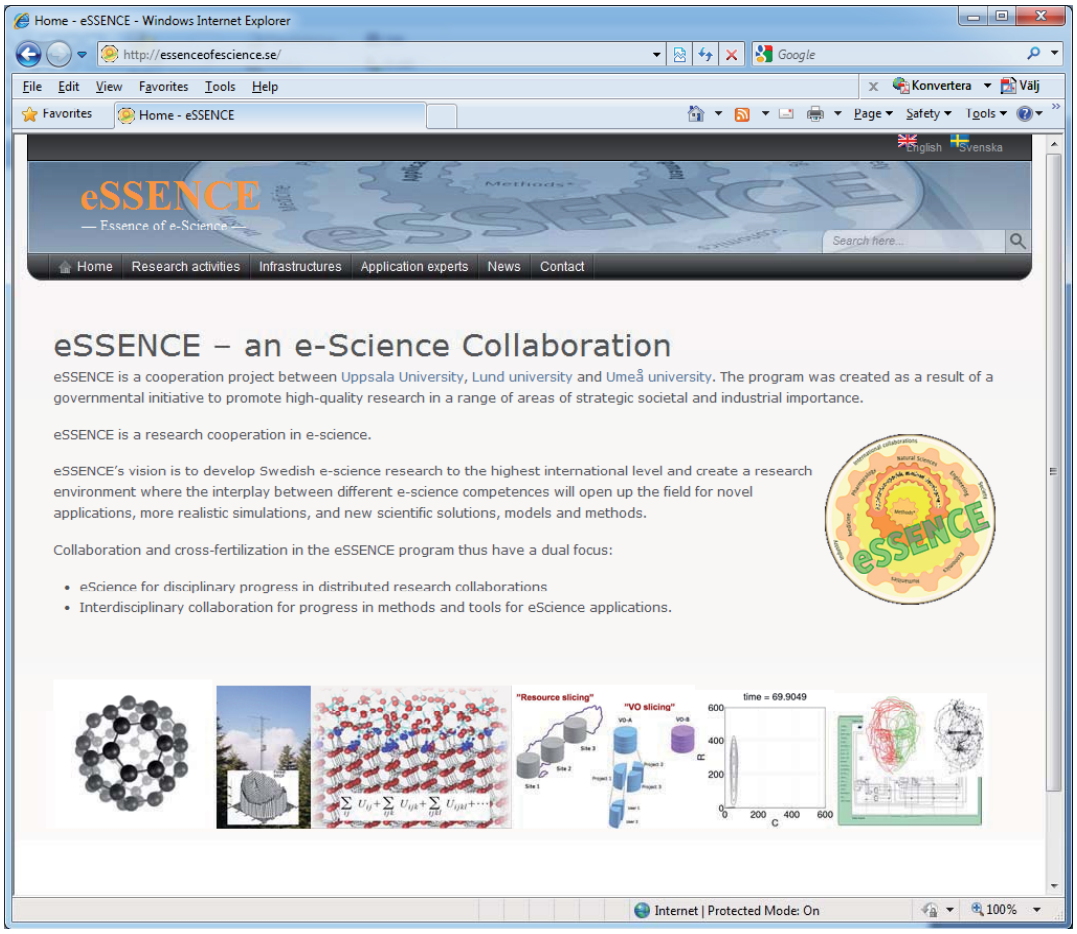
eSSENCE

An eScience collaboration

Göran Sandberg
Lund University

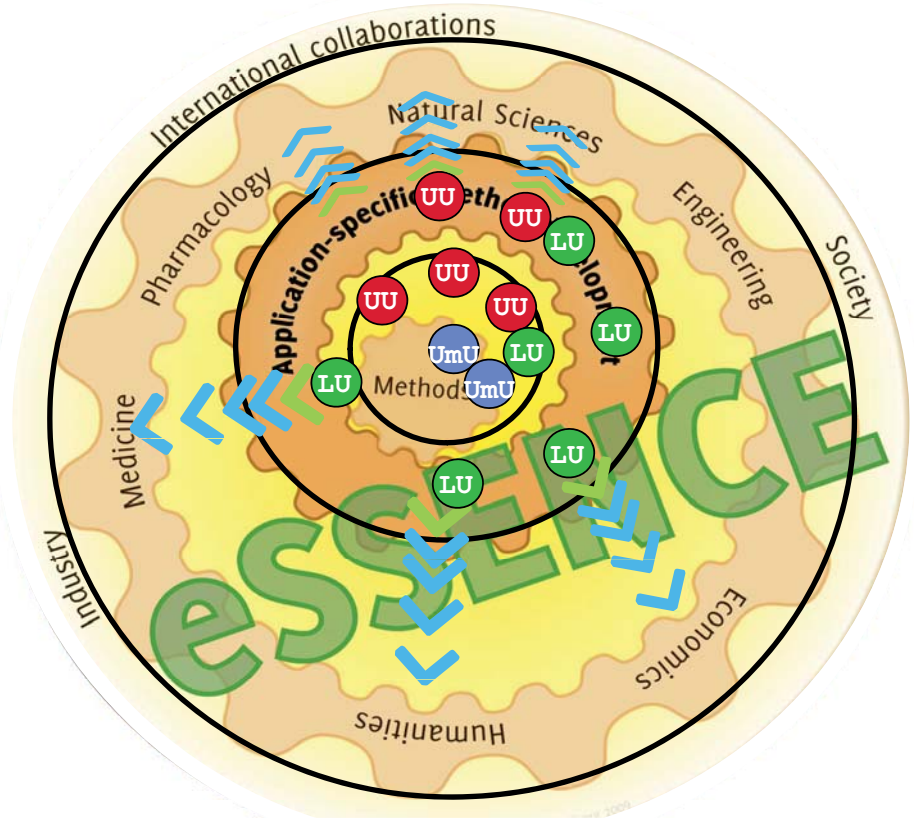


Two eScience challenges

People don’t know what eScience contains!

The people that knows what it’s all about!

eSSENCE organization and content



PIs and coordinators of eSSENCE

- Prof. Tord Ekelöf, Department of Physics and Astronomy, UU
- Prof. Hans Ellegren, Dept of Evolutionary Biology, UU
- Prof. Olle Eriksson, Department of Physics and Materials Science, UU
- Prof. Kersti Hermansson, Department of Materials Chemistry, UU
- Prof. Sverker Holmgren, Department of Information Technology, UU
- Prof. Tore Risch, Department of Information Technology, UU

- Prof. Bo Jönsson, Department of Theoretical Chemistry, LU
- Prof. Anders Lindroth, Department of Physical Geography and Ecosystem Analysis, LU
- Prof. Göran Sandberg, Department of Construction Sciences and LUNARC, LU
- Prof. Sven Strömqvist, Department of Linguistics and Phonetics, LU
- Assoc. Prof. Magnus Ullner, Department of theoretical chemistry and LUNARC, LU

- Prof. Erik Elmroth, Department of Computing Science and HPC2N, UmU
- Prof. Bo Kågström, Department of Computing Science and HPC2N

Underlined constitutes the “programberedning”

Local steering groups

Umeå

- Prof. Åsa Rasmuson-Lestander, Dean,Teknisk-naturvetenskapliga fakulteten vid UmU
- Prof. Bo Kågström, PI i eSSENCE,
- Prof. Erik Elmroth, PI i eSSENCE

Uppsala

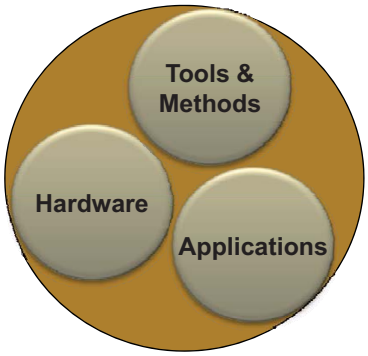
- Professor Kersti Hermansson, Inorganic Chemistry (materials chemistry)
- Professor Olle Eriksson, Theoretical Magnetism (materials physics)
- Professor Tord Ekelöf, Elementary Particle Physics (high energy physics)
- Professor Tore Risch, Database Technology
- Professor Johan Åqvist, Theoretical Chemistry (biochemistry)
- Professor Sverker Holmgren, Scientific Computing

Lund

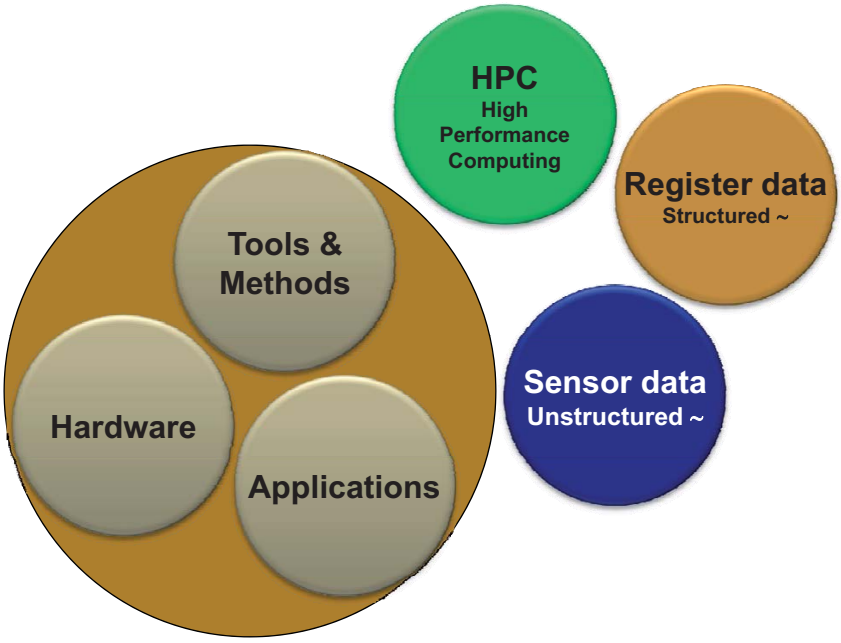
- Prof. Bo Jönsson, Department of Theoretical Chemistry
- Prof. Anders Lindroth, Department of Physical Geography and Ecosystem Analysis
- Prof. Sven Strömqvist, Department of Linguistics and Phonetics,
- Professor Freddy Ståhlberg, Radiation Physics, Faculty of Medicine
- Professor Kalle Åström, Mathematics
- Ass professor Oxana Smirnova, High energy physics
- Professor Tommy Bengtsson, Economic demography
- Ass professor Johan Revstedt, Fluid mechanics
- Professor Ulf Körner, Information technology
- Professor Göran Sandberg, Lunarc

eSSENCE – Mission & Goals

- Be part of the national responsibility within important eScience areas
- Create an efficient collaboration between methods & tools – hardware and applications.
- Create efficient collaboration between the nodes in the network
- Create efficient collaboration within each node.
- Strengthen new eScience areas.
- Insure future excellence through university education



eScience - essentials



Research areas

- Materials and Molecules
  - Materials Physics
  - Chemistry of complex materials
- Human interaction
  - Linguistics and visual information
  - Pattern recognition in the living brain
  - Economic demography
  - Ecosystems and climate change
- Computational biology
- "Datornära" method and tools development
  - Distributed IT Systems and Grid
  - Computational Algorithms, implementation also for GPU:s
  - High-Performance Parallel Computing
  - Database Technology

The Human Infrastructure Project

- Integrating various kinds of geographical time-varying information
  - soil quality, roads, costs-of living, hydrological and climate information, etc. to individual level time-varying data
- Graphical interface for users
- Information structure varies geographically and over time
- Makes it possible to trace individuals over time and across space

Includes the following partners

- Uppsala University
  - Database Technology
- Lund University
  - Economic demography
  - Physical Geography and Ecosystem Analysis

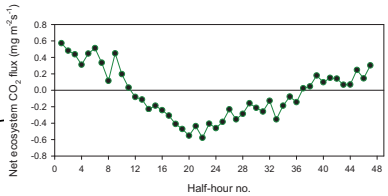
Background: The Scanian Demographic Database 1646-2010

- Nine rural parishes - one a small town today
- One town - today 5th largest in Sweden
- Total population - unmarried and married
- Based on
  - Church records, daily
  - Population registers after the 1820s, yearly
  - Land registers and tax records, yearly
  - Local prices and wages, yearly - later monthly
  - And more
- The database which previously covered the period 1646-1895 is now expanding to 1968 to be linked with national registers up to the present as part of a VR Linnaeus project (Centre for Economic Demography, Lund University)
- Approximately 250,000 individuals (up to 10 generations) when finished

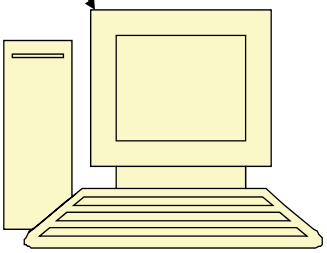
MERGE:
Near real-time presentation and retrieval of greenhouse gas exchanges

In situ data collection
100 values/second/flux system

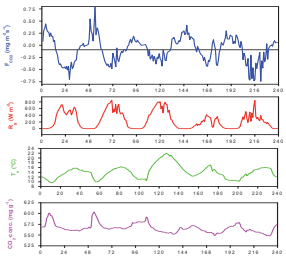
On-line advanced calculations and **near-real time** presentationfor measurement managers and data users



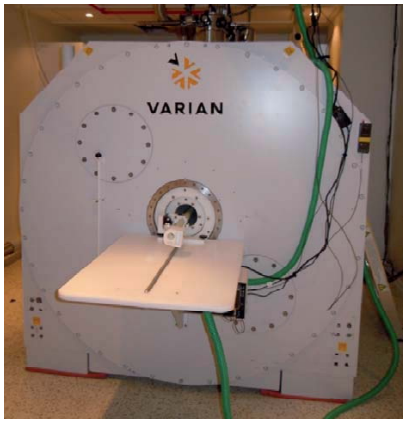
Interactive database…



.. with **graphic interface** for easy overview



Sensor data – Humanities & Medicin

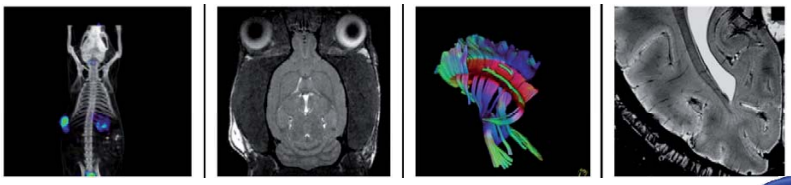


Humanities Laboratory and Lund Bio Imaging Centre

Humanities and Medicine have a lot of common practise that needs to be developed.

The base are the study of images of the brain.

- Workflow
- Larges sets of streaming data
- Subsequent analysis



Sensor data
Unstructured ~

Quantum Mechanics and Statistical Mechanics

Mutual interest areas

- Software development, methodology

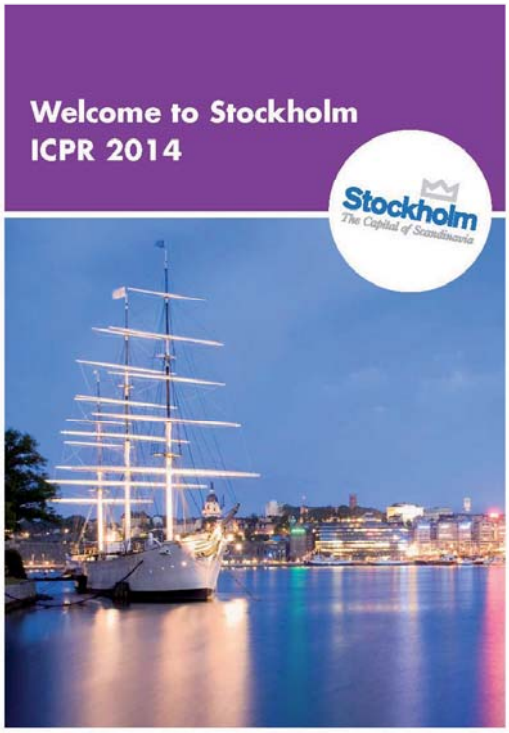
between

- Group in Quantum Mechanics incl
- Group in Statistical Mechanics

HPC
High
Performance
Computing

Conference

- International Conference on Pattern Recognition
- Organizers: Ingela Nyström (UU), Anders Heyden (LU), + Linköping
- *A consequence of collaboration*



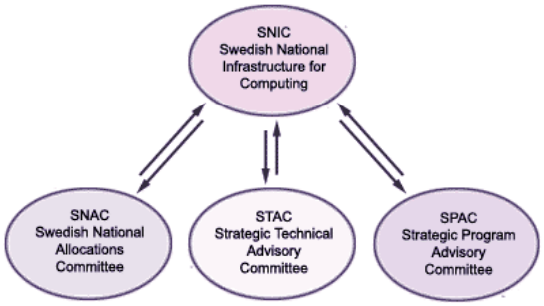
APPLIKATIONS-EXPERTER

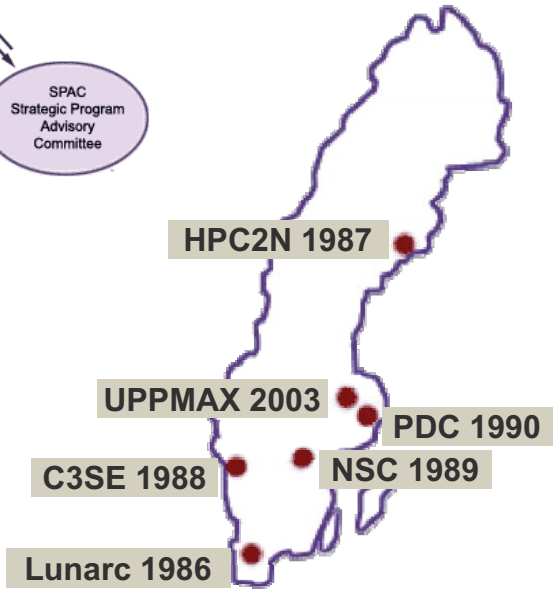
Avancerat nationellt användarstöd och utveckling; strategiska forskningsomr.

- Competence Group for GRID: collaborative effort between HPC2N, Lunarc, UPPMAX
- Support for massive parallellisation
- Support reg material modelling – material physics
- Support reg material modelling –material chemistry
- Storage
- Material science at Chalmers - C3SE

INFRA-STRUCTURE

SNIC – Swedish National Infrastructure for Computing





eSSENCE essentials

- Strat Res Area – Strong Brand for the Universities
- Effect of 5-10 MKR?????
- Pilot projects
- New employees in several projects
- New questions through
  - New collaboration
  - New combinations of scientfic areas
  - Will arrive at new generic capacities
- Link to several strategic research areas

eSience Ambitions in Sweden

Budgetpropositionen 2009

4.4 Forskning

Regeringens mål är att stärka Sveriges ställning som forskningsnation och därmed **stärka konkurrenskraften** i en globaliserad värld och bidra till ökad ekonomisk tillväxt och välfärd i Sverige.

Strategiska forskningsområden

Den **enskilt största satsningen** i forsknings- och innovationspropositionen är **satsningen på strategiska områden.** Regeringen menar att koncentrerade satsningar på **högkvalitativ forskning och forskning** av stor betydelse för samhället och näringslivet samt en **effektiv infrastruktur** för forskningen behövs för att behålla den internationella konkurrenskraften inom svensk forskning och svenskt näringsliv. Strategiska satsningar görs främst inom tre övergripande områden, medicin och livsvetenskaper, teknik och klimat.

Strategic Research Funding – eScience (MKR)

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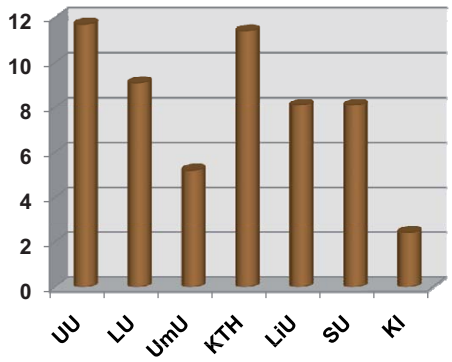
		2010	2011	2012	2013	2014	
Huvudsökande	UU	4,5	6,3	11,7	11,7	11,7	46
Medsökande	LU	3,5	4,9	9,1	9,1	9,1	36
Medsökande	UmU	2	2,8	5,2	5,2	5,2	20
		10	14	26	26	26	

Swedish e-Science Research Centre

		2010	2011	2012	2013	2014	
Huvudsökande	KTH	3,8	6,84	11,4	11,4	11,4	45
Medsökande	LiU	2,7	4,86	8,1	8,1	8,1	32
Medsökande	SU	2,7	4,86	8,1	8,1	8,1	32
Medsökande	KI	0,8	1,44	2,4	2,4	2,4	9
		10	18	30	30	30	



And the money comes from

Funding of national and international research infrastructure, 1of3

Rekommendationer om avsättning av medel till nationell och internationell infrastruktur inom ramen för utlysningen av de strategiska forskningsområdena	2010 (Mkr)	2011 (Mkr)	2012 ff (Mkr/år)	tre första åren	total budget, tre första åren	procentuell avsättning
Nanovetenskap och nanoteknik	8	11	20	39	80	49%
Cancerforskning	9	11	14	34	70	49%
Diabetes	9	11	14	34	70	49%
Molekylär biovetenskap	15	27	45	87	190	46%
IT och mobil kommunikation	9	11	16	36	80	45%
Effekter på naturresurser	5	7	10	22	50	44%
Epidemiologi	3	3	5	11	25	44%
E-vetenskap	5	8	14	27	70	39%
Neurovetenskap	5	8	14	27	70	39%
Materialvetenskap	5	7	13	25	65	38%
Havsmiljöforskning	1	1	2	4	20	20%
Klimatmodeller	1	2	3	6	30	20%
Stamceller och regenerativ medicin	2	4	6	12	65	18%
Säkerhet och krisberedskap	0	1	1	2	20	10%
Hållbart nyttjande av naturresurser	1	1	2	4	50	8%
Produktionsteknik	1	1	2	4	50	8%
Transportforskning	1	2	3	6	80	8%
Energi	0	0	0	0	160	0%
Politiskt viktiga geografiska regioner	0	0	0	0	20	0%
Vårdforskning	0	0	0	0	50	0%
	80	116	184	380	1315	29%

Funding goes to …

Forskningsfinansiärerna rekommenderar att avsättningar från de olika strategiska områdena görs enligt nedanstående tabell:				
Infrastruktur	2010 (Mkr)	2011 (Mkr)	2012 ff (Mkr/år)	tre första åren
Biobanker/BBMRI	11	17	28	56
BILS/ELIXIR	4	6	9	19
LifeWatch	6	8	14	28
MAX IV	26	35	55	116
MyFab	10	15	23	48
SNIC/PRACE	7	12	18	37
Teknikplattformar i medicin och livsvetenskap1	16	23	37	76
	80	116	184	380

Comparison between various strategic areas

	Total budget inom område år 2012* (Mkr)	Avsättning till infrastruktur (Mkr)	Infrastrukturer
Energi	160	-	-
Klimat och miljö	150	17	Lifewatch, **SNIC**
Medicin och livsvetenskap	540	98	BILS/ELIXIR, Biobanker/BBMRI, Teknikplattformar, **SNIC**, MAX IV
Teknik (inkl Säkerhet)	425	69	MyFab, **SNIC**, MAX IV

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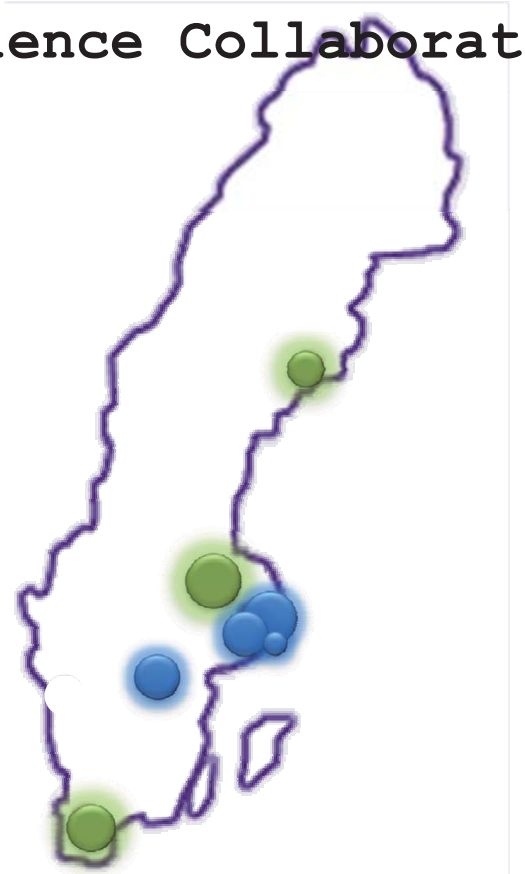
UMEÅ UNIVERSITET

UPPSALA UNIVERSITET

LUND UNIVERSITY



eSSENCE - an eScience Collaboration

LULEÅ TEKNISKA UNIVERSITET

IRF

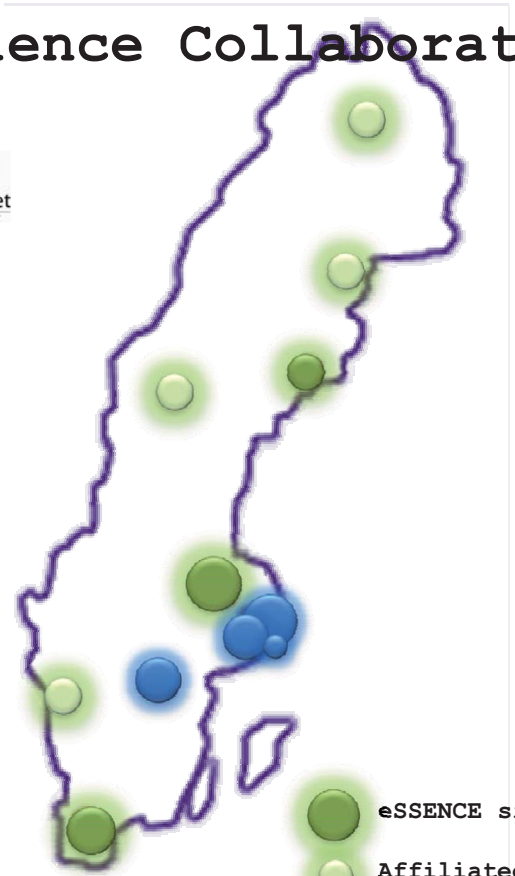
SLU

Mittuniversitetet MID SWEDEN UNIVERSITY

HPC2N

Uppsala Multidisciplinary Center Advanced Computational Science UPPMAX

LUNARC



eSSENCE site

Affiliated site

The national as well as the distributed perspective are two fundamental visions of eSSENCE.
The Project, the user support, and the hardware, all of this complement each other - In order to be an effective unit
Thus the key word are
*** National**
*** Distributed**
*** Balanced**

eSSENCE essentials

- advantage eScience – in many fields and at many locations
- ”No helpdesk solutions”
- We need “distributed”
- ... and “presence”

THANKS