



High Performance Computing

Research activities within Satanas



High Performance Computing at LaBRI

- The **SATANAS** LaBRI-CNRS Team = two INRIA projects
 - **Runtime (R. Namyst)**
 - High Performance Runtime Systems for Parallel Architectures
 - **Scalapplix (J. Roman)**
 - Algorithms and Methods for Grand Challenge Applications
- **Application domain = High Performance Simulations**
 - Seismology, molecular dynamics, laser plasma interaction, combustion, fluid flow, nuclear simulation...
- **Main partners**
 - CEA/DAM, EDF, IFP, Total, Bull, Myricom



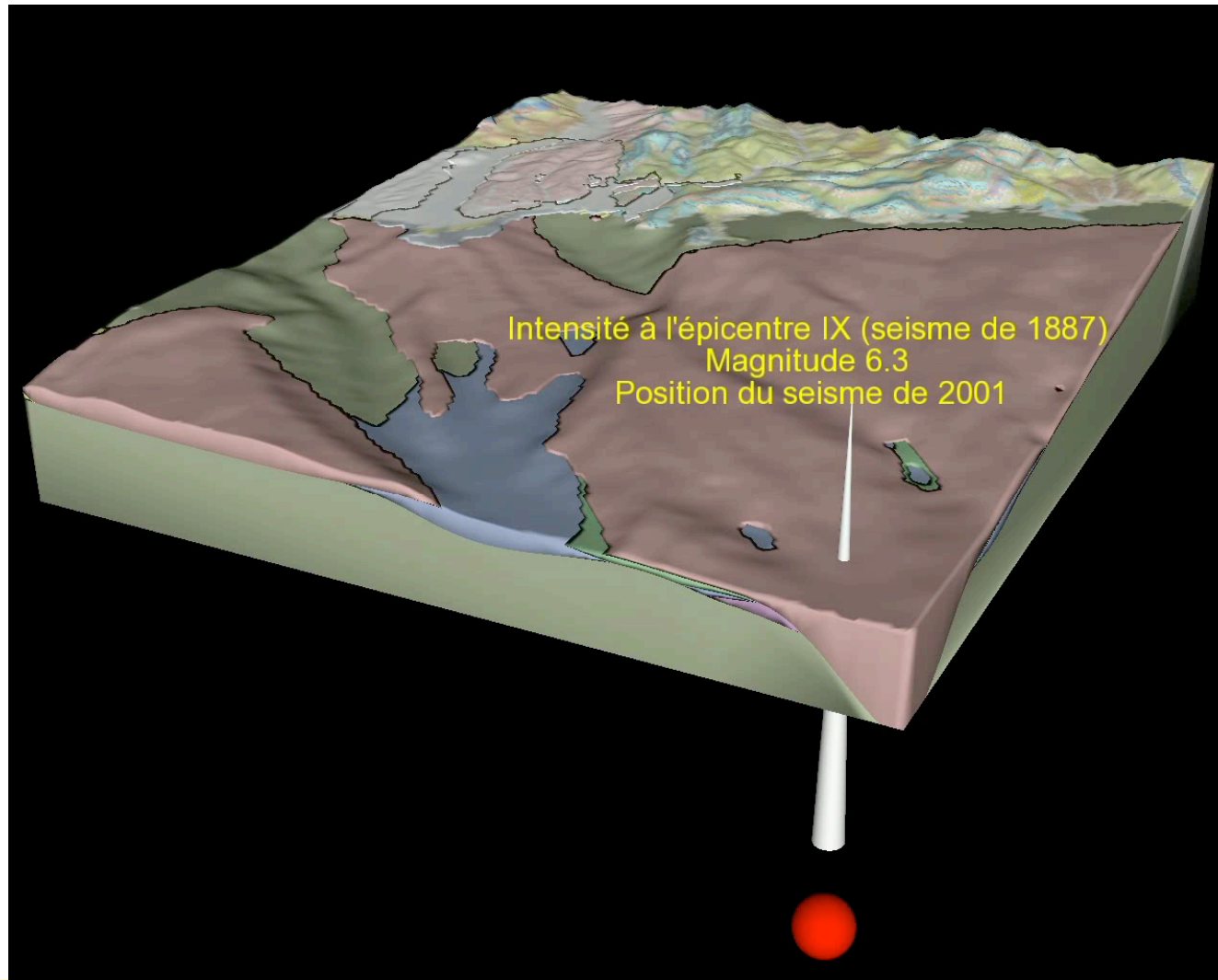
Falcon 7X (Dassault)

- 100% Computer Assisted Design





Seismic simulation





Target machines = parallel computers

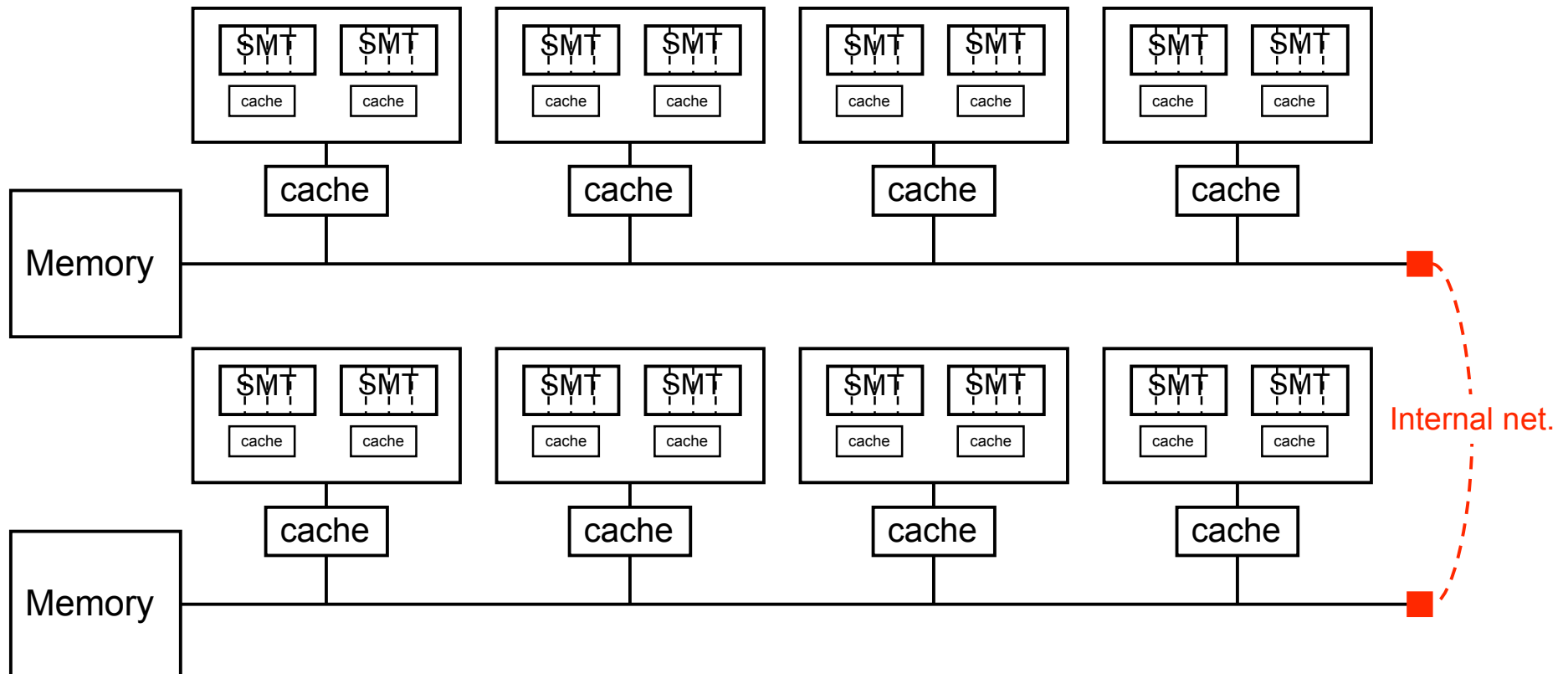
- Parallel computers
 - Typically many “off the shelf” processors...





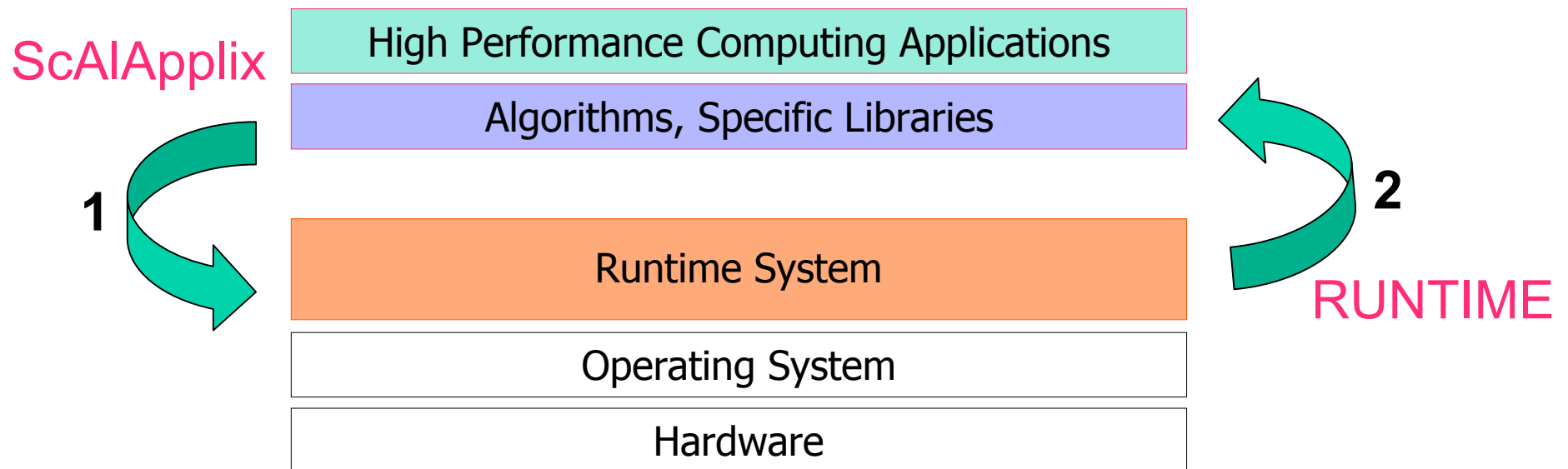
...organized in a very complex way!

- Parallel architectures are going increasingly hierarchical





Algorithms, methods and runtime systems for HPC



1 : give directives and hints about scheduling, communication schemes

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2 : provide high level abstractions to enhance “portability of performance”



Keywords

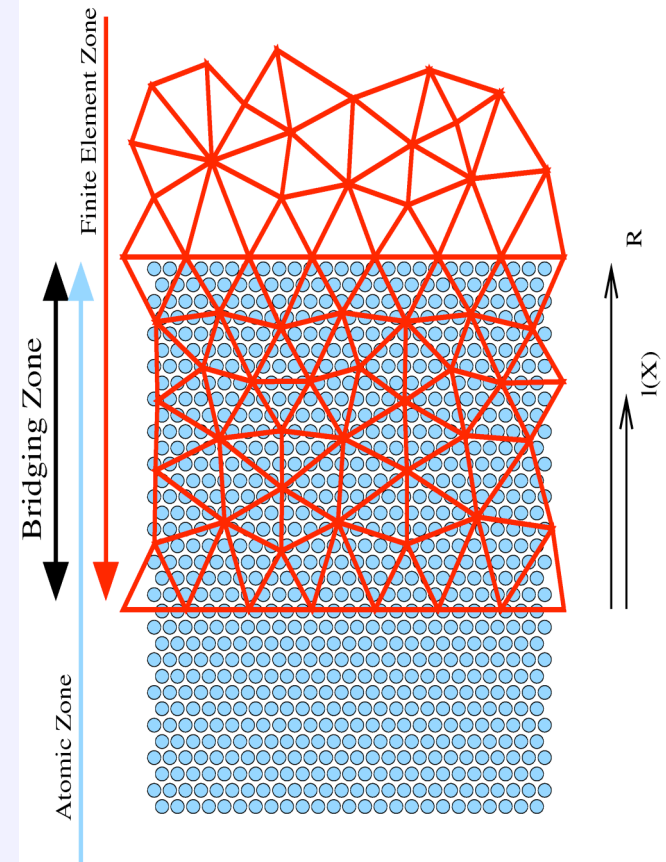
- Parallel algorithms
- Code-coupling frameworks
- Domains-specific libraries

- Parallel languages
- Communication over high speed networks and grids
- Thread scheduling & memory management over hierarchical architectures



Multi-scale approach for simulating materials

- **Mixing molecular dynamics with finite elements...**
 - Adapted model to exchange information between two different physical models (continuum elasticity VS. molecular dynamics)
- **Issues**
 - Different time/length scales
 - 100 nm³ of silicon crystal contains near billion atoms...
 - Need for smart data handling at the interface
 - Domain decomposition implies redistributing communication
 - Load balancing





Crack propagation application within an argon crystal

• Simulation

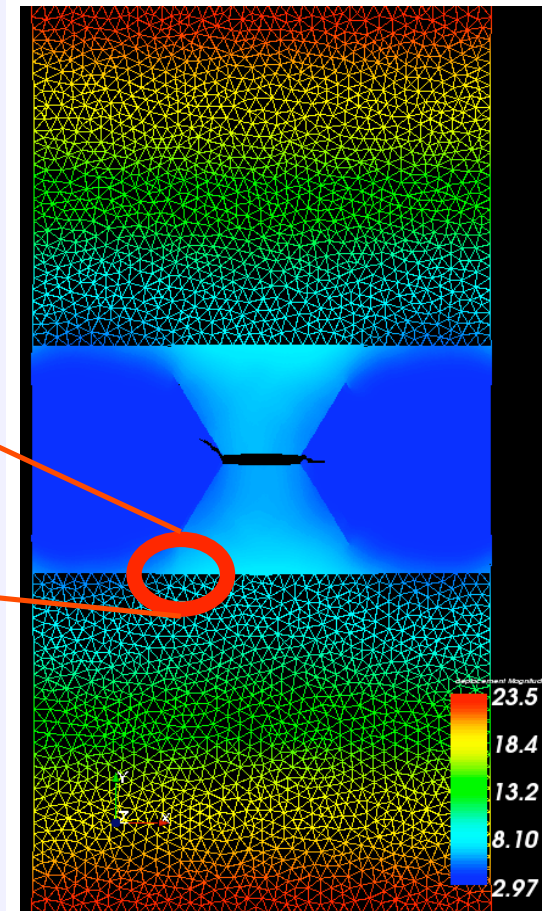
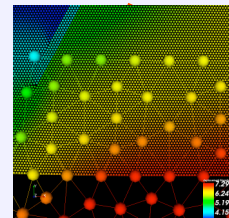
- 1/2 Million of Atoms, 100 processors – Cluster @ Bordeaux
- 5 000 Finite Elements, 20 processors – Cluster @ Sophia
- Visualization, 4 processors – Cluster @ Bordeaux

• Steering and Online Visualization

- Online visualization of intermediate results
- Parameter modifications on-the-fly
 - boundary conditions, checkpoint frequency, ...
- Advanced filters to plot relevant information

• Ongoing work

- Improving the physical model of the coupling
- Improving the communication volume by advanced mesh partitioning
- Use of MPICH/Madeleine to speed up communication over Grid'5000





Computational Steering

- **Steering of Parallel Numerical Simulations**

- Computational steering as a more interactive approach than batch mode
- Online visualization of intermediate results (monitoring)
- Change simulation parameters or data on-the-fly (steering)

- **Keypoints**

- Coupling of parallel simulations and parallel visualization systems
- Parallel data redistribution to avoid communication bottleneck

