Issues in HPC middlewares

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Last lecture: low-level HPC programming languages

Threads

- Thread programming models (user, kernel, mixed)
- PThread
- OpenMP

GPGPU

- Cuda
- OpenCL

MPI

Today lecture

Goals of the lecture

- understand links between OS and HPC middleware
- understand how HPC middleware can be improved
- think about some issues in HPC middleware

Methods

- lots of study cases
- some outdated, some still valid
- the way issues are solved are more important than the presented results

Extending OS interfaces for HPC

Improving low-level API

5. Optimizing communications
   - Optimizing communication methods
   - An experimental project: the Madeleine interface

6. Hierarchical plate-forms and efficient scheduling
   - Programming on current SMP machines
   - BubbleSched: guiding scheduling through bubbles

HPC implementation issues

7. Mixing threads and communications
   - Why?
   - Issues
   - A proposition
8. Asynchronous communications with MPI
   - MPI recall
   - MPI pathological behavior
9. Conclusion
   - High-performance parallel programming is difficult

Part I

Extending OS interfaces for HPC

An normalized API is not an implementation

- Even when normalized, an API can be implemented very differently
- Different possible focus: portability, performance, coverage (for optional parts of the standard)
- Examples: PThreads, MPI, OpenMP, etc.
- private extensions can be developed in order to offer new features or to guarantee better performances

Outlines: Extending OS interfaces for HPC

2. Linux POSIX Threads Libraries
   - History
   - Synchronization
3. Efficient network communications
4. Improving thread models

History: history

LinuxThread (1996) : kernel level, Linux standard thread library for a long time, not fully POSIX compliant

GNU-Pth (1999) : user level, portable, POSIX

NGPT (2002) : mixed, based on GNU-Pth, POSIX, not developed anymore

NPTL (2002) : kernel level, POSIX, current Linux standard thread library

PM2/Marcel (2001) : mixed, mostly POSIX compliant, lots of extensions for HPC (scheduling control, etc.)

From linuxthread to NPTL

LinuxThread: first “official” Linux thread library (1996)

- use available support (nearly none) from the Linux kernel
  - based on the `clone()` system call
  - implemented as processes that share their virtual memory
  - each thread has its own pid (and not tid)
  - no notion of multithreaded process from OS point of view

NPTL: developed in 2002 to have a real POSIX thread library

- based on new kernel features
  - notion of multithreaded processes introduced in the kernel
  - signals correctly handled
  - extension of `clone()` system call (synchronous notification of new thread, etc.)
  - new low-level synchronization service (*futex*)

Implementation of threads synchronizations

From signals. . .

- communication base of the linuxthread library
- the only support from the kernel at this time
- one 'manager' hidden thread
- race conditions and error prone
- not really efficient

. . . to futex

- synchronization in userspace (no system call) if no contention
- also allow synchronization between processes
- require specific support from the kernel used by NPTL
- since, kernel support improved for specific needs

Futex: powerful but complex interface

From the manpage:

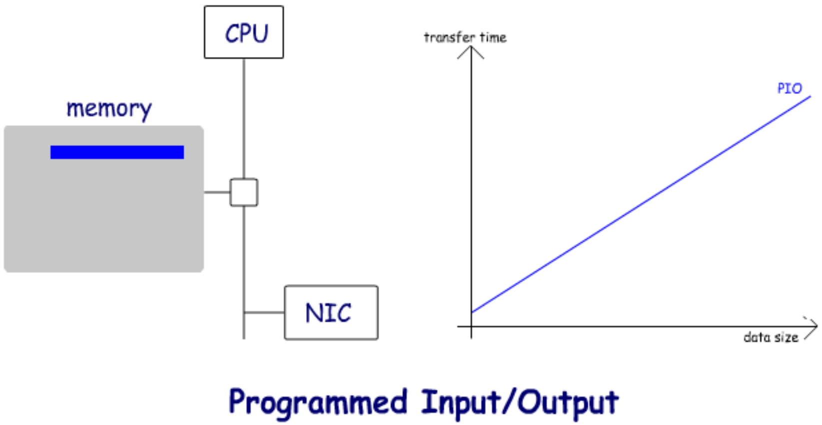
```
int futex(int *uaddr, int op, int val, const struct
          timespec *timeout, int *uaddr2, int val3);
[...]
Five operations are currently defined:
FUTEX_WAIT [...]
FUTEX_WAKE [...]
FUTEX_FD (present up to and including Linux 2.6.25)
   [...]
   Because it was inherently racy, FUTEX_FD has been
   removed from Linux 2.6.26 onward.
FUTEX_REQUEUE (since Linux 2.5.70)
   [...]
FUTEX_CMP_REQUEUE (since Linux 2.6.7)
   There was a race in the intended use of FUTEX_REQUEU
   so FUTEX_CMP_REQUEUE was introduced.
   [...]
```

Summary

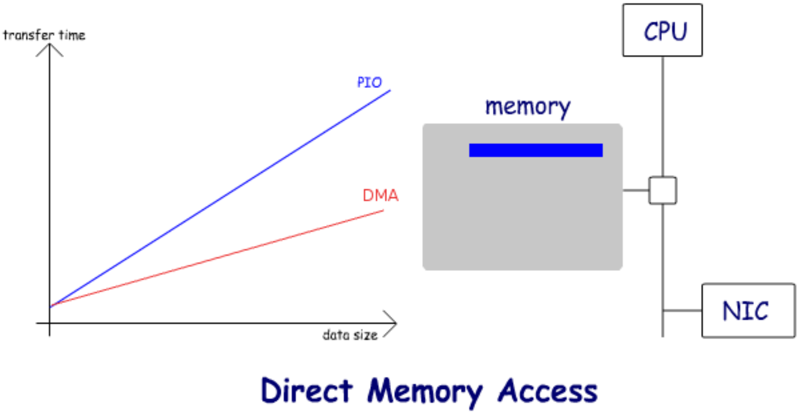
- without good OS support, no way to offer efficient and correct middleware
- designing the best OS support can be really tricky, especially for synchronization

Outlines: Extending OS interfaces for HPC

Interacting with the network card: PIO mode



Interacting with the network card: DMA mode



Zero-copy communications

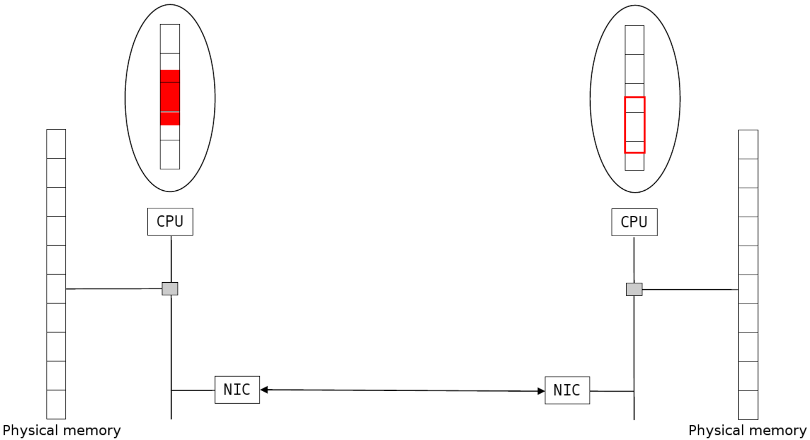
Goals

- Reduce the communication time
  - Copy time cannot be neglected
    - but it can be partially recovered with pipelining
- Reduce the processor use
  - currently, `memcpy` are executed by processor instructions

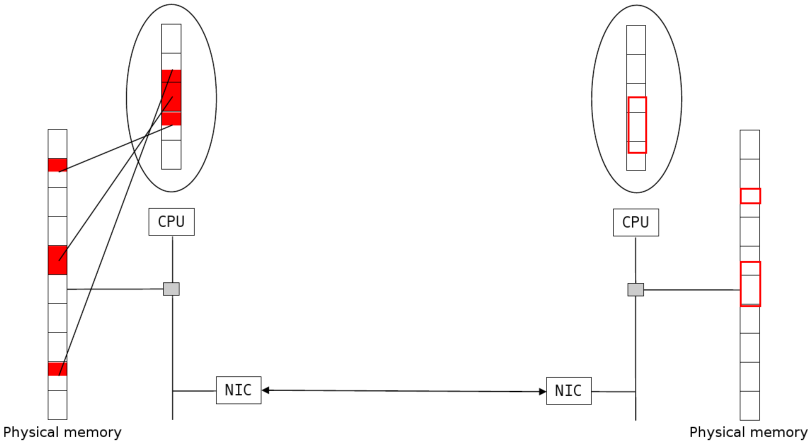
Idea

The network card directly read/write data from/to the application memory

Zero-copy communications



Zero-copy communications



Zero-copy communications for emission

PIO mode transfers

- No problem for zero-copy

DMA mode transfers

- Non contiguous data in physical memory
- Headers added in the protocol
  - linked DMA
  - limits on the number of non contiguous segments

Zero-copy communications for reception

A network card cannot “freeze” the received message on the physical media

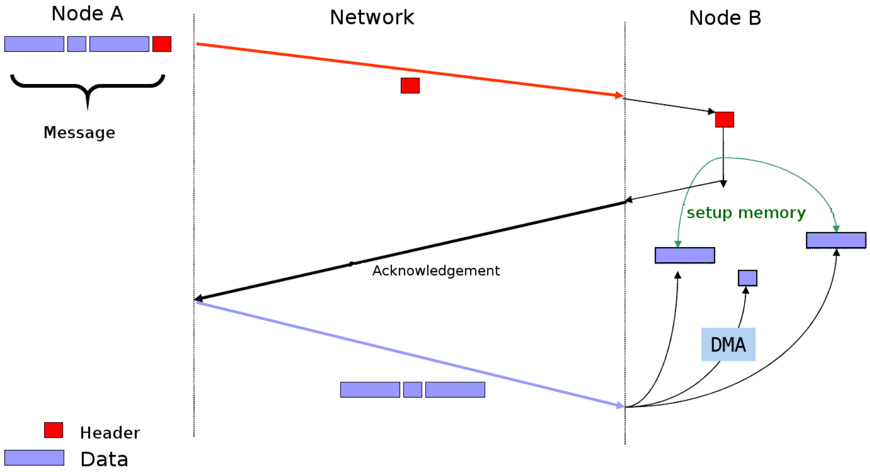
If the receiver posted a “recv” operation before the message arrives

- zero-copy OK if the card can filter received messages
- else, zero-copy allowed with bounded-sized messages with optimistic heuristics

If the receiver is not ready

- A handshake protocol must be setup for big messages
- Small messages can be stored in an internal buffer

Using a Handshake Protocol



A few more considerations

The receiving side plays an important role

- Flow-control is mandatory
- Zero-copy transfers
  - the sender has to ensure that the receiver is ready
  - a handshake (REQ+ACK) can be used

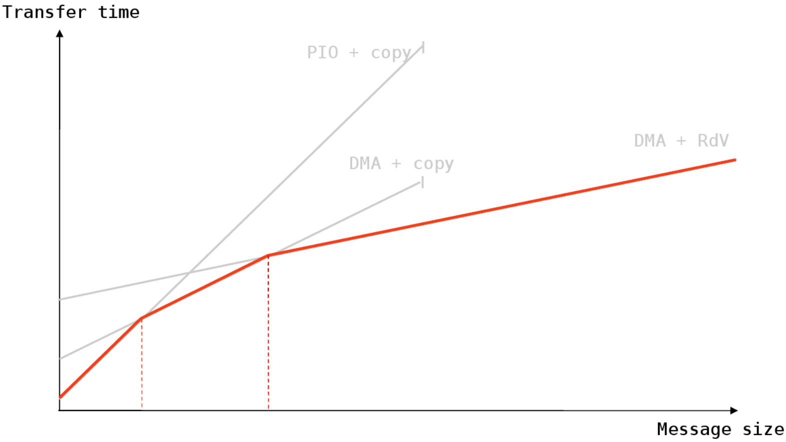
Communications in user-space introduce some difficulties

- Direct access to the NIC
  - most technologies impose “pinned” memory pages

Network drivers have limitations

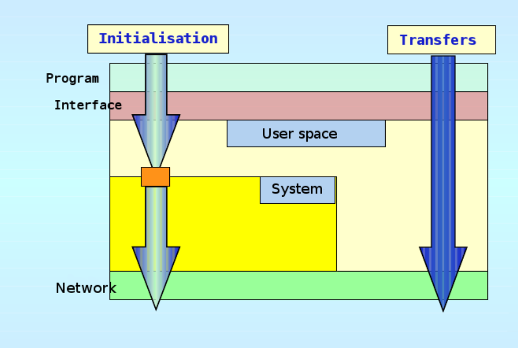
Communication Protocol Selection

Communication Protocol Selection



Operating System Bypass

- Initialization
  - traditional system calls
  - only at session beginning
- Transfers
  - direct from user space
  - no system call
  - “less” interrupts
- Humm. . . And what about security ?

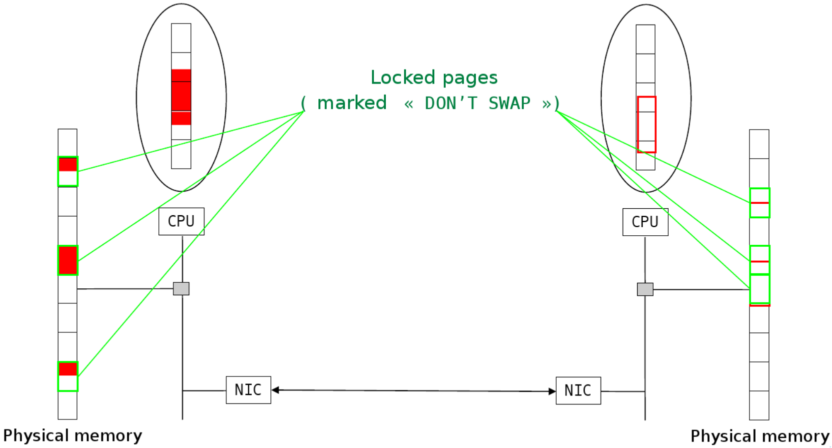


OS-bypass + zero-copy

Problem

- Zero-copy mechanism uses DMA that requires physical addresses
- Mapping between virtual and physical address is only known by:
  - the processor (MMU)
  - the OS (pages table)
- We need that
  - the library knows this mapping
  - this mapping is not modified during the communication
    - ex: swap decided by the OS, copy-on-write, etc.
- No way to ensure this in user space !

OS-bypass + zero-copy



OS-bypass + zero-copy

First solution

- Pages “recorded” in the kernel to avoid swapping
- Management of a cache for virtual/physical addresses mapping
  - in user space or on the network card
- Diversion of system calls that can modify the address space

Second solution

- Management of a cache for virtual/physical addresses mapping on the network card
- OS patch so that the network card is informed when a modification occurs
- Solution chosen by MX/Myrinet and Elan/Quadrics

Direct consequences

- Latency measure can vary whether the memory region used
  - Some pages are “recorded” within the network card
- Ideal case are ping-pong exchanges
  - The same pages are reused hundred of times
- Worst case are applications using lots of different data regions…

Outlines: Extending OS interfaces for HPC

2. Linux POSIX Threads Libraries
3. Efficient network communications
4. Improving thread models
   - Classical models
   - Scheduler Activations

Thread models characteristics

Library	Characteristics			
	Efficiency	Flexibility	SMP	Blocking syscalls
User	+	+	-	-
Kernel	-	-	+	+
Mixed	+	+	+	limited

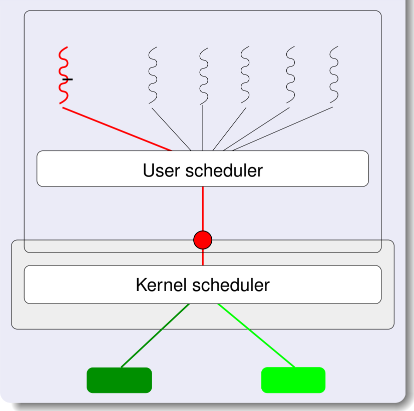
Summary

Mixed libraries seems more attractive however they are more complex to develop. They also suffer from the blocking system call problem.

User Threads and Blocking System Calls

User level library

Mixed library



Scheduler Activations

Idea proposed by Anderson et al. (91)

Dialogue (and not monologue) between the user and kernel schedulers

- the user scheduler uses system calls
- the kernel scheduler uses upcalls

Upcalls

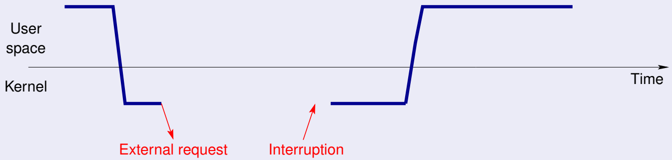
Notify the application of scheduling kernel events

Activations

- a new structure to support upcalls
  a kinf of kernel thread or virtual processor
- creating and destruction managed by the kernel

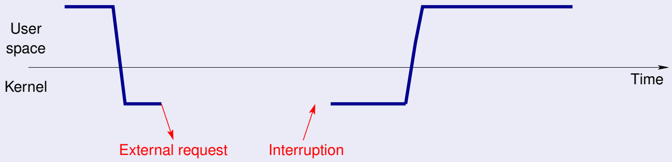
Scheduler Activations

Instead of:

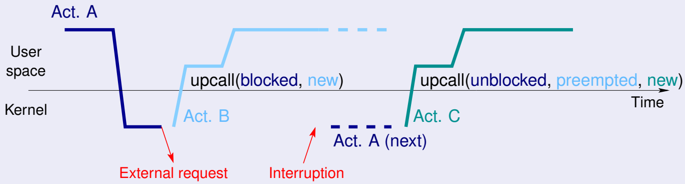


Scheduler Activations

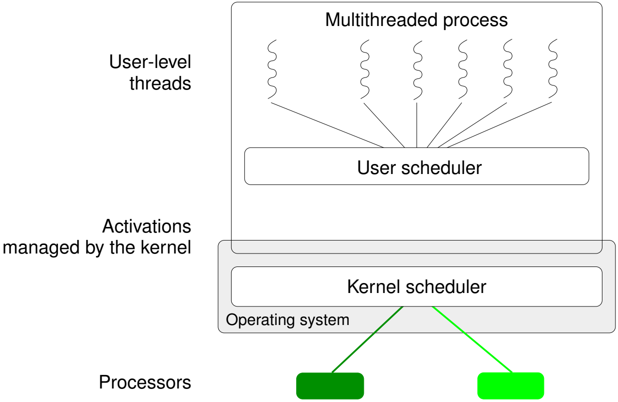
Instead of:



...better use the following schema:



Working principle



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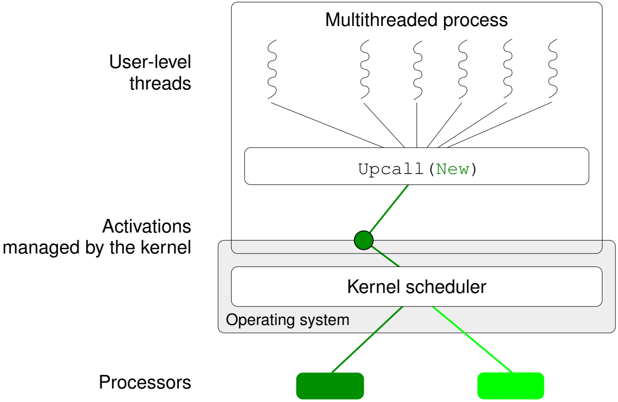

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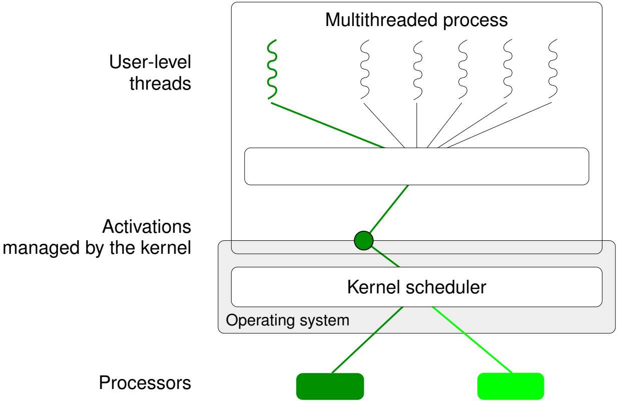

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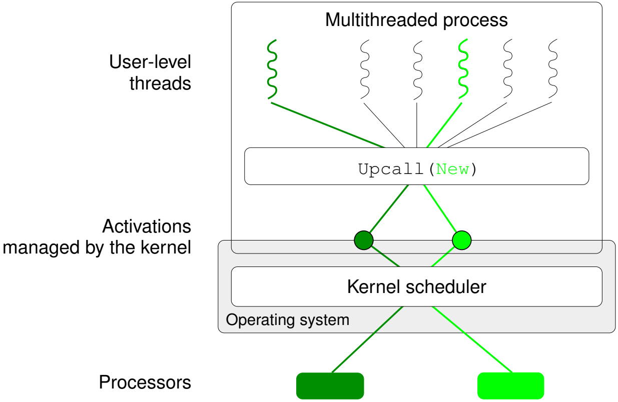
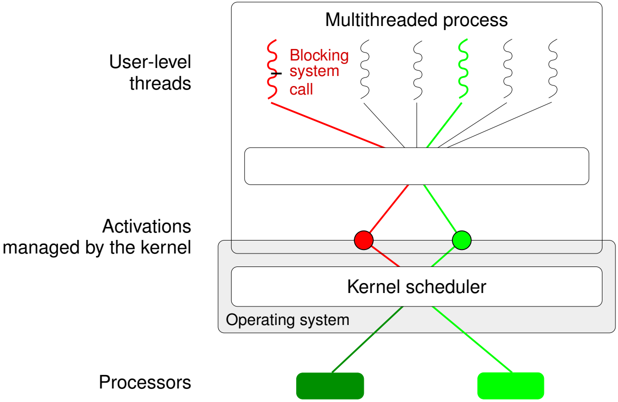
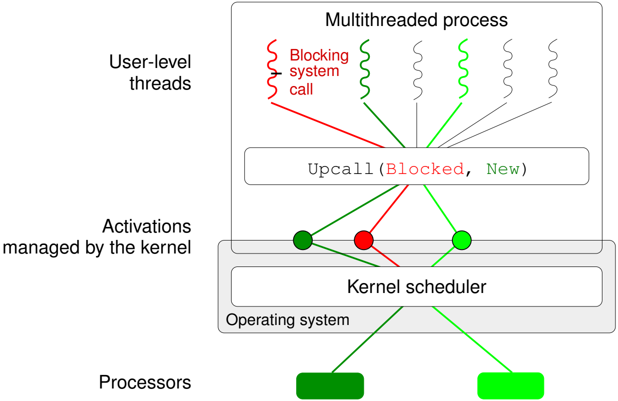


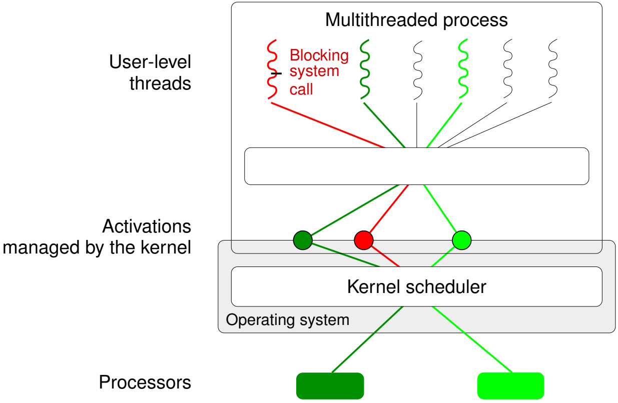
Working principle



Working principle



Working principle



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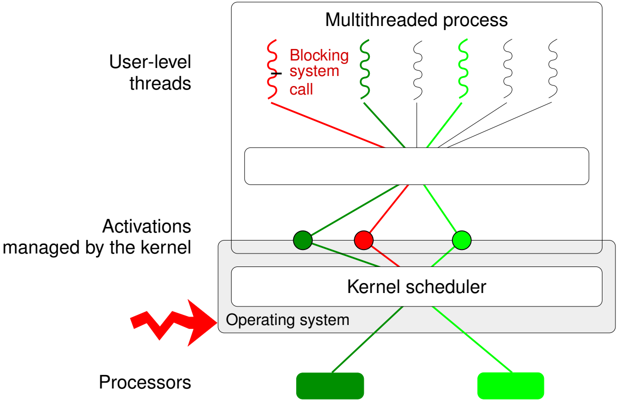

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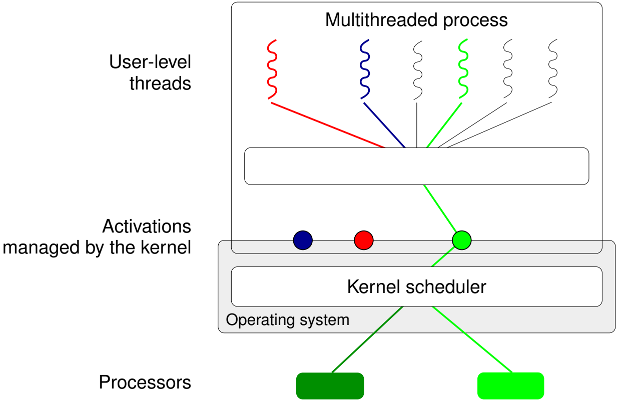

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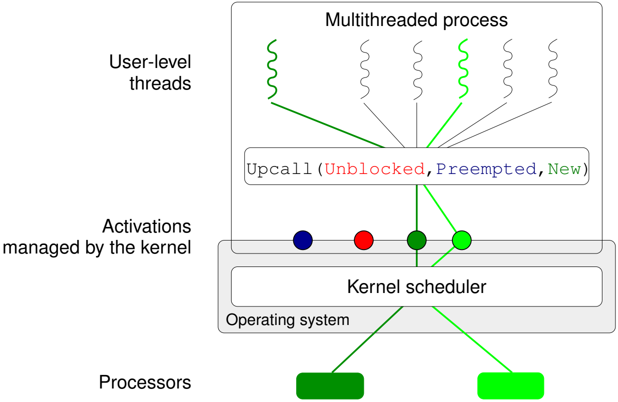


Summary on activations

The best thread model?

- efficient, flexible, SMP aware, **and** correctly handling blocking system calls
- patch for an old Linux kernel
- released for some time in FreeBSD

but a model not used nowadays

- complex to implement
- require a two-level thread library
  - very complex wrt POSIX for some features (signals, etc.)
  - not really efficient with multiple processes

Part II

Improving low-level API

Outlines: Improving low-level API

5 Optimizing communications
- Optimizing communication methods
- An experimental project: the Madeleine interface

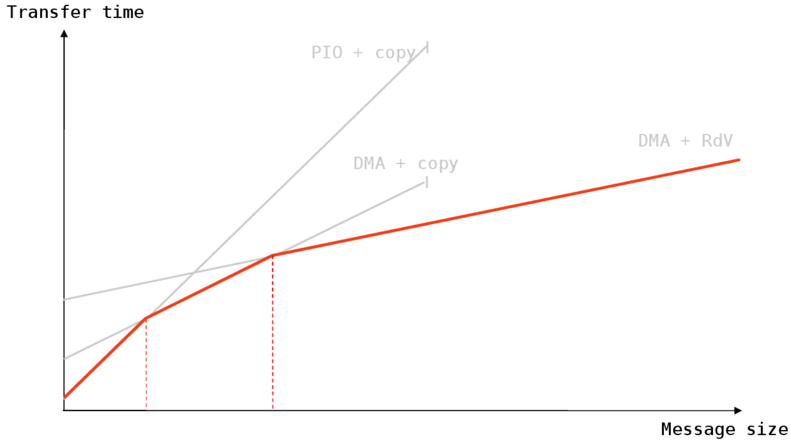
6 Hierarchical plate-forms and efficient scheduling

Optimizing communication methods

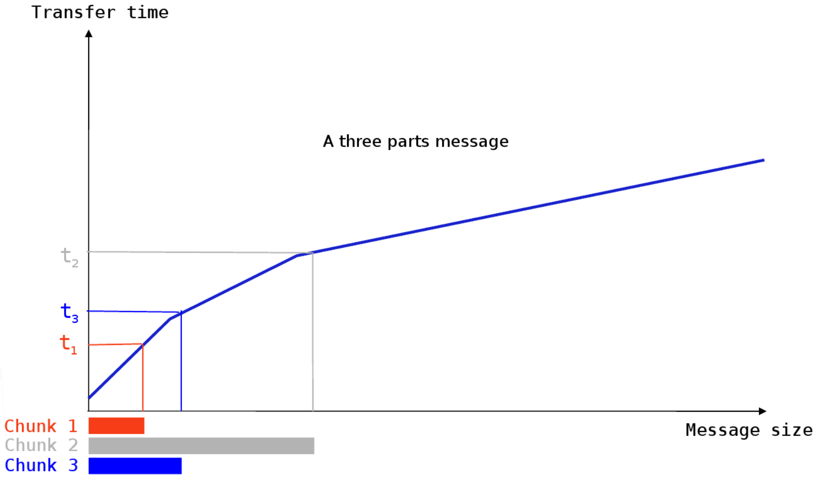
Low-level libraries sometimes prefer using the processor in order to guaranty low latencies

- Depending on the message size
  - PIO for small messages
  - Pipelined copies with DMA for medium messages
  - Zero-copy + DMA for large messages
- Example: limit medium/large is set to 32 KB for MX
  - sending messages from 0 to 32 KB cannot overlap computations

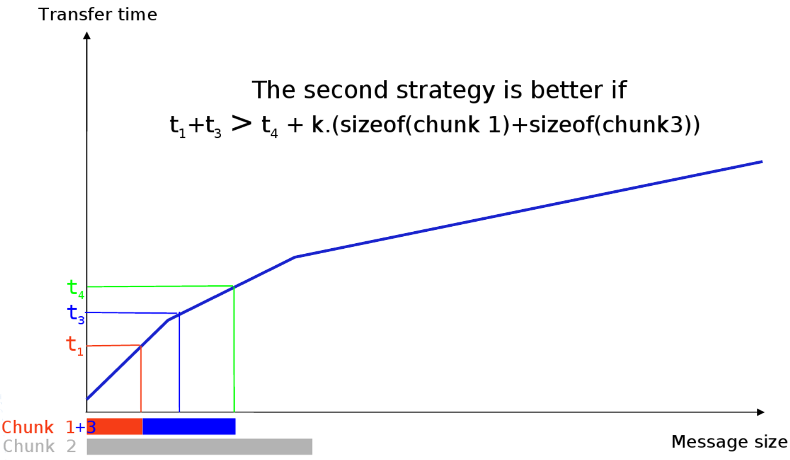
Choosing the Optimal Strategy



Choosing the Optimal Strategy



Choosing the Optimal Strategy



Choosing the Optimal Strategy

It depends on

- The underlying network with driver performance
  - latency
  - PIO and DMA performance
  - Gather/Scatter feature
  - Remote DMA feature
  - etc.
- Multiple network cards ?

But also on

- memory copy performance
- I/O bus performance

Efficient AND portable is not easy

An experimental project: the Madeleine interface

Goals

Rich interface to exchange complex message while keeping the portability

Characteristics

- incremental building of messages with internal dependencies specifications
  - the application specify dependencies and constraints (semantics)
  - the middle-ware automatically choice the best strategy
- multi-protocols communications
  - several networks can be used together
- thread-aware library

Message building

Sender

```
begin_send(dest)

pack(&len, sizeof(int))


pack(data, len)





end_send()
```

Receiver

```
begin_recv()

unpack(&len, sizeof(int))

data = malloc(len)
unpack(data, len)





end_recv()
```

Message building

Sender

```
begin_send(dest)

pack(&len, sizeof(int),
   r_express)

pack(data, len,
   r_cheaper)

end_send()
```

Receiver

```
begin_recv()

unpack(&len, sizeof(int),
   r_express)
data = malloc(len)
unpack(data, len,
   r_cheaper)

end_recv()
```

Message building

Sender

```
begin_send(dest)

pack(&len, sizeof(int),
  r_express)

pack(data, len,
  r_cheaper)

pack(data2, len,
  r_cheaper)

end_send()
```

Receiver

```
begin_recv()

unpack(&len, sizeof(int),
  r_express)
data = malloc(len)
unpack(data, len,
  r_cheaper)
data2 = malloc(len)
unpack(data2, len,
  r_cheaper)

end_recv()
```

How to implement optimizations ?

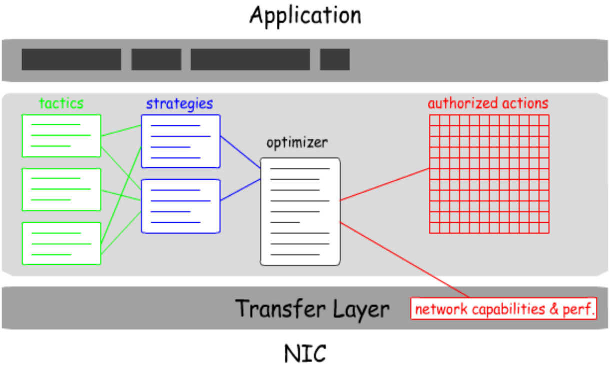
Using parameters and historic

- sender and receiver always take the same (deterministic) decisions
- only data are sent

Using other information

- allow unordered communication (especially for short messages)
  - can required controls messages
- allow dynamically new strategies (plug-ins)
- use “near future”
  - allow small delays or application hints

Optimisations « Just-in-Time »



Courtesy of Olivier Aumage

Why such interfaces ?

Portability of the application

No need to rewrite the application when running on an other kind of network

Efficiency

- local optimizations (aggregation, etc.)
- global optimizations (load-balancing on several networks, etc.)

But non standard interface

rewrite some standard interfaces on top of this one

- some efficiency is lost

Still lots of work

What about

- equity wrt. optimization ?
- finding optimal strategies ?
  - still an open problem in many cases
- convincing users to try theses new interfaces
- managing fault-tolerance
- allowing cluster interconnections (ie high-speed network routing)
- allowing connection and disconnections of nodes
- etc.

Outlines: Improving low-level API

5 Optimizing communications

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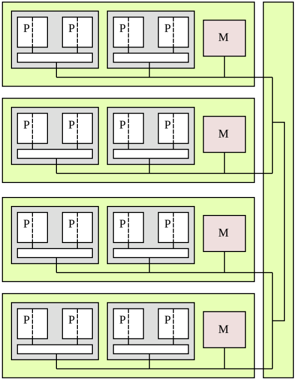
- Programming on current SMP machines
- BubbleSched: guiding scheduling through bubbles

Towards more and more hierarchical computers

- SMT

  (HyperThreading)
- Multi-Core
- SMP
- Non-Uniform Memory Access (NUMA)



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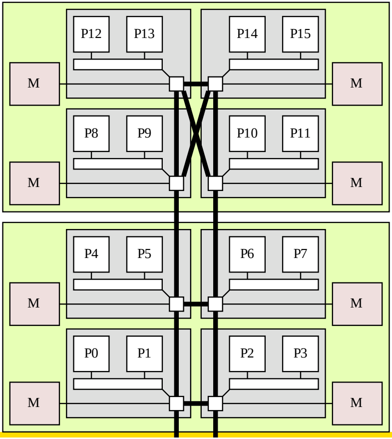
Hagrid, octo-dual-core

- AMD Opteron
- NUMA factor 1.1-1.5



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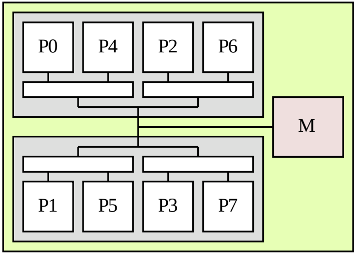
Aragog, dual-quad-core

- Intel
- Hierarchical cache levels



Courtesy of Samuel Thibault

How to run applications on such machines?

Courtesy of Samuel Thibault

How to program parallel machines?

- By hand
  - Tasks, POSIX threads, explicit context switch
- High-level languages
  - Processes, task description, OpenMP, HPF, UPC, ...
- Technically speaking, threads
- How to schedule them efficiently?

How to schedule efficiently?

- Performance
  - Affinities between threads and memory taken into account
- Flexibility
  - Execution easily guided by applications
- Portability
  - Applications adapted to any new machine

Courtesy of Samuel Thibault

Predetermined approaches

- Two phases
  - Preliminary computation of
    - Data placement [Marather, Mueller, 06]
    - Thread scheduling
  - Execution
    - Strictly follows the pre-computation
- Example: PaStiX [Hénon, Ramet, Roman, 00]

✔ Excellent performances

✗ Not always sufficient or possible: strongly irregular problems...

Courtesy of Samuel Thibault

Opportunistic approaches

- Various greedy algorithms
  - Single / several [Markatos, Leblanc, 94] / a hierarchy of task lists [Wang, Wang, Chang, 00]
- Used in nowaday's operating systems
  - Linux, BSD, Solaris, Windows, ...

✔ Good portability

✗ Uneven performances

  - No affinity information...

Courtesy of Samuel Thibault

Negotiated approaches

- Language extensions
  - OpenMP, HPF, UPC, ...

✔ Portability (adapts itself to the machine)

✗ Limited expressivity (e.g. no NUMA support)

- Operating System extensions
  - NSG, liblgroup, libnuma, ...

✔ Freedom for programmers

✗ Static placement, requires rewriting placement strategies according to the architecture

Courtesy of Samuel Thibault

Issues

- Negotiated approach seems promising, but
  - Which scheduling strategy?
    - Depends on the application
  - Which information to take into account?
    - Affinities between threads?
    - Memory occupation?
  - Where does the runtime play a role?
- But there is hope!
  - Programmers and compilers do have some clues to give
  - Missing piece: structures

Courtesy of Samuel Thibault

BubbleSched

Guiding scheduling through bubbles

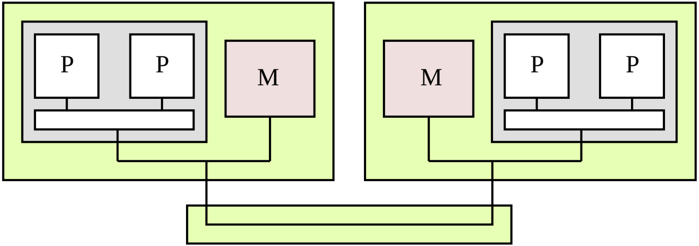
Idea: Structure to better schedule

Bridging the gap between programmers and architectures

- Grab the structure of the parallelism
  - Express relations between threads, memory, I/O, ...
- Model the architecture in a generic way
  - Express the structure of the computation power
- Scheduling is mapping
  - As it should just be!
  - Completely algorithmic
  - Allows all kinds of scheduling approaches

Courtesy of Samuel Thibault

Runqueues to model hierarchical machines



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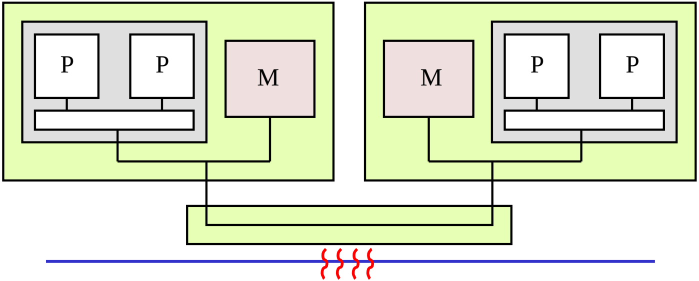

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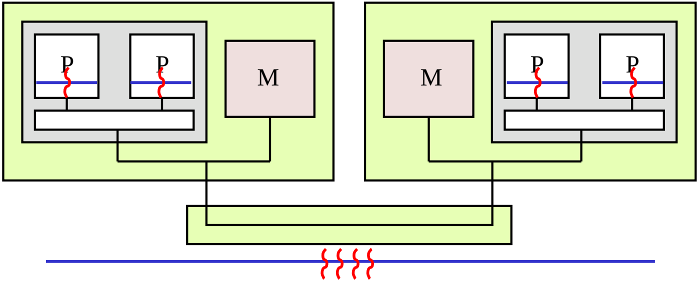

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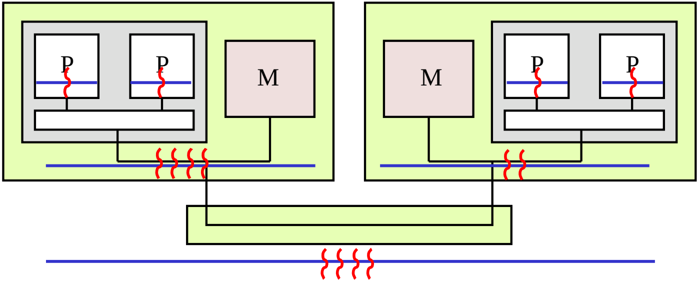
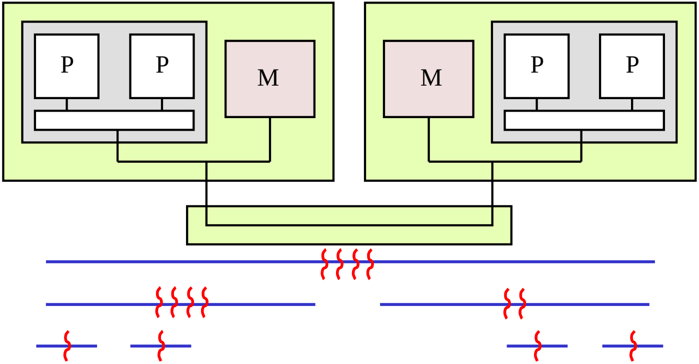
Runqueues to model hierarchical machines



Courtesy of Samuel Thibault

Runqueues to model hierarchical machines

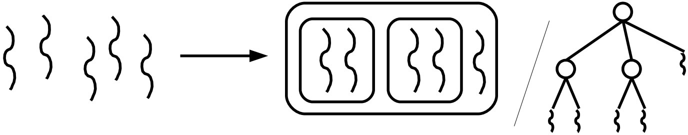


Courtesy of Samuel Thibault

Bubbles to model thread affinities

Keeping the structure of the application in mind

- Data sharing
- Collective operations
- ...



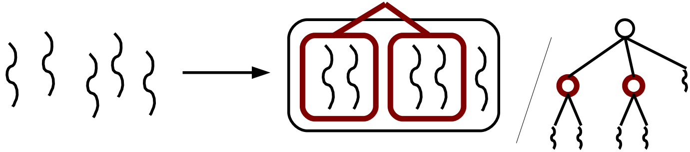
```
bubble_insert_thread(bubble, thread);
bubble_insert_bubble(bubble, subbubble);
```


Courtesy of Samuel Thibault

Bubbles to model thread affinities

Keeping the structure of the application in mind

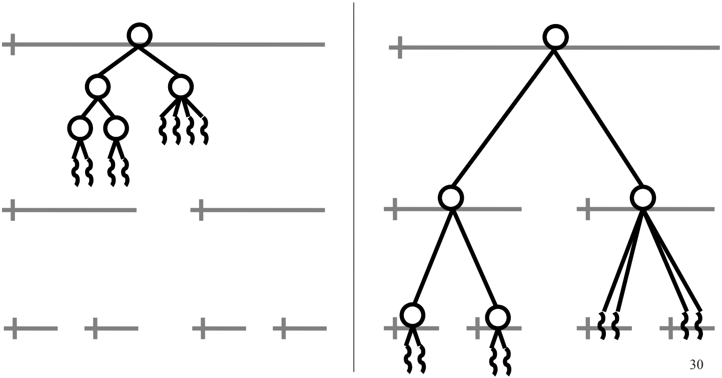
- Data sharing
- Collective operations
- ...




```
bubble_insert_thread(bubble, thread);
bubble_insert_bubble(bubble, subbubble);
```


Courtesy of Samuel Thibault

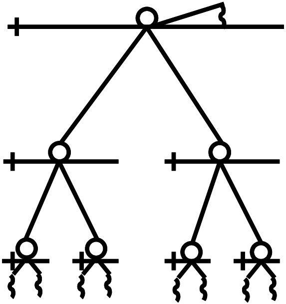
Examples of thread and bubble repartitions



Courtesy of Samuel Thibault

Implemented schedulers

- Full-featured schedulers
  - Gang scheduling
  - Spread
    - Favor load balancing
  - Affinity
    - Favor affinities (Broquedis)
    - Memory aware (Jeuland)
- Reuse and compose
  - Work stealing
  - Combined schedulers (time, space, etc.)



Courtesy of Samuel Thibault

Conclusion
A new scheduling approach

Structure & conquer!

- Bubbles = simple yet powerful abstractions
  - Recursive decomposition schemes
    - Divide & Conquer
    - OpenMP
- Implement scheduling strategies for hierarchical machines
  - A lot of technical work is saved
- Significant benefits
  - 20-40%

Courtesy of Samuel Thibault

Part III

HPC implementation issues

Outlines: HPC implementation issues

7. Mixing threads and communications
   - Why?
   - Issues
   - A proposition
8. Asynchronous communications with MPI
9. Conclusion

Mixing threads and communications

Problems: asynchronous communications required

- progression of asynchronous communications (MPI)
- remote PUT/GET primitives
- etc.

Solutions

- Using threads
- Implementing part of the protocol in the network card (MPICH/GM)
- Using remote memory reads

Multithreading

A solution for asynchronous communications

- computations can overlap communications
- automatic parallelism

But disparity of implementations

- kernel threads
  - blocking system calls, SMP
- users threads
  - efficient, flexible
- mixed model threads

Difficulties of threads and communications

Different way to communicate

- active polling
  - memory read, non blocking system calls
- passive polling
  - blocking system calls, signals

Different usable methods

- not always available
- not always compatible
  - with the operating system
  - with the application

An experimental proposition: an I/O server

Requests centralization

- a service for the application
- allow optimizations
  - aggregation of requests

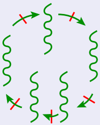
Portability of the application

- uniform interface
  - effective strategies (polling, signals, system calls) are hidden to the application
- application without explicit strategy
  - independence from the execution plate-form

I/O server linked to the thread scheduler

Threads and polling

- difficult to implement
- the thread scheduler can help to get guarantee frequency for polling
  - independent with respect to the number of threads in the application



instead of

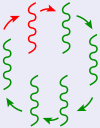


Illustration of such an interface

Registration of events kinds

`IO_handle=IO_register(params)`

- call-back functions registration
- used by communication libraries at initialization time

Waiting for an event

`IO_wait(IO_handle, arg)`

- blocking function for the current thread
- the scheduler will use the call-backs
  - communications are still manged by communication libraries

Example with MPI

Registration

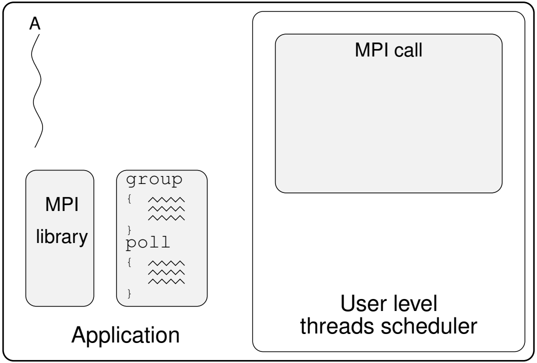
```
IO_t MPI_IO;
...
IO_register_t params = {
 .blocking_syscall:=NULL,
 .group=&group_MPI(),
 .poll=&poll_MPI(),
 .frequency=1
};

MPI_IO=
 IO_register(&params);
...
```

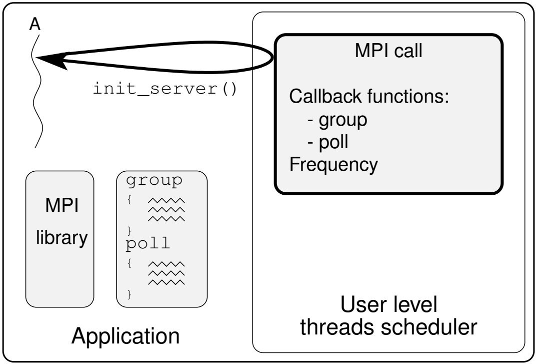
Communication

```
MPI_Request request;
IO_MPI_param_t param;
...
MPI_Irecv(buf, size,
    ..., &request);
param.request=&request;
IO_wait(MPI_IO, &param);
...
```

Running the scrutation server



Running the scrutation server



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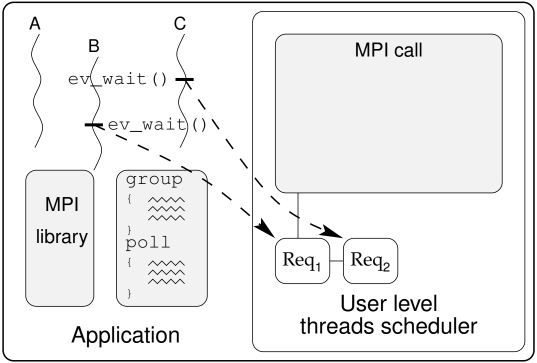

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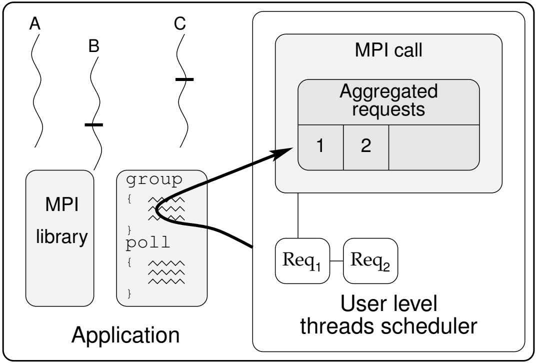

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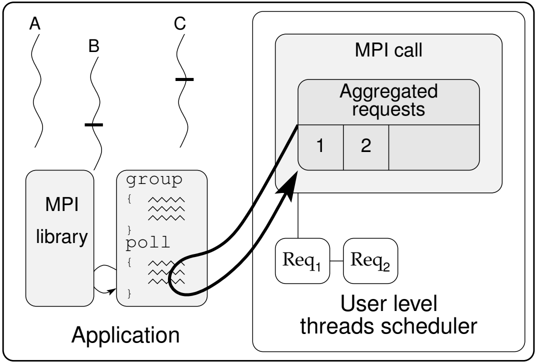

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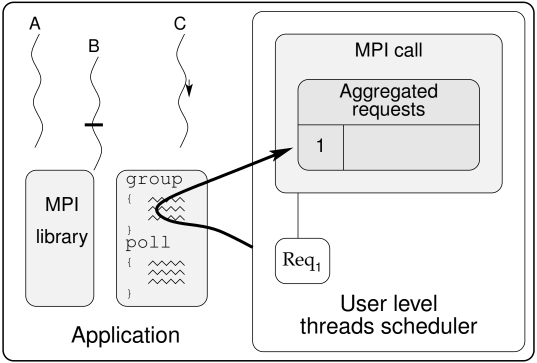

Key points

High level communication libraries needs multithreading

- allow independent communication progression
- allow asynchronous operations (puts/gets)

Threads libraries must be designed with services for communication libraries

- allow efficient polling
- allow selection of communication strategy

Mixing threads and communications

- mixing several efficient HPC libraries can lead to inefficient behaviors (conflictual optimizations)
- multi-criteria optimization is generally a good strategy
- this requires a co-design of all involved HPC libraries
- HPC programming is not a lego game

Outlines: HPC implementation issues

Message Passing Interface

Characteristics

- Interface (not implementation)
- Different implementations
  - MPICH
  - LAM-MPI
  - OpenMPI
  - and all closed-source MPI dedicated to specific hardware
- MPI 2.0 begins to appear

Several Ways to Exchange Messages with MPI

MPI_Send (standard)

- At the end of the call, data can be reused immediately

MPI_Bsend (buffered)

- The message is locally copied if it cannot be send immediately

MPI_Rsend (ready)

- The sender "promises" that the receiver is ready

MPI_Ssend (synchronous)

- At the end of the call, the reception started (similar to a synchronization barrier)

Non Blocking Primitives

MPI_Isend / MPI_Irecv (immediate)

```
MPI_request r;

MPI_Isend(..., data, len, ..., &r)

// Calculus that does not modify
'data'
MPI_wait(&r, ...);
```

These primitives must be used as much as possible

About MPI Implementations

- MPI is available on nearly all existing networks and protocols!
  - Ethernet, Myrinet, SCI, Quadrics, Infiniband, IP, shared memory, etc.
- MPI implementation are really efficient
  - low latency (hard), large bandwidth (easy)
  - optimized version from hardware manufacturers (IBM, SGI)
  - implementations can be based on low-level interfaces
    - MPICH/Myrinet, MPICH/Quadrics

BUT these “good performance” are often measured with ping-pong programs…

Asynchronous communications with MPI

Token circulation while computing on 4 nodes

```
if (mynode!=0)
  MPI_Recv();

req=MPI_Isend(next);
Work(); /* about 1s */
MPI_Wait(req);

if (mynode==0)
  MPI_Recv();
```

Asynchronous communications with MPI

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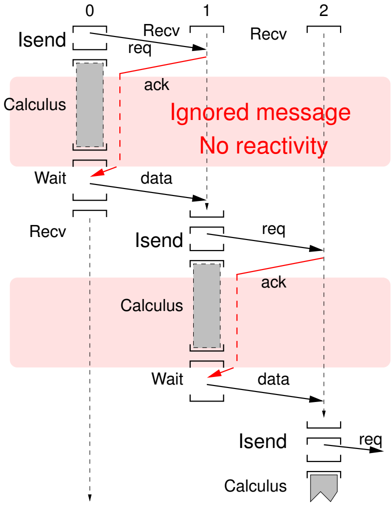
- expected time: ~ 1 s
- observed time: ~ 4 s

Asynchronous communications with MPI



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```

- expected time: ~ 1 s
- observed time: ~ 4 s

Lessons to learn

How to improve this behavior?

- requiring help from the programmer
- using the compiler
- using hardware RDMA
- using threads

Why not solved in all MPI implementations?

- threads not yet handled in all MPI implementations
- overhead to use (internal) threads in monothreaded applications
- not so many user interested (workaround already implemented, etc.)

Outlines: HPC implementation issues

7 Mixing threads and communications

8 Asynchronous communications with MPI

9 Conclusion
- High-performance parallel programming is difficult

High-performance parallel programming is difficult

Need of efficiency

- lots of efficient hardware available (network, processors, etc.)
- but lots of API

Need of portability

- applications cannot be rewritten for each new hardware
- use of standard interfaces (pthread, MPI, etc.)

On the way to the portability of the efficiency

- very difficult to get: still lots of research
- require very well designed interfaces allowing:
  - the application to describe its behavior (semantics)
  - the middle-ware to select the strategies
  - the middle-ware to optimize the strategies

- lots of criteria to optimize in real applications
  - scheduling, communication, memory, etc.
- multi-criteria optimization is more than aggregation of mono-criteria optimization
- other high-level interface programming for parallel applications ? (work-stealing, etc.)

Part IV

MPI Exercise

Matrix multiplication in MPI

How to write such a program?