

OpenEye Spring miniCUP April 2021

Introduction & Welcome

Anthony Nicholls

CEO, Founder



Customers, Users and Programmers



CUP

Santa Fe, early March
>20 years

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Santa Fe, early March
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EuroCUP, Various Chateaus



JCUP, Tokyo in May
> 10 years

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One-Day
miniCUPs
Live + Virtual



Fall (& Spring)

Customers, Users and Programmers



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One-Day
miniCUPs
Live + Virtual



Fall (& Spring)

AntiCUP

All OpenEye
Employees,
Early January



Spring miniCUP Presentations

- AntiCUP-derived:
 - Geoff Skillman – Science at OpenEye
 - Caitlin Bannan- Finite Temperature & Multicomponent Crystal Physics
 - Christopher Bayly- MD and Affinity
 - Jharrod LaFon, Matt Geballe – Cloud Technology at OpenEye
 - Bob Tolbert, Steve Muchmore, Jeff Grandy – Orion in motion
- Giovanna Scapin, *Nanolmaging Services* – CryoEM + Drug Discovery
- John Chodera, *Memorial Sloan Kettering* – COVID Moonshot

Live Q&A
& Discussions
Sessions

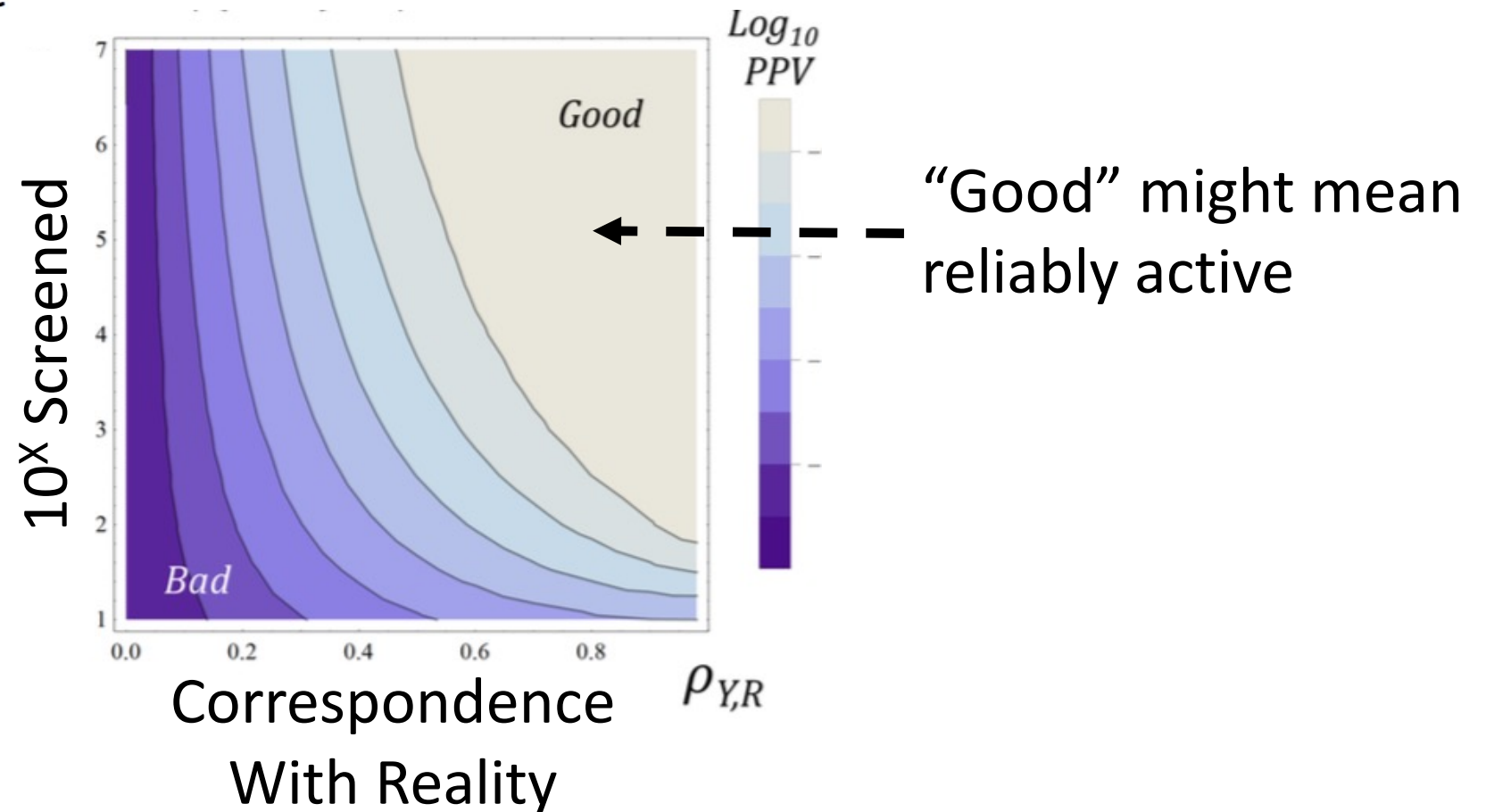
- Biomodeling, Proteins & Antibody Engineering
- Crystal Structure Prediction
- Small Molecule Discovery: Lead Optimization
- Small Molecule Discovery: Virtual Screening

Progress can be made with a lot of computers

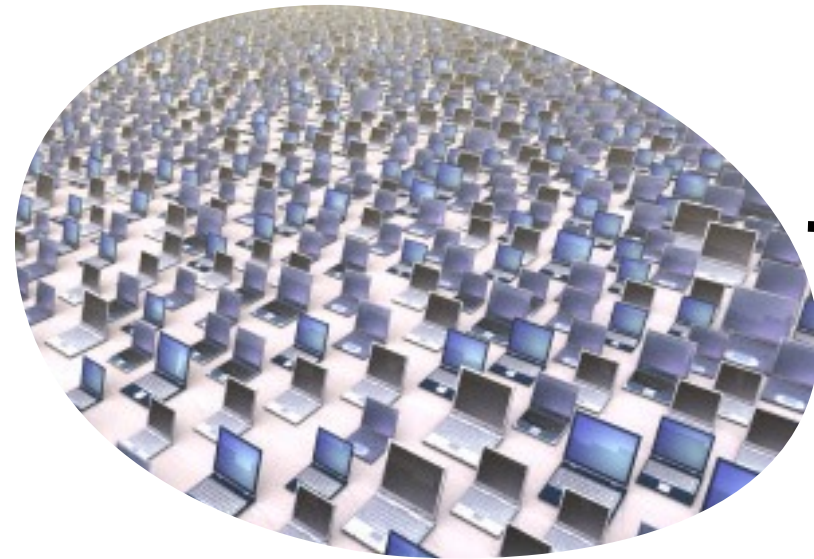
RESEARCH ARTICLE

When Quality Beats Quantity: Decision Theory, Drug Discovery, and the Reproducibility Crisis

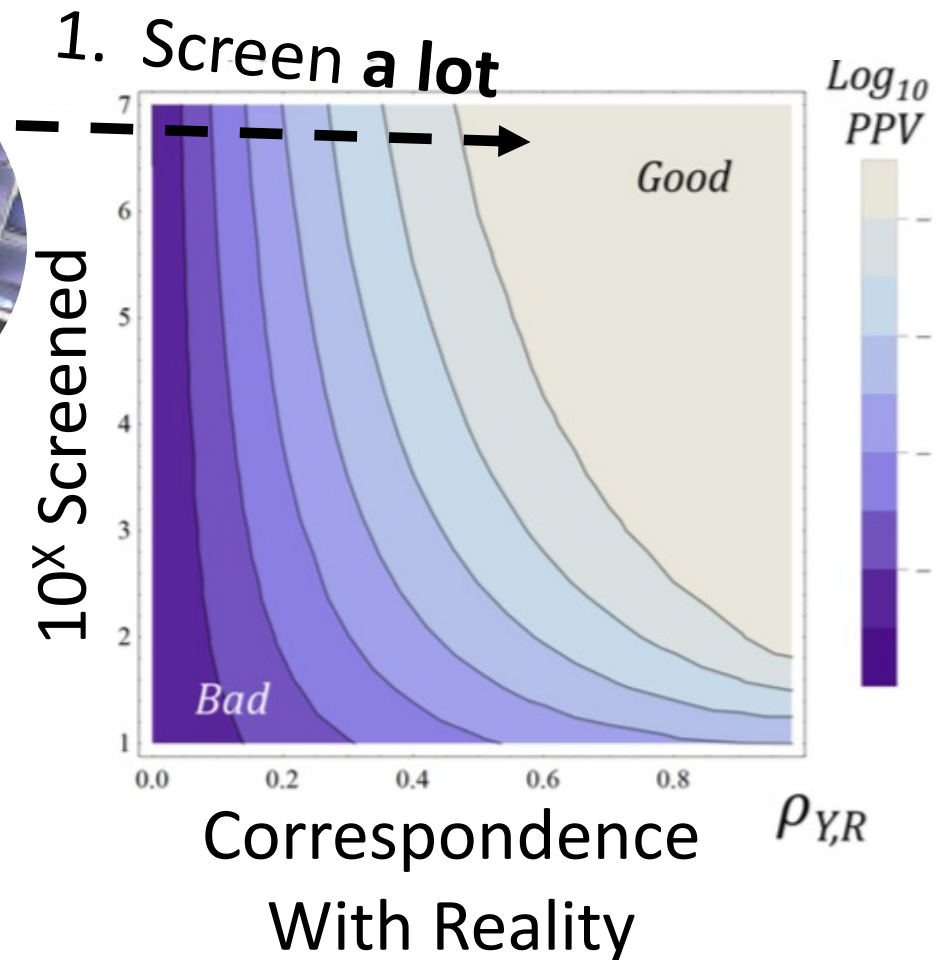
Jack W. Scannell^{1,2,3*}, Jim Bosley⁴



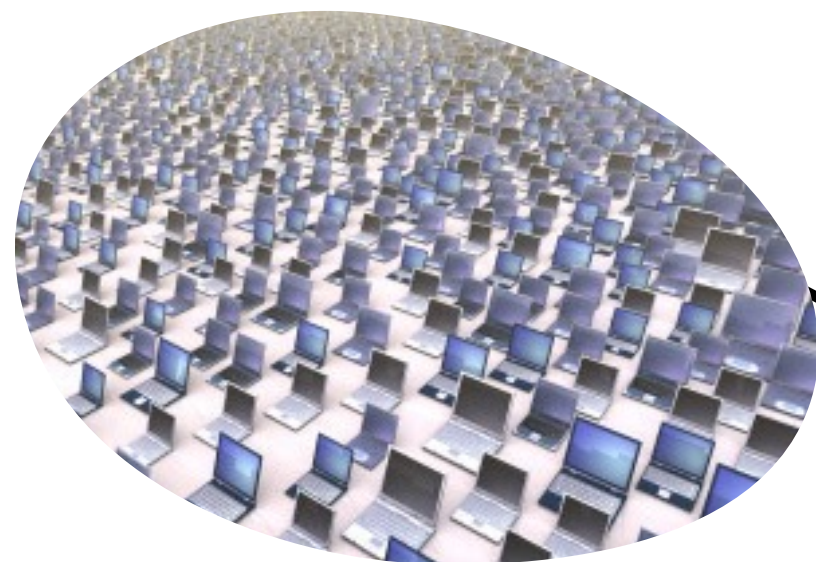
Progress can be made with a lot of computers



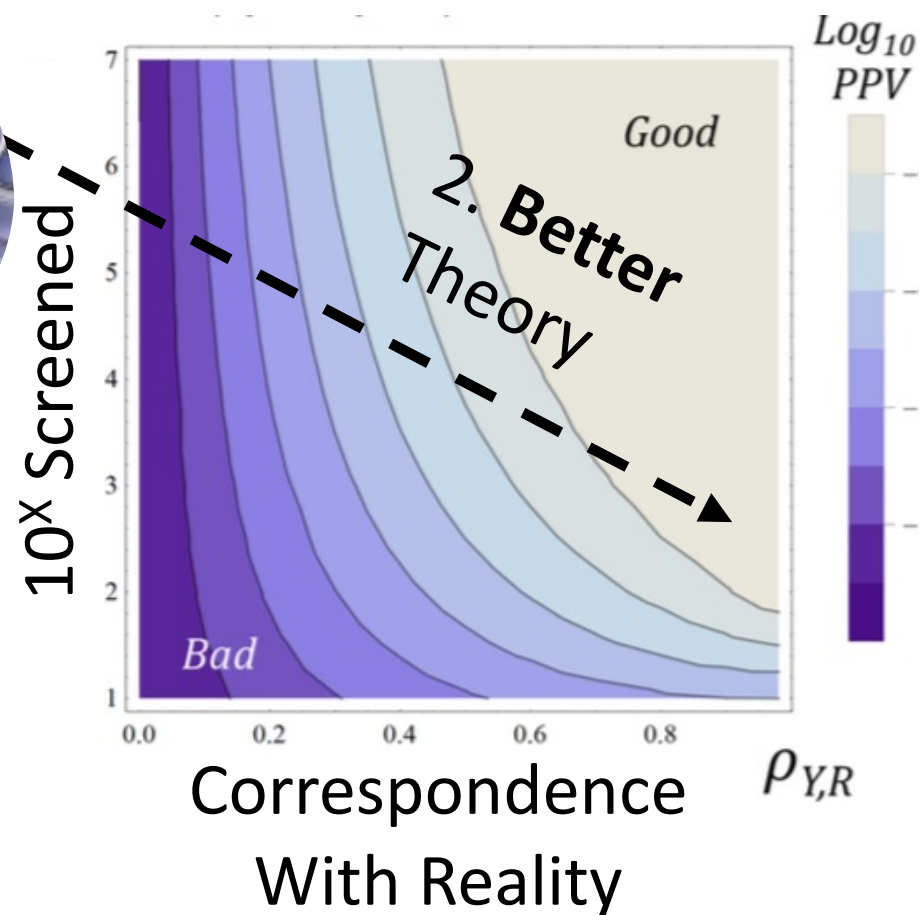
Small Fraction*
Large Number
=Enough





Progress can be made with a lot of computers










Crystal Structure Prediction



Exponential Growth of Scientific Computing

- X-ray refinement → CryoEM refinement
- BLAST searches → GWAS studies
- “Shaking the protein” → “ANTON”-scale Protein MD
- 2D corporate collection queries → 3D Enamine-scale search 
- Force-field Crystal simulation → Explicit QM simulation 
- FEP Lead Opt → FEP Screening tool
- “Threading” → AlphaFold

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Progress has been made
with a lot of computers



**Computational
Resource**



**Programming
Environment**



**Modeling
Environment**



**Scientific
Capabilities**

a lot of computers



**Computational
Resource**



**Programming
Environment**



**Modeling
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**Scientific
Capabilities**

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Coding the Technological Transformation of CADD

Molecular Modeling
Before The Cloud



Early Molecular Modeling
On The Cloud



Coding the Technological Transformation of CADD

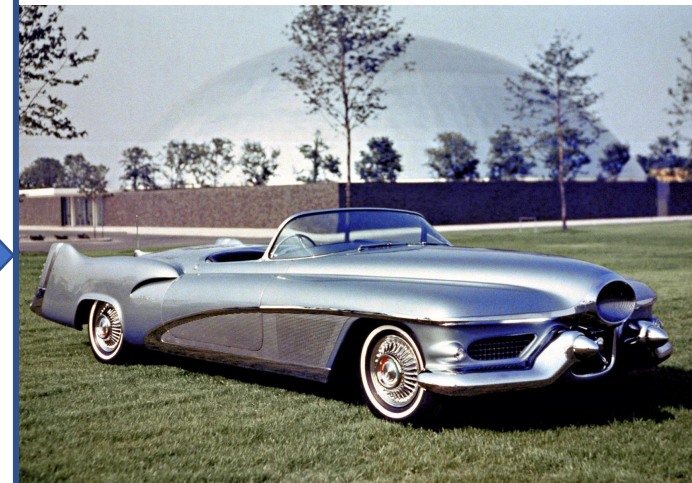
Molecular Modeling
Before The Cloud



Early Molecular Modeling
On The Cloud



Molecular Modeling
On The Cloud



“Why do we even use the term ‘horsepower’? Is that to further humiliate horses? The space-shuttle rockets have 20 million horsepower. Is there any point in still comparing it... to the horses?” -Jerry Seinfeld

Thanks! Hope miniCUP charges you up!

