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Project Title

An Advanced Distributed Computing Approach to High-Resolution Climate Modeling

Objectives

The primary objectives of the proposed work are three-fold:

1. *Realize an international distributed proof-of-concept testbed cyberinfrastructure consisting of multiple supercomputer systems coupled via 10G (or higher) lightpaths.*
2. *Using the proof-of-concept system, run large-scale & high-resolution coupled climate simulations to investigate the effect of ocean circulation changes on climate.*
3. *Use the resulting climate simulations as a basis for advanced computer science research on programming models for Jungle Computing Systems and Advanced Distributed Cyber-infrastructure.*

1. Organisation

Provide a complete overview of the project organization with roles and responsibilities for each location.

The project team consists of members from 4 countries: The Netherlands, United Kingdom, Germany, and United States. The team is inherently multi-disciplinary in nature, with researchers and specialists from the fields of High-Performance and Distributed Computing, Climate Research, and eScience. Team member roles range from coordinating tasks (for research, implementation, and supercomputer access and use) to software and hardware implementation tasks.

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2. Project details

Project title:

An Advanced Distributed Computing Approach to High-Resolution Climate Modeling

Summary of the proposed research (max. 500 words excluding references):

Advanced Distributed Multi-Model/Multi-Kernel Simulations

Many scientific applications are of such complexity and scale that solutions can be obtained only by using a wide variety of computing hardware – all at once. The need for *concurrent use* of e.g. multiple clusters, grids, clouds, and supercomputers has spawned much innovative research into Advanced Distributed Cyberinfrastructure [1] and Jungle Computing [2]. User-oriented programming models for such advanced systems are under constant development (e.g. P* [3], Ibis/Constellation [4]) with much proven success (e.g., awards at AAAI'07, SCALE'08, DACH'08, SCALE'10, EYR3'11). Examples of applications that benefit particularly well from these advances are so-called *multi-model/multi-kernel simulations* [5], in which multiple distinct models of real-world phenomena are coupled to form a single, large simulation of a physical system. Such simulations are common in climate research, where models of land, ocean, atmosphere, and sea ice are combined to simulate Earth's climate, e.g. using the Community Earth System Model (CESM) [6].

Collapse of the Atlantic Ocean Circulation

As an appealing and important application of the CESM we consider the problem of the strong weakening (collapse) of the Meridional Overturning Circulation (MOC) in the Atlantic Ocean. State-of-the-art Global Climate Models (GCMs) have indicated that a weakening of the MOC would lead to a strong cooling of the North Atlantic region [7]. Constrained by compute power, most GCMs operate at a horizontal resolution of about one degree for ocean (and sea-ice), and about two degrees for atmosphere (and land). As a result, the ocean component does not resolve many important oceanic features, including so-called eddies (vortices with scales ranging from 10-100 km). The same holds for many atmospheric features. Recent research [8, 9] has indicated that high spatial resolution in both ocean and atmospheric model components does improve the simulation of many features in the climate system. In particular, the impact of changes of the Atlantic MOC are significantly different in eddy-resolving ocean models compared to models in which these eddies are parameterized [10].

Aim and scope

This proposal focuses on large-scale and high-resolution CESM simulations that are at the moment not easily executed on a single supercomputer. To assess the impact of a severe reduction of the strength of the MOC on climate, we aim to run distributed coupled simulations at such high resolution that ocean eddies are fully resolved. Success of this project will be a first step towards running climate simulations at extreme spatial resolution. The simulations in turn will spawn further advanced research in our P* and Ibis/Constellation programming models.

While investigation of the impact of ocean circulation changes on climate is our primary scientific aim, many additional research questions serve as further driving forces for the proposed testbed cyberinfrastructure and work. A direct beneficiary of this proposal is the SCIHM project (http://scihm.org/), which focuses on new approaches to multi-model/multi-kernel predictive simulation of high impact hydrometeorological events. Another direct beneficiary involves the work performed by Oxford eResearch Centre on high-resolution regional simulations using the UK MetOffice coupled climate model.

References:

1. *S. Jha et al. The Research in Advanced Distributed Cyberinfrastructure and Applications Laboratory (RADICAL), Rutgers University, USA*
2. *F.J. Seinstra et al. "Jungle Computing: Distributed Supercomputing Beyond Clusters, Grids, and Clouds". In: Grids, Clouds and Virtualization, 167-197, Springer-Verlag, 2011.*
3. *A. Luckow et al. "P*: A Model of Pilot-Abstractions", IEEE eScience, 1-10, Oct. 2012*
4. *H.E. Bal et al. "Real-World Distributed Computing with Ibis". IEEE Computer, 43(8): 54-62, Aug. 2010 (see also: www.cs.vu.nl/ibis/)*
5. *N. Drost et al. "High-Performance Distributed Multi-Model / Multi-Kernel Simulations: A Case-Study in Jungle Computing". IPDPS / HCW 2012, Shanghai, China, May 2012.*
6. *P. Worley et al. "Performance of the Community Earth System Model", SC11, Nov. 2011.*
7. *Vellinga et al. "Impacts of Thermohaline Circulation Shutdown in the Twenty-First Century". Climate Change, 91 (1-2), 43-63, 2008.*
8. *F. Bryan et al. "Frontal Scale Air-Sea Interaction in High-Resolution Coupled Climate Models". Journal of Climate, 23, 6277-6291, 2010.*
9. *B. Kirtman et al. "Impact of Ocean Model Resolution on CCSM Climate Simulations". Climate Dynamics, 39, 1303-1328, 2012.*
10. *W. Weijer et al. "*Response of the Atlantic Ocean Circulation to Greenland Ice Sheet Melting in a Strongly-Eddying Ocean Model.*". Geophysical Research Letters. 39, L09606, 2012.*

Fields of research covered within the project: Climate Research, Computer Science

Keywords: Atlantic Ocean Circulation, Climate Models, Distributed Computing

3. Scientific outlook (max. 300 words)

Ambitions

Describe your scientific ambitions; what are the results you would like to achieve in your scientific work?

We aim to perform simulations of the climate system with such a high-resolution in the global ocean model component that a new level of detail is revealed. This level of detail, with many new phenomena to discover, is reached at the 2 km scale, when the so-called ocean eddies are resolved. We aim to reach this (simulation) level of detail by performing a climate model simulation (with the CESM climate model) over four different supercomputers in the world (The Netherlands, UK, Germany, and USA) using state-of-the-art distributed computing software and networking technology.

Breakthroughs

What would be achievable breakthroughs in your scientific domain?

By using eddy-permitting models (typical with a global horizontal resolution of 10-25 km) over the last decade, the view on the ocean circulation has changed from a steady relatively passive ocean driven by the atmosphere to an active highly variable ocean, which is able to influence the atmosphere. Even a one-year simulation of the climate system with a full eddy-resolving ocean model, as is aimed in this project, will likely lead the way to a second paradigm shift to understand the physics of ocean circulation. Resolving the eddies is expected to lead to a much better correspondence with available observational data, such as in situ and satellite data, in particular on sea surface height variability.

Challenges

Describe the challenges you expect to face in reaching the desired breakthroughs.

Main challenges are in the technology to perform a simultaneous simulation of the CESM model over the different computing systems. We do, however, have ample experience running such complex simulations in several domains – even at a world-wide scale (e.g. see [5] above, and Appendix A). Further challenges are the preparation of the high-resolution (2 km) global input (bathymetry) and surface forcing (e.g., wind) files.

4. Technical requirements (no maximum)

Please describe your project from a technical perspective, both in its current form and in the aspirational form that the project would take if EYR Global resources were granted. In particular, please answer the following questions (both for the current state and for the aspirational future state).

For proposals with workflows that move data without copying files, provide the following:

- *How is the data movement currently accomplished? (e.g. remote filesystem mount, use of native InfiniBand, RDMA over Ethernet, remote file I/O service, …)*
- *How much data is moved now?*
- *How often do the data movement operations occur? If the answer is "continuously" then how long is a run?*
- *What is the current performance?*
- *What is the desired performance?*
- *Are the systems resources at the end sites able to achieve the desired performance if the network provides the necessary capabilities?*
- *Is a change of tools or methodology required or anticipated in order to achieve the desired performance?*

For proposals that require lightpath or other virtual circuit services, provide the following:

- *Are all the site networks involved able to provide local lightpath services in support of the proposal?*
- *Do all the site networks involved have lightpath connectivity to regional or national providers?*
- *Are the systems resources at the sites able to use lightpath services for the proposal?*
- *Will the software tools (e.g. data transfer tools, workflow managers) be able to interface with the lightpath services when they are provisioned?*
- *Have system configuration aspects for ligthpaths such as additional interfaces, IP addressing, security, etc. been addressed?*

Situation sketch

[Insert a graphic of your current and proposed ICT infrastructure]

Describe the current eInfrastructure set-up and data flow at all proposed locations (preferably using illustrations or flow charts. Ask for help from the network coordinators if necessary).

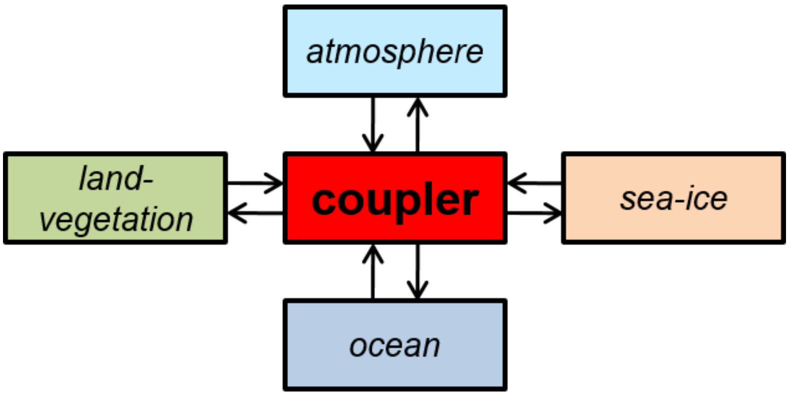
Describe the additional infrastructure set-up and data flows requested in your proposal.

Specify the current role of each of the partner institutes in the project, e.g. user, compute cluster, storage cluster, data provider.

[Insert a graphic of your current and proposed data flow illustrating input, processing steps and output (e.g. pipeline)]

Technical description of CESM

CESM is a multi-model/multi-kernel simulation consisting of 5 components: atmosphere, ocean, land, ice and coupler, as shown in the figure below. The coupler is the component that is responsible for the necessary data conversion between the models.

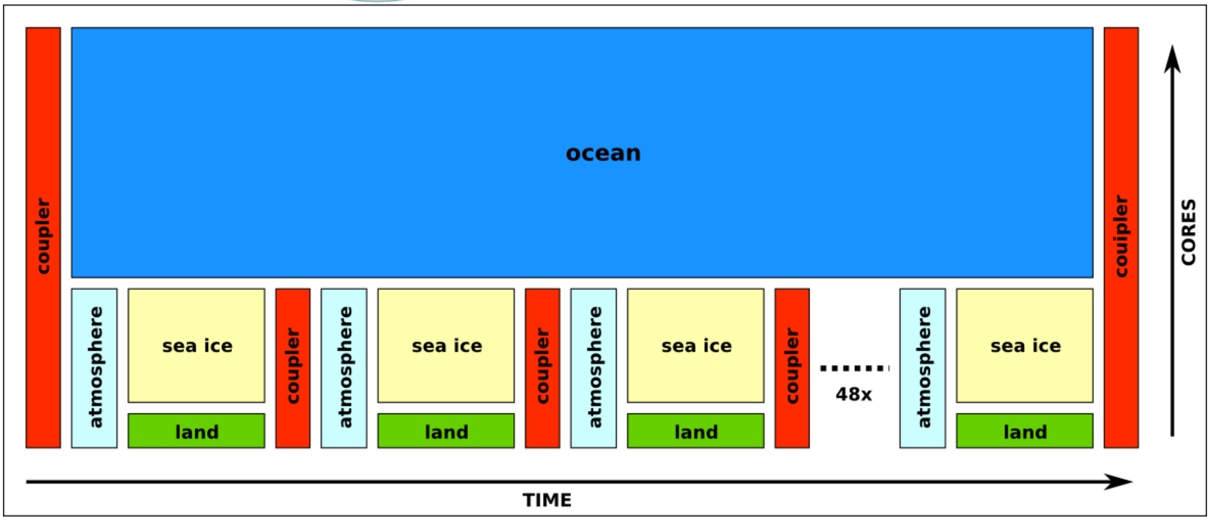


In its current form, the CESM climate model is run on a single supercomputer, typically on ten thousand cores or more, although some experiments use up to 200,000 cores [11]. When running a simulation, CESM internally divides the available cores over the 5 different models. It is up to the user of CESM to the assign cores to each model. Cores may be assigned to a single model, or shared by multiple models.

The amount of processing time required per model depends both on the resolution and the complexity of each model. For typical configurations, the ocean model requires by far the most processing time, followed by atmosphere and ice. Land only requires a small amount of processing due to its low complexity.

The coupling frequency is the number of times data is exchanged between models per simulated day. For typical configurations, data is exchanged between land, ice and atmosphere models every 30 simulated minutes, resulting in 48 couplings per simulated day. The ocean model only needs to exchange data with the other models once every simulated day.

Due to data dependencies between the atmosphere model and the land and ice models, these models cannot be run concurrently. The resulting workflow for CESM is shown below. This workflow illustrates a single simulated day (left to right) for all cores (bottom to top).



The day starts by a global coupling involving all cores. Next, both *ocean* and *atmosphere* models start their computation. While the ocean model continues to run separately for the rest of the simulated day, the atmosphere model stops after 30 simulated minutes. The *sea ice* and *land* models are then allowed to run concurrently, using the same set of cores as the atmosphere model. After they have completed their 30 simulated minutes, the coupler is run to exchange data between the atmosphere, sea ice and land models. This is repeated 48 times, after which a global coupling is performed to exchange data between the ocean model and the others. This completes the simulation of a single day.

The amount of data transferred between the models depends ***only*** on the resolution of the models. Changing the number of cores assigned to each model will only change the number of messages exchanged, not the total data volume. Data exchange between the models is performed using the MPI library. On supercomputers, MPI typically uses InfiniBand for communication, although some vendors (e.g. Cray or IBM) use their own network fabrics.

As explained in Section 3, our goal is to increase the resolution of simulations from the current state-of-the-art 0.1 degree (~10 km) ocean and 0.5 degree (~ 50 km) atmosphere to a currently unfeasible 0.02 degree (~ 2 km) ocean and 0.5 degree (~ 50 km) atmosphere. This will require *at least* 25x more processing time for the ocean model, although more pessimistic estimates go up to an increase of 100x or even more.

At these resolutions most (traditional) supercomputers do not have enough processing power available to fulfill our needs. We therefore propose several solutions, both pushing the state-of-the-art in climate modeling, as well as making a (computer science oriented) case for distributed computing solutions as an alternative to strictly centralized approaches:

a) **Distribute CESM over 2 supercomputers**. Since the ocean model is relatively loosely coupled to the other models, it can be run on a separate machine, provided the communication channel between the machines is fast enough for the data exchanges taking place once per model day. We have already performed small scale experiments that show that this approach works well for low resolution simulations.

b) **Distribute the ocean model over multiple supercomputers**. Internally, the ocean model partitions the work into blocks which are then distributed over the available cores. During the simulation, data must be exchanged between neighboring blocks, resulting in a large amount of communication. However, no communication is needed with neighboring blocks that only contain land. Hence, by taking geography into account when distributing blocks over multiple supercomputers, it is possible to reduce the amount of communication. In [12] we show that by using this approach, is it indeed possible to run the ocean model efficiently in a distributed fashion.

c) **Improve the performance of the ocean model using accelerators such as GPUs.** Many state-of-the-art supercomputers use accelerators such as GPUs or Xeon Phi to significantly improve their computational performance. By converting (part of) the ocean model to use such accelerators, its performance can be increased significantly. In [12] we have shown that converting part of the ocean model to GPUs indeed results in a much higher overall performance.

In this project we will use these three solutions to improve the performance and scalability of CESM, ultimately allowing us to run a simulation at ultra-high resolution (0.02 degree ocean and 0.5 degree atmosphere).

Experiment Scenarios

We have defined four scenarios, as shown below. For each scenario we will start with a high-resolution experiment (with 0.1 degree ocean) to prove that the technology works. This is then followed by the desired ultra-high resolution experiment (with 0.02 degree ocean). The four scenarios are:

1) A distributed run on 2 supercomputers in Europe, one running the ocean model, and one running the atmosphere, sea ice and land models.

2) A distributed run on 2 supercomputers, one in Europe, one in the US, with the same work distribution as on (1). *(This scenario is used to show that our approach also works on a global scale.)*

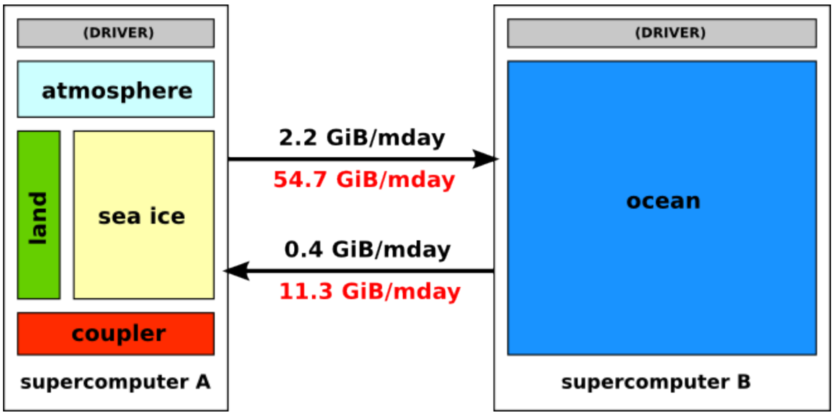
3) A distributed run on 3 supercomputers, one in the US (running the atmosphere, land and sea ice models) and two in Europe both running *half* of the ocean model.

4) A distributed run on 2 supercomputers in Europe, one running a GPU accelerated version of the ocean model, and one running the atmosphere, sea ice and land models.

Data Transfer Estimations

The figures below show an estimate for the data transfers required **per model day** in each scenario. High resolution data transfers are shown in black, while ultra-high resolution data transfers are shown in red.

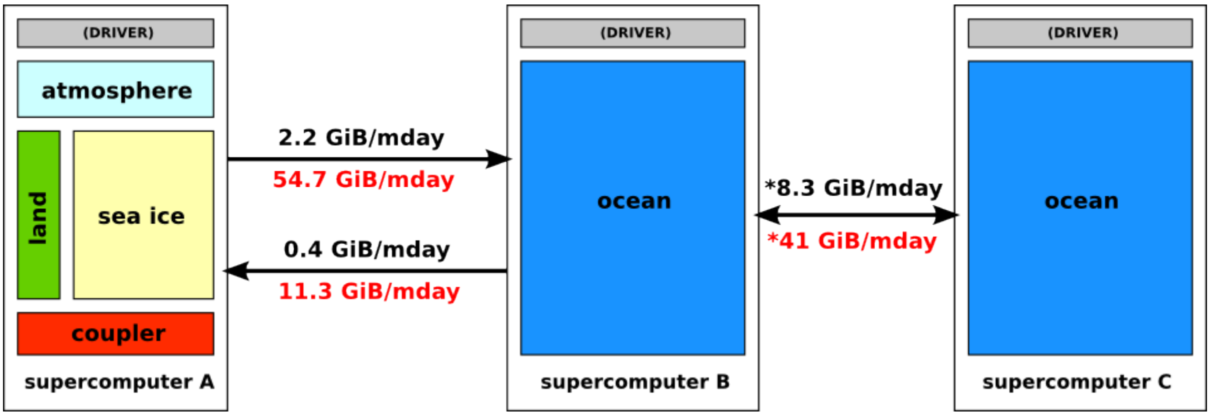
Scenarios 1, 2, and 4:



For scenarios 1, 2 and 4 the amount of data transferred between supercomputers is the same. The difference lies in the geographical location of the machines (all within Europe for 1 and 4, and in both Europe and the US in 2), and the use of GPUs as accelerators (only in 4).

The communication between the supercomputers is performed in bursts. That is, no communication is performed while the simulation is running. **Once a simulated day is completed the models must perform the data exchange, or coupling, as quickly as possible to minimize the communication overhead.** After completing the data exchange they continue simulating the next day.

Scenario 3:



For scenario 3, the left part is the same as in the previous scenarios. It shows the communication between the models that occurs once per model day. The right part illustrates the communication within the ocean model. This communication is continuous; it is spread out over the full time required to simulate a single day. As before, the data transfer volume **per model day** is shown, in black for the high resolution model, and in red for the ultra-high resolution model.

To estimate the required network capacity between the supercomputers, an estimate of the required compute time per model day is also needed. For high-resolution runs using 0.1 degree ocean, 0.5 degree atmosphere, Dennis et al [13] report a performance of 3.23 model years/24 hours on 19,812 cores of the Kraken supercomputer [14], or 73.3 seconds per model day. Kliphuis at al [15] report a performance 6.68 model years/24 hours on 4176 cores of the Cartesius supercomputer [16] for an ocean-only run, or 35.4 seconds per model day. Assuming the relative performance of the ocean model and the other models is similar on Kraken and Cartesius, we estimate that running CESM instead of POP on the latter will require approximately 6050 cores for a performance of 6 model year/24 hours. This clearly shows that the per-core performance of Cartesius is much higher that the (older) Kraken machine. We will therefore use Cartesius as a reference in our estimates below.

High-resolution experiments – scenarios 1, 2, and 4

The total amount of data that needs to be transferred between models (per model day) in scenarios 1, 2 and 4 in the **high-resolution experiments** is:

2.2 + 0.4 = 2.6 GiB/mday (or 22.3 Gbit/mday)

Assuming the data transfers cannot be performed concurrently (which is overly pessimistic), the minimum time to transfer this data will be:

1 Gbit/s link:	22.3 seconds
10 Gbit/s link:	2.2 seconds

This assumes that the link can reach 100% utilization (which is overly optimistic). Since the compute time on a Cartesius class machine is 35.4 seconds per model day on 6K cores, the percentage of time spent in communication will be at least:

1 Gbit/s link:	100 * (22.3 / (22.3 + 35.4)) = 38.6%
10 Gbit/s link:	100 * (2.2 / (2.2 + 35.4)) = 5.8%

These numbers clearly show that for a 1 Gbit/s link, the communication overhead is unacceptably high. For a 10 Gbit/s link, however, it is acceptable.
When simulating a single model year, the total amount of data transferred over the lightpath will be:

2.6 * 356 = 949 GiB

The estimated runtime for one model year when using a 10 Gbit/s link will be:

(2.2+35.4) * 365 = 13724 seconds (= 3.8 hours)

High-resolution experiments – scenario 3

Communication within the ocean model in scenario 3 requires approximately 8.3 GiB/mday (or 71.3 Gbit/mday). The minimum time to transfer this data is:

1 Gbit/s link:	71.3 seconds
10 Gbit/s link:	7.1 seconds

Assuming communication and computation cannot be overlapped (which is pessimistic) the overhead of communication will be at least:

1 Gbit/s link:	100 * (71.3 / (71.3 + 35.4)) = 66.8%
10 Gbit/s link:	100 * (7.1 / (7.1 + 35.4)) = 16.7%

As before, the communication overhead is unacceptably high for a 1Gbit/s link, while for a 10Gbit/s link it is still acceptable.

When simulating a single model year, the total amount of data transferred over the lightpath will be:

8.3 * 356 = 3030 GiB (= 3.0 TiB)

Note that this is in addition to the transfer described in scenario above.

The estimated runtime for one model year when using a 10 Gbit/s link will be:

(2.2 + 7.1 + 35.4) * 365 = 16315 seconds (= 4.5 hours)

Note that this adds both the extra time caused by the exchange between model (2.2 sec) and the extra time cause by the exchange within the ocean model (7.1 sec) to the time observed on one machine (35.4 sec).

Ultra-high resolution experiments – scenarios 1, 2, and 4

Since the communication volume exchanged between models in scenarios 1, 2, and 4 increases linearly with the number of grid points, the **ultra-high resolution experiments** require 25x more data to be transferred than the high resolution experiment:

54.7 + 11.3 = 66.0 GiB/mday (or 566.9 Gbit/mday)

The minimum time to transfer this data will be:

1 Gbit/s link:	566.9 seconds
10 Gbit/s link:	56.7 seconds

The communication overhead depends on how much the required processing time increases with the increase in resolution. If the processing time is assumed to also increase linearly with the number of grid points (an optimistic assumption), an increase of processing time of 25x is expected and the overhead remains unchanged:

1 Gbit/s link:	100 * (566.9 / (566.9 + 25*35.4)) = 39.0%
10 Gbit/s link:	100 * (56.7 / (56.7 + 25*35.4)) = 6.0%

(Note that the slight difference in overhead compared to the high resolution model estimations on the previous page is caused by round-off errors). As before, the communication overhead when using a 1 Gbit/s link is unacceptably high.

The total amount of data transferred per simulated model year will be:

66.0 * 365 = 24090 GiB (= 23.5 TiB)

The estimated processing time per simulated model year will then be:

(56.7 + 25*35.4) * 365 = 343720 seconds (= 95.5 hours)

If we more pessimistically (but realistically) assume that the processing time is increased by 100x, the overhead will become:

1 Gbit/s link:	100 * (566.9 / (566.9 + 100*35.4)) = 13.8%
10 Gbit/s link:	100 * (56.7 / (56.7 + 100*35.4)) = 1.6%

In other words, the communication overhead drops if the required processing time grows more than linearly with the number of grid points. The estimated processing time per simulated model year will increase to 365 hours.

Ultra-high resolution experiments – scenario 3

For scenario 3, the communication within the ocean model grows linearly with only one dimension of the grid. Therefore, the increase in data transfer from the high resolution to the ultra-high resolution is only 5x instead of 25x; 41 GiB/mday (or 352.2 Gbit/mday). The minimum time to transfer this data is:

1 Gbit/s link:	352.2 seconds
10 Gbit/s link:	35.2 seconds

If we assume an increase in processing time of 25x, the communication overhead becomes:

1 Gbit/s link:	100 * (352.2 / (352.2 + 25*35.4)) = 28.5%
10 Gbit/s link:	100 * (35.2 / (35.2 + 25*35.4)) = 3.8%

As before, the overhead on a 10 Gbit/s link is acceptable. If we assume an increase in processing time of 100x the communication overhead will become:

1 Gbit/s link: 100 * (352.2 / (352.2 + 100*35.4)) = 9.0%
10 Gbit/s link: 100 * (35.2 / (35.2 + 100*35.4)) = 1.0%

In this case even a 1 Gbit/s link has acceptable overhead. The total data transfer per simulated model year is:

41 * 365 = 14596 Gib (= 142.6 TiB)

The estimated processing time per simulated model year will be:

25x increase: (56.7 + 35.2 + 25*35.4) * 365 = 356569 seconds (= 99 hours)
100x increase: (56.7 + 35.2 + 100*35.4) * 365 = 1325643 seconds (= 368 hours)

Note that this estimate add both the time needed to transfer data between models and within the ocean model.

Importantly, the ultra-high resolution estimates above all assume that the number of cores used for processing is fixed. However, due to the increase in processing time, the speed of the simulation (measured in model days computed per 24 hours) drops significantly, from approximately 6.7 model years/24h down to 24 model days/24h (for a 100x increase in processing time). Therefore, it makes sense to increase the number cores to increase the speed of the simulation. The machines participating in this project (see below) have more than ample cores available to scale the application in this way. As a result, the processing time will drop, and the communication overhead will increase again. Finding the optimal balance between simulation speed and communication overhead is one of the open research questions of this project.

Hardware Infrastructure

For this project we have access to the following supercomputers:

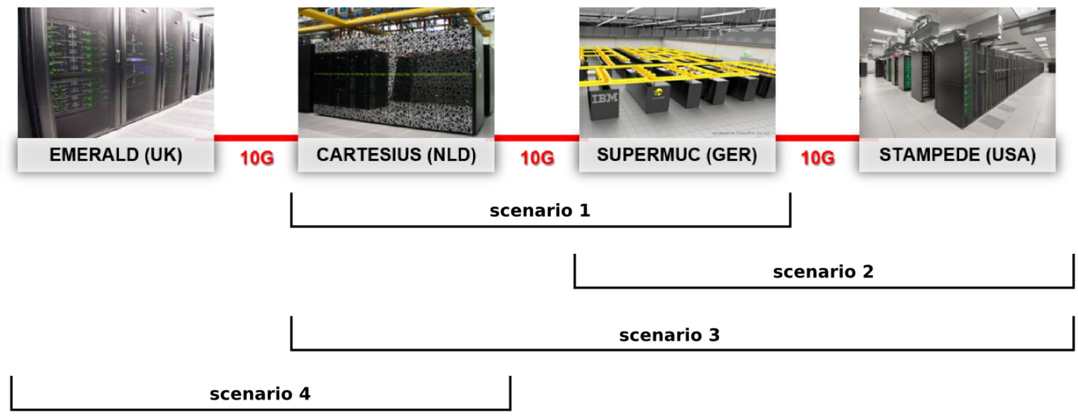
Stampede (#6 Top500)
Texas Advanced Computing Center (TACC)
Austin, Texas, USA
102,400 cores + 6880 Xeon Phi + 128 NVIDIA GPUS, 5.2 PFlop/s
http://www.tacc.utexas.edu/

SuperMUC (#9 Top500)
Leibniz-Rechenzentrum (LRZ)
Garching, Germany
155,656 cores, 2.9 PFlop/s
https://www.lrz.de/services/compute/supermuc/

Cartesius (not yet listed in Top500)
SURFsara
Amsterdam, The Netherlands
13984 cores, 271 TFlops/s
https://www.surfsara.nl/systems/cartesius

Emerald (#379 Top500)
Science and Technology Facilities Council (STFC) Rutherford Appleton Laboratory
Didcot, United Kingdom
1008 cores + 372 NVIDIA Tesla GPUS, 114 TFlop/s
http://www.einfrastructuresouth.ac.uk/cfi/emerald

The figure below illustrates how we intend to use these machines for each of the scenarios:



For the first scenario we intend to connect Cartesius to SuperMUC. These machines are geographically close (approximately 700 km). This will allow us to run the ocean model on SuperMUC, and the other models on Cartesius.

In scenario 2 we replace Cartesius with Stampede. These machines are much further apart (approximately 8800 km). This will result in a significant increase in latency during communication between the models. However, since the models are loosely coupled we do not expect this to be a problem.

In scenario 3, we combine the three machines used in the previous two scenarios. We distribute the (relatively tightly coupled) ocean model over Cartesius and SuperMUC (which are close) and run the other models on Stampede (which is much further away).

In scenario 4, we use the GPUs of Emerald to run our GPU-implemented version of the ocean model. The other models are run on Cartesius. These machines are geographically close (approx. 400 km).

Wide-area network infrastructure

In total **three point-to-point connections** between supercomputers are needed, as shown in the figure above. These three connections are sufficient to run all four scenarios. The data flows between sites are described in detail in the first part of this section. As explained, for scenarios 1, 2, and 4 the communication between the supercomputers is performed in bursts. It is therefore important that the bandwidth during the communication phase is sufficient, and that there is limited interference from other traffic. We expect that **10G links** (or faster) provides sufficient bandwidth to run our simulations.

For scenario 3, the communication within the ocean model is more tightly coupled. As a result, low latency and limited jitter on the communication link between Cartesius and SuperMUC are of additional importance in this scenario.
Since the wide area links are not used in all scenarios, and only as part of actual simulations, we believe that **dynamic 10G lightpaths** would suit our needs best. These provide high bandwidth, low latency, low jitter, and no interference from other traffic. In addition, they can be set up on demand, before a simulation is run, and released afterwards. As a result, only the used links would be active.

Static lightpaths would serve our needs equally well, although they would not be in fulltime use. Other solutions may also be acceptable, provided that they offer high bandwidth, and relatively low latency and low jitter for the link between Cartesius and SuperMUC used in scenario 4.

For each of the sites the lightpath connectivity with regional or national providers is as follows:

Stampede (TACC)
TACC has internet2 up to Houston, then fiber from Houston via Austin (UT main campus) to

TACC. Therefore, lightpaths are available up to Houston but some work must be done to forward it to the systems at TACC.

SuperMUC (LRZ)
LRZ is connected to X-WIN.

Cartesius (SURFsara)
SURFsara is connected to SURFNet.

Emerald (STFC)
STFC is connected to JANET.

To the best of our knowledge all participating sites are capable of supporting lightpath services. LRZ, STFC and SURFsara already run other projects that use lightpaths.

For this project we propose to use a dedicated service node in each of the sites which are connected to the lightpath, and configured such that they are in a small private subnet. This allows them to communicate directly with each other (via the lightpaths) and with the other nodes in the machine (using MPI via the local network interface such as infiniband). These nodes can then be used as gateway nodes when running CESM. Alternative solutions may also be used if the use of a dedicated node would be a problem.

Software Infrastructure

From a software perspective we need the following components:
Community Earth System Model (CESM)
The climate models are available under an open-source license from:
http://www2.cesm.ucar.edu/models/current

eSALSA MPI
The MPI wrapper needed for communication between the machines is available under an open source license from:
https://github.com/NLeSC/eSalsa-MPI

This is a prototype that has been successfully tested in smaller scale experiments. Some further development and performance tuning may be necessary to use this solution on the target machines of this project.

eSALSA POP
The ocean model with GPU extensions is available under an open source license from:
https://github.com/NLeSC/eSalsa-POP

This is a stand-alone version of the ocean model. The changes to this version must be ported to the CESM ocean model which is also based on POP. As there is very little difference between these two implementations, this will be straightforward.

Next to hardware and software, we also need an input data set for the ultra-high resolution experiments. This data set contains, for example, description of the geography of the earth. These data sets will be generated by extrapolation of the existing high-resolution data sets.

References:

11. *P.H. Worley, A.P. Craig, J.M. Dennis, A.A. Mirin, M.A. Taylor, and M. Vertenstein. Performance of the Community Earth System Model. Proceedings of 2011 International Conference for High Performance Computing, Networking, Storage and Analysis (SC'11), Seattle, Washington, November 12-18, 2011*
12. *B. van Werkhoven, J. Maassen, M. Kliphuis, H.A. Dijkstra, S.E. Brunnabend, M. van Meersbergen, F.J. Seinstra, and H.E. Bal. A distributed computing approach to improve the performance of the Parallel Ocean Program (v2.1). Currently under public discussion at Geoscientific Model Development (an open access journal).*
13. *J.M. Dennis, M. Vertenstein, P.H. Worley, A.A. Mirin, A.P. Craig, R. Jacob, and S. Mickelson. Computational performance of ultra-high-resolution capability in the Community Earth System Model. International Journal of High Performance Computing Applications, 2012, 26: 5.*
14. *NICS Kraken. http://www.nics.tennessee.edu/computing-resources/kraken*
15. *Performance tests with POP on Cartesius, Michael Kliphuis, 2013.*
16. *SURFsara Cartesius. https://www.surfsara.nl/nl/systems/cartesius*

5. Project plan (no maximum)

Todo's

List per location what needs to be realized, and specify the required steps, who is responsible for each step and an estimated time of delivery (when starting the project early 2014)

Emerald (STFC Rutherford Appleton Laboratory)

Result: Provisioning the lightpath and connect it to Emerald.

What	Who	When
Roll out additional fiber	Scientific Computing / Nick Hill	Once the project starts
Connect service node to POP	STFC Site Telecoms	Once the lightpaths have been provisioned
Configure firewall/switch	STFC Central Networking and Scientific Computing / Nick Hill	Once the lightpaths have been provisioned to the Point of presence on the STFC(RAL) site.

Cartesius (SURFsara)

Result: Connect the lightpaths to one of the service nodes of Cartesius.

What	Who	When
Connect service node to POP	SURFsara / Sander Boele	Once the lightpaths are available.

Stampede (TACC)

Result: Provisioning the lightpath from Houston to TACC and connect it to Stampede.

What	Who	When
Forward lightpath from internet2 (Houston) to main campus at TACC	TACC / Yaakoub El Khamra	Start of project
Connect service node to POP	TACC / Yaakoub El Khamra	Once lightpath is available

SuperMUC (LRZ)

Result: Connect the lightpaths to one of the service nodes of SuperMUC.

What	Who	When
Connect service node to POP	LRZ / Dr. Christian Grimm	Once lightpaths are available
Configure firewall/switch	LRZ / Dr. Christian Grimm	

Preconditions

List any conditions (technical, financial, human resources, external dependencies etc.) that have to be met throughout the project in order to successfully carry out and complete the project.

Depending on the bandwidth required the project is likely to require some additional NICs in the hosts at STFC (Didcot) that will connect to the lightpaths.

TACC has internet2 up to Houston, then fiber from Houston via Austin (UT main campus) to TACC. Therefore, lightpaths are available up to Houston but some work must be done to forward it to the systems at TACC. At the moment it is unclear how much work is needed.

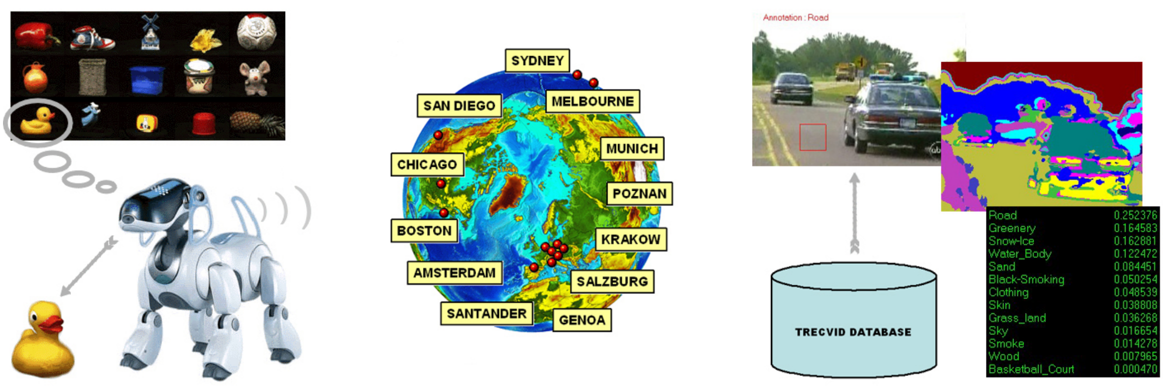
Appendix A

Below we describe two example applications developed by members of the project team in previous years. These examples are included to indicate that we have ample experience in successful deployment of scientific applications on a wide variety of hardware, even on a world-wide scale. Although we have more successful examples, the applications described below a.o. were demonstrated **live** at previous ACM/IEEE Supercomputing (SC) conferences.

High-performance Distributed Multimedia Content Analysis (2004+)

Multimedia Content Analysis (MMCA) considers all aspects of the automated extraction of knowledge from multimedia data. In the last decade, MMCA applications have been gaining importance along with deployment of public digital TV archives, and surveillance cameras in public locations. MMCA has become a problem of phenomenal proportions, with digital video even producing data at rates beyond 100 Mbytes/sec, and multimedia archives steadily running into Petabytes of storage space. For example, the Dutch Institute for Sound and Vision has archived over 700,000 hours of TV data waiting to be analyzed and searched. Distributed sets of surveillance cameras generate even larger quantities of data.

Clearly, for MMCA problems there is an urgent need for speed and scalability, with large-scale distributed supercomputing being one way of pushing forward the state-of-the-art in MMCA. In [17] we have shown that a distributed system comprising hundreds of massively communicating heterogeneous resources located in Europe, USA, and Australia, can bring efficient solutions for off-line applications and (soft) real-time problems (see figure below). Despite the 'toy' nature of the robot application, the applied algorithmic, parallelization, and distribution approaches are exemplary for (soft) real time applications in the domain.



Real-time (left) and off-line (right) distributed multimedia computing on a world-wide scale. The (soft) real-time application constitutes a visual object recognition task performed by a robot dog. The off-line application was our contribution to the 2005 international TRECVID competition.

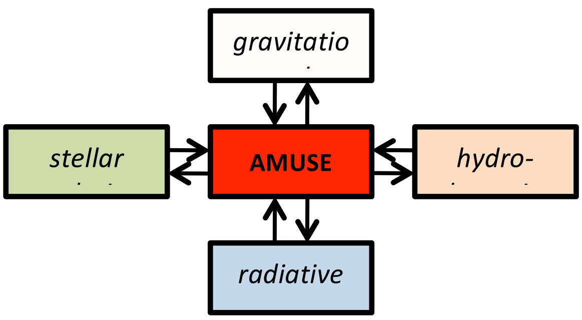
Our distributed MMCA applications have been successful. For the off-line application we obtained a '**Best Technical Demo Award**' at ACM Multimedia 2005. The robot application was demonstrated **live** – under slight variations in the underlying hardware infrastructure - at ICME'05, ECCV'06, SC'07, and HPDC'08. The robot application was awarded the '**Most Innovative Research Award**' at AAAI'07, '**First Prize'** in the Scalable Computing Challenge at CCGrid'08, and was shown on Dutch National Television in December 2012. A video demonstration of the robot application is found at: www.cs.vu.nl/~fjseins/aibodemo.shtml.

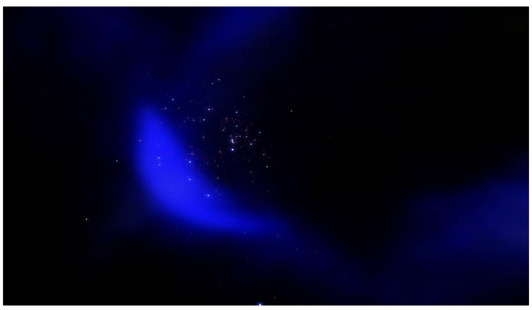
As an aside, it must be noted that in current solutions to similar MMCA problems we also incorporate state-of-the-art GPUs. This was not yet the case in the above demonstrations.

High-performance Distributed Simulation of Star Cluster Evolution (2010+)

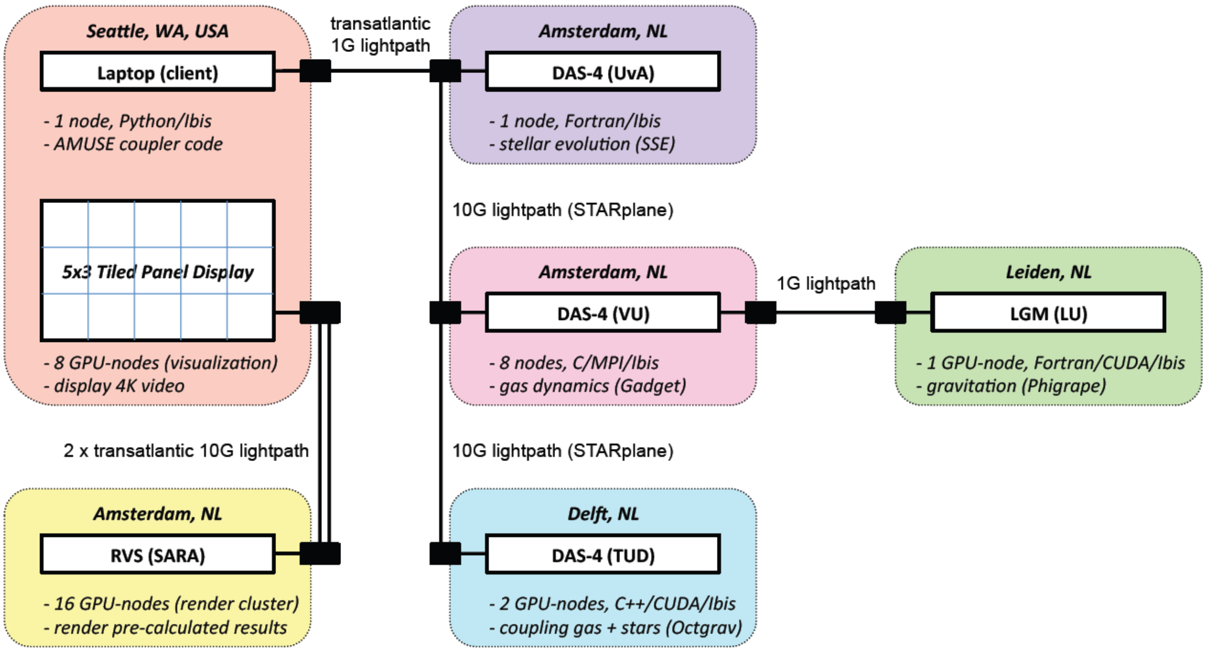
As explained in Section 2 of this proposal, multi-model/multi-kernel simulations are a prime target for Advanced Distributed Cyberinfrastructure and Jungle Computing. Whereas this proposal aims for a solution for the domain of Climate Research, in the recent past we have implemented a very similar (albeit smaller scale) solution for a multi-model/multi-kernel problem from the domain of Computational Astrophysics.

To simulate the early evolution of star clusters (or many other phenomena) in the universe, the domain of Computational Astrophysics combines and integrates several physical models in a very similar manner as in the field of Climate Research. The AMUSE system developed at Leiden University (see [18] and figure below) is a software framework for large-scale astrophysics simulations that couples distinct models for a.o. gravitational dynamics, hydrodynamics, radiative transfer, and stellar evolution. Each of the distinct models is best executed on a different hardware platform. Stellar evolution, for example, is an embarrass-singly parallel problem which is best executed on a cluster computer or cloud system. Gravitational dynamics, on the other hand, is an N-body problem, which is best executed on a GPU cluster. Other models, in turn, are best executed on a supercomputer system.





High-level overview (left) of the AMUSE system, comprising a central coupler component and multiple connected models. Note the similarity with the CESM system for Climate Research described *in Section 4. Visualization (right) of star cluster evolution with stars (dots) and gas (blue) visible.*



High-level overview of our distributed AMUSE simulation demonstrated live at SC'11, Seattle, USA.

Using Jungle Computing technologies, we have build a distributed version of AMUSE capable of vastly scaling up simulations using large-scale, distributed, heterogeneous, and hierarchical computing systems. Our proof of concept system has been demonstrated **live** at SC'11, with the central coupler being executed in Seattle, and all connected models executed using 4 different high-performance computing systems in Europe (see figure above). Transatlantic connectivity was provided through a 1G lightpath, with further connectivity between the computing systems comprising of both 1G and 10G lightpaths. The system was the basis for the '**Sustainability Prize**' awarded to us in the EYR3 competition in December 2011. Video presentations of this work are found at www.cs.vu.nl/ibis/demos.html.

17. *F.J. Seinstra, J.M. Geusebroek, D. Koelma, C.G.M. Snoek, M. Worring, and A.W.M. Semulders. High-Performance Distributed Video Content Analysis with Parallel-Horus. IEEE Multimedia, 14(4):64-75, October-December 2007.*
18. *F.I. Pelupessy, A. van Elteren, N. de Vries, N. McMillan, N. Drost, and S. Portegies Zwart. The Astrophysical Multipurpose Software Environment. Astronomy & Astrophysics, in press, 2013.*

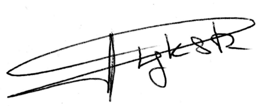
Appendix B: Letters of consent

Date: 10/11/2013

Dear EYRG committee member,

I will take the responsibility as the PI for the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", and I have reserved one million core hours on the Cartesius machine (within the budget allocated to the Netherlands eScience Center project eSALSA) to carry out the computations mentioned in this proposal.

Sincerely,



Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy,
Utrecht University
The Netherlands

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Dr. Frank J. Seinstra
Netherlands eScience Center
Science Park 140
1098 XG Amsterdam, The Netherlands

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Dr. Jason Maassen
eScience Engineer

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Henri Bal
Professor in Computer Science

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Michael Kliphuis
Ir.

Date: 10/11/2013
Prof. Dr. ir. H. A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Sandra-Esther Brunnabend
Dr. rer. nat.

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: “An Advanced Distributed Computing Approach to High-Resolution Climate Modeling”, with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Sander Boele
Senior Network Engineer at SURFsara

Date: 10/11/2013

Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Jules Wolfrat

Dr. Jules Wolfrat
Sr. Consultant SURFsara

Date: 10/11/2013

Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Maarten van Meersbergen, MSc.
eScience Engineer (CESM Visualization)

Date: 10/11/2013

Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Ben van Werkhoven
Msc

OXFORD e-Research CENTRE

UNIVERSITY OF OXFORD

Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dr David C. H. Wallom
Oxford eResearch Centre
University of Oxford,
7 Keble Road
Oxford
OX1 3QG
United Kingdom

Date: 07/10/2013

Dear Prof. Dijkstra,

I would like to confirm that I will be participating in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

As a researcher from within an organization that is a core member of the SES5 consortia which operates the Emerald GPU enables HPC system I have a research account approved on the system already. As part of this there is no strict allocation of CPU hours etc. on the system though I have already engaged the systems operations team representative in my organization and they are excited to have a project that could possibly utilize the whole system at once and will make whatever necessary arrangements are needed to allow us to successfully utilize the system.

Sincerely,

Dr David Wallom

Associate Director - Innovation

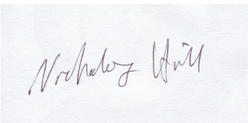
Scientific Computing Department
Rutherford Appleton Laboratory
Chilton
Didcot
Oxon
OX11 0QX
UK

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

I am happy to confirm my desire to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,



Nicholas Hill
Group Leader
STFC Scientific Computing Department

Leibniz-Rechenzentrum
der Bayerischen Akademie der Wissenschaften

Prof. Dr. Dieter Kranzlmüller
Leibniz-Rechenzentrum, Boltzmannstraße 1, 85748 Garching

Garching, den 10.10.2013

Telefon: 089 / 35831-8703
Telefax: 089 / 35831-9700
E-Mail: kranzlmueller@lrz.de

Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University
The Netherlands

Intention of participation in
„An Advanced Distributed Computing Approach to High-Resolution Climate Modeling"

Dear Prof. Dijkstra,

With pleasure I would hereby want to express our intention to participate in the project "*An Advanced Distributed Computing Approach to High-Resolution Climate Modeling*", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

The request for core hours on LRZ's supercomputer SuperMUC as mentioned in the above mentioned project proposal is subject to approval of a respective proposal (under preparation) by the scientific reviewing committee of LRZ and the technical feasibility on SuperMUC.

Yours sincerely,

Prof. Dr. Dieter Kranzlmüller
(Member of the Board of Directors)

DFN
Deutsches
Forschungsnetz

Contact: Angela Lenz

DFN-Verein, Alexanderplatz 1, 10178 Berlin

Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University

The Netherlands

Berlin, 10. October 2013

DFN, the National Research and Education Network in Germany, is deeply involved in high-capacity data communications and novel networking technologies for the scientific community. With its newest incarnation of the German Research Network X-WiN today DFN provides a multi terabit platform to R&E in Germany. Recent extensions such as 100G connectivity to GÉANT as well as hosting of the PRACE core switch in Frankfurt build the ideal environment to get LRZ connected to its partners. With these reasons, DFN gives a strong support to this submission from the International Earth Sciences Community.

Sincerely,

C. Grimm

C. Grimm
Managing Director, DFN

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition. Furthermore, I'd like to confirm that as part of our XRAC allocation (MCB090174), we are making available upto 1 Million computing-hours on XSEDE (primarily Stampede) for climate-science simulations in collaboration with you.

Sincerely,

Shantenu Jha
Assistant Professor

Rutgers University

http://radical.rutgers.edu

Date: 10/9/2013

Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Mark Santcroos
PhD Candidate
Research in Advanced Distributed Cyberinfrastructure and Applications Laboratory (RADICAL)
Rutgers, The State University of New Jersey

UNIVERSITY OF MIAMI
ROSENSTIEL SCHOOL of MARINE & ATMOSPHERIC SCIENCE

Meteorology and Physical Oceanography
Rosenstiel School of Marine and Atmospheric Science
University of Miami
4600 Rickenbacker Causeway
Miami, FL 33149, USA

Phone: 305-421-4046 Email: bkirtman@rsmas.miami.edu

24 September 2013

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to confirm my role as a US team co-applicant in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", as mentioned in the final proposal which will be submitted to the Enlighten Your Research Global competition (deadline October 14). It is clear that this research will benefit climate model improvement and help drive the climate modeling enterprise to produce more actionable results.

Sincerely,

Ben Kirtman
Professor and Associate Dean for Research
Division of Meteorology and Physical Oceanography
Rosenstiel School of Marine and Atmospheric Sciences
Program Director, Physical Sciences and Engineering
Center for Computational Science
University of Miami

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

National Center for Atmospheric Research
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Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With this letter I want to confirm my role as a US team co-applicant in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", as mentioned in the final proposal which will be submitted to the Enlighten Your Research Global competition. As you know, I have been involved in several efforts using very high-resolution versions of the Community Earth System Model to investigate the role of ocean mesoscale processes in the climate system. The project described in this proposal will advance both our technical capabilities in achieving useful high-resolution climate integrations and our scientific insight into the role of small scale ocean processes in the global climate system. I look forward to continued discussions as the proposal and project move forward.

Sincerely,

Dr. Frank O. Bryan
Head, Oceanography Section
Climate and Global Dynamics Division
National Center for Atmospheric Research

Date: 10/11/2013
Prof. dr. ir. H.A. Dijkstra
Department of Physics and Astronomy
Utrecht University, The Netherlands

Dear Prof. Dijkstra,

With pleasure I want to participate in the project: "An Advanced Distributed Computing Approach to High-Resolution Climate Modeling", with the role as mentioned in the final proposal that will be submitted to the Enlighten Your Research Global competition.

Sincerely,

Yaakoub Y. El Khamra

Ressearch Engineer/Scientist Associate IV

Texas Advanced Computing Center TACC

The University of Texas at Austin