SeRC Annual meeting Skåvsjöholm, June 2-3, 2016

Thursday 2/6

10.45	**Chartered buses** leaves from KTH, Lindsteds väg 3 (registration needed)
12.15	**Lunch**
13.00-13.30	**Welcome** Dan Henningson, SeRC Director, KTH
13.30-14.15	**Organizing the human e-cloud at EPCC** Mark Parsons, Executive director, EPCC
14.15-14.45	**SICS ICE a datacenter that offers analytics tools and compute & storage** Tor Björn Minde, Chief executive officer, SICS North Swedish ICT AB
14.45-15.15	**Coffee**
15.15-15.45	**SeSSI: SeRC Exascale Simulation Software Initiative** Stefano Markidis, Berk Hess & Philipp Schlatter, KTH
15.45-16.15	**FAST Big data for climate science** Rodrigo Caballero, SU & Lars Kroll, KTH
16.15-16.45	**Visualization in e-Science applications** Ingrid Hotz, Tino Ebbers and Mathieu Linares, LiU
16.45-17.45	**Panel discussion**
19.00	**Dinner**

Friday 3/6

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11.20-11.50	**Data-driven computational materials design** Igor Abrikosov, LiU, Rickard Armiento, LiU, Anna Delin, KTH & Patrick Lambrix,
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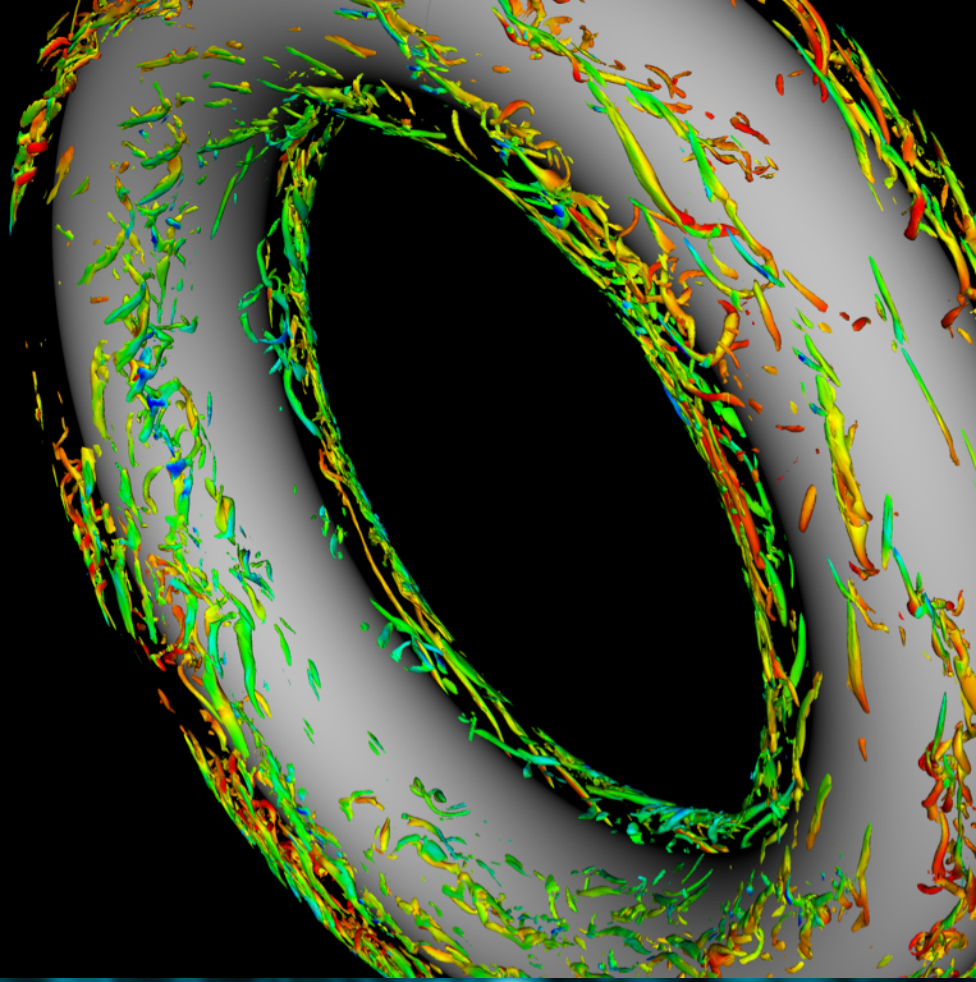
SeRC
Swedish e-Science Research Centre
Five-year progress
Organisation
Future plans

What is e-Science?

- e-Science = using digital information and the processing of this information to gain new scientific insights

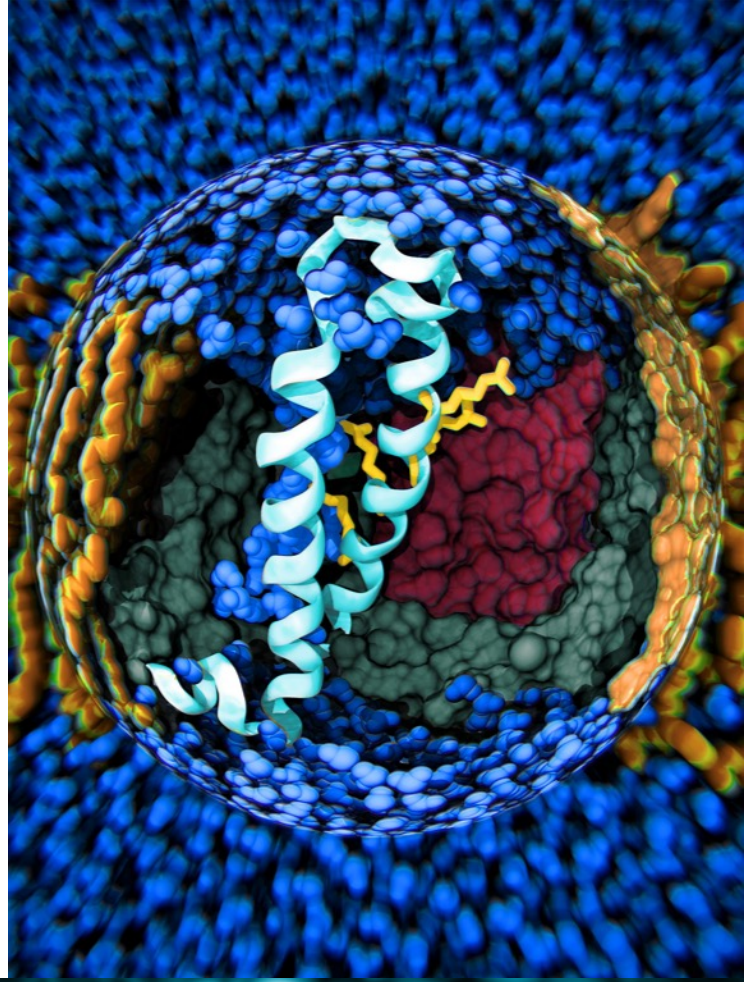


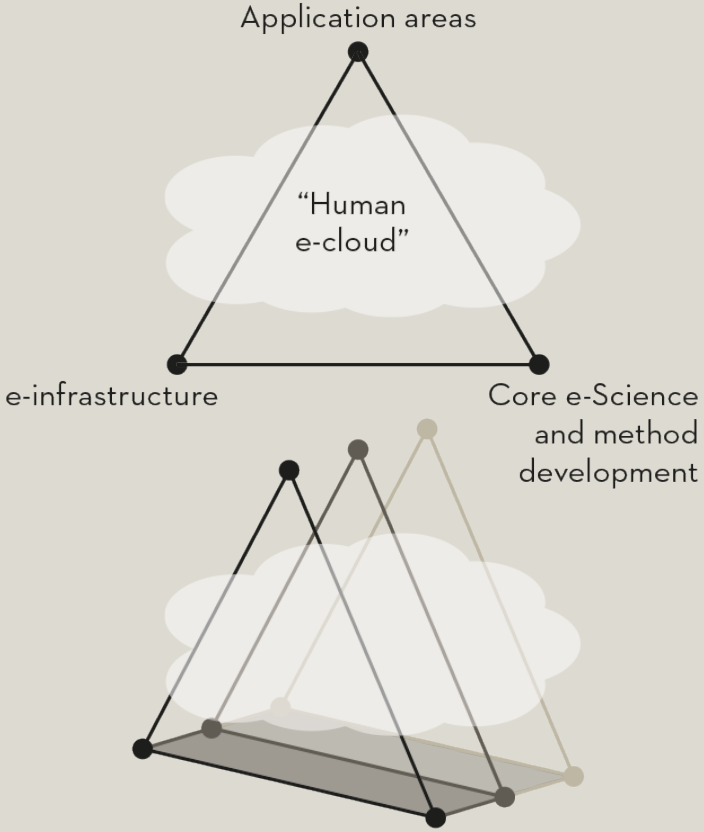
What is SeRC?

- A strategic research centre within the strategic research area (SRA) of e-Science …
- … which is one of 24 SRAs
- Funded by the Swedish government Strategic Research Area Initiative
- Founded in 2010 resulting from the Swedish Government Bill on Research Policy
- Based on a collaboration between KTH, SU, KI, and LiU

SeRC's scope

- To address problems that go beyond standard solutions …
- … with the help of:
  - e-infrastructure
  - core e-Science and method development



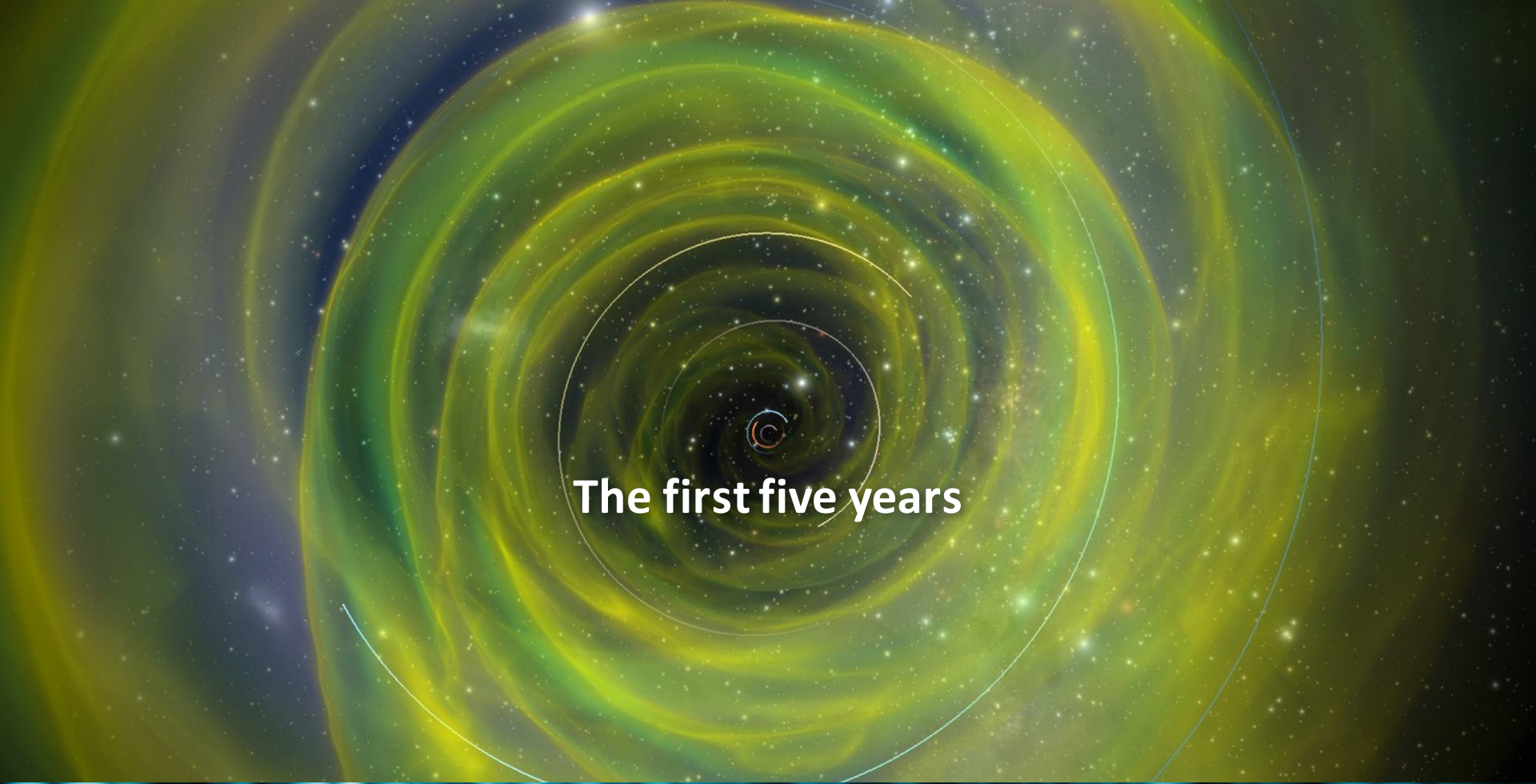


SeRC's three-pillar model

- Pillar 1 – application areas
- Pillar 2 – e-infrastructure
- Pillar 3 – core e-Science and method development
- "Human e-cloud" facilitate interaction
- Bottom pillars mutual for different several application areas

e-Science infrastructure

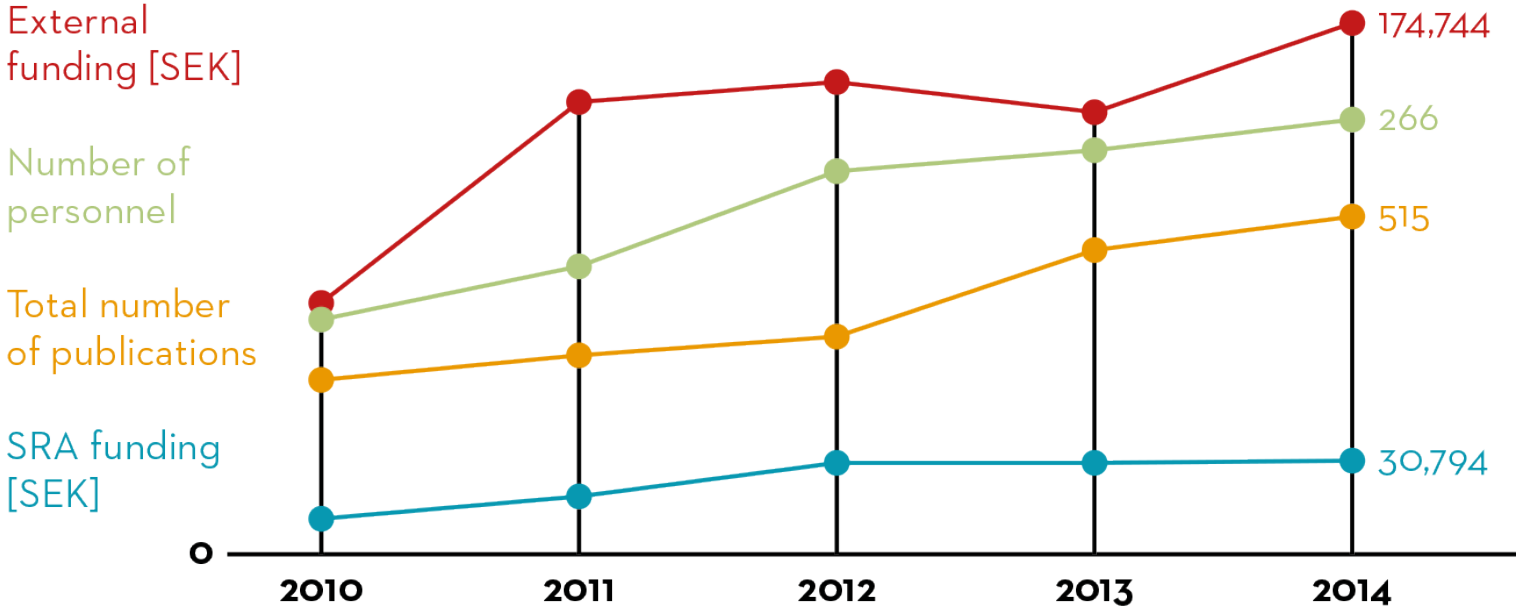
- Two supercomputer centres:
  - PDC, KTH
  - NSC, LiU
- Two visualisation centres:
  - Visualization Center C, Norrköping
  - Visualisation Studio, KTH
- A number of e-Science experts part of the "Human e-cloud"


The first five years

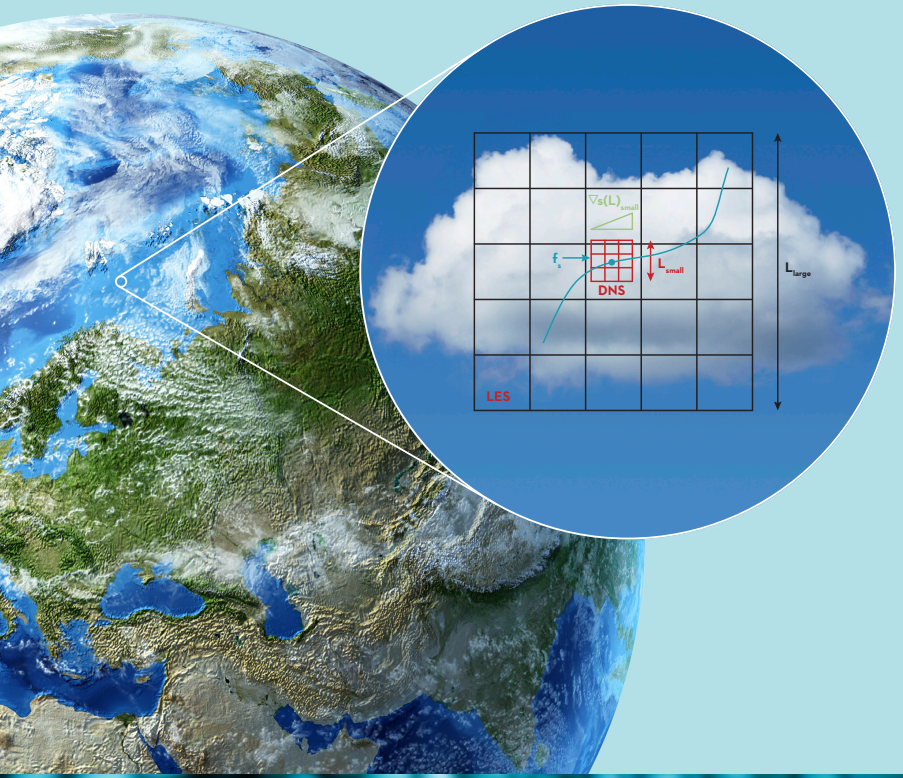
Evaluation

- SRA evaluation:
  - “KTH has … excellent … SRAs”. (One of the two acknowledged was SeRC.)
  - SeRC = "… a strong national network …"
- SeRC evaluation:
  - "… appears to be internationally competitive …"
  - "… systematically bridged the gap between tool developers and the actual users …"
  - "… appears to have been particularly strategic …” (Refers to Flagships)

Progress


External funding [SEK]
Number of personnel
Total number of publications
SRA funding [SEK]
174,744
266
515
30,794
0
2010
2011
2012
2013
2014

Success story: Climate modelling



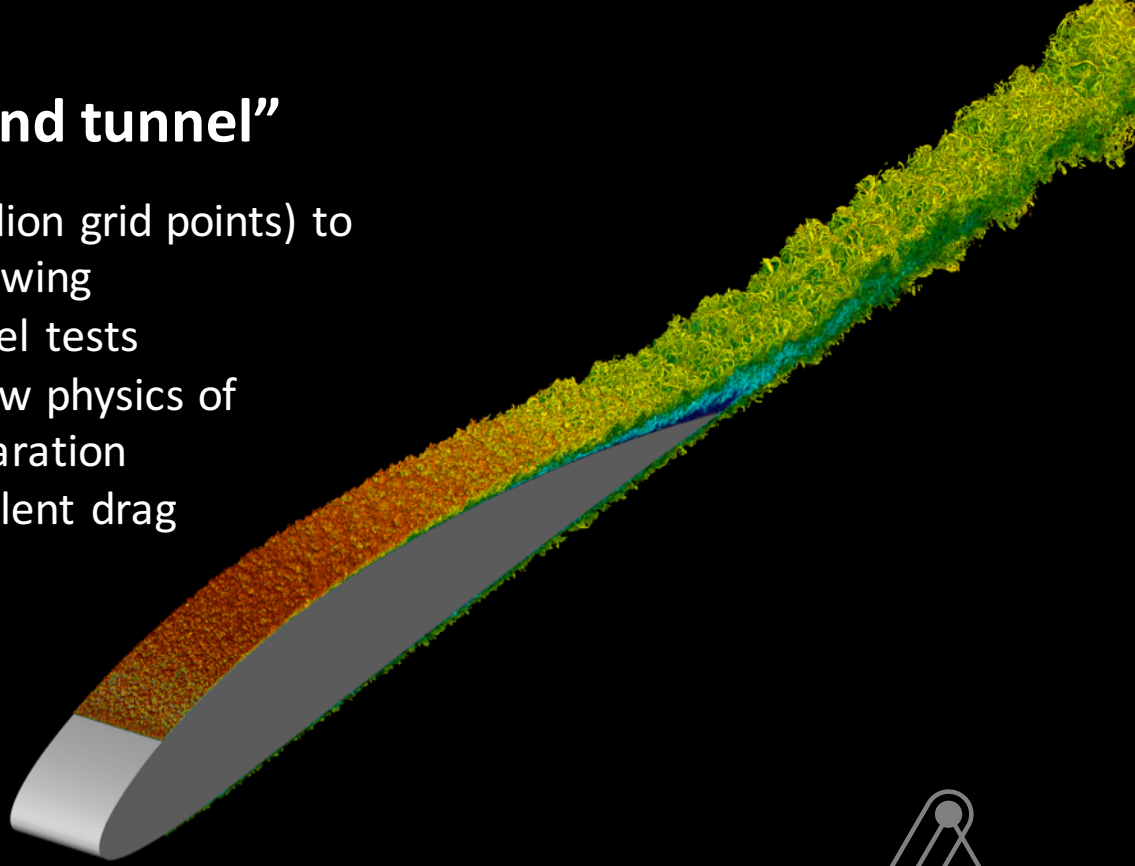
- Contributed to the development of the EC-Earth global climate model (www.ec-earth.org)
- Conducted global-scale simulations contributing to the IPCC Report 2013
- Collaboration with FLOW to understand cloud turbulence

Success story: **Personalised cancer screening – eCPC**

- Goal is to design trials and evaluate public policy for cancer screening using micro-simulation
- Integrates scientific expertise in computer science, statistics, and mathematics with molecular medicine and clinical epidemiology
- Contributed to landmark STHLM3 study for improved screening of prostate cancer

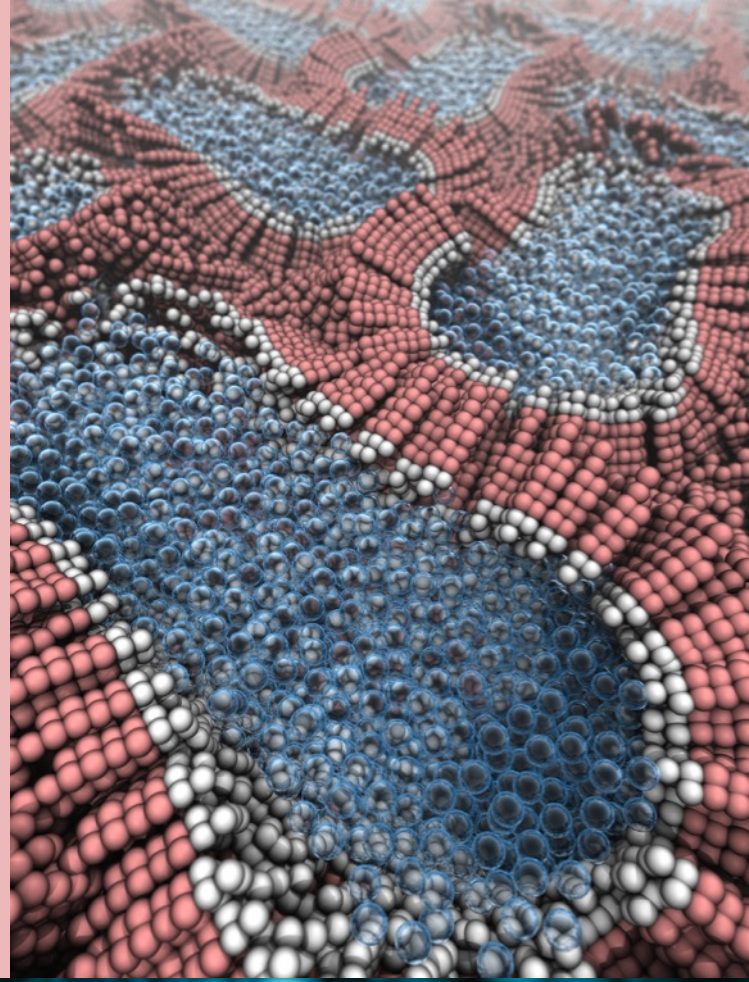
Success story: “Virtual wind tunnel”

- Large-scale simulations (3.2 billion grid points) to analyze turbulent flow around wing
- Replacing university wind tunnel tests
- Detailed characterization of flow physics of transition, turbulence and separation
- Important for decreasing turbulent drag



Success story: GROMACS – molecular simulation

- Cornerstone in materials and biomolecular research
- SU/KTH developed GROMAX code 1000's of users world wide
- Optimization resulting in world-leading simulation performance
- Understanding how outer layer of skin forms

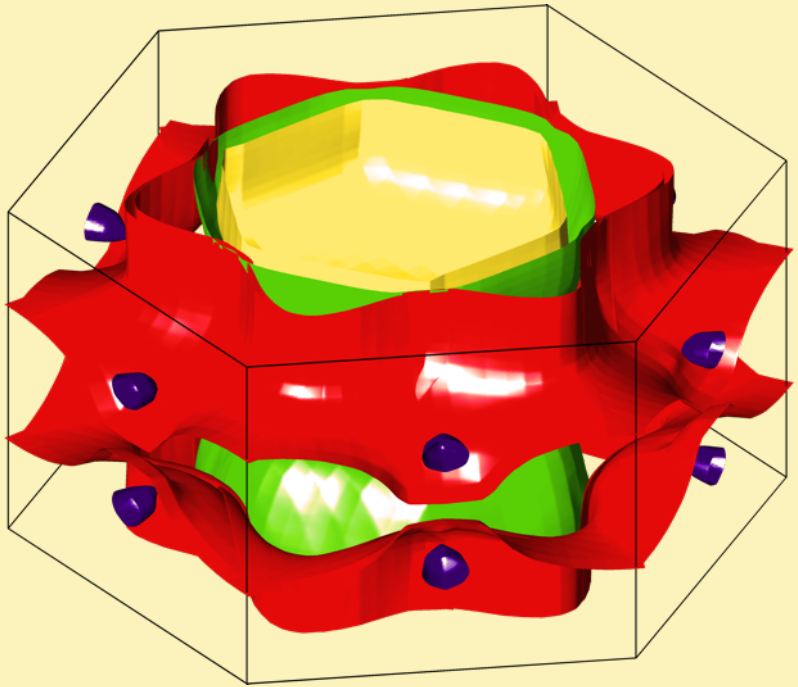


Success story: **Visualisation**

- An essential tool for accessing and understanding large generated data of use for most SeRC communities
- Development of advanced visualization tools
- Development of virtual autopsies in regular use at hospitals and police

Success story: **Electronic structure**

- Simulation of material science properties using quantum mechanics methods
- Brand new states of matter simulated
- Valence electron surface give important properties of Osmium metal



The future

e-Science agenda

- Recommendations from Vetenskapsrådet *(Swedish Science Case for e-Infrastructure)*:
  - Development of methods, tools, and software to meet increasing demand for e-Science methods
  - Advanced and long-term user support and human infrastructures key to e-Science adoption
  - A complementary and more data-centric aspect of e-Science needed
  - Active support to e-social science and e-humanities needed

Initiative: **Multidisciplinary collaboration programmes**

- Development of multidisciplinary collaboration programmes in strategic areas with high potential gain, by consolidating the SeRC efforts into larger constellation
  - eCPC Flagship
  - Visualisation In e-Science Applications
  - SeRC Exascale Simulation Software Initiative
  - Data-Driven Computational Materials Design
  - FAST Climate Science
  - Brain-IT

Initiative: **Scientific computing lab**

- Prototyping a scientific computing lab on international examples such as NCSA at UIUC
- Integrating researchers in the three pillar, with collaboration between application areas, e-infrastructure and methods
- Nucleus of the "human e-cloud”
- A physical interaction space created close to PDC a key component

Initiative: **Data-driven science**

- A data deluge from scientific instruments and large simulations require new analysis methods
- SeRC will help transfer knowledge of methods and tools from data science to SeRC communities
- Initial emphasis on data from life-science applications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