SNIC SWEDISH NATIONAL INFRASTRUCTURE FOR COMPUTING

SNAC SWEDISH NATIONAL ALLOCATION COMMITTEE

Philipp Schlatter Chairman SNAC KTH Mechanics, Stockholm, Sweden



Outline for today

- Short intro about me
- SNIC
- SNAC
- Large-scale applications
- PRACE and HPC-Europa3
- Questions and (hopefully) answers





Who am I?



Philipp Schlatter

PhD in Technical Sciences, ETH Zürich, Switzerland (2005)

Moved as postdoc to KTH Stockholm, now Professor in Fluid Dynamics, KTH Mechanics

Member of SNAC since 2009

Chairman of SNAC since 2018

Involved in "supercomputing" since Master's thesis at KTH (1999), at that time running on CRAY J90 (PDC) and SIG Origin 2000 (NSC)





The Linné FLOW Centre and the Swedish e-Science Reserach Centre

- Centre of excellence in Fluid Mechanics at KTH Stockholm (Sweden), 2007 – …
- Approx. 30 faculty and 50 PhD students



www.flow.kth.se

- Strategic research area in Sweden → e-Science
- Collaboration with visualisation, numerics, application experts...



www.e-science.se





Swedish e-Science Research Centre (SeRC)

CONTENTS

Welcome to SeRC!. 1. e-Science and SeRC...

- 2. The first five years Success story: Personalised cancer screening (eCPC) . Success story: "Virtual wind tunnel" Success story: "Virtual wind tunnel" Success story: GROMACS - Molecular simul:
- Success story: Visualisation. cess story: Electronic structure.....
- 3. The future. Initiative: Multidisciplinary collaboration prog Initiative: Scientific computing lab..... Initiative: Data-driven science

THE CONCEPT OF e-SCIENCE In its most basic form, the concept of e-Science information and the processing of this informati

SeRC LEADERSHIP

Dan Henningson Director, KTH Erik Lindahl Co-director, SU Olivia Eriksson Coordinator, KTH Morten Daelen Chairman of the board, University of Anders Ynnerman Vice chairman of the board, LiU Juni Palmgren University representative, KI Gunilla Svensson University representative, SU info@e-science.se, www.e-science.se

Text: @ SeRC. The contents may be quoted provided the tion data based on Thomson Reuters databases. Photo/rendering: 05 SAPC except & Andrey/Copow/Stor Photo/rendering: 05 SAPC except & Andrey/Copow/Stor Thinkstock, pz.Xze/Stock/Thinkstock Thinkstock Stock/Thinkstock 19 parumas nikomkai//Stock/Thinkstock Editing, form, layout, illustrations: Gunnar Linn, Linnko Print: Atta.45 Tryckeri AB, Järfälla, 2016



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SUCCESS STORY: "VIRTUAL WIND TUNNEL"

utomotive, aeronautic, and maritime Atransport of people and goods play important roles in the globalised world, but are also using up about five billion barrels of oil per year. Roughly half of the energy being spent worldwide in such transport activities is dissipated by undesired turbulent motion in the interface between moving objects and surrounding fluid. The knowledge of the behaviour of turbulence dose to these surfaces is of paramount importance if optimal design and perhaps drag reduction via flow control is attempted.

Accurate numerical simulations allow the characterisation, with the highest level of detail, of the multiple physical phenomena present in complex flow cases such as around airplane wings. The physics

Figure 5. Three-dimensional visualisation of turbulent vortices in the flow around a NACA4412 wing section simulated in the "virtual wind tunnel".

includes the change from laminar to turbulent flow, developed turbulence, separation and the structure of the turbulent wake. In this project we use large-scale numerical simulations (so far with up to 3.2 billion grid points) to analyse the flow around an idealised wing.

Numerical experiments in a "virtual wind tunnel" and the concept of "virtual wind tunnel" aims at replacing, in the future, some real wind-tunnel experiments by corresponding simulations, which will yield a much larger wealth of data relevant for design purposes.

Read more on www.e-science.se/flow

September 2019



Why are we here...?

- "When a sufficiently advanced computer becomes available, we believe it will replace the wind tunnel as the principal facility for providing aerodynamic flow simulations"
- "If past trends continue, such computer performance should be available in the mid-1980s..."

Chapman, D. R., Mark, H., Pirtle, M. W., "Computers vs. wind tunnels for aerodynamic flow simulations", Astronautics & Aeronautics **13**(4):22-30, 1975 (NASA Ames)





SNIC Swedish National Infrastructure for Computing



Philipp Schlatter

September 2019

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Swedish National Infrastructure for Computing SNIC

The **Swedish National Infrastructure for Computing** is a science enabling e-infrastructure for Swedish research.

SNIC makes available resources for large scale **computing** and **storage**, and provides advanced **user support** in order to facilitate efficient use of the SNIC resources.

SNIC provides these services for Swedish researchers at universities and research agencies, but not commercial companies.



Setting the context...

Go to <u>www.menti.com</u> and use the code 27 07 71.

Cost of a core hour including everything

https://www.mentimeter.com/s/b854d9dafae78f0aaf3e9eba04337ab5/2a395b8ad9df/edit



SNIC

- SNIC was founded in 2003 as a collaboration between six computing centra with funding from the Swedish Research Council (Vetenskapsrådet – VR) and participating universities
- In 2012 Uppsala University became the host for SNIC
- From 2018 SNIC is organized as a consortium of ten universities
- SNIC is the second largest national research infrastructure (largest ist MAX-IV)



SNIC



SNIC is being reorganized from a collaboration between **six computing centra** ...

SNIC

- Umeå (HPC2N)
- Uppsala (UPPMAX)
- Stockholm (PDC)
- Linköping (NSC)
- Gothenburg (C3SE)
- Lund (LUNARC)

The SNIC consortium



- ...to consortium of **ten universities**:
- Umeå University
- Swedish University of Agricultural Sciences (SLU) Uppsala
- Uppsala University
- KTH Stockholm
- Stockholm University
- Karolinska Institute (KI)
- Linköping University
- Chalmers Göteborg
- Gothenburg University
- Lund University



SNIC funding 2018-2022



100 MSEK/year from the Swedish Research Council VR.

64 MSEK/year **in-cash** participation and usage fees from the members in the consortium.

32 MSEK/year **in-kind** contributions in the form of provisioning of user support for the general SNIC national services.

Total ~200 MSEK/year + additional projects



SNIC Governance



SNIC National Collaboration



Common resources

Nationally available storage (Swestore) Common resource allocation (SNAC) Advanced user support Shared competences

International collaborations PRACE (Tier0/Tier1), EUDAT, EGI, NeIC, EOSC, EuroHPC, HPC Europa.

Collaboration with other national RI

Max IV, Scilifelab, Onsala, WLCG, ...



SNIC Board

SNIC board until end of 2019:

- Mille Millnert (LiU), chairman
- Per Dannetun, (LiU)
- Bjørn Hafskjold (NTNU, Norway)
- Kristina Edström, (UU), deputy chairman
- Kristina Gold (Ericsson)
- Annika Stensson Trigell (KTH)
- Stefan Eriksson (KI)
- Katrine Riklund (UmU)
- Anders Karlhede (SU)



SNIC Office

SNIC Office at Uppsala University during 2019:

- Hans Karlsson, director
- Anna-Helena Brandhammar, accountant
- Ann-Charlotte Sonnhammer, technical coordinator
- Lars-Owe Ivarsson, technical coordinator
- Mathias Brännvall, coordinator
- Per-Olov Hammargren, SNAC coordinator
- Nils Daniels, security coordinator



SNAC

SNAC – Swedish National Allocation Committee:

- Philipp Schlatter, chairman (KTH): Fluid dynamics, HPC, numerics, climate
- Johan Revstedt (LU): Fluid dynamics, Mechanics, climate
- Lynn Kamerlin (UU): *Biology, chemistry*
- Mattias Marklund, deputy chairman (GU): Physics, electromagnetics, plasma and atomic physics, quantum dynamics
- Leif Eriksson (GU): Theoretical chemistry
- Paul Erhart (Chalmers): condensed matter physics



SNAC Working Group

SNAC - WG:

- Philipp Schlatter, KTH, Chair SNAC
- Anders Sjöström, LUNARC
- Thomas Svedberg, C3SE
- Peter Münger, NSC
- Henric Zazzi, PDC
- Marcus Lundberg, UPPMAX
- Jerry Eriksson, HPC2N
- Dejan Vitlacil, PDC (Swestore)
- Jens Larsson, NSC (Swestore)



SNIC Computing Resources



SNIC computing resources

Name	Partner	Approx. performance	Size
Aurora	LUNARC, LU	115 TFLOPS	1.3 Mch/month
Beskow	PDC, KTH	2000 TFLOPS Tenger: GPU, fat	40 Mch/month
Hebbe	C3SE, Chalmers	180 TFLOPS (GPU, fat)	3.4 Mch/month
Kebnekaise	HPC2N, UmU	629-1000+ TFLOPS (GPU, fat, KNL)	11 Mch/month
Rackham	UPPMAX, UU	347 TFLOPS (fat)	4.3 Mch/month
Tetralith	LiU	4335 TFLOPS	46 Mch/month

Specialized systems

- SNIC Science Cloud (UPPMAX, C3SE, HPC2N)
- SNIC Sens (Bianca UPPMAX, PDC)
- Life sciences (UPPMAX)
- WLCG (HPC2N, NSC, LUNARC)



SNIC Storage



SNIC provides generally available national services for storage and management of *active research data*.

10 PetaByte national storage available, and capacity for 44 PetaByte tape storage (2018).

- Nationally available storage (dCache and iRODS)
- Center storage
- Backup
- Sensitive data

Long-term storage however duty of universities, not SNIC.
→ Next allocation period will include storage!



SNIC Storage



Usage of SNIC resources



- Researchers from all major Swedish Universities make use of SNIC resources
- SNIC has approximately 800 + projects, with more 3000 users. The number of projects and users increases every year.
- The largest usage (core-hours ch) is by researchers in the fields of condensed matter physics, fluid mechanics, theoretical chemistry, climatology and biosciences (Gromacs, Gaussian, Vasp, Nek5000, EC Earth, OpenFOAM...)
- During 2015 four universities used 81% of available SNIC resources: KTH (33%), Uppsala University (21%), Linköping University (15%), Stockholm University (12%)



SNIC Usage



Data summarized over the period January 2012 – May 2018.



Usage 2016 (thousand core hours - kch)



Usage 2016 (thousand core hours - kch)



Usage of SNIC resources

SNIC computing resources are allocated as Large, Medium or Small projects

Large projects

- More than ~100 000 ch/month (1.2 Mch/year)
- Two application rounds per year
- Allocation is based on scientific need, merit, feasibility, efficiency of use, previous use/experience and availability (more later)
- There are 57 projects using 75 % of the SNIC resources
- The ten largest groups used 48 % of the SNIC resources



Usage of SNIC resources

Medium projects (5000 – 80 000 ch/m)

- In 2015 there were 349 Medium projects corresponding to approximately 24 % of the total usage of SNIC resources
- Application is possible throughout the year

Small projects (< 5000 ch/m)

- "Long tail of science"
- Testing of new architectures
- About 28 fields of research utilizing SNIC resources, including archeology, linguistics, political science, and economics
- The number fields of research utilizing SNIC resources is growing





SNAC Policy

- <u>http://snic.se/about/governance/policies/</u> (approved 2018)
- Allocations valid for **one year**, **twice a year**.
- the PI must be a senior scientist in Swedish academia (including research agencies such as FOI, SMHI), at least at the level of assistant professor (forskarassistent), however preferred permanent faculty (continuity). Grey zones (e.g. researcher position): SNIC Director
- Needs to have a formal affiliation at that university/agency (official homepage)
- Only one large allocation per PI, medium allocations stop when a large one is allocated. Small ones (to test hardware for instance) can still be granted.
- Preferred to have larger "consortia" rather than many "smaller" applications
- SNAC gets around 40-50 applications per round, ~200-300% of available resources.





Next SNAC LARGE call

- Autumn 2019 call, deadline October 11 2019
- Distribution of referees: October 16, 2h phone
- Referee work, reminders, collection of grades
- Committee Meeting: December 4, 6h in person. All time distributed!
- Review of referee answers, notification of applicants: December 10, 2h phone
- Begin of allocation: January 1 2020

Centre	Resource	Fall 2019	Minimum
C3SE	Hebbe	600 000	100 000
HPC2N	Kebnekaise	3 200 000	200 000
	Kebnekaise Large Memory	450 000	20 000
Lunarc	Aurora	500 000	100 000
NSC	Tetralith	16 000 000	200 000
PDC	Beskow	11 200 000	200 000
UPPMAX	Rackham	1 000 000	100 000



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- CV of the PI principal investigator (Maximum 2 pages)
- Publication list of the principal investigator
- SNIC Project Description (Maximum 5 pages)
- Activity report (**Maximum 8 pages**)
- Filled in form at SUPR (supr.snic.se) with some technical details





SNIC Project Description (Maximum 5 pages)

Overview (0.5 page)
Provide an abstract of the proposed research and computations.

Resource usage, codes and performance (1.5 pages)

Describe how your applications can make efficient use of the requested resources. Give numbers and/or indicate measures of scalability and performance (for example a graph of execution time versus number of cores).

Include records of usage only if this project is not a direct continuation of a previous one, or if you have not been granted time for a similar project(s) in previous allocation rounds. If the requested time differs significantly from earlier allocations and/or used time, please explain the difference. Also motivate if specific resources (such as large memory, GPUs, etc.) are requested.

Scientific challenges (2 pages)

Describe how the proposed project relate to the state of the art of the scientific area, has the potential to increase the knowledge within its scientific area, and how the proposed project uses adequate computational methods to address scientific questions.

Research group and management (0.5 page)

Describe the complete research group that will be working on the proposed project: name of member, HPC experience, position, and roles. Indicate how the allocated time will be managed within the group. \rightarrow also in SUPR



References (0.5 page)

Include a list of references for the project description.

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Activity report. (Maximum 8 pages)

Please note that the activity report is compulsory for all applicants.

Summary

The report must include an account of the major scientific achievements emanating from the use of the allocated SNIC resources / comparable resource outside of Sweden. If this is your first application for SNIC resources, but you have previously been using comparable resources abroad, please also provide allocation and usage statistics in the activity report.

Publications list

The activity report must include a list of publications from the **last two years** of all publications that acknowledge the use of SNIC resources. You may include forthcoming / in press publications (NOT submitted articles)

Academic achievements

The activity report must include achievements such as theses defended and graduate degrees completed.

HPC related developments

The activity report must include any developments related to programming, code optimization, visualization etc.

What not to include

Please note that publications that do not acknowledge the use of SNIC resources shall not be included in the activity report.





Acknowledging SNIC

Acknowledging SNIC:

Please note that you must give SNIC credit for research facilitated by SNIC resources. SNIC should be acknowledged as follows:

"The computations/simulations/[SIMILAR] were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at [CENTRE NAME (CENTRE ABBREVIATION)]."



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What is the decision based on:

- a peer review procedure is used with both internal (SNAC) and external reviewers. We have a list of 50+ reviewers for different topics. Anybody with interest to review for SNAC please contact me.
- Conflict of interest is handled as in VR
- Technical and scientific assessment
- SNAC evaluates the applications and decides on the allocations at the meeting
- The evaluation is based on scientific merit, need for the resources, feasibility and efficient use of the requested resources, and impact.
- Consideration of availability of suitable resources.
- Apply for the time you need!
- Previous experience and running statistics are also considered. This is mainly to ensure good usage of the resources (resource management, correct usage numbers)





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What happens then?

- The decision letter contains the granted amount of time on each machine
- Some referee comments are posted, these are mainly thought as help for the next rounds.
 Each application is discussed in detail during the meeting.
- The allocation starts July 1 or January 1
- Comments are welcome to <u>snac.chair@snic.se</u>, but note that typically the time is distributed.
- The project list on the SNIC webpage is updated
- Abstract/allocations publicly available



SUPR

SNIC Projects Large Medium Small SENS UPPNEX Projects User Agreement Login Your are not logged in.

Start / Current Large SNIC Projects / SNIC 2018/2-4

Large-scale Simulations in Stability, Transition, Turbulence and Control

Dnr:	SNIC 2018/2-4
Туре:	SNAC Large
Principal Investigator:	Dan Henningson
Affiliation:	Kungliga Tekniska högskolan
Start Date:	2019-01-01
End Date:	2020-01-01
Primary Classification:	20306: Fluid Mechanics and Acoustics
Secondary Classification:	10508: Meteorology and Atmospheric Sciences
Tertiary Classification:	10501: Climate Research
Webpage:	http://www.flow.kth.se/

Allocation

- Tetralith at NSC: 2500 x 1000 core-h/month
- Beskow at PDC: 2500 x 1000 core-h/month
- Kebnekaise at HPC2N: 300 x 1000 core-h/month
- Kebnekaise Large Memory at HPC2N: 200 x 1000 core-h/month
- Tegner at PDC: 41 x 1000 core-h/month

Abstract

In this proposal we list our individual projects which rely on HPC resources, grouped into six focal areas. We actively promote collaboration within our large user group to facilitate HPC support, sharing of simulation methods and codes, and user experience. We have thus found it beneficial to apply with a large-level request instead of multiple medium-level requests. I. Turbulent wall-bounded flows: Simulations of small- and large-scale turbulent motion close to walls, including heat transfer and pressure-induced separation. Simulations of turbulent pipe flow with and without bends and constrictions. Turbulent flows over walls with curvature. Turbulent boundary layers. 2. Receptivity and transition to turbulence: Receptivity of wall flows to external disturbances, growth and breakdown of disturbances close to solid walls. Dynamical-systems approach to study transition in Blasius and suction boundary layers; bypass transition to study percolation models. 3. Flow control, global modes and shape optimisation: Control and optimisation of flows exploiting modern methods of control theory; reduced-order models based on various global modal decompositions. 4. Wind turbines: Interference and breakdown of wind-turbine wakes and atmospheric turbulence. 5. Large-eddy simulations (LES) and reactive flows: Model development and validation for LES of high Reynolds number wall-bounded flows and simulations of turbulence.



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Future plans

- Implement large-scale storage allocations
- Include AI/ML machine into SNIC
- Heterogeneous systems
- EuroHPC
- Nationally available advanced user support
- Implement multi-year projects
- Include publication reporting via SUPR?
- "Local" users meetings (some already in place)



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Access through PRACE Peer-Review www.prace-ri.eu/call-announcements/



Free-of-charge required to publish results at the end of the award period

Preparatory Access (2 to 6 months)

SHAPE Programme (2 to 6 months)



Project Access (12, 24 or 36 months)





Centers of Excellence : 0,5 % of the total resources available for CoE



DECI: Only Tier-1 systems and 10% of each system+5% for external projects (12 months) – <u>NOT through Peer review</u>



HPC-Europa3 EU project

http://www.hpc-europa.eu/

- Gives access to world-class HPC systems
- Provides funding for travel and accommodation expenses for the visit and gives subsistence
- Provides support and training to visitors
- Creates opportunities for scientific collaborations
- Has a very easy application procedure

Application portal is always open with closing dates 4 times per year.

Questions to: staff@hpc-europa.org



HPCE3 Partners:

- 1. CINECA
- 2. UEDIN-EPCC
- 3. BSC
- 4. USTUTT-HLRS
- 5. SURFsara
 - 6. CSC
 - 7. GRNET
- 8. KTH-PDC
- 9. NUIG-ICHEC
- 10. CNRS (not participating in the Transitional Access activity)



Questions?

 In case of any comments, please contact me: pschlatt@mech.kth.se

 <u>snac.chair@snic.se</u> for a larger group including SNIC Office (for official matters)

