A Parallel Direct Search Algorithm

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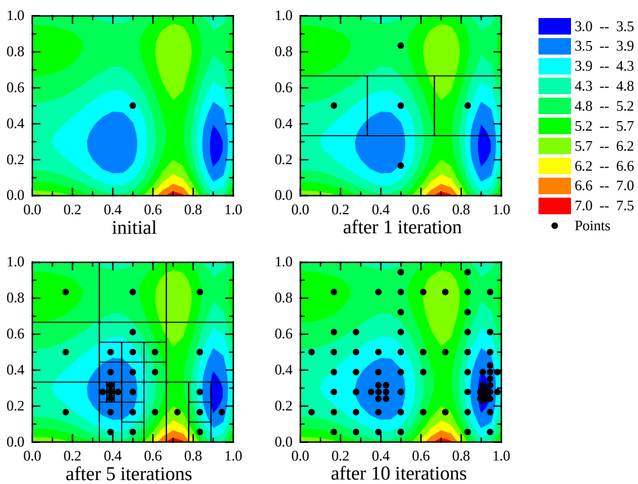
Outline

1. DIRECT Global Search Algorithm (Jones, Perttunen, and Stuckman, 1993)
   - DIviding RECTangles in action
   - Algorithm description
   - Global convergence property
2. Parallel Scheme and Implementation
   - Design challenges
   - Dynamic data structures
   - A dynamic parallel scheme
3. Applications
   - Cell cycle modeling
   - Aircraft design: HSCT (high speed civil transport)
   - Wireless communication system design
4. References

DIRECT Global Search Algorithm

DIviding-RECTangles in action



DIRECT Global Search Algorithm

Algorithm description

Given an objective function f and the design space $D = D_0$:

Step 1. Normalize the design space D to be the unit hypercube. Sample the center point c_i of this hypercube and evaluate $f(c_i)$. Initialize $f_{\min} = f(c_i)$, evaluation counter $m = 1$, and iteration counter $t = 0$.

Step 2. Identify the set S of potentially optimal boxes.

Step 3. Select any box $j \in S$.

Step 4. Divide the box j as follows:

(1) Identify the set I of dimensions with the maximum side length. Let δ equal one-third of this maximum side length.

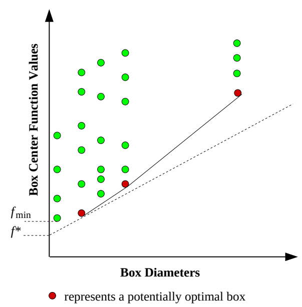
(2) Sample the function at the points $c \pm \delta e_i$ for all $i \in I$, where c is the center of the box and e_i is the ith unit vector.

(3) Divide the box j containing c into thirds along the dimensions in I, starting with the dimension with the lowest value of $w_i = \min\{f(c+\delta e_i), f(c-\delta e_i)\}$, and continuing to the dimension with the highest w_i. Update $f_{\min}$ and m.

Step 5. Set $S = S - \{j\}$. If $S \neq \emptyset$ go to Step 3.

Step 6. Set $t = t + 1$. If iteration limit or evaluation limit has been reached, stop. Otherwise, go to Step 2.

DIRECT Global Search Algorithm
Global convergence property



- Box selection rule: box j is potentially optimal if

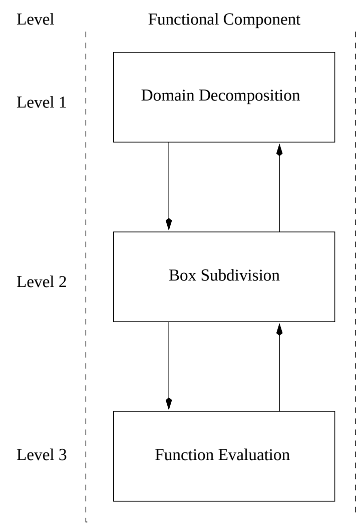
$$f(c_j) - \tilde{K}d_j \le f(c_i) - \tilde{K}d_i,$$

$$f(c_j) - \tilde{K}d_j \le f_{\min} - \epsilon|f_{\min}|,$$

for some $\tilde{K} > 0$ and $i = 1, \ldots, m$ (the total number of subdivided boxes)

- Lipschitz continuity is required in the domain.

Parallel Scheme and Implementation
Design challenges



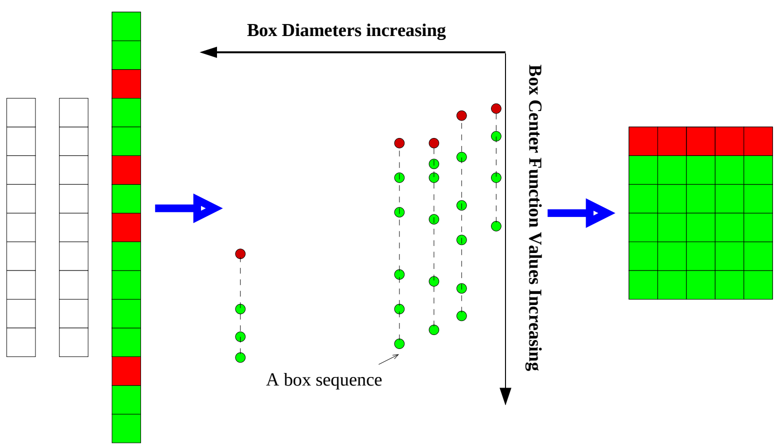
1. Unpredictable storage requirement
2. A single starting point
3. Unpredictable workload
4. Strong data dependency

A 3-functional level dynamic parallel scheme:

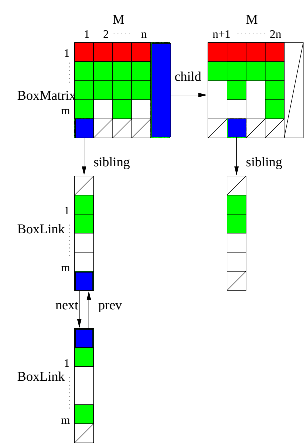
1. Dynamic data structures
2. Single-start to multi-start
3. Dynamic load balancing
4. Dynamic process role change

Parallel Scheme and Implementation
Dynamic data structures

From 1-D data structures to a 2-D data structure.

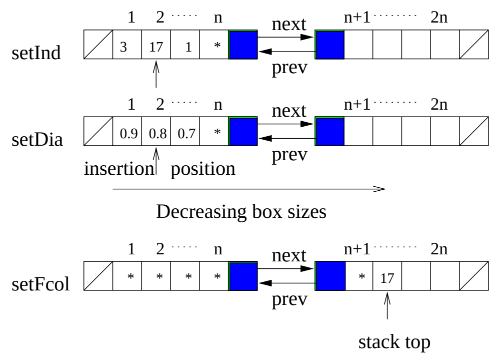


Parallel Scheme and Implementation
Dynamic data structures—box structures



- Two-dimensional dynamic structure
- Priority queue vs. sorted list

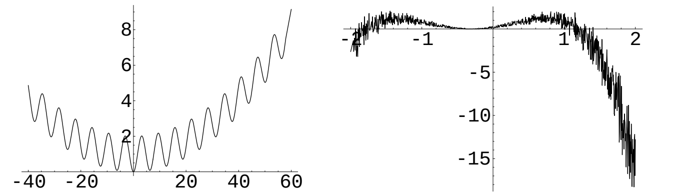
Parallel Scheme and Implementation
Dynamic data structures—Linked list structures



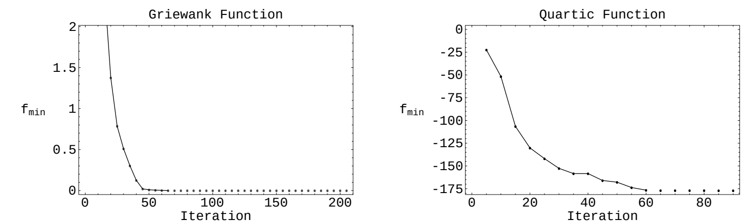
- Maintain 2-D structure
- Recycle box sequence columns

Parallel Scheme and Implementation
Performance studies

- Objective function convergence tolerance τ

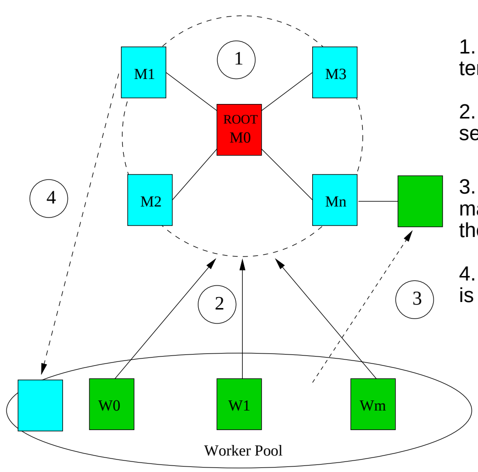


One-dimensional Griewank function and quartic function



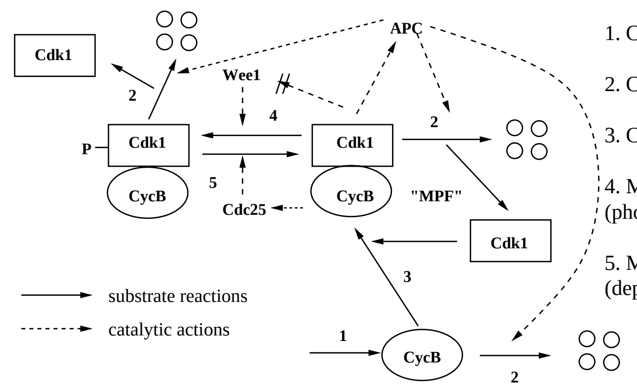
Comparison of $\tau = 0.0001$ (solid) and $\tau = 0$ (dotted)

Parallel Scheme and Implementation
A dynamic parallel scheme



1. Masters decompose the domain, control global termination, and merge the results to the root master.
2. Masters share a worker pool, where each worker sends requests to randomly selected masters.
3. A randomly selected worker becomes a new master to share the box subdivision tasks with the memory overloaded master.
4. A master becomes a worker when the search is done in its subdomain.

Applications
Cell cycle modeling—the wiring diagram for frog eggs



1. CycB synthesis
2. CycB degradation (APC)
3. CycB + Cdk1
4. MPF inactivation (phosphorylation by Wee1)
5. MPF reactivation (dephosphorylation by Cdc25)

Applications

Cell cycle modeling—the ODE system

Apply mass-action kinetics and Michaelis-Menten rate laws to the wiring diagram.

$$\frac{dM}{dt} = \big(v_d'(1-D) + v_d''D\big)(C_T - M) - \big(v_w'(1-W) + v_w''W\big)M, \quad (1)$$

$$\frac{dD}{dt} = v_d\left(\frac{M(1-D)}{K_{md} + (1-D)} - \frac{\rho_d D}{K_{mdr} + D}\right), \quad (2)$$

$$\frac{dW}{dt} = v_w\left(-\frac{MW}{K_{mw} + W} + \frac{\rho_w(1-W)}{K_{mwr} + (1-W)}\right), \quad (3)$$

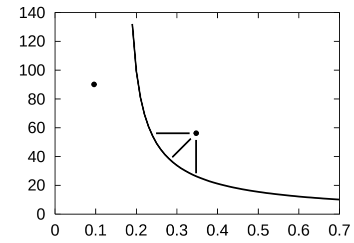
where

M = [MPF]/[total Cdk1],
D = [Cdc25P]/[total Cdc25],
W = [Wee1]/[total Wee1],
C_T = [total cyclin]/[total Cdk1].

M, D, W, and C_T represent scaled concentrations of active MPF, active Cdc25, active Wee1, and total cyclin in the extract, respectively. The parameters v_d', v_d'', v_w', v_w'', v_d, K_{md}, ρ_d, K_{mdr}, v_w, K_{mw}, ρ_w, and K_{mwr} are also scaled, making the system dimensionless.

Applications

Cell cycle modeling—the objective function



$$y_i = f_i(x_i;\beta), i = 1\ldots n,$$

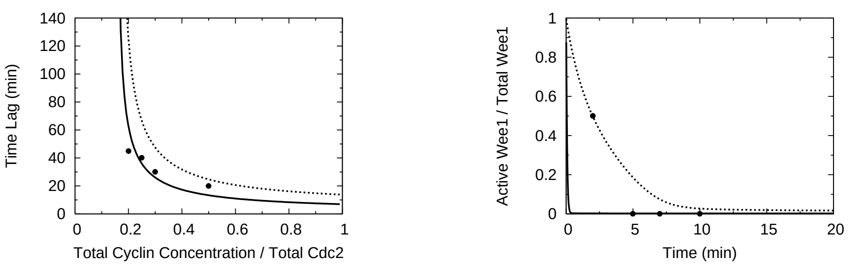
$$E_{min} = \min_{\beta,\delta}\left(\sum_{i=1}^{n} \epsilon_i^T w_{\epsilon_i}\epsilon_i + \delta_i^T w_{\delta_i}\delta_i\right),$$

subject to the constraints

$$\epsilon_i = f_i(x_i + \delta_i;\beta) - y_i, i = 1,\ldots,n.$$

Applications

Resulting goodness-of-fit for frog eggs



generated by the optimal parameters

generated by the parameters known in literature: Marlovits et al. (left) and Moore (right).

Applications

Parallel efficiency for frog eggs

The parallel efficiency E is defined as

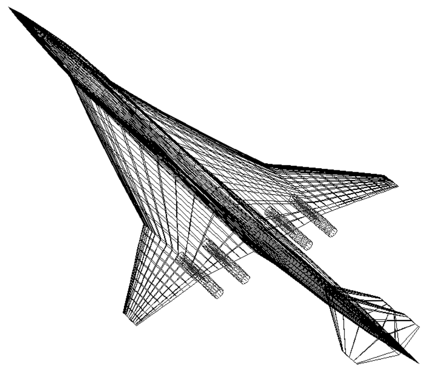
$$E = \frac{S_r}{p/base},$$

where $S_r = \mathrm{Time}_{base}/\mathrm{Time}_p$ is the relative speedup.

	Frog Egg Model				
I	3	6	$E(6)$	15	$E(15)$
10	1432	1152	0.62	372	0.77
20	3939	2267	0.87	1045	0.75
40	8657	4936	0.88	1960	0.88

Application in Aircraft Design: HSCT (high speed civil transport
Problem scenario

Optimization objective: minimize takeoff gross weight (TOGW) for a range of 5500 nautical miles and a cruise Mach number of 2.4, while carrying 251 passengers.



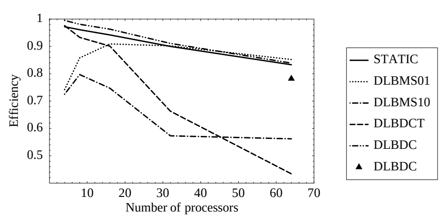
Typical high speed civil transport (HSCT) configuration.

Application in Aircraft Design: HSCT
Optimization design variables and constraints

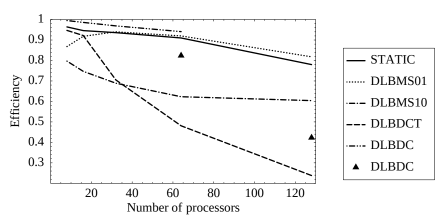
1. **28 design variables:**
- Geometry of the aircraft: 24 variables in 6 categories
  wing planform,
  airfoil shape,
  tail areas,
  nacelle placement,
  and fuselage shape.
- Idealized cruise mission: 4 variables
  mission fuel,
  engine thrust,
  initial cruise altitude,
  and constant climb rate.

2. **68 constraints in 3 categories:**
- Geometry
- Performance
- Aerodynamic

Application in Aircraft Design: HSCT
Parallel efficiency comparison



Original DIRECT.



Aggressive DIRECT.

Application in Wireless Design: S^4W
Problem scenario

1. **Transmitter placement optimization:** ensuring an acceptable level (*threshold*) of wireless system *performance* within a *geographical area* of interest at a minimum *cost*.

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2. **Problem abstraction:**

$$\min_{x \in D} f_0(x),$$

$$D = \{x \in D_0 \mid f_j(x) \leq 0,\ j = 1, \ldots, J\},$$

where $D_0 = \{x \in E^n \mid \ell \leq x \leq u\}$ is a simple box constraint set.

Application in Wireless Design: S⁴W

Objective formulation

1. **Power coverage:**

$$\frac{\text{Number of receivers with received power above threshold}}{\text{Total number of receivers}}$$

2. **Bit error rate (BER):**

$$\frac{\text{Number of incorrectly received bits}}{\text{Total Number of received bits}}$$

3. **Observation:** Discrete vs. continuous.
4. **Reformulation:**

- **Decision variables for n transmitters over m receivers:**

$$X = (x_1, y_1, z_1, x_2, y_2, z_2, \ldots, x_n, y_n, z_n),$$

where $z_i = z_0$.

Application in Wireless Design: S⁴W

Objective formulation (cont.)

- **Objective function**

Average shortfall of the estimated performance metric from the given threshold T:

$$f(X) = \begin{cases} \frac{1}{m}\sum_{i=1}^{m}(T - p_{ki})_+, & \text{coverage,} \\ \frac{1}{m}\sum_{i=1}^{m}(p_{ki} - T)_+, & \text{BER.} \end{cases}$$

p_{ki}: performance metric of transmitter (k,i) evaluated at the ith receiver location, where transmitter (k,i), located at $(x_k, y_k, z_0),\ 1 \le k \le n$, generates the highest power level $P_{ki}(x_k, y_k, z_0) \ge P_{ji}(x_j, y_j, z_0),\ 1 \le j \le n$, at the receiver location $i,\ 1 \le i \le m$.

Power coverage optimization:

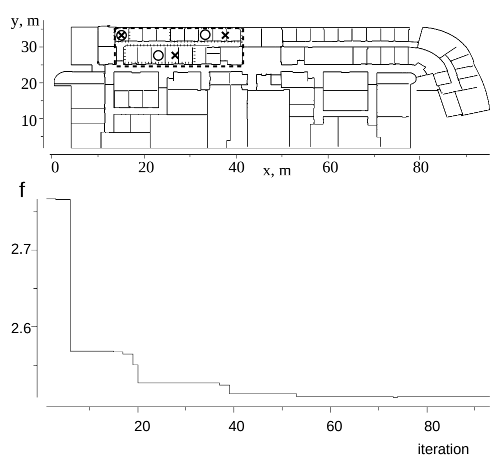
$p_{ki} = P_{ki}(x_k, y_k, z_0), (T - p_{ki})_+$ is the penalty for a low power level.

BER optimization:

$p_{ki} = \log_{10}(\mathrm{BER}_{ki}), (p_{ki} - T)_+$ is the penalty for a high bit error rate.

Application in Wireless Design: S⁴W

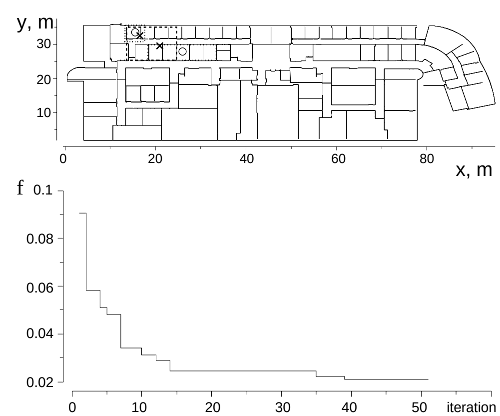
Optimization results



Power coverage optimization results for three transmitters. The starting (optimal) locations are marked with circles (crosses).

Application in Wireless Design: S⁴W

Optimization results



BER optimization results for two transmitters. The starting (optimal) locations are marked with circles (crosses).

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