

Interactive Molecular Studies in VR

Technische Universiteit Delft / Opening VRLab

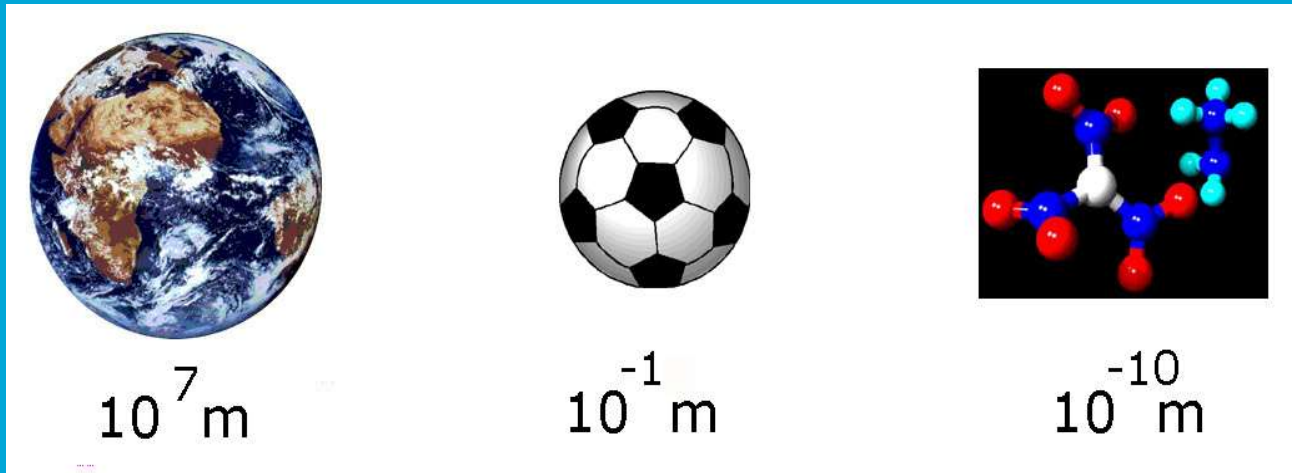
Ir. Gerwin de Haan

September 16, 2005

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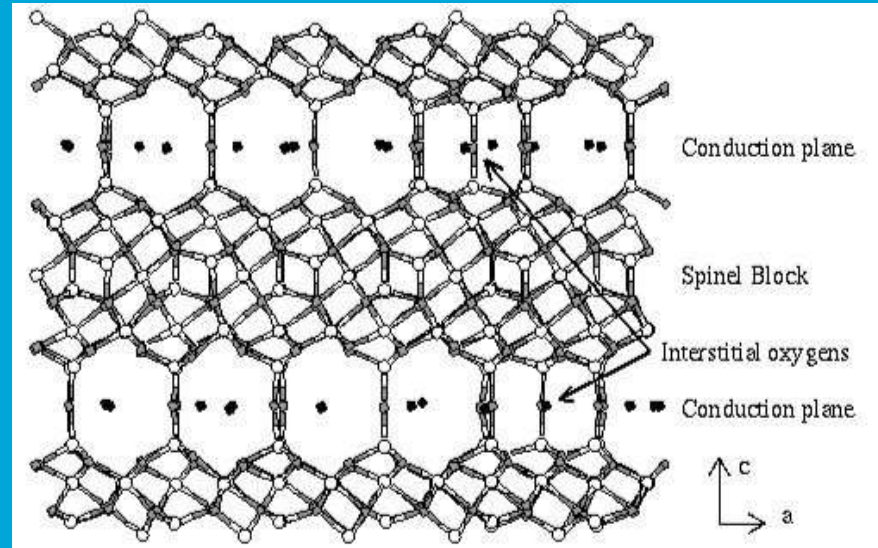
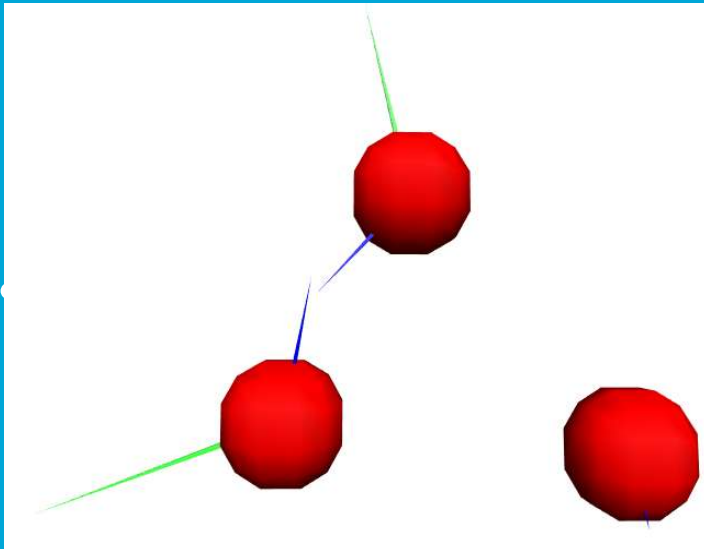
Studying molecular structures

- Material properties, protein behavior
- Small scales
 - Spatial : from nano meters
 - Time : from pico seconds

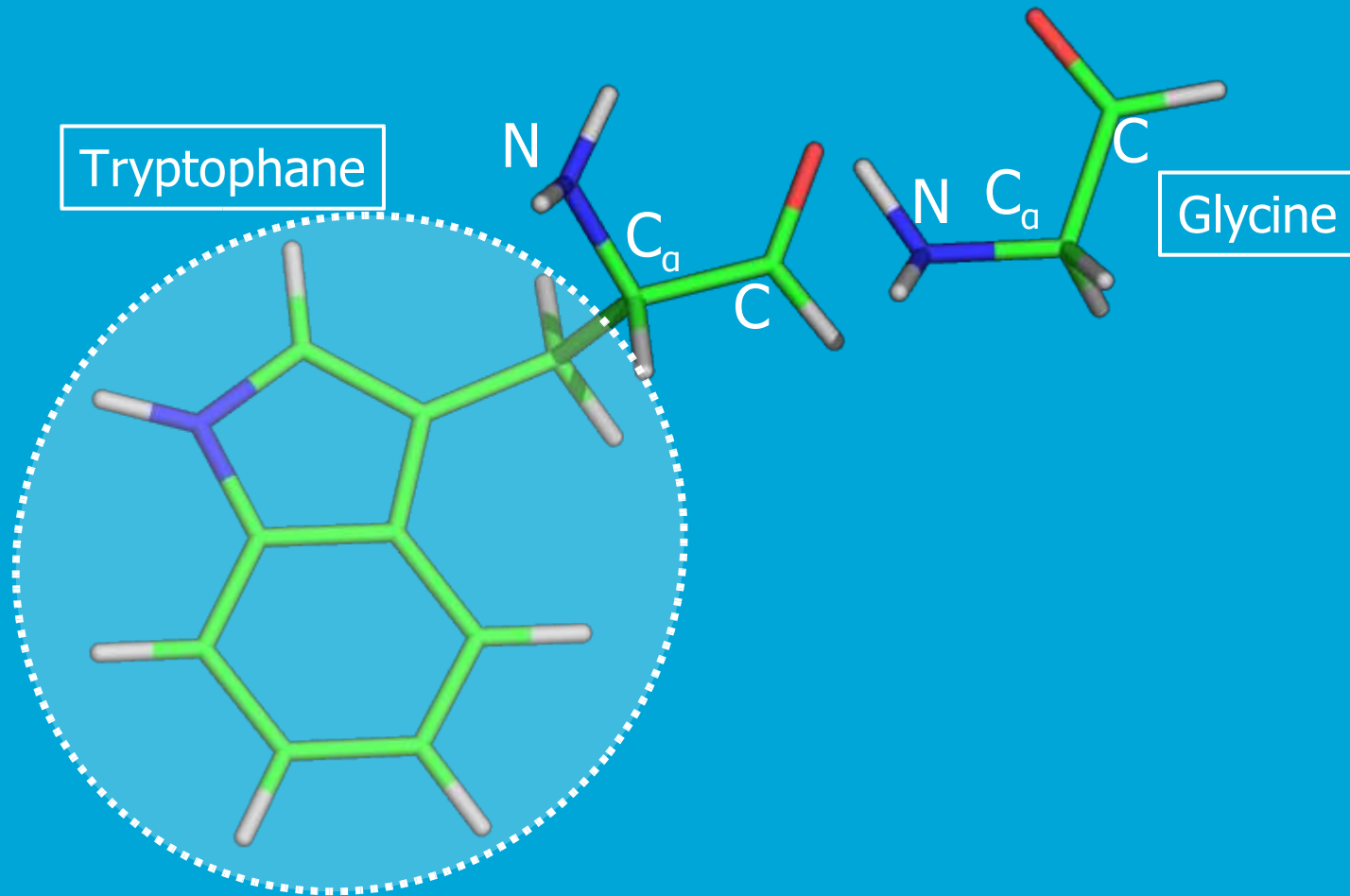


Molecular Dynamics (MD)

- Computer simulation of "Newtonian" behavior



Molecular Dynamics



Molecular Dynamics

- **Input:** Molecular structure, force field
- **Process:** MD simulation
- **Output:** Trajectory file

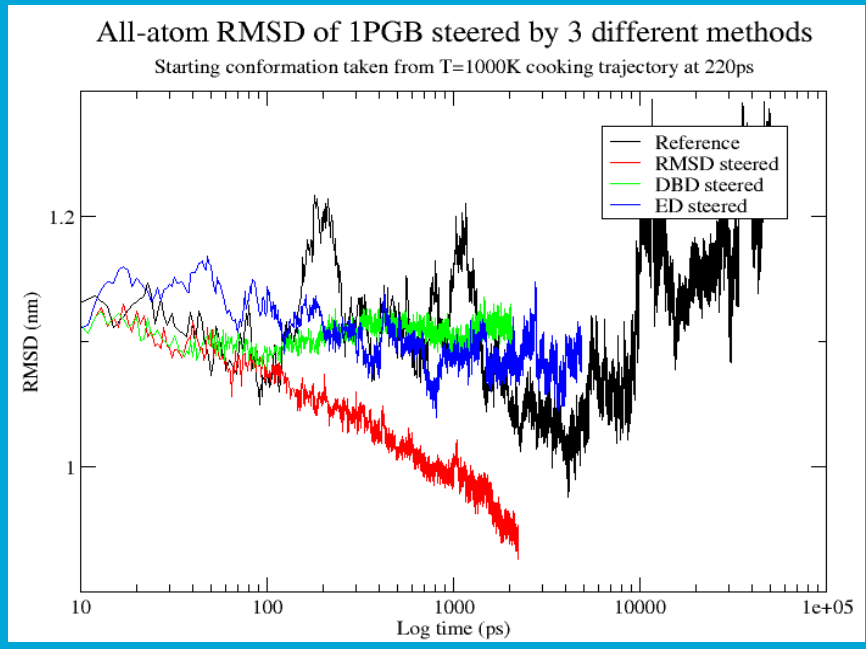
Typical MD toolchain

- **Input creation**
 - Databases, Molecular modellers
- **Simulations**
 - Amber, CHARMM, DEMMPSI, GroMACS
- **Output analysis tools**
 - Plotting, statistics, animations

Typical MD toolchain

```

1AKS A SWS P00761 134 - 231 NOT IN ATOMS LIST
1AKS B SWS P00761 1 - 133 NOT IN ATOMS LIST
S A 16 145 SWS P00761 TRYP_PIG 9 133
S B 146 245 SWS P00761 TRYP_PIG 134 231
S ASN B 165 SWS P00761 ASP 153 CONFLICT
S GLN B 186 SWS P00761 GLU 175 CONFLICT
A 125 ILE VAL GLY GLY TYR THR CYS ALA ALA ASN SER ILE PRO
A 125 TYR GLN VAL SER LEU ASN SER GLY SER HIS PHE CYS GLY
A 125 GLY SER LEU ILE ASN SER GLN TRP VAL VAL SER ALA ALA
A 125 HIS CYS TYR LYS SER ARG ILE GLN VAL ARG LEU GLY GLU
A 125 HIS ASN ILE ASP VAL LEU GLU GLY ASN GLU GLN PHE ILE
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A 125 ILE SER GLY TRP GLY ASN THR LYS
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B 98 GLN GLN THR ILE ALA ALA ASN
112 1
CA CALCIUM ION
CA CA1 2+
HOH *111(H2 O1)
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H2 ASN B 165 SER B 171 1 7
H3 VAL B 231 ASN B 233 5 3
H4 VAL B 235 ALA B 244 1 10
    
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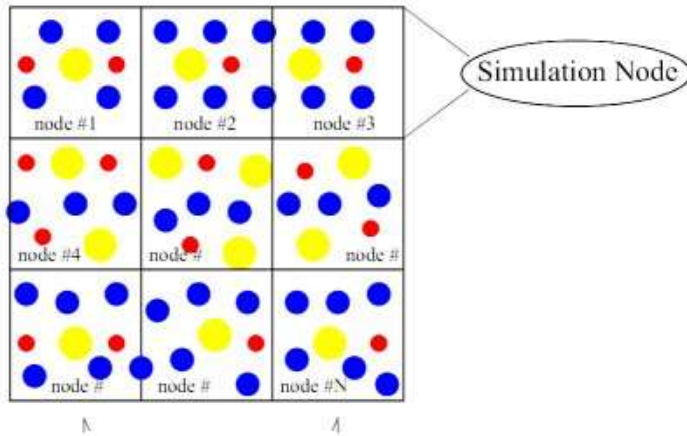
Towards VR tools, why?

- From desktop to VR
 - Display
 - Interaction

“Explore 'real-time' simulation experiments”

Parallel Remote Simulation

SUPER COMPUTER:
 1) CRAY T3E 128 nodes
 2) BEOWULF CLUSTER 54 nodes
 3) Origin 2000 8 nodes



Internet



Simulation Server

Shared Memory

Control data	
Visualization data	
Comm. data	Comm. data
Particle data #1	Particle data #1
Particle data #N	Particle data #N
Grid data	Grid data

Read buffer

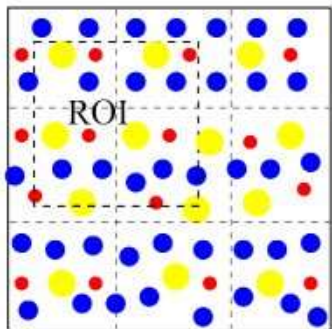
Write buffer

Pointer Switch

XML Configuration File

MoIDRIVE Manager

VIRTUAL REALITY WORKBENCH
 - SGI ONYX 2 workstation
 - 4 processors
 - Infinity Reality 2 graphics

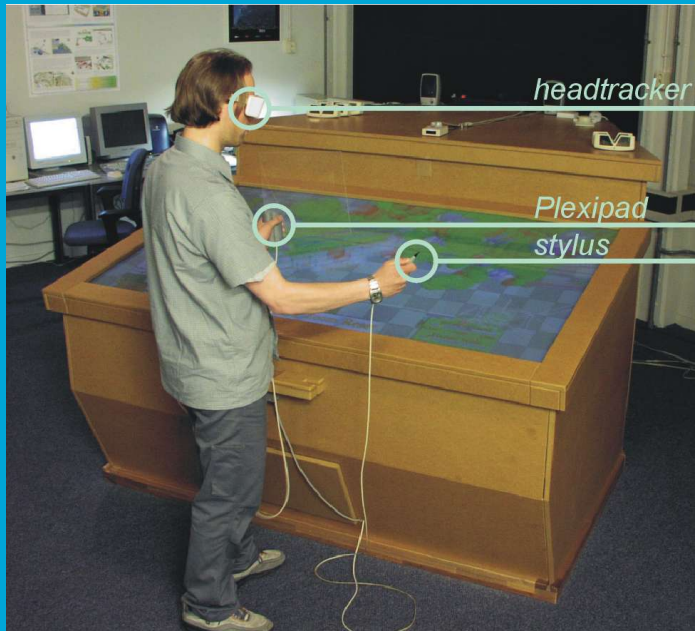


User Interaction

Visualization Client

MoIDRIVE

- Approach
 - VR to applic.
 - XML protocol
- Simulation in VR
 - Stored files
 - Running sims
 - Distributed
 - Steering



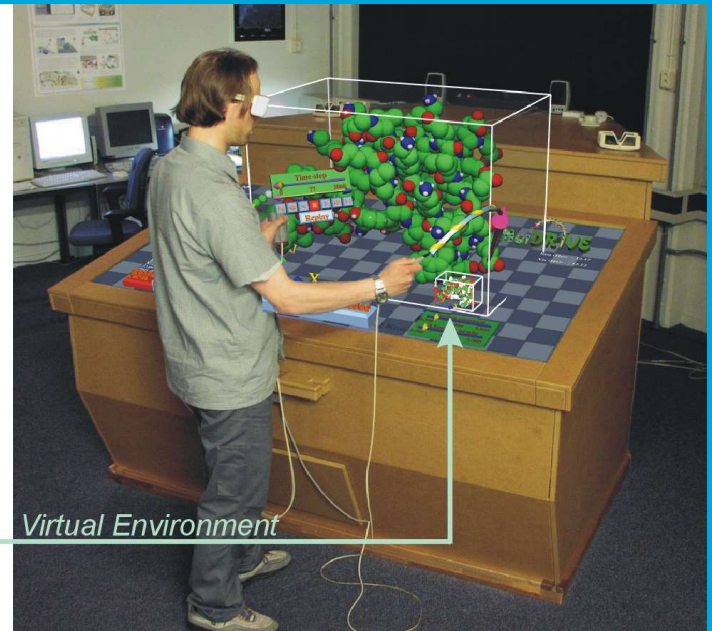
headtracker

Plexipad
stylus



Tracking system

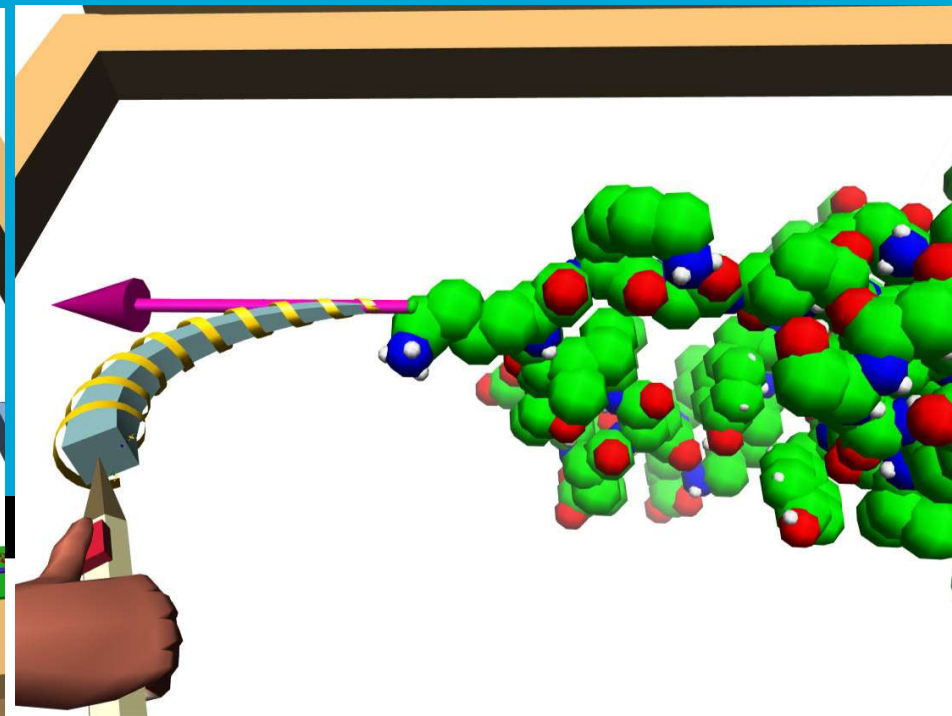
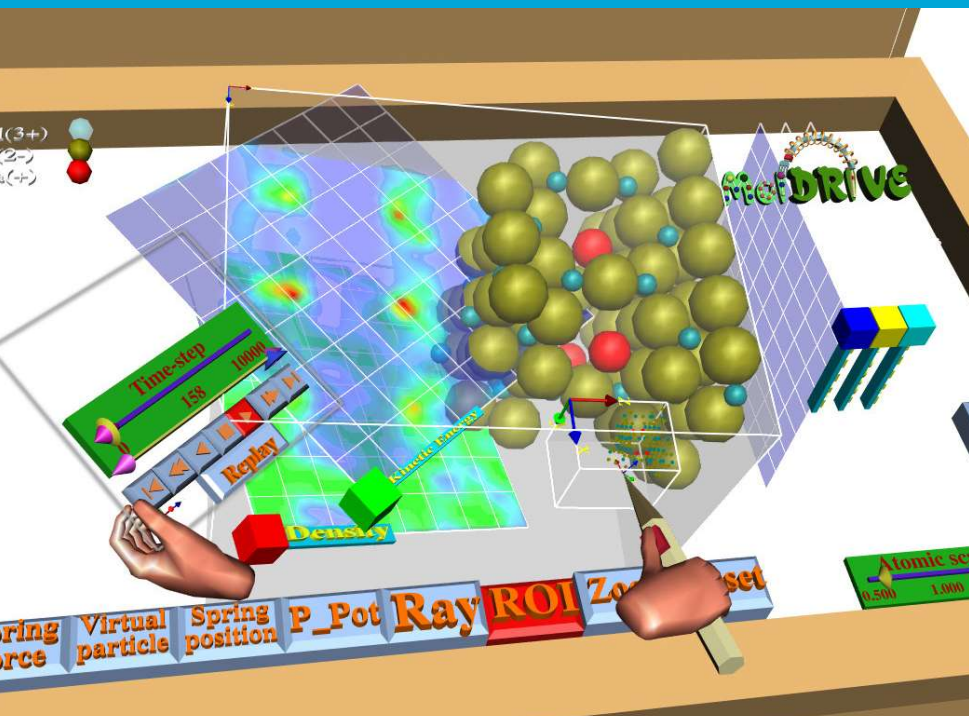
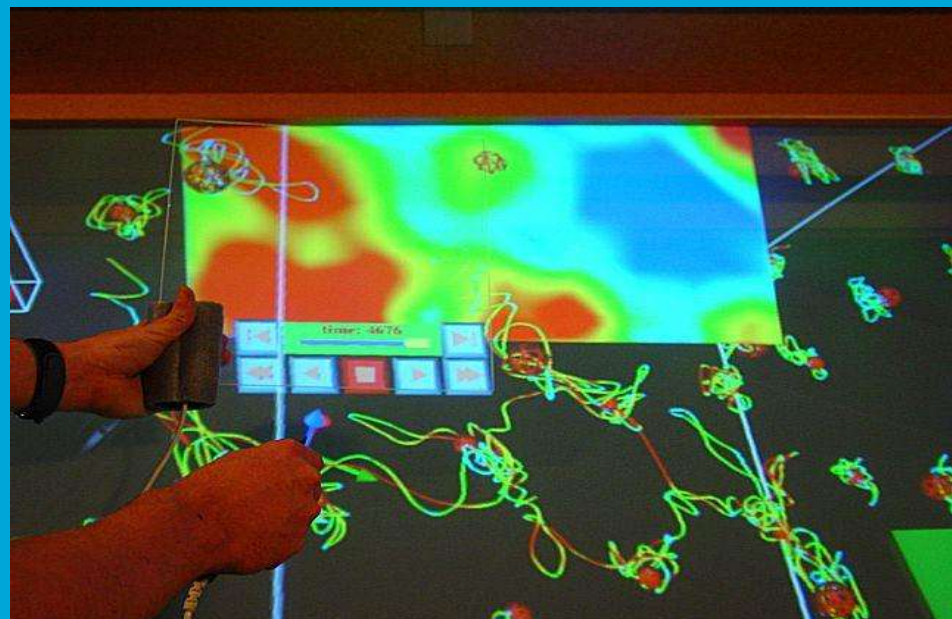
Graphics server



Virtual Environment

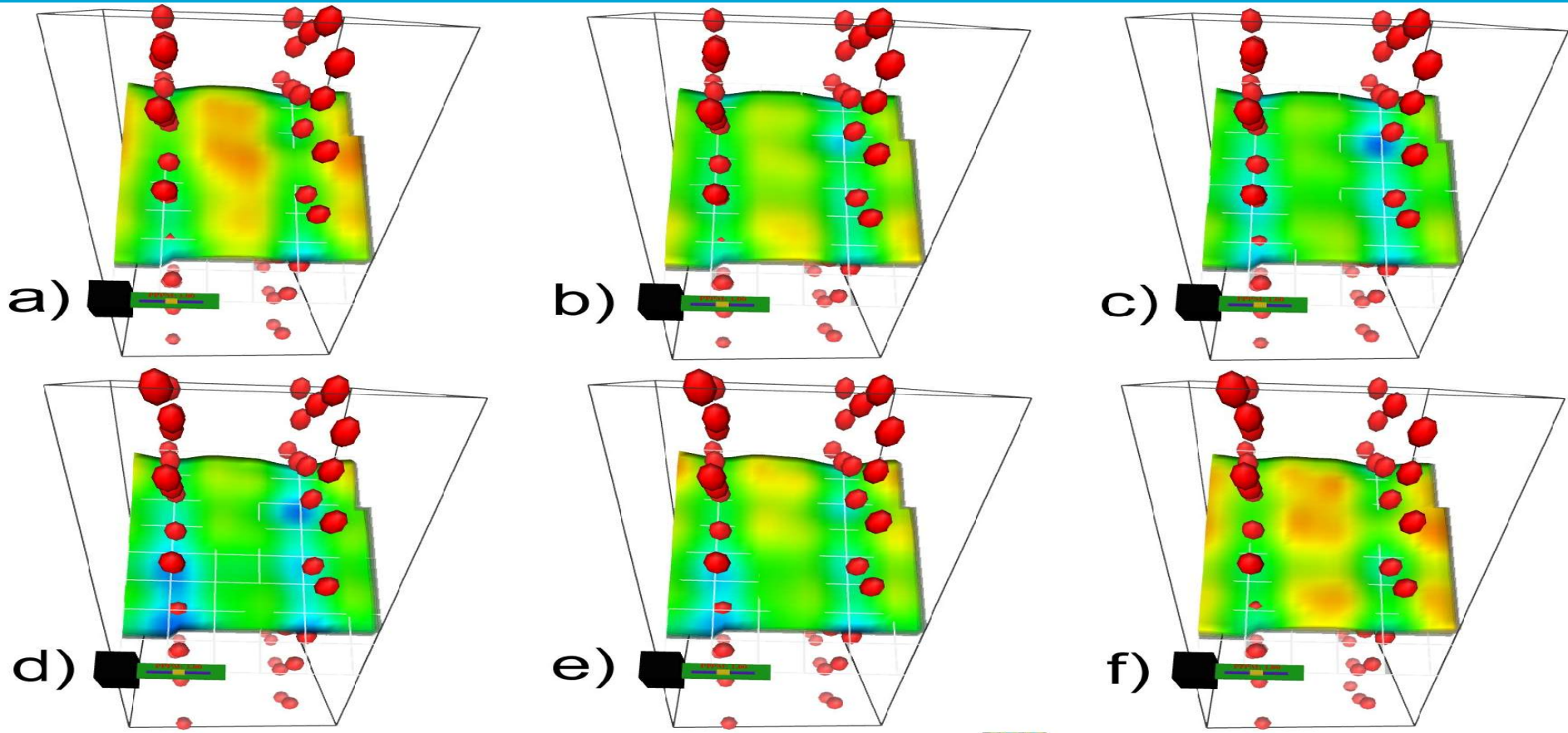
MoIDRIVE, now

- Visualization
 - Particle properties
 - Derivative data
 - Steering



MoIDRIVE, results?

- Educational value
- Observation of properties, behavior
- Visual prototyping

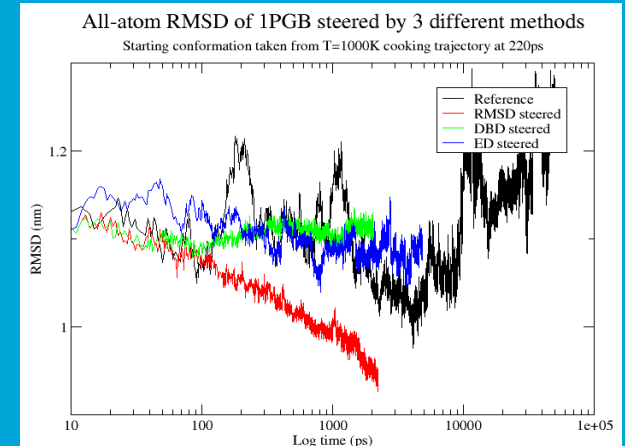


MoldRIVE, Problem areas

- **Fundamental**
 - Small timescale
 - Jitter
- **Technical**
 - Clusters
 - Compatibility
- **User Interface**
 - High setup time
 - Interfacing, Representations

Where do we want MoIDRIVE to go?

- Live vs. Recording
- Transparent Distribution
- Application specific interface
- From early prototyping to experimental setup



“Integration in the toolchain”

Where do we want VR-vis to go?

- Distribution
- Application specific interface
- From early prototyping to experimental setup
- Recording/Reproducing sessions

“Integration in the toolchain”

Your application ?

?!

MoDRIVE Workbench Demo after the opening