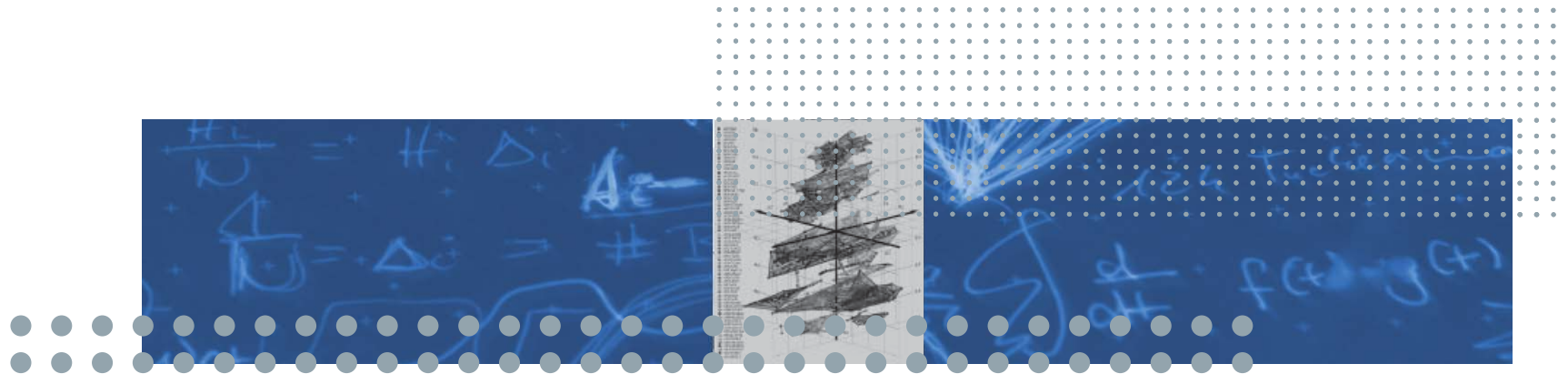


## Conference Site:

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## ADVANCED DISCUSSION From Atoms to Continuum

ICAMS  
INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION



## From Atoms to Continuum

09:00	Arrival / Coffee	13:45-15:00	Panel discussion: "From Atoms to Continuum"
09:25	Opening		Introductory statements: <i>M. Finnis (Imperial College, London), A. Hartmaier (ICAMS)</i>
09:30-10:15	<i>W. Curtin (EPFL, Lausanne):</i> From atoms to autos: Successes and challenges		Chair of discussion: <i>I. Steinbach (ICAMS)</i>
10:15-11:00	<i>D. Raabe (Max-Planck-Institut für Eisenforschung, Düsseldorf):</i> Scale hopping materials simulations and real atoms	15:00-15:30	Coffee break
11:00-11:30	Coffee break	15:30-17:10	Presentations from ICAMS
11:30-12:15	<i>E. Busso (Onera National Aerospace Research Centre, Paliseau Cedex):</i> On the incorporation of environmental effects on multi-scale modelling approaches		<i>G. Diaz Leines (ICAMS):</i> Nucleation during solidification in Ni: Atomistic insight from transition path sampling simulations
12:15-13:00	<i>E. Kozeschnik, A. Redermeier, D. Reith, T. Kerschner, R. Podlucky (Technische Universität, Wien):</i> Monte Carlo study of Cu precipitation in Fe – From temperature-dependent cluster expansion to local chemical environment potentials		<i>C. Begau (ICAMS):</i> Free energy function of dislocation densities in large scale atomistic simulations
13:00-13:45	Lunch		<i>O. Shchyglo, M. Mikolaychuk, I. Steinbach (ICAMS):</i> Stress-strain sensitive Gibbs energy of alloys
			<i>S. G. Fries (ICAMS):</i> Thermodynamic descriptions for solid phases
		17:10	End