Distributed Supercomputing for climate modeling?

Dr. Jason Maassen
Technology Lead Efficient Computing
Netherlands eScience Center

netherlands eScience center

by SURF & NWO

Netherlands eScience Center

By Frits Ahlefeldt

Bridging the gap between research and e-infrastructure

30 eScience Research Engineers

Broadly oriented scientists

at the interface of research and ICT

Close collaboration with researchers

to implement eScience projects and technology

Developing usable & sustainable tools

suitable for a broad range of users

eScience center

Background: eSalsa Project

(2012-2015)

Predict **local** sea-level changes (caused by climate change) with an unprecedented level of detail.

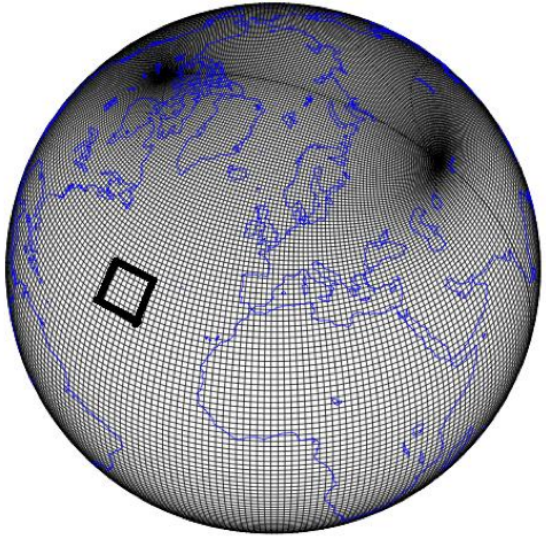
Utrecht University (IMAU)
Prof. Henk Dijkstra (Ocean Modeling)
Dr. Sandra Brunabend

VU University (CS-HPDC)
Prof. Bal (GPU computing)
Dr. Ben van Werkhoven

Netherlands eScience Center
Dr. Jason Maassen (Distributed Computing)
Drs. Maarten van Meersbergen (Visualization)

Source: Actueel Hoogtebestand Nederland

Typical Supercomputer application



Source: Los Alamos National Laboratory

Catresius Supercomputer (source: SURFSara)

POP at 0.1° resolution (10x10 km)

3600 x 2400 x 42 ≈ 360 million grid points

Single 100 year simulation takes **weeks** on 2~4K cores. Need ensemble of 10's.

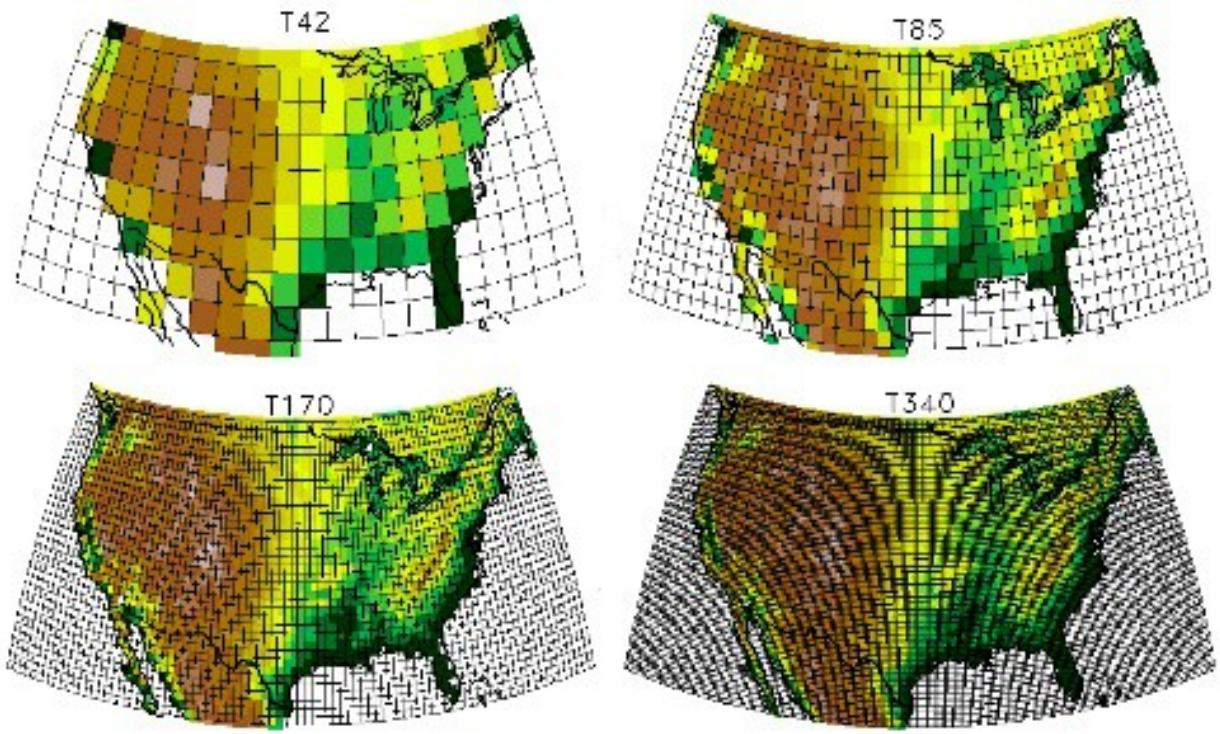
Quest for Higher Resolution

Scientists want higher model resolution (this gives more detailed results).

Ultimate goal:

0.01° resolution (1x1 km)
fully eddie resolving

100~250x increase in compute time!



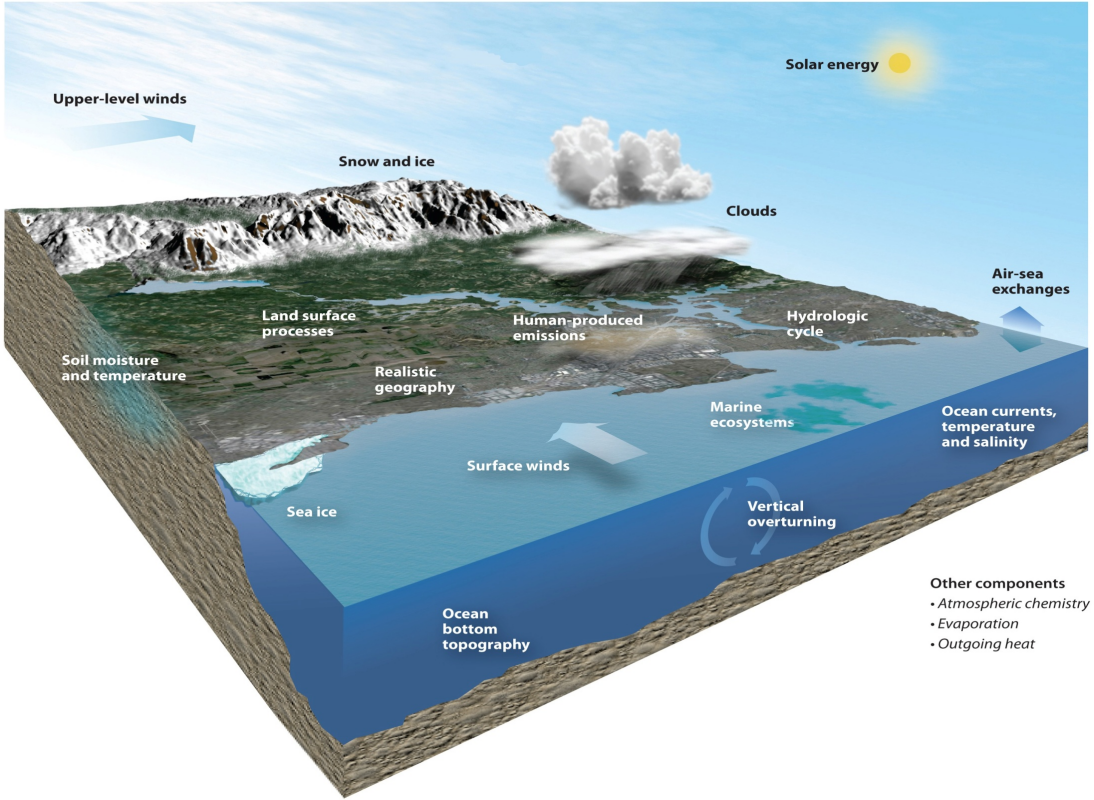
Source: Illustration courtesy Warren Washington, NCAR

Earth System Modeling

Climate is more than just ocean!

Scientist also want to **combine** ocean, land, ice and atmosphere models (to simulate the interactions)

2~3x increase in compute time.



Where do we get the compute power?

Accelerators

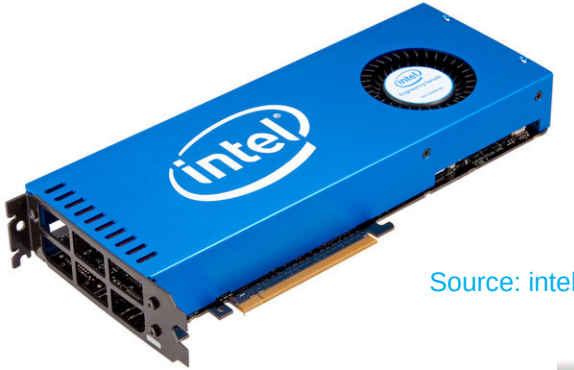
- for more compute power per node
- success, but slow progress!
- model implementations are diverging (CPU, GPU, Xeon Phi)

Source: nvidia

Distributed Computing

- for more overall compute power
- allows use of heterogeneous system

(focus of this presentation)



Source: intel

ENLIGHTEN YOUR RESEARCH GLOBAL

Spinoff of the eSalsa project at the Netherlands eScience Center

Our a submission to **Enlighten Your Research global** competition in 2013

…. and we where one of the winners!

Enlighten Your Research Global 2013/14

Top 500 #10
2.9 PFlop/s

SUPERMUC (GER)

10G

Top 500 #184
223 Tflop/s

CARTESIUS (NLD)

10G

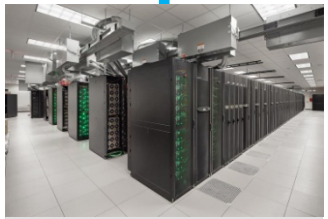
114 TFlop/s

EMERALD (UK)

GPUs

10G

GPUs



STAMPEDE (USA)

Top 500 #7
5.1 PFlop/s

Xeon Phi

Extremely ambitious goal: combine 2 or 3 supercomputers from Europe and the US to run Earth System Model at 0.02° (2x2 km) resolution!

Requires a lot of international cooperation!

19 project members:

- *5 climate researchers*
- *9 computer scientist*
- *5 system and network specialist*

4 countries (NL, US, UK, DE)

4 research institutes

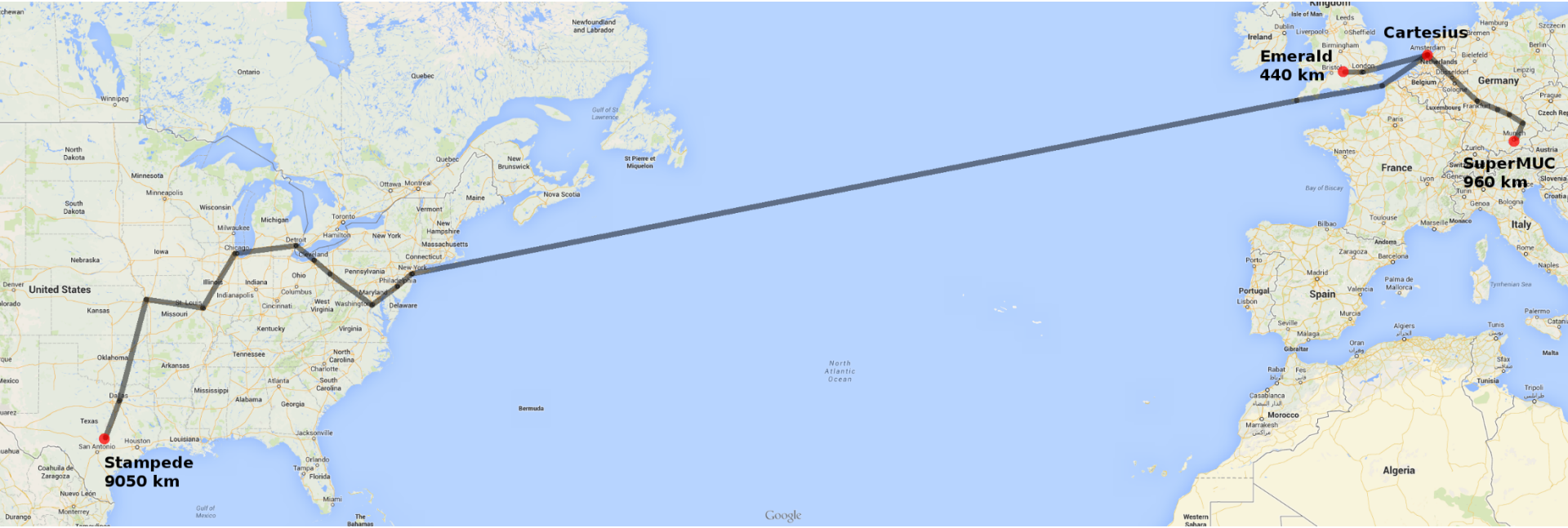
6 universities

4 supercomputing centers

PRACE & XSEDE

… and this does not even include the NRENs yet!

World wide 10G network links



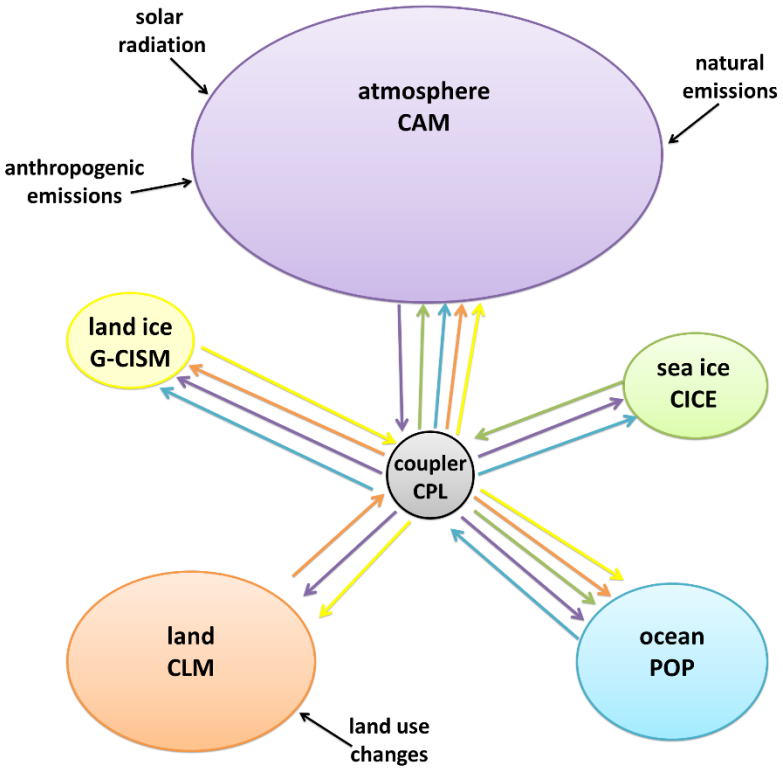
NRENs provide the essential 10G network links between the sites.

CESM & model coupling

We use the **Community Earth System Model** (CESM).

CESM combines 5 simulations each simulating a different aspect of the climate (ocean, atmosphere, land, etc).

Models regularly **exchange data** to model the influence on each other.

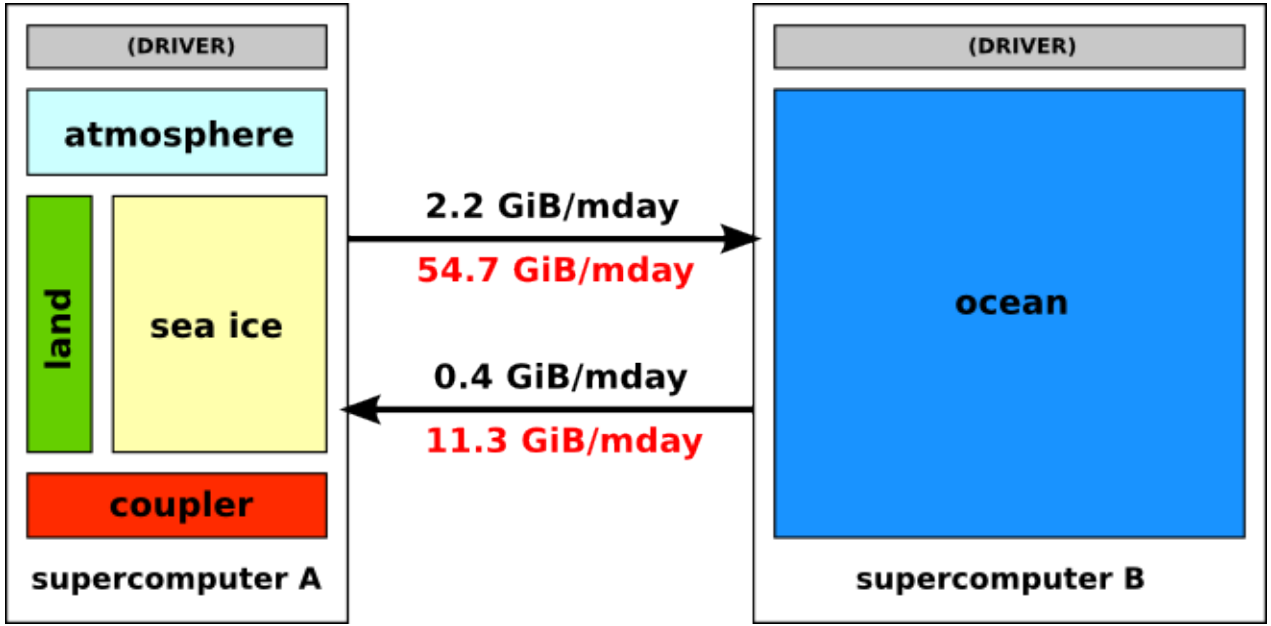


Source: climatesight.org

Distributed CESM

We can run the ocean model **separately!**

Coupling occurs 4x per simulated day (once every **~30 sec**) and **data volume** is limited.

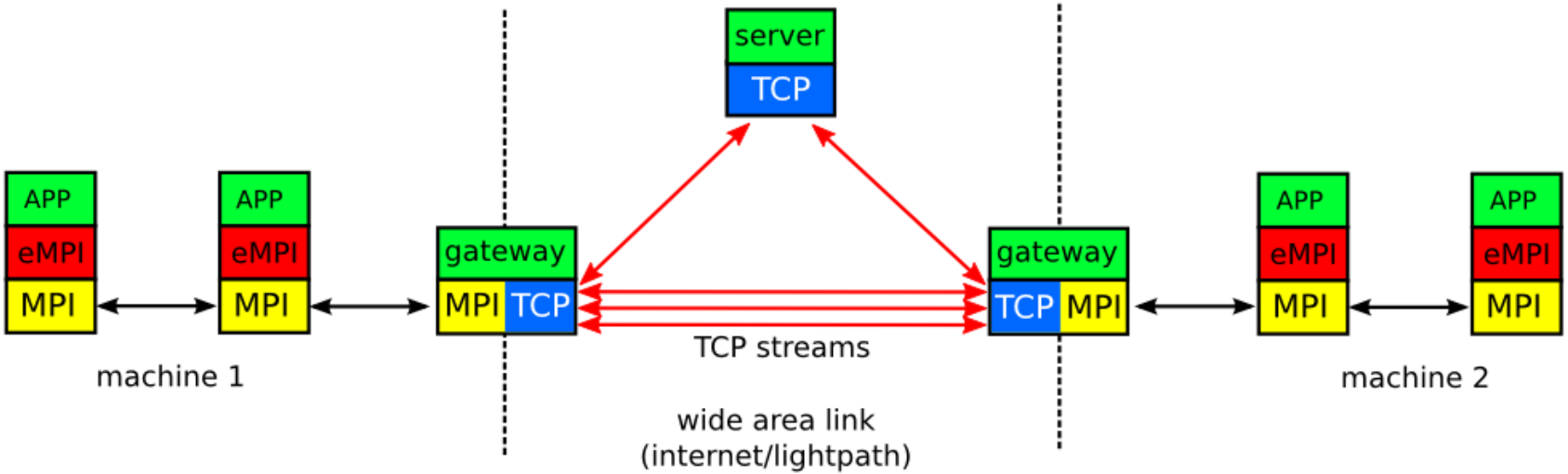


2.6 Gigabyte per exchange for 10 km resolution

66 Gigabyte per exchange for 2 km resolution

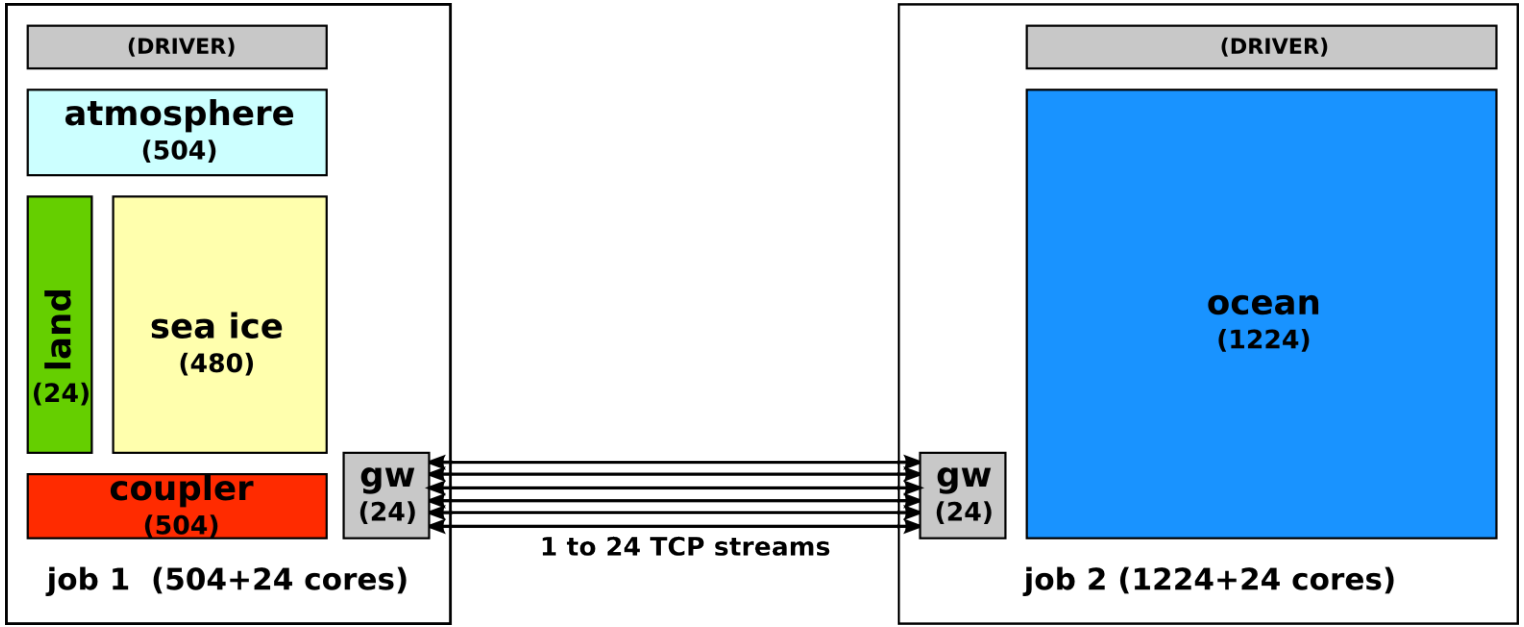
bursty traffic, not latency sensitive!

Coupling sites using eSalsa-MPI



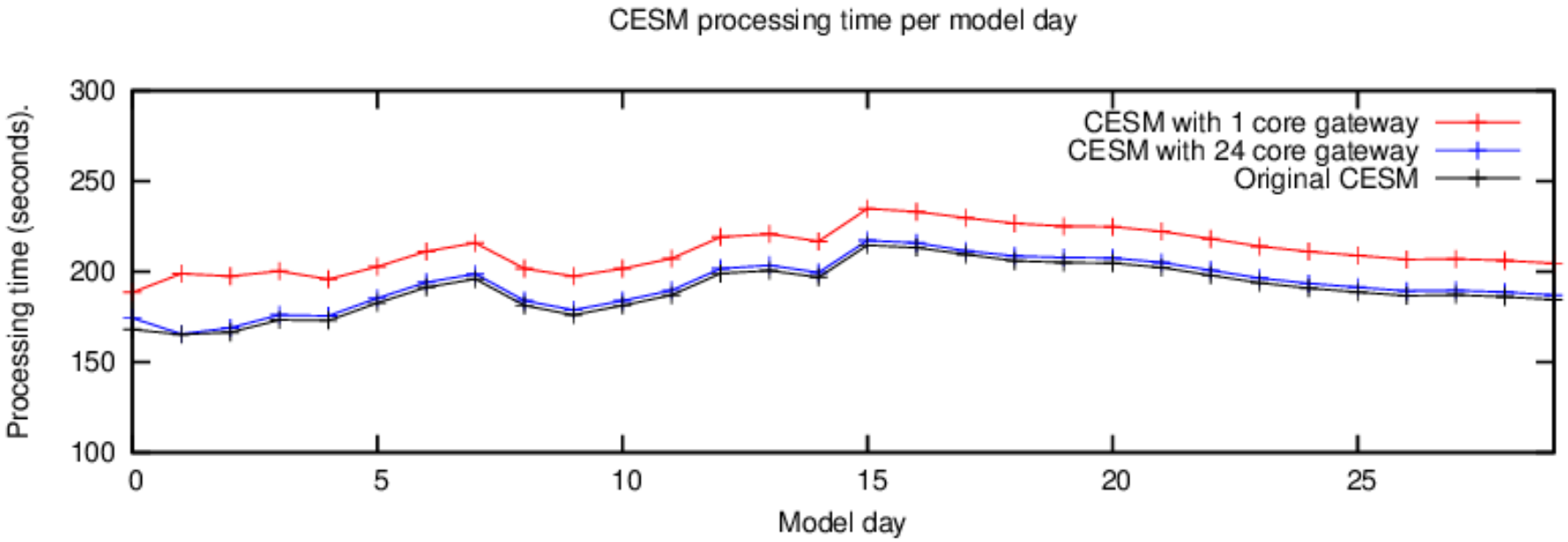
eSalsa-MPI is an **MPI wrapper library** that can combine two MPI runs on different supercomputers, and presents it as a **single set of processes** to the application. An extra **gateway node** is requires at each site.

Single site test: Two jobs on Cartesius



We combine two MPI jobs (504 and 1224 cores) by using two **gateway nodes**. All traffic between jobs goes through these gateways.

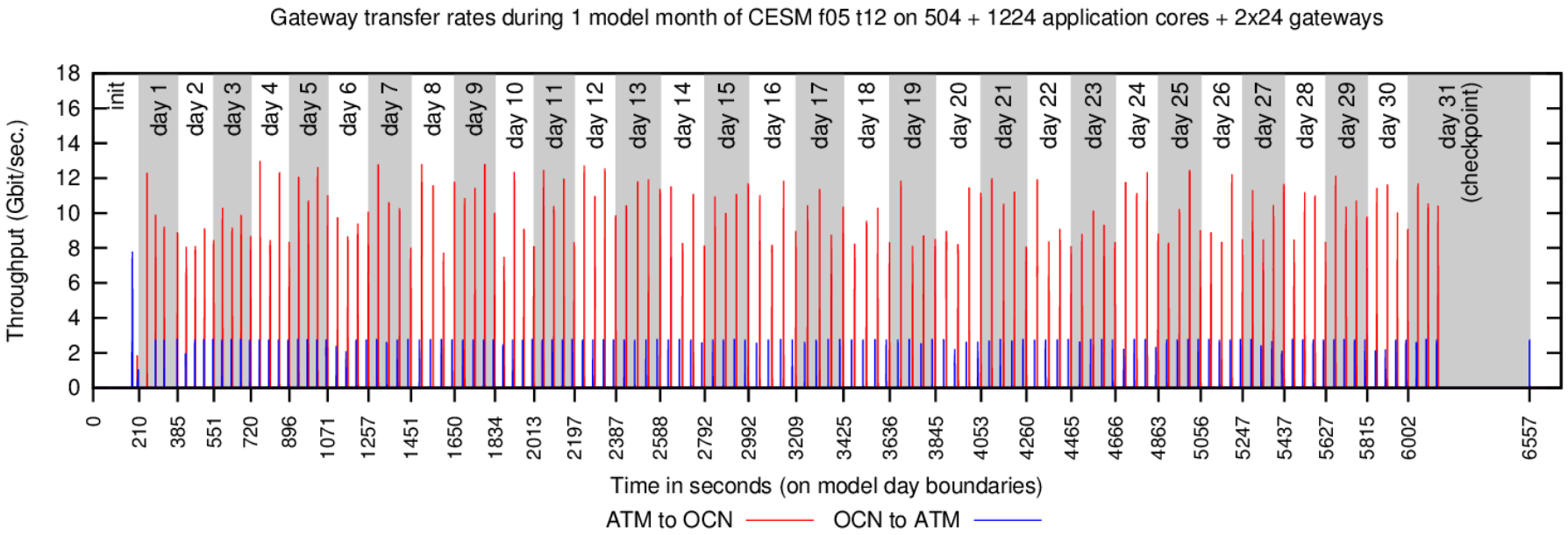
Single site test: time per model day



Two separate jobs (Cartesius 504+1224 cores) connected via eSalsa-MPI

Overhead 10%-1.5% dep. on number of TCP streams between gateways

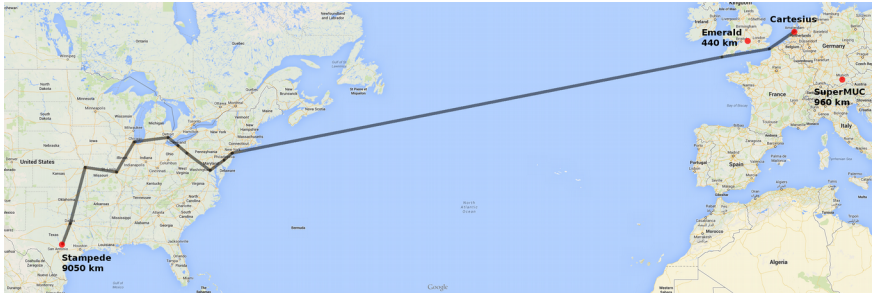
Single site test: gateway throughput



Bursty traffic pattern clearly visible. ATM to OCN uses about 8-12 Gbit/s, OCN to ATM uses about 2.5 Gbit/s (sends less data).

Lightpath setup

Cartesius (NL) – Stampede (US)



Atlantic lightpath was up pretty quickly

- Last mile took longer, as TACC wasn't connected at 10G yet

Setup of gateway node was quite difficult!

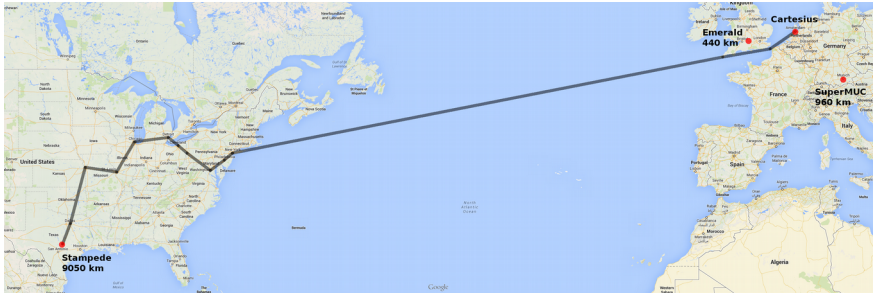
- Unclear who to contact, unclear how to set to up hardware and network
- Colliding IP ranges complicate matters
- Finally a Stampede service node was configured to use a Cartestius IP adres!

Initial run worked nicely, but then we had a **break in the cable**!

- Lost the Stampede node while repairs where taking place
- Replaced node by VM, which had unreliable performance

Lightpath benchmarks

Cartesius (NL) – Stampede (US)



Low level performance benchmarks:

RTT: 126 ms

TCP throughput:

32MB buffer, 1 stream	: 1.57 Gbit/s
32MB buffer, 3 or more streams	: 4.52 Gbit/s

UDP throughput:

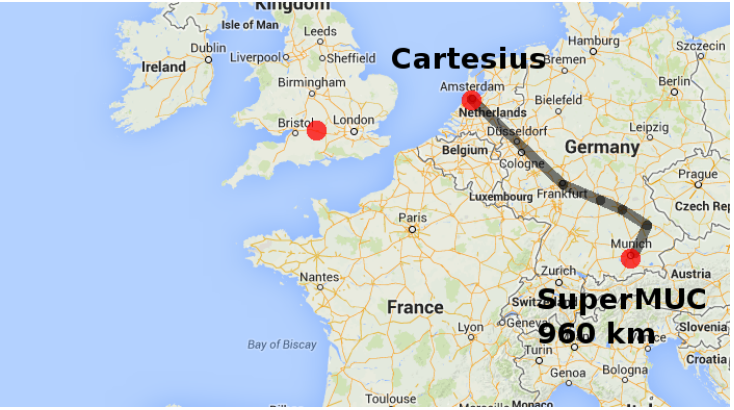
32K packets	: 9.7 Gbit/s (almost zero packet loss)

UDT throughput:

9K packets, 150 MB buffer	: 9.5 Gbit/s (no packet loss)

Lightpath setup

Cartesius (NL) – SuperMUC (DE)



Lightpath already available

- Re-use the existing **PRACE** link

Setup of gateway node again quite difficult!

- Took a bit of convincing to get support
- Network hardware issues limited the performance initially
- Required a change of the network setup at SuperMUC
- Jumbo frames do not seem to work on this link – still unclear why...

But we did end up with a working setup!

Lightpath benchmarks

Cartesius (NL) – SuperMUC (DE)

Low level performance benchmarks:

RTT: 14.9 ms

TCP throughput:

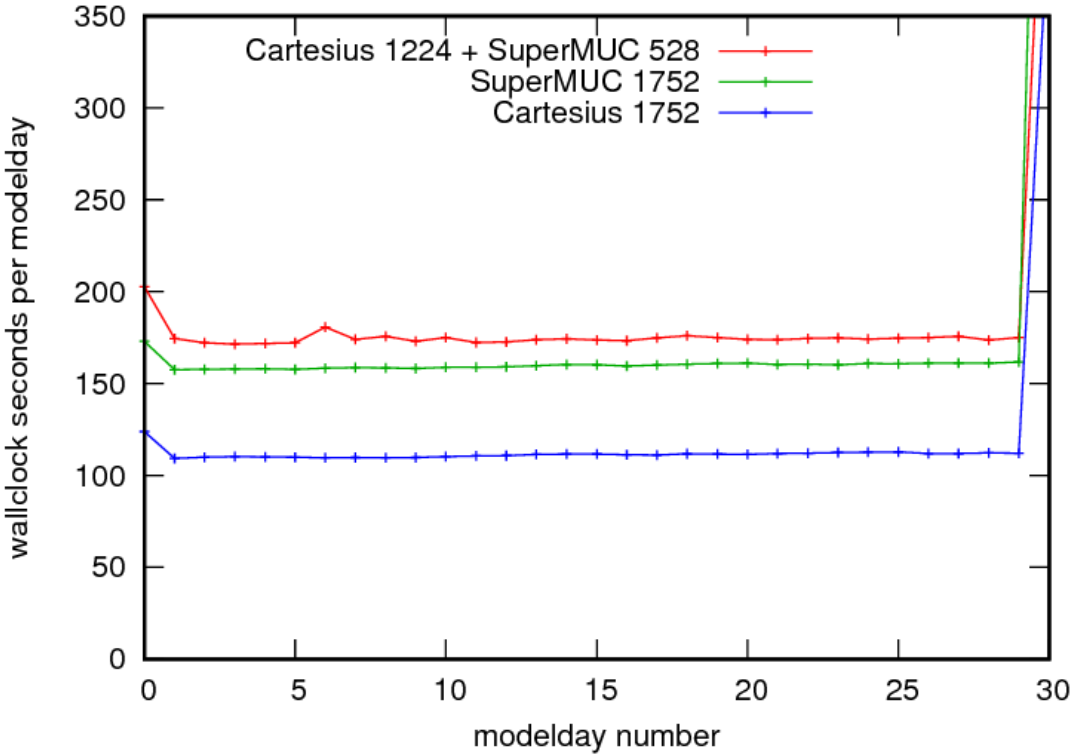
1 stream : 5.3 Gbit/s

Multiple TCP streams does not help due to relatively low latency

UDP / UDT not usable due to lack of jumbo frames

Application run

Cartesius (NL) – SuperMUC (DE)



It runs!

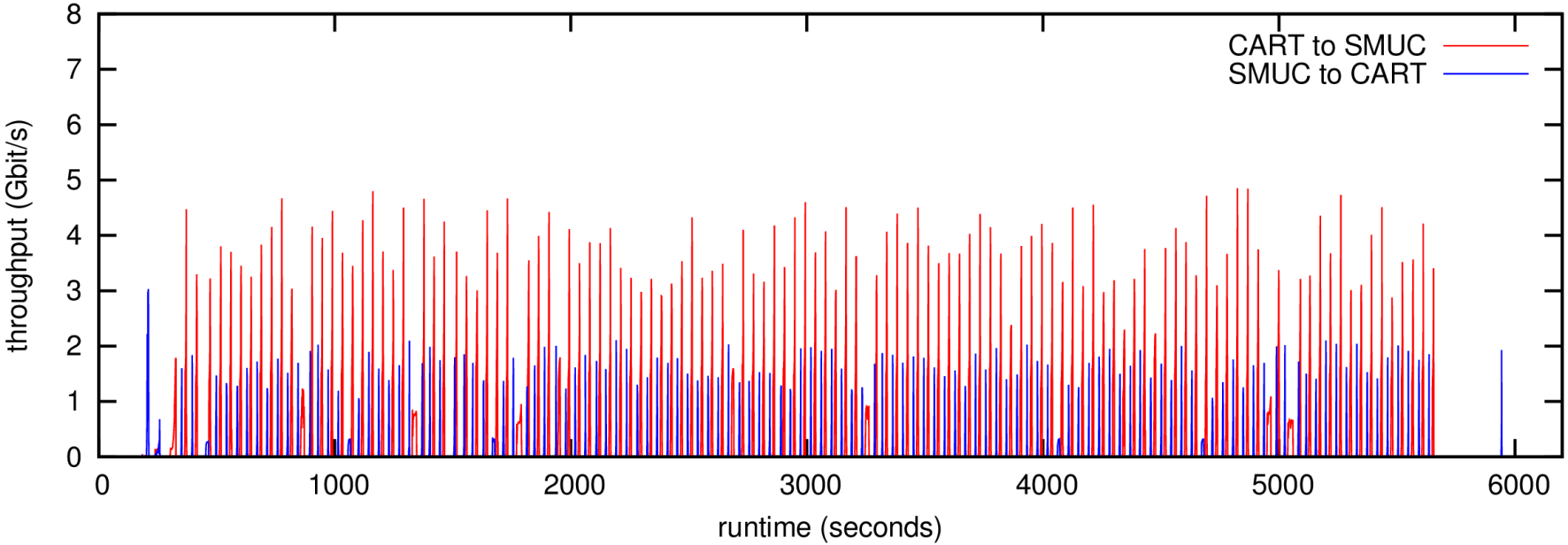
Performance tuning needed:

Already 44% performance difference between Cartesius-only and SuperMUC-only.

Distributed adds extra 10%

Gateway thoughput

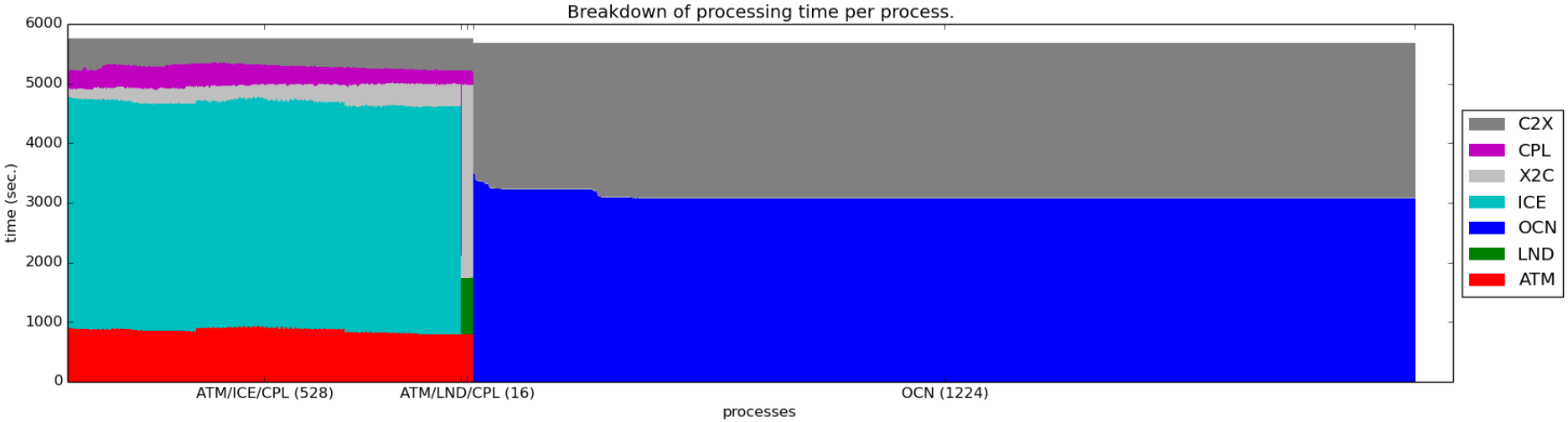
Cartesius (NL) – SuperMUC (DE)



Wide area network behavior seem fine...

Load balance

Cartesius (NL) – SuperMUC (DE)

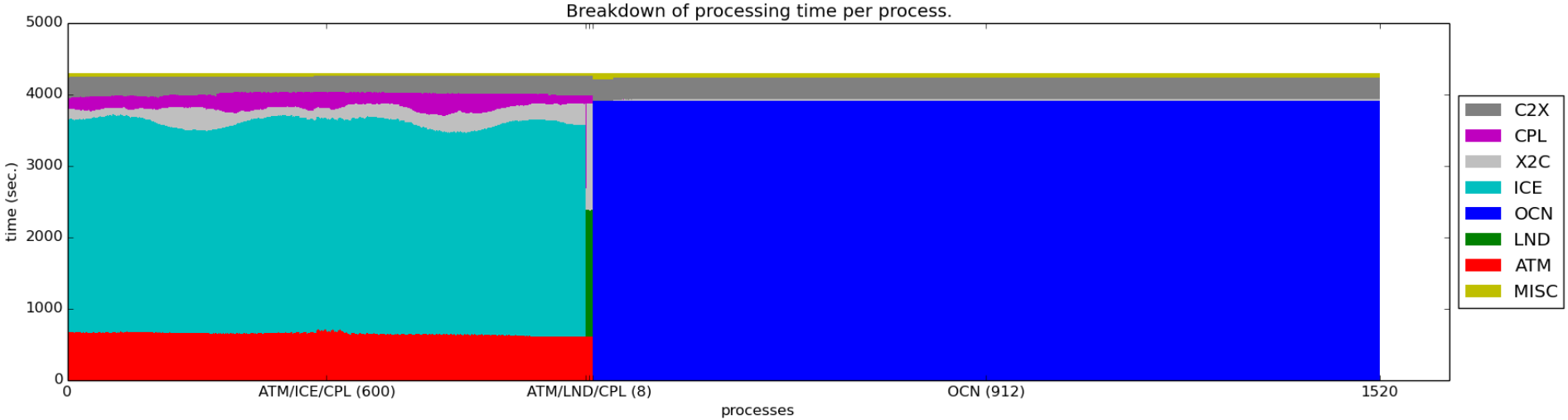


Desparately needs better load balancing!

Ocean is running too fast (too many cores)

Fixed load balance

Cartesius (NL) – SuperMUC (DE)

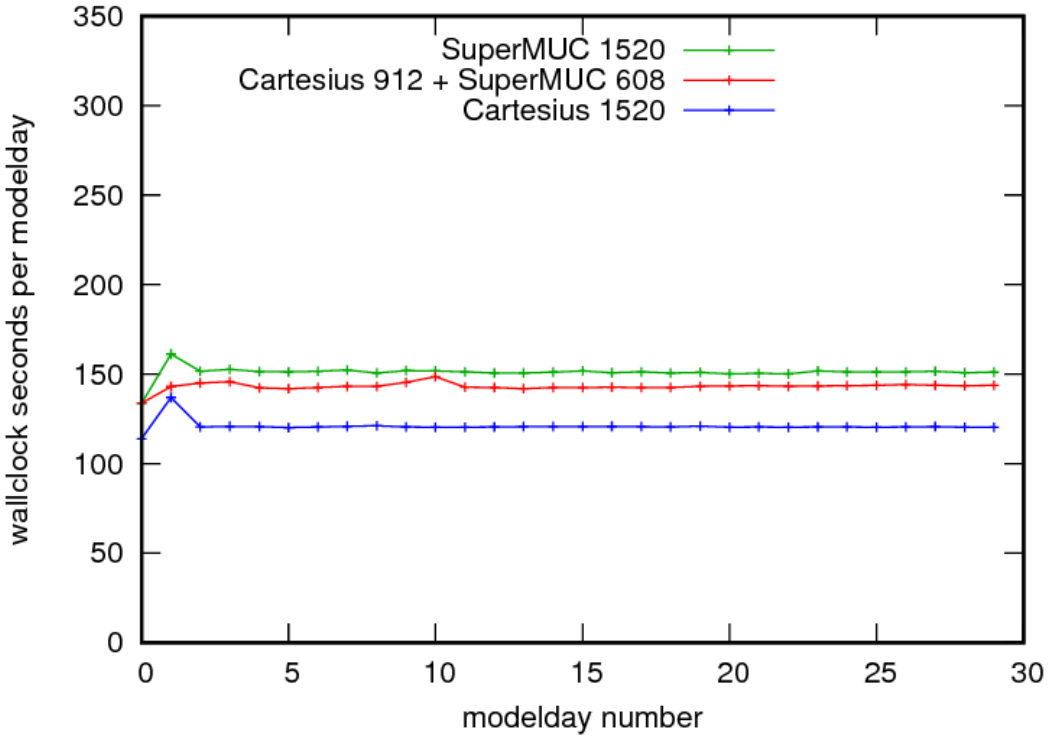


Less cores on Cartesius (-312), more on SuperMUC (+80)

Much better load balance between the systems!

Application run (retry)

Cartesius (NL) – SuperMUC (DE)



25% performance difference between Cartesius-only and SuperMUC-only.

Distributed in between the two!!

…. and then we ran out of time

Working on this (on-and-off) for two years

- Parent project had finished long before
- Core hours started disappearing
- People started disappearing
- Machines started disappearing (Emerald was gone)

What *did* we do

Distributed MPI: we managed to get the eSalsa MPI up and running with reasonable performance

Small scale experiments: we managed to run small scale experiments on combinations of 2 machines O(2K) cores at 10km resolution.

Published a paper on our experiences:

On the complexities of utilizing large-scale lightpath-connected distributed cyberinfrastructure (DOI: 10.1002/cpe.3853)

What *didn't* we do

US link: we did not managed to get the US link stable for long enough to run real experiments in that direction

Large scale experiments: we did not managed to run large scale high resolution experiments on O(50K) cores and 1~2 km resolution

Heterogeneous runs: we did not managed to run experiments with heterogeneous combinations of machines (CPU/GPU/XeonPhi)

3 site runs: we did not managed to run experiments on more that 2 sites

Lessons learned

It works!

We can run an climate model on a distributed system with acceptable performance!

But tuning the wide-area TCP links is still an issue ?

Balancing the number of cores on the sites is black magic!

The **hardest part** (by several orders on magnitude) is the **last 10 feet!**

Lessons learned

Even if you have a 9000 km lightpath up and running with ends up in the datacenter, actually getting it connected to the supercomputer is **hard!**

- Weird usecase
- Initially goes against the gut feeling of the sysadmins and network admins
- No standard way to do it
- Need to bridge networks (requires some gateway machine) and tuning

System and network admins were **very helpful**, but support time still became an issue when quick fixes were not enough!

Possible solutions

Providing infrastructure (network & core hours) is not enough. Need to add **person hours** for setup and support

Provide standardized way to **connect running simulations**, which is different from the existing storage-to-storage data transfers

Co-scheduling would be great, although we managed amazingly well without

Many thanks to:

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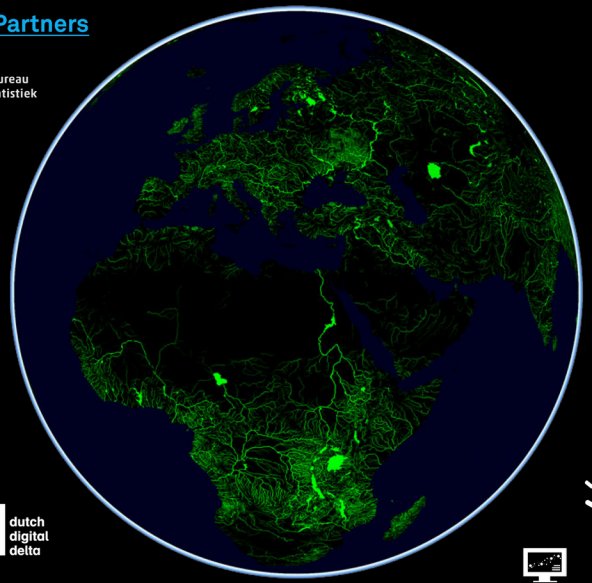

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