Interactive Biomedical Problem Solving on the Grid:

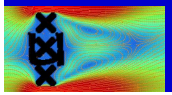
Peter Sloot

sloot@science.uva.nl

Computational Science

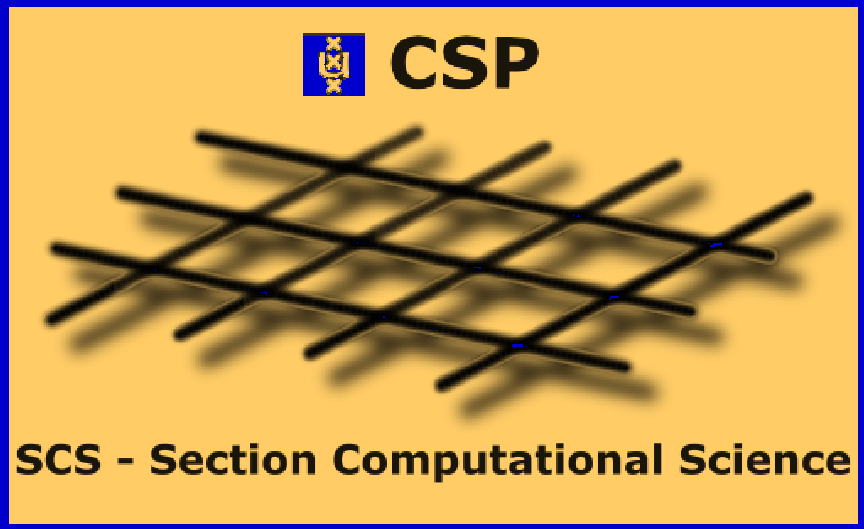
http://www.science.uva.nl/research/scs

University of Amsterdam, The Netherlands



The CrossGrid Project
Information Society

HealthGRID


CSP
SCS - Section Computational Science

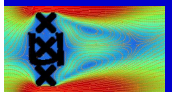
A prototypical killer application

The Grid is not about Science… it is about Engineering…

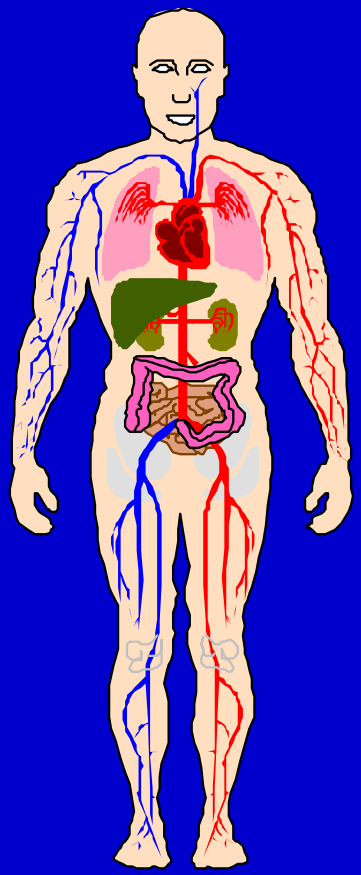
The science is in the application…
-lots on High Energy Physics etc… but…

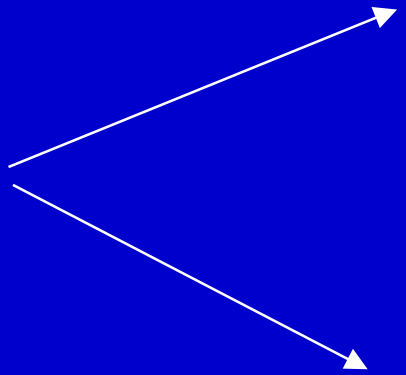
-let's forget the 'Rocket Science' for a while

☺



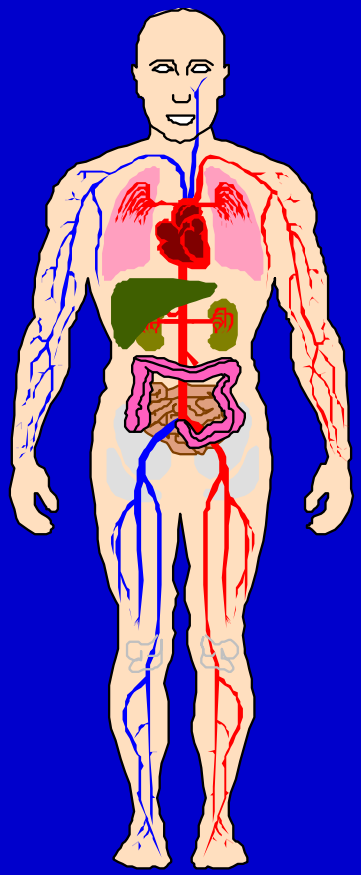
Changing the Paradigm

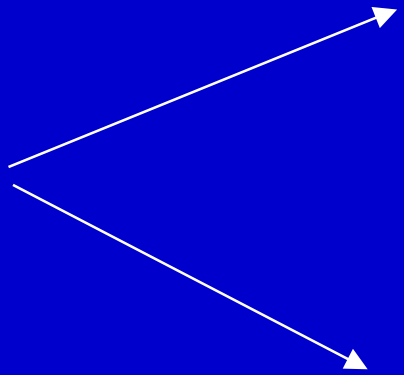


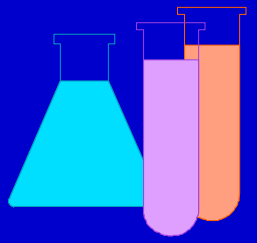


In Vivo

Changing the Paradigm



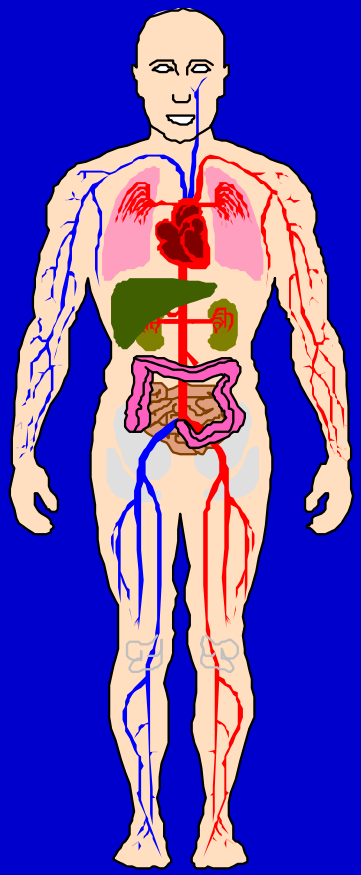




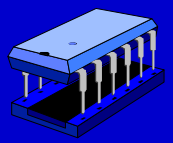
In Vitro

In Vivo

Changing the Paradigm



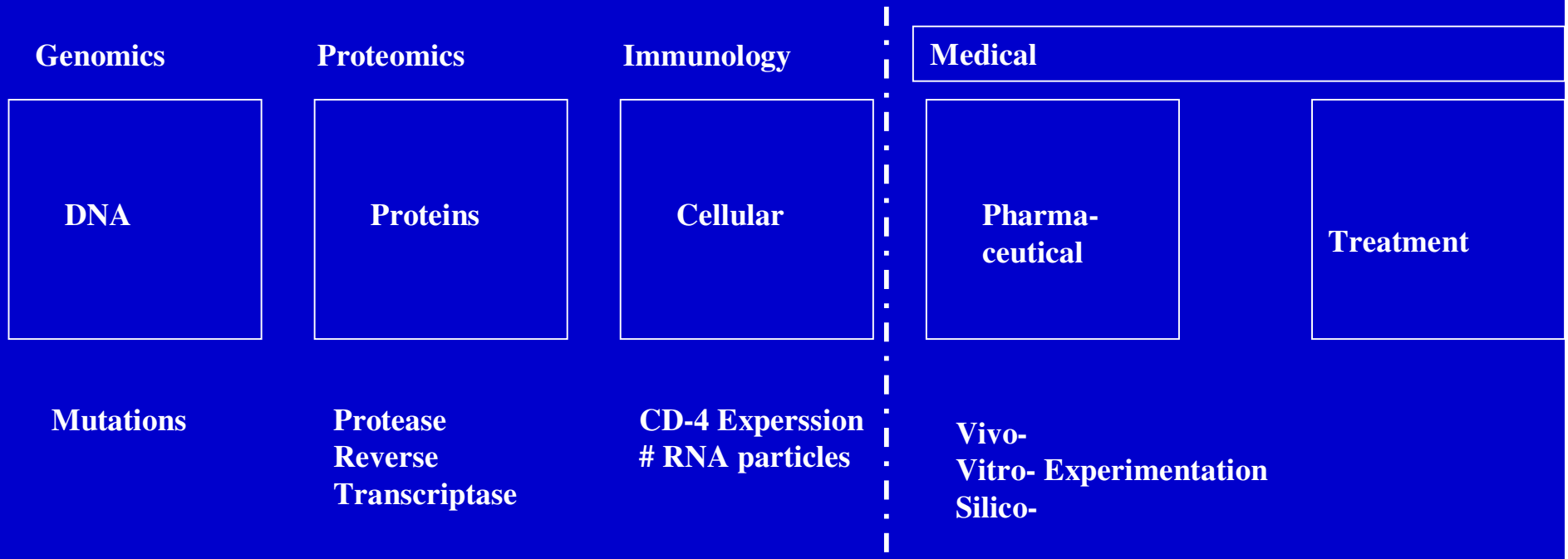
In Vitro



In Vivo

In Silico

From Molecule to Man…



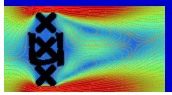
From Molecule to Man…Cont

- **First Principle Modeling**
  - **Genetic Regulatory Networks**
  - **Metabolic Networks**
  - **Immunological Networks**
  - **… Silicon Cell**

Analytic
Molecular Dynamics
Monte Carlo
Mesoscopic

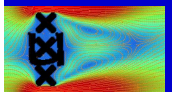
- **Hierarchical data Modeling**
- **G-P-M & Patient Dbases**

AI – GA's, NN's, Fuzzy L.



From Molecule to Man…PSE/G

- **Mesoscopic Simulation → High Performance Computing**
- **Parameter Space Exploration → High Throughput Computing**
- **Data Disclosure → Dbase Federation and Integration**
- **Data Fusion → Hierarchical Parameter Transfer**
- **Access → Visualization/VR && Roaming &&PDA**

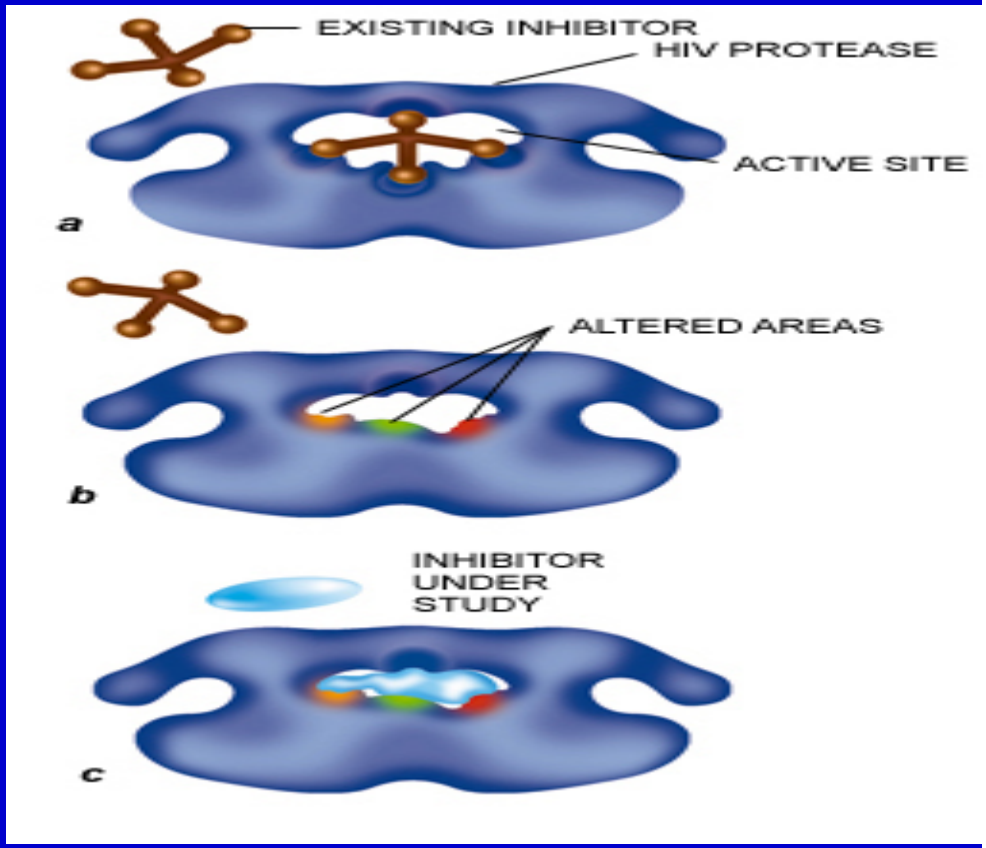


Two Projects

5th International Conference on Cellular Automata for Research and Industry, ACRI 2002, Geneva, Switzerland, October 9-11, 2002. Proceedings, in series *Lecture Notes in Computer Science*, vol. 2493, pp. 282-293. October 2002.

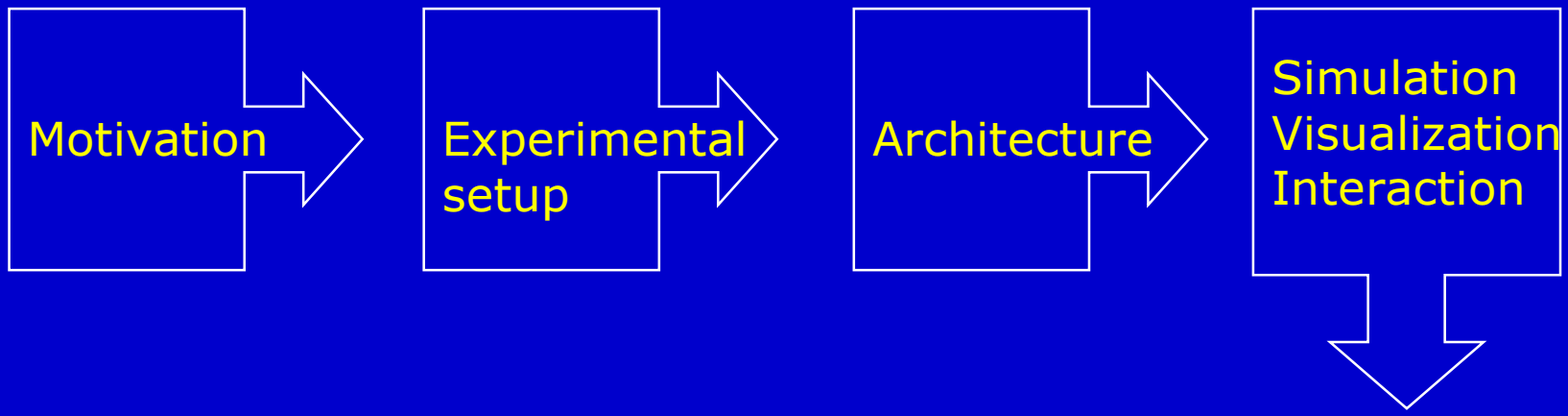
Computational Science - ICCS 2003, Melbourne, Australia and St. Petersburg, Russia, Proceedings Part I, in series *Lecture Notes in Computer Science*, vol. 2657, pp. 125-135. Springer Verlag, June 2003. ISBN 3-540-40194-6.

Abdominal Aortic Aneurysm

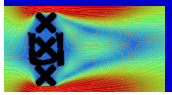


HIV Expert System

Ariadne's red rope



Status: Some 'hot' results



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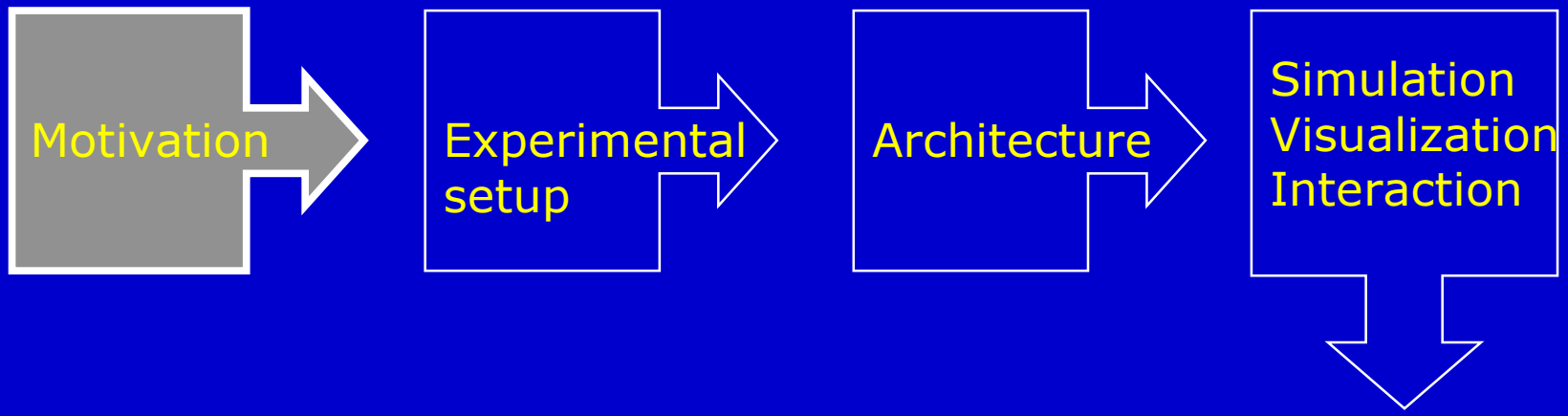

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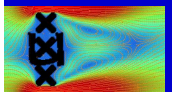
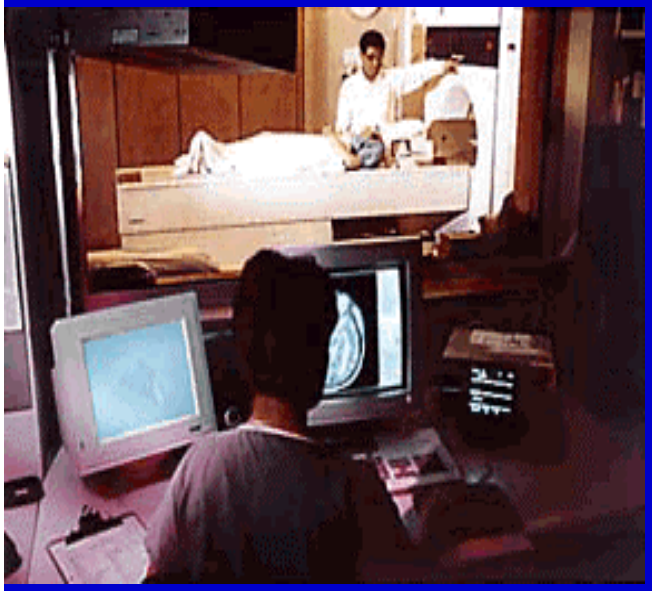


Current Situation

Diagnosis & Planning

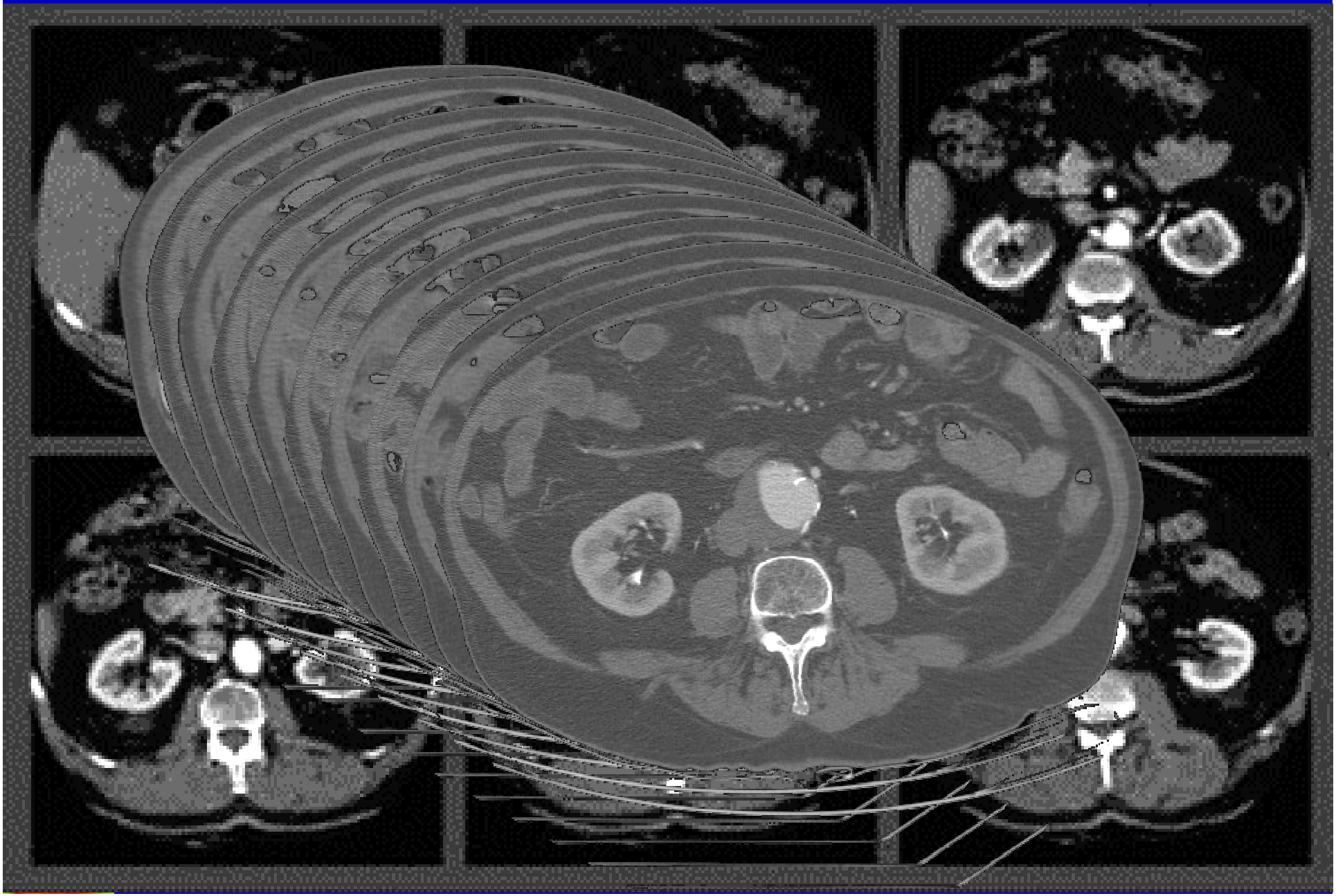
Treatment



Observation

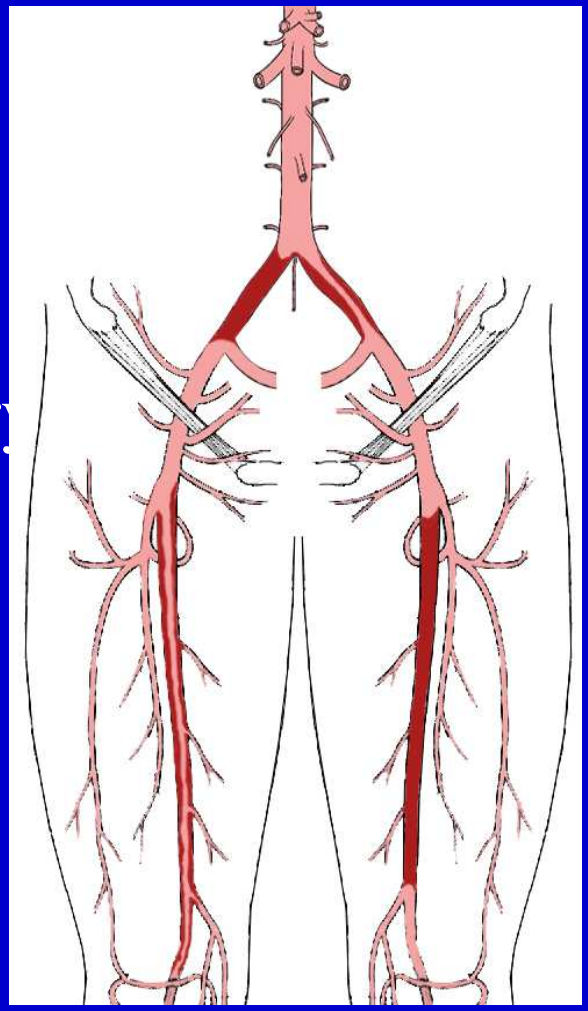
Nature March 2002

Salami...

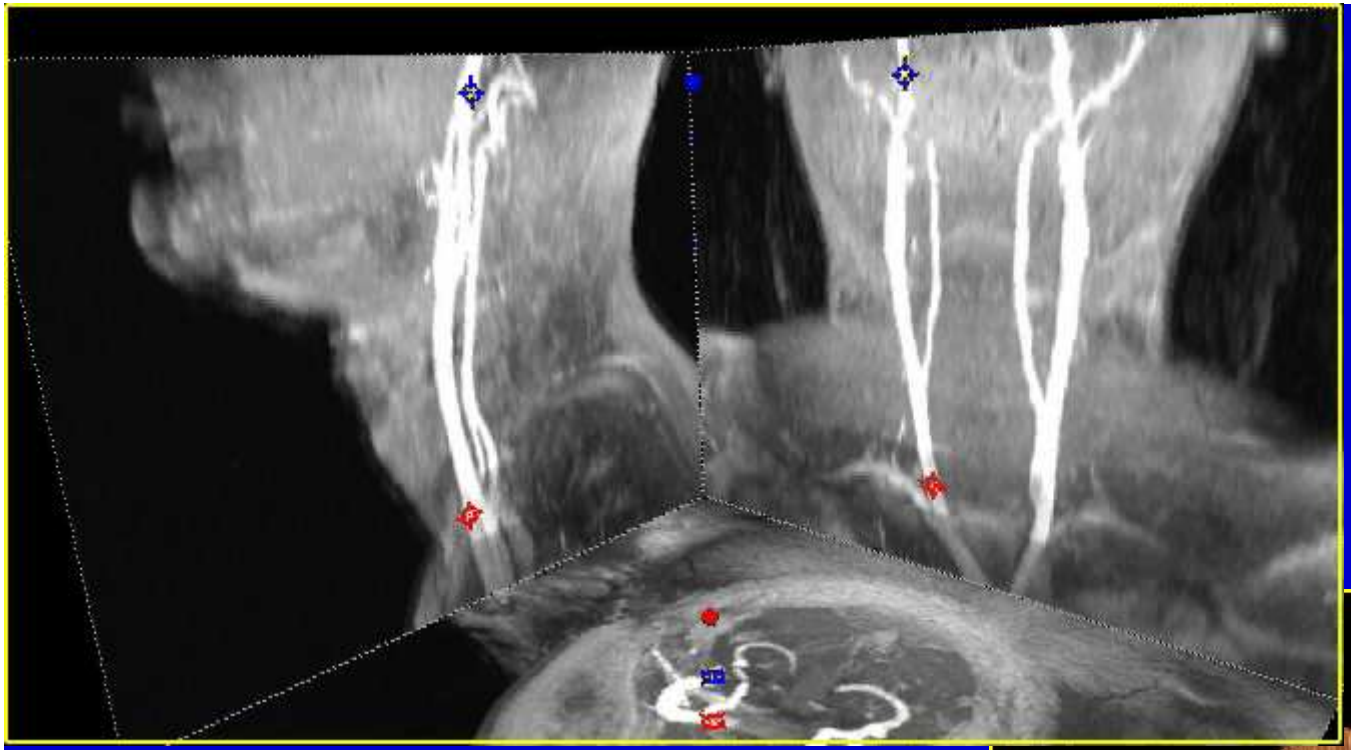


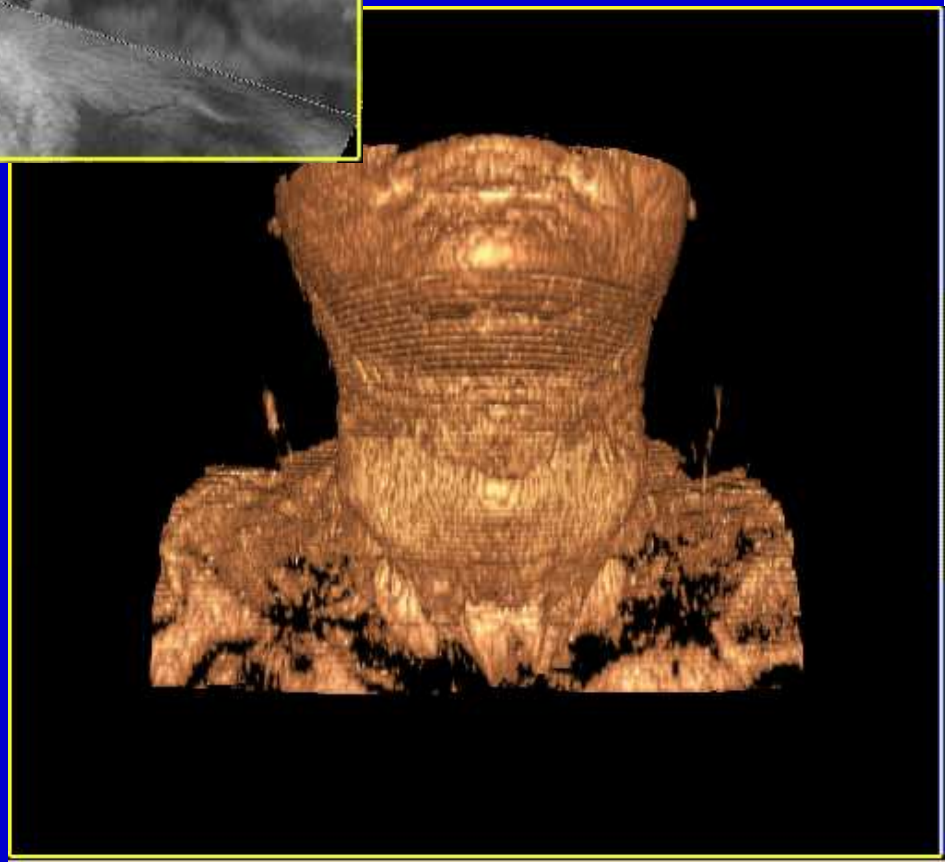
Example: Proof is in the pudding...

- Diagnostic Findings
  - Occluded right iliac artery
  - 75% stenosis in left iliac artery
  - Occluded left SFA
  - Diffuse disease in right SFA

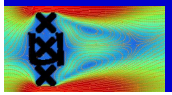


Computer Assisted Radiology and Surgery (Excerpta Medica, International Congress Series 1230), pp. 938-944. Elsevier Science B.V., Berlin, Germany, June 2001.



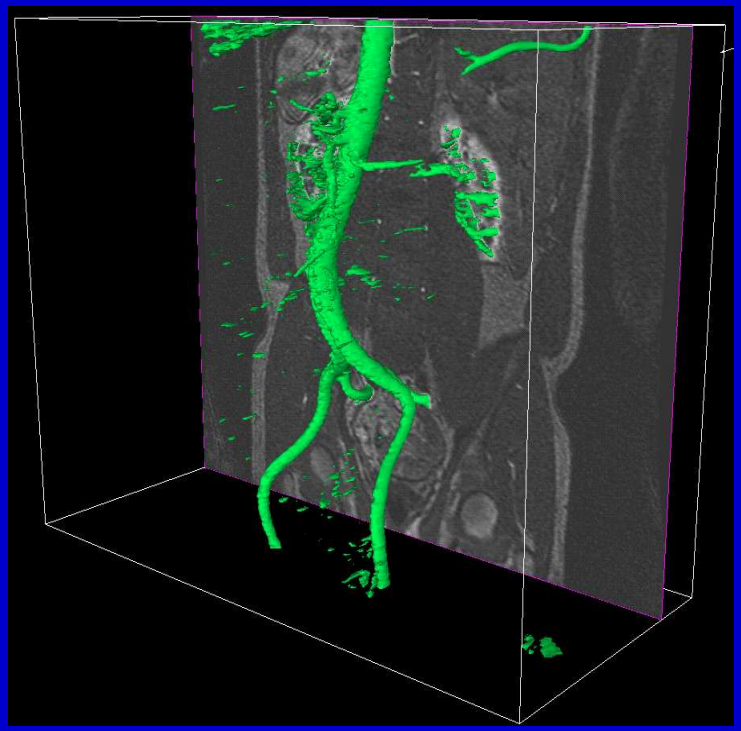


Segmentation Through Wave Propagation

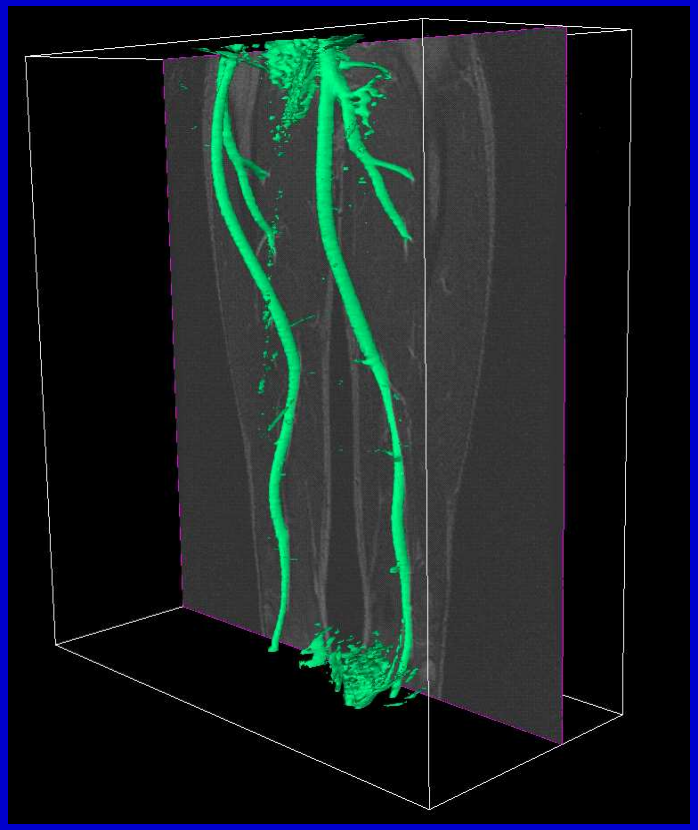


Peter Sloot: Computational Science, University of Amsterdam.

Methods - MR Imaging

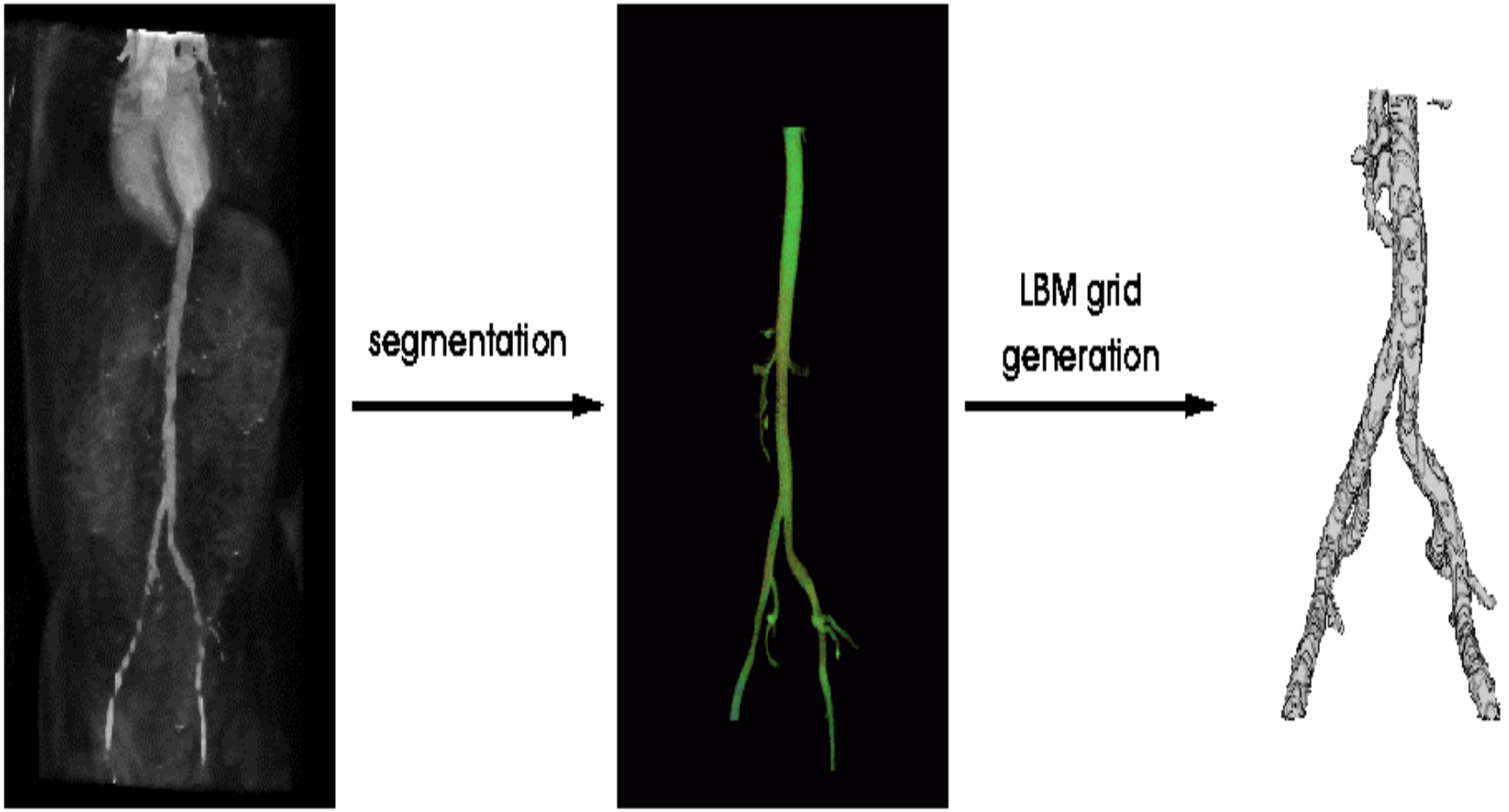


MR Scan of Abdomen

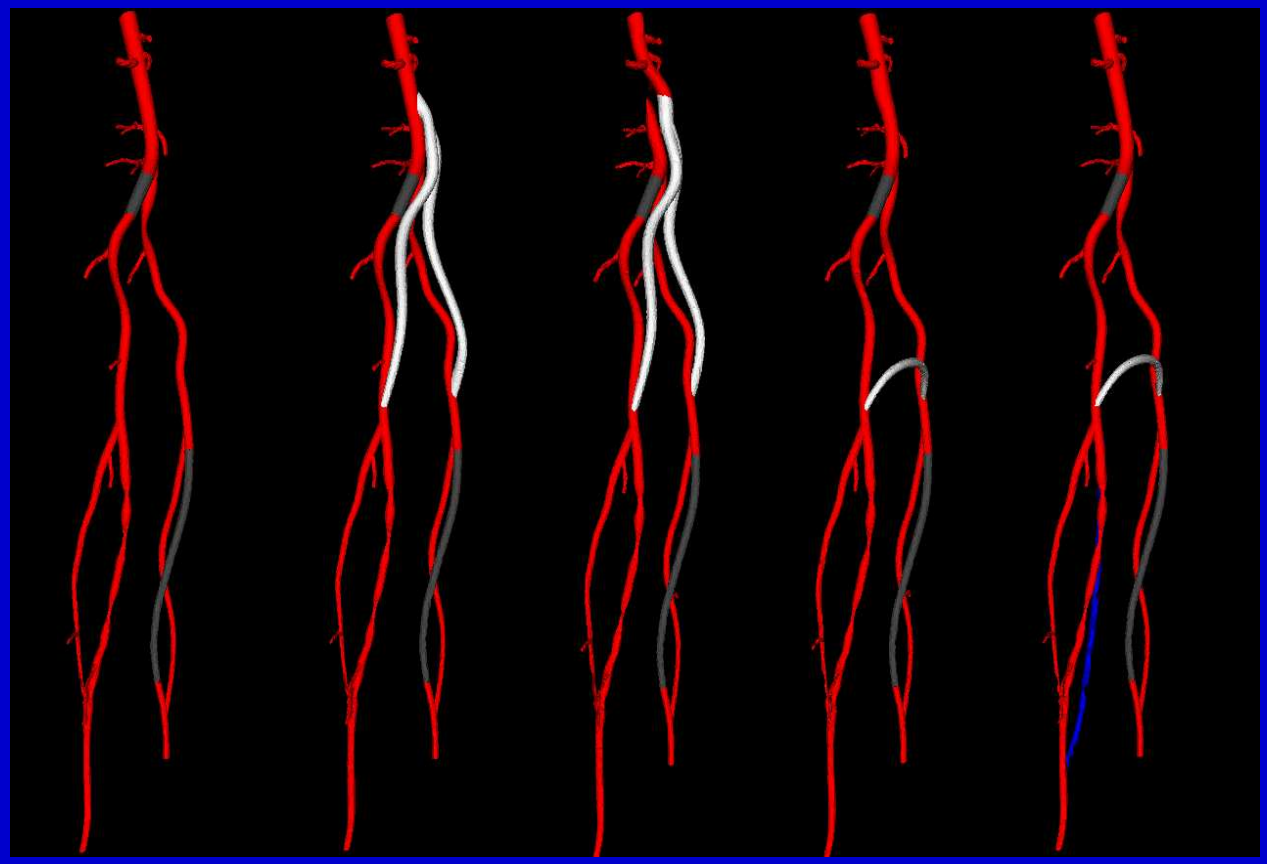


MR Scan of Legs

Methods - Geometric Models



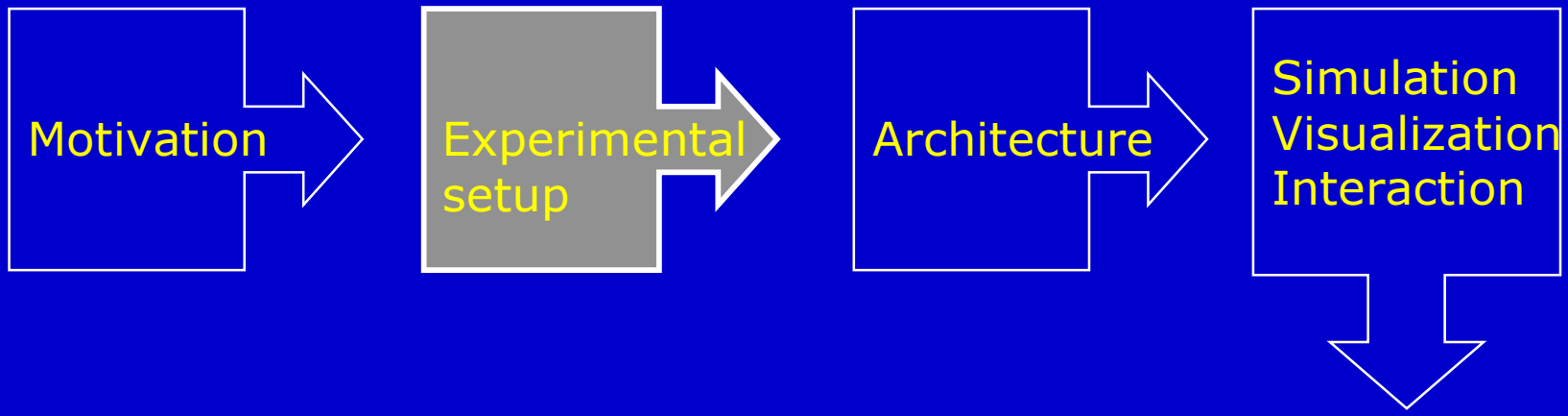
Alternate Treatments



Preop | AFB w/ E-S Prox. Anast. | AFB w/ E-E Prox. Anast. | Angio w/ Fem-Fem | Angio w/ Fem-Fem & Fem-Pop

Courtesy Prof. C. Taylor

Ariadne's red rope



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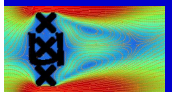
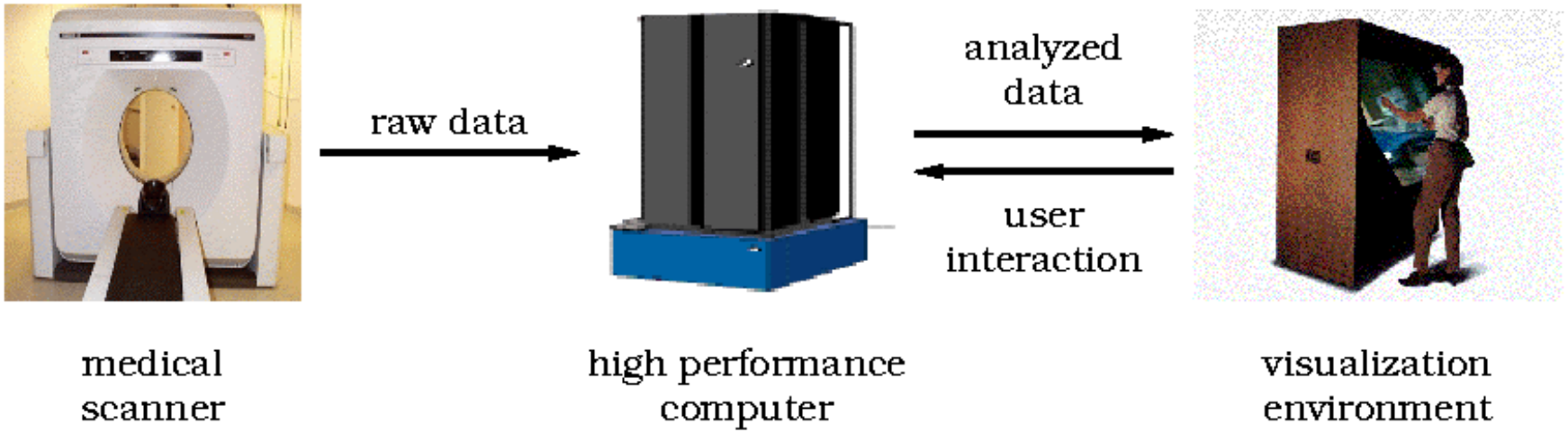


Experimental set-up

Advanced Infrastructures for Future Healthcare, pp. 275-282. IOS Press, 2000.

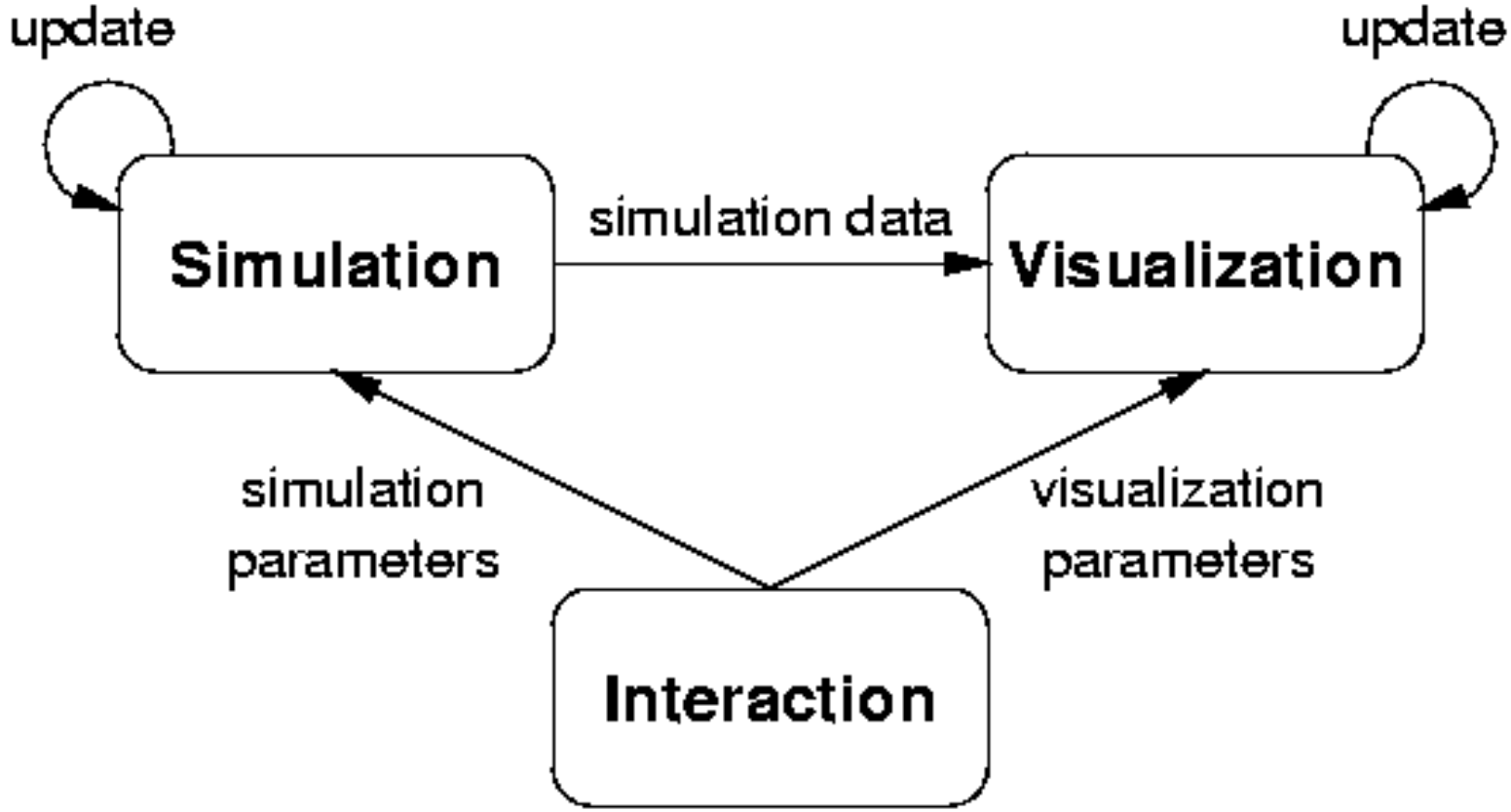


MRI, PET

Monolith, Cluster

Cave, Wall, PC, PDA

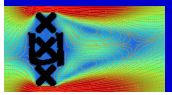
Design Considerations



Provoking a bit…

Progress in natural sciences comes from taking things apart ...

Progress in computer science comes from bringing things together...



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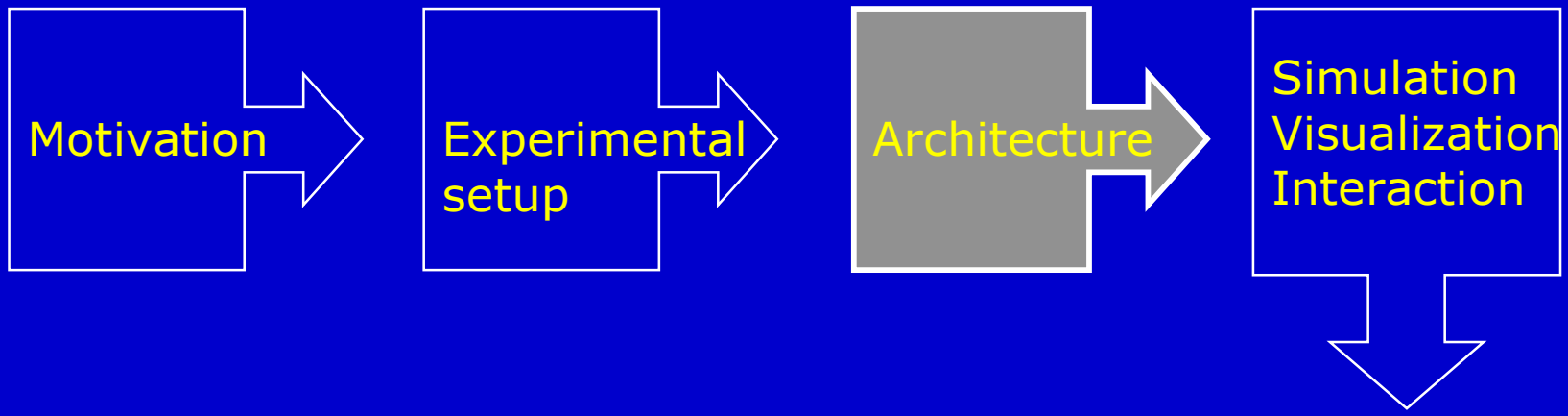

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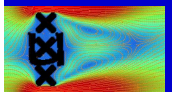
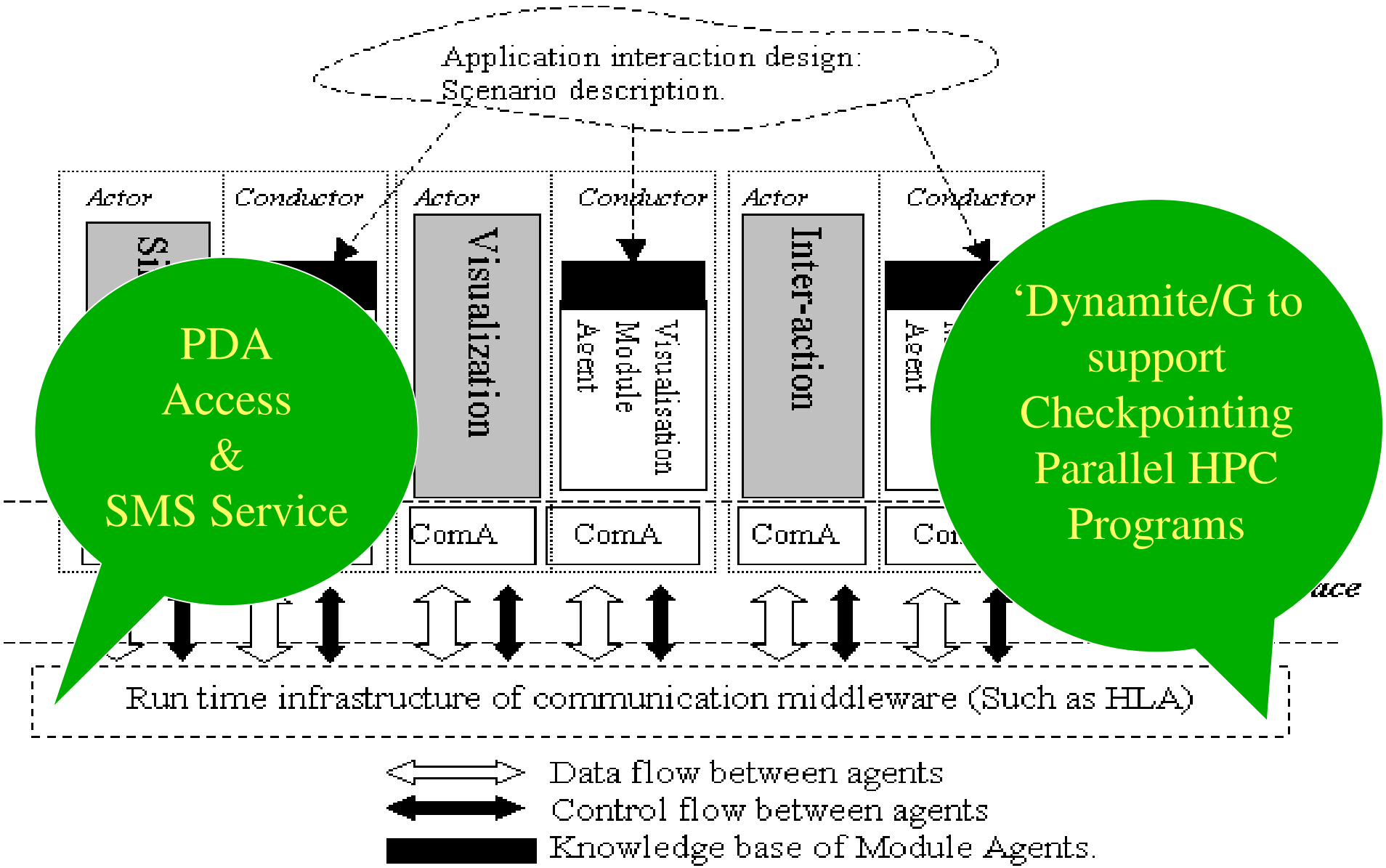


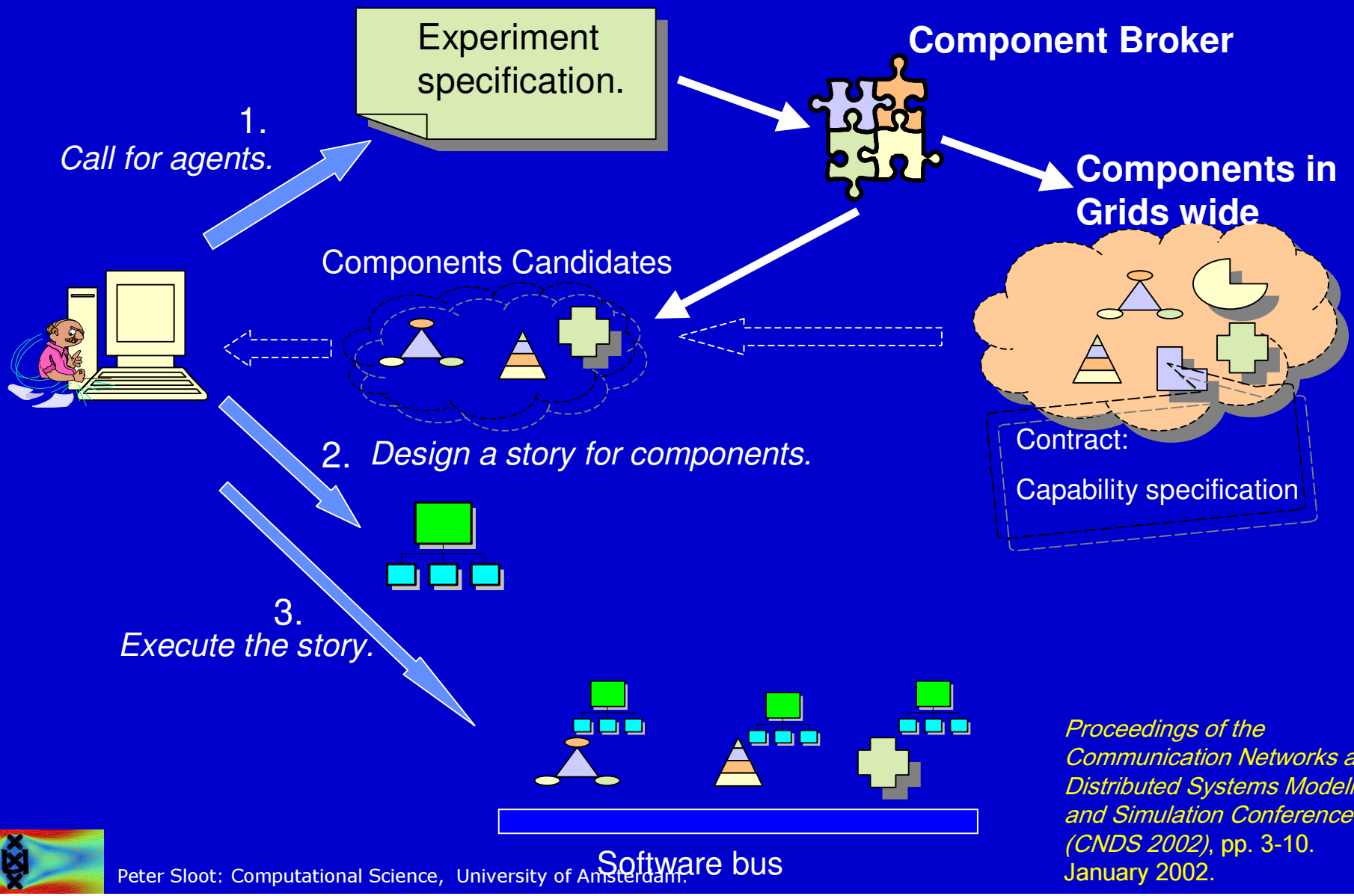
PSE/G Architecture

Concurrency and Computation: Practice and Experience, ((Special Issue on Grid Computing Environments)) vol. 14, pp. 1313-1335. John Wiley and Sons, 2002.

Lecture Notes in Computer Science, vol. 1971, pp. 203-213. Springer-Verlag, December 2000

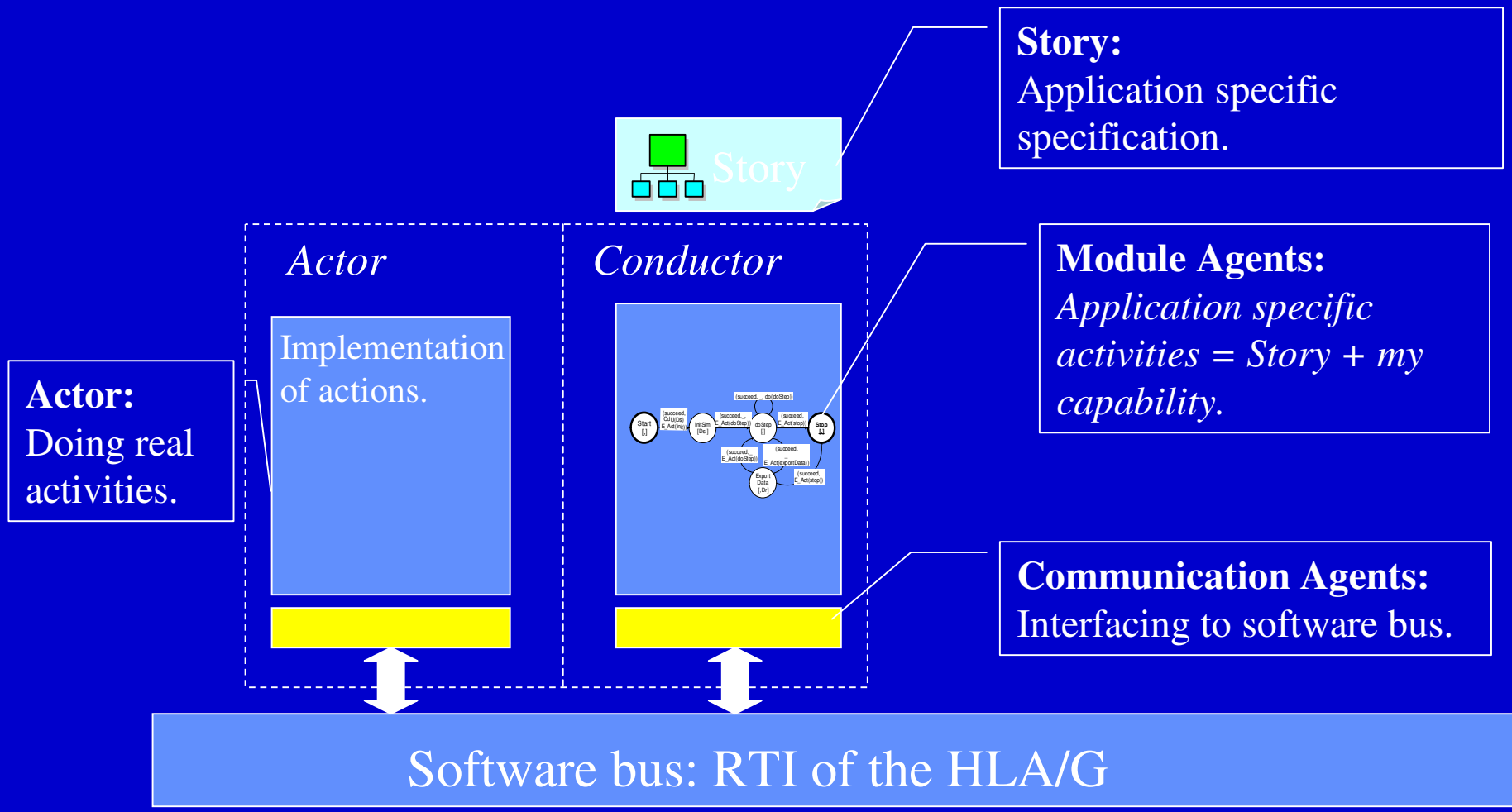


Building the workflow



Proceedings of the Communication Networks and Distributed Systems Modeling and Simulation Conference (CNDS 2002), pp. 3-10. January 2002.

Actors setting the scene



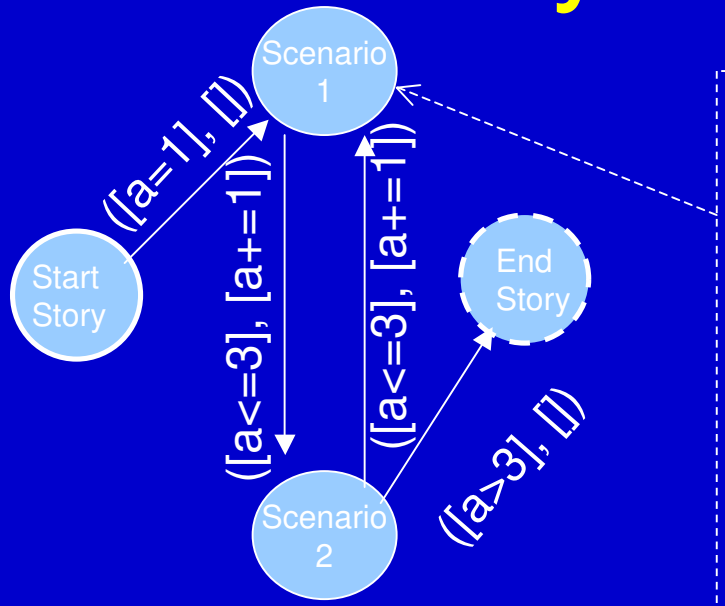
Story:
Application specific specification.

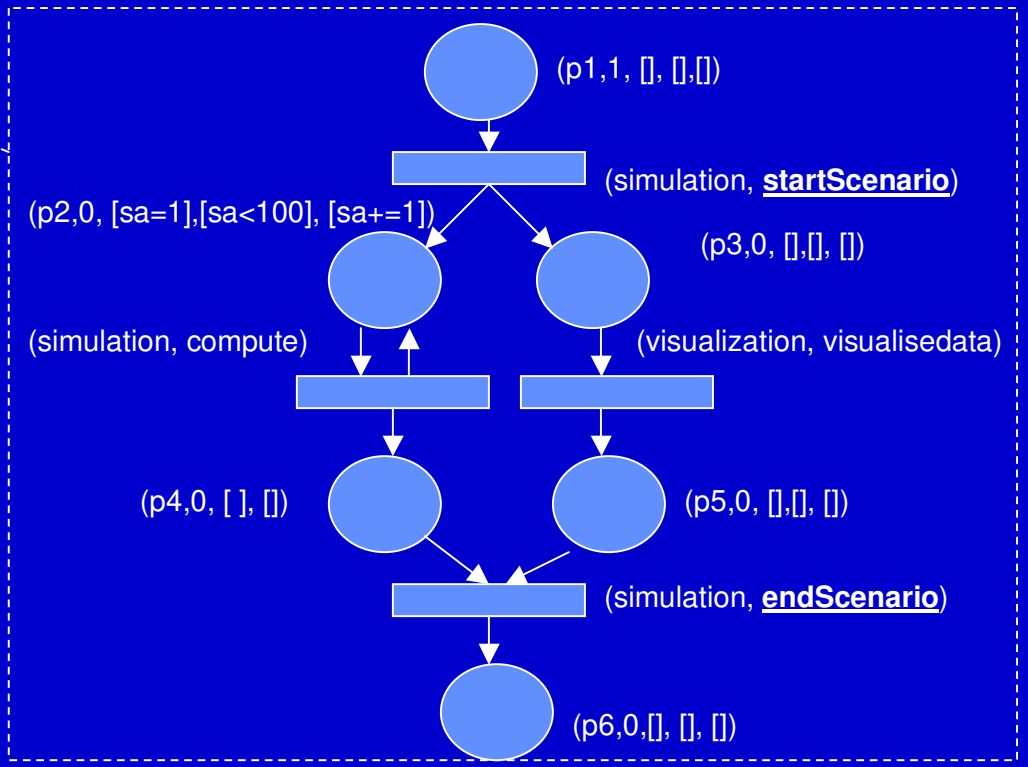
Module Agents:
Application specific activities = Story + my capability.

Communication Agents:
Interfacing to software bus.

Actor:
Doing real activities.

Story = {Scenarios}





Story: scenario transition graph.

Nodes: {scenarios};

Transitions: {([Ee], [Eq])};

[Ee]: expression when entering;

[Eq]: expressions when leaving.

Scenario: P/T net:

Places: {(name, token, [Ei], [Ee], [Eq])}

[Ei]: expressions when init the P/T net;

[Ee]: expressions when enter a place;

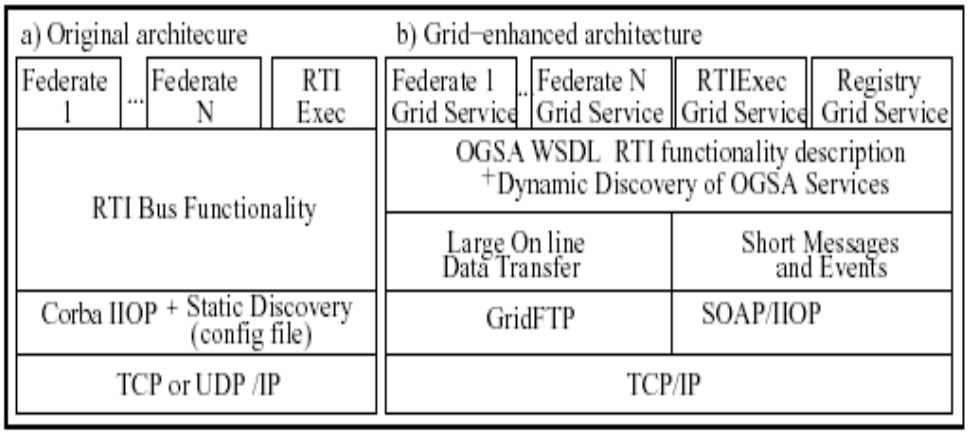
[Eq]: expressions when leave a place.

Transitions: {(role, action)}

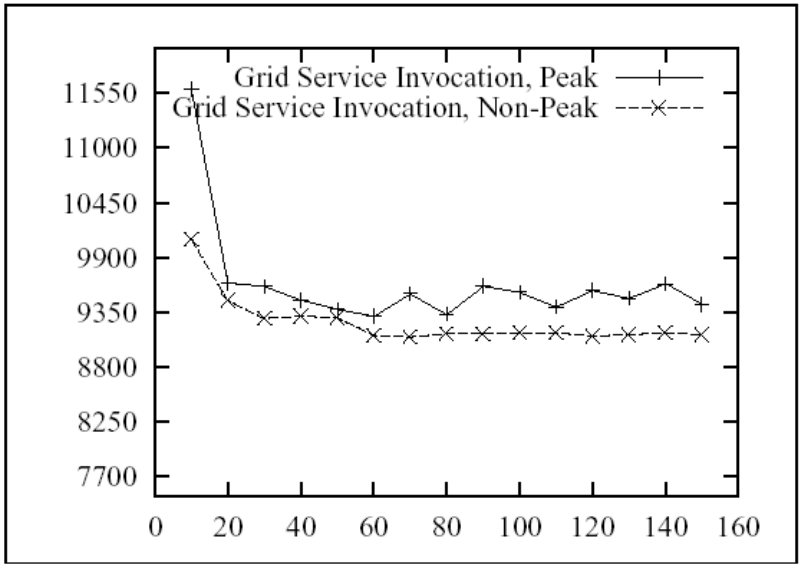
Grid Services and HLA

Grid Services for HLA-based Distributed Simulation Frameworks, in *First European Across Grids Conference, Santiago de Compostela, Spain*, Springer-Verlag, Heidelberg, February 2003.

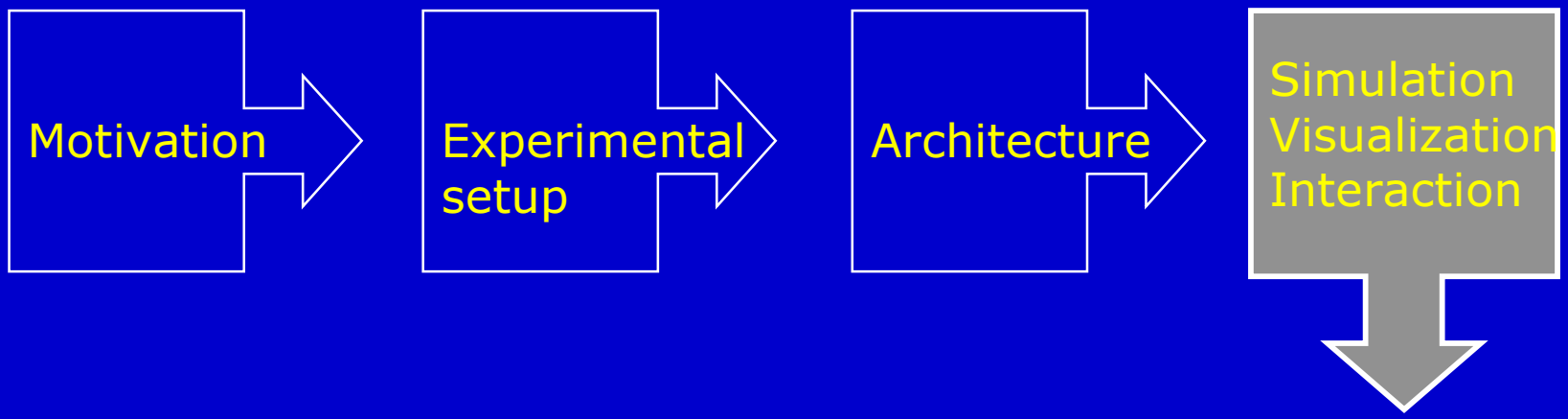
- Why HLA:
  - Simulation modules aggregation and reuse; Large and mature user base; legacy
- But:
  - HLA requires explicit description of data and event objects that will be exchanged before the actual federation starts execution
  - Static bootstrapping process required to enable RTI system communication
- Our approach:
  - GT3 index service and data transfer infrastructure evaluated to assess capabilities and limitations with HLA integration
  - Performance of GT3 GIS infrastructure for querying and modifying RTIexec endpoint information and RTI bootstrap
  - Current GT3 GIS performance demonstrates the feasibility of the GT3/HLA based GIS for HLA runtime information query, RTI dynamic modification of HLA Federates, and bootstrapping
  - Added features to HLA like security, extensibility, scalability, and decentralized maintenance.
- Implementation: RTI 1.3 NG V5, Amzi Prolog



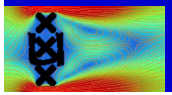
Migration approach from HLA to GS



Ariadne's red rope



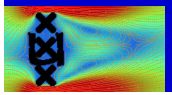
Status: Some 'hot' results



Flow through complex geometry

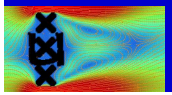
- After determining the vascular structure simulate the blood-flow and pressure drop…

- Conventional CFD methods might fail:
  - Complex geometry
  - Numerical instability wrt interaction
  - Inefficient shear-stress calculation



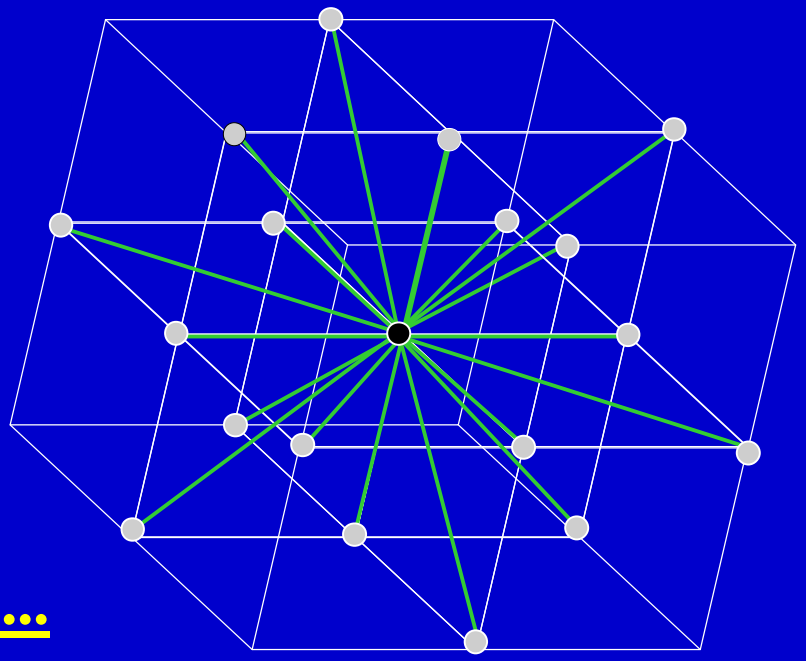
Solution to interactive flow simulation

– Use Cellular Automata as a mesoscopic model system:
  - Simple local interaction
  - Support for real physics *and* heuristics
  - Computational efficient

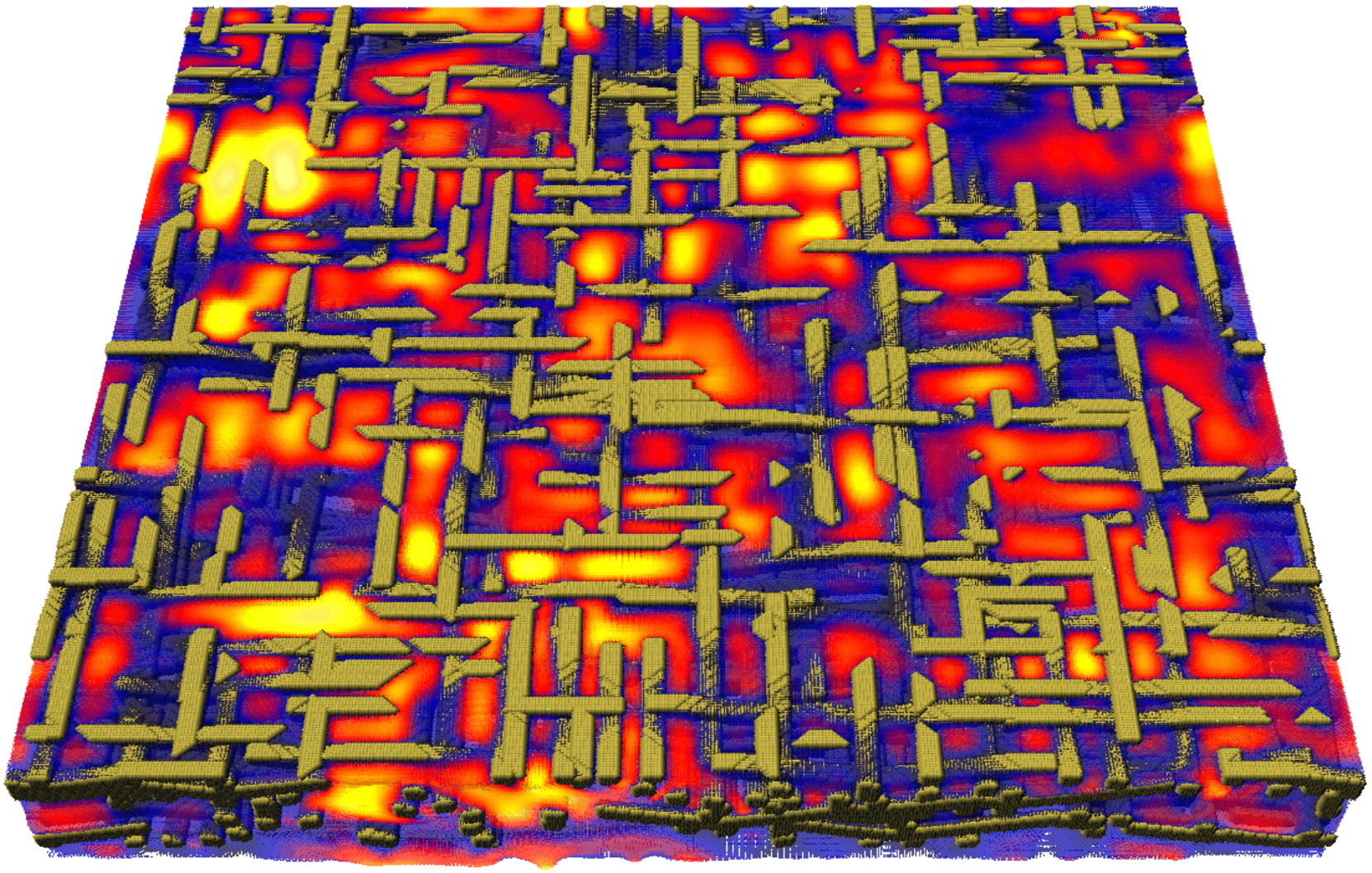


Mesoscopic Fluid Model

- Fluid model with Cellular Automata rules
- Collision: particles reshuffle velocities
- Imposed Constraints
  - Conservation of mass
  - Conservation of momentum
  - Isotropy



Details...



Efficient Calculation of Shear-Stress

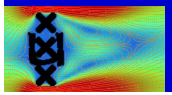
Perpendicular momentum transfer:

$$\sigma_{\alpha\beta} \sim \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}$$

From LBE scheme: $\rho = \sum_i f_i$ $\rho \mathbf{u} = \sum_i f_i \mathbf{c}_i$

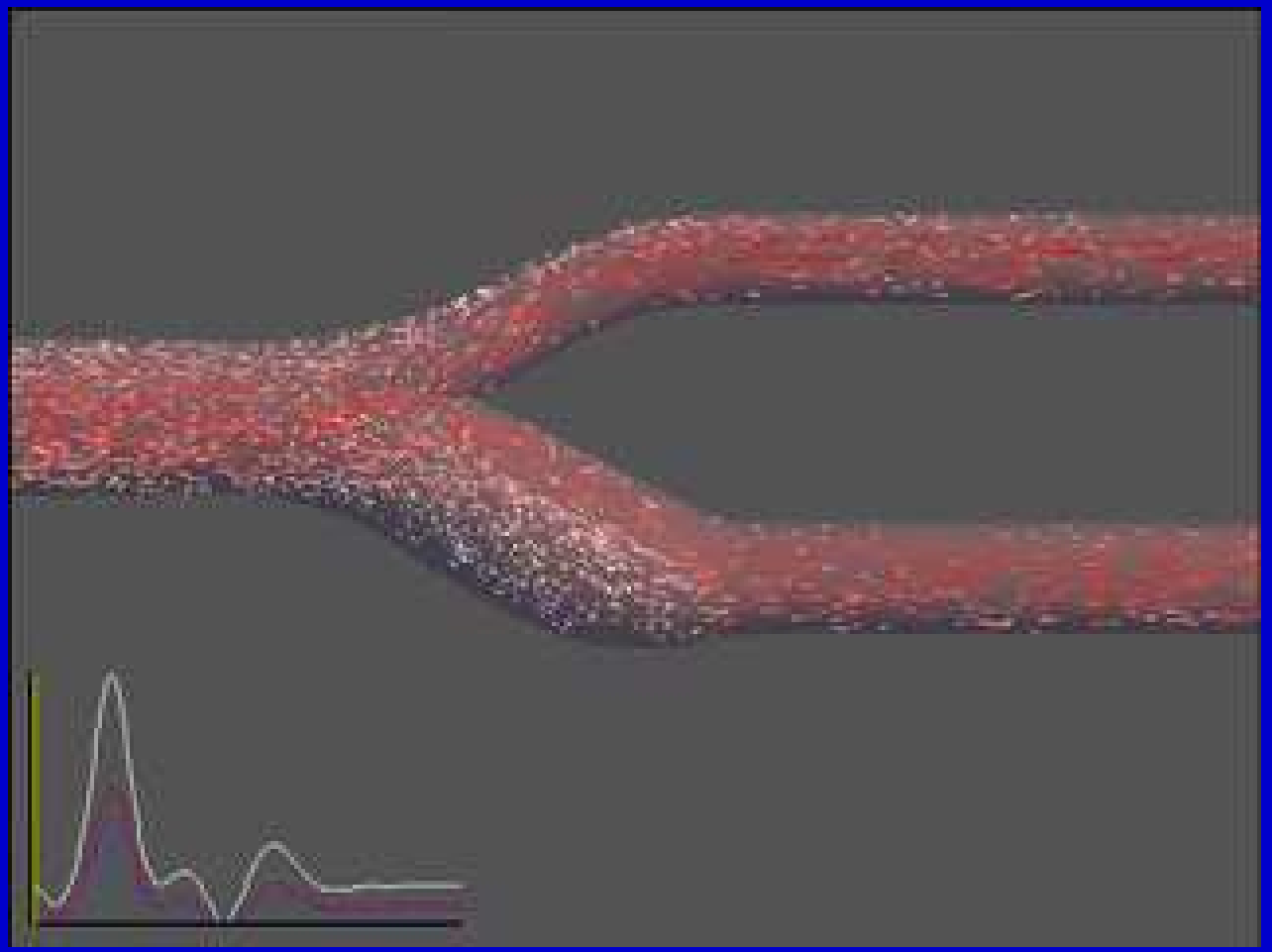
AND the momentum stress tensor Π that is linearly related to the shear stresses $\sigma_{\alpha\beta}$

$$\mathbf{\Pi}_{\alpha\beta} = \sum_i f_i \mathbf{c}_{i_\alpha} \mathbf{c}_{i_\beta}$$



International Journal of Modern Physics B, vol. 17, nr 1&2 pp. 95-98. World Scientific Publishing Company, January 2003.

International Journal of Modern Physics C, vol. 13, nr 8 pp. 1119-1134. October 2002.



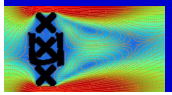
Visualization Courtesy J. Steinman

T.S. Elliot

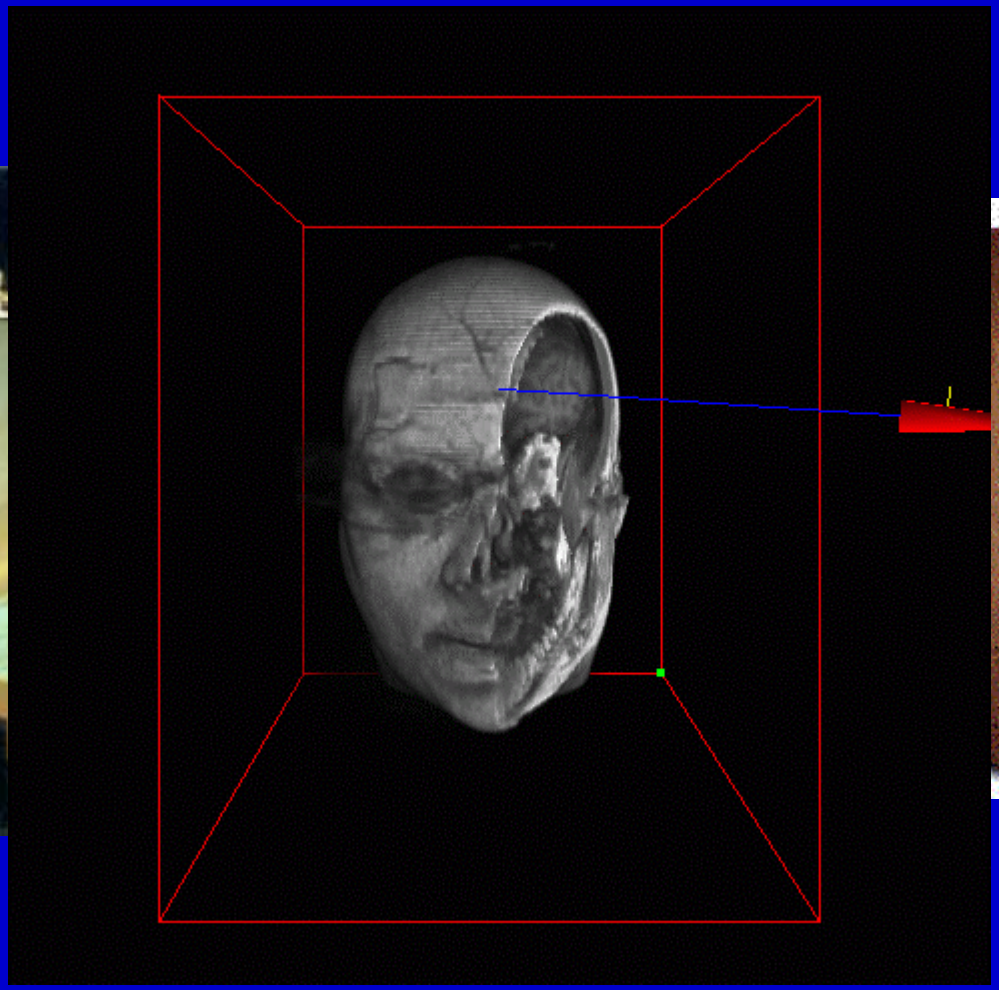
‘How much wisdom has been lost in knowledge and how much knowledge has been lost in information...’

How much Information has been lost in Data!!

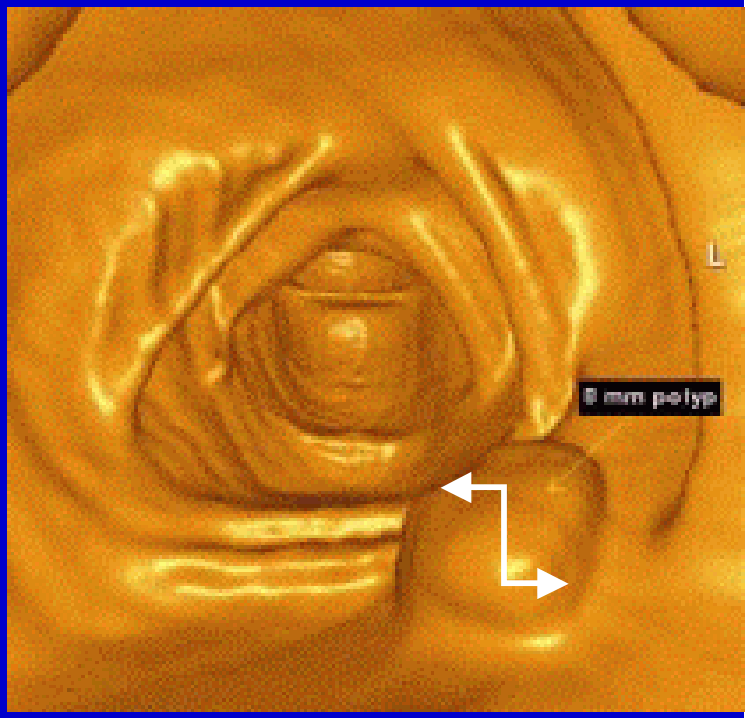
Fourth IEEE ACMI'02 International Conference on Multimodal Interfaces, Pittsburgh, Pennsylvania, 14-16 October 2002, pp. 313-318. IEEE Computer Society, Los Alamitos, California, USA, 2002.

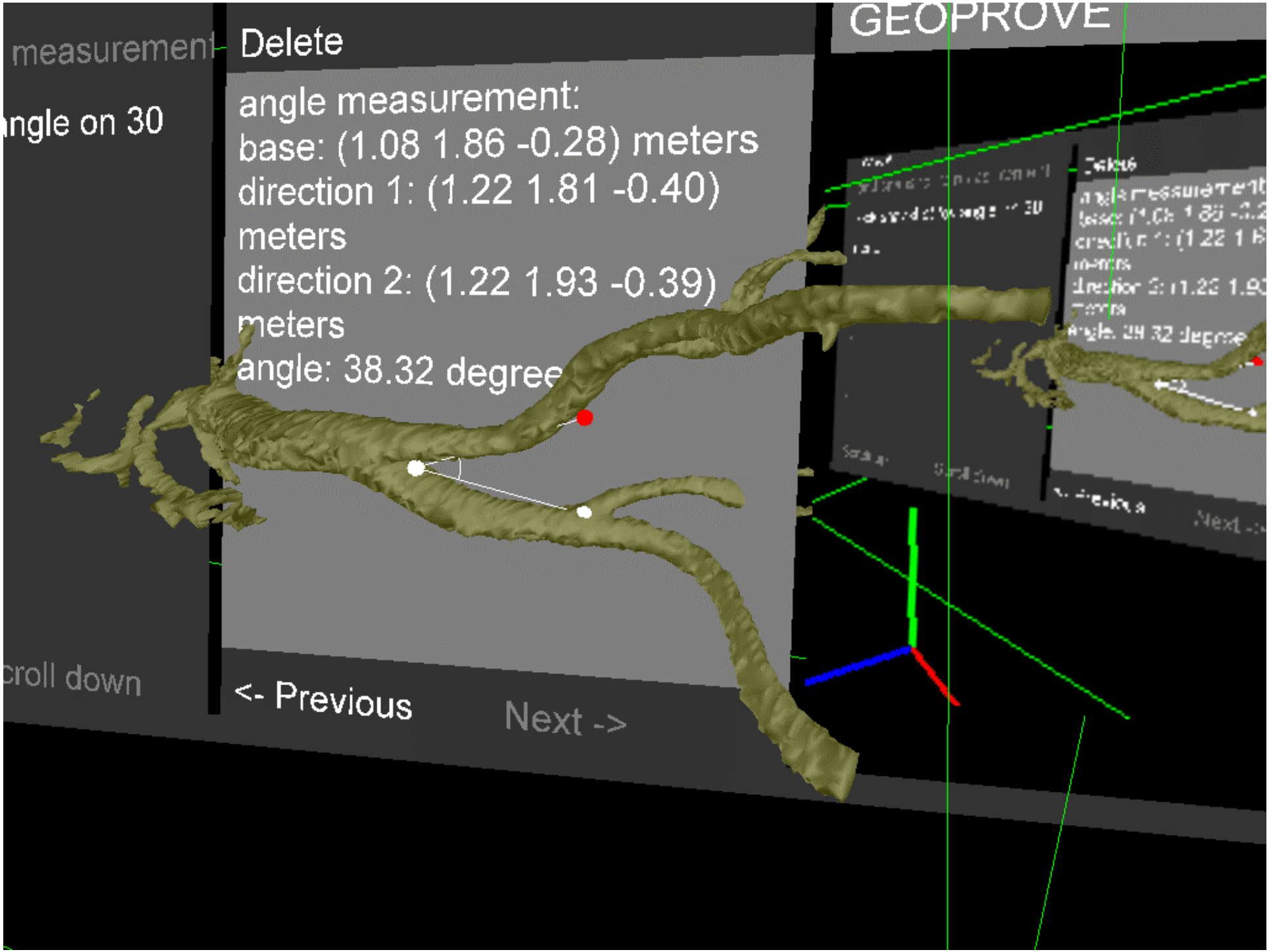


Immersive Environments

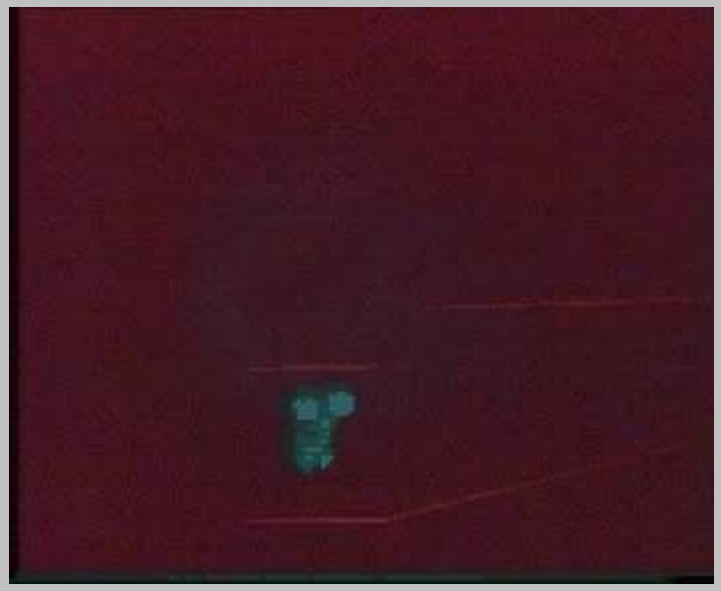


3D Information and Interaction

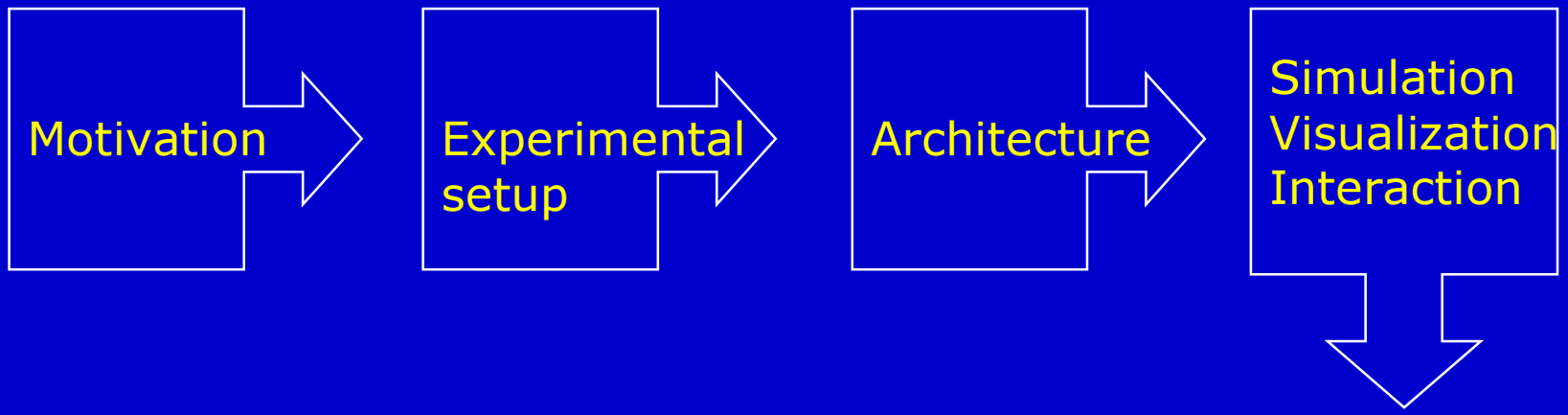



measurement
ngle on 30
Delete
angle measurement:
base: (1.08 1.86 -0.28) meters
direction 1: (1.22 1.81 -0.40)
meters
direction 2: (1.22 1.93 -0.39)
meters
angle: 38.32 degree
GEOPROVE
croll down
<- Previous
Next ->

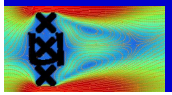
VR Portal



Ariadne's red rope



Status: Some 'hot' results



The Specs

- DAS2 SEs
  - Storage Elements (SE) in UvA, NIKHEF, and Leiden
  - EDG 2.0 release candidate with VDT-1.1.8-6, installed and configured manually instead of LCFG, because is a shared system
  - No R-GMA running, using the MDS interface on port 2135
  - Distributed ASCI Supercomputer 2 **(DAS-2)**
  - Myrinet multi-Gigabit wide-area distributed computer of 200 Dual Pentium-III nodes
  - Fast Ethernet used as OS network
  - Each node contains:
    - Two 1-Ghz Pentium-IIIs
    - At least 1 GB RAM
    - At least 20 GByte local IDE disk
    - A Myrinet and Fast Ethernet interface cards
    - Linux 2.4.7-10

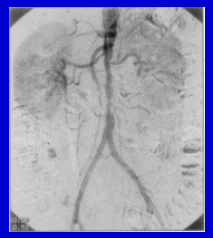
- CrossGrid CEs
  - Currently EDG 1.2.2 and 1.2.3 deployed in the production testbed
  - EDG 1.4.3 being tested at several validation sites
  - Production testbed resources:
    - 15 Computing Elements
    - 69 Worker Nodes
    - 115 CPUs
    - 2.7TB Storage Capacity

- MD
  - Local repository for remote navigation, data transfer and D-VRE initialization
  - Requirements:
    - Web Browser
    - Java Plugin 1.4 or newer with JAR cache disabled
    - Firewalls open for 8080 port
    - Pool 13000-17000 and port 2811 open in both directions between local workstation and remote SE (se.crossgrid.man.poznan.pl)
    - Valid x509 certificate credentials

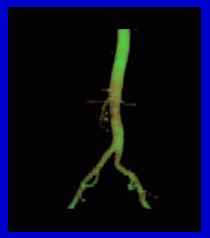
The Scenario

Proceedings of the First European HealthGrid Conference, January, 16th-17th, 2003, pp. 57 - 66.

Patient at MRI scanner

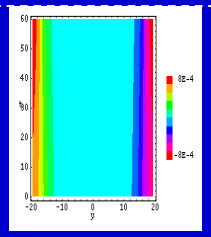


MR image



MR image Segmentation (soon a GS!)

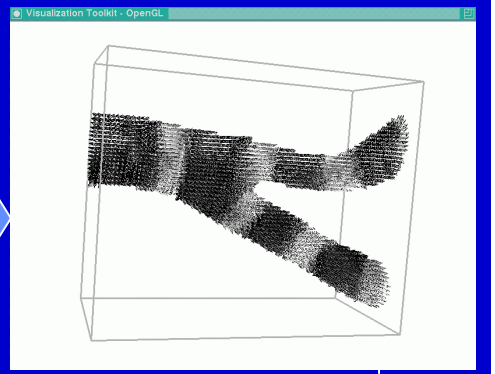
se1 (e.g., Leiden)



Shear stress, velocities, masses, etc.

LB Solver

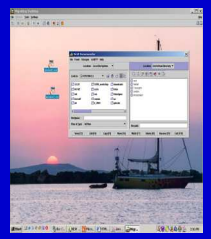
ce (CrossGrid)



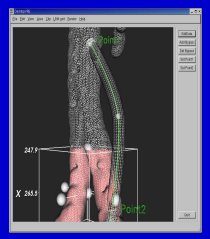
GVK

ce (CrossGrid)

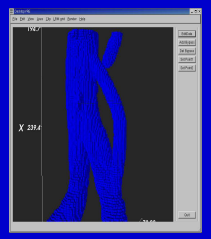
MD login and Grid certificates submission



Virtual Node Creation

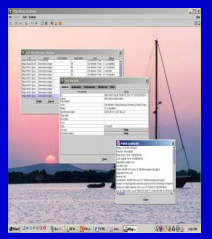


Bypass creation

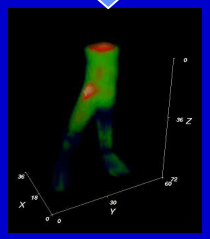


LB mesh generation

Job submission



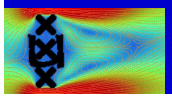
Job monitoring



Simulated flow

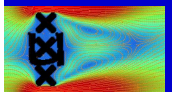
D-VRE

se2 (D-VRE machine)

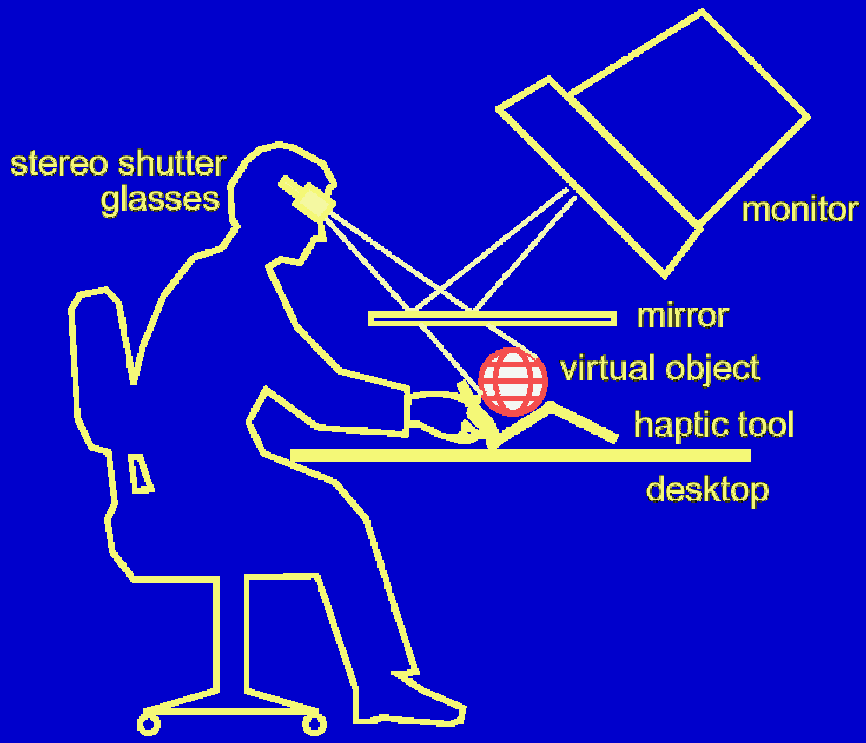


Recorded Session

September 25th 2003



A peek in the kitchen…

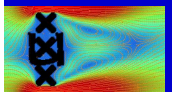


CRUIZ

Wrapping up

- Agent based iPSE (Simulation, Interaction and Visualization)
- Vascular Reconstruction
- Dynamic task Migration support for HPC on the Grid
- Migrating Desktop X# integrated with VRE

- Working on:
  - Human Machine Interaction (trial in 3 Hospitals)
  - Stent Placement
  - Alternative VR: DesktopVR
  - OGSA and HLA-Grid



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U. Wisconsin

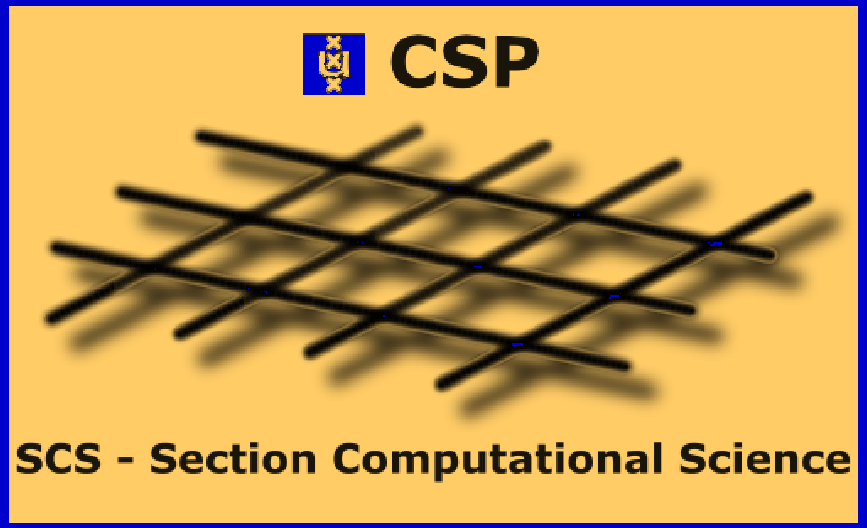
M. Livney, PhD

SARA:

A. de Koning, PhD.

Krakow

Marian Bubak, PhD

Katarzyna Zajac

http://www.science.uva.nl/research/scs