Algorithms for modern shared-memory parallel architectures

Providing efficient HPC for everybody

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Overview

What my research is all about

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- In order to continue getting *faster*, programs need to become *more parallel*.
- Unfortunately, most current parallel approaches do not scale well.
- Better exploiting parallelism is possible, but requires completely re-thinking the algorithms we use.
- Doing things right can lead to performance gains of more than a factor of ten.
  $\longrightarrow$ Better use of existing and future infrastructure.
- Applied to interdisciplinary problems, which provide interesting computational questions, and require close collaborations to produce immediately useable software.
- In summary: Providing efficient High-Performance Computing for everybody.

Not faster, but more parallel

Increasingly parallel hardware

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- Until a few years ago, we could rely on computer processors getting faster every year (Moore's Law).
- Now, due to the physical limitations on individual processor speeds, computers are not getting *faster*, but *more parallel*.
- Instead of relying on increasing processor speeds to make codes continuously faster, we now need to rely on exploiting increasing parallelism.
- As a consequence, many problems that do not scale well or have reached their maximum degree of parallelism, won't get any faster. Ever.

Not faster, but more parallel

Distributed-memory parallelism

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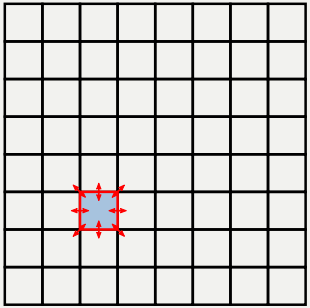
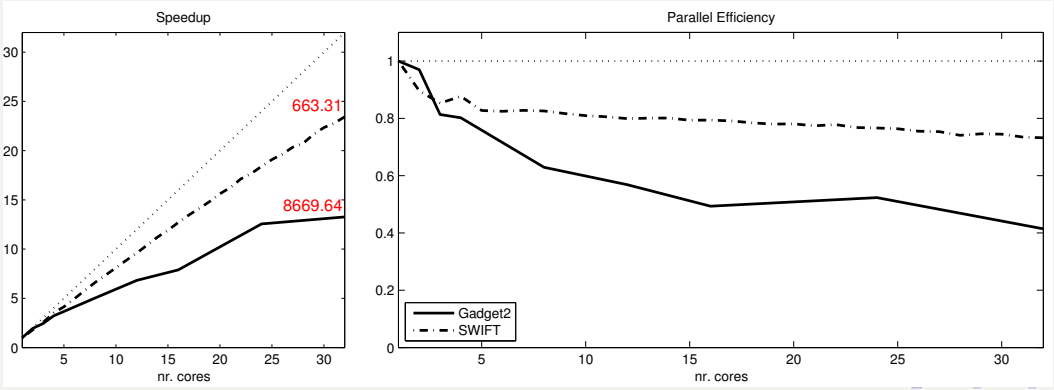
- Distributed-memory parallelism, e.g. using MPI, is based on data decomposition, i.e. each processor is assigned part of the problem to work on and communicates with its neighbours.
- Surface-to-volume ratio problem: As the number of cores increases, the amount of computation per core (volume) decreases while the relative amount of communication (surface) increases.
- The entire computation is then dominated by communication, thus seriously degrading parallel efficiency.



Case in point

Good vs. bad scaling

- Cosmological simulation (galaxy formation) with 1.8 M particles in a cubic box of 6.25 Mpc on a 4 $\times$ Intel Xeon X7550 with 32 cores, 2 GHz.
- GADGET-2, MPI-based, used for multi-billion particle simulations.
- SWIFT, my own code for the same problem. 13$\times$ faster on 32 cores.



Case in point
Performance benefits

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- Better value for money from existing computing infrastructure.
- Lowering the hardware costs makes HPC accessible to a much wider audience.
- Faster generation of research outputs in the application domain.
- Ability to study new problems beyond the range of what is currently possible.

Task-based parallelism

What it is

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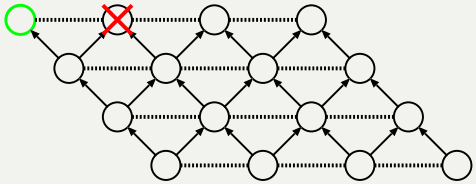
- Shared-memory parallel programming paradigm in which the computation is formulated in an implicitly parallelizable way that automatically avoids most of the problems associated with concurrency and load-balancing.
- We first reduce the problem to a set of inter-dependent tasks.
- For each task, we need to know:
  - Which tasks it depends on,
  - Which tasks it conflicts with.
- Each thread then picks up a task which has no unresolved dependencies or conflicts and computes it.



Task-based parallelism

Why it is good

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- The order in which the tasks are processed is dynamic and adapts automatically to load imbalances.
- If the dependencies and conflicts are specified correctly, we do not have to worry about concurrency at the level of the individual tasks.
  $\longrightarrow$ No need for expensive explicit locking, synchronization, or atomic operations.
- The same approach can be applied to more unconventional many-core systems such as general-purpose Graphics Processing Units (GPUs), making code reuse between different platforms easier.
- However, this usually means that we have to re-think our entire computation, e.g. redesign it from scratch to make it task-based.

My work in this area

Four main topics

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- Task-based computational models, i.e. develop memory-efficient, task-based algorithms for specific computational problems.
- Algorithms for task-based parallelism, i.e. task sorting, task clustering, task selection, and efficient task queues.
- New architectures, i.e. algorithms for emerging high-performance/low-cost many-core architectures, e.g. GPUs, the Intel MIC, or Adapteva's Epiphany IV.
- Hybrid shared/distributed-memory schemes, i.e. use both MPI and task-based parallelism on clusters of multi-cores, interleaving communication and computation such as to hide communication latencies.

My work in this area

Interdisciplinary research and applications

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- Tight coupling between theory and practice: all algorithms are implemented as part of specific interdisciplinary applications.
- I am currently working on two such software projects:
  - `mdcore`: An flexible and efficient library for shared-memory parallel Molecular Dynamics simulations on multi-cores and GPUs.
  - SWIFT: A hybrid shared/distributed-memory SPH and gravity simulation software for large-scale cosmological simulations.
- Interdisciplinary projects require close collaboration with a counterpart in the domain of application such as to make the results immediately useful.

My work in this area

Research outlook

- Continue work on `mdcore` and SWIFT, adding functionality as it becomes necessary by the application areas.
- Extend both software projects to emerging architectures, e.g. newer GPUs, the Intel MIC, and Adapteva's Epiphany IV architecture.
- Actively look for new interdisciplinary collaborations, both within and outside of traditional high-performance computing areas.

  $\longrightarrow$ Developing new, better, and useful algorithms, both for task-based parallelism in general, and for specific applications.

Conclusions
In summary

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- In order to continue getting *faster*, programs need to become *more parallel*.
- Task-based parallelism is a simple and efficient, cross-platform paradigm for shared-memory parallel computing.
- Speedups of ten times faster and more are possible.
- Theoretical results applied to interdisciplinary applications which provide interesting computational challenges.
- Much work still needs to be done, both in developing better task-based algorithms…But also in teaching the next generation of Computer Scientists to use them.
- In summary: Providing efficient High-Performance Computing for everybody.

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Thank you for your attention!