An Introduction into Parallelization

Part II - Design

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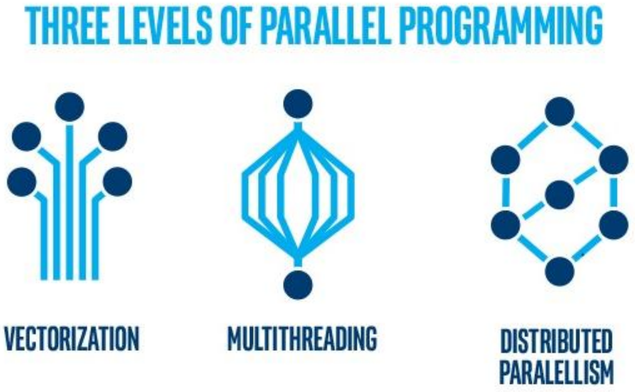
Outline

1. Parallel Programming Models (cont.)
   - Recap: Computer Architectures
   - Distributed Parallelism with Message Passing
   - Hybrid Models
2. Designing Parallel Programs
   - Understand your problem and tools
   - Partitioning - Domain vs functional decomposition
   - Data Dependence / Race conditions
   - Synchronization
   - Communication
   - Load balancing
   - I/O
   - Performance Analysis & Tuning
   - Conclusions / tl;dr

Parallel Programming Models

Parallel Programming Models - Overview



Distributed Parallelism with Message Passing

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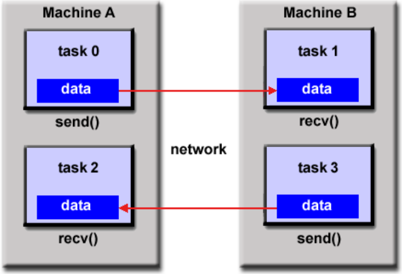

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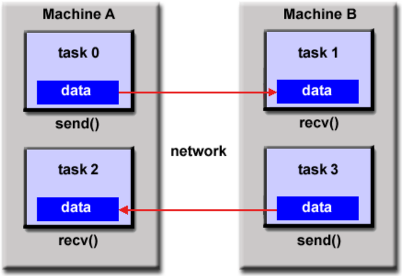

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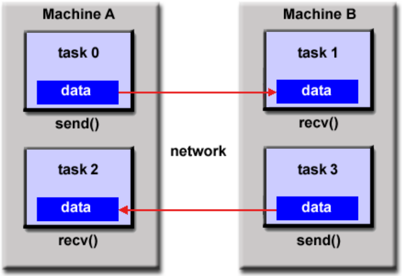

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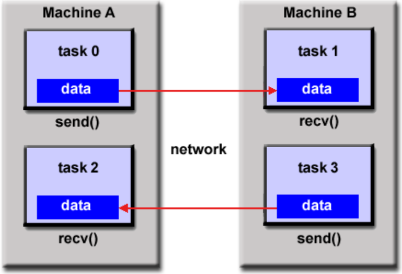

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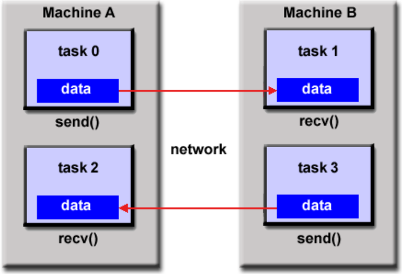
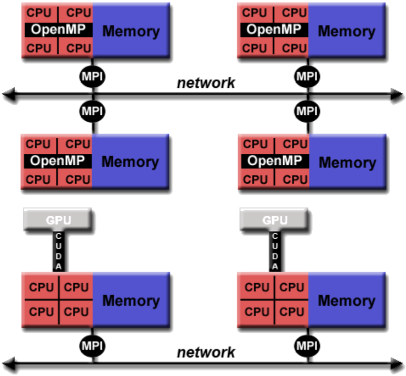
- *MPI* is the "de facto" standard



Hybrid Models

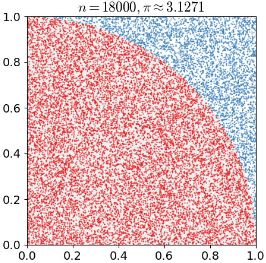
- Allows to make best use of locally shared memory or hardware, while still allowing for a good scalability across multiple nodes
- Comes with a significant increase in complexity/costs
- certain incompatibilities between libraries may exist (e.g. lack of thread-safety of MPI library)



Designing Parallel Programs

Understand your problem (!)

- some problems can be easily parallelized e.g. calculation of π by Monte-Carlo sampling



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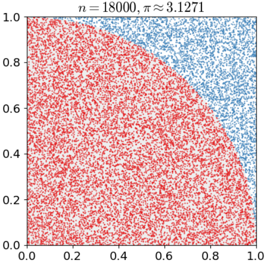

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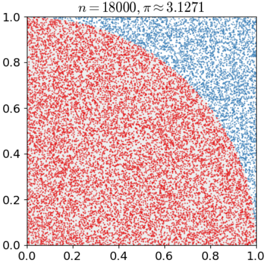

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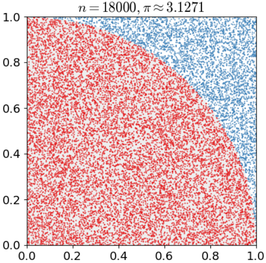

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- Consider replacing your algorithms with equivalent ones better suited for parallelism

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- identify hotspots in your program, i.e. routines where program spends lots of time in and check for improvement in parallelism ($\rightarrow$Amdahl's Law/Scaling)

Partitioning - Domain decomposition

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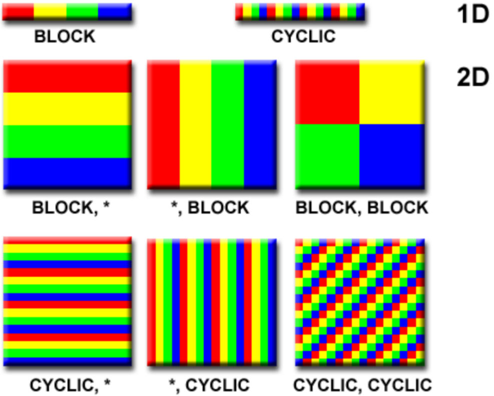

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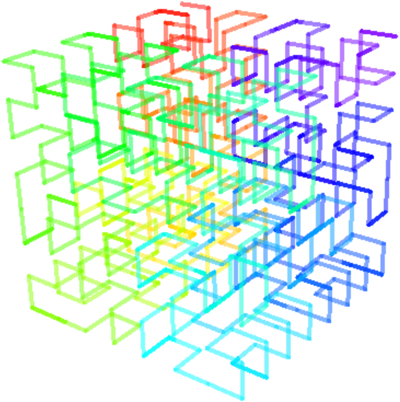

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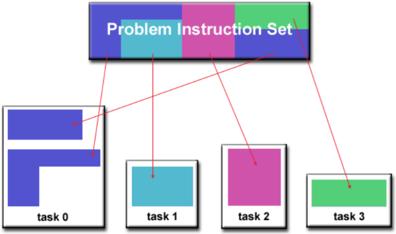

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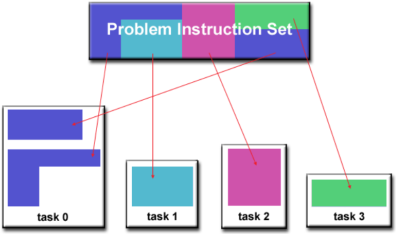

- implemented e.g. in master/slave paradigm (see exercises)

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- Dependencies are important to parallel programming because they are one of the primary inhibitors to parallelism (cf. Fibonacci series).
- This can also cause a so called race condition:

Thread 1	Thread 2		Integer value
			0
read value		←	0
increase value			0
write back		→	1
	read value	←	1
	increase value		1
	write back	→	2

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- ... or to synchronize the calculations of processes (using barriers) for communication to exchange results or to redistribute the workload

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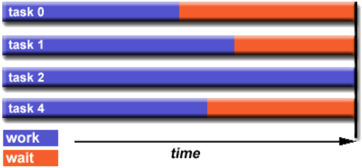
  - Point-to-Point vs. collective communications

Load balancing

- Load balancing needed to ensure that processors are optimally i.e. minimizing idle times at synchronization points



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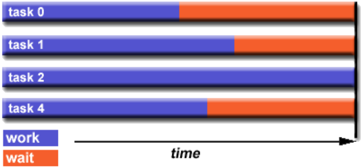

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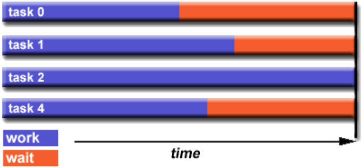
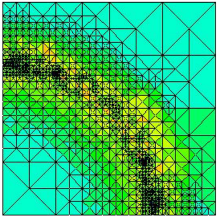


- requires well-balanced workload distribution between processors
- difficult in heterogeneous, dynamic problem sets with incomplete information about the actual workload



Load balancing (cont.)

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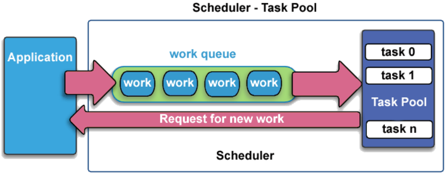
- alternatively, use asynchronous approach with scheduler-task pool with smaller workload packages



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- more on this in the "HPC & (Big) Data" talk!

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- profilers do **NOT** tell you **HOW** to optimize your code, they merely tell you **WHERE** to (potentially) do so for the best yield.

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```
Function stats for (_MainThread) (0)

Clock type: WALL
Ordered by: totaltime, desc

name                                  ncall  tsub      ttot      tavg
..hon3.8/threading.py:859 Thread.run  2      0.000017  44.09970  22.04985
..eads_revisited/helper.py:26 runall  2      0.002906  44.09969  22.04984
time_trials_threading.py:11 worker    10     0.052127  44.09676  4.409676
..ads_revisited/helper.py:10 foreach  1      0.000022  22.06303  22.06303
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..:1017 Thread._wait_for_tstate_lock  2      0.000014  22.06240  11.03120
time_trials_threading.py:23 g         10     0.084264  9.152582  0.915258
..._trials_threading.py:24 <listcomp> 10     7.603336  9.068318  0.906832
time_trials_threading.py:26 h         10     7.371068  8.857567  0.885757
time_trials_threading.py:19 f         10     5.973178  5.973178  0.597318
..ges/numpy/core/numeric.py:144 ones  10     0.000200  0.045074  0.004507
..ray_function__ internals>:2 copyto  10     0.000135  0.044414  0.004441
..n3.8/threading.py:834 Thread.start  2      0.000023  0.000501  0.000250
..hon3.8/threading.py:540 Event.wait  2      0.000014  0.000375  0.000188
...8/threading.py:270 Condition.wait  2      0.000027  0.000350  0.000175
..._revisited/helper.py:52 <listcomp> 1      0.000011  0.000091  0.000091
..8/threading.py:761 Thread.__init__  2      0.000039  0.000080  0.000040
...8/threading.py:505 Event.__init__  2      0.000006  0.000021  0.000010
..mpy/core/multiarray.py:1043 copyto  10     0.000018  0.000018  0.000002
..n3.8/threading.py:944 Thread._stop  2      0.000014  0.000016  0.000008
..hreading.py:222 Condition.__init__  2      0.000014  0.000014  0.000007
..reading.py:261 Condition._is_owned  2      0.000005  0.000009  0.000005
..8/threading.py:1306 current_thread  4      0.000008  0.000009  0.000002
..n3.8/_weakrefset.py:81 WeakSet.add  2      0.000007  0.000008  0.000004
..reading.py:246 Condition.__enter__  2      0.000004  0.000006  0.000003
..ing.py:255 Condition._release_save  2      0.000004  0.000005  0.000002
..hreading.py:249 Condition.__exit__  2      0.000005  0.000005  0.000002
..ython3.8/_weakrefset.py:38 _remove  2      0.000004  0.000004  0.000002
...py:258 Condition._acquire_restore  2      0.000001  0.000003  0.000002
..ython3.8/threading.py:734 _newname  2      0.000003  0.000003  0.000002
..ng.py:1177 _make_invoke_excepthook  2      0.000003  0.000003  0.000002
..reading.py:1095 _MainThread.daemon  4      0.000002  0.000002  0.000000
..n3.8/threading.py:513 Event.is_set  4      0.000001  0.000001  0.000000
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..n3.8/_weakrefset.py:81 WeakSet.add  2      0.000007  0.000008  0.000004
..reading.py:246 Condition.__enter__  2      0.000004  0.000006  0.000003
..ing.py:255 Condition._release_save  2      0.000004  0.000005  0.000002
..hreading.py:249 Condition.__exit__  2      0.000005  0.000005  0.000002
..ython3.8/_weakrefset.py:38 _remove  2      0.000004  0.000004  0.000002
...py:258 Condition._acquire_restore  2      0.000001  0.000003  0.000002
..ython3.8/threading.py:734 _newname  2      0.000003  0.000003  0.000002
..ng.py:1177 _make_invoke_excepthook  2      0.000003  0.000003  0.000002
..reading.py:1095 _MainThread.daemon  4      0.000002  0.000002  0.000000
..n3.8/threading.py:513 Event.is_set  4      0.000001  0.000001  0.000000
```

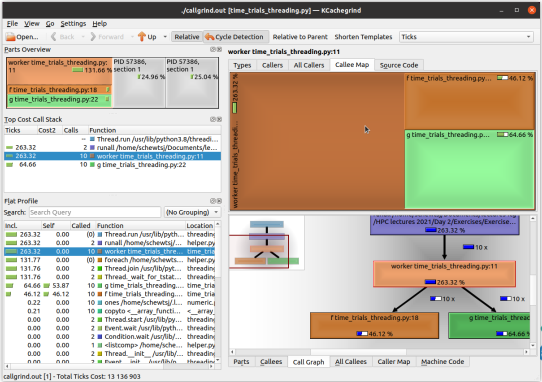

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- often, there are already "low-hanging fruits" in the serial code (reduction of I/O, amount of function calls, object conversions, etc.); demands in-depth knowledge of how things work "under the hood".
- tools like profilers can help you to identify what to optimize, but you still need the knowledge on how to do this.