Program Third Annual Meeting

Tuesday 24/4

12.00	**Lunch**
13.00-14.00	**Welcome and presentation of SeRC faculty** Dan Henningson (SeRC Director, KTH) Olof Runborg (SeRC faculty)
14.00-14.45	**The Challenges of Petascale Computing** William T.C. Kramer (NCSA, University of Illinois)
14.45-15.15	**Coffee**
15.15-15.45	**UNINETT Sigma and SNIC** Jacko Koster (New SNIC director)
15.45-16.30	**Visualization in Data Intensive Domains** Timo Ropinski (SeRC Visualization Community,
16.30-17.15	**CFD in Hollywood** Marcus Nordenstam (Exotic Matter)
17.15-19.00	**Cross-community meetings and poster session**
19.30	**Dinner**

Wednesday 25/4

07.30	**Breakfast**
08.30-09.00	**Infrastructure** Bengt Persson (NSC Director, LiU) Erwin Laure (PDC Director, KTH)
09.00-09.45	**e-Science at Science for Life Laboratory** Mathias Uhlén (SciLifeLab)
09.45-10.15	**Coffee**
10.15-10.45	**eCPC, e-Science for Cancer Prevention and Cure** Ola Spjuth (eCPC project leader, KI) Sampsa Hautaniemi (Complex Diseases Community, Un
10.45-11.30	**e-Science and Bioinformatics** David Jones (University College London)
11.30-12.00	**Closure**
12.00	**Lunch**

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Annual Meeting Report

Skogshem & Wijk, Lidingö, April 24-25, 2012

Dan Henningson

Director SeRC

SeRC Vision

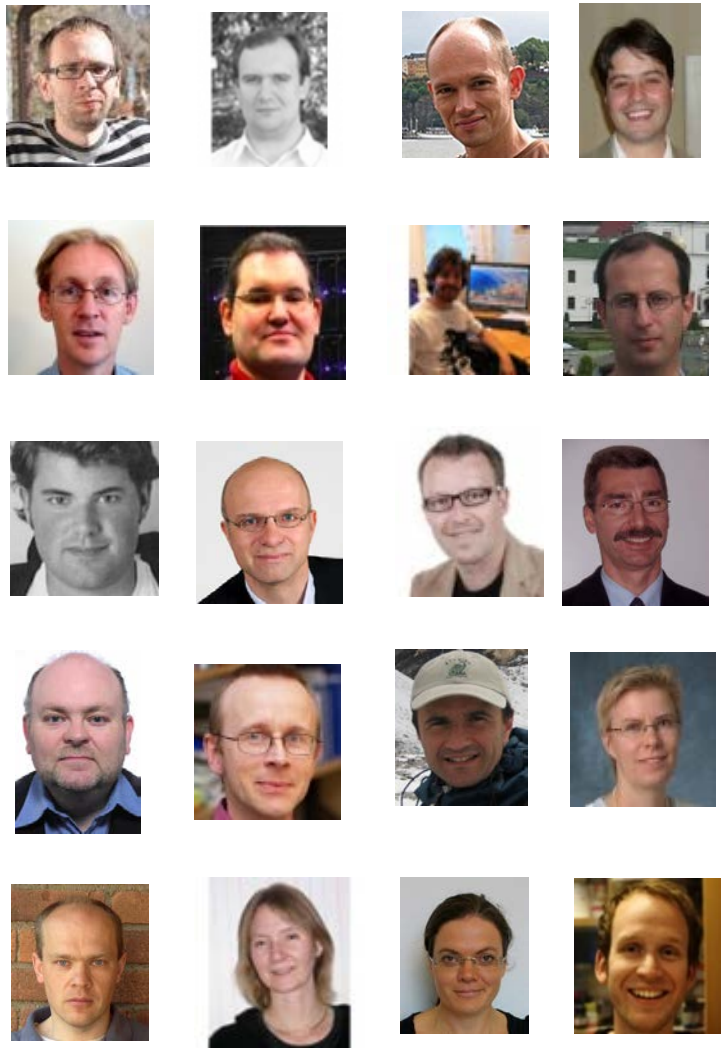
Through e-Science enable world leading research within strategically important areas

We realize our vision by

- recruiting faculty within the strategic research areas
- forming e-Science communities where collaboration between applications, core e-Science and computer centers are promoted
- forming a strong European e-infrastructure node through close collaboration between PDC and NSC
- creating an interface with industry and society
- creating a strong e-Science curriculum at the partner universities

20 SeRC faculty

- ***Lars Bergqvist***, ELEC, KTH
- ***Zilvinas Rinkevicius***, ELEC, KTH
- ***Berk Hess,*** MOL, KTH
- ***Philipp Schlatter***, FLOW, KTH
- ***Olof Runborg***, NA, KTH
- ***Erwin Laure*** DPT, KTH 2012
- ***Mathieu Linares, Leonid Pourovskii***, ELEC, LiU
- ***Björn Wallner,*** *BIO,* LiU
- ***Tino Ebbers, Timo Ropinski,*** VIZ, LiU
- ***Christoph Kessler, Patrick Lambrix,*** DM/DPT, LiU
- ***Lars Arvestad***, BIO, SU
- ***Rodrigo Caballero, Gunilla Svensson***, CLIM, SU
- ***Keith Humphreys,*** COM, KI
- ***Jeanette Hellgren-Kotaleski***, COM, KTH
- ***Olivia Eriksson***, SeRC, KTH, ***Ola Spjut***, eCPC/DM, KI



e-Science Communities

- Applied communities:
  - Bioinformatics
  - Climate Modeling
  - Complex Diseases
  - Electronic Structure
  - FLOW
  - Molecular Simulation
- Core communities:
  - Data Management
  - Distributed and Parallel Techniques
  - Numerical Analysis
  - Visualization

e-infrastructure goal

- Prioritize collaboration between NSC and PDC in order to optimize user support and establish the capacity to host large HPC systems at the European Tier 1 level.
- Integrate application experts at centers in e-Science communities to provide advanced user support

PDC/NSC host about 70-80% of Swedish HPC-resources, including Cray Lindgren and coming Triolit cluster

SNIC provides 50% funding, KTH and LiU 30% (40 MSEK)

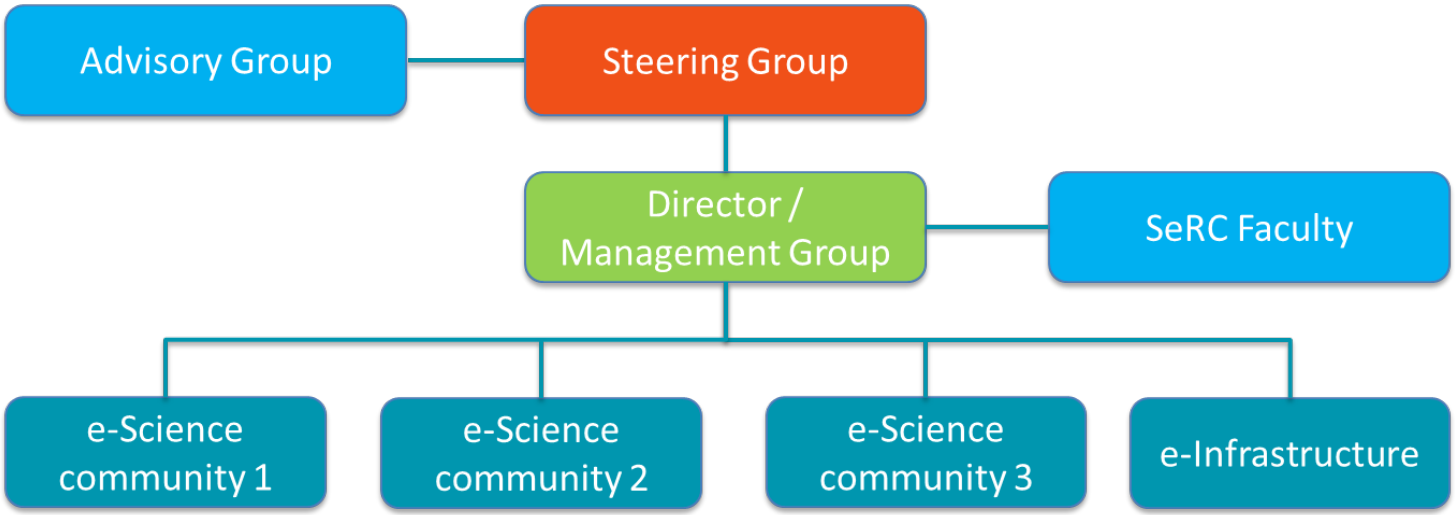
13 SeRC Application Experts

- Rossen Apostolov rossen@kth.se
- Lilit Axner lilit@kth.se
- Chandan Basu cbasu@nsc.liu.se
- Mikael Djurfeldt djurfeldt@gmail.com
- Jing Gong jing.gong@gmail.com
- Joel Hedlund yohell@ifm.liu.se
- Soon-Heum ("Jeff") Ko sko@nsc.liu.se
- Peter Larsson pla@nsc.liu.se
- Weine Olovsson weiol@nsc.liu.se
- Johan Raber raber@nsc.liu.se
- **Torben Rasmussen** torbenr@nsc.liu.se
- Olav Vahtras vahtras@pdc.kth.se
- Jonathan Vincent jonvin@pdc.kth.se

Interface with Industry and Society

- External Advisory Group with international experts and representatives from industry and society
- Representatives from industry and society in e-Science communities, *only in a few cases so far*
- Develop software of industrial interest *when possible*, e.g. participating in open source code development
- Spin-off companies in electromagnetics, material science, medical visualization, etc., *when possible*
- Production of PhDs of interest to industry

SeRC Organization



- Steering Group (SG) decides about budget and strategic directions
- Advisory Group (AG) gives external advice
- Management Group (MG) help Director deal with day-to-day activities
- SeRC Faculty (SF) has internal advisory role and coordinates between communities (core/applied), *researchers with substantial funding from SeRC*

SeRC management

Steering Group

Dan Henningson

Anders Ynnerman

Juni Palmgren

Anna Delin

Gunilla Svensson

Erik Lindahl

Olof Runborg

Bengt Persson

Erwin Laure

Jan-Eric Litton










Coordinators

Olivia Eriksson

Philipp Schlatter

Ola Spjut

Berk Hess

Jeanette Hellgren

Timo Ropinski

Tino Ebbers

Lars Bergquist

Rodrigo Caballero

Björn Wallner










Management Group in Red

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Advisory Group

- Niklas Blomberg (AstraZeneca)
- Morten Dæhlen (University of Oslo); *Chairman*
- Björn Engquist (KTH)
- David Jones (University College London)
- Claes Lundström (Sectra)
- Mattias Sillén (SAAB Group)
- Nicola Spaldin (ETH Zürich)
- Anne Trefethen (UK e-Science)

First two years of SeRC

- 150 researchers involved, including many PhD students
- 18 faculty positions recruited/identified
- About 40 SeRC funded projects defined, additional 150 Milj/year external funding
- 13 application experts financed and national portal organized
- 10 e-Science communities formed
- Flagship program on data management and modelling for cancer research
- External Advisory Group with international experts and representatives from industry and society established
- Three annual meetings and various community meetings
- MOU between LiU and KTH regarding cooperation of PDC and NSC
- First Swedish Tier 1 PRACE computer funded by VR and KTH
- Organization of IEEE e-Science conference, Dec 5-8, 2011
- Initiative to from international e-Science coordination/collaboration
- Web site launched http://www.e-science.se/

Examples of SeRC funded projects

- Directly funded SeRC projects 2010 and 2011
- Some of the research performed by SeRC funded faculty during 2010 and 2011

Bioinformatics

Modeling of membrane proteins.
Arne Elofsson, Stockholm University

Goal: To develop methods that can accurately generate protein structure from protein sequences.

- Drugs act primarily against membrane proteins
- Difficult to study experi
- Structural information
- Sequence databases gr

Collaborations with core and core parallel computi

People: Prof Arne Elofsso Peters, Marcin Skwark

Highlight publication: Nat

SeRC BIO Project:
High-throughput prediction of disease-causing SNPs

- Goal: Develop automated methodology to predict molecular consequences of disease-causing SNPs
  - Mapping structural effects of mutations
  - Use information about pathways to get a
  - Apply new methods on biomedically inte proteins associated with cancer developn important membrane proteins.
- Background:
  - Many diseases are caused by single nucle cause an amino acid in a protein to be m not cause a disease.
  - Today SNPs are readily detected in large s genetic variation.
  - Thus, improved prediction techniques wil

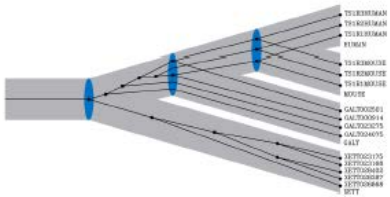
Collaboration with Complex Disease community and SeRC Flagship project.

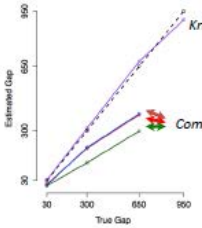
SeRC BIO Community:
Bengt Persson (LiU)
Linus Östberg (LiU/KI)
SeRC COM Community
SeRC FLAGSHIP Project

Stockholms universitet

Computational Evolution & Genomics

- **Goals**
  - Tools for inferring evolutionary history
  - Better understanding of gene evolution
  - Improved and specialized tools for genome assembly
- **Results**
  - Best gene tree inference when species tree is known
  - Accurate estimation of distance between genome "pieces"





- **Collaborators**
  - Jens Lagergren, Bengt Sennblad, Joakim Lundeberg, et c.
- **Core collaboration interests**
  - Distributed and parallel computing
  - Data management
  - Visualization
- **Group**
  - Mehmood Alam Khan, PhD student
  - Hashim Ali, PhD student
  - Kristoffer Sahlin, PhD student
  - Francesco Vezzi, postdoc

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Complex Disease & Data Management

SeRC COM Project: Modeling heterosynaptic events in the striatum

d models of plasticity-related intracellular signaling dynamics in the striatal neurons
grate with upper-levels in a multi-scale framework.

lenge experimenter's verbal models
ore experimentally inaccessible regions
st in the rational development of therap

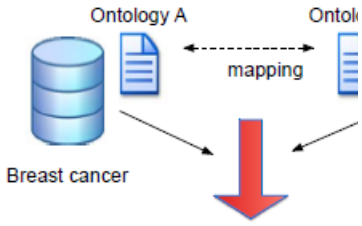
topologies, parameters and phenotype
ublic repositories.
nd fit preliminar ODE-based models,
to spatially explicit stochastic models
te with upper level models
els regulating electrical properties)

ant extension of a previous model to
e ERK activation and cholinergic modula

eRC COM Community:
eanette Hellgren-Kotaleski
KTH, KI), Omar Gutierrez-
Arenas (KTH), Olivia
Erickssson (KTH)

SeRC COM Project: Data integration in complex diseases

- Goal: Develop methods for integrating data between heterogeneous data sources relevant to research in complex diseases, such as:
  - Quality registries
  - Biobanks
  - Local study datal



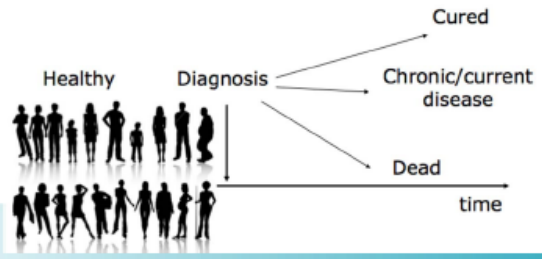
Project members: **Ola Spjuth (KI)**, Juni Pal
Jesper Tegnér (KI), Maria Krestyaninova (E

e-Science for Cancer Prevention and Cure

- a SeRC flagship project

Use statistical modeling and data integration in cancer research

- Individualized prevention strategies
- Individualized treatments



Stora prostata-cancerstudien:
STHLM 2

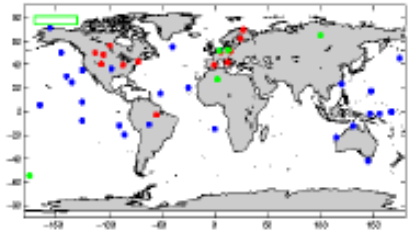
Stora nationella bröstcancerstudien:
Karma

CRisP
The Cancer Risk Prediction Center

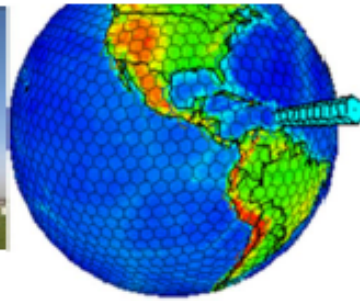
SeRC
Swedish e-Science Research Centre

Climate

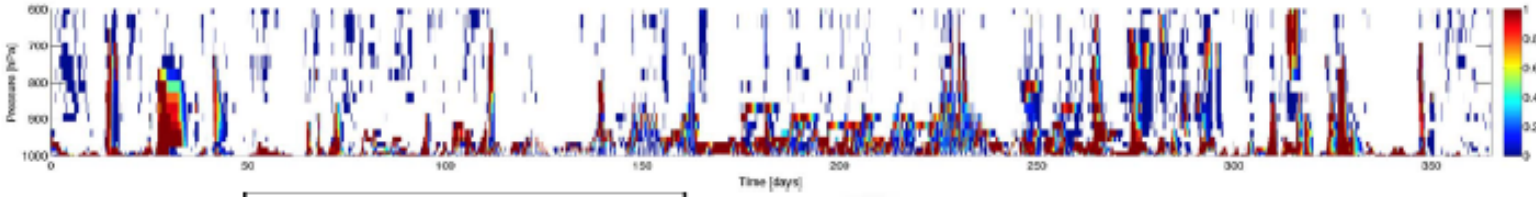
An Ensemble Single Column Model System



- Goal: To develop a user-friendly single column model of the global climate model EC-Earth that can run simultaneously at numerous locations from a web interface
  - ideal for studying sub-grid scale parameterizations
  - computationally much less expensive than the global climate model and, one-year integration <2 min
  - massively parallel: each column is run on a single processor means that one can instantly evaluate a change in the model physics at many different sites to find strengths and weaknesses in direct comparison with observations
  - easy to run without HPC experience



A year of cloud fraction in the Arctic region (70N, 160W), forced by "observed climate" (ERA-Interim re-analysis data)



SeRC Climate Modeling community
Anders Engström (Postdoc, SU)
Gunilla Svensson (SU)
Rodrigo Caballero (SU)

EC EARTH

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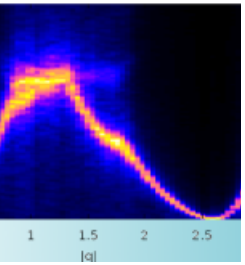
Electronic structure

Atomistic spin dynamics

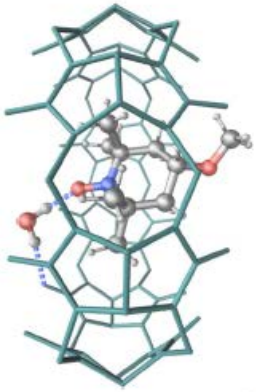
velop and apply methods to study magnetization dynamics on the atomic scale
ormation technology (storage, next-generation memory devices)
nomagnets (wires, clusters and nanostructures)
erplay with thermal gradients (spin-calometry)
ite temperature properties of magnets

onal methods:
ic structure calculatic
al theory to extract m
c spin dynamics simu
program
g the stochastic Lanc
ve parallel implemen
ectures (ongoing wor



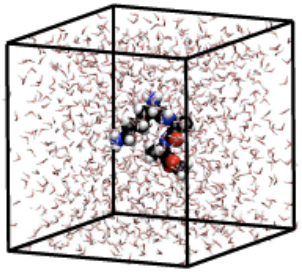
SeRC Electronic Structure Project: Multiscale Modeling Methods for Biomolecules

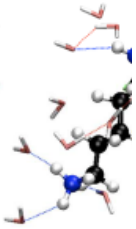
- Goal: Develop novel hybrid quantum mechanics/molecular mechanics (QM/MM)methods for computation of various spectroscopic properties of the biomolecules
  - Relevant for various simulations of various biomarkers in proteins and cellular



SeRC Electronic Structure Project: Conformational averaging for ECD spectra calculations

- Goal: Develop an efficient method to obtain ECD spectra for flexible molecules
  - Spectra calculation for flexible molecules is a challenging task
  - MD simulations are performed to study the conformation at different temperatures
  - Snapshot extract from the MD trajectory are used to compute the ECD spectra with state of the art QM/MM response theory





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SeRC Project: *Ab initio* simulation of st correlated materials: methods and appl

- Goal: Development of an efficient first-principles framework for simulating strongly-correlated materials and applying it to materials of technological and fundamental interest
  - Combining ab initio band structure methods with an advanced treatment of electronic correlations provided by the dynamical mean-field theory (DMFT)
  - Implementing simulation of various properties: ground-state and free energy, spectral function, magnetic properties, elastic modules
  - Applications mainly to transition metal systems: Fe, Co, Ni, Mn at ambient and extreme conditions (high temperature/pressure).

- Large scale calculations
  - Use of GROMACS (MM/MD) for lon
  - Use of DALTON (QM/MM response
    (solvent) on the electronic respons

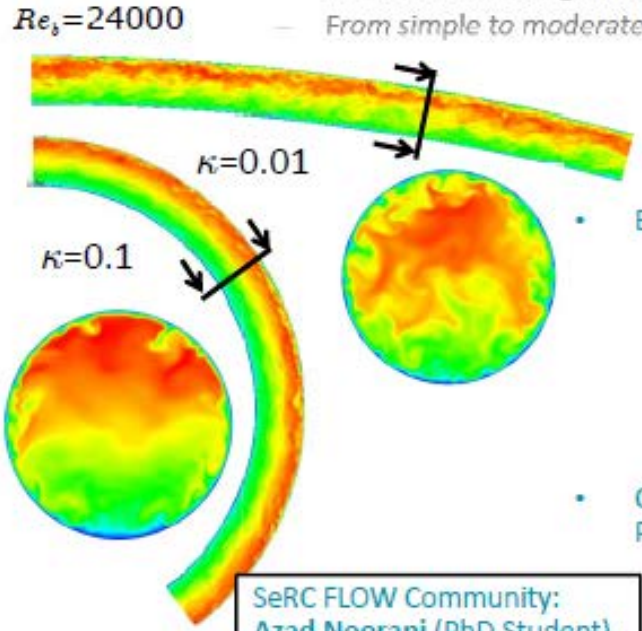
Current results:
- *A package combining DMFT with the electronic structure Wien-2k*
- *Applications to describing an electronic topological transition of*

Mathieu Linares (LIU),
Zilvinas Rinkevicius (KTH),

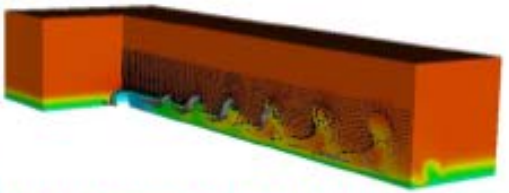
FLOW

SeRC FLOW Project: Methods for Lagrangian particles in complex geometries

- Goal: Develop, implement and apply methods for efficient Lagrangian particle tracking suitable for complex geometries
  - Relevant for various transport processes (drug delivery in blood flow), pollutants, *etc.*
  - Turbulence in straight and bent pipes as flow cases (never studied in detail!)
  - *From simple to moderately* complex geometries: Stenotic flow with particles



- Efficient coupling Lagrangian-Eulerian solver
  - Massively parallel code Nek5000 (up to 200'000 cores), optimal performance on Lindgren (PDC)
  - On-going: Methods for millions of particles in flow domain.



- Collaboration with Core activities: Parallelisation (DPT), Visualisation (VIS), Argonne National Lab (Algorithms)

SeRC FLOW Community: **Azad Noorani** (PhD Student), Philipp Schlatter, Luca Brandt (KTH), Matts Karlsson (LiU)

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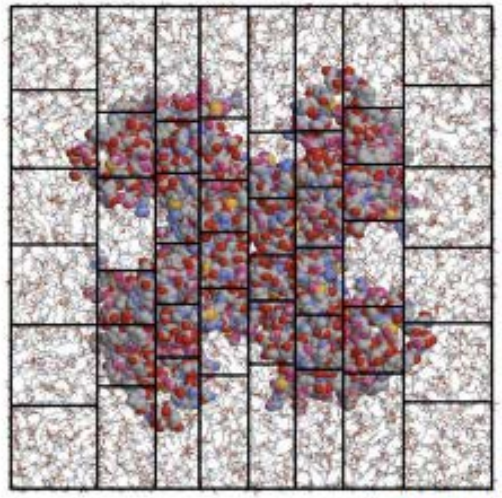
Molecular simulation

SeRC Molecular Simulation Project: Algorithms for parallel molecular dynamics simulations

- Goal: Develop algorithms to allow molecular simulation of 100 000 to 10 million atoms on 1000 – 100 000 cores on heterogeneous computer architectures
  - Simulations of protein, DNA and RNA can take months of simulation time
  - Computers are getting more and more cores, as well as GPUs
  - New algorithms are required to tackle challenges in life sciences



- Tightly coupled algorithms
  - Hybrid MPI+OpenMP parallelization
  - Domain decomposition with dynamic load balancing
  - Efficient non-bonded kernels using SSE and CUDA (GPUs)
  - Electrostatics are non-local -> limits scaling
- Collaboration with Core activities:
  Numerical Analysis (accurate parallel electrostatics solvers)

This SeRC project:
Szilárd Páll (PhD-student)
Berk Hess

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Distributed and parallel techniques

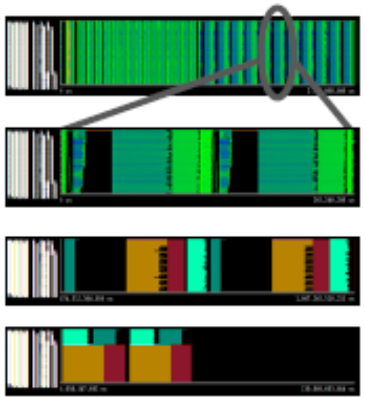
SeRC project OpCoReS

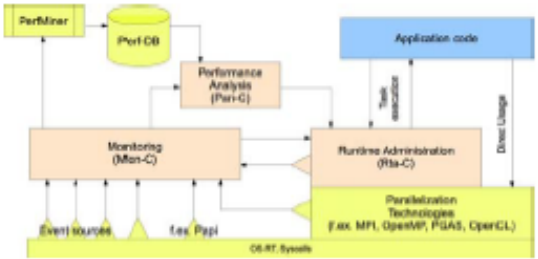
Optimized Component Runtime System for e-Science

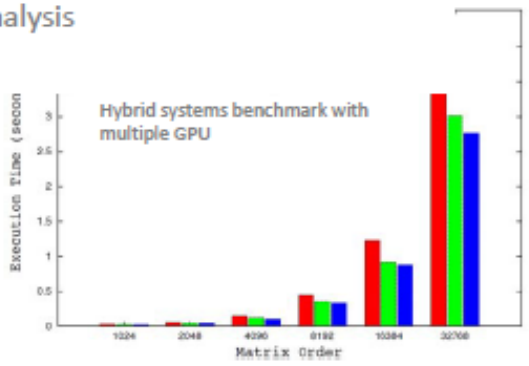
A project of the Community Distributed and Parallel Techniques

Develop, implement and apply methods allowing efficient use of hybrid computer systems as well as large-scale clusters in numerical simulations

- Use of component-based, task-oriented programming models and high-level equation-based object-oriented textual/graphical programming models
- Efficient compilation of such models and composition of applications from components
- Exploitation of multi-level parallelism in application development as well as during runtime and associated performance monitoring and analysis







Community cooperations:
Electronic Structure, FLOW, Numerical Analysis

encore! CREST PEPPHER

EU FP7 Involvement & Cooperation

Erwin Laure, Mats Brorsson
PhD students: Xavi Aguilar, Michael Schliephake

Christoph Kessler, Peter Fritzson
PhD students: Mahder Gebremedhin, Mudassar Majeed

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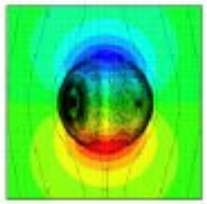
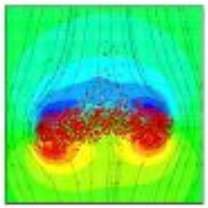
Numerical analysis

Sedimentation of point cloud

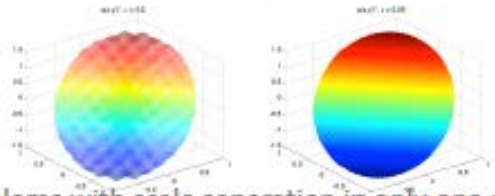
SeRC NA Project: Multiscale Problems in Fluid Dynamics

- General goal: Develop and analyze numerical methods which couple micro- and macroscopic descriptions of fluid flow
  - Target applications: complex flow (sedimentation of fibers/particles in a fluid), geophysical flow (cloud parameterization)
  - Coarse behaviour depends significantly on fine scale details in model
  - Use primarily the Heterogeneous Multiscale Methods (HMM) framework





- Model problem: Elliptic PDEs with rapidly varying coefficients
  - Mathematically similar to Stokes equations, easier to analyze
  - Improved HMM efficiency by reducing the coupling errors from microscale solver



  - HMM for problems with scale separation in only one coordinate direction
- Collaboration with FLOW, Micro and complex fluids area.

SeRC NA Community: **Doghonay Arjmand** (PhD Student), Olof Runborg, Anna-Karin Tornberg (KTH)

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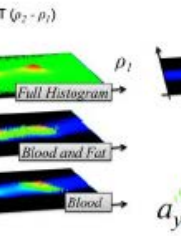
Visualization

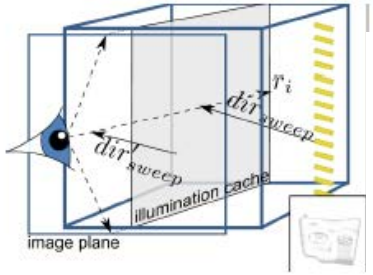
Clinically Applied Multivariate Volume Rendering

- Goal: Improved material separation in medical volume data
  - Relevant for image-based medical diagnosis and organ-based analysis
  - Enable anatomical transfer function design



Efficient Methods for Volumetric Illumination

- Goal: Improve spatial comprehension of volume rendered images
  - Currently used illumination models are local
  - Global models are demanding with respect to computing
  - Interactive data exploration, which requires interactive frame rates

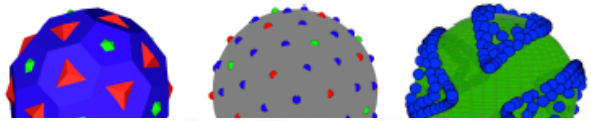


SeRC VIS Co
Stefan Lindl
Student), Cl
(CMIV), And
(CMIV), And

SeRC Project: Visualization of MR Diffusion Data

Goal: Develop a common theoretical framework for sampling, representation and visualization of in vivo diffusion processes

- Nested Rotationally Invariant Sampling Scheme for Diffusion MRI



- A mathematical
representation o
tensor pairs

SeRC VIS Community:
Daniel Jönsson (PhD Student), **Erik Sunden** (
Timo Ropinski (LiU), An
Ynnerman (LiU)

Fat-Water Imaging

- Aims
  - Quantitative fat water imaging
  - Atlas based whole body image segmentation
  - Searchable database of human high resolution quantitative datasets
  - Quantitative image visualization

- Monomial filter
order tensor rep
of orientation or

- Clinical Applications
  - Abdominal fat quantification

Program

Tuesday 24/4

12.00	**Lunch**
13.00-14.00	**Welcome and presentation of SeRC faculty** Dan Henningson (SeRC Director, KTH) Olof Runborg (SeRC faculty)
14.00-14.45	**The Challenges of Petascale Computing** William T.C. Kramer (NCSA, University of Illinois)
14.45-15.15	**Coffee**
15.15-15.45	**UNINETT Sigma and SNIC** Jacko Koster (New SNIC director)
15.45-16.30	**Visualization in Data Intensive Domains** Timo Ropinski (SeRC Visualization Community,
16.30-17.15	**CFD in Hollywood** Marcus Nordenstam (Exotic Matter)
17.15-19.00	**Cross-community meetings and poster session**
19.30	**Dinner**

Wednesday 25/4

07.30	**Breakfast**
08.30-09.00	**Infrastructure** Bengt Persson (NSC Director, LiU) Erwin Laure (PDC Director, KTH)
09.00-09.45	**e-Science at Science for Life Laboratory** Mathias Uhlén (SciLifeLab)
09.45-10.15	**Coffee**
10.15-10.45	**eCPC, e-Science for Cancer Prevention and Cure** Ola Spjuth (eCPC project leader, KI) Sampsa Hautaniemi (Complex Diseases Community, Un
10.45-11.30	**e-Science and Bioinformatics** David Jones (University College London)
11.30-12.00	**Closure**
12.00	**Lunch**