Novel Materials Discovery: NOMAD

Rubén Jesús García-Hernández
Leibniz Supercomputing Centre,
Bavarian Academy of Sciences

Dissemination Session
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Who I am

What I work on

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
Dissemination activities that worked well

- Summer of Simulation 2017 at the Leibniz Supercomputing Centre of the Bavarian Academy of Sciences (25 October 2017)
- Increased awareness of NOMAD VR at LRZ
- NOMAD VR is used at Technical University of Munich Theoretical Chemistry Chair
- NOMAD VR also used to visualize Fluid Dynamics at TUM.
Dissemination activities that did not work well and why


- Lots of interest in testing the VR setup
- However, no follow-up communications
Dissemination activities in preparation

- Talk at the LRZ Extreme Scaling Workshop
- Early 2019, 3 day event
- Presentations regarding SuperMUC NG

- 30 minute talk with NOMAD and NOMAD VR overview.
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