

Making hardware, software, and people collaborate

Building scalable e-Infrastructures for research

David Groep, Nikhef November 10, 2020 Physics-DKE colloquium

Scaling & the 'data deluge' ... with data comes processing



Building Scalable e-Infrastructures for Research

Data is distributed – but collaboratively interpreted





>170 institutes in >42 countries and economic regions



- Computing
- On-line disks
- Archival

~ 1,000,000 cores > 310 PB > 390 PB egi Ş Running jobs: 441353 Active CPU cores: 630003 Transfer rate: 35.32 GiB/sec



The High Luminosity Challenge



Source: D. Lange Source: Andrea Sciaba et al. for the WLCG Resource Evolution WG, CHEP2019

dwide LHC Cor

Scaling across all science domains

Dutch-only (!)

compute requirements for LHC, KM3NeT, and SKA, until 2030

Even then, it will be sufficient if and only if

- GPU and parallelism are fully exploited
- throughput per core continues to increase
- data access patterns will match system design



Source: FuSE, the Fundamental Sciences E-infrastructure, 2019 for Research https://fuse-infra.nl

Building Scalable e-Infrastructures for Research

Infrastructure: dealing with data processing at scale

1: matching algorithms and systems design

- designing for high-performance processors
- rethinking design patterns for work & data orchestration



people - systems

2: collating compute, storage, and networks

- building 'facilities'
- peering and global networks
- stressing networks
- research 'cloud' services



systems - systems

3: accessing services, collaboratively & securely

- community building in a multi-national federation
- global trust and identity
- securing the infrastructure of an open science cloud
- our National e-Infrastructure





"It's just hardware"

performance goes up, doesn't it?

- processor performance
- memory bandwidth and on-die caching
- accelerators (GPU, &c)



- wider and faster PCI bus throughput
- faster storage and global interconnects



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Atlas image source: Simone Campana for WLCG, 135th LHCC Meeting Open Session, September 2018

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What we knew was coming ...



Helge Meinhard, Bernd Panzer-Steindel, Technology Evolution, https://indico.cern.ch/event/555063/contributions/2285842/ Figure left: Herb Sutter, Dr.Dobbs Journal 2004, updated 2009, see http://www.gotw.ca/publications/concurrency-ddj.htm

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Yet exploiting even these improvements need people and implementations that take 'hardware' into account

Application performance ("HEPSPEC06") diverging from system capability ("SpecINT")

High level C++ code \rightarrow			if (abs(point[0] - origin[0]) > xhalfsz) return FALSE;					
Assembler inst	ructions	→ an con jbe	ovsd 16(%rsi bsd 48(%rdi) dpd _2il0floa misd 24(%rd eB5.3 #), %xmm0 , %xmm0 // lo tpacket.1(%rip), i), %xmm0 // lo Prob 43% // jun	ad & subtra %xmm0 / ad and com p if FALSE	act / and with a npare	a mask	
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2007 Core 2 efficiency: Sverre Jarp, CHEP 2007 (!)



SPEC benchmark: spec.org, «Rate Base» (R/B) measures throughput under full load of all cores

Graph: measured HS06 and registered SpecINT06 Rate (base) performance per core, with SMT disabled, for the Nikhef Data Processing Facility NDPF (HTC compute) line is not mononotically increasing because of other design choices (power efficiency) and price-performance optimisation chosen



And of course depends on hardware & CPU architecture

AMD "Naples to Rome" – boost in application ("HS06") performance due to new memory (I/O) architecture and direct access to all memory banks



"Zen" Based EPYC" Processors



"Zen 2" Based EPYC Processors

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etrieved from https://www.nextplatform.com/2018/11/06/amds-long-road-from-naples-to-milan-centers-on-rom

And why some changes will not impact performance at all



ps://m.hexus.net/tech/news/cpu/135479-amd-shares-details-zen-3-zen-4-architectures/



Bigger is Better - if you keep it together

Common element: moving data is 'expensive', so 'keep on computing as long as you can, and don't move data around'

- e.g. AMD (and for others: single-socket systems), are better since there are no (useless) cache coherency delays and improved direct memory access
- similarly, keep your GPU busy ... as data comes from (slow) RAM

Getting to be a quite specialised field – use **frameworks** to implement key code



The GPU is specialized for compute-intensive, highly parallel

computation (exactly what graphics rendering is about)

... or just ask Daniel Campora et al.



DVIDIA

and if it doesn't quite fit ...





SuperMicro (branded as 'Lambda Blade') 4U chassis, supporting 10 consumer-grade GPUs with a bump





Image source: https://lambdalabs.com/products/blade

Beyond the single box

Luckily, many things in this world are *conveniently parallel*

- HEP events & simulation
- structural biochemistry

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33149132.korf.nikhef.n	lhcbpi08	lhcb	1	1	5120m	41:59:57	R	32:36:49	wn-mars-057
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challenge is not in the parallelism itself, but in **global compute with data** *just like difference between SI06 and HS06 showed data as the driving factor*



Conveniently parallel: a global infrastructure for research



shared multi-community infrastructure Already EGI e-infra has >250 communities just doing HTC

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Right-hand graphic: EGI operations portal, https://operations-portal.egi.eu/vo/ Building Scalable e-Infrastructures for Research

Nikhef Data Processing Facility – multi-community service

'just one of these sites'



NDPF HTC platform

- member of a federated service with SURFsara, Nikhef, RUG-CIT
- high-throughput storage at SURFsara and Nikhef,
- long-term storage at SURFsara,
- interconnected by SURFnet, and authentication by TCS and IGTF



Getting the data to process ... in the right place







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ESCAPE

Rucio FTS image: "The ESCAPE Datalake" Aris Fkiaras, CERN, February 26th, 2020 ESCAPE WP2 eDIOS https://indico.in2p3.fr/event/20203/sessions/12778/#20200226 DIRAC image from: A. Tsaregorodtsev, CPPM IN2P3, ECL Webiner, 7, June 2016, https://indice.org.ou/ovent/2027

Nikhef storage infrastructure

Storage as infrastructure – even a few PBytes requires some organization

- management challenge is #files, not capacity
- cost challenge is throughput, not capacity

for the management software, see https://dcache.org alternatives exist, like DPM https://lcgdm.web.cern.ch/dpm

ATLAS Federation ATLAS Federation DESY ATLAS Federation, Munich CA-TRIUMF CH-CERN CHIPP CMS Federation DESY RWTH Aachen CPPM, Marseille Canada-East Federation DESY RWTH Aachen DE-KIT DE-Tier3s ES-PIC FR-CCIN2P3 FR-Tier3s
 FZUAS Prague GRID LAB, KAVALA Institute of Technology GRIP, Paris Great Lakes ATLAS T2 (CEPP, Tokyo HEP, Beijing IL-HEP) Ter-2 Federation INN T2 Federation INN

source: https://monit-grafana.cern.ch/d/000000420/fts-transfers-30-day

Structuring of frameworks impacts systems design

pre-staging all data locally supports latency hiding, posix-style access with lseek(2), '\$TMPDIR' e.g. why there are Data Transfer Nodes (DTNs) in the 'Science DMZ' concept

but, recently, pre-staging starts coming at a cost, when using SSDs as local data 'scratch' area ... because of their unique element: 'endurance'

WORN storage – Write Once Read Never

Frequency distribution observed on the NDPF execution nodes for outside ('grid') access (blue) and local access (orange)

Access pattern is rather different. But why?

- external users pre-stage, because that is built into the frameworks (like DIRAC, Athena), where local users can use streaming access ('dCache NFSv4') yet there are changes in pre-stage streaming behaviour over time
- different types of workload: ntuple-data analysis vs (re)processing

Data: NDPF execution nodes, based on SSD SMART data, integrated over total device lifetime lot shows number of local analysis nodes scaled to DNI-WLCG count; collected using smartctl on 2020-10-28

Data comes from somewhere, and has to go somewhere ...

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STBC Analysis

Left: IBR-LAN (1996) in H1.40; Right: Nikhef peering visualisation (medio 2020)

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Desktops and

servers 10Gbps

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Analysis Storage

SURF DNI Compute & Storage

Interface: ae66, Enabled Encapsulation: ethernet, Traffic statistics: Input bytes: Output bytes: Input packets: Output packets:	d, Link is Up , Speed: 1200000mbps 491308044270834 (5226505855 55684866 (49256 bps) 7676688082851 (1020790999 418932 (48 pps)	Current delta 76 bps) [455708529457430] pps) 1.02 Bpps 7872] [
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ballenbak.nikhef.nl Image: Tristan Suerink Nikhef

Our science data looks akin to a DoS

evaluating resilience to cyberattack – in a cooperative way

Segmentation: a network of 'private domain' clouds within

open-core research network model implements the enclave structure

protects against overload by no stateful components in the network path

and allows open research federated cloud using eVPN overlays

although you'll always have some (reputational) risks even if you advertise the block as 'customer network devices'

Nikhef cloud – targeting high-throughput use cases

There is NO CLOUD, just other people's computers

Nobody wants a cloud ... you want a solution! research community overlays and 'virtual clusters'

at scale: container computing, yet with curated application images - slateci.io

Cross-organisation infrastructure we need an 'ecosystem' more than a cloud

on-prem cloud, or research cloud, is oft better

- very cost-efficient if utilised at capacity
- effective as it can provide more than 'laaS'
- can leverage our own R&E federated access

and not all 'cloud' is what you think it is

PROMPTING AN EOSC IN PRACTICE

"We are creating a European Open Science Cloud now. It is a trusted space for researchers to store their data and to access data from researchers from all other disciplines. We will create a pool of interlinked information, a 'web of research data'. Every researcher will be able to better use not only their own data, but also those of others. They will thus come to new insights, new findings and new solutions."

Ursula von der Leyen, European Commission President World Economic Forum in Davos, January 2020

EOSC – the European Open Science Cloud more an ecosystem (or 'web of data') than a 'cloud'

sources: https://www.eoscsecretariat.eu/eosc-symposium-programme/

An ecosystem built on federated infrastructures

EOSC Portal (https://www.eosc-portal.eu/) – as built by EOSChub

Whence we came: the long road to federated access

From disparate systems in ~2000

separated authentication and authorisation, splitting *identity sources, community membership,* and *services*

Federated Access

Login via the Nikhef service proxy to *gitlab, ifosim.org, ...*

"Where are you from"

discovery screen showing entities from the eduGAIN global interfederation

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ifosim federated AAI integration implementation

Nik]

eduGAIN

Challenges of scaling federation

Beyond 'enterprise' services, it becomes challenging!

Collaborations - by design - have their services distributed and

- not that many collaborations are a legal entity
- or not 'legally authoritative' for constituent services
- or run into risk-averse, or slow, 'home organisations'

Scaling community and institutional trust

eduGAIN (global R&E) Entity Categories	e-Infrastructure IGTF Authentication Profiles	Use of proxy bridging components
Curated grouping of entities 'REFEDS R&S' this is a research service	Common baseline and profiles co-defined by relying parties	SP SP SP
'DP CoCo' abides by GDPR	user-centric ID harmonisation with unique global naming	Identity and access 'proxy'
cares for security response	<i>real person with real name</i> 'DOGWOOD'	based on entity categories
slower adoption process	persistent linkable identifier	leverage Sirtfi and 'R&S' proxying is bi-directional
action at all 60+ Feds & 4k+ IdPs	research-specific user base	responsibility on the proxy operator

Research-friendly federation: REFEDS R&S ... or SRAM

🏀 REFEDS Spaces 🛩	Search Q	Log in			'a scie	nce co	llabor	ation zo	one'
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-	Research and Scholarship			Us Memb	er Account Registry	Members Managem	hip ient	h	
Pages	Created by Nicole Harris, last modified on Apr 30, 2020				ипла	- Service			
99 Blog	For IdP Operators				8 Î	Existing	Existing	Newly piloted	Existing services
CHILD PAGES	What attributes should be released by a	an R&S IdP	?	17 in	MataData	sources	federation	FIAM INITASUUCTURE	consume federated IDs
Entity-Categories Home	The Decearch & Scholarship energification define	a a hundlar c	of attributes the	Identit	ty HUB Service	-	SURF CONEXT .	Proxy	and groups
Research and Scholarship FAQ	Providers are encouraged to release to R&S ser	vices:		Disco Ser	overy 2FA vice	UMCs 1	50 institutions	Athenies	And ODC Hattand Hat
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	a significant subset of its user population	, release all re	equired attributes in						

https://refeds.org/SIRTFI https://refeds.org/assurance https://refeds.org/category/research-and-scholarship

Bridges and Token Translation Services

GEANT Trusted Certificate Service

TCS (today: Sectigo) acts as SAML Service provider to eduGAIN: eligible authenticated users can obtain client certificate for access and delegation to services

Building Scalable e-Infrastructures for Research https://cert-manager.com/customer/surfnet/idp/clientgeant https://www.geant.org/Services/Trust_identity_and_security/Pages/TCS.aspx/

Interoperable Global Trust Federation IGTF

3 regional chapters: EMEA, Americas, AP

- ~ 90 Identity Providers (some leveraging a R&E federation)
- ~ 10 international major relying parties
- ~ 60 countries / economic areas / extra-territorial orgs
- > 1000 relying service provider collaborations

Managing complexities of distributed identity sources

their own 'proxy' model to abstract complexity

each of which had to manage federation complexity

Community images: Romain Wartel, CERN; Mikael Linden, CSC; Lukas Hammerle, SWITCH

Community First' AARC Blueprint Architecture: the Proxy

... user and group ID same across services ... minimize discovery 'wayf' & info screens

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https://aarc-community.org/guidelines/

Linking the providers and users together - AAI

AARC BPA's 'community-first' model does not cover all EOSC cases, e.g. *infrastructures acting as providers* **and** *suppliers* **and** *as attribute authority*

Now what have we built?!

We have federation and single sign-on but can we share security information when needed? ... timely and confidentially, protecting everyone's reputation?

Assessing risk ... in a collaborative infra

InfoSec **risk assessment framework** for (EOSC) services based on WISE SCI

abolices values, care on en HDP* pervises in the tope of the DDM* instance is associated coordinated by SURF, and partners in theread in instance uses in which INMAN participates and in have been designated as an in-scope target autence by exploit designation or by default, in scope Services are those services that are managed and operated by or provided under the authority of the Computer Technology (CT) group and/or the Physics Data Processing (PDP) programme that are in addition interface to be used by the Target Audience (Target (Target Audience (Target (Target (Target (Target (Target

Contents

Introduction and scope		
A.5 Information security policies		
A.6 Organization of information security		
A.6.1 Internal organization		
A.6.2 Mobile devices and teleworking		
A.7 Human resource security		

e.g. ISO27001 can help structure or identify gaps in your knowledge, but ISO27002 should not be blindly applied without *considering the federated interactions*

	SCI version 2.0, 31 May 2017
	L Florio ¹ , S Gabriel ¹ , F Gagadis ¹ , D Groep ¹ , W de Jong ¹ , U Kalla ¹ , D Kelsey ¹ , A Moens ¹ , I Neilson ¹ , R Niedorberger ² , R Guick ² , W Raquel ¹¹ , V Ribaillier ¹¹ , M Sallé ¹ , A Scicchtano ¹ , H Short ¹⁷ , A Slagell ¹¹ , U Steworic ¹¹ , G Venekamp ² and R Warte ¹⁰
	The WISE SCIv2 Working Group - e-mail: david kelsey@stfc.ac.uk, sci@lists.wise-community.org
A	B CÉANT Association, Ameteriam, The Netherlands: ² Nikhof, Amsterdam, The Netherlands: ² CEANT
1 Infrastructure Name:	Fermilab, Ltd., Cambridge, United Kingdom; ⁴ SURFsara, Amsterdam, The Netherlands; ⁵ CSC, IT Center for
2 Prepared By:	Keith Chait Science Ltd., Espoo, Finland; " STFC Rutherford Appleton Laboratory, Didcot, United Kingdom; "SURFnet, Utrecht, The Netherlands; "Forschungszentrum Jülich GmbH (FZJ), Jülich, Germany;
3 Reviewed By:	Indiana University, Indianapolis, USA; ¹⁰ National Center for Supercomputing Applications, University Indiana
5 SCL Operatio	ropean
	wise=community_oro/
8 SCI-053 - Vul	
9 SCI-OS4 - Introsion Detection	18
10 SCI-OS5 - Regulate Access	X (WISE) trust community. SCIV2-WG members include information security officers from several large-scale distributed Research Infrastructures and e-Infrastructures
11 SCI-OS6 - Contact Information	X The aims of the trust framework defined in this document are to enable
12 SCI-OS7 - Policy Enforcement	interoperation of collaborating Infrastructures and to manage cross-Infrastructure
13 SCI - Incident Response [IR]	operational security risks. It also aims to build trust between Infrastructures by
14 SCI-IR1 - Contact Information	security policy documents cannot be shared.
15 SCI-IR2 - Response Procedure	The second se
16 SCI-IR3 - Collaboration	X for the management, operations and security of a Research Infrastructure or an
17 SCI-IR4 - Assurance of Compliance	X e-Infrastructure.
18 SCI - Traceability [TR]	© Owned hy the authors and made systemic increase https://reastworownone.com/increase/hy-on-self 0/
15 SCI-TR1 - Traceability DP12	1 User Designation
20 SCI-TR2 - Data Retention DP5 - User Personal Data	PR12/Development activities of the sources / Attribution / Acknowledgements: The "SCI version 2" document, "A Trust Framework for Security PR12/Development for Security
21 SCI-TR3 - Document Controls	Cotat PR12 3 - 1 Ser Sispersion Kesey, K Chatack Maturity, U Kata, C. Kanelopoulos,
22 SCI - Particpant Responsibilites [PR]	J. Injectioner Technologies and the proceedings of The Database Strength and the proceedings of The proceedings of Thernational Symposium of Grids and Clouds – ISGC 2013* P S/ISGC2013/011.
24 SCI-PR1 DP3 - Moniton mg Data 24 SCI-PR2 - User Awareness & Agree	https://pos.see.PR12.4.setUser-Removal-%202013_011.pdf
25 SCI-PR3 Partnership Communication	Alternate
DP2 - User Registration Data SCI-PR11 - Collections of Users Process	PR12.5 - User Banning maturity
27 SCI-PR12 - Infrastructure Policies	See https://wile-community.org/
20DPgI-PAccounting Diaticy for Actions	PR13 - Responsibility for Actions
29 SCI-PR14 - User Identification	Authentication Policy
30 SCI-PR15 - Logs of Membership Management Act	tions OSE Baseline
ny Additional Restriction on Aims & Purposes	PR14 - User IdentificationCome Page - http://fermigrid.fna
32 SCI-PR21 - Vulnetability Patching	Fermilab Patching Timeline
SCI-PR22 - Incident Reporting	PR15 - Logs of Membership
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LI4 -Dispute Handling and	PR16 - Define Common Aims &
SCI- segar issues [Li]	Fermilab Policy on Computing
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re sci-Li3-iSoftware Licensing	
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39 Sci-US - iSaftware Licensing L12 - Liability, Responsibilities 8	PR22 - Incident Reporting

A Trust Framework for Security Collaboration

this spider diagram is fictional - based on a idea by Urpo Kaila, CSC

Containment & segmentation

matching the 'open core' research network community data & systems 1st class citizens

impression Nikhef network-level segmentation

CORE Critical CII segment

BYOD, laptops and self.

Information segment IKOHEF

Community Data

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beeld stynting vesting Bourtange

A question of when, not if

A federated community security challenge

Can we coordinate our collective R&E response? 'challenges' based on the *Sirtfi* contact model

Security Incident Response Trust Framework for Federated Identity

One Service Provider discovers a compromised user and alerts the Identity Provider of this user. Additional affected services are identified and hould be able to see activity by the Identity in their logs.

PARTIES INVOLVED IN RESPONSE CHALLENGE

REPORT-OUTS SEE HTTPS://WIKI.GEANT.ORG/DISPLAY/AARC/SIRTFI+COMMUNICATIONS+CHALLENGES%2C+AARC2-TNA3.1

INFN IdP

Sharing threat intel – working with our community

AARC I-051 Guide to federated incident response https://aarc-community.org/guidelines/aarc-i051/

e-Infrastructures: EGI, EUDAT, GEANT, PRACE, ... and DNI!

imagery: EGI.eu

'DNI coordinated by SURF'

Coordinated Dutch National e-Infrastructure

- Single application portal (at SURF and NWO)
- Resources allocated at most-suitable partners
- Federated management and common innovation

Home	Systems 🔻		About this site
▶ Cartesius	Svste	em sta	atus
▶ Lisa	Status update S	UREsara system	ns:
 Custom Cloud Solutions 	System	Status	Remarks
Data Archive	Cartesius	Up and running	21-10-2020: The scratch file system was I/O on scratch at that time.
Data Repository	Lisa CPU	Up and running	
EPIC PID	Lisa GPU	Up and running	
Research Drive	Data Archive	Up and running	Maintenance 2020-11-10 08:00 till 14:00
DP - Grid	EPIC PID	Up and running	
DP - Spider	ResearchDrive	Up and running	
▶ HPC Cloud	B2SAFE	Up and running	
 Collaboratorium 	Grid	Up and running	National e-Infrastructure Grid Downtime
 Visualization 	HPC Cloud	Up and running	See Maintenance Calendar
 System status 	Hathi Hadoop Lucy Elasticsearch	Discontinued Discontinued	
 General info 	SURFdrive	Up and running	

Nik

https://servicedesk.surfsara.nl/jira/plugins/servlet/desk/portal/1

Connecting resources – people – organisations – data

The definition distinguishes between hardware resources and services available to all researchers in the Netherlands (Category I), and those made available to a selected subset (Category II). The Category I e-Infrastructure, outlined below, is formed by the hardware resources and services provided and maintained by SURFsara, SURFnet, DANS, and - in part - also by Nikhef and RUG-CIT.

https://www.nwo.nl/onderzoek-en-resultaten/programmas/Rekentijd+nationale+computersystemen

Contact

Balanced infrastructure - based on our joint science cases

FuSE – Fundamental Sciences E-infra an integrated infrastructure for algorithms, hardware, networking, and collaboration

... since some things are fun, but not quite that scalable ...

Nik hef

GSKILL

Liquid CO₂ cooling test bench, 24.33% overclocked using CineBench R20 best sustained, i.e. without LN2... In a Nikhef-AMD collaboration

	SCORE	USER		FREQUENCY	HARDWARE	COOLING	HW		
1.	23323 pts		Splave	5400.2 MHz	AMD Ryzen Threadripper 3970X	LN2	0pts		0 💭
2.	23081 pts		Alex@ro	5375 MHz	AMD Ryzen Threadripper 3970X	LN2	0pts	()	1 💭
3.	22064 pts		Hiwa	5050.6 MHz	AMD Ryzen Threadripper 3970X	LN2	0pts	()	0 💭
4.	21601 pts		keeph8n	5000.4 MHz	AMD Ryzen Threadripper 3970X	LN2	0pts	()	0 💭
5.	20022 pts		Nikhef	4600.1 MHz	AMD Ryzen Threadripper 3970X	SS	0pts	\square	0 💭

T Suerink, K de Roo: https://hwbot.org/submission/4539341_nikhef_cinebench___r20_with_benchmate_ryzen_threadripper_3970x_20022_pts

Let It All Collaborate!

David Groep

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Nikhef