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Scaling the Geneva library collection to large HPC clusters

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Gemfony scientific UG (haftungsbeschränkt)

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of GSI Darmstad

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Who we are

- Gemfony scientific
  - A spinoff from Steinbuch Centre for Computing at Karlsruhe Institute of Technology
- With particular experience in the fields of
  - Optimization of complex systems
  - Technical- and Science-Consulting
  - Implementation of IT-Solutions
  - Technical Marketing, PR and Training
- Long standing bacground in parametric optimiuation
  - Gemfony maintains the Geneva library collection of distributed optimization algorithms

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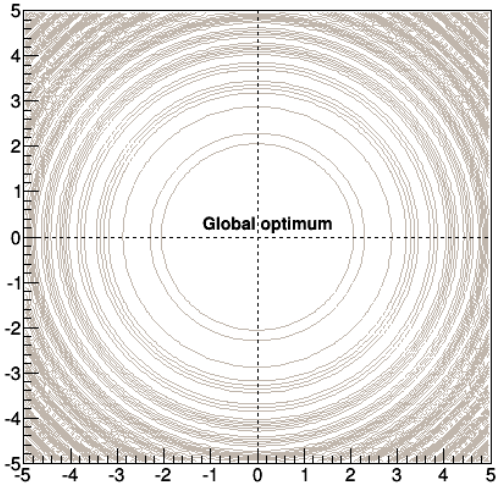
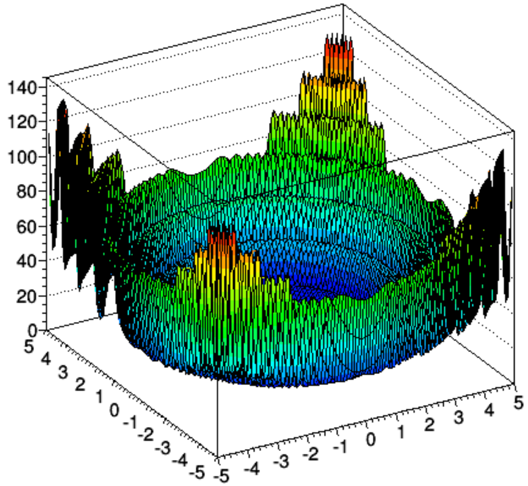
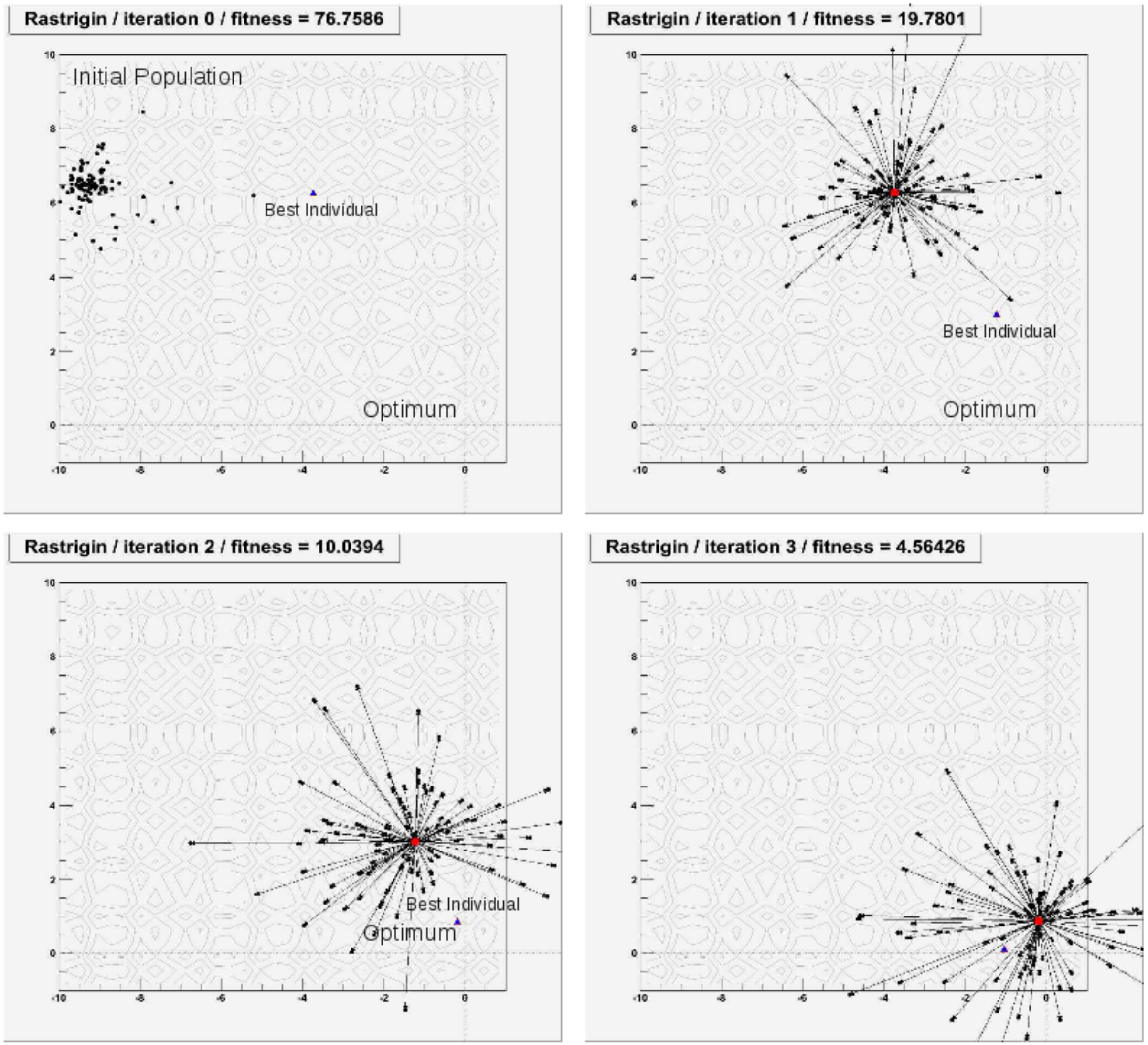
Parametric Optimization: Finding maxima or minina of $\vec{Q} = \vec{f}(x_1, x_2, \ldots, x_n)$





- Any mapping „f“ from input parameters to one or more numeric evaluations can be optimized
- For one evaluation criterion: optimization == finding suitable minima or maxima of solver „f“
  - Very similar to the search for extreme values of mathematical functions
  - „Solution space“ for multiple criteria
- However In the general case, „f“ will be a computer program
- Hence standard mathematical procedures cannot be applied easily
- Solvers may be computationally expensive
- As optimization algorithms will typically call the solver hundreds or thousands of times, such optimization problems will greatly benefit from parallelization

Parallelizability on the Example of Evolutionary Algorithms

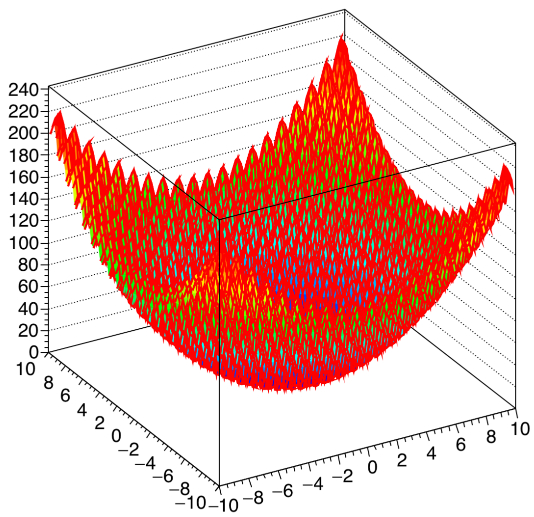

Rastrigin / iteration 0 / fitness = 76.7586

Rastrigin / iteration 1 / fitness = 19.7801

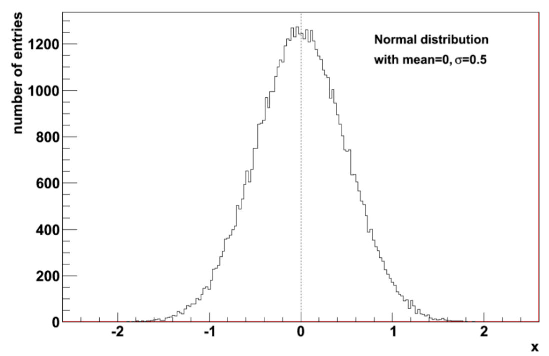
Rastrigin / iteration 2 / fitness = 10.0394

Rastrigin / iteration 3 / fitness = 4.56426

Surface plot of the Rastrigin function



„Gauss-Mutation“

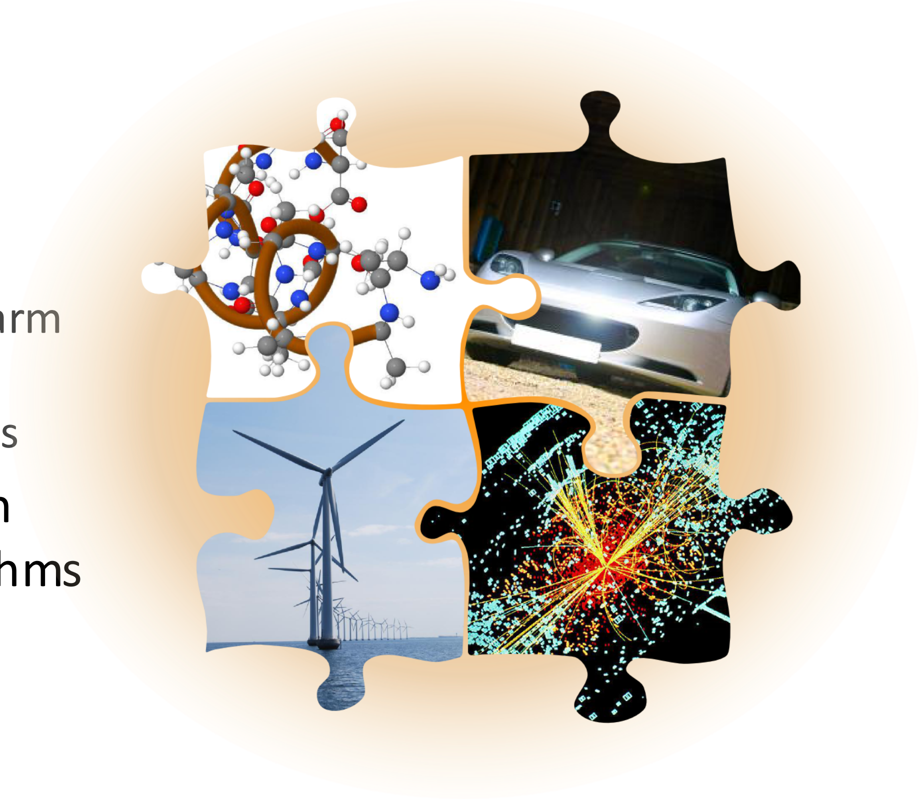


Why in „Massively Distributed Computing and Citizen Sciences“

- While this is probably not an exact fit:
  - Geneva is commercially supported Open Source (see http://www.launchpad.net/geneva)
  - Geneva particularly targets distributed and parallel execution
  - As optimization is a generic topic, application scenarios target just about every aspect of daily life
  - Free (simulation-)tools, along with cheap cloud resources, allow research to be performed by all scientifically interested parties

The Geneva Library Collection

- Generic solution for the search for **optimized solutions** of technical and scientific problems
- **„Metaheuristic“ Optimization**
  - Covering **Evolutionary Algorithms**, Swarm Algorithms, Simulated Annealing, Parameter Scans and Gradient Descents
- Data structures allow direct interaction between different optimization algorithms with **just one problem description**
- Written in portable C++
  - Uses the Boost library collection
  - Runs on different Unix variants (Linux, MacOS, ...) and Windows (experimental!)
- > 130.000 LOC (.hpp, .cpp, scripts, ...)



Sources:

- Car: Image courtesy of Simon Howden at FreeDigitalPhotos.net
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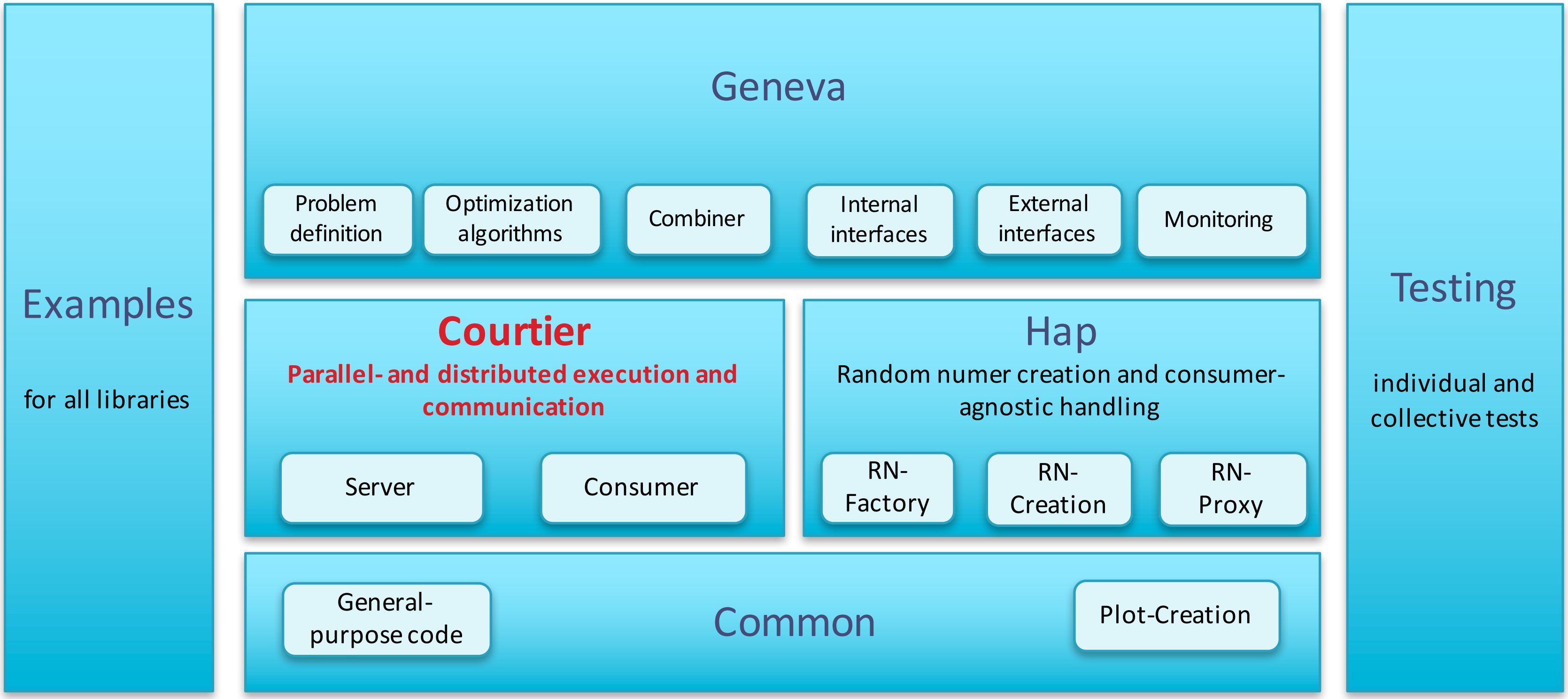
Library Components

Strong modularization allows for an efficient decoupling of evaluation and optimization!



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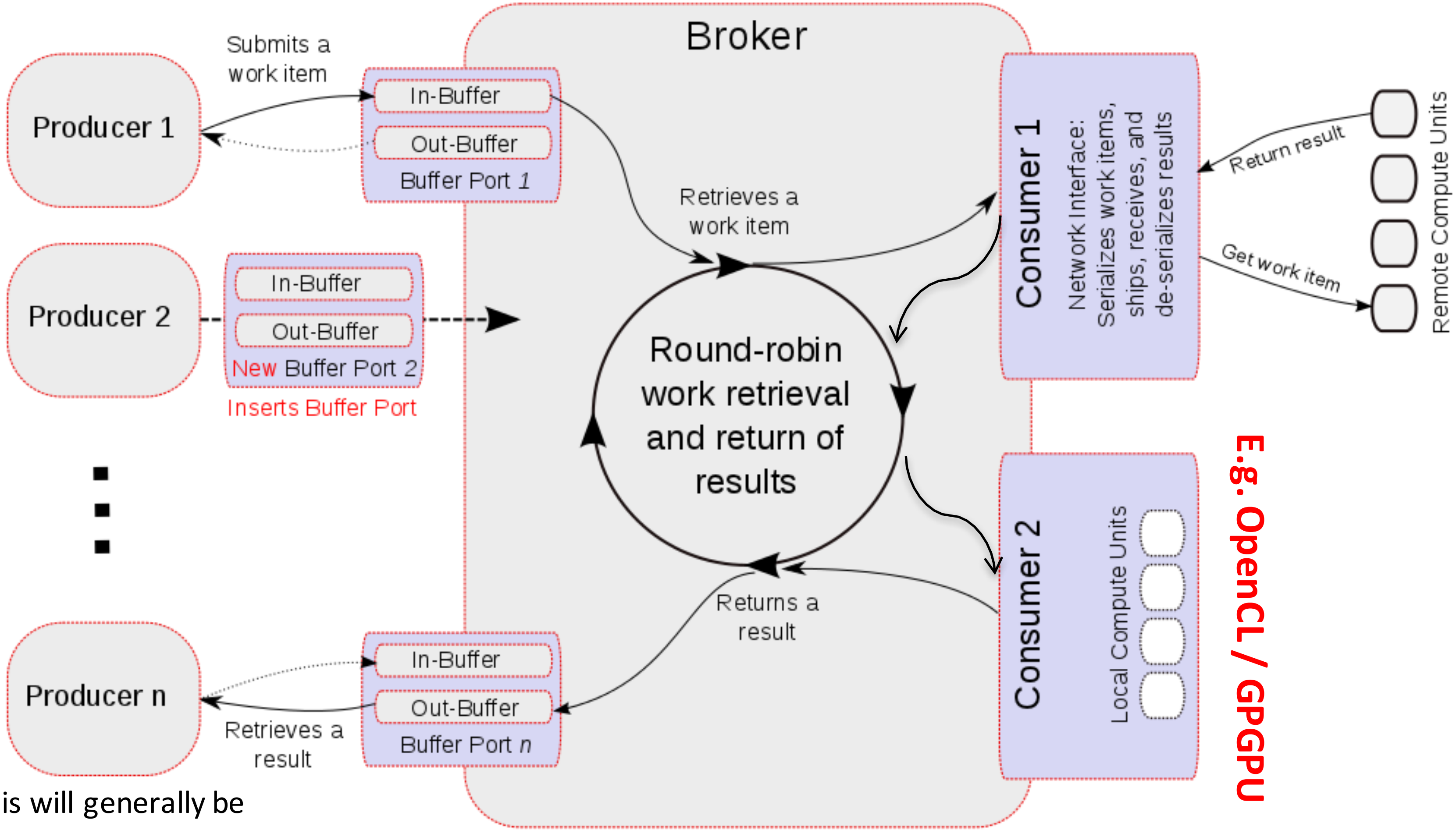
Source: Gemfony

Tuning Scalability

- „Performance“ is very problem-dependent
- In a nutshell, on the same hardware, performance improvements may be achieved in numerous ways, e.g.
  - Making the Geneva code more efficient
    - BUT: Focus on long-running evaluation-functions mandates focus on core-library stability rather than performance
    - Reducing run-time of the solver(s). But: task for the user
  - Making optimization algorithms converge faster
    - Minimization of Iterations needed to reach a given optimum
- But in particular: Parallelization of parallelizable parts
  - Reducing parallelization-overhead: „Amdahl“ may have a major impact on performance → Asynchronous transfer of candidate solutions
  - May need to cater for potentially thousands of clients, running for hours or days
- Reducing protocol overhead and improving stability is crucial

The „Courtier“ Library: Problem-Independent Parallelization

Source: Gemfony



E.g. OpenCL / GPGPU

This will generally be
An optimization algorithm

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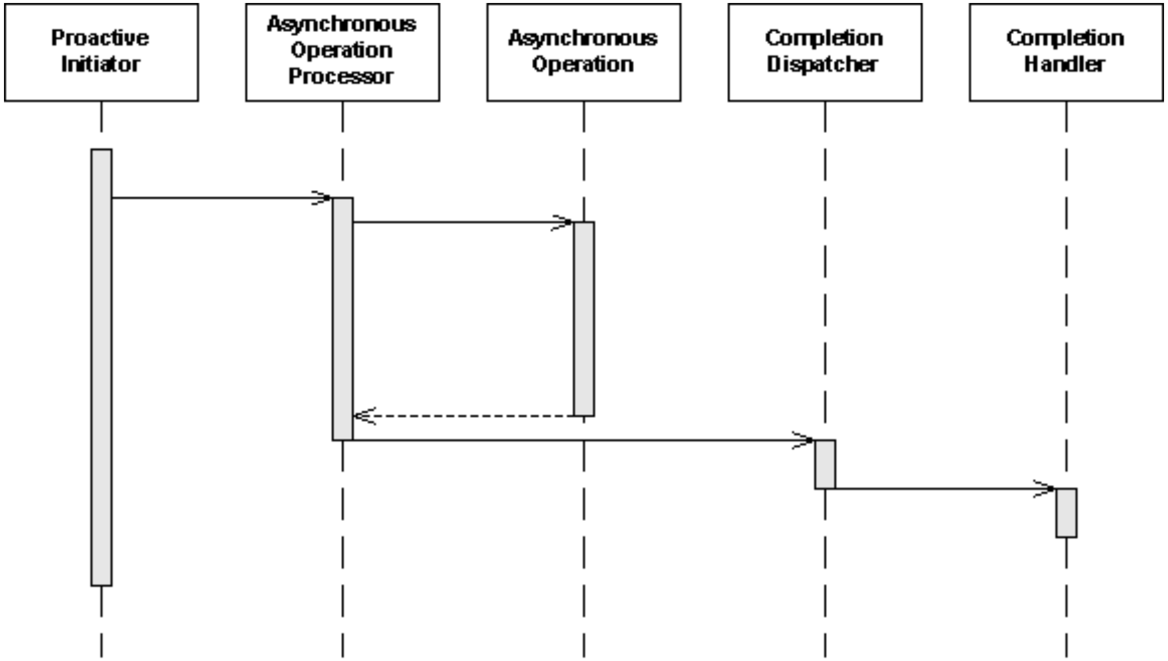
Proactor Pattern



- Boost.ASIO
  - Uses operating system parallelization
    - Thus very efficient
  - Will likely be part of the next standard C++17
  - Main usage: tcp networking in C++
    - Need to deal with TCP oddities on the lowest level

Picture source: Wikipedia „Proactor“, License CC-BY-SA 3.0, Author UlrichAAB

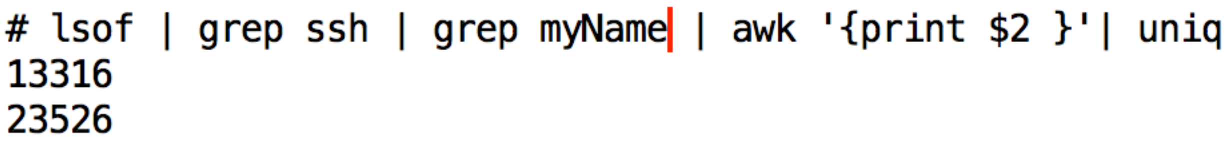
Dissecting the Network Mode (1)

- Current usage pattern in the release version (pull-mode!)
  - Client connects, retrieves work item, disconnects, does calculation, reconnects, transfers a result and retrieves the next work item
  - Many sockets are opened and closed
  - If calculation time and speed of clients is similar, connections may happen within a very small time window → long idle times for the server, followed by short periods of very high traffic
  - From the server-perspective, the problem may be quite similar to a high-load web-server
- Chosen, as, from the library perspective, there is no information about the length of an evaluation -- may take seconds or days
  - Server must cater for missing responses
  - Timeout must be calculated and possibly clients resubmitted, which may be problematic
- Scales to approx. 100 clients, but shows many problems beyond this

Dissecting the Network Mode (2) / How to tune a frequent-access Linux server ?

Follows http://www.lognormal.com/blog/2012/09/27/linux-tcpip-tuning/

- Simultaneously open files per process:
  - E.g. on MacOS: „ulimit –n“ returns 256. Even on a stock Ubuntu: only set to 1000
  - But every new socket requires a file handle ...
  - ... and even when a socket is closed, the handle is kept around, possibly for minutes, depending on the TCP/IP implementation
- Supply of “short-lived“ ports
  - By default 32768 – 61000 (range may be slightly increased)
  - Every new connection consumes a new port
    - E.g. two ssh connections to a server yields



```
# lsof | grep ssh | grep myName | awk '{print $2 }'| uniq
13316
23526
```

  - Unused ports are recycled ... after some time

Dissecting the Network Mode (3) / How to tune a frequent-access Linux server ?

- TIME_WAIT
  - Purpose: Packages returning after a connection is closed do not confuse TCP
  - May last long ... 2 minutes not uncommon
  - Affects open files, ephemeral ports
- iptables / Connection Tracking
  - iptables needs to allow two-way communication through the firewall
  - Needs to track connections
  - Keeps a list of connections, whose state is kept in a list
  - The list may not exceed a given limit
  - Will lead to silent failures if it does

Dissecting the Network Mode (4) / How to tune a frequent-access Linux server ?

- „nf_conntrack_tcp_timeout_established“
  - Timeout for established connections
  - Has very high default value of 432000 seconds
- Saturation of server by many simultaneous connections
  - De-Serialization in C++ (using Boost.Serialization) may be very costly
  - Must make sure (de-)serialization is disconnected from accepting new connections, or the server may not be responsive
- Queue-flooding in pull-mode
  - Where a timeout is reached, work items may need to be resubmitted.
  - Resubmission happens through a queue
  - Where timeout-values are not coupled (correctly) to the average compute time of clients, the queue will be flooded with work items
  - Need to make sure consumption rate is higher than submission rate

In summary, problems relate to …

- TCP/IP oddities
- Firewall deficiencies
- Internal architecture of Geneva

→ Not an easy problem

→ Need to reduce complexity!

→ Current design goal: Use a Websocket-type server architecture. May solve MANY of the above problems

Websockets (1)

- Client never disconnects
  - Reduces complexity on the TCP level
  - Reduces overhead for handshakes
  - May even allow a push-mode, without fear of queue-flooding
  - May inform clients about shutdowns (formerly they would have to terminate, when the server became unrechable)
- Must deal with TCP-timeouts
  - "Paylod-communication" may still only happen in very long intervals, as the client may just sit there, doing calculations
  - Will need a „heart-beat"

Websockets (2)

- Current implementation derived from „eidheim / Simple-Websocket-Server“ (see https://github.com/eidheim/Simple-WebSocket-Server)
  - MIT-licensed
  - Based on Boost.ASIO
  - Pure C++11
- Removed the pure „Websocket“ part, but kept part of the architecture

Websockets (3)

- Communication now happens on two levels:
  - Administrative (initial hand-shake, keep-alive in regular intervals)
  - Payload (exchange of work-items and results)
- Payload-protocol is implemented on top of the message-transfer
- Administrative and payload-messages enter the same queue → submission in the order they entered the queue
- Payload processing needs to happen in own thread-pool to keep client and server responsive

Summary

- High-throughput / high frequency TCP communication in C++ is CHALLENGING
- Current Design seems to be far more responsive
- Not yet part of a stable release
- Needs further tests
- Will be part of Geneva 2.0, which also represents a major redesign (C++14, simpler creation of new optimization algorithms, Broker-only architecture for parallelization, ...)

Thank you / Contact

Thanks
to the audience and the GSI team!

If you want to try Geneva:

http://launchpad.net/geneva

You may reach us at

contact@gemfony.eu

The project-team wants to thank Karlsruhe Institute of Technology, Steinbuch Centre for Computing as well as the Helmholtz-Association for supporting our work!

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