HPC@SC

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DLR, Simulation and Software Technology (SC)

High Performance Computing – Survey of Topics

Parallel algorithms and data structures

- Numerical libraries
- Optimization algorithms and tools
- Pre- and post-processing

Cooperation partner for the development of parallel applications

- HPC simulation codes

Parallelization techniques for modern architectures

- Parallel programming (MPI, OpenMP, OpenCL, OpenACC, PGAS, Python, …)
- Tools for parallel software systems
- Software engineering for HPC codes

Project Survey

- Exascale Computing
  - CRESTA
  - ESSEX
- DLR Aeronautics and SPACE
  - THERMAS
  - Free-Wake
  - BACARDI
- BMBF Inverse Problems
  - HPC-FLiS

EC Project CRESTA

- Three year EU-funded collaborative project, 13 partners, €12 million costs, €8.5 million funding, start: October 2011
  - **Collaborative Research into Exascale Systemware, Tools and Applications**
  - Project coordinator: EPCC at The University of Edinburgh
- CRESTA has a very strong focus on exascale software challenges
- Uses a co-design model of applications with exascale potential interacting with systemware and tools activities
- The hardware partner is Cray
- Applications represent broad spectrum from science and engineering
- CRESTA will compare and contrast incremental and disruptive solutions to Exascale challenges

Consortium & Applications

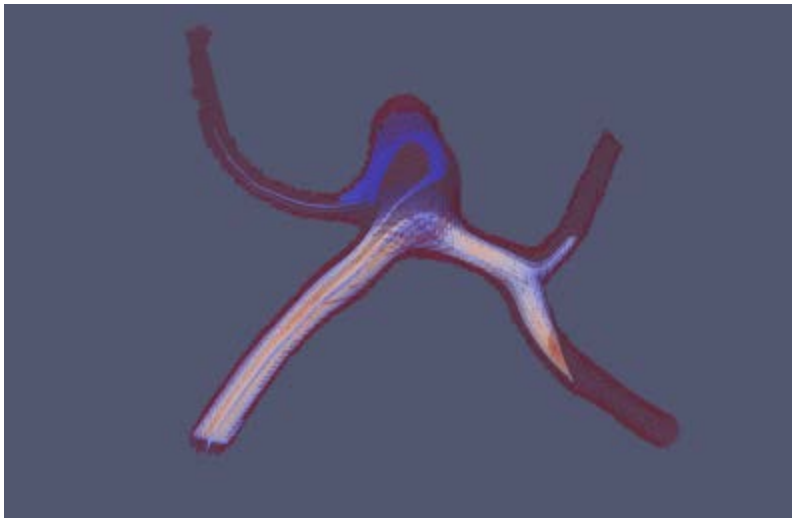
- Leading European HPC centres
  - EPCC, HLRS, CSC, PDC
- A world leading vendor
  - Cray
- World leading tools providers
  - TUD (Vampir), Allinea (DDT)
- Exascale application owners and specialists
  - ABO, JYU, UCL, ECMWF, ECP, DLR

Application	Grand challenge	Partner responsible
GROMACS	Biomolecular systems	KTH (Sweden)
ELMFIRE	Fusion energy	ABO (Finland)
HemeLB	Virtual Physiological Human	UCL (UK)
IFS	Numerical weather prediction	ECMWF (International)
OpenFOAM	Engineering	EPCC / HLRS / ECP
Nek5000	Engineering	KTH (Sweden)

SC´s Task: Pre- and Post-Processing

Challenges in exascale post-processing

- Huge amount of data to be processed and visualized
- Not possible to store data on disk
- Moving data is costly
- Memory issue
- Efficiency of parallelization with respect to visualization techniques
- Latency



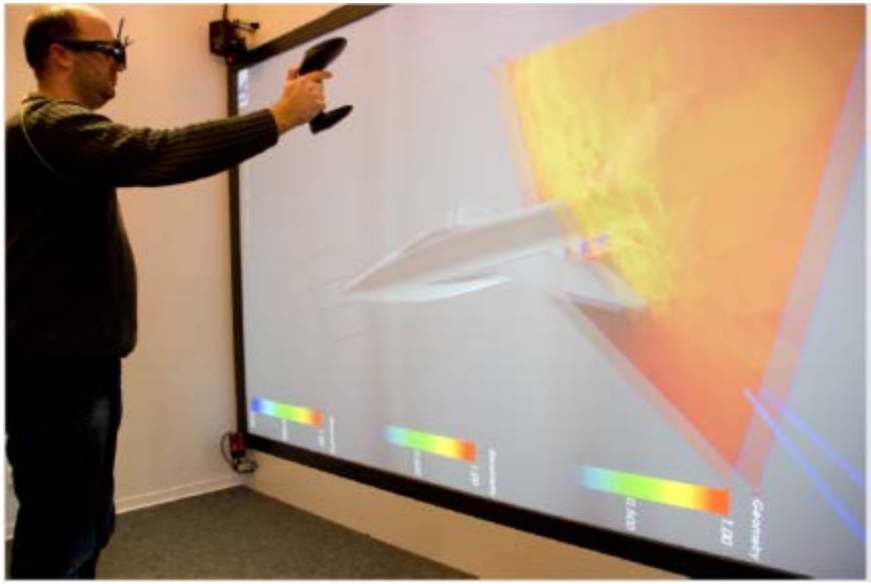
Application: blood flow simulation for aneurysm study

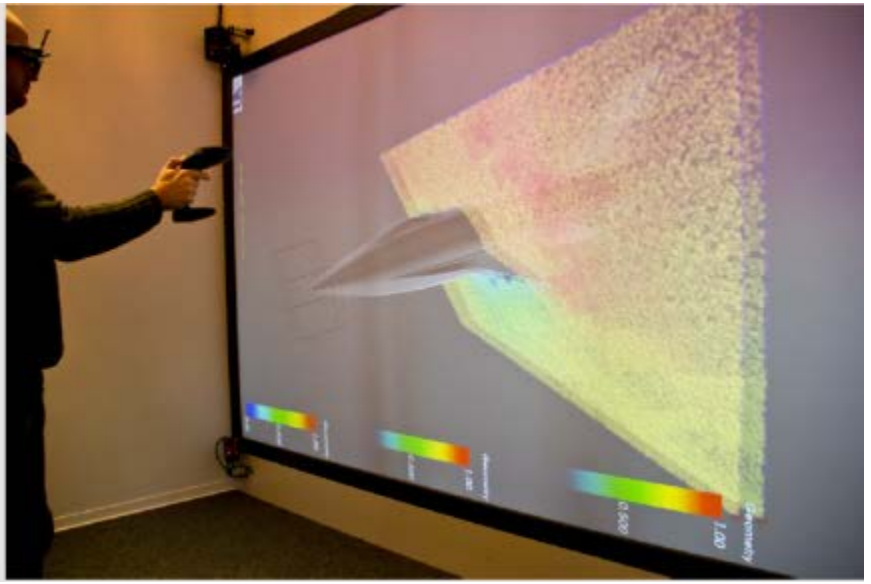
Approaches

- In-situ visualization
- Interactive visualization
- Multi-resolution data visualization

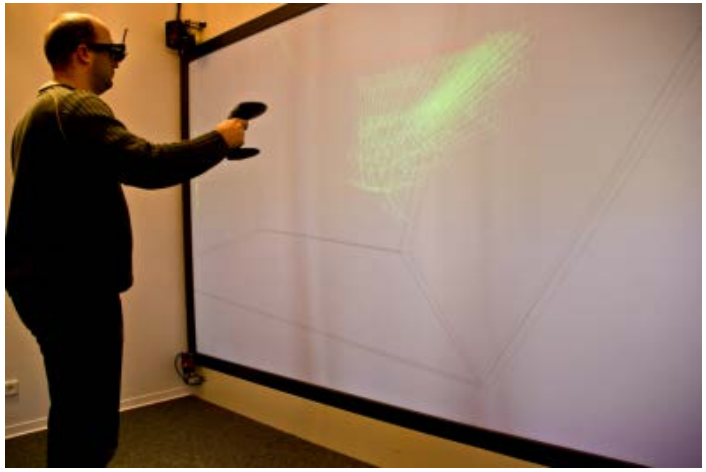
Using Virtual Reality

- Power-wall, display-wall systems
- Immersive visualization
- Provide great details
- Enhanced depth perception in VR
- Enable user to explore their data in a natural way





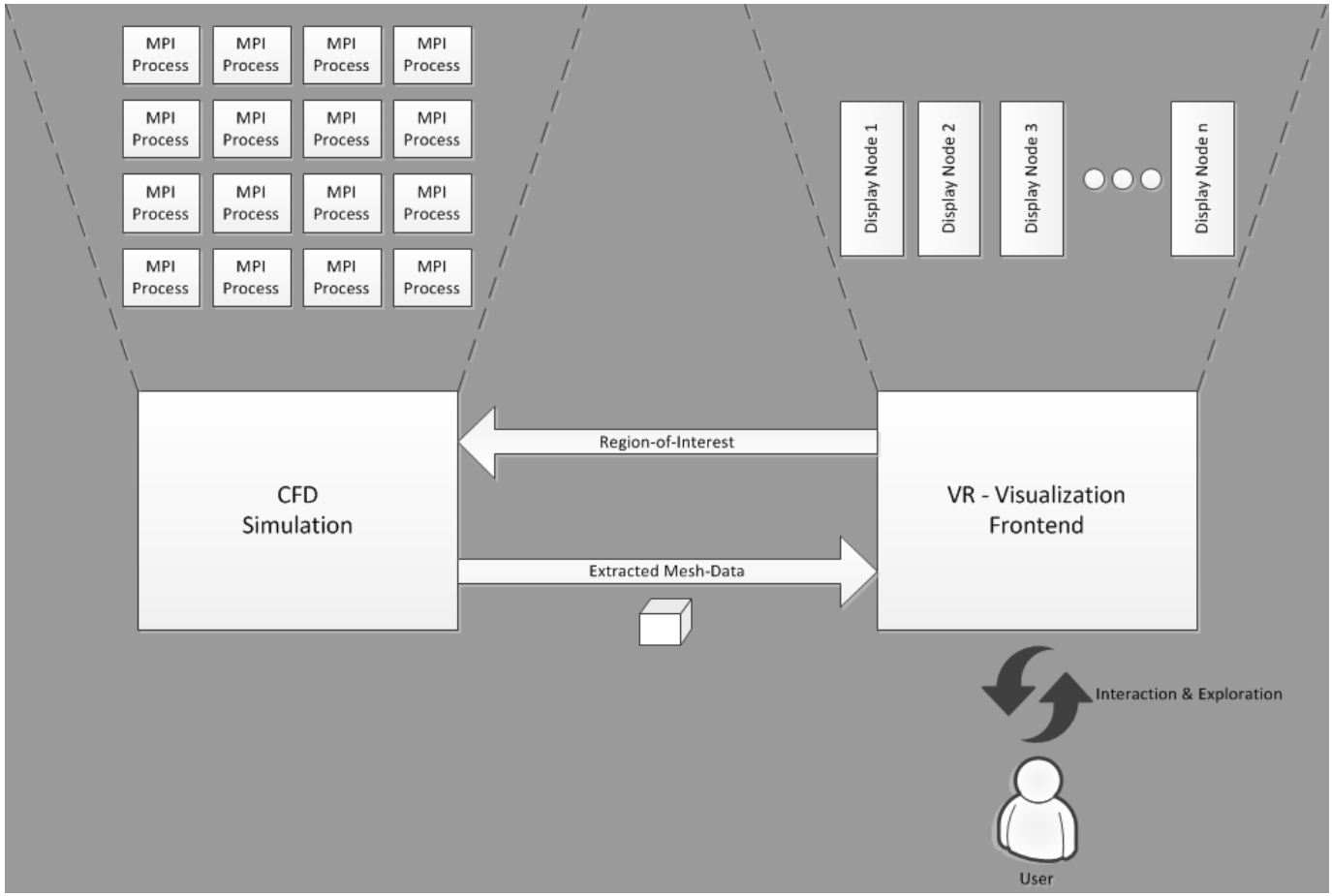
Computational Steering



- Steer mesh or simulation parameters
- Based on provided in-situ visualization
- Carry out steering while simulation is running
- Prevent failure
- Achieve better convergence for the solver
- Saving time

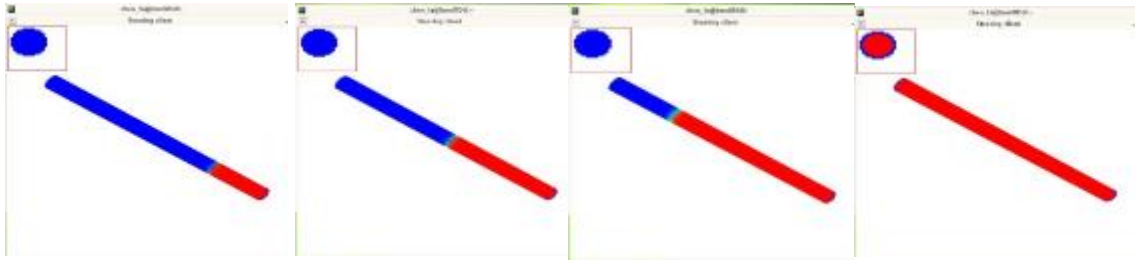
Post-processing: system survey

- Interactive data post-processing
- In-situ processing
- Enable computational steering



Post-processing: co-design with HemeLB

- Prototype for post-processing with testing dataset
- Cylinder simulation with various number of lattice points,
  1k-2M
- Performance evaluation on different datasets
- Visualization and steering overhead, approximately 20%.



The prototype of cut plane visualization

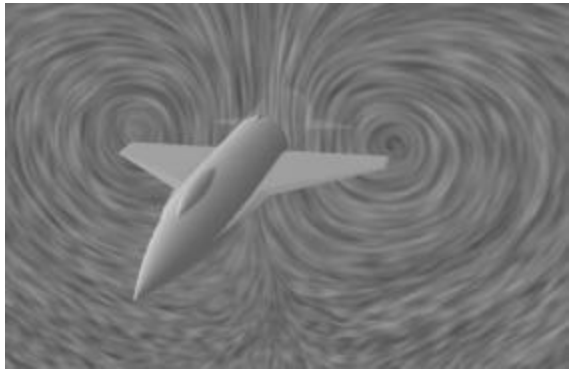
Number of lattice points / Time required	1k	16k	128K	256K	1M	2M
Simulation alone	0.0001	0.0021	0.0083	0.0146	0.011	0.021
With vis. and steering	0.00012	0.00219	0.00837	0.0158	0.0149	0.026

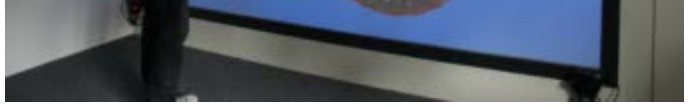
(256 processes)

Post-processing: co-design with HemeLB

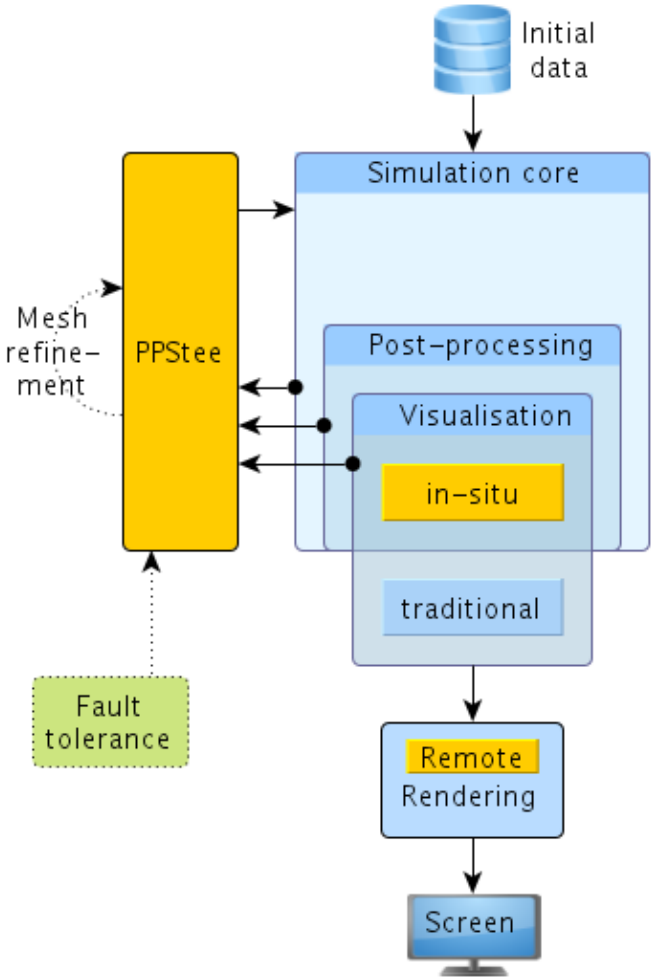
On-going work:

- Bifurcation dataset
- Implementing LIC (line intergral convolution) for the vector field
- Possible intergration to DLR´s VR system

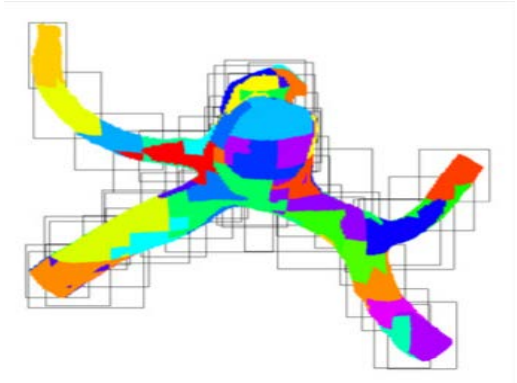




PPSTee: A Pre-Processing Interface for Steering Exascale Simulations

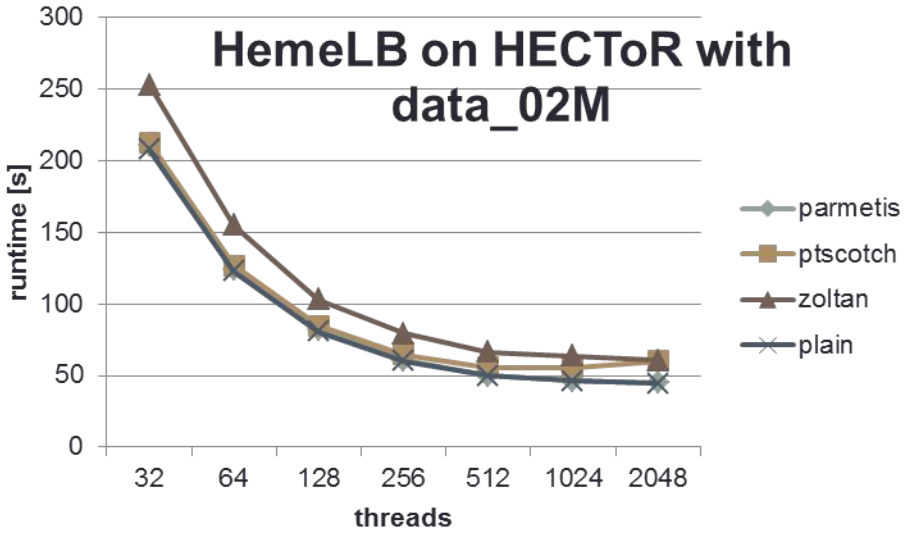


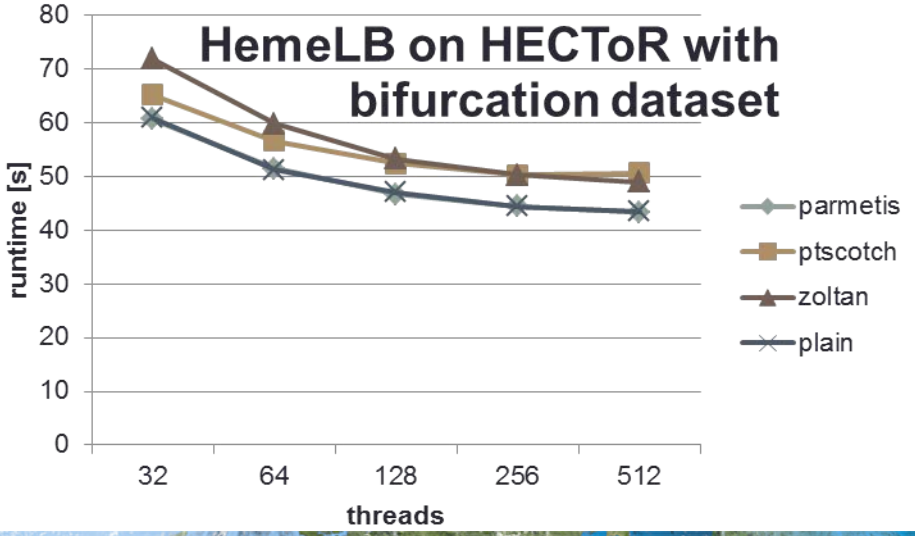
- Swappable external partitioning tool (ParMETIS, PTScotch, Zoltan)
- Flexible data format
- Incorporates different simulation stages like computation and visualization
- Easily adjustable to
  - new partitioning tools
  - different kinds of stages
  - fault tolerance
  - mesh refinement



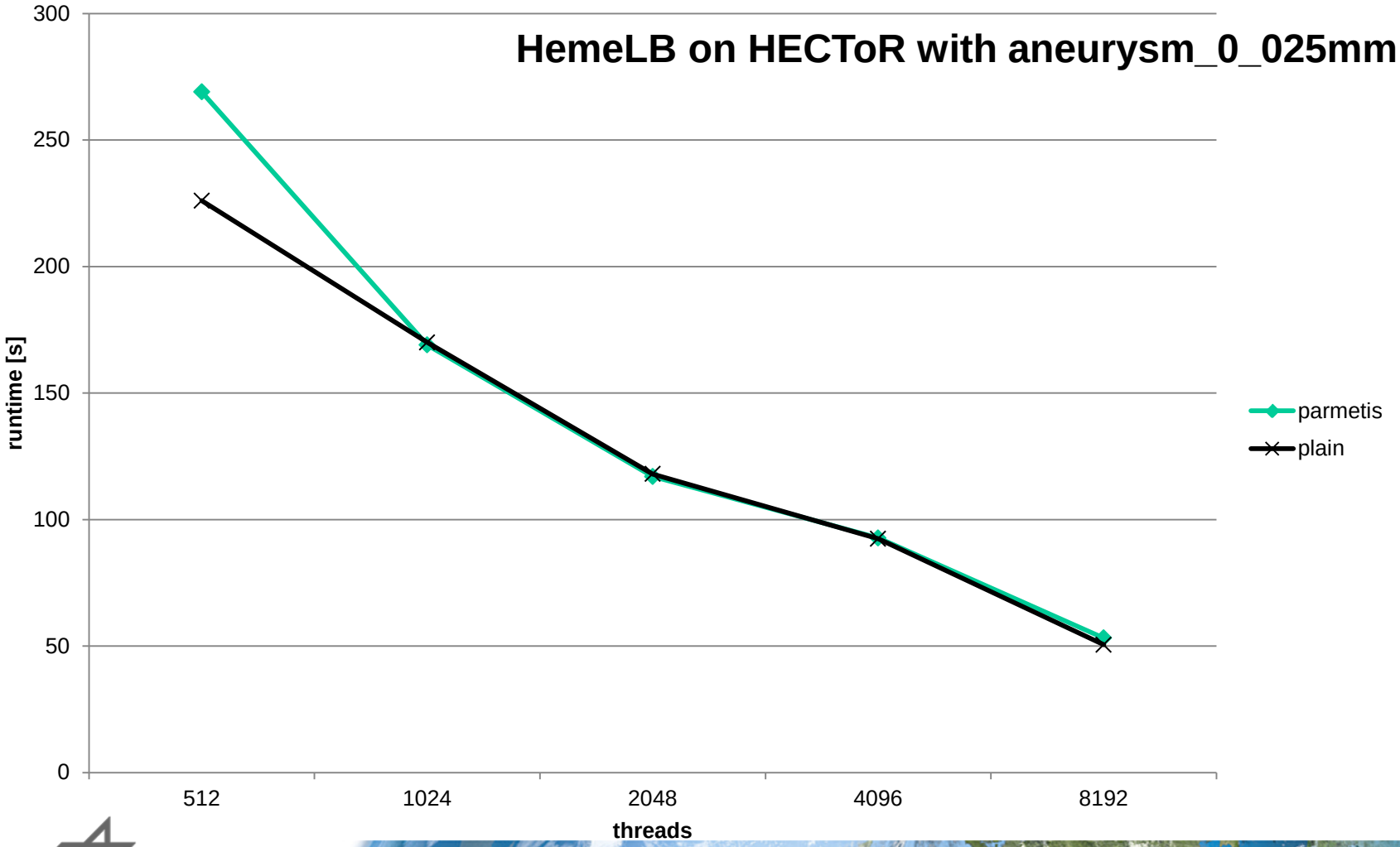
Pre-processing: HemeLB using PPStee on HECToR (1)

- Close match of HemeLB and PPStee with ParMETIS
- PPStee with PTScotch shows a similar behaviour, but is worse for larger thread counts (and shows scaling problems starting at 512 cores)
- PPStee with Zoltan shows a constant overhead





Pre-processing: HemeLB using PPStee on HECToR (2)



Future work

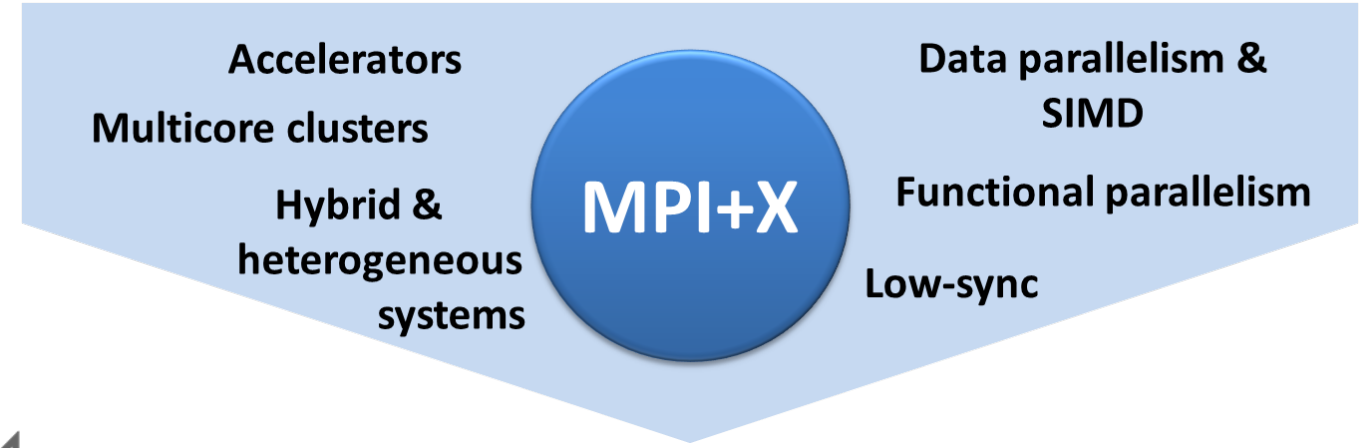
- Final tool development

- Co-design: tool integration into CRESTA applications
  - Pre- and post-processing: HemeLB
  - Pre- and post-processing: Nek5000
  - Post-processing: Elmfire
  - Post-processing: OpenFOAM

- Co-design: tool evaluation with CRESTA applications
  - Pre- and post-processing: HemeLB
  - Pre- and post-processing: Nek5000
  - Post-processing: Elmfire
  - Post-processing: OpenFOAM

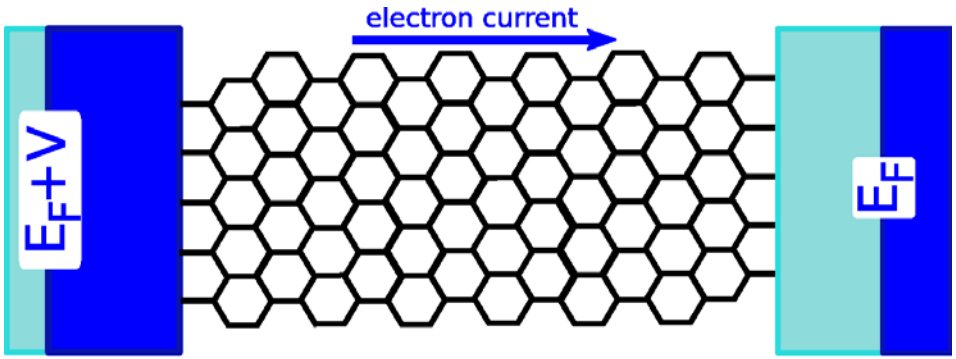
DFG Project ESSEX (Start: January 2013): Equipping Sparse Solvers for the Exascale

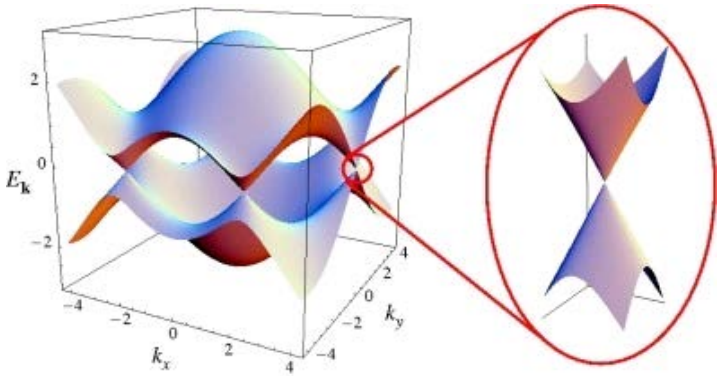
Parallelization targets	
Basic building blocks	Algorithms
spMVM BLAS	Preconditioners
	KPM, ChebTP, JaDa, FEAST, CFET



ESSEX Application: Complex Quantum Systems

Example: DC current through graphene nano-ribbon





Hard eigenproblems:

- Find a few extreme eigenpairs
- Find many interior eigenpairs

Pipelined Hybrid-Parallel Jacobi-Davidson

Iterative solver for a few extreme eigenpairs

- Based on (block) Jacobi-Davidson
- Uses highly optimized MPI+X kernels
- Dynamic scheduling to optimize cache usage and reduce latency effects

Technology for Computing Interior Eigenpairs

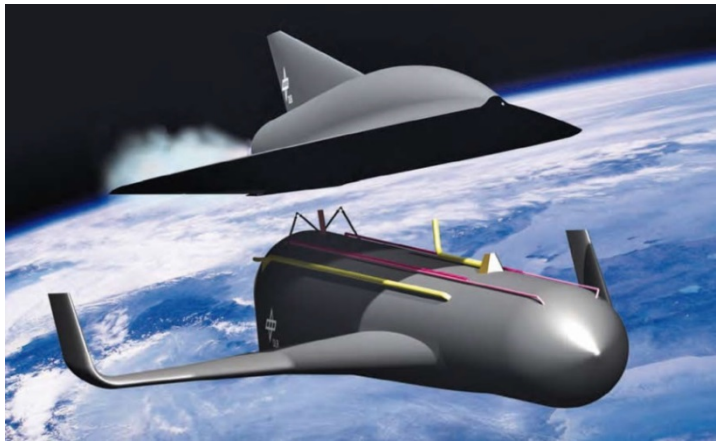
- Block Krylov methods to be used in the FEAST eigensolver
- Robust and scalable incomplete factorization preconditioners for indefinite matrices
- The hard linear systems force us to rethink the way we do numerics on parallel computers.

DLR Project THERMAS : Analysis and Optimization of the Spaceliner Pre-Design

- Development of a hypersonic passenger spacecraft for long distance flights

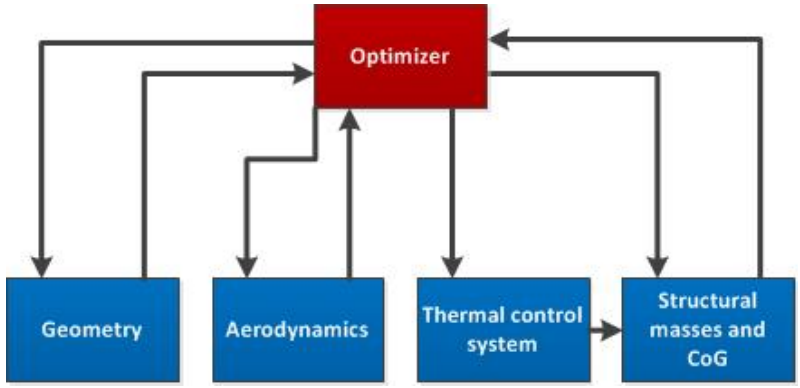
- Descent should be accomplished in gliding flight

- **New research focus:** development of a hybrid structure with integrated thermal control units involving magnetohydrodynamic (MHD) effects with cooled magnets

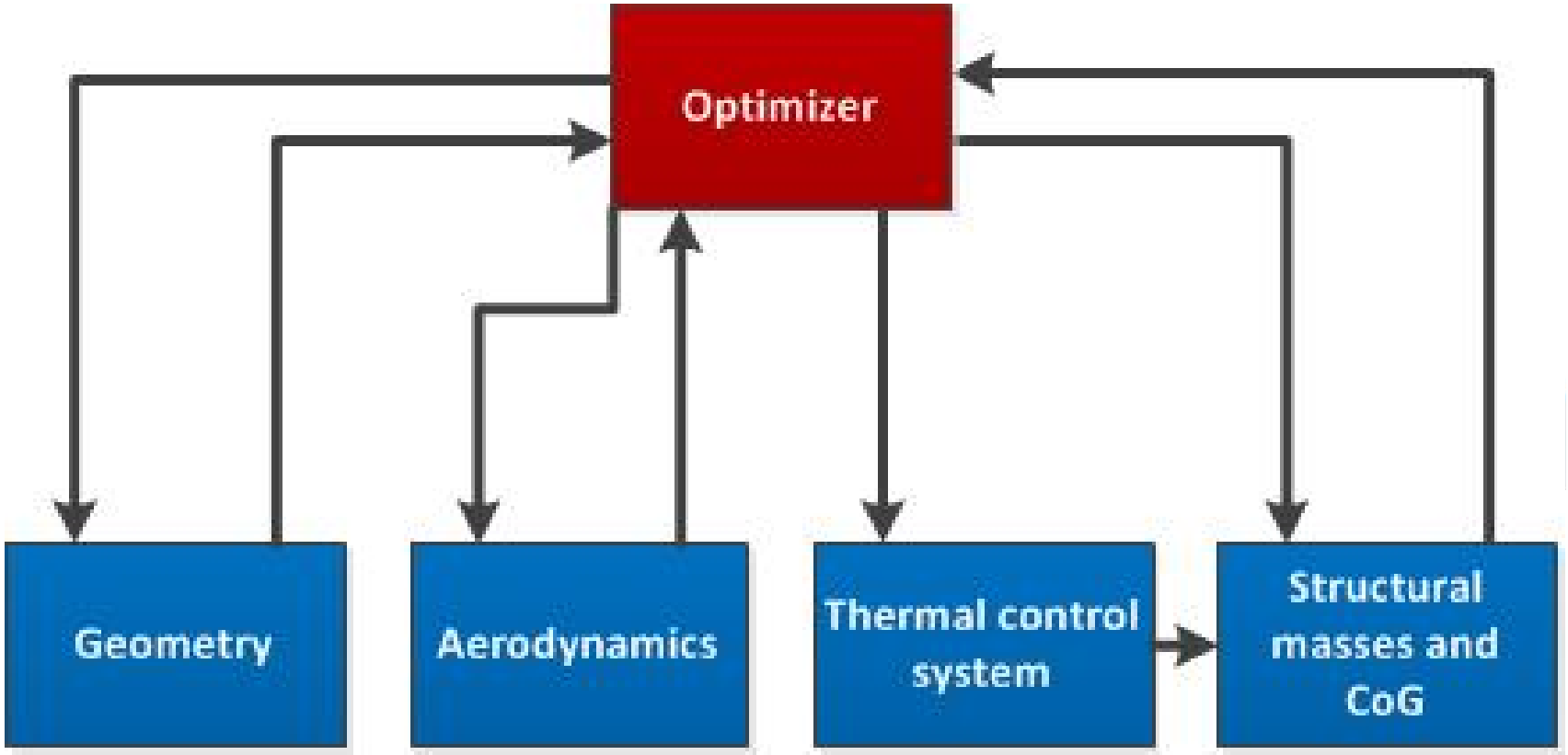


Multidisciplinary Design Optimization: Sequential IDF (Individual Design Feasible)

- **Geometry** (e.g., maximum length or nose radius of the space craft)
- **Aerodynamics** (e.g., lift and drag coefficients)
- **Thermal management** (e.g., the choice or combination of the cooling system and its parameters)
- **Structural sizing** (e.g., the computation of structural masses and center of gravity)

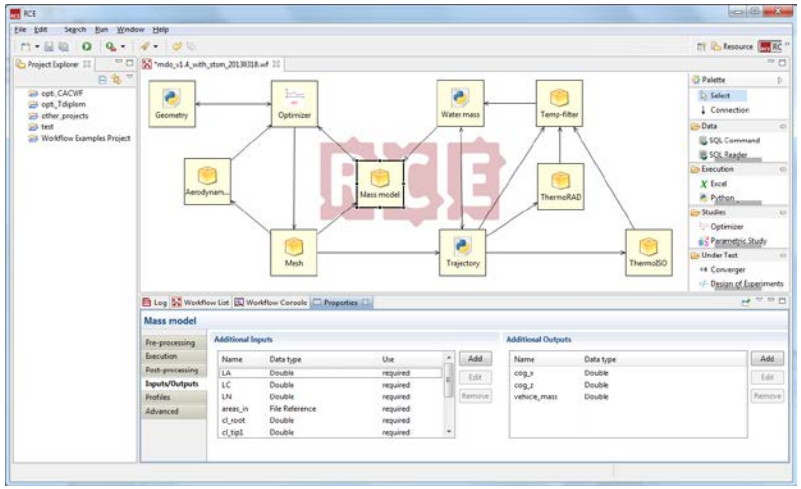


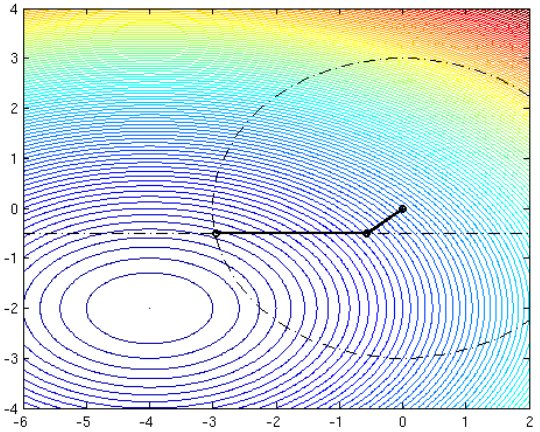
Multidisciplinary Design Optimization: Sequential IDF (Individual Design Feasible)

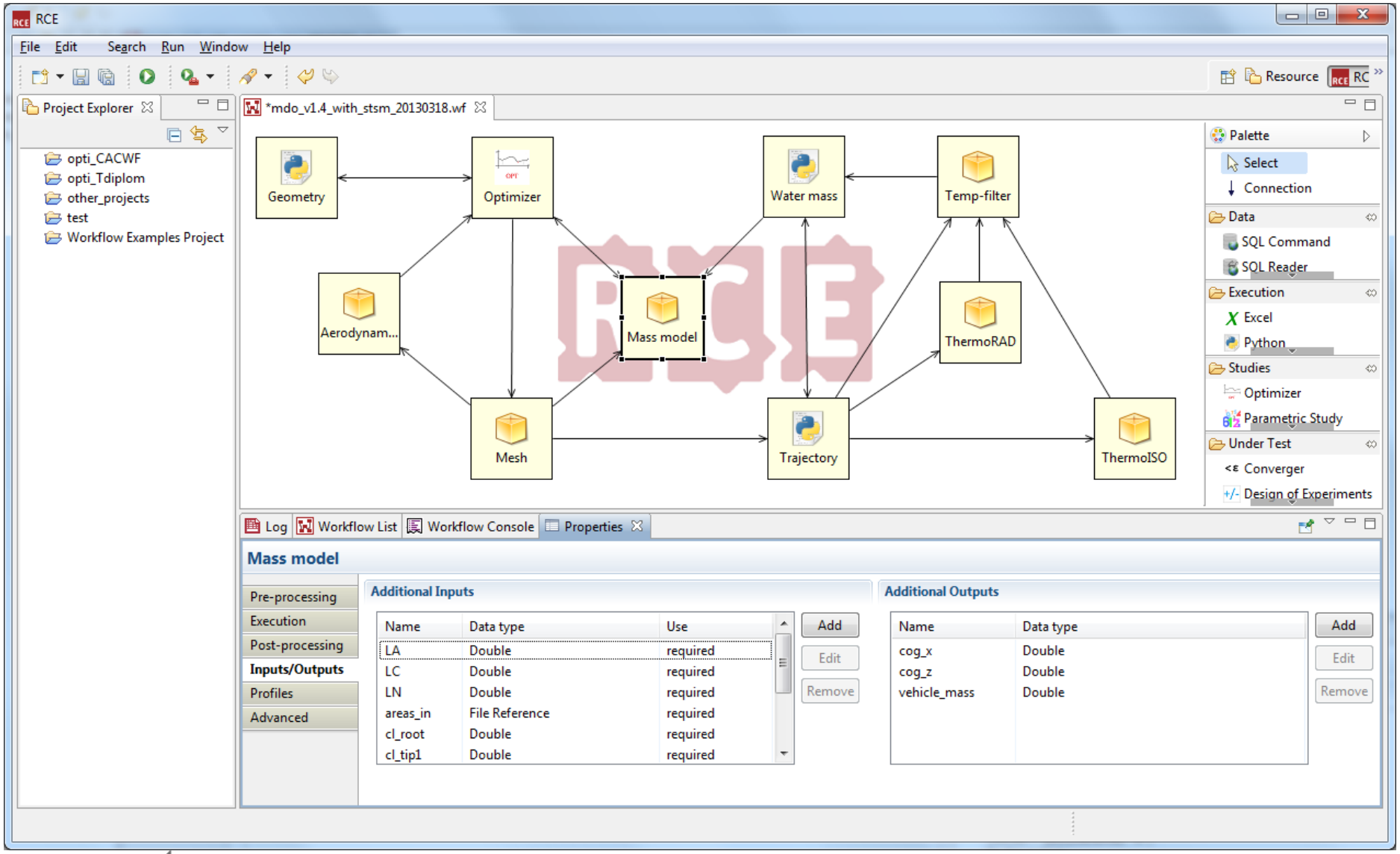


Implementation of a Multidisciplinary Optimization Loop

- Implementation of the design process graph in the software platform **RCE** (remote component environment) coupling tools from different disciplines
- Problem: no derivatives available
- Up to now: use of derivative-free optimizers from toolbox **DAKOTA**
- **Current development:** new algorithm for nonlinear derivative-free constrained optimization
  - Derivative-free trust-region **SQP**-method






RCE
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Temp-filter
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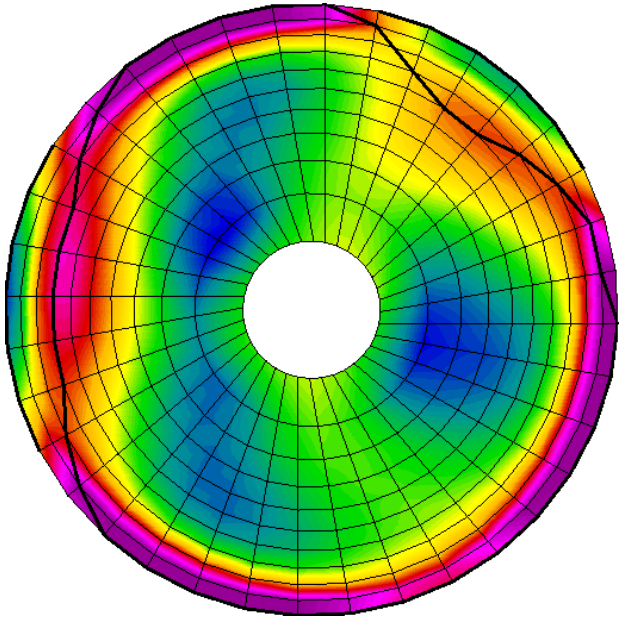
ThermoRAD
Mesh
Trajectory
ThermoISO
Palette
Select
Connection
Data
SQL Command
SQL Reader
Execution
Excel
Python
Studies
Optimizer
Parametric Study
Under Test
Converger
Design of Experiments
Log
Workflow List
Workflow Console
Properties
Mass model
Pre-processing
Execution
Post-processing
Inputs/Outputs
Profiles
Advanced
Additional Inputs
Name Data type Use
LA Double required
LC Double required
LN Double required
areas_in File Reference required
cl_root Double required
cl_tip1 Double required
Add
Edit
Remove
Additional Outputs
Name Data type
cog_x Double
cog_z Double
vehicle_mass Double
Add
Edit
Remove

DLR Project Free-Wake



- Free-Wake code developed at the DLR-Institute of Flight Systems, Rotorcraft department
- Simulates the flow around a helicopter's rotor
- Discretizes complex wake structures with a set of vortex elements
- Models the interaction between wakes and rotor blades
- Based on experimental data (from the international HART-program 1995)
- MPI-parallel implementation in Fortran
- **SC´s task: porting Free-Wake to GPUs using OpenACC**

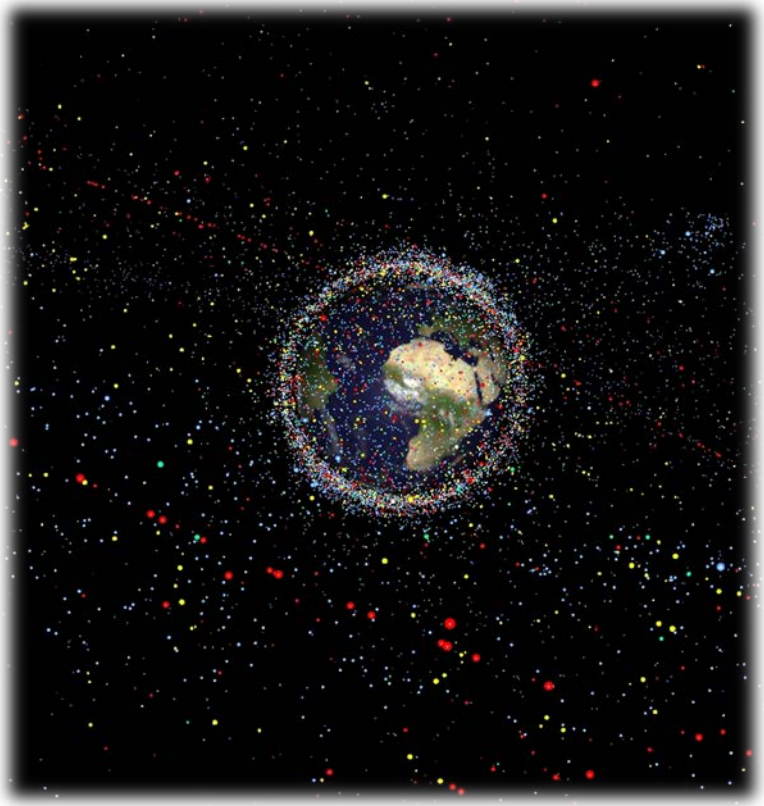
GPU Computing with OpenACC

- Directive based
- Similar to OpenMP
- Explicit data movement between host and GPU (bottleneck!)
- Supported by CAPS-, CRAY- and PGI-compilers (C, C++, Fortran)
- Recently: also supported by gcc

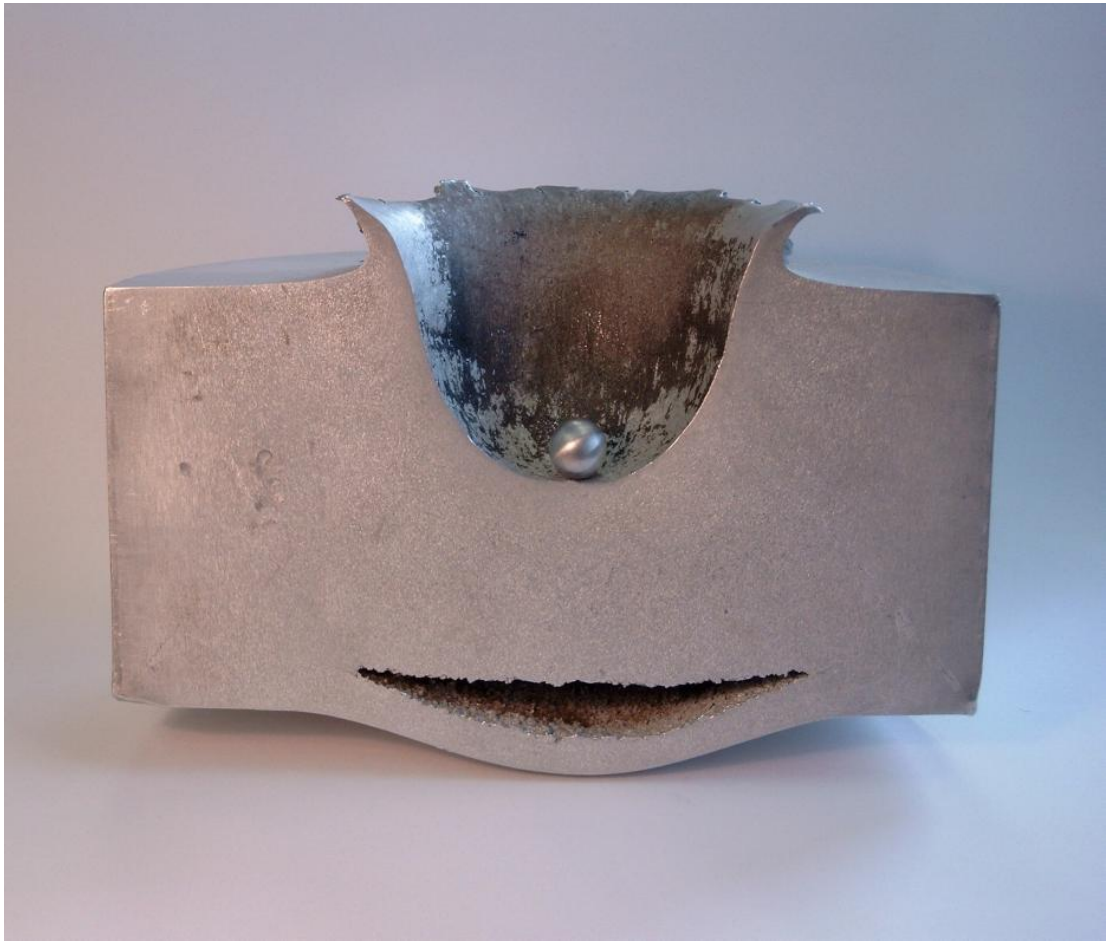
```
program main
   integer :: a(N)
   …
!$acc data copyout(a)
   ! computation on the GPU in several loops:
!$acc parallel loop
   do i = 1, N
      a(i) = 2*a(i)
   end do
!$acc parallel loop
   …
!$acc end data
   ! Now results available on the CPU
   …
end program main
```

DLR Project BACARDI: Backend Catalog for Relational Debris Information

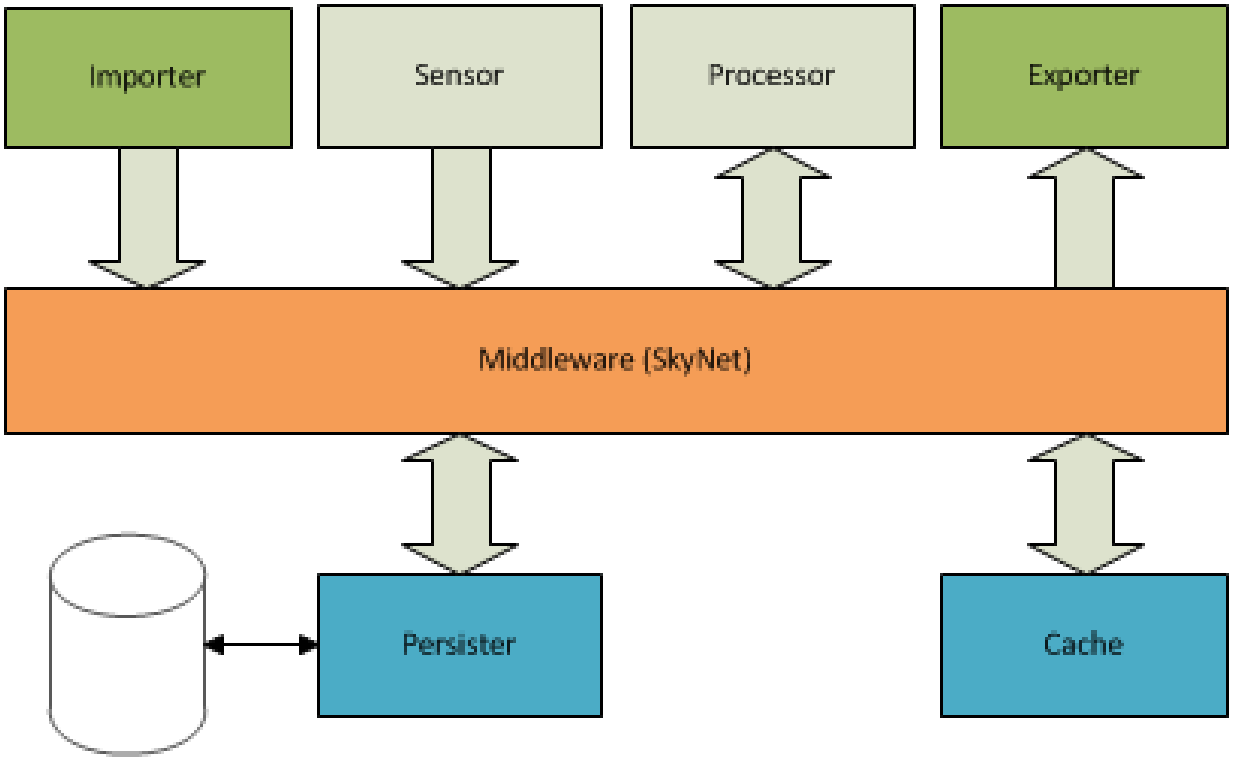
- Increasing number of space debris
  - 26,000 known objects > 10 cm
  - Objects > 1 cm problematic
- Current capabilities at DLR, GSOC
  - Orbit propagation
  - Collision detection
  - Observation planning and correlation
- Composition of a DLR database
  - TLE unprecise
  - Precise data restricted



Big Damage through Small Debris Particles



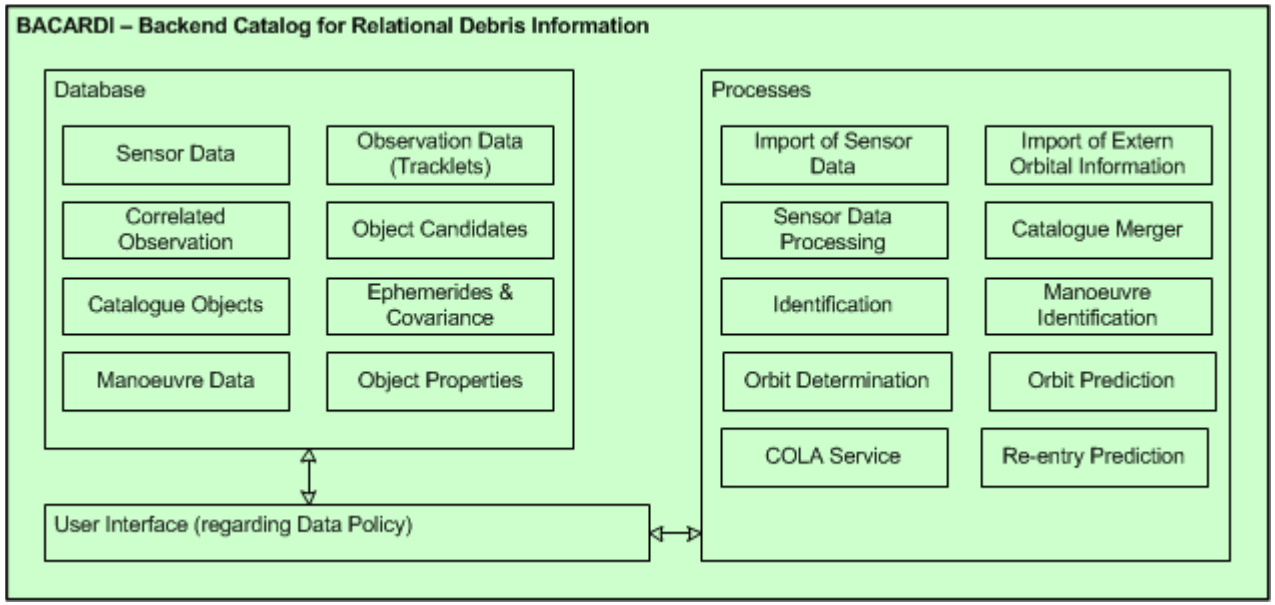
BACARDI Architecture Layers



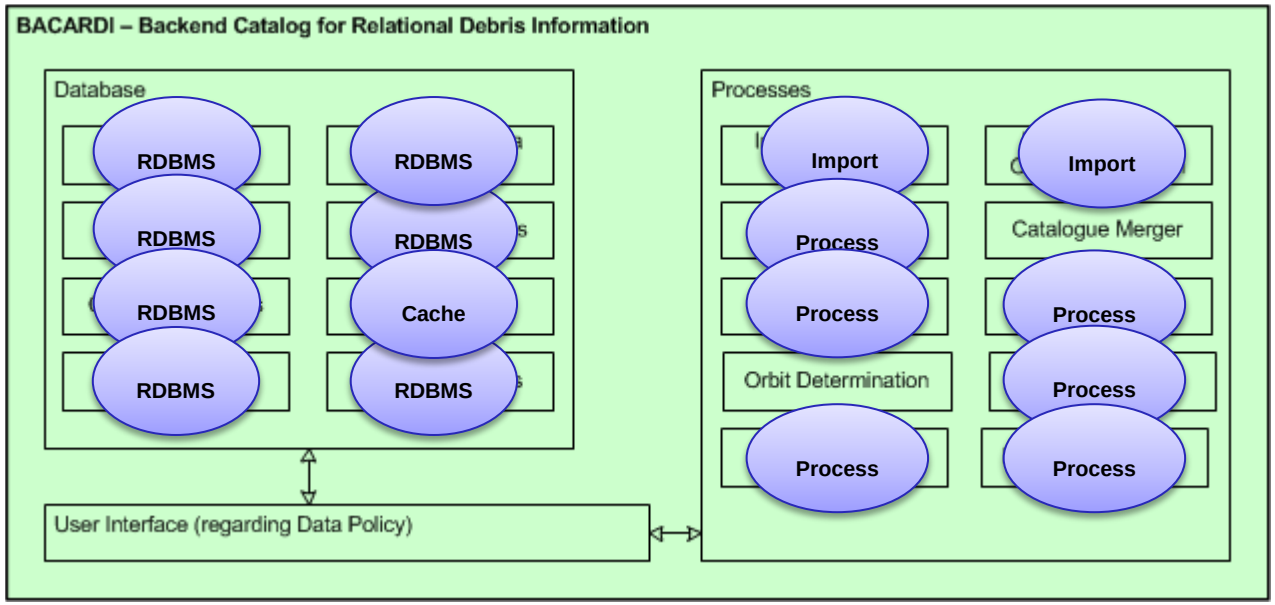
HPC technology and methods for

- processing of orbit data from sensor data
- processing of correlation operations with the data base

System Analysis (1)

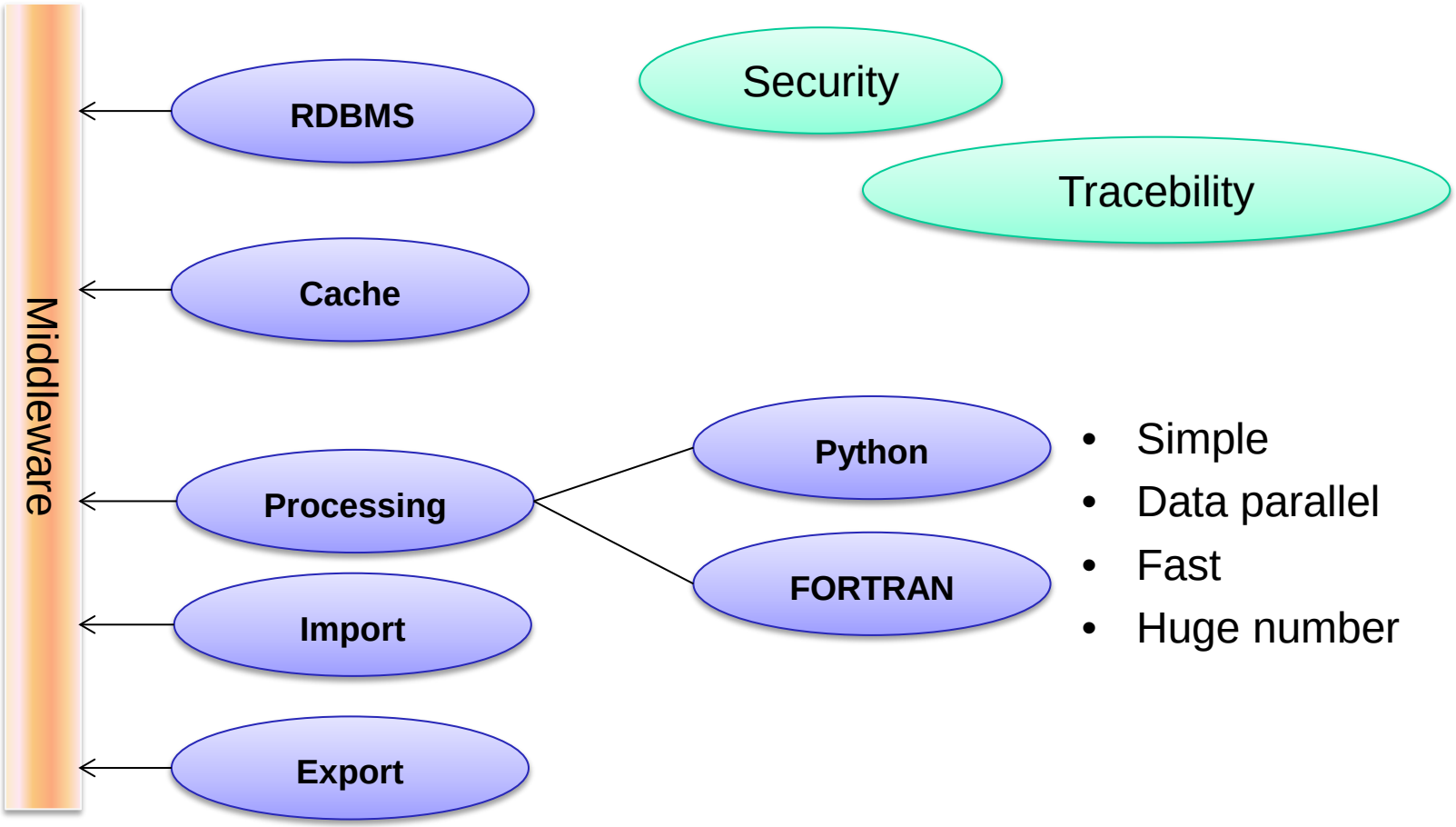


System Analysis (1)



Goal: scalability to 1,000,000 objects

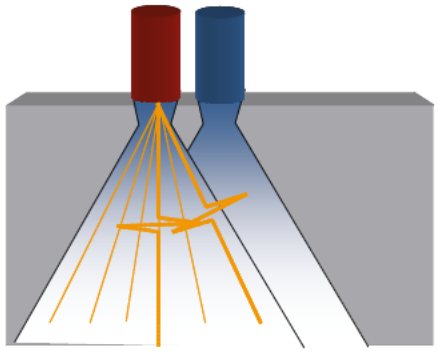
System Analysis (2)



- Simple
- Data parallel
- Fast
- Huge number

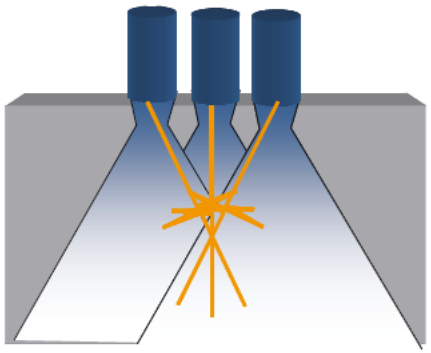
BMBF Project HPC-FLiS: An HPC Framework for the Solution of Inverse Problems

- Applications: material testing and medical diagnostics
- Industry partner: SIEMENS Corporate Technology
- SC´s task: software test
  - Unit tests
  - System tests
    - HPC specific quality tests: scalability, communication efficiency
    - Use of HPC profiling and performance analysis tools



Ultrasonic Inspection Setup

Result of conventional inspection
(Image of Cross Section = „B-View“)



Desired: One focused indication instead of a crescent shaped indication
→ Each location is focused individually by calculation („Synthetic probe“)

DLR

Questions?


SOFIA
STRATOSPHERIC OBSERVATORY FOR INFRARED ASTRONOMY
NASA
DLR
N747NA