SOLVING COMPLEX APPLIED GLOBAL OPTIMIZATION PROBLEMS IN A DISTRIBUTED ENVIRONMENT

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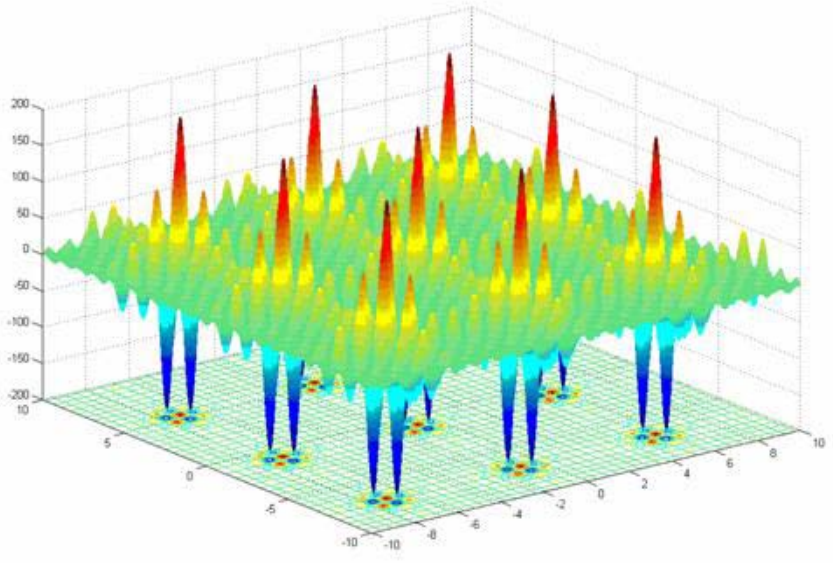
GLOBAL OPTIMIZATION

$$f(x) \to \min,\ x \in G \subseteq \Re^n$$



Basic types:
- continuous;
- discrete;
- mixed.

Possible problem statement:
- find global minimum (maximum),
- find all local minima (maxima) points,
- find all stationary points.

APPLICATION OF GLOBAL OPTIMIZATION

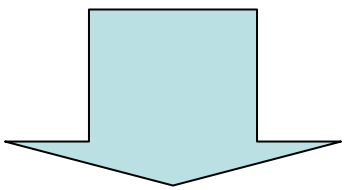
- Computational chemistry.
- Design automation (VLSI design).
- Construction of transport networks.
- Mathematical economy problems.
- Scheduling problems (train scheduling, optimization of work-flows)
- ……

METHODS FOR SOLVING GLOBAL OPTIMIZATION PROBLEMS

- Methods with the prove of optimality (to a given precision)
  - Branch-and-bound;
  - Branch-and-cut;
  - …
- Heuristic methods
  - Stochastic methods;
  - Genetic methods;
  - Tabu search;
  - …

COMMON GLOBAL OPTIMIZATION METHODS

- Different GO algorithms have a lot in common
- High complexity
- Decompositional structure



UNIVERSAL HIGH-PERFORMANCE SOLUTIONS ARE NEEDED

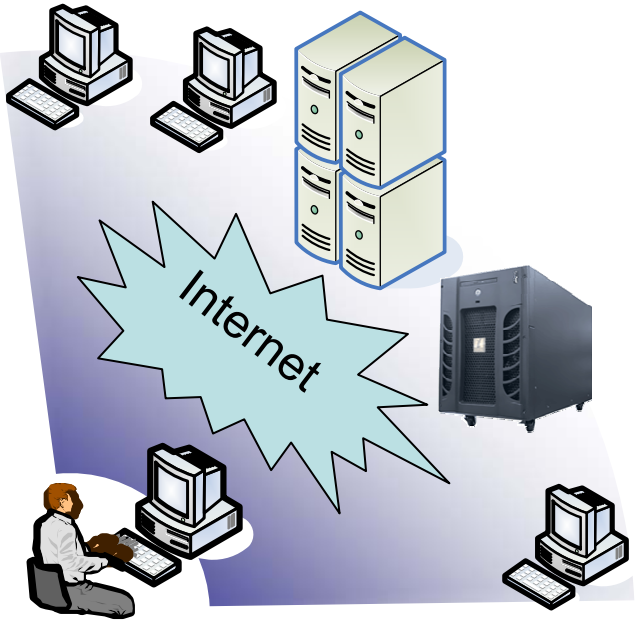
DISTRIBUTED PROGRAMMING ENVIRONMENT FOR SOLVING LARGE-SCALE GLOBAL OPTIMIZATION PROBLEMS

Features:

- Use in computations heterogeneous geographically distributed computing resources;

- Solve different kinds of GO problems;

- Support for long-running computations with control points, restart and fault-tolerance.

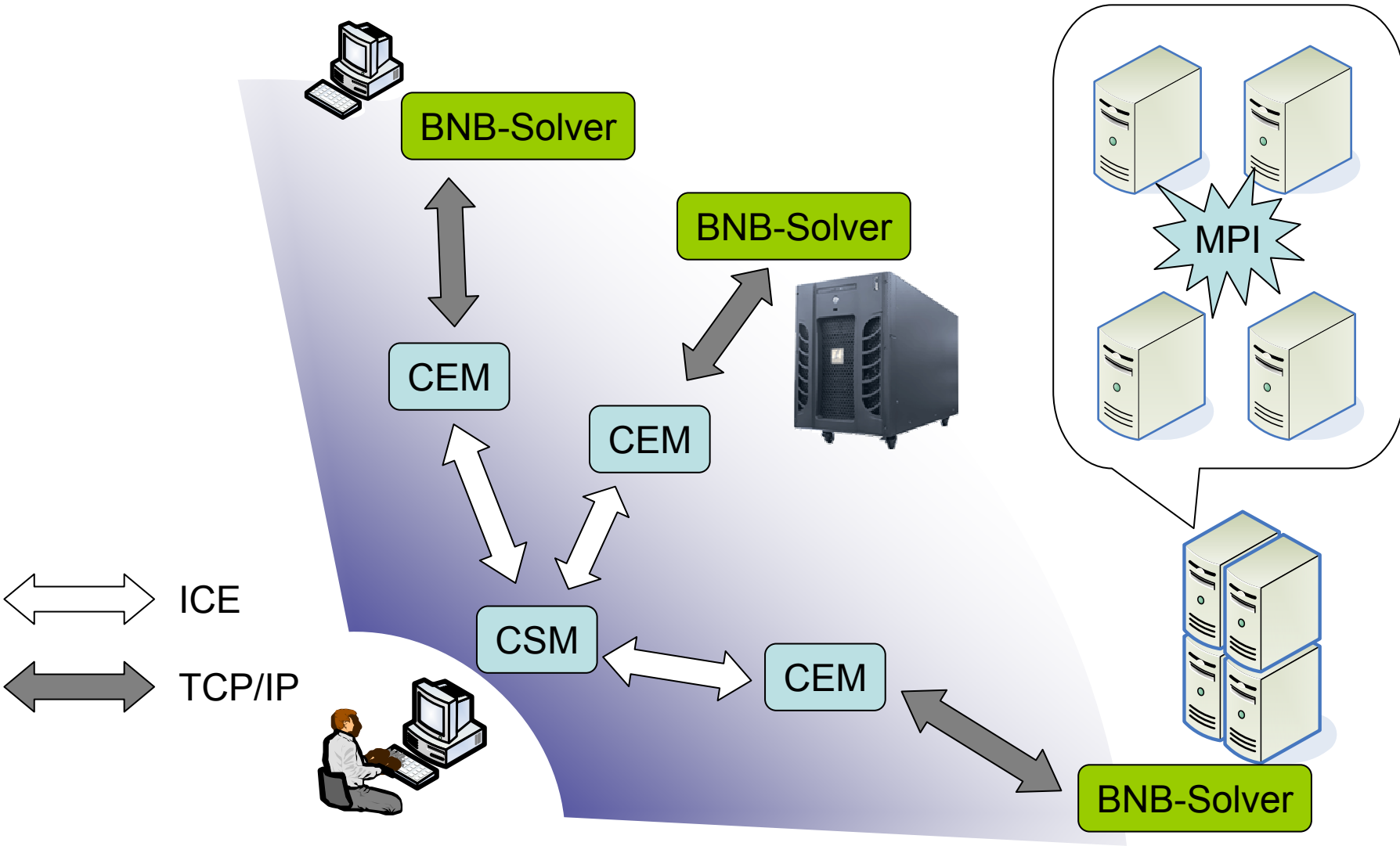


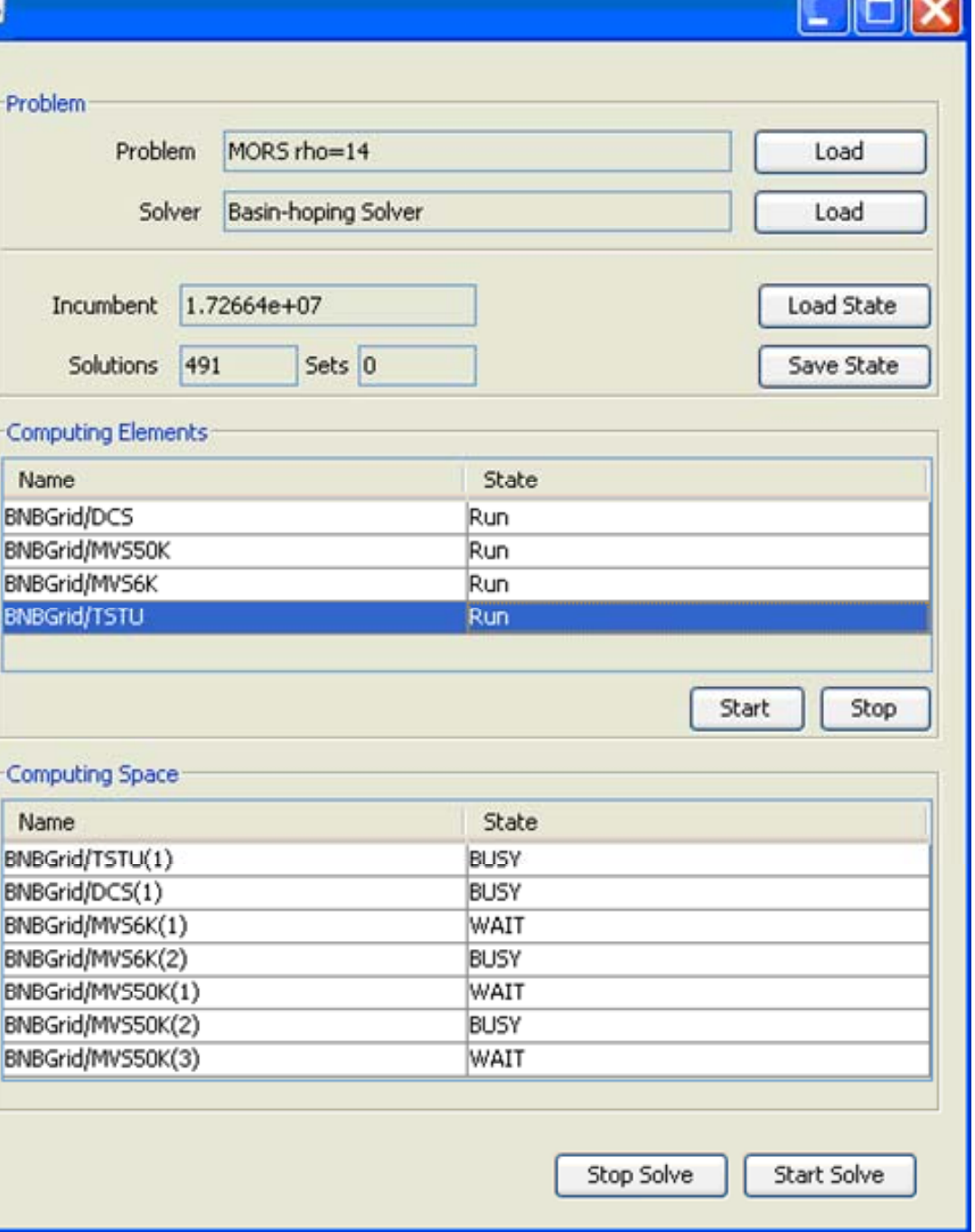
SUPPORTED PROBLEMS

Flexible infrastructure. Implementing of a new problem or resolution method requires minimal efforts: only problem-specific parts should be implemented. Problem-independent modules for computing space management, interactions, load-balancing remain intact.

Currently
- Knapsack problem (exact and heuristic algorithms).
- Continuous Global optimization (branch-and-bound, multi-start, basin-hoping).

ARCHITECTURE





Исходные данные
и состояние задачи

Список вычислительных
узлов

Список запущенных приложени
(вычислительное пространств

SEARCHING FOR OPTIMAL MOLECULAR CONFORMATION

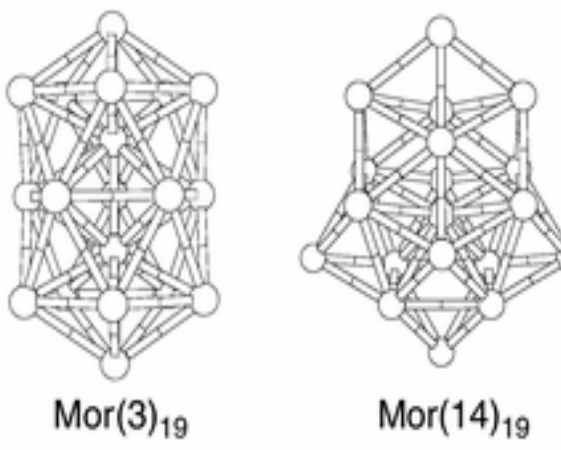
$$F(x) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} v\left(\left\| x^{(i)} - x^{(j)} \right\|\right) \rightarrow \mathbf{min}$$

$\left\| x^{(i)} - x^{(j)} \right\|$ - distance between atom i and j;

$v(r)$ - pair potential;

$v_{LJ}(r) = \frac{1}{r^{12}} - \frac{2}{r^{6}}$ - Lennard-Jones potential;

$v_M(r;\rho) = e^{\rho(1-r)}\left(e^{\rho(1-r)} - 2\right)$ - Morse potential.



COMPUTATIONAL EXPERIMENTS

Environment

Название	Архитектура процессора	Число процессоров	Местоположение	Наличие системы пакетной обработки
MVS50K	Clovertown (4 core), 3 GHz	940	МСЦ РАН (Москва)	+
MVS6K	Itanium II, 2.2 GHz	256	ВЦ РАН(Москва)	+
TSTU	Pentium IV, 3.2 GHz	8	ТГУ (Тамбов)	-
DCS	Pentium IV, 3.2GHz	1	ИСА РАН (Москва)	-

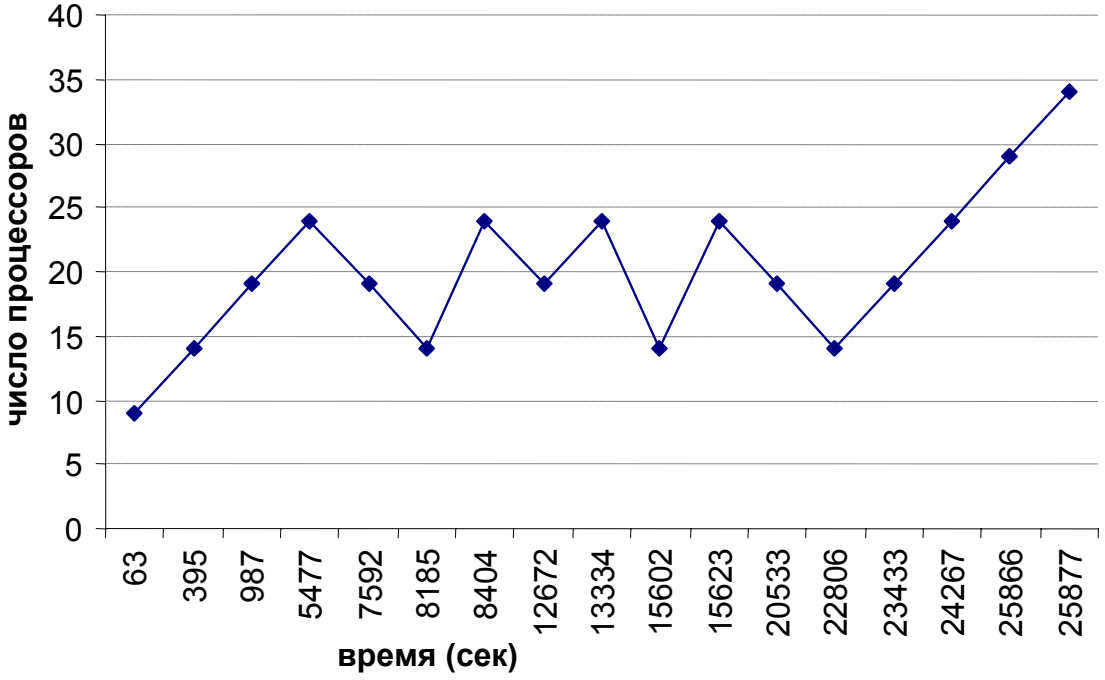
METHODS: MULTI-START + BASIN-HOPING (with Conjugate Gradient)

Most complex conformations for

Morse potential $\rho = 14$

50-80 atoms were found.

Number of atoms	Time to reach minimum	Value
50	19 m	-198.456
60	26 m.	-244.579
70	2 hours 11 m.	-292.463
80	4 hours 32 m.	-340.811



Number of processors as a function of talk

THANK YOU !