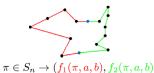


### Multiobjectivization

Some problems are easier to solve in a multiobjective scenario

example: TSP [Knowles et al. 2001]





### Multiobjectivization

by addition of new "helper objectives" [Jensen 2004] job-shop scheduling [Jensen 2004], frame structural design [Greiner et al. 2007], theoretical (runtime) analyses [Brockhoff et al. 2009]

by decomposition of the single objective

TSP [Knowles et al. 2001], minimum spanning trees [Neumann and Wegener 2006], protein structure prediction [Handl et al. 2008a], theoretical (runtime) analyses [Handl et al. 2008b]

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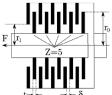
### **Innovization**

Often innovative design principles among solutions are found

example:

clutch brake design
[Deb and Srinivasan 2006]

min. mass + stopping time

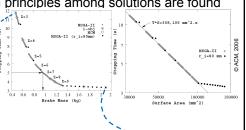


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### **Innovization**

Often innovative design principles among solutions are found

example: clutch brake design [Deb and Srinivasan 2006]



Solution					$x_5$	<i>3</i> ~	$f_2$
Min. $f_1$	70	90	1.5	1000	3	0.4704	11.7617
Min. $f_2$	80	110	1.5	1000	9	2.0948	3.3505

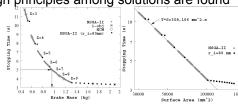
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### **Innovization**

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example:

clutch brake design [Deb and Srinivasan 2006]



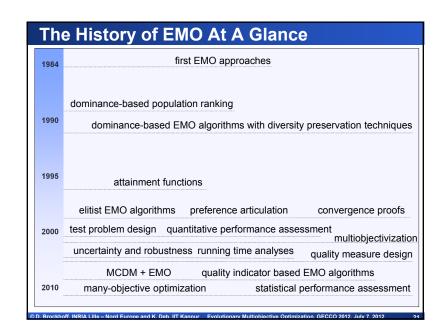
### Innovization [Deb and Srinivasan 2006]

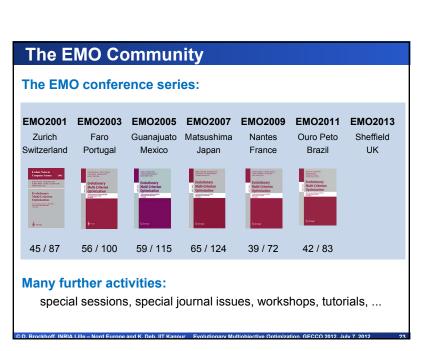
- = using machine learning techniques to find new and innovative design principles among solution sets
- = learning about a multiobjective optimization problem

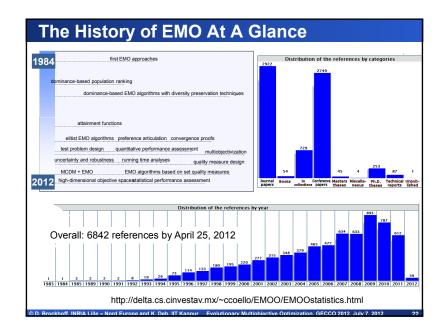
### Other examples:

- SOM for supersonic wing design [Obayashi and Sasaki 2003]
- biclustering for processor design and KP [Ulrich et al. 2007]

Described BIDIA III. New Forces and V. Deb HT Venues. Fundamental Multiplication Optionistics CECCO 2010. 10th 7 2010







### **Overview**

### The Big Picture

### **Basic Principles of Multiobjective Optimization**

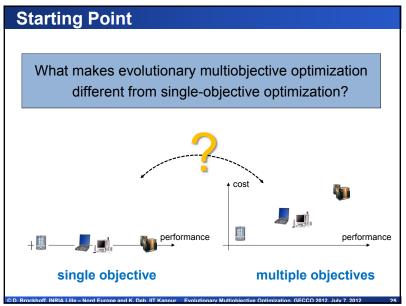
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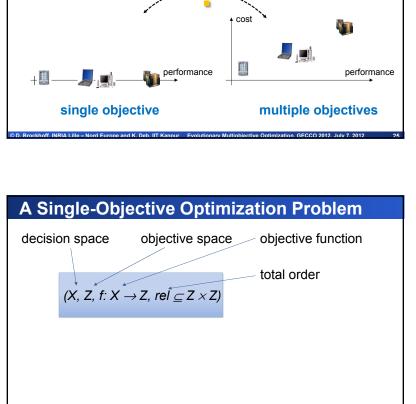
### Selected Advanced Concepts

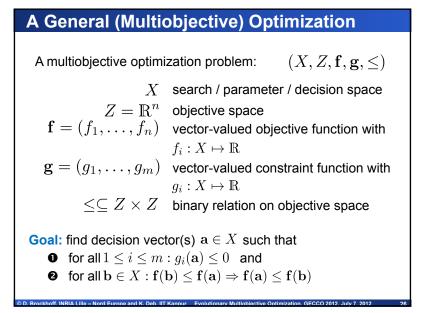
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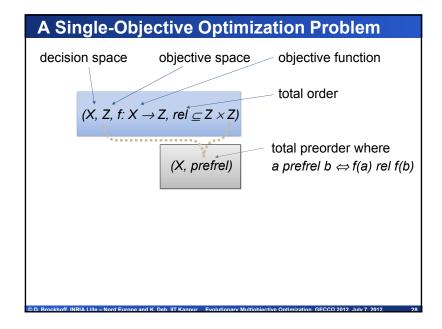
A Few Examples From Practice

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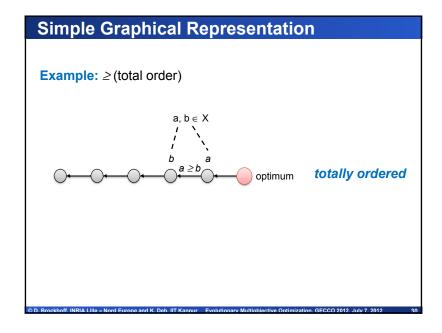


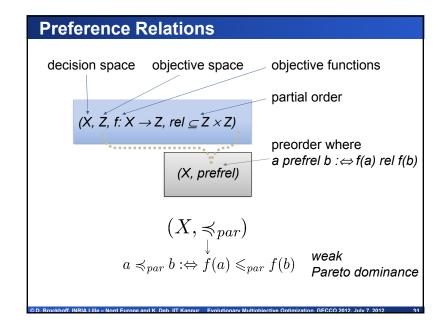


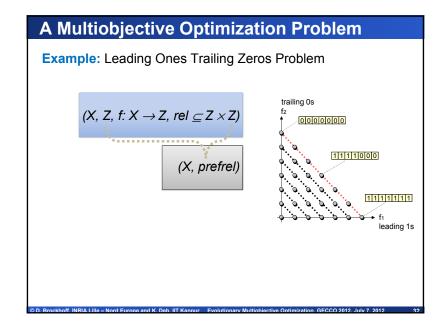


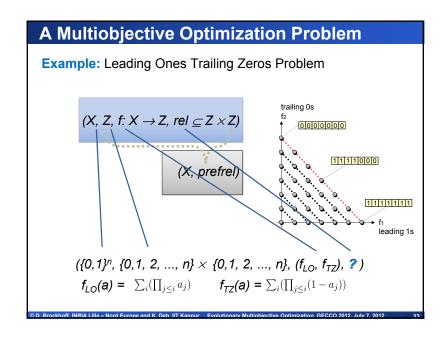


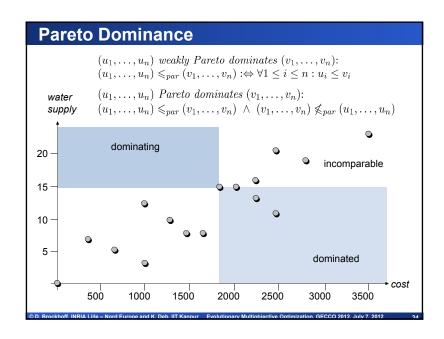
### Example: Leading Ones Problem $(X, Z, f: X \to Z, rel \subseteq Z \times Z)$ $(\{0,1\}^n, \{0,1,2,...,n\}, f_{LO}, \ge) \qquad \text{where } f_{LO}(a) = \sum_i (\prod_{j \le i} a_j)$

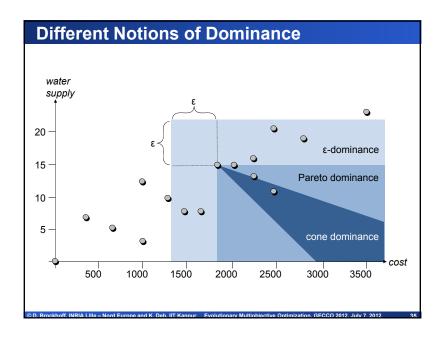


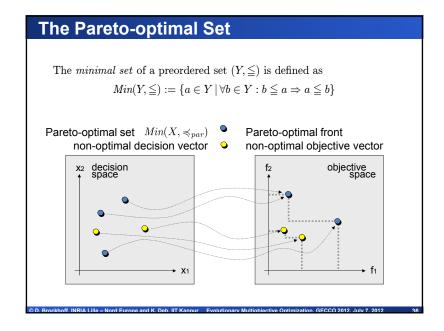




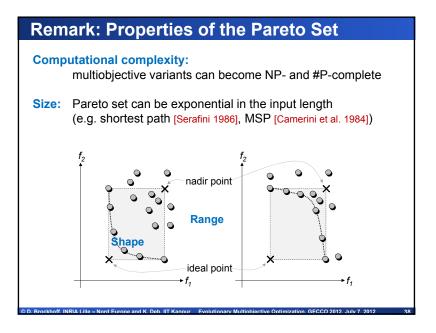








# Visualizing Preference Relations $(f_{\text{cost}})$ $(f_{\text{water supply}})$ $(X, \preccurlyeq par)$ $(x, ; f_{\text{water supply}})$ $(x, ; f_{\text{water supply})$ $(x, ; f_{\text{$



### **Approaches To Multiobjective Optimization**

A multiobjective problem is as such underspecified ...because not any Pareto-optimum is equally suited!

Additional preferences are needed to tackle the problem:

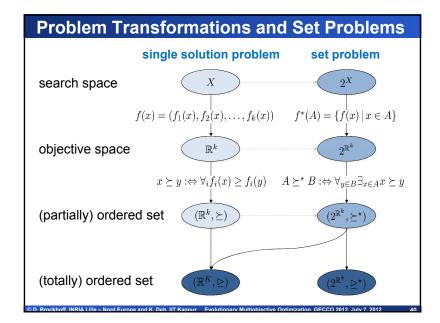
### **Solution-Oriented Problem Transformation:**

Induce a total order on the decision space, e.g., by aggregation.

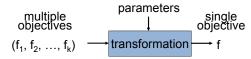
### **Set-Oriented Problem Transformation:**

First transform problem into a set problem and then define an objective function on sets.

Preferences are needed in any case, but the latter are weaker!

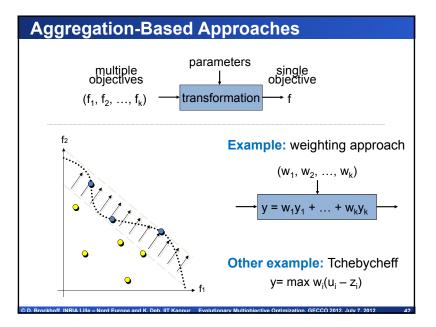


### **Solution-Oriented Problem Transformations**



A *scalarizing function s* is a function  $s: Z \mapsto \mathbb{R}$  that maps each objective vector  $(u_1, \ldots, u_n) \in Z$  to a real value  $s(u_1, \ldots, u_n) \in \mathbb{R}$ .

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### **Set-Oriented Problem Transformations**

For a multiobjective optimization problem  $(X, Z, \mathbf{f}, \mathbf{g}, \leq)$ , the associated *set problem* is given by  $(\Psi, \Omega, F, \mathbf{G}, \leq)$  where

- $\Psi = 2^X$  is the space of decision vector sets, i.e., the powerset of X,
- $\Omega = 2^Z$  is the space of objective vector sets, i.e., the powerset of Z,
- F is the extension of f to sets, i.e.,  $F(A) := \{f(\mathbf{a}) : \mathbf{a} \in A\}$  for  $A \in \Psi$ ,
- $\mathbf{G} = (G_1, \dots, G_m)$  is the extension of  $\mathbf{g}$  to sets, i.e.,  $G_i(A) := \max \{g_i(\mathbf{a}) : \mathbf{a} \in A\}$  for  $1 \le i \le m$  and  $A \in \Psi$
- $\leq$  extends  $\leq$  to sets where  $A \leq B : \Leftrightarrow \forall \mathbf{b} \in B \; \exists \mathbf{a} \in A : \mathbf{a} \leq \mathbf{b}.$

Pareto Set Approximation (algorithm outcome) = set of (usually incomparable) solutions

Performance

A weakly dominates B = not worse in all objectives and sets not equal

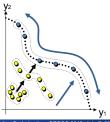
C dominates D = better in at least one objective

A strictly dominates C = better in all objectives

B is incomparable to C = neither set weakly better

### What Is the Optimization Goal (Total Order)?

- Find all Pareto-optimal solutions?
  - Impossible in continuous search spaces
  - ▶ How should the decision maker handle 10000 solutions?
- Find a representative subset of the Pareto set?
  - Many problems are NP-hard
  - What does representative actually mean?
- Find a good approximation of the Pareto set?
  - What is a good approximation?
  - How to formalize intuitive understanding:
    - close to the Pareto front
    - well distributed



### **General Remarks on Problem**

### Idea:

Transform a preorder into a total preorder

### Methods:

- Define single-objective function based on the multiple criteria (shown on the previous slides)
- Define any total preorder using a relation (not discussed before)

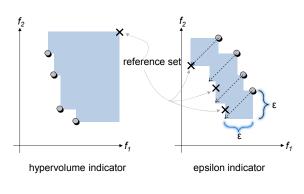
### Question:

Is any total preorder ok resp. are there any requirements concerning the resulting preference relation?

⇒ Underlying dominance relation *rel* should be reflected

### **Quality of Pareto Set Approximations**

A (unary) quality indicator I is a function  $I: \Psi \mapsto \mathbb{R}$  that assigns a Pareto set approximation a real value.



### **Refinements and Weak Refinements**

● ≼ refines a preference relation ≼ iff

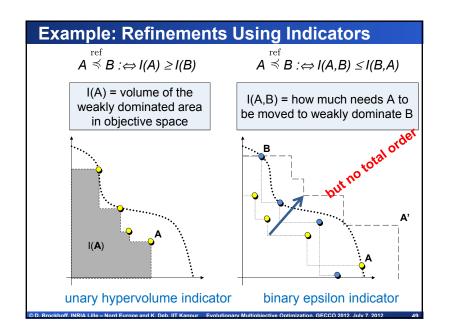
$$A \preceq B \land B \not\preceq A \Rightarrow A \preceq B \land B \not\preceq A$$
 (better  $\Rightarrow$  better)

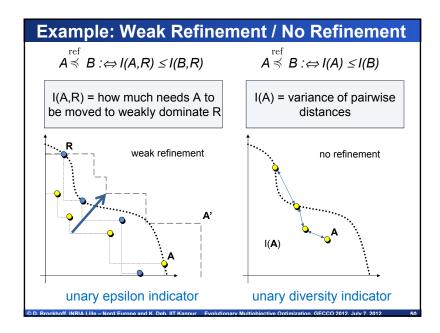
- ⇒ fulfills requirement
- $oldsymbol{2} \stackrel{\mathrm{ref}}{\preccurlyeq}$  weakly refines a preference relation  $\preccurlyeq$  iff

$$A \preccurlyeq B \land B \nleq A \Rightarrow A \stackrel{\text{ref}}{\preccurlyeq} B$$
 (better  $\Rightarrow$  weakly better)

 $\Rightarrow$  does not fulfill requirement, but  $\leq$  does not contradict  $\leq$ 

...sought are total refinements...





### **Overview**

The Big Picture

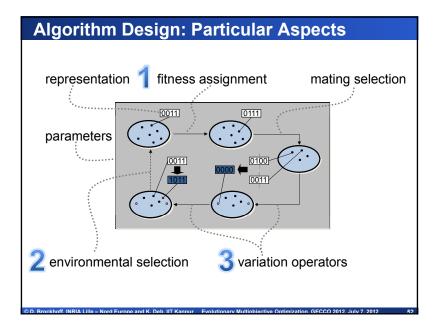
Basic Principles of Multiobjective Optimization

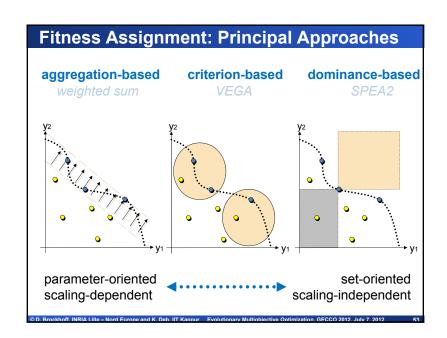
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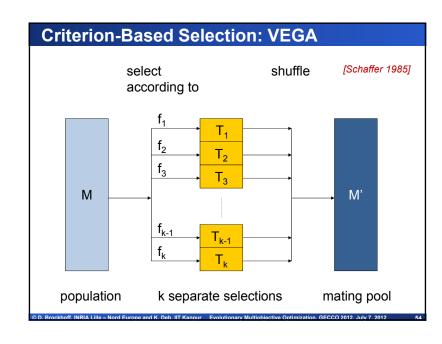
Selected Advanced Concepts

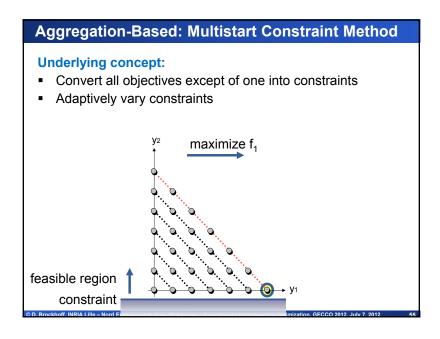
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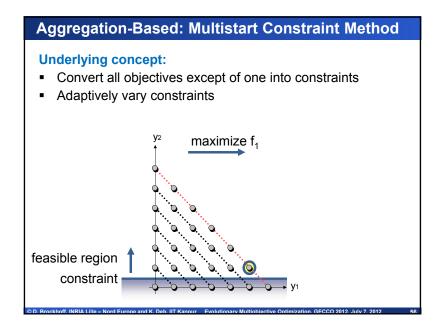
A Few Examples From Practice



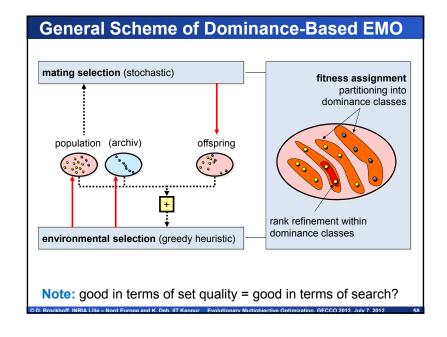


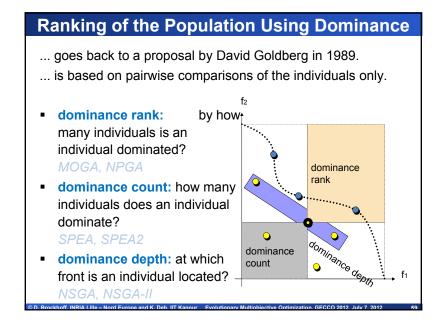


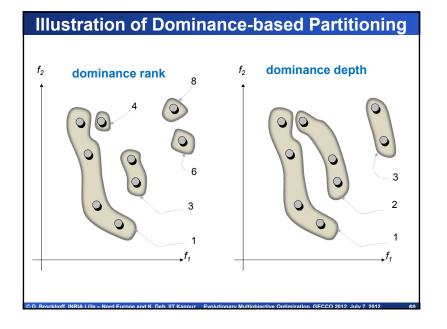




# Aggregation-Based: Multistart Constraint Method Underlying concept: Convert all objectives except of one into constraints Adaptively vary constraints maximize f constraint feasible region constraint







### **Refinement of Dominance Rankings**

Goal: rank incomparable solutions within a dominance class

• Density information (good for search, but usually no refinements)

### Kernel method

density = function of the distances



### k-th nearest neighbo density = function of distance

to k-th neighbor

### k-th nearest neighbor Histogram method

density = number of elements within box



2 Quality indicator (good for set quality): soon...

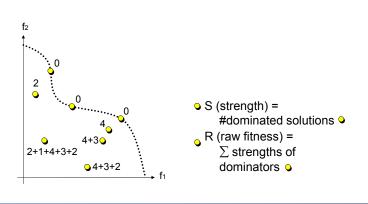
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### **Example: SPEA2 Dominance Ranking**

Basic idea: the less dominated, the fitter...

**Principle:** first assign each solution a weight (strength),

then add up weights of dominating solutions

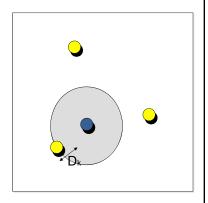


### **Example: SPEA2 Diversity Preservation**

### **Density Estimation**

k-th nearest neighbor method:

- Fitness = R + 1 / (2 + D<sub>k</sub>)
- D<sub>k</sub> = distance to the k-th nearest individual
- Usually used: k = 2



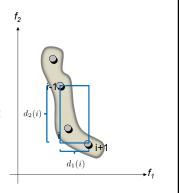
**Example: NSGA-II Diversity Preservation** 

### **Density Estimation**

crowding distance:

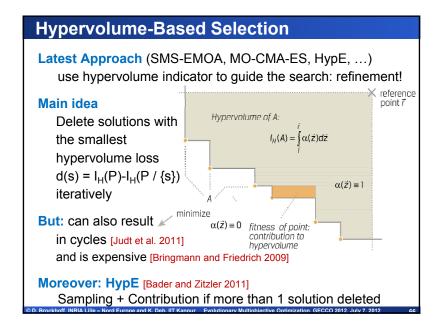
- sort solutions wrt. each objective
- crowding distance to neighbors:

$$d(i) - \sum_{\text{obj. } m} |f_m(i-1) - f_m(i+1)|$$



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# SPEA2 and NSGA-II: Cycles in Optimization Selection in SPEA2 and NSGA-II can result in deteriorative cycles Indicate the company of the co

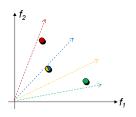


### **Decomposition-Based Selection: MOEA/D**

MOEA/D: Multiobjective Evolutionary Algorithm Based on Decomposition [Zhang and Li 2007]

### Ideas:

- Optimize N scalarizing functions in parallel
- Use only best solutions of "neighbored scalarizing function" for mating
- keep the best solutions for each scalarizing function
- use external archive for nondominated solutions



### **Variation in EMO**

- At first sight not different from single-objective optimization
- Most algorithm design effort on selection until now
- But: convergence to a set ≠ convergence to a point

### **Open Question:**

how to achieve fast convergence to a set?

### Related work:

- multiobjective CMA-ES [Igel et al. 2007] [Voß et al. 2010]
- set-based variation [Bader et al. 2009]
- set-based fitness landscapes [Verel et al. 2011]

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### **Overview**

The Big Picture

Basic Principles of Multiobjective Optimization

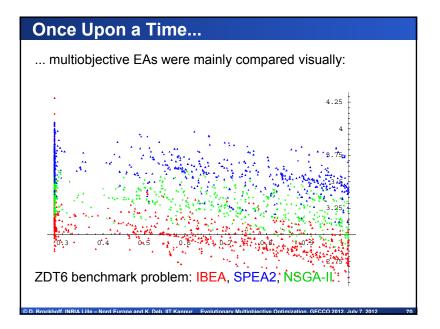
- algorithm design principles and concepts
- performance assessment

**Selected Advanced Concepts** 

- indicator-based EMO
- preference articulation

A Few Examples From Practice

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### **Two Approaches for Empirical Studies**

### **Attainment function approach:**

- Applies statistical tests directly to the samples of approximation sets
- Gives detailed information about how and where performance differences occur

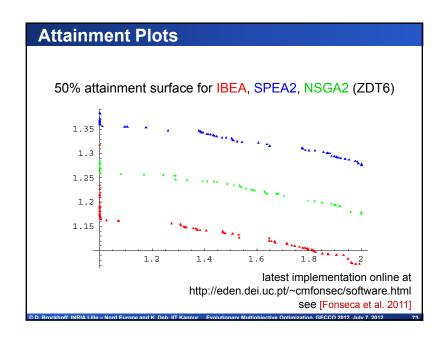
### A attains B attains

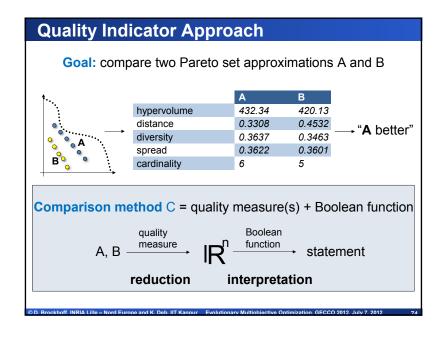
### **Quality indicator approach:**

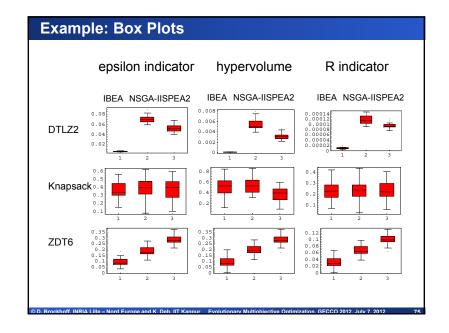
- First, reduces each approximation set to a single value of quality
- Applies statistical tests to the samples of quality values

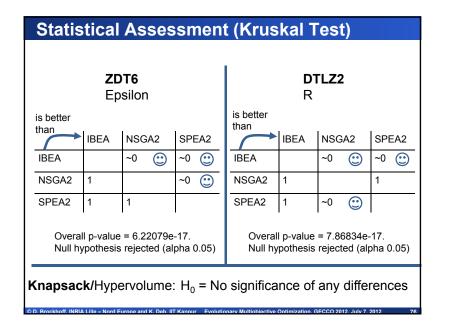
Indicator	A	В
Hypervolume indicator	6.3431	7.1924
$\epsilon$ -indicator	1.2090	0.12722
$R_2$ indicator	0.2434	0.1643
$R_3$ indicator	0.6454	0.3475

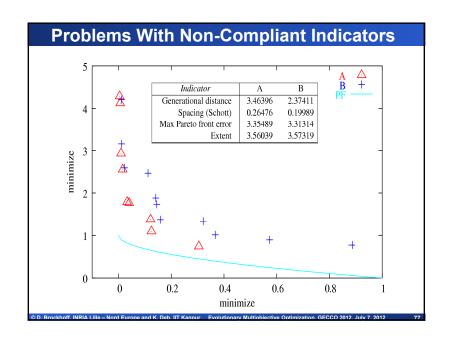
see e.g. [Zitzler et al. 2003]

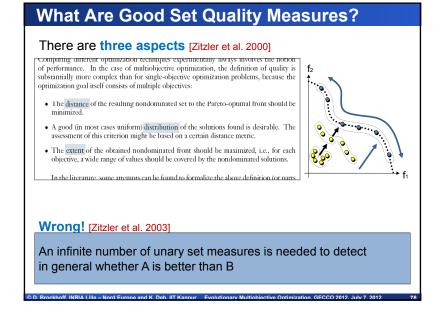












### **Set Quality Indicators**

### **Open Questions:**

- how to design a good benchmark suite?
- are there other unary indicators that are (weak) refinements?
- how to achieve good indicator values?

### **Overview**

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### **Indicator-Based EMO: Optimization Goal**

### When the goal is to maximize a unary indicator...

- we have a single-objective set problem to solve
- but what is the optimum?
- important: population size μ plays a role!

Multiobjective Indicator Single-objective Problem

### Optimal µ-Distribution:

A set of  $\mu$  solutions that maximizes a certain unary indicator I among all sets of  $\mu$  solutions is called optimal  $\mu$ -distribution for I. [Auger et al. 2009a]

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### Optimal µ-Distributions for the Hypervolume

Hypervolume indicator refines dominance relation

 $\Longrightarrow$  most results on optimal  $\mu\text{-distributions}$  for hypervolume

### Optimal µ-Distributions (example results)

### [Auger et al. 2009a]:

- contain equally spaced points iff front is linear
- density of points  $\propto \sqrt{-f'(x)}$  with f' the slope of the front

### [Friedrich et al. 2011]:

optimal  $\mu$ -distributions for the hypervolume correspond to E-approximations of the front

OPT  $1 + \frac{\log(\min\{1/3, b/5\})}{n}$ HYP  $1 + \frac{\sqrt{A/a} + \sqrt{B/b}}{n - 4}$  $\log$ HYP  $1 + \frac{\sqrt{\log(A/a)\log(B/b)}}{n}$ 

! (probably) does not hold for > 2 objectives

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### **Overview**

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A Few Examples From Practice

What we thought: EMO is preference-less

Given by the Divi.

Search before decision making: Optimization is performed without any preference information given. The result of the search process is a set of (ideally Pareto-optimal) candidate solutions from which the final choice is made by the DM.

Decision making during search: The DM can articulate preferences during

What we learnt: EMO just uses weaker preference information

environmental selection

3 out of 6

Preferable?

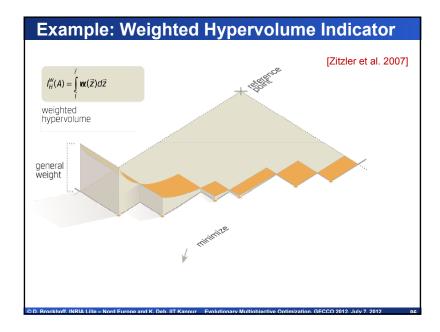
### Incorporation of Preferences During Search Nevertheless... • the more (known) preferences incorporated the better • in particular if search space is too large [Branke 2008], [Rachmawati and Srinivasan 2006], [Coello Coello 2000]

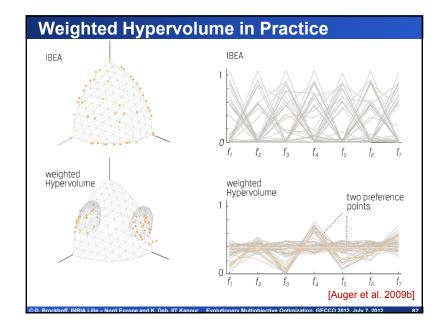
- Refine/modify dominance relation, e.g.:
  - using goals, priorities, constraints [Fonseca and Fleming 1998a,b]
  - using different types of cones [Branke and Deb 2004]

### 2 Use quality indicators, e.g.:

- based on reference points and directions [Deb and Sundar 2006, Deb and Kumar 2007]
- based on binary quality indicators [Zitzler and Künzli 2004]
- based on the hypervolume indicator (now) [Zitzler et al. 2007]

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### **Overview**

The Big Picture

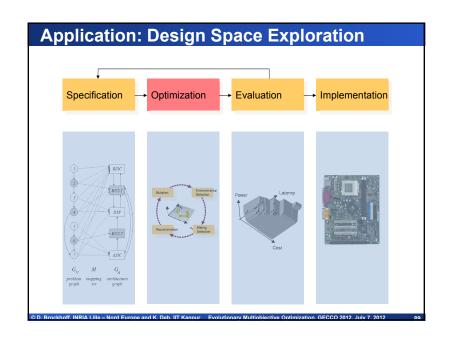
Basic Principles of Multiobjective Optimization

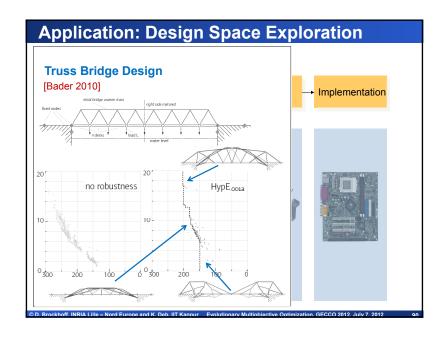
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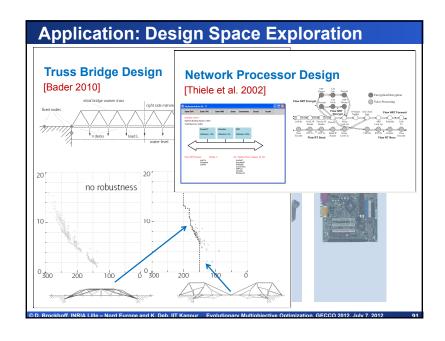
Selected Advanced Concepts

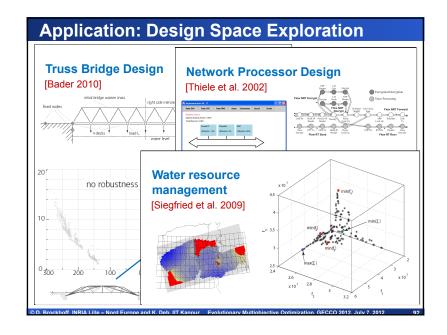
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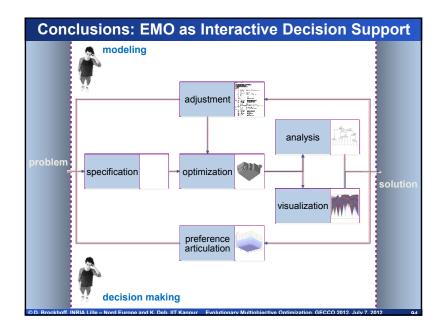








### **Application: Trade-Off Analysis** Module identification from biological data [Calonder et al. 2006] Find group of genes wrt GE f, vs. GE f, GE f<sub>1</sub> vs. PPI f<sub>2</sub> different data types: → GE f₁ vs. metabolic f₂ 0.7 similarity of gene expression profiles 0.4 overlap of protein interaction partners 0.2 metabolic pathway map distances distance objective f, (A.U.)



### **The EMO Community**

### Links:

- EMO mailing list: http://w3.ualg.pt/lists/emo-list/
- EMO bibliography: http://www.lania.mx/~ccoello/EMOO/
- EMO conference series: http://www.shef.ac.uk/emo2013/

### **Books:**

- Multi-Objective Optimization using Evolutionary Algorithms
  Kalyanmoy Deb, Wiley, 2001
- Evolutionary Algorithms for Solving Multi Evolutionary Algorithms for Solving Multi-Objective Problems Objective Problems, Carlos A. Coello Coello, David A. Van Veldhuizen & Gary B. Lamont, Kluwer, 2<sup>nd</sup> Ed. 2007
- Multiobjective Optimization—Interactive and Evolutionary Approaches, J. Branke, K. Deb, K. Miettinen, and R. Slowinski, editors, volume 5252 of *LNCS*. Springer, 2008 [many open questions!]
- and more...

PISA: http://www.tik.ee.ethz.ch/pisa/

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### **Additional Slides**

D. Brockhoff, INRIA Lille - Nord Europe and K. Deb. IIT Kanpur Evolutionary Multiobjective Optimization, GECCO 2012, July 7, 2012

### **Instructor Biography: Kalyanmoy Deb**

### Kalyanmoy Deb

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He holds Deva Raj Chair Professor at Indian Institute of Technology Kanpur in India. He is the recipient of the prestigious MCDM Edgeworth-Pareto award by the Multiple Criterion Decision Making (MCDM) Society, one of the highest awards given in the field of multi-criterion optimization and decision making. He has also received prestigious Shanti Swarup Bhatnagar Prize in Engineering Sciences for the year 2005 from Govt. of India.

He has also received the `Thomson Citation Laureate Award' from Thompson Scientific for having highest number of citations in Computer Science during the past ten years in India. He is a fellow of Indian National Academy of Engineering (INAE), Indian National Academy of Sciences, and International Society of Genetic and Evolutionary Computation (ISGEC). He has received Fredrick Wilhelm Bessel Research award from Alexander von Humboldt Foundation in 2003. His main research interests are in the area of computational optimization, modeling and design, and evolutionary algorithms. He has written two text books on optimization and more than 240 international journal and conference research papers. He has pioneered and a leader in the field of evolutionary multi-objective optimization. He is associate editor of two major international journals and an editorial board members of five major journals.

Brockhoff, INRIA Lille - Nord Europe and K. Deb. IIT Kanpur Evolutionary Multioblective Optimization, GECCO 2012, July 7, 2012

### **Instructor Biography: Dimo Brockhoff**

### **Dimo Brockhoff**

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After obtaining his diploma in computer science (Dipl.-Inform.) from University of Dortmund, Germany in 2005, Dimo Brockhoff received his PhD (Dr. sc. ETH) from ETH Zurich, Switzerland in 2009. Between June 2009 and October 2011 he held postdoctoral research positions---first at INRIA Saclay Ile-de-France in Orsay and then at Ecole Polytechnique in Palaiseau, both in France. Since November 2011 he has been a junior researcher (CR2) at INRIA Lille - Nord Europe in Villeneuve d'Ascq, France . His research interests are focused on evolutionary multiobjective optimization (EMO), in particular on many-objective optimization, benchmarking, and theoretical aspects of indicator-based search.

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