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NOVEL MATERIALS DISCOVERY

V2C VR and Visualisation Centre

lrz

Novel Materials Discovery: NOMAD

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Application enabling at exascale
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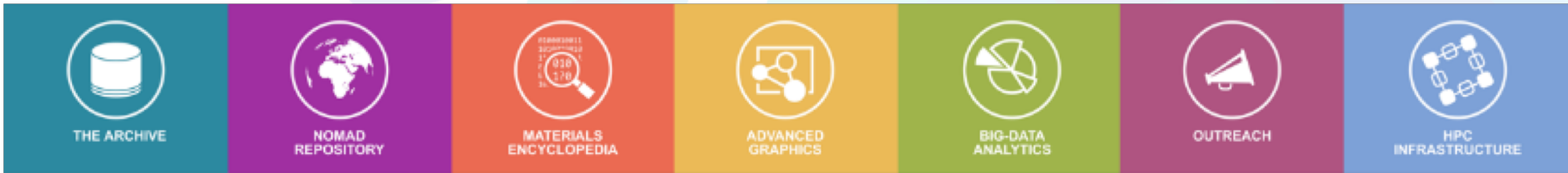
Who I am
What I work on

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



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Terascale - Petascale

- Current chemistry calculations for a specific compound:
  - Small complexity (one single desktop for a short time)
  - Middle complexity
  - High complexity
    (simulating quantum processes with high accuracy)
    - Take months of calculations on a current petascale system

Petascale – Exascale+

- Computational screening (overview)
  - Calculate properties for thousands or millions of different compounds
    - The space of interesting compounds is practically infinite, but it can be reduced by the aggressive filtering that the screening process adds.
    - Use Artificial Intelligence, Machine Learning to obtain accurate predictions for rest of compounds
  - Adds 3 to 6 orders of magnitude to previous calculatons
    - Petascale -> Exascale or zettascale

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Exascale+

- Computational screening
  - Calculations are completely independent
    - Not “classic exascale”
  - Possibly also used in other application domains using big-data techniques
- Future:
  - More complex methods
  - More compounds

Increased computational demands

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