

Welcome to NCMC-3: A Workshop on Combinatorial and High-Throughput Informatics

May 22-23, 2003

National Institute of Standards and Technology
Gaithersburg, MD



NIST
Combinatorial
Methods Center

<http://www.nist.gov/combi>

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Center for Theoretical and Computational Materials Science

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The NCMC Research Team

Polymers Division Core Group & Affiliates



Workshop Goals:



- 1) **Elucidate** issues in combinatorial and high-throughput informatics
- 2) **Consider** needs for further NIST research in combinatorial informatics
- 3) **Begin a process** for the establishment of combi informatics data interchange standards

Workshop Structure:

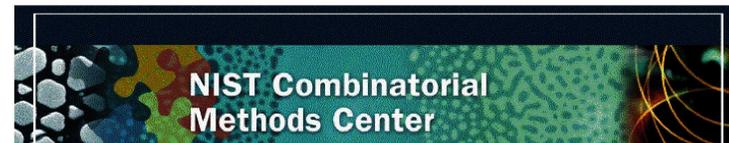
Elucidating issues in combi informatics

- Plenary Presentations:

Laurel Harmon
President, StriatuS Inc

David Rothman
Corporate R&D
The Dow Chemical Company

Prof. Krishna Rajan
Rensselaer Polytechnic
Institute



NCMC-3: Combinatorial Informatics
May 22-23, 2003 Bldg. 101 / Lecture Rm. A

Thursday, May 22 nd , 2003		Friday, May 23 rd , 2003	
8:30 am	Registration <i>Coffee & Doughnuts</i>	3:15 pm	<i>Coffee Break</i>
9:00 am	Welcome and Introductions Alamgir Karim, Eric Amis	3:30 pm	Standards Development Strategy John Barkley, Barbara Guttman, NIST
9:15 am	Combinatorial Materials Research: Challenges for Data Interchange and Analysis Laurel Harmon, StriatuS, Inc.	4:00 pm	Panel Discussion: NIST Role in Combinatorial Informatics Standards Development Mike Fasolka, NIST MSEL
10:00 am	<i>Coffee Break</i>	5:30 pm	Dinner Summit Station Restaurant & Brewery (227 East Diamond Ave, Gaithersburg)
10:15 am	Informatics in Materials Science and Basic Chemicals Research Dave Rothman, Dow Chemical	Friday, May 23rd, 2003	
11:00 am	Combinatorial Experimental Strategies Z. Q. John Lu, NIST ITL	8:30 am	<i>Coffee & Doughnuts</i>
11:30am	MatML: Definition, History, Results Ed Begley, NIST BFRL	9:00 am	An Informatics Infrastructure for <i>in-silico</i> Materials Science Krishna Rajan, Rensselaer Polytechnic Institute
12:00 pm	Lunch (NIST cafeteria, Bldg. 101)	9:45 am	Interoperability Standards in the Future Steven Ray, NIST MEL
1:15 pm	Statistical Software for Gradient Experiments Walter Liggett, NIST ITL	10:15 am	<i>Coffee Break</i>
1:45 pm	Electrostatic Coating process for Depositing Combinations of Nanoparticles from Dry as well as Wet Media Ajay P. Malshe, University of Arkansas	10:30 am	Discussion on Informatics Standards Working Groups
2:15 pm	XML Standards for Analytical Chemistry Gary Kramer, NIST CSTL	10:50 am	NCMC Informatics Project Wenhua Zhang, NIST MSEL
2:45 pm	NeXus: Interchange formats for scattering data Przemek Klosowski, NIST MSEL	11:20 am	NCMC Focused Projects Kathryn Beers, NIST MSEL Steve Hudson, NIST MSEL Christopher Stafford, NIST MSEL Focused Project Q&A
		12:20 pm	Lunch (NIST cafeteria, Bldg. 101)
		1:30 pm	NCMC Members Tours/Demos
		3:00 pm	Meeting Over

This meeting is co-sponsored by the NIST CTCMS

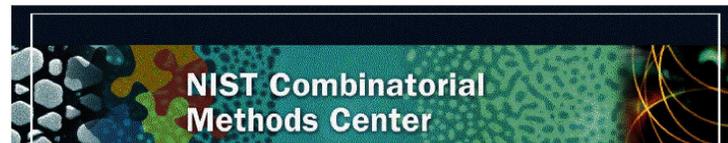
CTCMS www.ctcms.nist.gov
Center for Theoretical and Computational Materials Science

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Workshop Structure:

Beginning a data standards establishment process

- XML-based data interchange format examples
- Development and advancement strategies for interchange and interoperability standards
- Discussion and formation of *Combinatorial Materials Research Data Standards Working Group*



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