Swedish e-Science Research Centre (SeRC)

Advancing e-Science in Sweden

Dan Henningson

Director

e-Science

- "systematic development of research methods that exploit advanced computational thinking"
  Professor Malcolm Atkinson, UK e-Science Envoy

- Scientific research that is carried out using advanced computer based research tools

- Three main ingredients
  - Methods and tools: *numerics, visualization, databases, …*
  - Application areas: *climate, materials, life science, …*
  - Infrastructure: *supercomputers, networks, …*

e-Science in UK

- Belfast e-Science Centre (BeSC)
- Cambridge e-Science Centre (CeSC)
- STFC e-Science Centre (STFCeSC)
- e-Science North West (eSNW)
- National Grid Service (NGS)
- OMII-UK
- Lancaster University Centre for e-Science
- London e-Science Centre (LeSC)
- North East Regional e-Science Centre (NEReSC)
- Oxford e-Science Centre (OeSC)
- Southampton e-Science Centre (SeSC)
- Welsh e-Science Centre (WeSC)

National e-Science call

- One of 20 strategic research areas to which applications were solicited during spring 2009

- Consortium KTH – LiU – SU – KI
  - KTH main applicant
  - 30 Milj/yr research: 38%, 27%, 27%, 8%
  - 20 Milj/yr infrastructure: 50% KTH, 50% LiU

- Consortium include
  - Core of methods development
  - Strong application centers and research groups
  - Majority of Swedish e-infrastructure (PDC, NSC)

Main applicants

- ***Dan Henningson***, Mekanik, KTH
- ***Hans Ågren***, Teoretisk Kemi, KTH
- ***Anna Delin***, Materialvetenskap, KTH
- ***Anna-Karin Tornberg***, Numerisk Analys, KTH
- ***Anders Ynnerman***, NVIS, LiU
- ***Bengt Persson***, Bioinformatik, LiU/KI
- ***Igor Abrikosov***, Materialvetenskap, LiU
- ***Juni Palmgren***, Matematisk statistik, SU/KI
- ***Anders Lansner***, NADA, SU
- ***Erik Lindahl***, Bioinformatik, SU









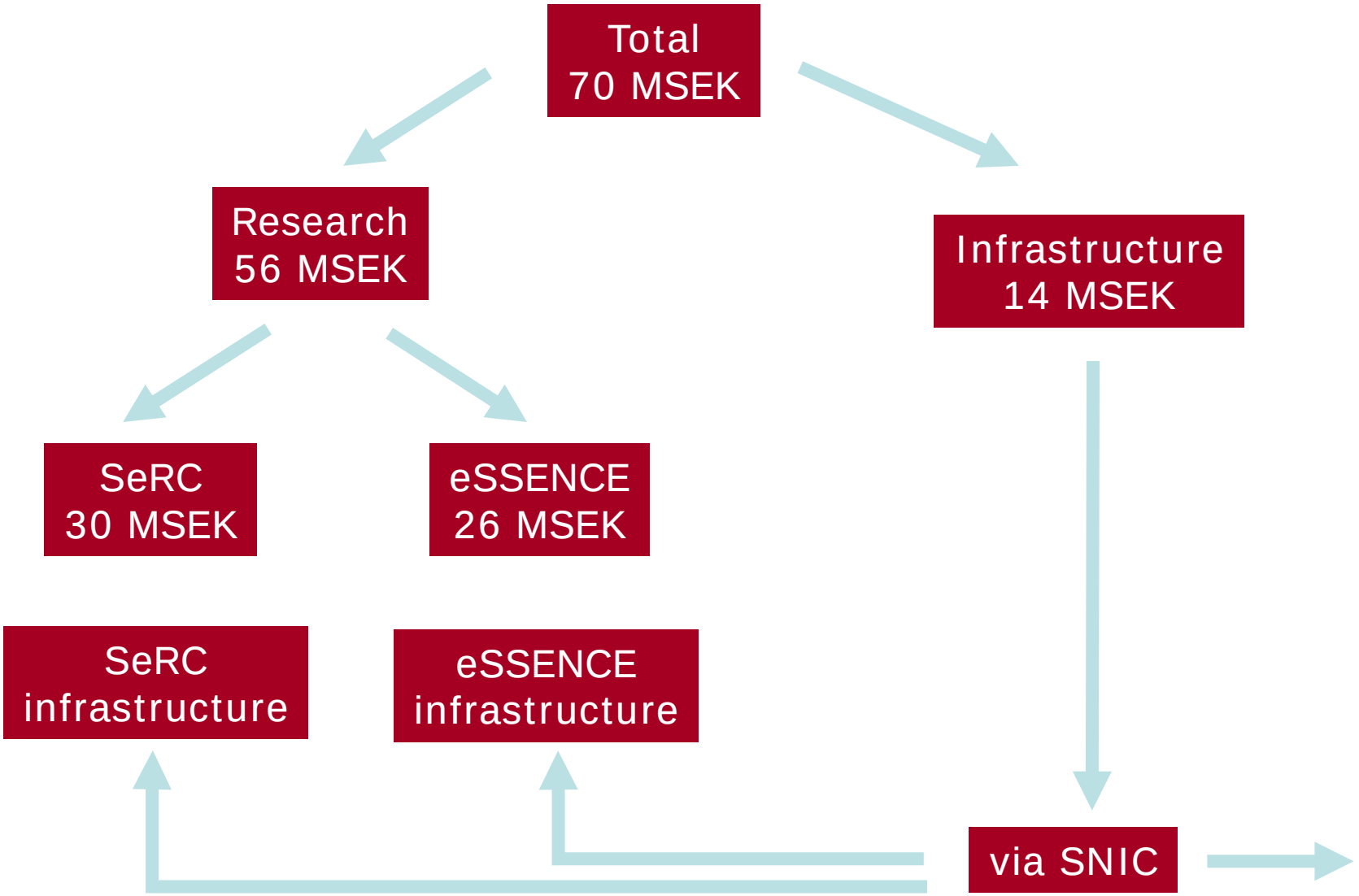

Strengths of the consortium

- Ten centers of excellence (5 Linné, 4 SSF, 1 Berzelii)
  - Seven additional research centers
- 54 key researchers named
  - Six members of KVA
  - Five ERC grants
  - Five ”rådsforskare”
- Majority of computer capacity for academic research at PDC and NSC
- Software development
  - DALTON, EMTO, GROMACS, PENCIL, SIMSON, SUPERFLUID, FEniCS
- Participation in EU/National projects
  - SweGrid, NDGF, EGEE, DEISA, PRACE, ELEXIR, BBMRI, INCF, IS-ENES
- Industrial support
  - SAAB, SCANIA, SKF, BOMBARDIER, AstraZeneca, SECTRA, LightLab, Portendo, SMHI

Application granted

- Highest ranked application
- Full research budget of 30 milj/year granted
- Additional research funding of 26 milj/year to eSSENCE, a UU-Lund-Umeå consortium
- Infrastructure part treated separately

Strategic funding for e-Science



What will SeRC do?

- Form e-Science communities; collaboration between
  - e-Science applications
  - core e-Science
  - computer experts at PDC/NSC
- Research in core e-Science areas of importance for e-Science applications
- Form strategic collaboration between PDC och NSC
  - national responsibility for largest computer infrastructure
  - strong partner in European collaborations
- Interface with industry and society

Strategy

use e-Science communities as e-Science enablers

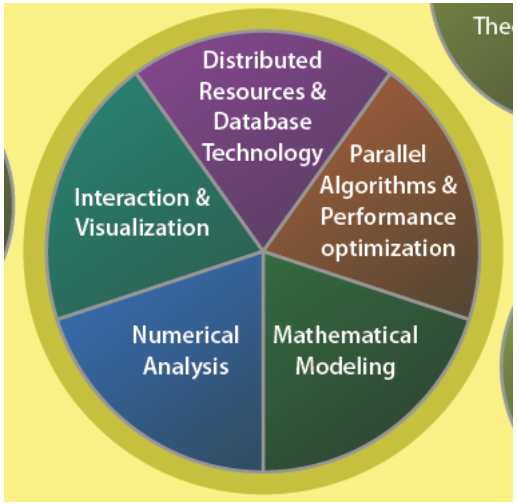
- Enhanced collaboration between application areas, core e-Science and computer experts by having
  - Forum for meetings and interactions
  - Application experts integral part of research projects
  - Projects in application areas contain method development
  - Core projects associated with e-Science communities
  - Collaborative projects with e.g. twinning of PhDs

e-Science communities

- Computational fluid dynamics
- Climate and the Environment
- Bioinformatics: mapping and analyzing DNA and protein sequences
- Complex Diseases: merging of molecular and medical data
- Particle Simulations and Molecular Dynamics
- Electron structures: DFT and Hartee-Fock methods
- Waves: aero-acoustics and electromagnetics

Core e-Science areas

- Numerical Analysis
- Visualization and Image Science
- Mathematical Modeling
- Distributed resources
- Database technology
- Parallel Algorithms and Performance Optimization



Infrastructure

SeRC will continue to take national responsibility for major parts of Swedish e-infrastructure through the two major HPC-centers PDC and NSC

- Host additional large scale HPC resources e.g. new Cray PRACE computer
- Finance application experts, typically PhD in an e-Science core or application area, with excellent computational skills
- Finance software engineers, typically consultants with excellent programming background
- Transition of HPC-centers to e-Science enablers through nationally available advanced user support

Future HPC hardware poses challenges

- A major shift in hardware is approaching fast
- Largest machines today have ~300,000 cores
- Top500 #2 is a streaming architecture (Nvidia GPU)
- Around 2020, we can expect 10^9 “core” elements

- *All* applications must become extremely parallel
- Requires entirely new approaches to scaling
- Sweden needs to focus research on Exaflop scale
- Integrate research & infrastructure in SeRC
- Research must start NOW to be ready in time

Interface to industry and society

- External advisory committee with international experts and representatives from industry and society
- Representatives from industry and society in e-Science communities; establish e-Science industry forum
- e-Science software and spin-offs
  - Open Source software of industrial interest
  - Spin-off companies in electromagnetics, material science, medical visualization, …
  - Establish software curation unit
- Production of PhDs of interest to industry

SeRC management structure

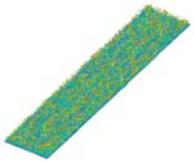
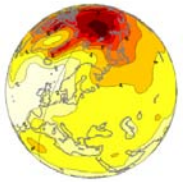
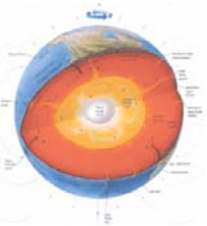
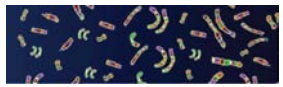
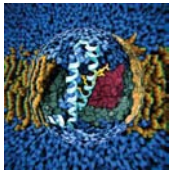
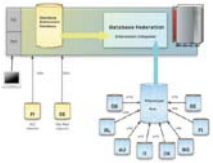
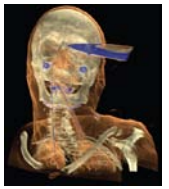
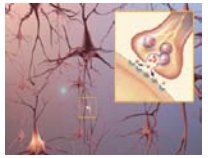
- Director: Dan Henningson
- Co-director: Anders Ynnerman
- Coordinator: Mattias Chevalier

Current status

- 10 faculty positions hired
- 3 additional during 2011
- 4 positions for advanced user support financed by SNIC are being hired
- 1.5 additional positions for PRACE
- MOU underway between KTH-LiU regarding collaboration between PDC-NSC, including cross representation in boards
- Kick-off April 22-23, Häringe Slott
- Managing group meetings once a month
- Coordinator started August 1
- Work within 7 e-Science communities started
- 4 additional communities start 2011

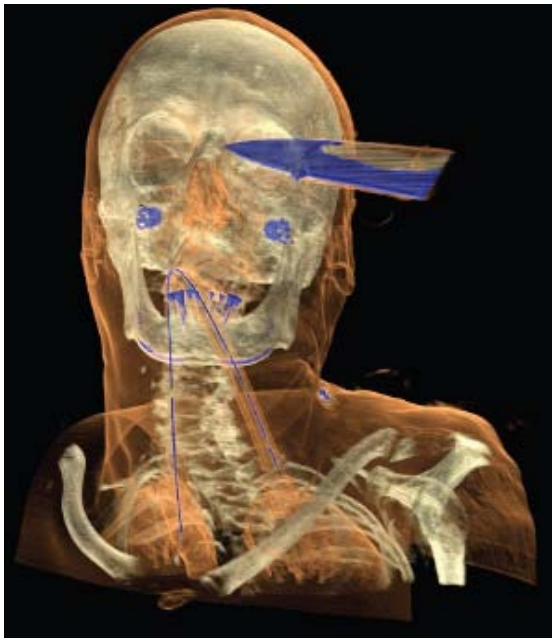
Research showcases

- FLOW: massively parallel turbulence simulations
- ENVIRONMENT: simulations of global climate change
- MATERIALS: simulations give structure of iron in earths core
- GENOMIC MEDICINE: Identification of genome variation increasing risk of prostate cancer
- MOLECULAR MODELING: distributed computing enable the longest ever ion channel simulations
- MOLECULAR EPIDEMIOLOGY: ”Twin-Net data federation” – distributed database model for European infrastructure
- VISUALIZATION: Interactive full-body scan possible through smart handeling of data
- BRAIN MODELING: New method enables largest simulation of memory network

Virtual autopsies

- Research at the Center for Medical Image Science and Visualization, LiU
  - Algorithms for data reduction that handle the enormous data from the CAT-scans
- Crime Scene Investigators (CSI)
  - Detailed 3D images where layer after layer can be removed
  - Virtual autopsies are regularly performed in Linköping
- Recently reported in The Economist



The Economist

Log in | Register | My account

Home | World | Business & finance | Science & technology | Markets

Virtual autopsies

A cut from CSI

A CT scanner and gaming technology opens up a body

Dec 10th 2009

From *The Economist* print edition

PERFORMING a postmortem on a murder victim can take days, delaying any criminal investigation. Moreover, pathologists sometimes get only one chance to look for clues when dissecting a body. But Anders Persson, director of Linköping University's centre for medical image science and visualisation in Sweden, hopes to change that. Along with his colleagues Thomas Rydell and Anders Ynnerman of the Norrköping Visualisation Centre, they have created a virtual autopsy system.

The body needing to be examined is first scanned using a computed tomography (CT) machine, a process which takes about 20 seconds and creates up to 25,000 images, each one a slice through the body. Different tissues, bodily substances and foreign objects (such as bullets) absorb the scanner's X-rays in varying amounts. The software recognises these and assigns them a density value. These densities are then rendered with the aid of an NVIDiA graphics card, of a type used for high-speed gaming, into a 3-D visualisation of different colours and opacities. Air pockets are shown as blue,

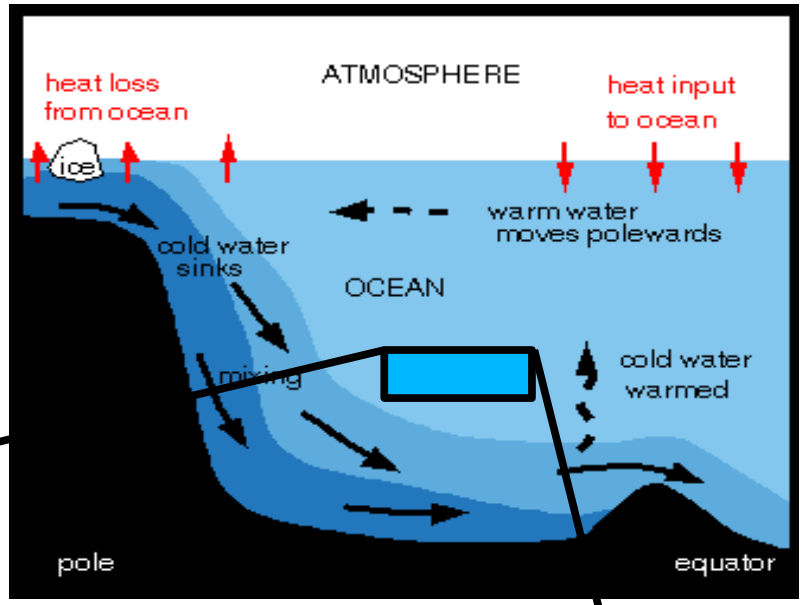
Quantum-chemical simulations used to design new materials

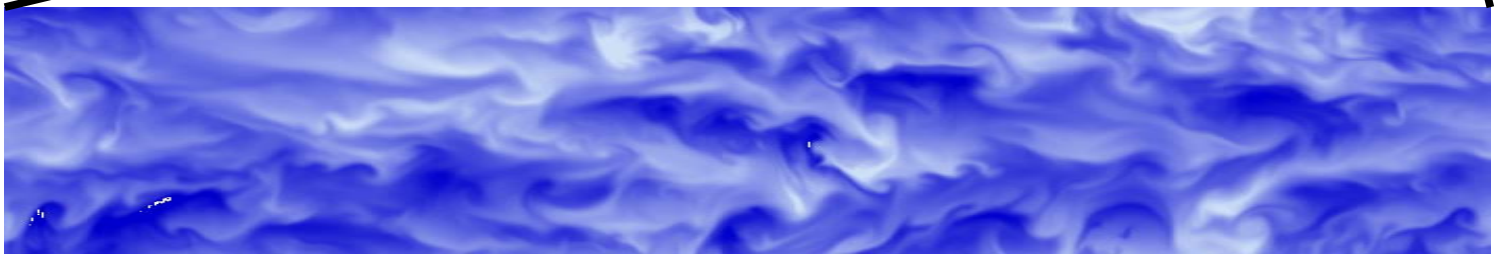
- Innovative self activating material which protects the eyes from strong lasers
- Collaboration KTH, LiU, FOI

Ocean turbulence influences future climate

Supercomputer simulations at KTH predicts how turbulence properties influences heat transfer in the oceans

- important to understand consequences of global warming

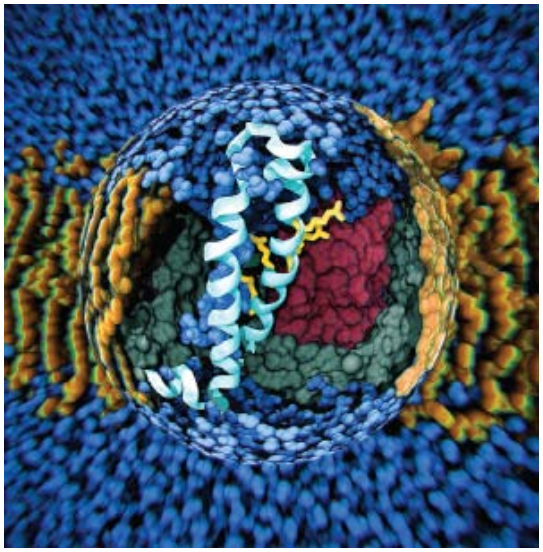


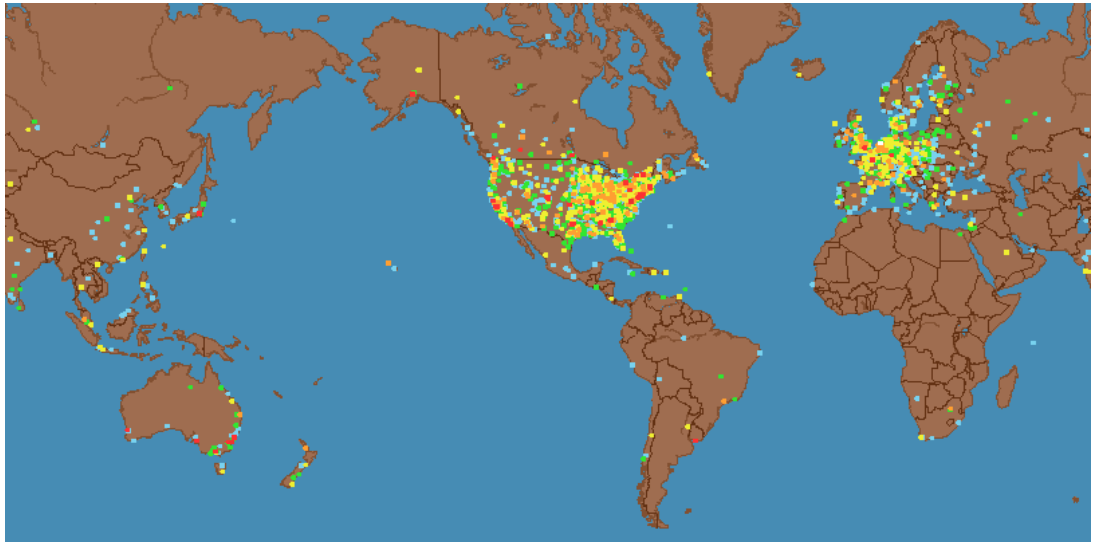


Hundreds of thousands computers connected in global network

Folding@Home: Over 400.000 computers work continuously in simulations of new protein structures

Collaboration between Stanford and Stockholm University

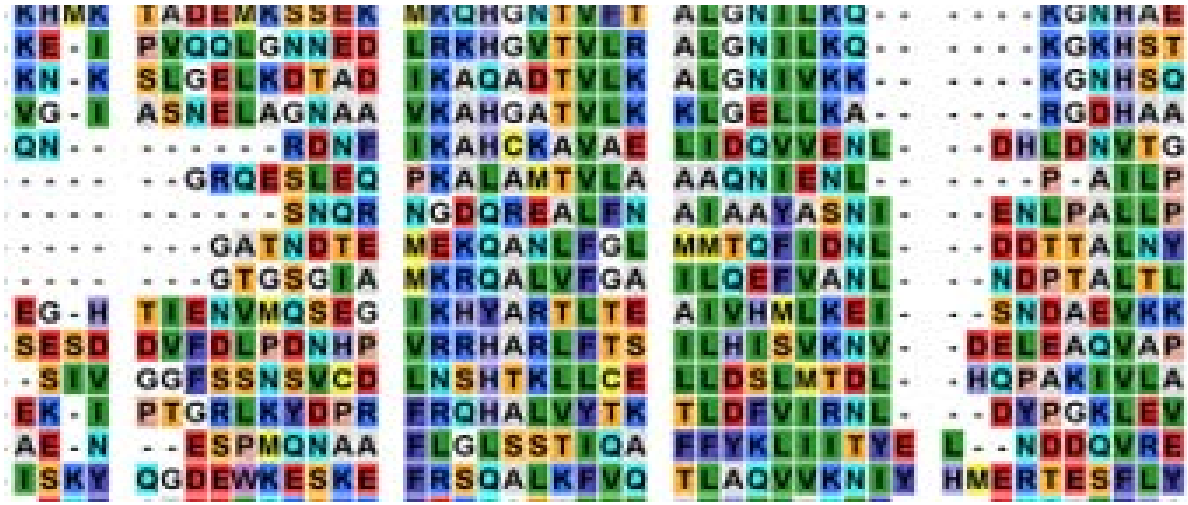




Future pharmaceuticals are designed using computers

Within SeRC we combine sequence data (SciLifeLab), patient data (KI) and advanced bioinformatics (SU,KTH,LiU) with the aim of individualized medicine

Sequence data grow faster than super computer power



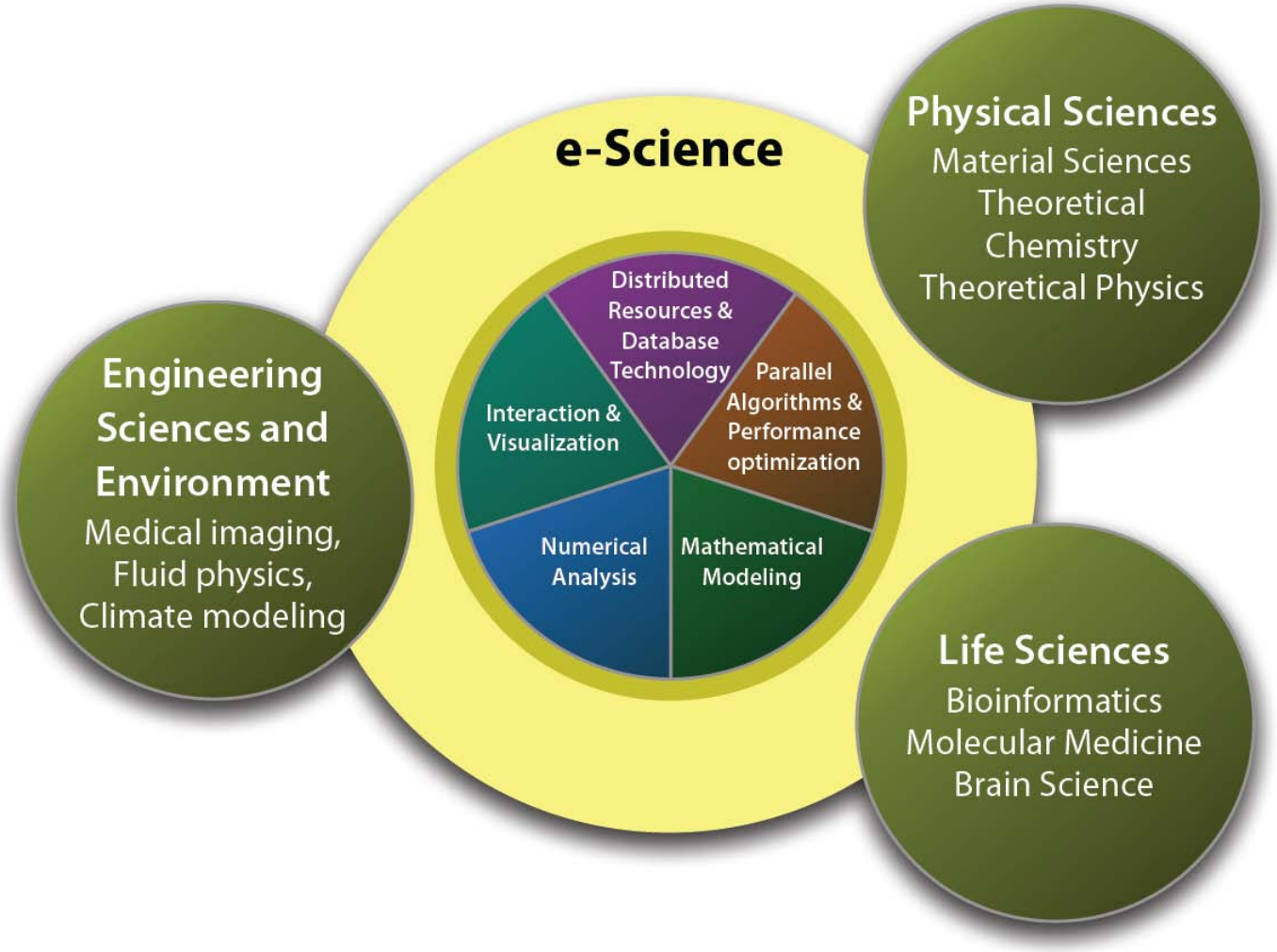
Swedish e-Science Research Centre (SeRC)

KTH VETENSKAP OCH KONST

Linköpings universitet

Stockholms universitet

Karolinska Institutet



Enhancing e-Science through e-Science communities

Swedish e-Science Research Centre