A birds eye view of a decade of

efficient computing

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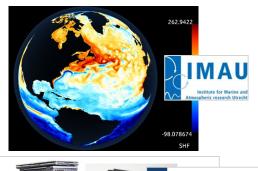


Dr. Jason Maassen

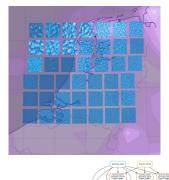
My background



Method Invocation Based **Communication Models** for **Parallel Programming** in Java Jason Maassen









1993-1998 MSc Computer Science HPC

1998-2012
PhD / Postdoc Computer Science
HPC / Grid computing

2012+Research Software Engineer
Ocean Modelling / Digital Forensics

2016+Technology Lead
Efficient Computing





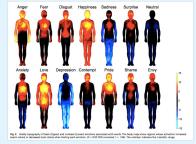






netherlands Science center?





325 projects

(on many different topics)

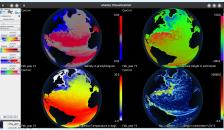


Humanities & Social Sciences

incl. SMART cities. text analysis, creative technologies



incl. astronomy, high-energy physics, advanced materials

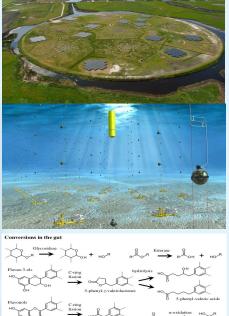


Sustainability & Environment

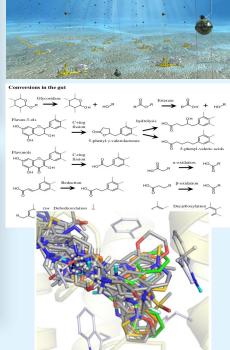
incl. climate, ecology, energy, logistics, water management

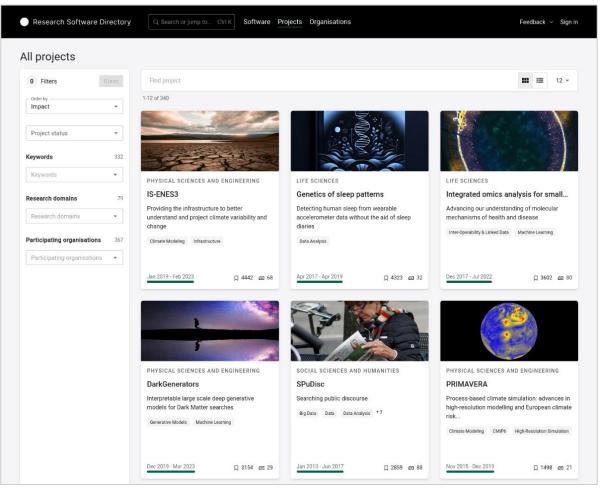


incl. bio-imaging, next generation sequencing, molecules









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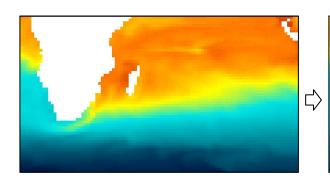
FORTRAN is here to stay

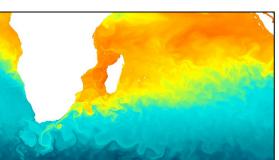
eSalsa (2012-2016)

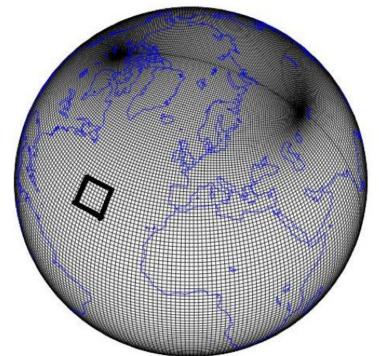
Ocean modelling using Parallel Ocean Program (POP)

Very traditional Fortran/MPI application (1992)

Goal: go from 1° to 0.1° resolution (100x100km to 10x10km)







Source: Los Alamos National Laboratory





PHYSICAL SCIENCES AND ENGINEERING eSALSA

Predicting local sea level changes

Climate Modeling GPU Ocean-Circulation-Models

Jan 2012 - Feb 2016 □ 79 🖃 27



PHYSICAL SCIENCES AND ENGINEERING

Extreme climate changes due to...

Showcasing an extreme high resolution climate simulation

Climate Change Climate Modeling High Performance Computing

Nov 2012 - Dec 2013



LIFE SCIENCES, PHYSICAL SCIENCES AND.

Summer in the City

Forecasting and mapping human thermal comfort in urban areas

Data Analysis

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Jan 2013 - Sep 2016 □ 266 🖃 31



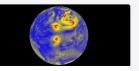
PHYSICAL SCIENCES AND ENGINEERING

Towards Large-Scale Cloud-Resolvin...

Understanding the interaction between clouds and the large-scale circulation

Atmospheric Physics Clouds Convection + 2

Dec 2015 - Oct 2019 □ 200 □ 38



PHYSICAL SCIENCES AND ENGINEERING

PRIMAVERA

Process-based climate simulation; advances in high-resolution modelling and European climate

Climate Modeling CMIP6 High-Resolution Simulation

Nov 2015 - Dec 2019 □ 1497 21



LIFE SCIENCES

Blue-Action

Arctic impact on weather and climate

Climate Change

Dec 2016 - Feb 2021 □ 97 🔳 11



PHYSICAL SCIENCES AND ENGINEERING

MAGIC

Metrics and Access to Global Indices for Climate Projections

Optimized Data Handling Workflow Technologies

Oct 2016 - Mar 2019

□ 0 ■ 4



PHYSICAL SCIENCES AND ENGINEERING

EUropean Climate Prediction system...

An innovative European regional ensemble climate prediction system

Visualization

Dec 2017 - May 2022



LIFE SCIENCES

MOSAIC

Modelling sea level and inundation for cyclones Multi-Scale & Multi Model Simulations

Dec 2018 - May 2024



PHYSICAL SCIENCES AND ENGINEERING

ESiWACE2

predictions



For future exascale climate and weather

Jan 2019 - Dec 2022 □ 120 □ 41



PHYSICAL SCIENCES AND ENGINEERING

ESiWACE3

Centre of Excellence in Simulation of Weather and Climate in Europe

Climate Change Climate Modeling GPU +1

Jan 2023 - Dec 2025 □0 ■ 5



PHYSICAL SCIENCES AND ENGINEERING

eTA0C

Tipping of the Atlantic Ocean Circulation

High Performance Computing

Multi-Scale & Multi Model Simulations

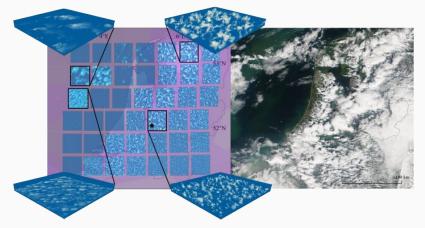
Rare Event Simulations

Jan 2023 - Sep 2027

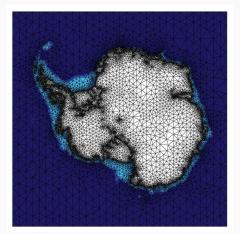
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Since then ... a long string of FORTRAN based projects!

□ 748 24



DALES: Atmospheric Large Eddy Simulation



UFEMISM 2.0 Ice sheet modelling

HADDOCK3: High Ambiguity Driven protein-protein DOCKing





Computational Structural Biology group focusing on dissecting, understanding and predicting biomolecular interactions at the molecular level.

- Email
- Twitter
- O Github
- Youtube

 Subscribe

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Research within the computational structural biology group focuses on the development of reliable bioinformatics and computational approaches to predict, model and dissect biomolecular interactions at atomic level. For this, bioinformatics data, structural information and available biochemical or biophysical experimental data are combined to drive the modelling process. This is implemented and further developed in the widely used HADDOCK solvance for the modelling of biomolecular complexes. By following a holistic approach integrating various experimental information sources with computational structural biology methods we aim at obtaining a comprehensive description of the structural admension of the structural admension to interaction networks and opening the route to systematic and genome-wide studies of biomolecular interactions.

HADDOCK

HADDOCK is a pioneer software in data-driven (or integrative) modelling of protein interactions and our flagship project. Developed since QOSI nour lah, it has been cited more than 1500 times, A user-friendly web server is also available. HADDOCK is well-known for its ability to integrate data in the modelling calculations, such as:

- Nuclear Magnetic Resonance: H/D Exchange, CSPs, RDCs (SANI, VEAN), PREs, PCSs, NOEs, Relaxation data (DANI)
- Mutagenesis
- Mass Spectromety: H/D Exchange, Cross-linking, scoring based on Ion Mobility-MS shape data
- Small Angle X-ray Scattering: Radius of Gyration, scoring based on experimental SAXS curves
- Bioinformatics predictions: evolutionary conservation and co-evolving amino acids

Other interesting features of HADDOCK include:

- Unambiguous Distance Restraints
- Ambiguous Interaction Restraints
- Flexibility of the backbone/sidechain atoms at the interface
 (Simultaneous) Multibody Docking (up to 6 molecules)
- Symmetry restraints (C2, C3, C4, C5, C6, D2, ...)
- Support for proteins, DNA, RNA, peptides, and small ligands (via PRODRG)
- Solvated Docking protocol to model wet interfaces

Binding Affinity Prediction

Interactions between proteins are a beautifully orchestrated event that underlie cellular function. The binding affinity, as defined in physics-chemical terms by the disociation constant (Risk), what determined in flux control in control in the control control in the control control in the control control in control in the control control in control in control in the control control in the con

CADDI

The Borwin lab participates in the Critical Assessment of Prediction of Interactions (CAPRI). This is a fun experiment in which research groups are given the sequence (and sometimes partial structures) of an unknown biomolecular complex (e.g. protein-protein, protein-DNA,...) and are tasked with modelling it using their software. The results are then compared to the unreleased structures that only the CAPRI committee holds (and their authors obviously). This serves not only as perfect playpround for HADDOCK but also as a medium for improvement and development of new features. Currently, HADDOCK and the Bonvin Lab rank #1 in CAPRI, an archivement that makes us all proud!

© 2025 Alexandre Borwin & CSB lab, design by João Rodrigues.

Poscered by Jekyll using an adanted Minimal Mistakes theme.



HPC = GPU

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)	
1	El Capitan - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DDE/NNSA/LLNL	11,039,616	1,742.00	2,746.38	29,581	
	United States			AMD	GPU	
2	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 26Hz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE	9,066,176	1,353.00	2,055.72	24,607	
	DOE/SC/Oak Ridge National Laboratory United States			AMD	GPU	
3	Aurora - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU	9,264,128	1,012.00	1,980.01	38,698	
	Max, Slingshot-11, Intel DDE/SC/Argonne National Laboratory United States			Intel	GPU	
4	Eagle - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure	2,073,600	561.20	846.84		
	Microsoft Azure United States		N	IVIDIA	GPU	
5	HPC6 - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11,	3,143,520	477.90	606.97	8,461	
	RHEL 8.9, HPE Eni S.p.A. Italy			AMD	GPU	
6	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu	7,630,848	442.01	537.21	29,899	
	RIKEN Center for Computational Science Japan			ARM	<u>CPU</u>	
7	Alps - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Stingshot-11, HPE Cray 0S, HPE	2,121,600	434.90	574.84	7,124	
	Swiss National Supercomputing Centre [CSCS] Switzerland		N	IVIDIA	GPU	
8	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE	2,752,704	379.70	531.51	7,107	
	EuroHPC/CSC Finland			AMD	GPU	
9	Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN	1,824,768	241.20	306.31	7,494	
	EuroHPC/CINECA Italy		N	IVIDIA	GPU	
10	Tuolumne - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE	1,161,216	208.10	288.88	3,387	
	DOE/NNSA/LLNL United States			AMD	GPU	



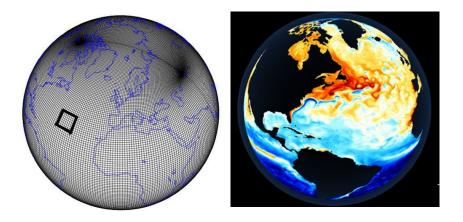
The best illustration of this ...



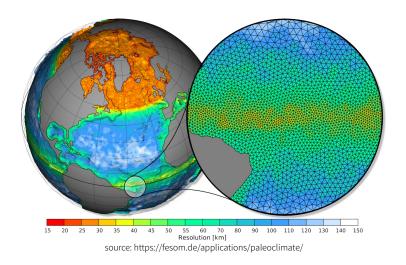
1997 ASCI Red 1.3 teraflops 850 KW / \$46M 150 m2



2025 AMD Radeon RX 9070 XT 1.5 teraflops 317 W / €799 0.04 m2

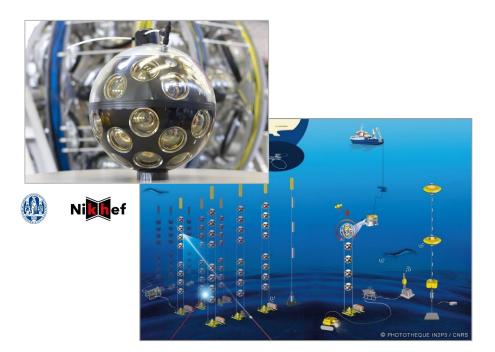


eSalsa (2012-2016) Porting an Ocean Model to GPU



ESiWACE2 (2019-2022)
Porting an Ocean Model to GPU

(yes, we've seen a lot of repeated efforts over the years!)



KM3NeT neutrino detector

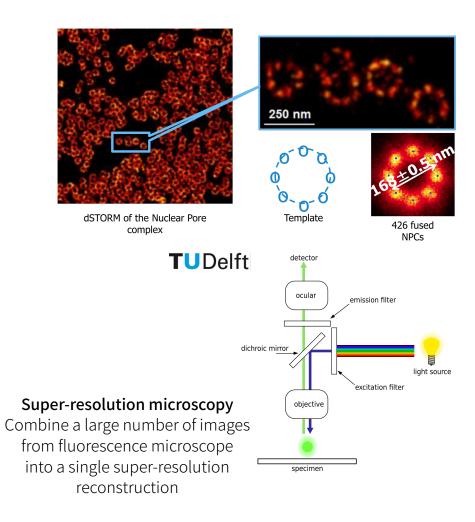
12.000 spheres with 31 photo detectors on 600 strings in the Mediterranean. Filter 55 GB/s in real time to detect neutrinos



APERTIF Westerbork Synthesis Radio Telescope 12 telescopes produce 500 GB/s Processed in real time to detect fast radio bursts



Real-time processing of Synthetic Aperture Radar (SAR) data Energy budget is limited to 50W



(Portable) performance is hard!

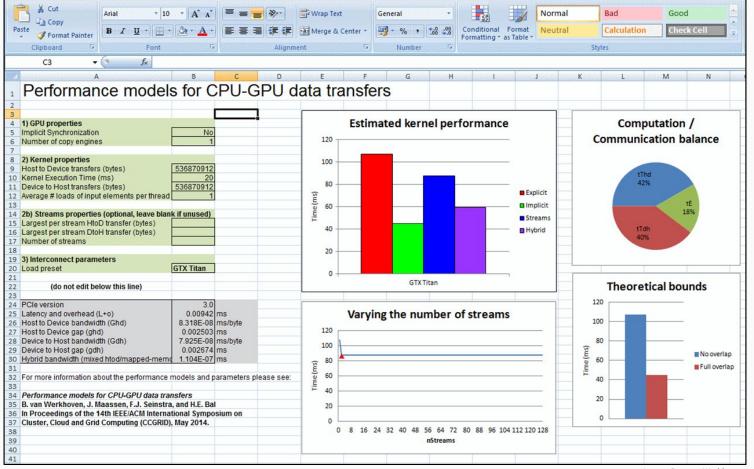
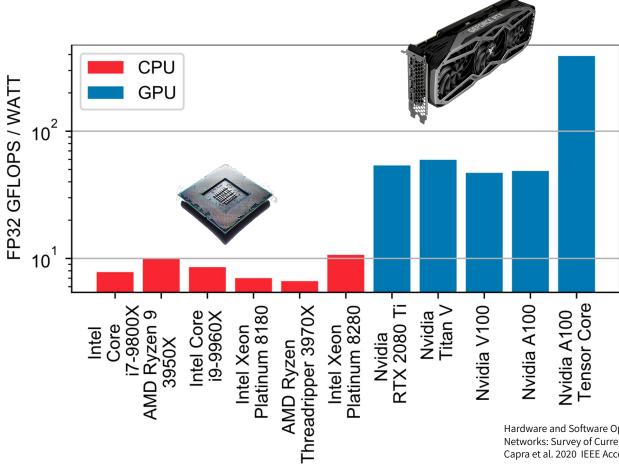


Image: Ben van Werkhoven

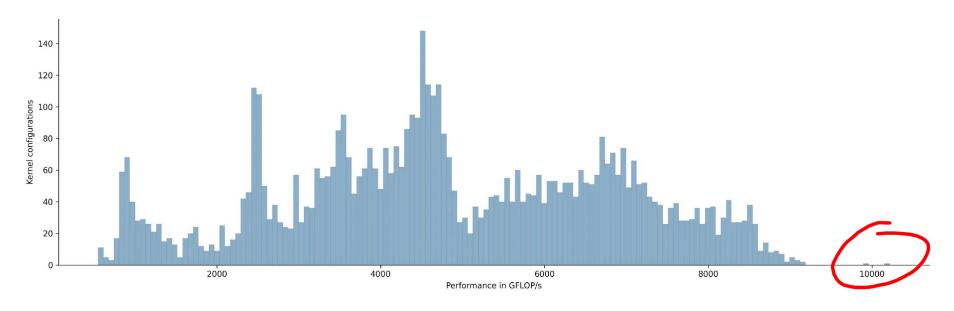
Today, performance depends on hardware...



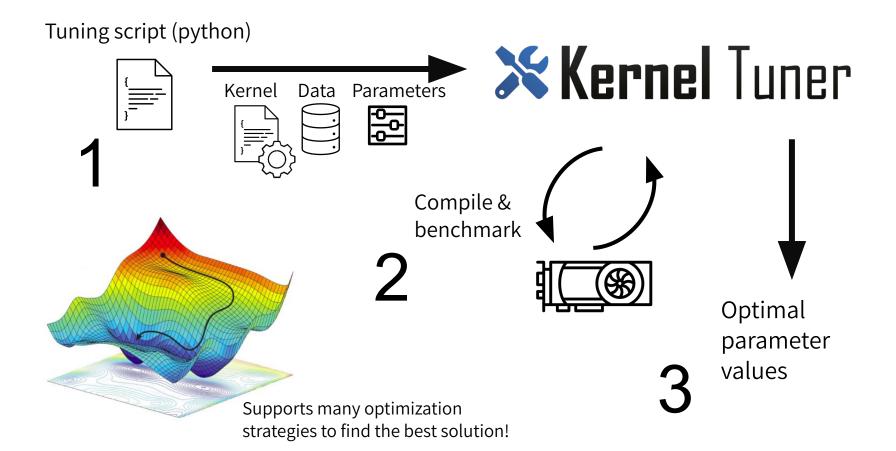
Hardware and Software Optimizations for Accelerating Deep Neural Networks: Survey of Current Trends, Challenges, and the Road Ahead Capra et al. 2020 IEEE Access

... and on the configuration of the software!

Different configurations of a convolution program on an Nvidia A100 GPU



Solution: Autotuning of GPU kernels!





A tool for automatic performance tuning of GPU kernels

Developed open source since 2016 Used by 10+ universities & organizations Funded by several NL and EU projects Supports:

> CUDA, HIP, OpenCL, C++, Fortran, OpenACC 20+ search optimization algorithms Energy measurement of GPU kernels Many different use cases





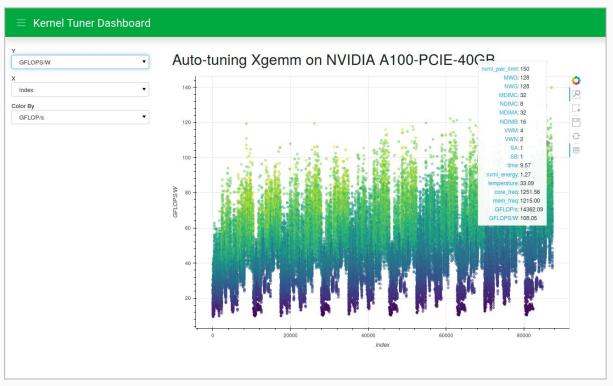






https://github.com/KernelTuner/kernel_tuner

Kernel Dashboard





Extracts & integrates auto-tuned kernels into C++ applications

cudawrappers

Portable API for resource management on NVIDIA & AMD GPUs

https://github.com/KernelTuner/dashboard

Think about energy use!

Energy cost of supercomputers

Frontier:

#2 in TOP500 list

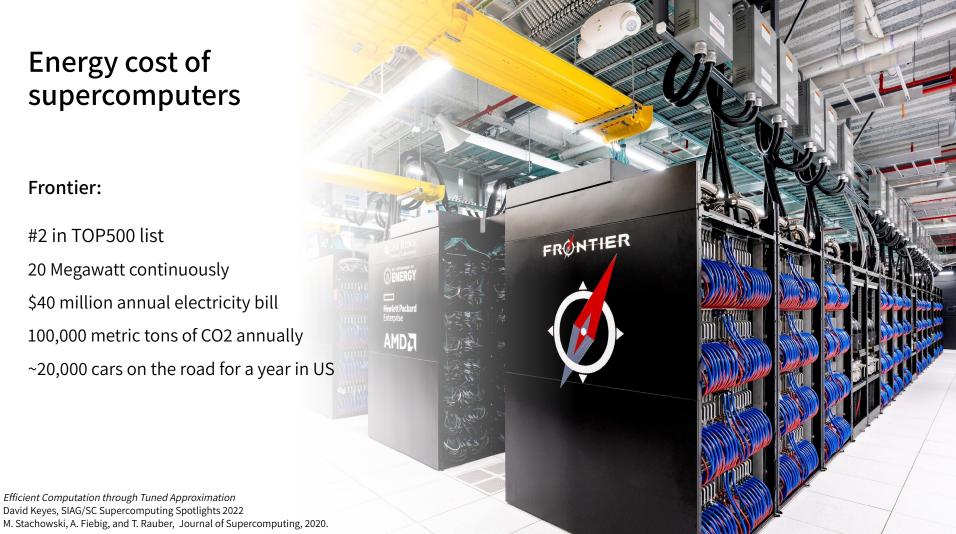
20 Megawatt continuously

Efficient Computation through Tuned Approximation David Keyes, SIAG/SC Supercomputing Spotlights 2022

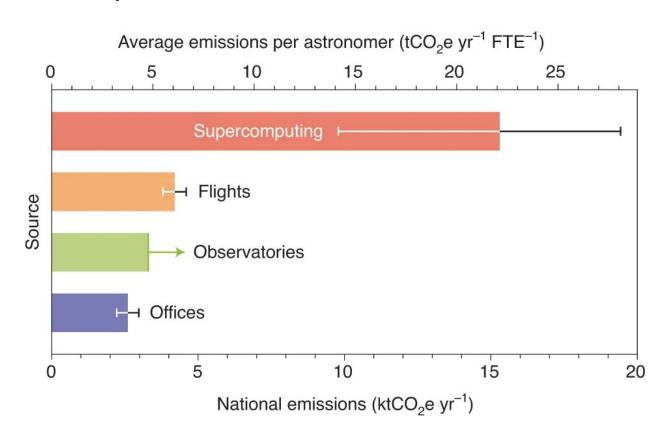
\$40 million annual electricity bill

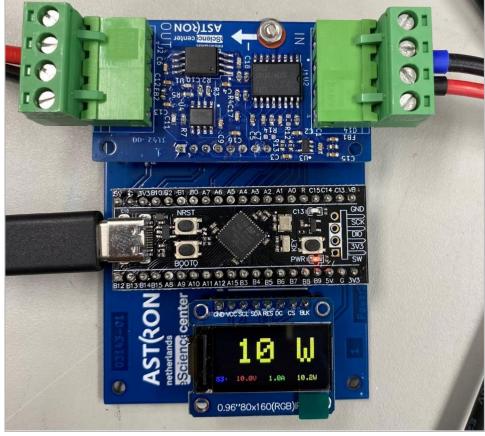
100,000 metric tons of CO2 annually

~20,000 cars on the road for a year in US



The carbon footprint of an astronomer

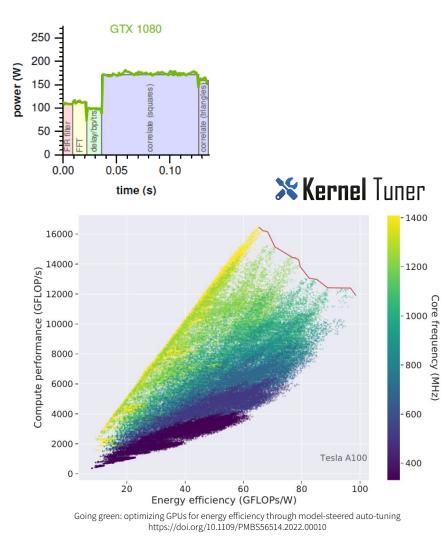




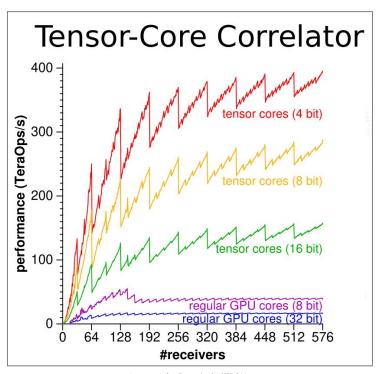
source: https://casper.astro.berkeley.edu/workshop2023/agenda/presentations/day3/11_SV.pdf

powersensor3





Less precision for more performance?





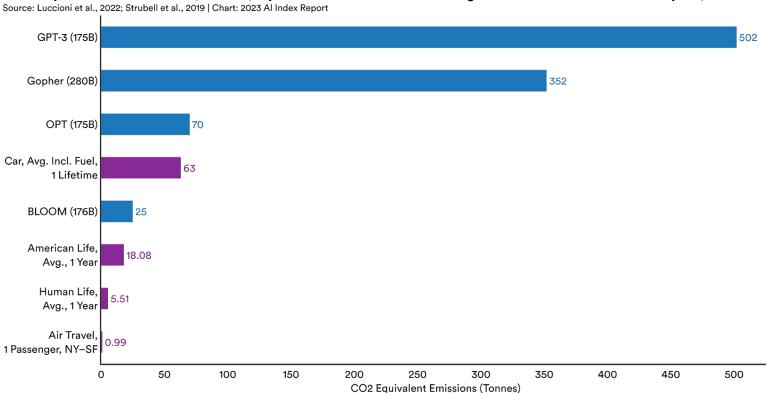
C++ data types for mixed-precision GPU kernel programming

Image: John Romein / ASTRON

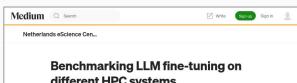
Al is the new HPC?

LLM Training emissions

CO2 Equivalent Emissions (Tonnes) by Selected Machine Learning Models and Real Life Examples, 2022



Source: Stanford AI Index report 2023



different HPC systems



Authors: Flavio Hafner (Netherlands eScience center), Mattie Niznik (Princeton Research Computing), Malte Lüken (Netherlands eScience center), Alessandra Maranca (Princeton University), Matthew Salganik (Princeton University).

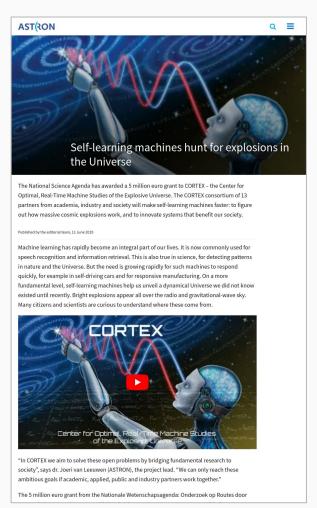
We have developed a benchmark that compares the compute performance of fine-tuning LLMs on multiple high-performance computing (HPC) systems, including systems designed for working with sensitive data. In this blog post, we introduce the benchmark, describe the lessons learned developing it and make it open-source so that it can be used and improved by others.



Photo by Nana Dua on Unsplash

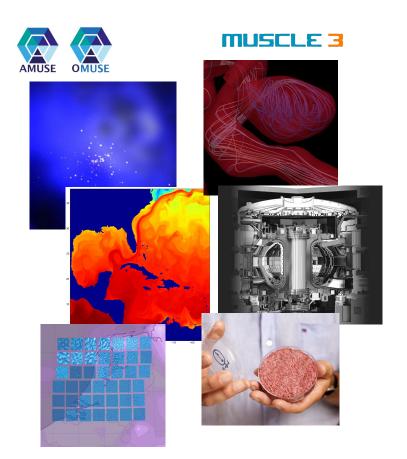
Our use case

Our team researches how Large Language Models (LLMs) can be leveraged to predict social outcomes with large-scale social and survey data. We use the ODISSEI Secure Supercomputer (OSSC), which SURF operates in the Netherlands. The OSSC is a virtual private cluster running on the hardware of Snellius, the Dutch national supercomputer. The OSSC makes it possible to use GPU and CPU nodes to analyze sensitive data from Statistics Netherlands. This makes the OSSC one among very few systems globally that bring the power of national computing clusters to large-scale social data.

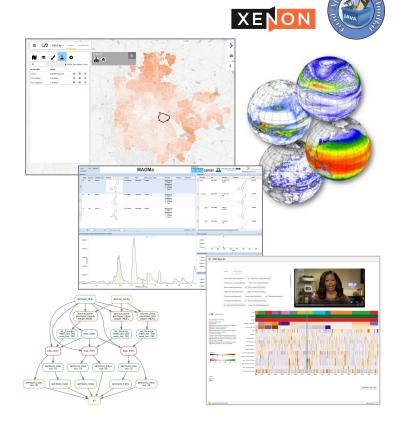


Sign in Sign up AMS@ Journals JOURNALS BROWSE PUBLISH SUBSCRIBE ABOUT Q Search Editorial Type: Article Article Type: Research Article Extended-Range Arctic Sea Ice Forecast with Convolutional Long Short-Term Memory Networks Yang Liu 6, Laurens Bogaardt, Jisk Attema, and Wilco Hazeleger Online Publication: 05 May 2021 Print Publication: 01 Jun 2021 DOI: https://doi.org/10.1175/MWR-D-20-0113.1 Page(s): 1673-1693 Article History Download PDF © Get Permissions Open access @ ① Abstract/Excerpt Full Text PDF Supplementary Materials Abstract Operational Arctic sea ice forecasts are of crucial importance to science and to society in the Arctic region, Currently, statistical and numerical climate models are widely used to generate the Arctic sea ice forecasts at weather time scales. Numerical models require near-real-time input of relevant environmental conditions consistent with the model equations and they are computationally expensive. In this study, we propose a deep learning approach, namely convolutional long short-term memory networks (ConvLSTM), to forecast sea ice in the Barents Sea at weather to subseasonal use of historical records and spatial and temporal relations ConvLSTM is able to learn t concentration skillfully at we LSTM Cell between predictors and predictors persistence, and a statistical with different climate fields predictors on the quality of t budget components have a la This method is a promising future Supplemental information relate https://doi.org/10.1175/MWR-D-20-0113.s1-Denotes content that is immediately available upon publication as open access. This article is licensed under a <u>Creative Commons Attribution 4.0 license</u> (http:// creativecommons.org/licenses/by/4.0/). © 2021 American Meteorological Society.

Interesting Crossovers



multi-model multi-scale simulations



deployment & workflows

What's next for the

roaring 20's?

HPC will get bigger ... and smaller

(because hardware will diversify further)

The role of autotuning will only get bigger

AI will grow up

(scientific AI, physics informed AI, explainable AI, ...)

Digital twins are the new hype

(multi-model + data assimilation + visualization)

FORTRAN will still be here!