



a PTEC project

PHARMAHUB

COLLABORATION FOR PHARMACEUTICAL ENGINEERING AND SCIENCE

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ERC

Structured Organic Particulate Systems

Manufacturing Science
Composite Structuring & Characterization
Particle Formation & Functionalization

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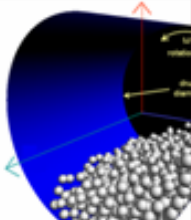
1 2 3 4 5 6

Flow Regime Models

Rotating Drum

1 Introduction → 2 Drum Diagram → 3 Describe Drum → 4 Describe Drum

Properties of the Drum	
Drum Diameter (meters):	50e-3
Drum Length (meters):	10e-3
Rotations/Minute:	100
Rotations:	2
Young's Modulus (SI units):	1e9



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NIPTE

The National Institute for Pharmaceutical Technology and Education

Improving quality and lowering the costs of

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Tools

- [Roller Compactor Johanson's Model](#)
- [Dynamic Roller Compactor](#)

Resources

- [Particle-based Computations Visualization Series](#)

Tags

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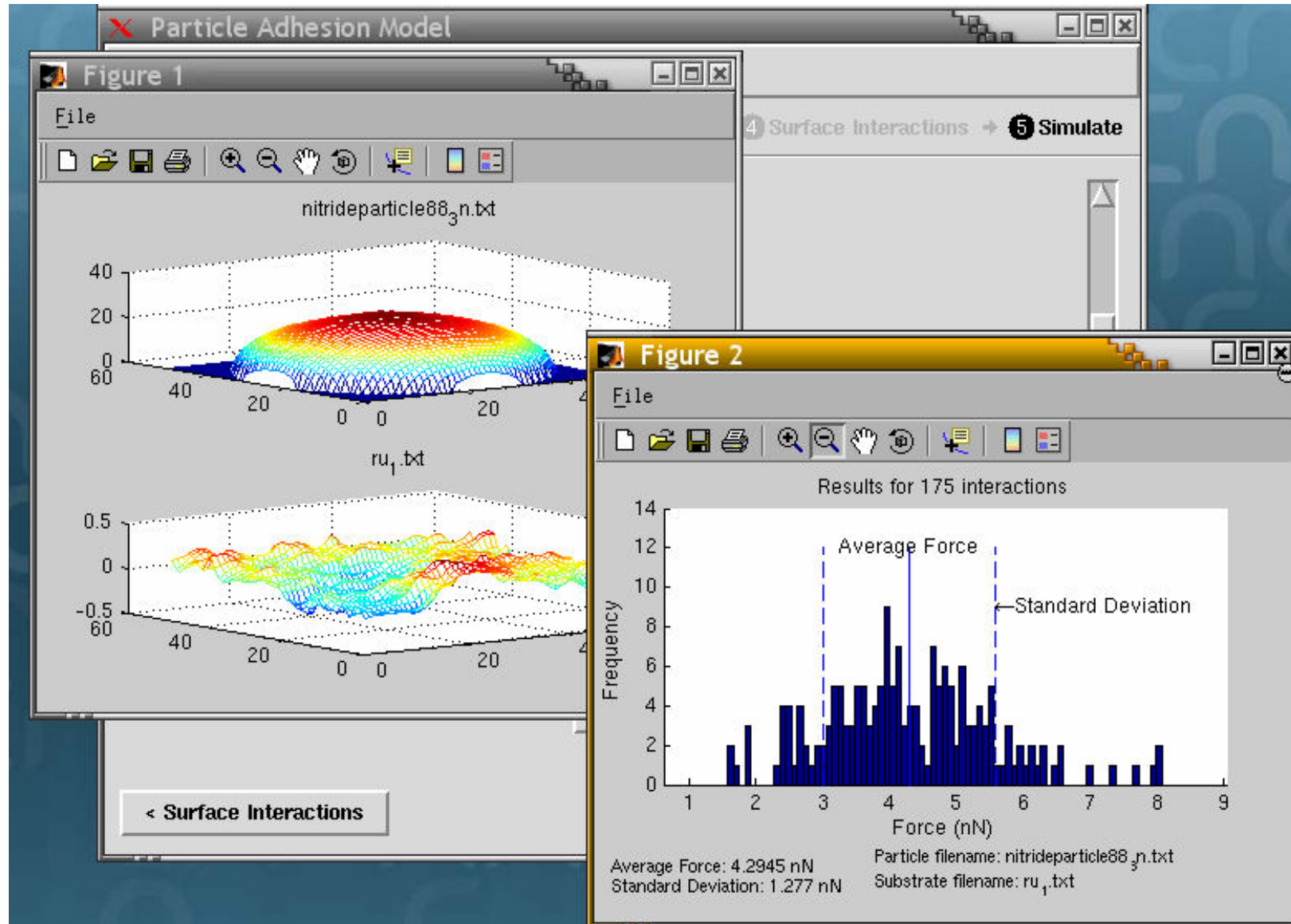
pharmaHUB Mission

- EVO tool: Resource for collaboration and sharing:
 - Science and engineering research on innovations in *pharmaceutical manufacturing*.
 - Information, knowledge, modeling & decision support tools for *drug product & process design*
 - Educational materials & experiences for education and training of *pharmaceutical technologists*.
- Sharing of research output of national projects
 - NSF ERC Structured Organic Particulate Systems
 - National Institute for Pharmaceutical Technology & Education (FDA support)

Tools Available

Particle-Surface Adhesion
Hopper Flow Discharge (DEM)
Rotating Drum (DEM)
High Shear Mixer (DEM)
Continuous Mixer (Compartment Model)
Roller Compactor
Dynamic Roller Compactor
SWOOP Ontology Browser
MOPP: Multipurpose Operation Production Planner
Level Set Dissolution

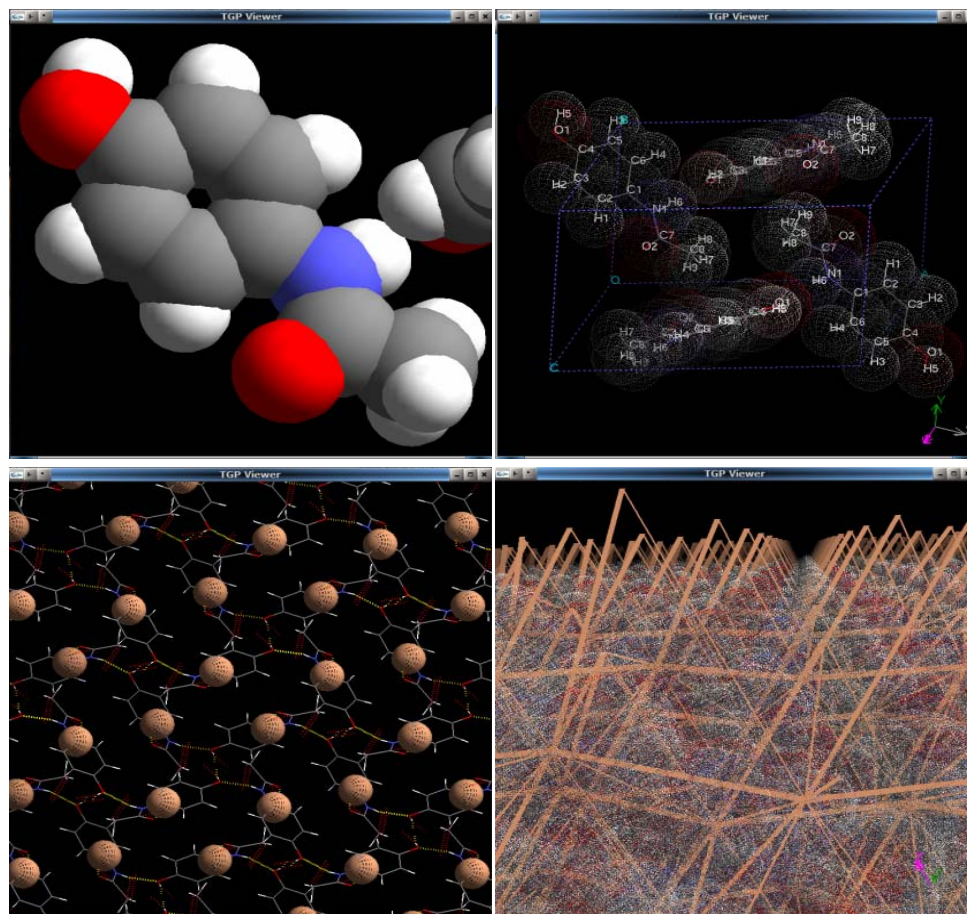
Particle adhesion simulation



ViewStruct: Visualization of Crystal Structures

S Boerrigter, *IPPH*

- Unit cells, labels
 - View range
- Representation Options
 - Wire frame
 - Covalent
 - Corey-Pauling-Koltun
 - Van der Waals
- Contacts and Interactions
 - Hydrogen bonds
- Crystal Graph
 - Growth Units
- View Options
 - Lighting, Perspective, Depth







Current: Download
Future: Hub-based tool


Online Presentations

Basic Forces in Particle Adhesion

Stephen Beaudoin
 Purdue University
 School of Chemical Engineering
 West Lafayette, IN 47907


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**ENGINEERING RESEARCH CENTER FOR
STRUCTURED ORGANIC PARTICULATE SYSTEMS**







RUTGERS UNIVERSITY
PURDUE UNIVERSITY
NEW JERSEY INSTITUTE OF TECHNOLOGY
UNIVERSITY OF PUERTO RICO AT MAYAGÜEZ



shortcourseforceintrowithwords

Outline	Thumb	Notes	Search
Slide Title		Duration	
▶ Basic Forces in Particle A...		00:35	
Course Outline		00:22	
Forces of Adhesion: Dry ...		01:40	
van der Waals (vdW) For...		01:23	
Describing vdW Forces		02:52	
Electrostatic (ES) Forces		01:45	
Forces of Interest: Aque...		01:56	
Solvation Forces		02:12	
Solvation Force		02:42	
Hydration Force		02:07	
Describing vdW Forces		01:59	

32 Minutes 26 Seconds Remaining




Slide 1 / 17 | Stopped
00:11 / 00:35




Long Term Development

- Visualization of particulate systems
- Model-based decision support
 - Generation and visualization of design space in process development
- Innovative learning modules for Pharma Engr degree
 - Convenient development, linking and use of complex modules involving simulations, presentations, videos, homework problems
- Growth of pharmaHUB community
 - Increase numbers of users, developers, contributors
 - New content, incentives
- New funding is being sought

pharmaHUB Usage (12/2007-6/2008)

Deployed on	12/11/2007
Hits	431,580
Visitors	1,411
Visits	3,671
Registered Accounts	118 (Current=163)
Simulation Users	82
Simulation Sessions	984
Elapsed Time	723 days
CPU Time	43 days
Interactive Time	81 days