Parallel Computing in R using the snowfall Package

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Structure of This Talk

1. Overview of Parallel Computing and The snowfall Package in These Slides

2. Demonstration of R Code
   A. Basic Examples
      - Simple example code designed to introduce the programming techniques.

   B. Advanced Examples
      - Code from real (and realistic) examples of how you might *actually* use the techniques.
        - Two examples of how to parallelize simulation studies.
        - An example of how snowfall interfaces with OpenMx.

Philosophy of Materials Included in this Presentation

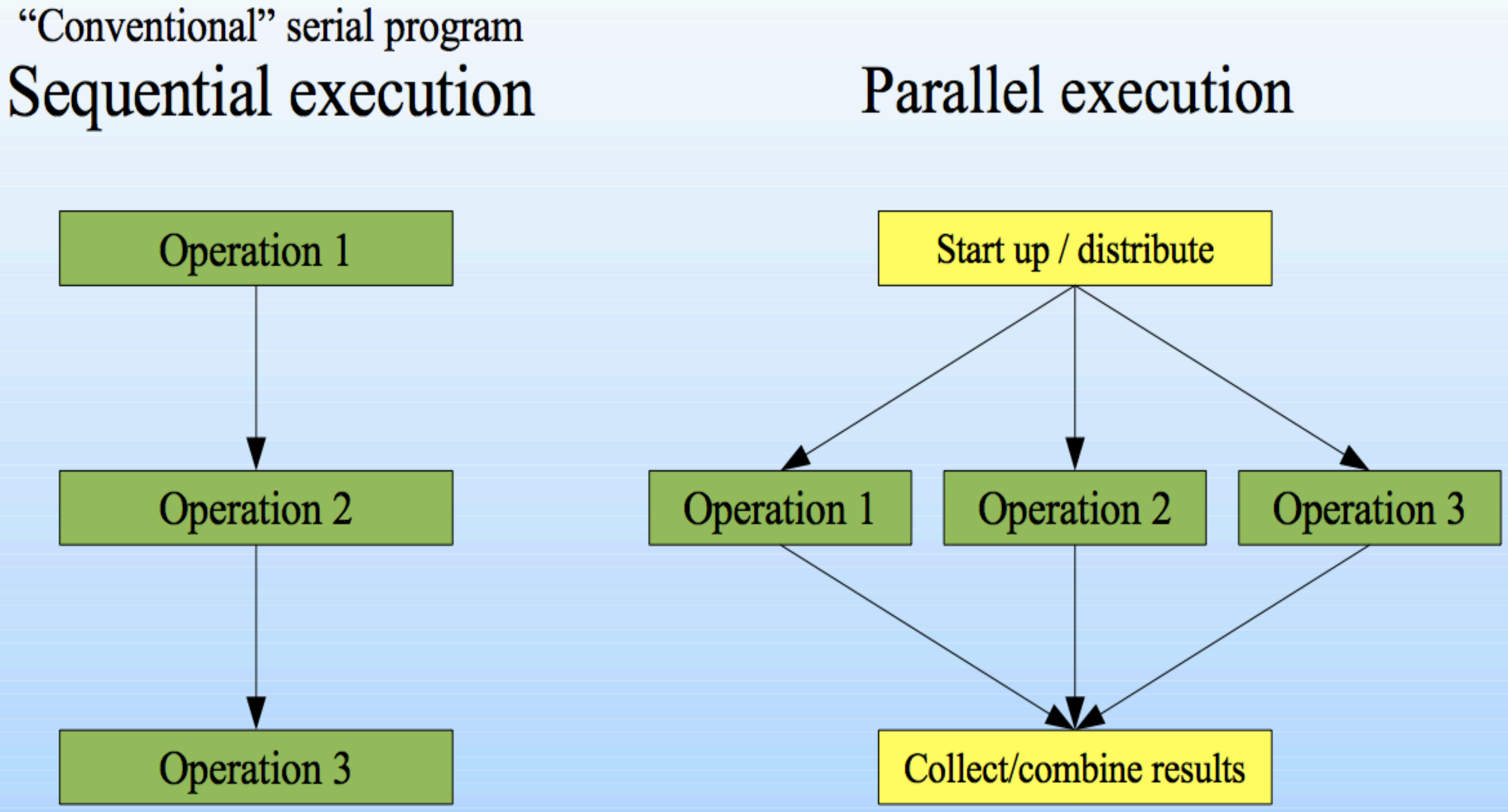
- These materials (including this slide show) are designed to be ***your future references***.

- Thus, they are a bit more text heavy than "good presentation etiquette" might dictate … but hopefully they will be more useful later.

Obligatory Introductory Section:

THE PROMISE OF PARALLEL COMPUTING

Parallel programs



From Knaus, 2008

Amdahl's Law: Theoretical maximum speedup with multiple processors

$n \in N$	the number of CPU cores
$B \in [0,\ 1]$	the serial portion of the algorithm
$T(n)$	the time to solution

$$T(n) = T(1)\left(B + \underbrace{\frac{1}{n}(1 - B)}\right)$$

Total time to solution if executed in parallel.

Total time to solution when executed serially.

This rescales proportions in units of time.

Proportion of algorithm that is **serial**.

Proportion of algorithm that is **not serial** divided by the number of cores.

http://en.wikipedia.org/wiki/Amdahl%27s_law

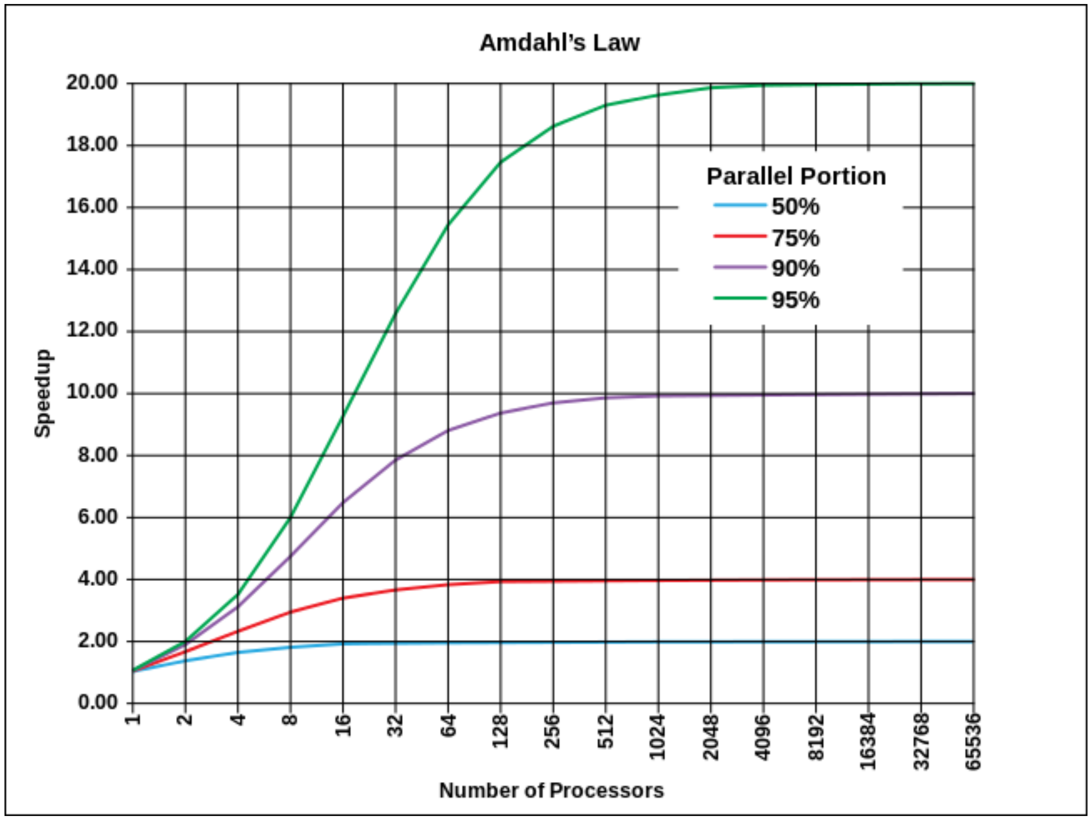
Amdahl's Law: Theoretical maximum speedup with multiple processors

Theoretical speedup gained by executing algorithm on a system capable of executing *n* threads in parallel:

$$S(n) = \frac{T(1)}{T(n)} = \frac{T(1)}{T(1)\left(B + \frac{1}{n}(1-B)\right)} = \frac{1}{B + \frac{1}{n}(1-B)}$$

Serial execution time (without parallel) divided by execution time with parallel

http://en.wikipedia.org/wiki/Amdahl%27s_law



"The speedup of a program using multiple processors in parallel computing is limited by the sequential fraction of the program. For example, if 95% of the program can be parallelized, the theoretical maximum speedup using parallel computing would be 20× as shown in the diagram, no matter how many processors are used."

http://en.wikipedia.org/wiki/Amdahl%27s_law

How Much Speedup Can You Get From Parallel Programming with the HPC?

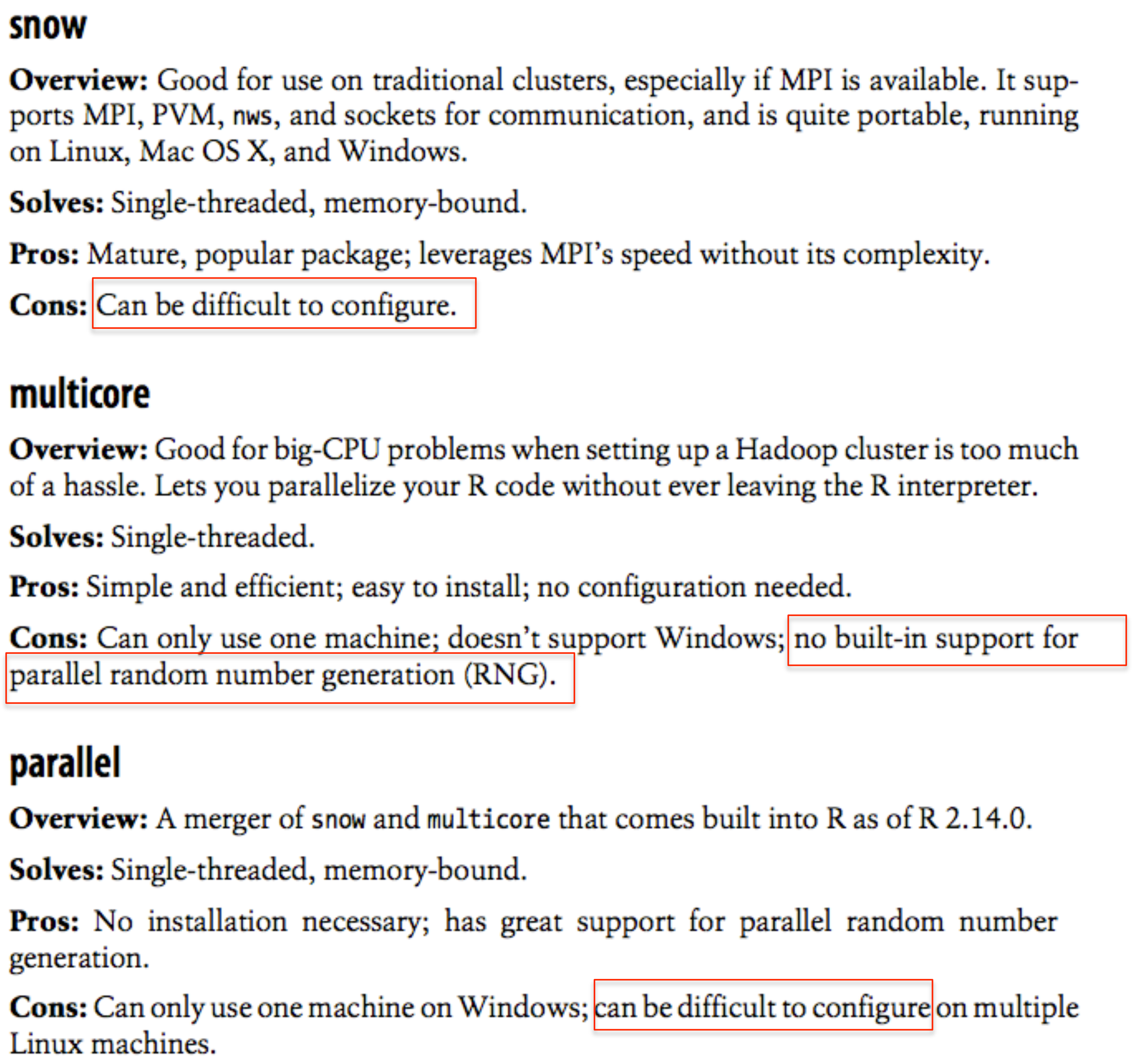
- Many HPCC nodes have as many as 16 cores.
- From experience, you can comfortably request ~6 nodes at a time.
- If you request 6 nodes with 16 processors per node, that is 6*16 = **96 operations running in parallel at any one time … <u>if you write your script in parallel.</u>**

Section 2

PARALLEL COMPUTING USING R

Parallel Computing in R

- Several packages are currently available to facilitate parallel computing in R:
  - `Multicore` (Urbanek, 2009)
  - `Parallel` (R-Core/Eddelbuettel, 2014)
  - `Snow` (<u>S</u>imple <u>N</u>etwork <u>o</u>f <u>W</u>orkstations in R; Tierney, Rossini, Sevcikova, 2003)



snow

Overview: Good for use on traditional clusters, especially if MPI is available. It supports MPI, PVM, `nws`, and sockets for communication, and is quite portable, running on Linux, Mac OS X, and Windows.

Solves: Single-threaded, memory-bound.

Pros: Mature, popular package; leverages MPI's speed without its complexity.

Cons: Can be difficult to configure.

multicore

Overview: Good for big-CPU problems when setting up a Hadoop cluster is too much of a hassle. Lets you parallelize your R code without ever leaving the R interpreter.

Solves: Single-threaded.

Pros: Simple and efficient; easy to install; no configuration needed.

Cons: Can only use one machine; doesn't support Windows; no built-in support for parallel random number generation (RNG).

parallel

Overview: A merger of `snow` and `multicore` that comes built into R as of R 2.14.0.

Solves: Single-threaded, memory-bound.

Pros: No installation necessary; has great support for parallel random number generation.

Cons: Can only use one machine on Windows; can be difficult to configure on multiple Linux machines.

McCallum & Weston, 2012

Snowfall (Knaus, 2010)

- Usability wrapper for the snow package.
- Interfaces with OpenMx.
- Relies on similar programming conventions to virtually all other parallel R packages, so easy to learn other packages after learning.
- Relatively thorough/helpful documentation available at:
  - https://www.imbi.uni-freiburg.de/parallel/

Some Highly Unfortunate Parallel Computing Terminology (Knaus, 2008)

- **Master:** Calculation is started on this node and the control program (start/init) is running here.
- **Slave (Worker):** CPU on which a raw parallelized calculation part is running.
- **CPU/Core:** Single calculation unit.
- **Node:** Single computer accessible in a cluster.
- **Universe:** All machines which can possibly be used as a node in a concrete cluster.
- **Cluster:** subset from the universe for specific use.

How does parallel computing in snowfall work? It’s simple…

In a bit more detail:

- Parallelization generally follows the following steps (Knaus, Porzelius, Binder, Schwarzer, 2009):
  1. Initialize the cluster using sfInit().
  2. Wrap parallel code in a wrapper function callable by an R list function.
  3. Export objects, packages, and/or source code to cluster nodes.
  4. Start a network random number generator if need be.
  5. Distribute the calculation to the cluster by using a parallel list function.
  6. Stop the cluster via sfStop().

snowfall functions corresponding to these steps:

- Cluster initialization
  - **sfInit**: initializes cluster with # of cpus set by user
- Exporting Objects, Libraries, and Packages
  - **sfLibrary**: load library on the slaves.
  - **sfSource**: source file on the slaves.
  - **sfExport**: export variables (objects) to slaves.
  - **sfExportAll**: export all variables (objects) in workspace.
  - **sfRemove**: remove specific objects from slaves
  - **sfRemoveAll**: remove anything from slave memory.
- Generating Parallel Random Numbers
  - **sfClusterSetupRNGstream:** set up parallel random number generation.
- Cluster Apply Functions for Actual Computations
  - **sfClusterLapply, sfClusterSapply, sfClusterApply**: Parallel apply functions that work on lists (first two) and arrays (last one) respectively.
  - **sfClusterApplyLB:** load balanced version of clustered Lapply (roughly speaking). Documentation: "If a node finished it's list segment it immediately starts with the next segment. Use this function in infrastructures with machines with different speed."
  - **parMM:** parallel matrix multiplication (I have not used this, but it seems extremely useful).

A Practical Perspective on Setting up Parallel Programs

- Researchers often "think in serial mode" and have a plan for how they would normally execute a script – e.g., a big, nested for loop.
- If so, these serial scripts will need to be rewritten to make them suitable for parallel computation (read: put a list on it).
- Because people don't typically "think in parallel list mode" the challenge, in practice, becomes figuring out where best to intervene in existing sequential programs to ***parallelize*** those programs effectively.

Where to Parallelize

- Where in your script should you intervene to parallelize your code?
  - Search for two requirements:
    1. Independent operations that are
    2. Computationally intensive and time consuming.

Where to Parallelize

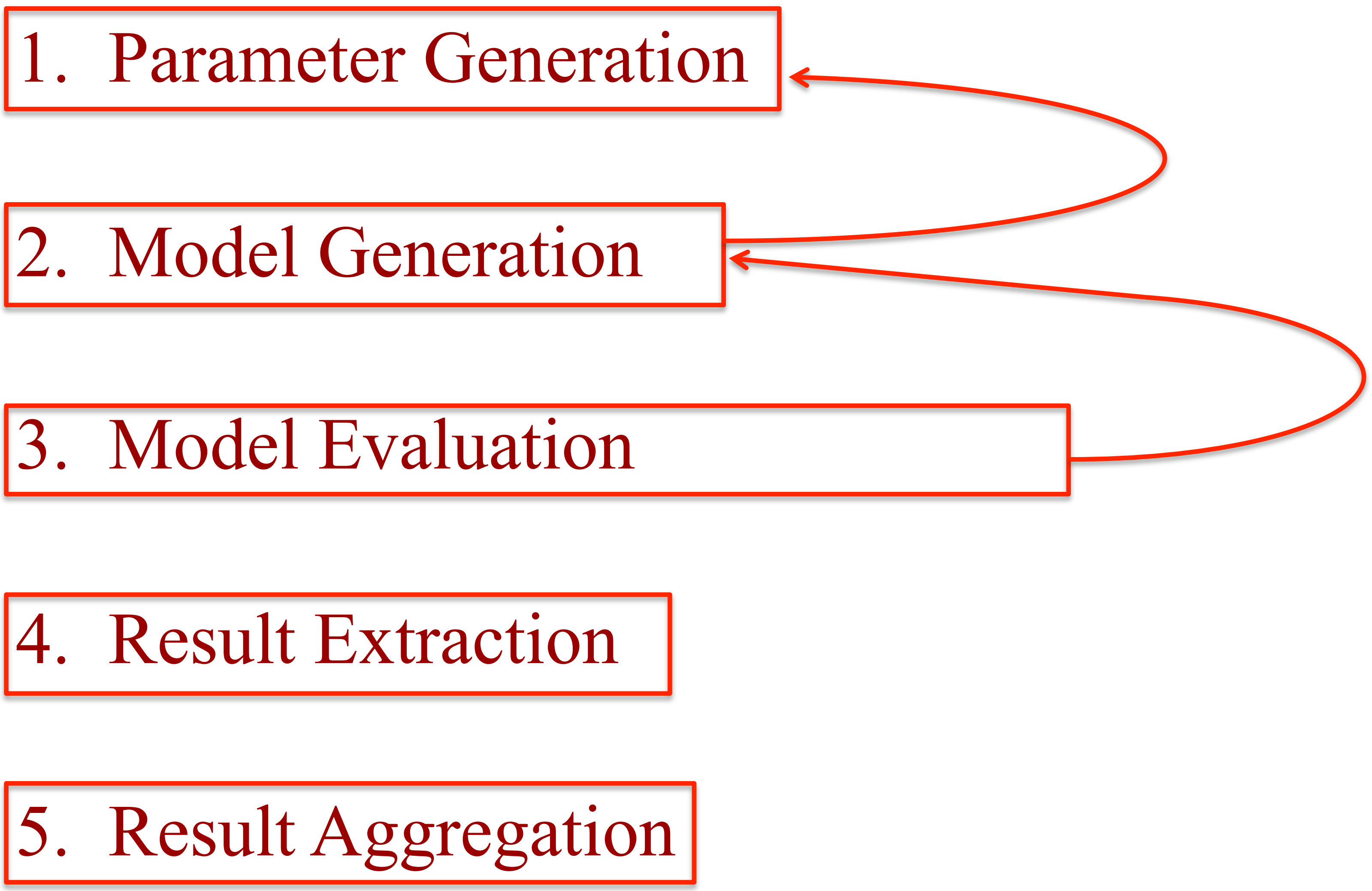
- Some blocks of code may involve independent operations and these blocks of code may even *look* computationally intensive (i.e., the code could look "big" in the script), but in practice they may only take fractions of a second to compute in serial mode.

- Thus, don't parallelize for parrallelization's sake. Intervene where it really matters.

- With that said, sometimes you will be faced with multiple ways to parallelize computationally time-intensive blocks of code, and this is where creativity and programming savvy come in.

Where to Parallelize

- Simulation Steps:



1. Parameter Generation
2. Model Generation
3. Model Evaluation
4. Result Extraction
5. Result Aggregation