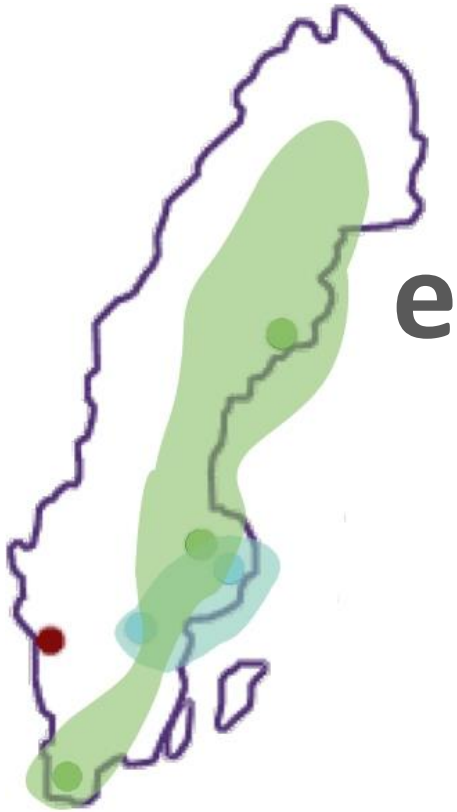
eSSENCE
THE e-SCIENCE COLLABORATION



Welcome to eSSENCE Academy 2013!

Lund October 16—17, 2013

Ingela Nyström, Professor
Coordinator of eSSENCE

UPPSALA UNIVERSITET

LUND UNIVERSITY

UMEÅ UNIVERSITET

Nobel Prizes 2013 to e-Science

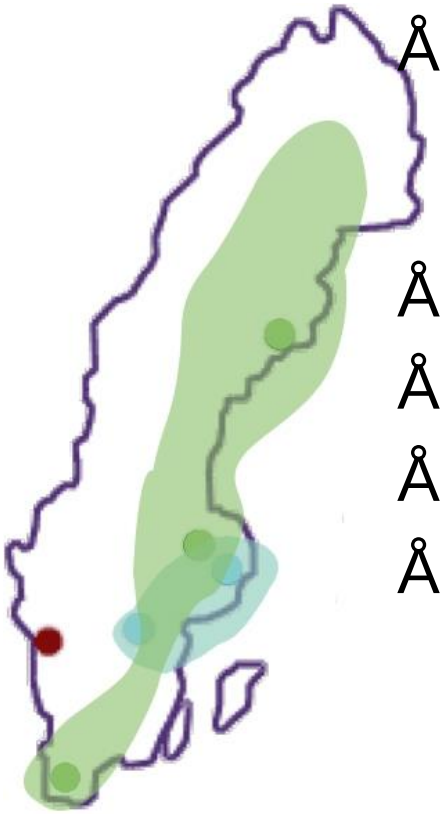
- **The Nobel Prize in Physics 2013 was awarded jointly to François Englert and Peter W. Higgs**
- *for the theoretical discovery of a mechanism that contributes to our understanding of the origin of mass of subatomic particles, and which recently was confirmed through the discovery of the predicted fundamental particle, by the ATLAS and CMS experiments at CERN's Large Hadron Collider*

Nobel Prizes 2013 to e-Science

- **The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt, and Arieh Warshel**

- *for the development of multiscale models for complex chemical systems*

Strategic Research Area: e-Science



- e-Science is one of 20 strategic research areas funded by the Swedish government during 2010—2014
- SeRC Swedish e-Science Research Centre — **KTH** – LiU – SU – KI, *30 MSEK/year*
- eSSENCE THE e-SCIENCE COLLABORATION — **UU** – Umeå – Lund, *26 MSEK/year*
- CHALMERS *e-Science Centre*
- Infrastructure funded separately by SNIC HPC centra
  - PDC and NSC part of SeRC
  - UPPMAX, HPC2N, and Lunarc part of eSSENCE
  - C3SE part of CheSC

UPPSALA UNIVERSITET · LUND UNIVERSITY · UMEÅ UNIVERSITET · CHALMERS · KTH VETENSKAP OCH KONST · Linköpings universitet · Stockholms universitet · Karolinska Institutet

Swedish e-Science builds on Swedish e-Infrastructure

Å **Swedish National Infrastructure for Computing (SNIC),** www.snic.se

Å **Swedish University Computer Network (SUNET**), www.sunet.se

Å SNIC and SUNET are bodies of the Swedish Research Council (**Vetenskapsrådet, VR**), www.vr.se

e-Science…

- has emerged as the third pillar underlying research, complementing theory and experiments
- builds on developing, implementing and using computer-based tools in research where traditional experimental and theoretical approaches are not sufficient
- provides new opportunities for collaboration in academia and industry, within the same and different disciplines, and over short and long geographical distances
- is connected to the development of computational tools and methods, as well as to the readiness of application areas to novel paradigms and to meet challenges from new directions

Vision

Provide excellence and scientific solutions at all stages of the e-Science process

- e-Science for disciplinary progress in distributed research collaborations
- Interdisciplinary collaboration for progress in methods and tools for e-Science applications

Advancing science through leading computation, information and communication technologies

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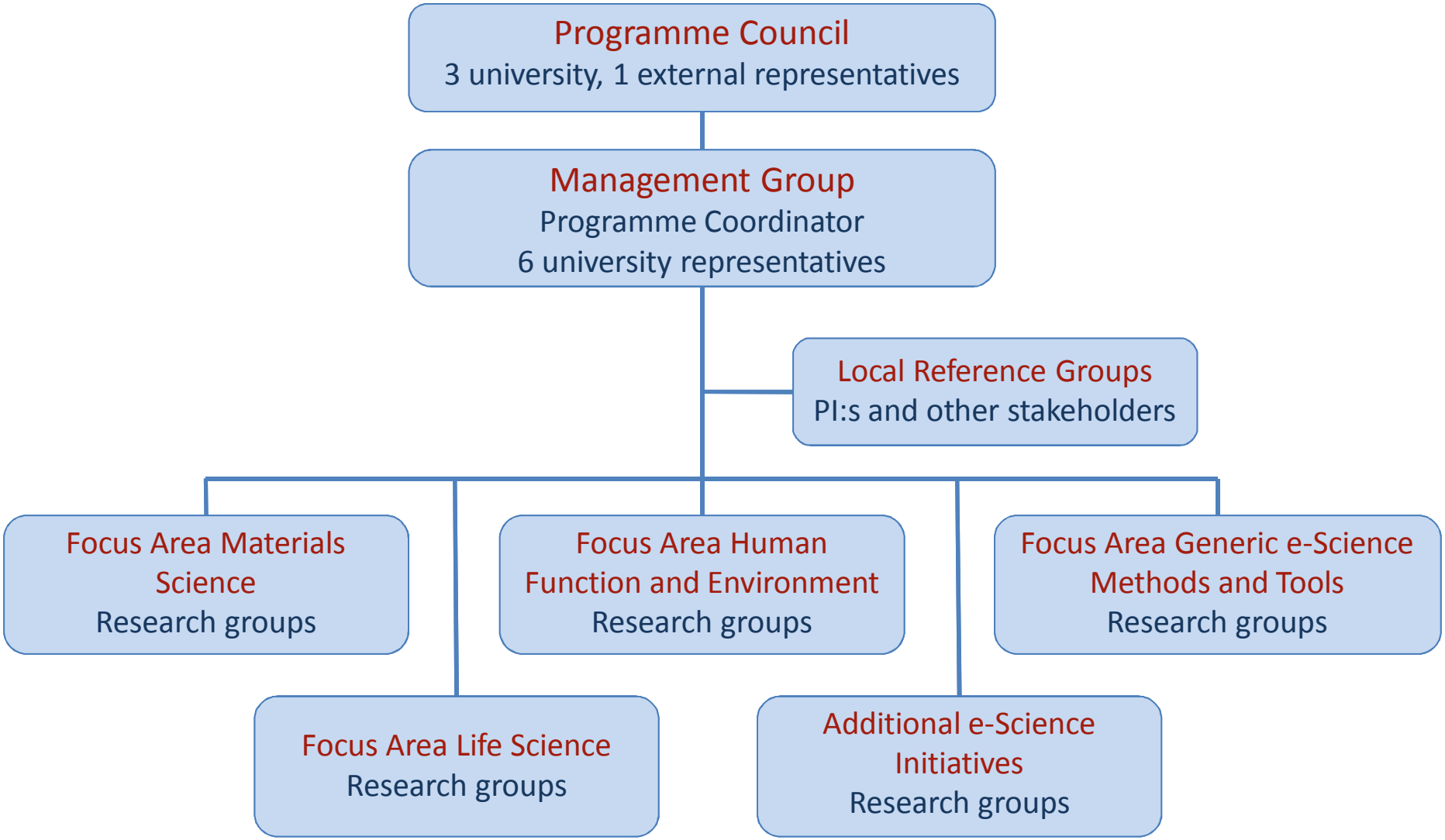
Research Areas & Programs

with collaboration between Universities

Materials Science	• Materials physics • Chemistry of complex materials • Nano materials
Human Function and Environment	• Linguistics and visual information • Pattern recognition in the living brain • Economic demography • Ecosystems and climate change
Life Science	• Computational biology • Bioinformatics
Generic e-Science Methods and Tools	• Distributed computing services and grid • Computational algorithms, implementation also for GPU:s • High-performance parallel computing • Database technology

Funding some 25 projects

Organisation



Principal Investigators

- Prof. Tord Ekelöf, Physics and Astronomy, UU
- Prof. Hans Ellegren, Evolutionary Biology, UU
- Prof. Erik Elmroth, Computing Science, UmU
- Prof. Olle Eriksson, Physics and Materials Science, UU
- Prof. Kersti Hermansson, Materials Chemistry, UU
- Prof. Bo Jönsson, Theoretical Chemistry, LU
- Prof. Bo Kågström, Computing Science, UmU
- Prof. Tore Risch, Information Technology, UU
- Prof. Anders Lindroth, Physical Geography & Ecosystem Analysis, LU
- Prof. Sven Strömqvist, Linguistics and Phonetics, LU

Program Council

- Å Ingemar Kaj, UU, Chair
- Å Sven Strömqvist, Dean LU
- Å Åsa Rasmuson-Lestander, Dean UmU
- Å Martin Norin, Kancera
- Å Ingela Nyström, UU
- Å Carmen Medina, research secretary UU

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Management Group

- Göran Sandberg, LU
- Magnus Ullner, LU
- Bo Kågström, UmU
- Erik Elmroth, UmU
- Gunilla Kreiss, UU
- Johan Åqvist, UU
- Ingela Nyström, UU, Chair
- Carmen Medina, research secretary UU

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Budget (in kSEK)

University	2010	2011	2012	2013	2014
LU (35 %)	3 500	4 900	9 100	9 100	9 100
UmU (20 %)	2 000	2 800	5 200	5 200	5 200
UU (45 %)	4 500	6 300	11 700	11 700	11 700
Total	**10 000**	**14 000**	**26 000**	**26 000**	**26 000**

- 90 % of the budget
  - Distributed to researchers at each University
  - How this distribution is performed is evaluated in the Management Group to identify possibilities for collaboration
- 10 % of the budget
  - Used for joint activities such as workshops, conference participation, involvement in higher education, coordination, etc.

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Current Status

- A set of *focus areas* has been selected for funding of eSSENCE *programs*
- Several *PostDoc projects* initiated after application rounds
- A group of SNIC advanced application experts supports researchers in usage of HPC
- Workshops
- Seminars
- www.essenceofescience.se

Thanks go to Pavlin Mitev!

Swedish e-Science Education

- Courses in e-Science for PhD students
- SeSE is a collaboration between the two national strategic research initiatives eSSENCE and SeRC, originating from the e-Science graduate schools NGSSC and KCSE
- Information about upcoming courses with syllabus and further information can be found at www.sese.nu

AIMday e-Tools & Methods

- On November 27, 2013
  in Uppsala
- www.aimday.se
- **Companies:**
  Folksam,
  Prosilico,
  ABB Crane Systems,
  Vegesack Arkitekter,
  Watty, SMHI, and more
- ***Registration is open!***

Academy Workshops

- It has become an annual opportunity to meet and acquaint ourselves with the exciting research that is happening within eSSENCE
- October 16—17, 2012 in Uppsala (Sigtuna)
  - 60 participants
- October 16—17, 2013 in Lund
- October 2014 in Umeå

Academy days 2013

- 82 participants
- 12 oral presentations
- 50 posters
- Panel discussion
- Lunches, dinner, coffees

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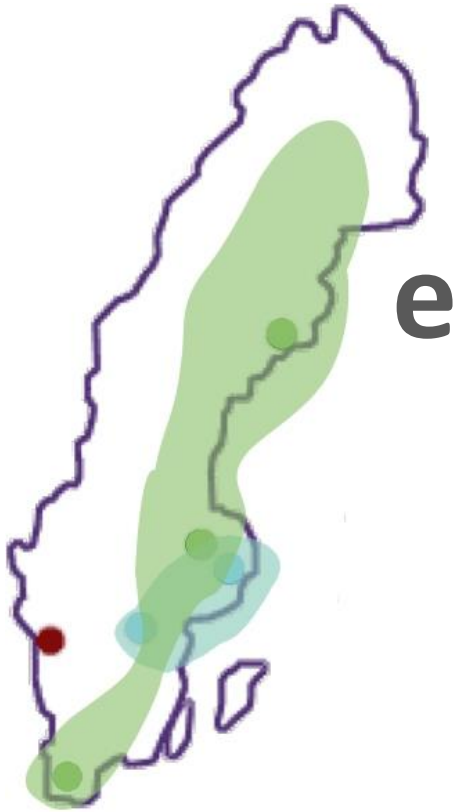

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