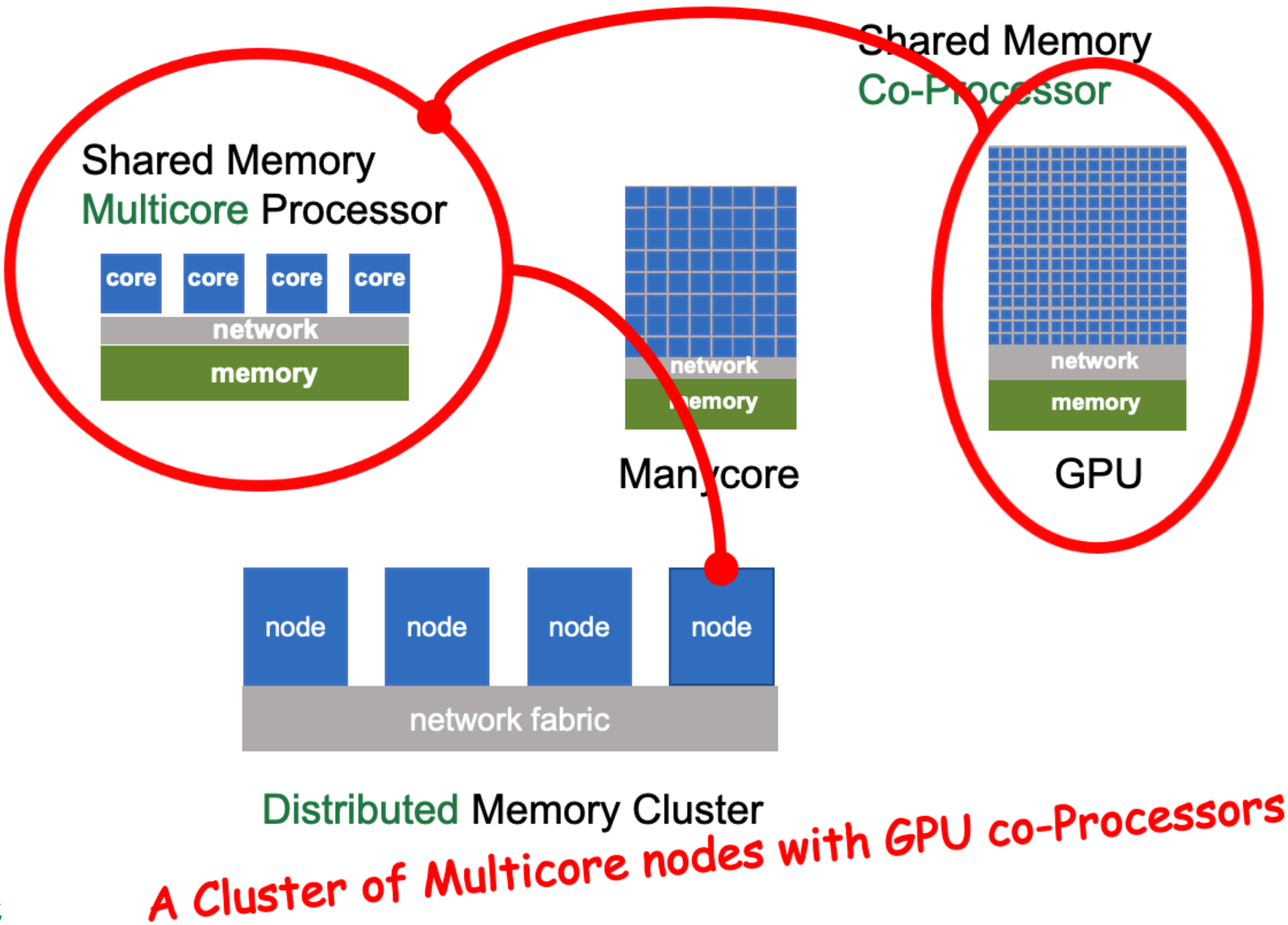

Shared Memory
Co-Processor
Shared Memory
Multicore Processor
core
core
core
core
network
memory
network
memory
Manycore
network
memory
GPU
A Cluster of Multicore nodes
node
node
node
node
network fabric
Distributed Memory Cluster



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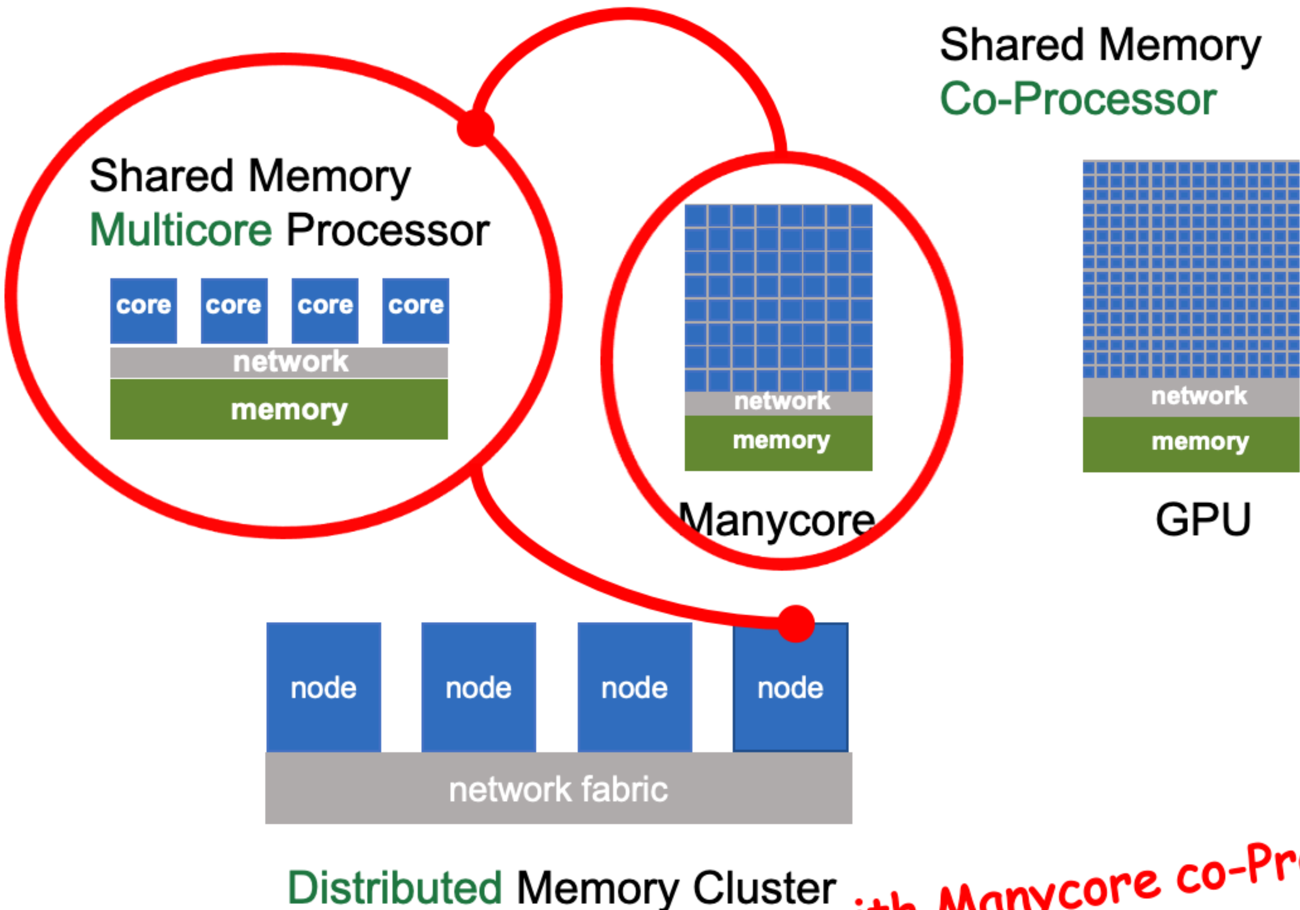

A Cluster of Multicore nodes with Manycore co-Processors

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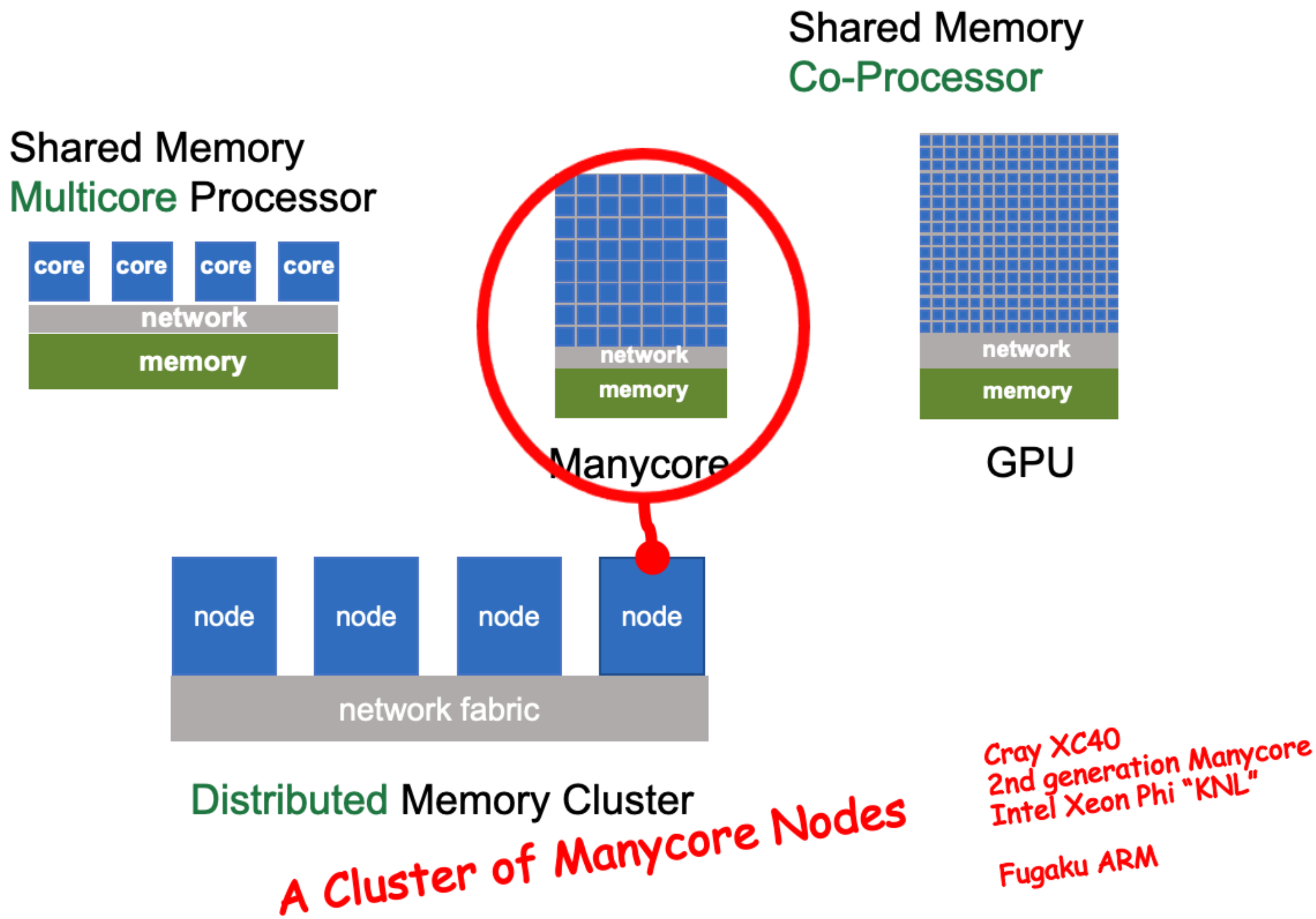
Shared Memory
Co-Processor
Shared Memory
Multicore Processor
core
core
core
core
network
memory
network
memory
Manycore
network
memory
GPU
node
node
node
node
network fabric
Distributed Memory Cluster
A Cluster of Manycore Nodes
Cray XC40
2nd generation Manycore
Intel Xeon Phi "KNL"
Fugaku ARM

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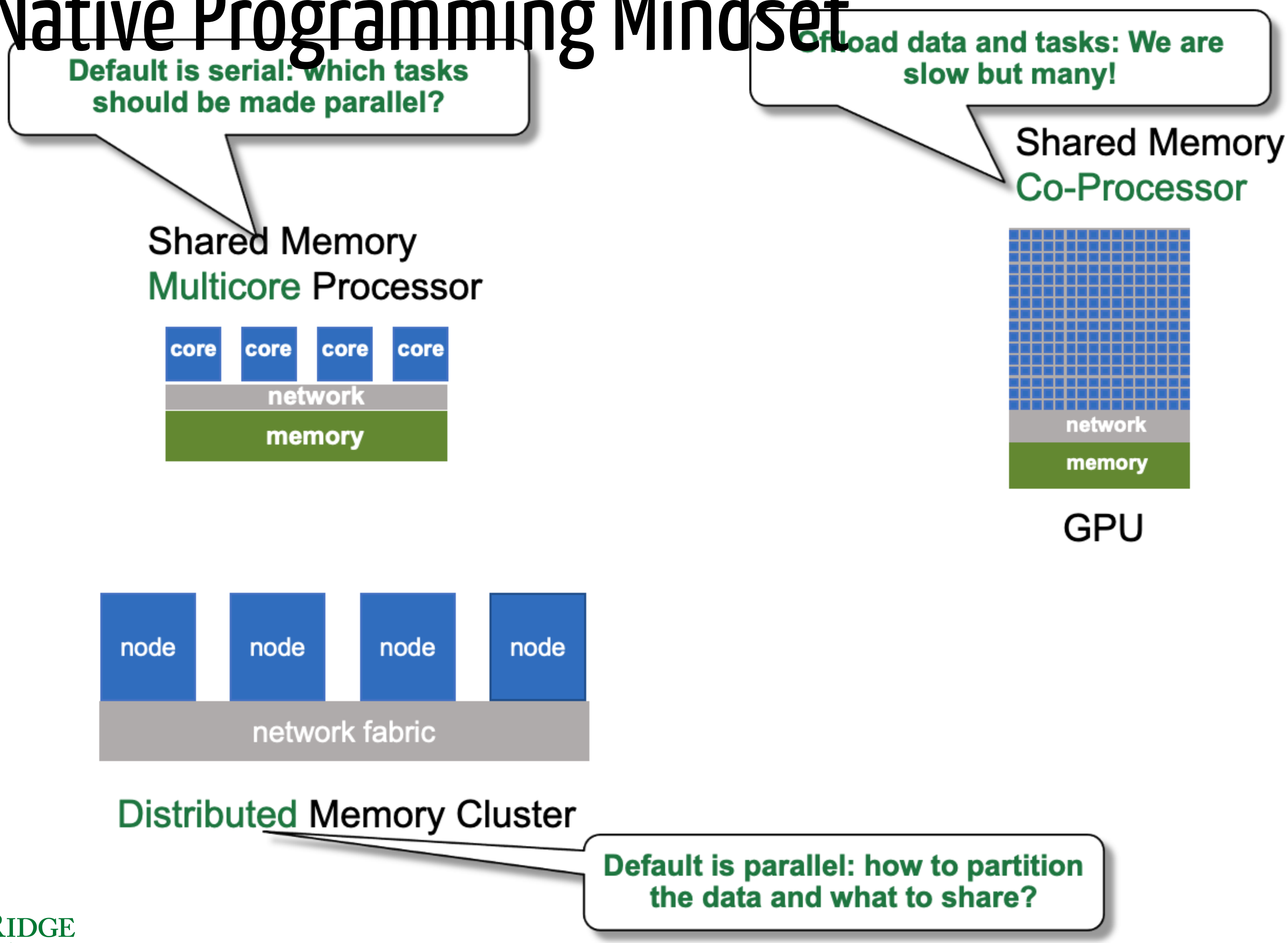
Section III:

Parallel Software

Native Programming Mindset



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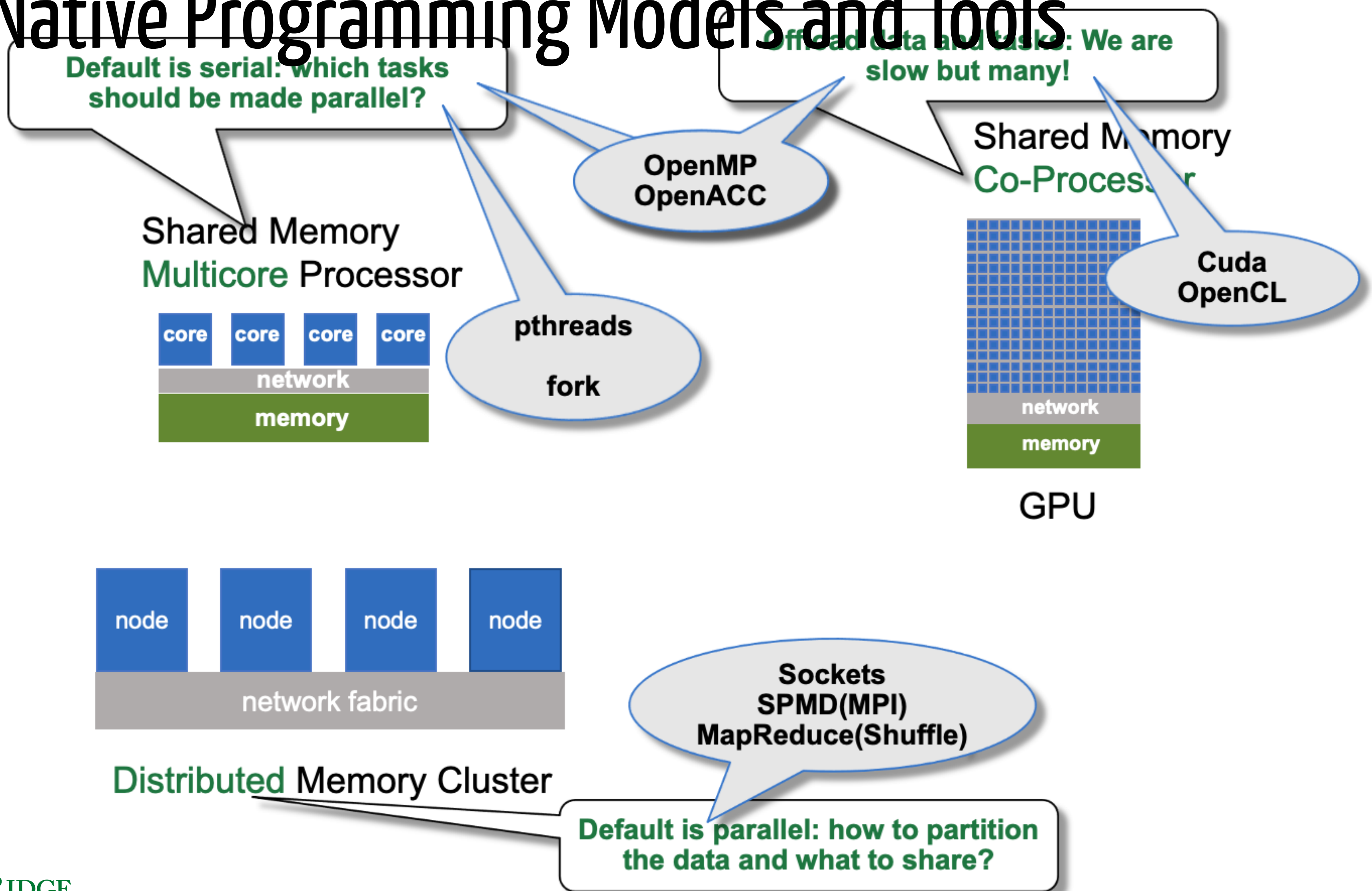
Native Programming Models and Tools



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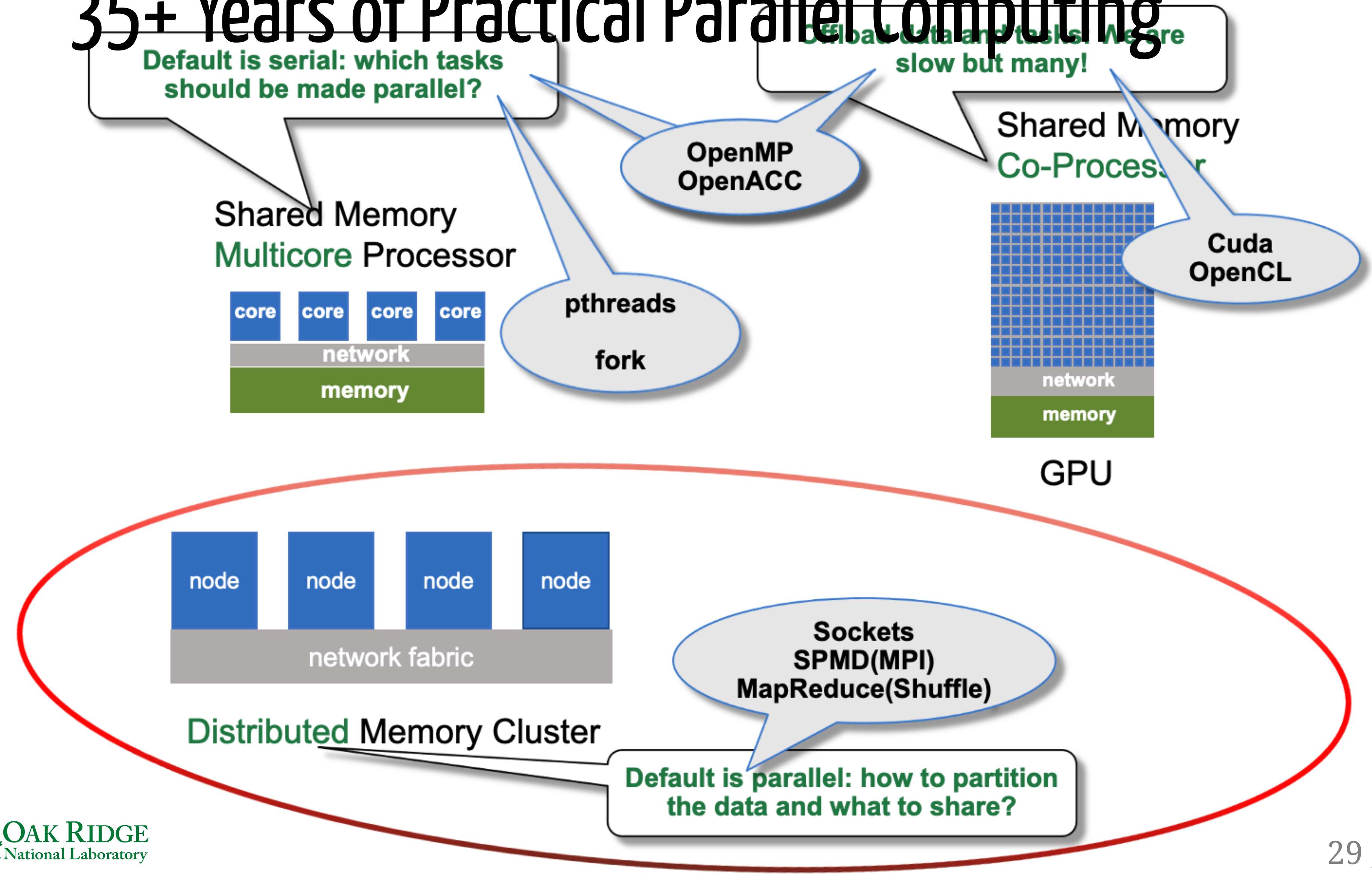
35+ Years of Practical Parallel Computing



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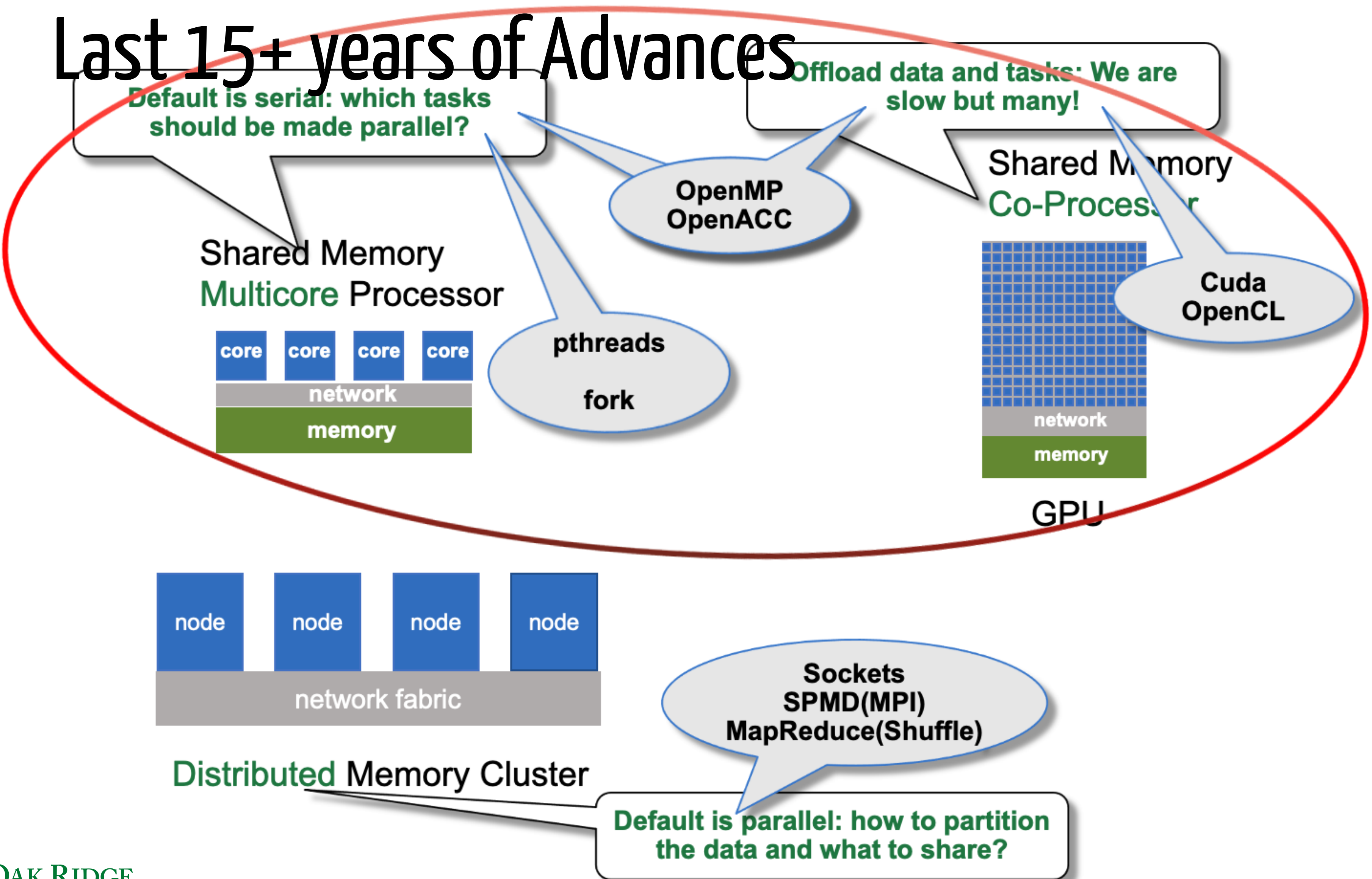
Last 15+ years of Advances



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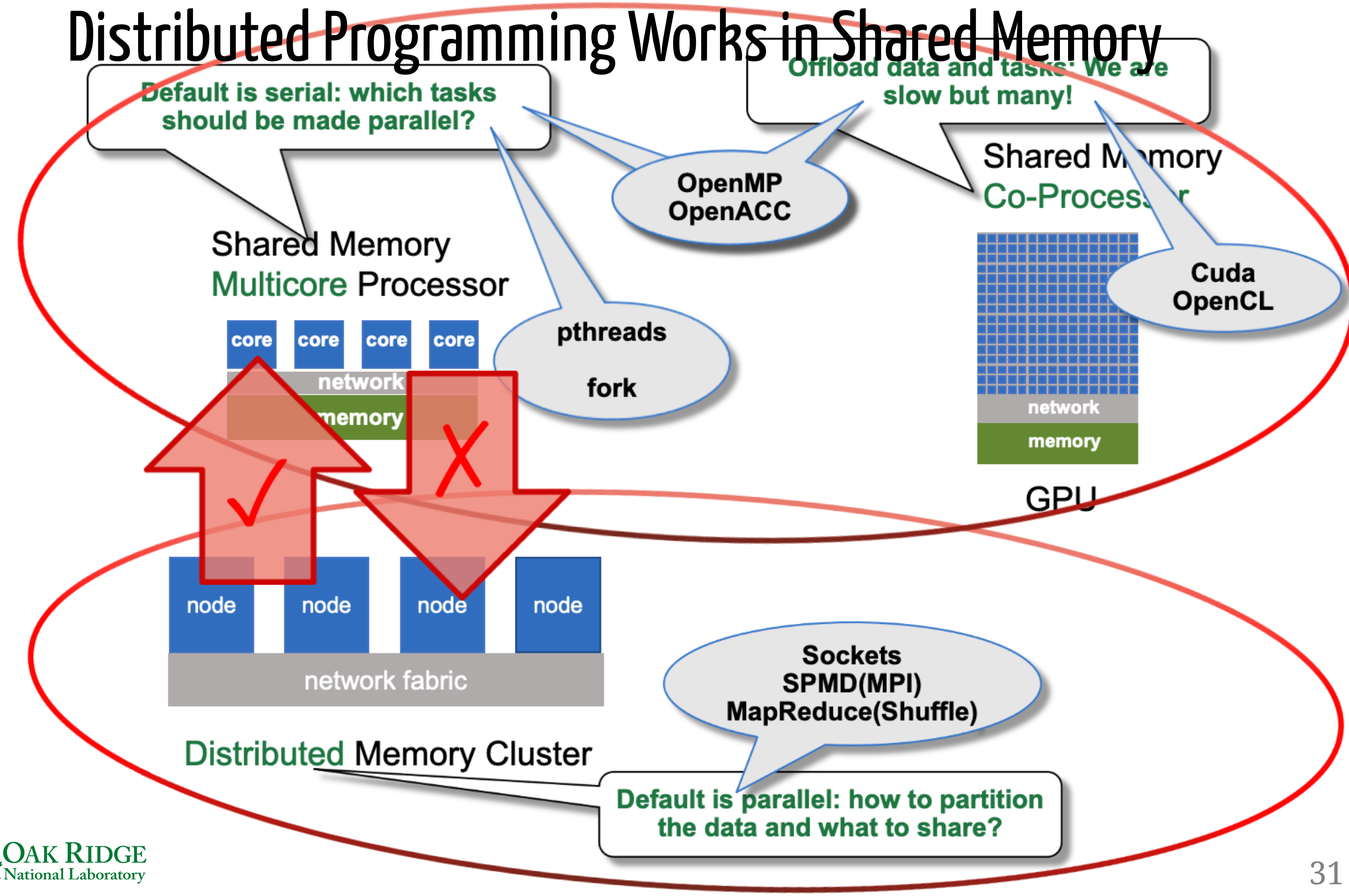
Distributed Programming Works in Shared Memory



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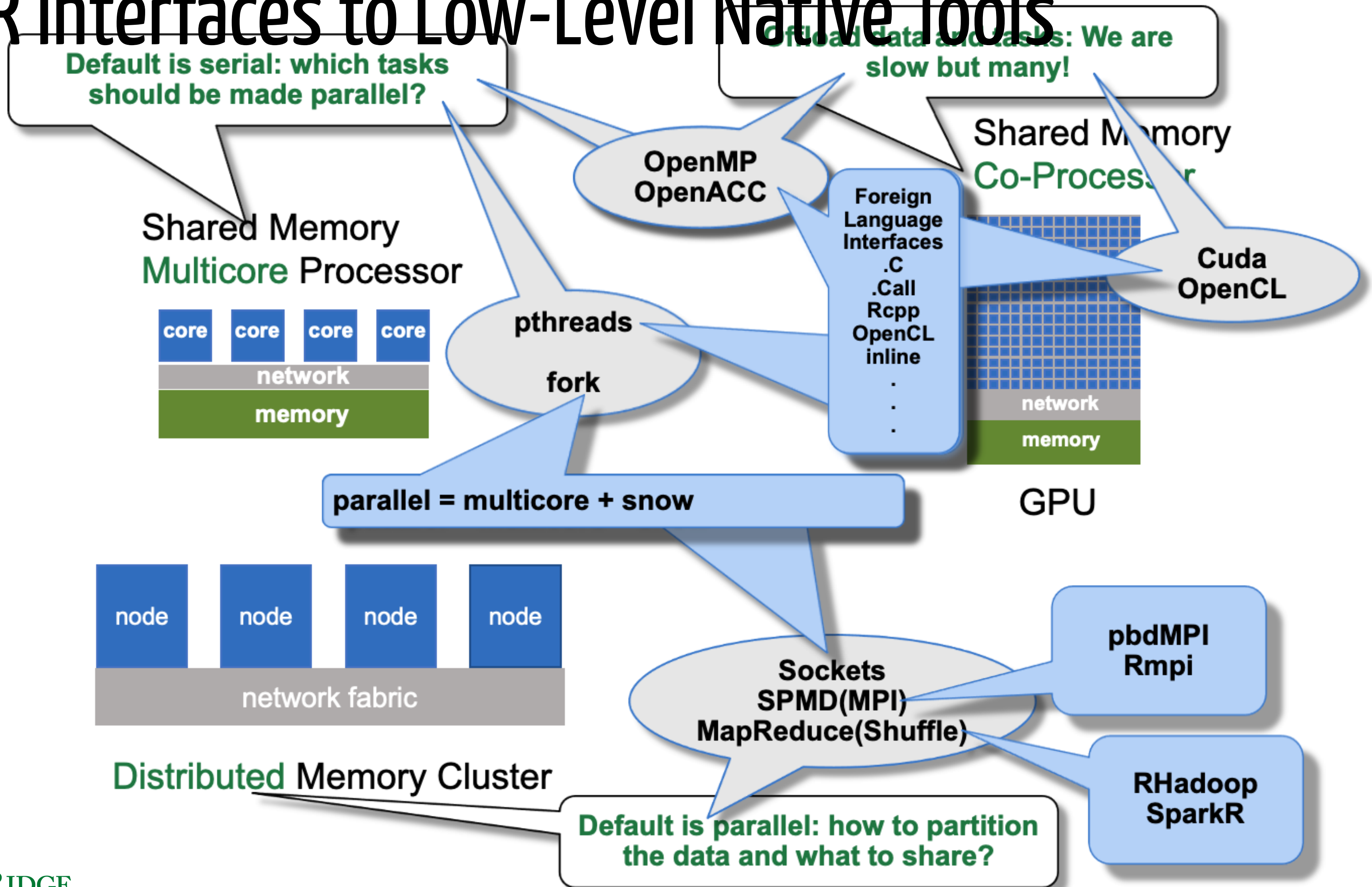
R Interfaces to Low-Level Native Tools



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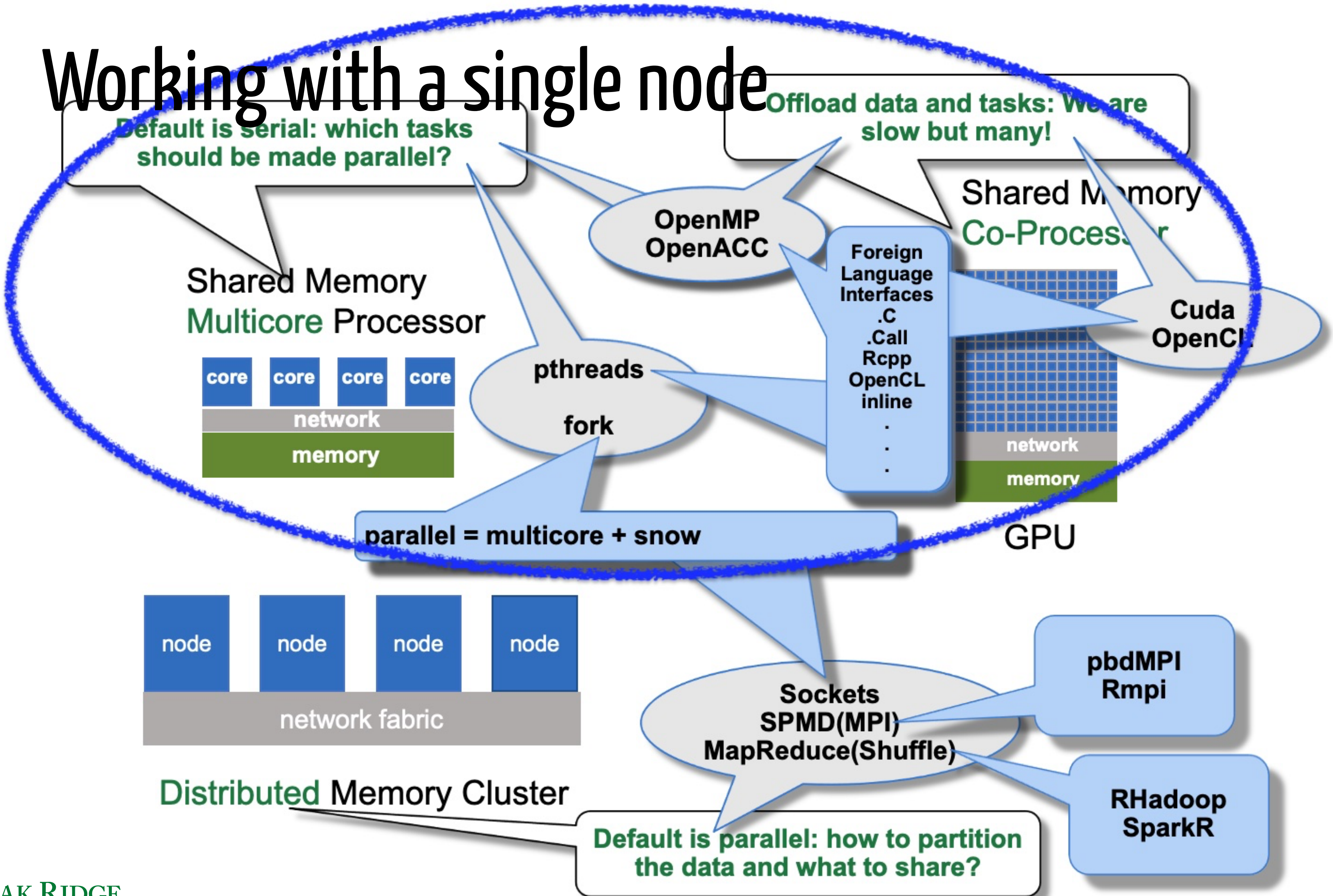
Section IV:

Shared Memory Tools

Working with a single node

Working with a single node



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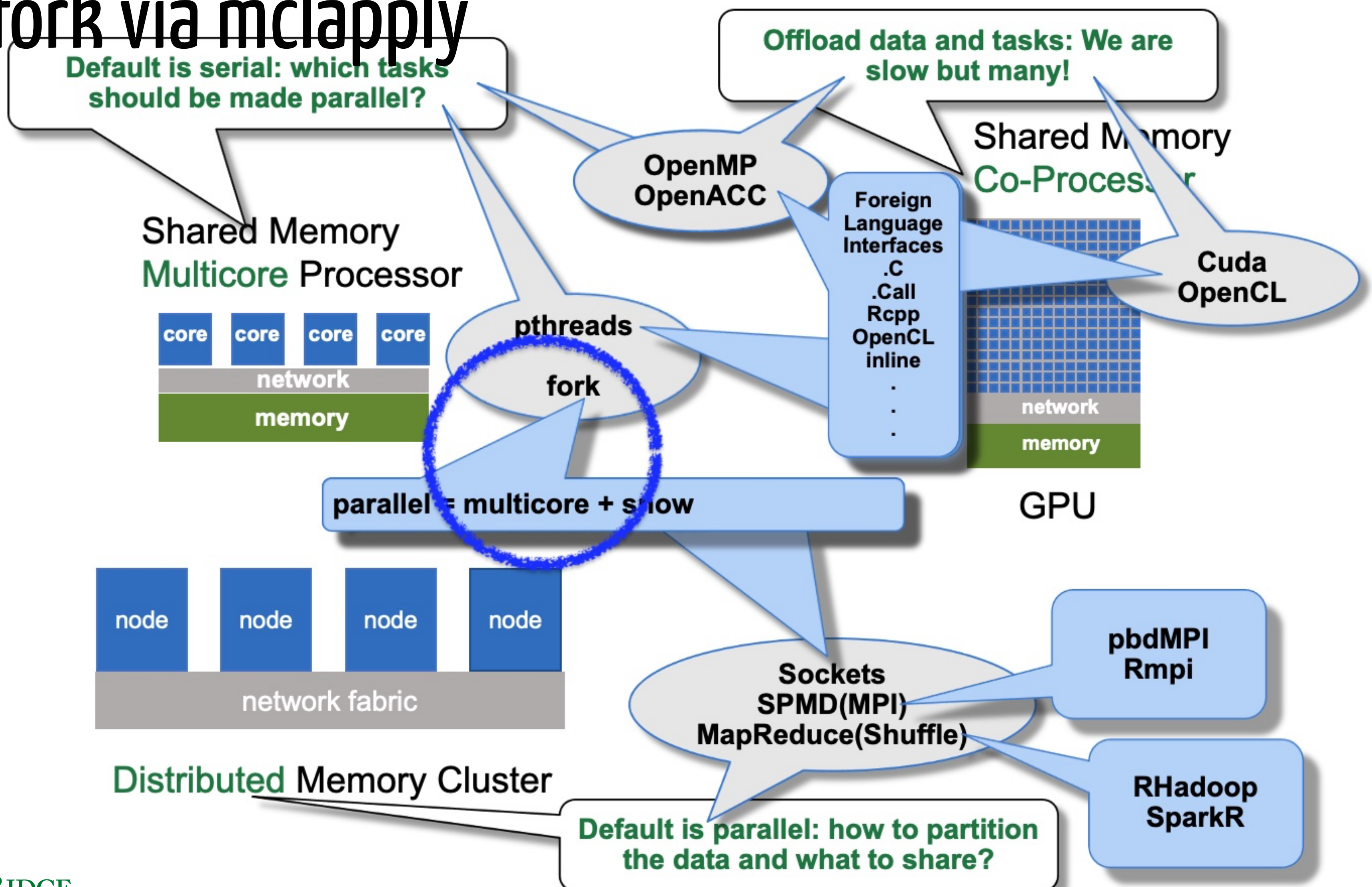
fork via mclapply



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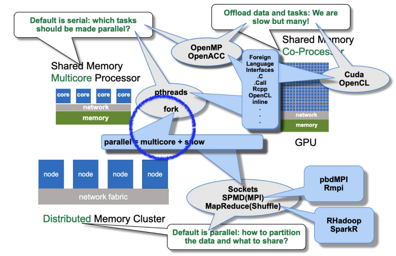
Unix `fork`



- A memory efficient parallelism on shared memory devices
- Copy-on-write: copy page if forked process tries to write
- R: **parallel** package `mclapply` and friends
  - Use for numerical sections only
  - Avoid GUI, I/O, and graphics sections
- Convenient for data (not modified)
- Convenient for functional languages like R
- Careful with nested parallelism
  - OpenBLAS takes all cores by default
  - data.table switches to single threaded mode upon fork

A deeper discussion of `fork` memory (if you have interest) on YouTube by Chris Kanich (UIC)

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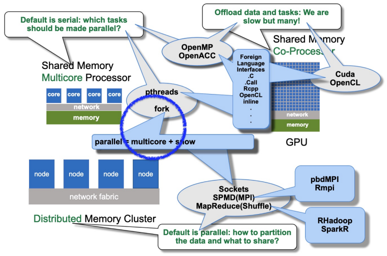
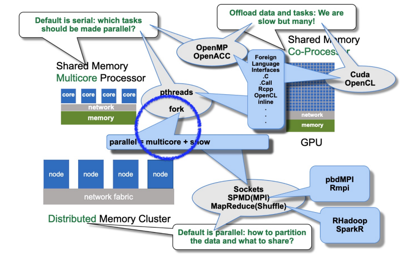


Copy-on-write



Mapping Threads to Cores

Theory and Reality

- Operating system manages core affinity
- OS tasks can compete and core switching occurs frequently

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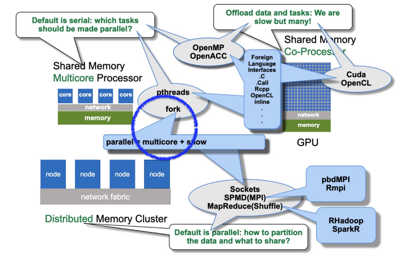

R: Drop-in replacements (almost) for `lapply`, `mapply`, and `Map`

```
mclapply(X, FUN, ..., mc.preschedule = TRUE, mc.set.seed = TRUE,
mc.silent = FALSE, mc.cores = getOption("mc.cores", 2L),
mc.cleanup = TRUE, mc.allow.recursive = TRUE, affinity.list =
NULL)
```

```
mcmapply(FUN, ..., MoreArgs = NULL, SIMPLIFY = TRUE, USE.NAMES =
TRUE, mc.preschedule = TRUE, mc.set.seed = TRUE, mc.silent =
FALSE, mc.cores = getOption("mc.cores", 2L), mc.cleanup = TRUE,
affinity.list = NULL)
```

```
mcMap(f, ...)
```

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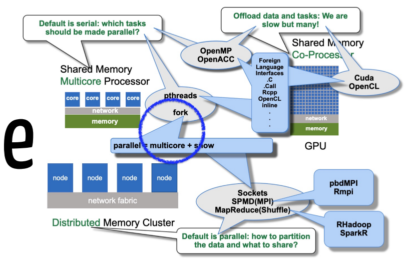
Hands-on Session 2 - Multicore Random Forest

- Go to `R4HPC/code_2` directory
- Look at the `rf_serial.R` and `rf_mc.R` codes

Hands-on Session 2 - Example Random forest Code



Letter recognition data ($20\,000 \times 17$)

```
[,1] lettr capital letter
[,2] x.box horizontal position of box
[,3] y.box vertical position of box
[,4] width width of box
[,5] high height of box
[,6] onpix total number of on pixels
[,7] x.bar mean x of on pixels in box
[,8] y.bar mean y of on pixels in box
[,9] x2bar mean x variance
[,10] y2bar mean y variance
[,11] xybar mean x y correlation
[,12] x2ybr mean of x^2 y
[,13] xy2br mean of x y^2
[,14] x.ege mean edge count left to right
[,15] xegvy correlation of x.ege with y
[,16] y.ege mean edge count bottom to top
[,17] yegvx correlation of y.ege with x
```

Figure 1: Letter Recognition data (image: [Frey and Slate, 1991], description: **mlbench** package).

*Parallel Statistical Computing with R: An Illustration on Two Architectures
arXiv:1709.01195

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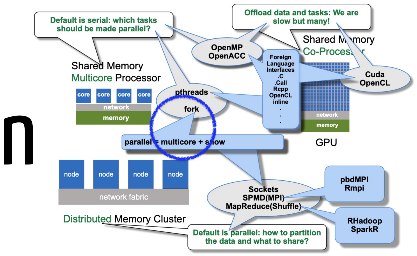
Hands-on Session 2 - Random Forest Classification



Build many decision trees

Each tree built from

- random subset of variables: subset of columns
- resampled (with replacement) data: same number of rows

Use their majority votes to classify

Hands-on Session 2 - R4HPC/code_2/rf_serial.R

```
suppressMessages(library(randomForest))
data(LetterRecognition, package = "mlbench")
set.seed(seed = 123)

n = nrow(LetterRecognition)
n_test = floor(0.2 * n)
i_test = sample.int(n, n_test)
train = LetterRecognition[-i_test, ]
test = LetterRecognition[i_test, ]

rf.all = randomForest(lettr ~ ., train, ntree = 500, norm.votes = FALSE)
pred = predict(rf.all, test)

correct = sum(pred == test$lettr)
cat("Proportion Correct:", correct/(n_test), "\n")
```

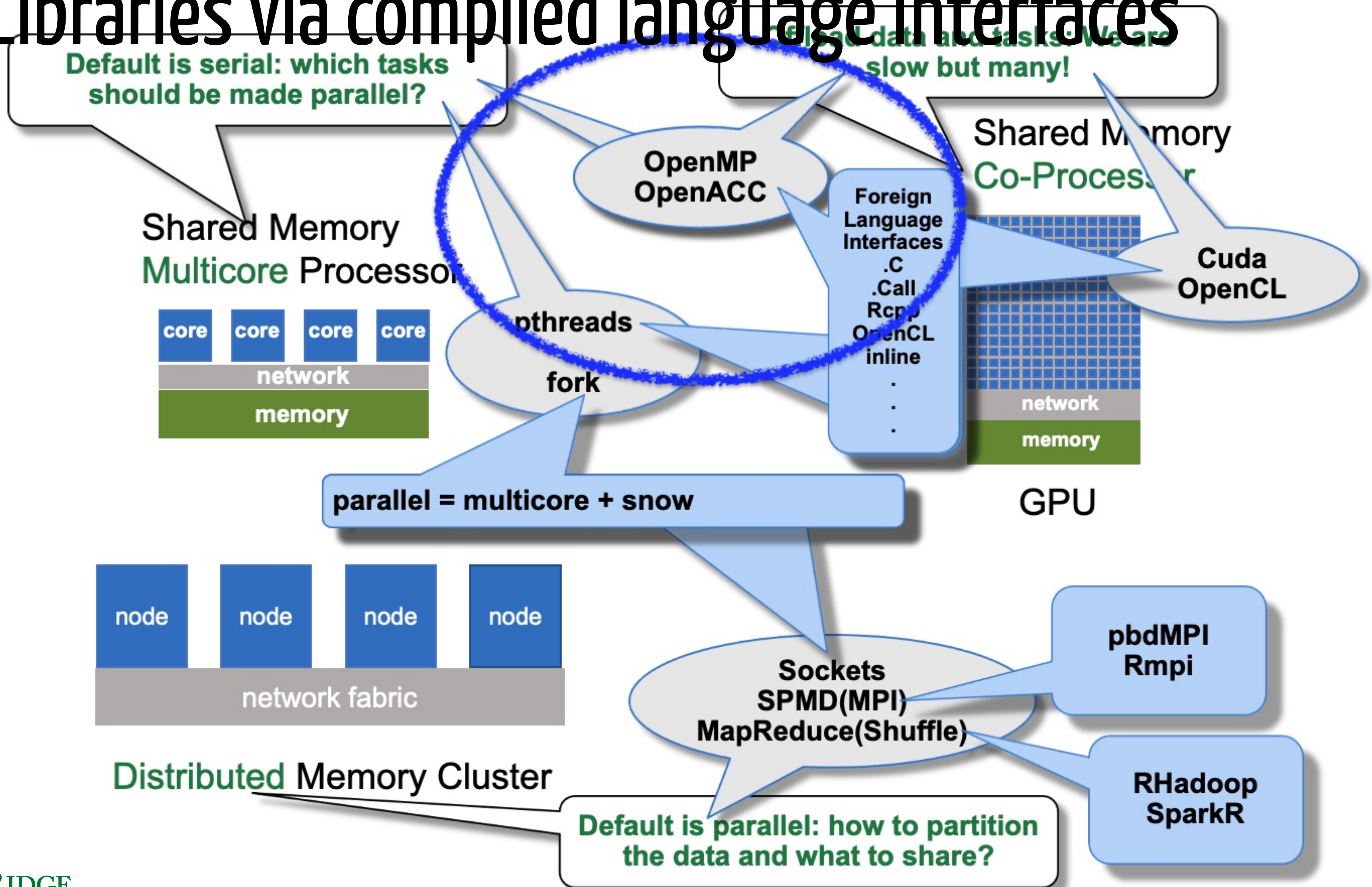
Hands-on Session 2 - R4HPC/code_2/rf_mc.R

```
library(parallel)
library(randomForest)
data(LetterRecognition, package = "mlbench")
set.seed(seed = 123, "L'Ecuyer-CMRG")

n = nrow(LetterRecognition)
n_test = floor(0.2 * n)
i_test = sample.int(n, n_test)
train = LetterRecognition[-i_test, ]
test = LetterRecognition[i_test, ]

nc = as.numeric(commandArgs(TRUE)[2])
ntree = lapply(splitIndices(500, nc), length)
rf = function(x, train) randomForest(lettr ~ ., train, ntree=x,
                                     norm.votes = FALSE)
rf.out = mclapply(ntree, rf, train = train, mc.cores = nc)
rf.all = do.call(combine, rf.out)

crows = splitIndices(nrow(test), nc)
rfp = function(x) as.vector(predict(rf.all, test[x, ]))
cpred = mclapply(crows, rfp, mc.cores = nc)
pred = do.call(c, cpred)

correct <- sum(pred == test$lettr)
```

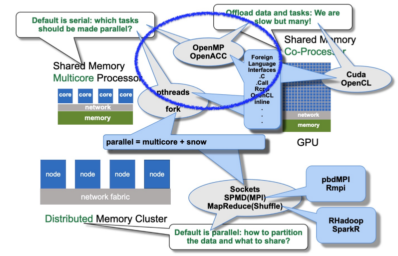
Hands-on Session 2 - Assignment

Time the random forest code `rf_mc.R` for 1 through 32 cores by modifying the `rf_MACHINE_slurm.sh` script.

Libraries via compiled language interfaces



R-LAPACK-BLAS



- BLAS: Basic Linear Algebra Subroutines - A matrix multiplication library
  - `%*%`, `crossprod()`, `sweep()`, `scale()`, and many more
- LAPACK: dense and banded matrix decomposition and more
  - `svd()`, `La.svd()`, `prcomp()`, `princomp()`, `qr()`, `solve()`, `chol()`, `norm()`, and many more
  - But not `lm()`, careful with `qr(x, LAPACK = TRUE)`: column pivoting
- Implementations: OpenBLAS, Intel MKL, Nvidia nvBLAS, Apple vecLib, AMD BLIS, Arm Performance Libraries
- **FlexiBLAS**: A BLAS and LAPACK wrapper library with runtime exchangeable backends
  - Great for benchmarking implementations
  - Great for dynamic core assignment

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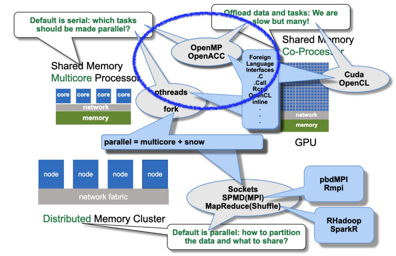
OpenBLAS



OpenBLAS is an optimized BLAS library based on GotoBLAS2 (2010, Kazushige Goto).

- openblas.net
- Optimizes algorithm to chip microarchitecture details of memory hierarchies (L1 cache, L2 cache, etc.) and register vector length
- IT4I FlexiBLAS: "OPENBLAS" backend

Wang Qian, Zhang Xianyi, Zhang Yunquan, Qing Yi, AUGEM: Automatically Generate High Performance Dense Linear Algebra Kernels on x86 CPUs, In the International Conference for High Performance Computing, Networking, Storage and Analysis (SC'13), Denver CO, November 2013.

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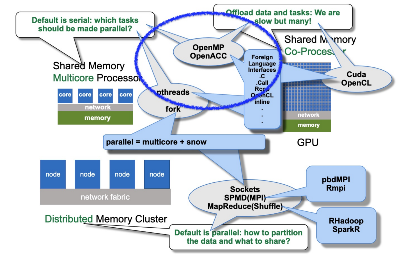


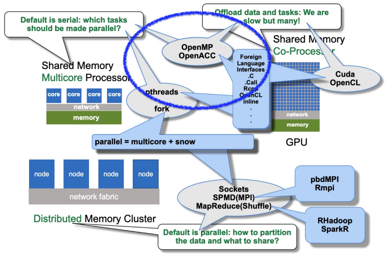
FlexiBLAS

flexiblas_setup.r

```
library(flexiblas)
flexiblas_avail()
flexiblas_version()
flexiblas_current_backend()
flexiblas_list()
flexiblas_list_loaded()

getthreads = function() {
  flexiblas_get_num_threads()
}
setthreads = function(thr, label = "") {
  cat(label, "Setting", thr, "threads\n")
  flexiblas_set_num_threads(thr)
}
setback = function(backend, label = "") {
  cat(label, "Setting", backend, "backend\n")
  flexiblas_switch(flexiblas_load_backend(backend))
}
```

https://github.com/Enchufa2/r-flexiblas
https://cran.r-project.org/package=flexiblas



Hands-on Session 3 - FlexiBLAS

- Go to `code_3` directory

Appendix: Faster BLAS For Faster R on your macOS Laptop

```
## Default BLAS from Netlib
> x = matrix(rnorm(1e7), nrow = 1e4)
> system.time(crossprod(x))
   user  system elapsed
  6.752   0.023   6.801
```

```
## vecLib
> system.time(crossprod(x))
   user  system elapsed
  0.666   0.003   0.120
```

```
## OpenBLAS
   > system.time(crossprod(x))
      user  system elapsed
     0.822   0.042   0.121
```

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Appendix: FlexiBLAS For BLAS Control on your macOS Laptop

- Install Xcode and command line tools
- Install Homebrew: https://brew.sh/
- In a terminal window:
  - `brew install cmake`
  - `brew install openblas`
- cmake needs to be told about OpenBLAS:
  - `export CMAKE_PREFIX_PATH=/usr/local/opt/openblas:$CMAKE_PREFIX_PATH`
- Install FlexiBLAS: https://www.mpi-magdeburg.mpg.de/projects/flexiblas
  - See Install section in its README.md
- After installation, link to R (terminal window):
  - `ln -sf /usr/local/lib/libflexiblas.dylib /Library/Frameworks/R.framework/Resources/lib/libRblas.dylib`
- In R, `install.packages("flexiblas")` and test if it works:
  - `flexiblas_avail()`
  - `flexiblas_list()`

R can now swap OpenBLAS and APPLE vecLib dynamically.

Appendix: For faster R on your Windows laptop

Assessing R performance with optimized BLAS across three operating systems link

Building R 4+ for Windows with OpenBLAS link