NOMAD

NOVEL MATERIALS DISCOVERY

V2C

VR and Visualisation Centre

lrz

Novel Materials Discovery: NOMAD

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Links with industry Session

PRACE-CoEs-FETHPC-EXDCI Workshop

Brühl, Germany. 30 October 2018

Who I am
What I work on

NOVEL MATERIALS DISCOVERY

- Rubén García - Specialization in Virtual Reality
  Deputy PI of NOMAD Advanced Graphics

- NOMAD Repository: largest collection of materials science simulations
- Code-independent view (archive)
- Material-centric property view (encyclopedia)
- Machine learning to discover new properties and descriptors (big-data analytics)
- Advanced graphics for interactive data exploration

Example VR datasets and supported devices

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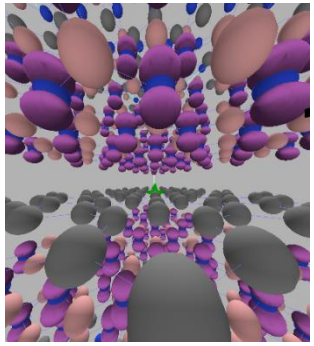

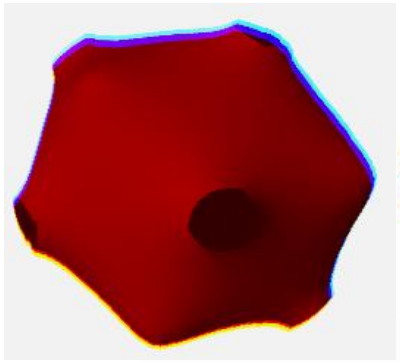

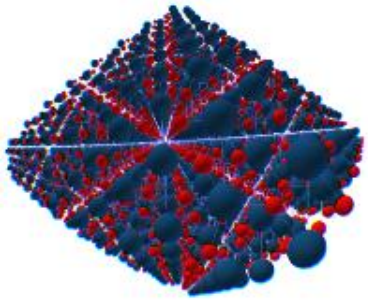

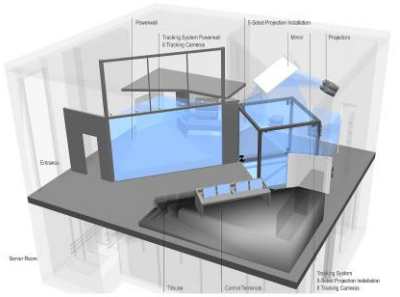

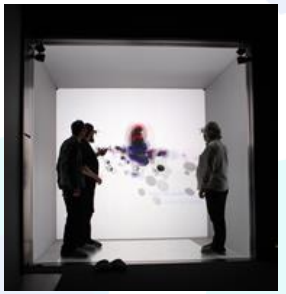

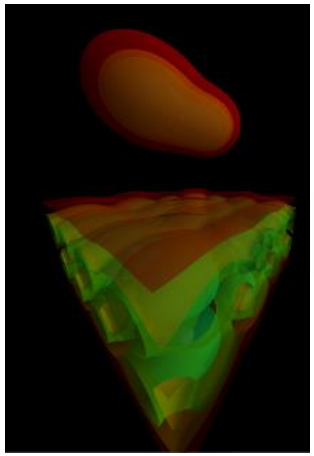

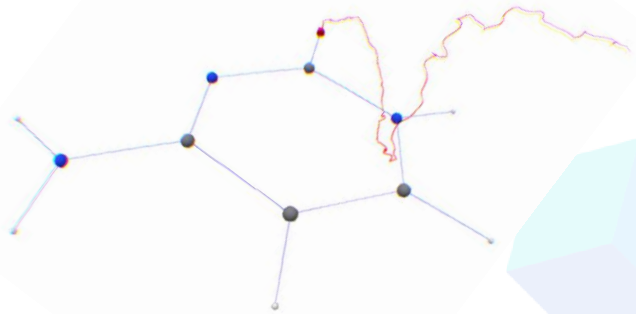

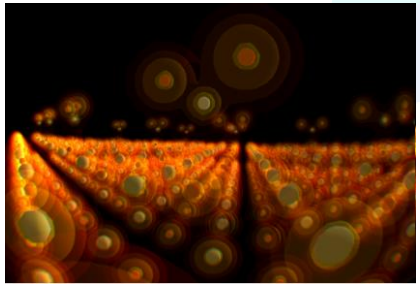

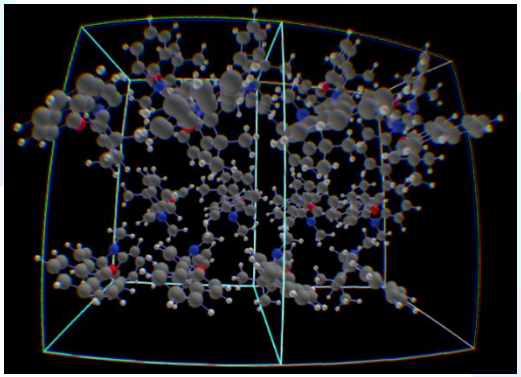

Shell-NOMAD Collaboration

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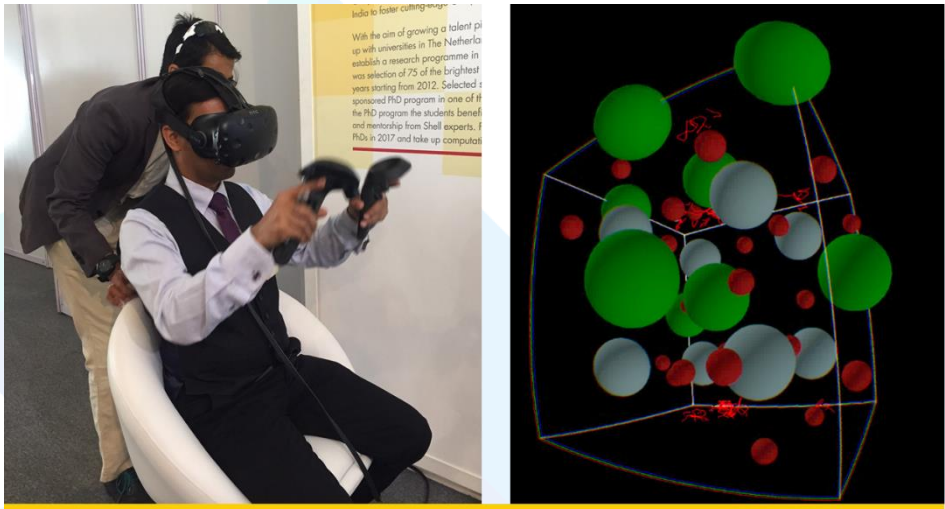
- The NOMAD General VR viewer was used with Shell dataset of barium zirconate simulation
- Inauguration of Shell Technology Center Bangalore, India, on 31st March, 2017
- Shell requested some additional functionality which was satisfactorily added to the VR viewer
- Development time: 3 weeks



"Being an atom": audience enjoying the VR Experience of moving through the structure of a membrane material as an atom. Image on the right shows a snapshot of Barium Zirconate, the material shown in VR. Blue balls denote Barium atoms, Green balls denote Zirconium and Red balls denote Oxygen atoms.

- On-going collaboration on various topics

TATA TCS-NOMAD Collaboration

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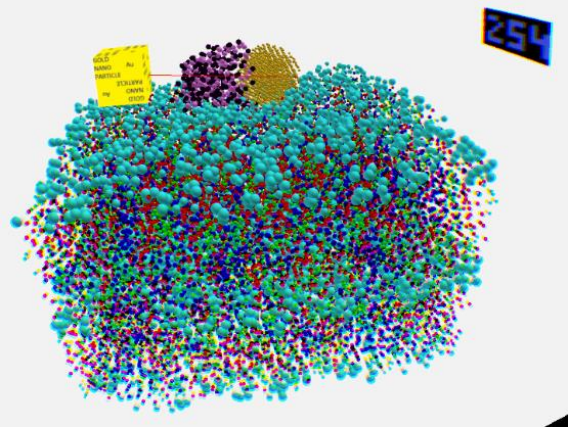
- TATA Consultancy Services used NOMAD VR in 13 events since March 2018
- More events planned for the future

- Ongoing collaboration

Example TATA TCS Dataset used as NOMAD VR Tutorial



In-Silico Skin Model – A molecular model for the top layer (Stratum Corneum) of human skin, by Deepak Jain and Rakesh Gupta (Tata Consultancy Services, Physical Sciences Research Area, Pune, India).
Showcasing the use of NOMAD VR for organic chemistry.
From Deepak Jain's (TATA Consultancy Services) presentation at the Second NOMAD Data Workshop

Thanks

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