Optimus: A Parallel Optimization Framework with Topology Aware PSO and Applications

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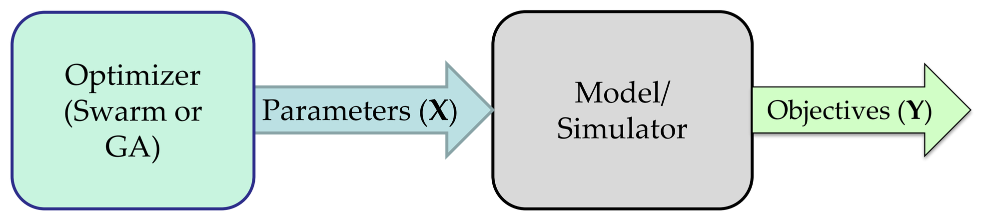
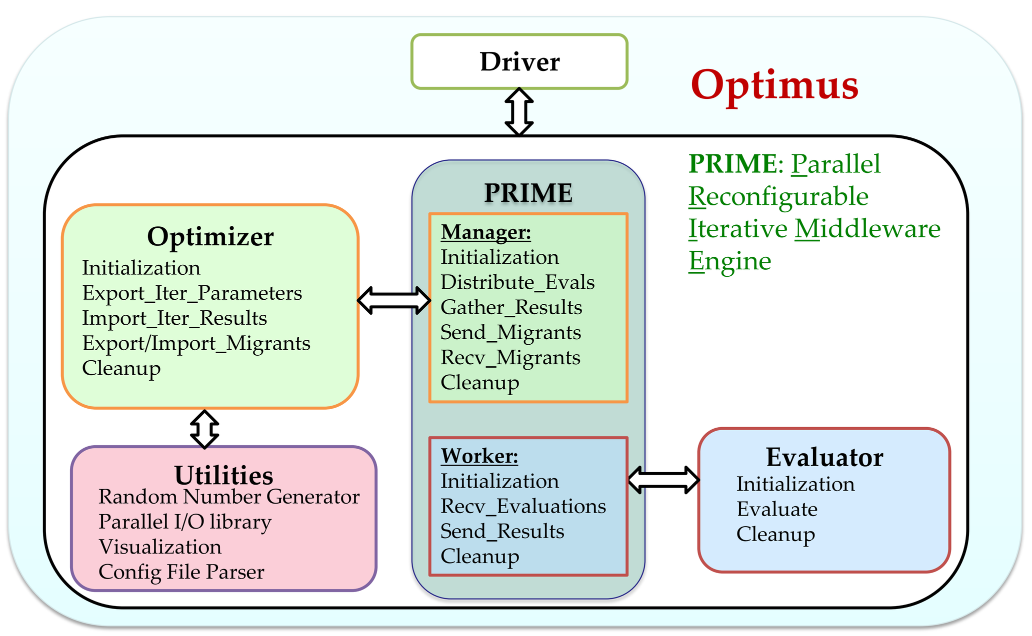
Simulation - Optimization



- Find optimal parameters(X*) to minimize/maximize objectives (Y)

Optimus: Optimization Methods for Universal Simulators



Contributions

- Optimus, a parallel platform for algorithmic exploration coupling optimization methods with target applications
- PRIME, scalable middleware component for effective deployment on leadership class supercomputers
- CoMSO, cooperative multi-swarm approach to achieve faster convergence and better solutions for difficult multi-modal problems
- TAPSO, new technique for graph based optimization problems

Particle Swarm Optimization(PSO)

- Emulates swarming behavior in nature
- Particle → Candidate solution
- Particles *fly* across parametric space
- Movement governed by mathematical rules

Flock of birds in Italy forming curious shapes
Courtesy: National Geographic

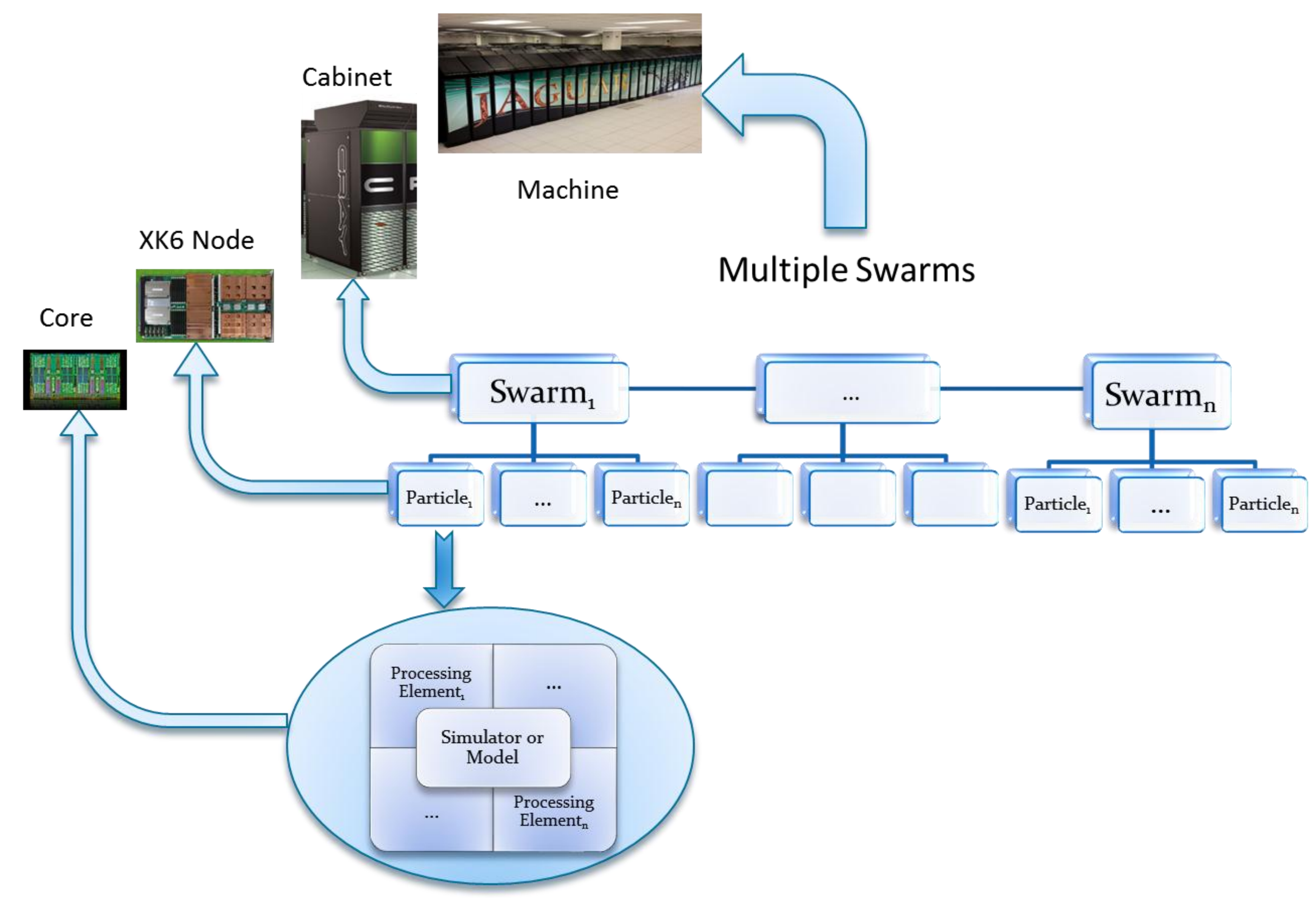
PSO Operations

$$\vec{v}_i^t = w^t \vec{v}_i^{t-1} + c_1\psi_1(\vec{p}_i - \vec{X}_i^{t-1}) + c_2\psi_2(\vec{p}_g - \vec{X}_i^{t-1})$$

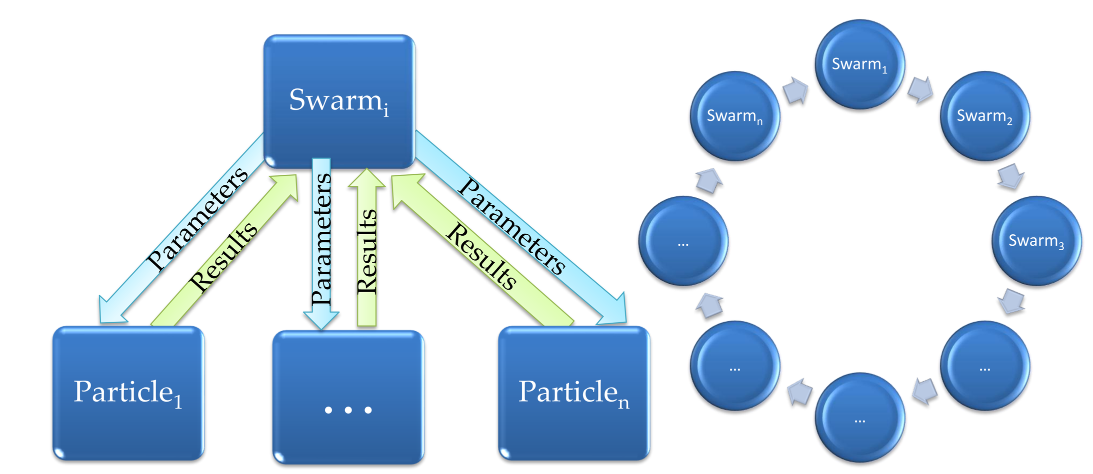
$$\vec{X}_i^t = \vec{X}_i^{t-1} + \underbrace{\Delta\vec{X}_i^t}_{\chi\vec{v}_i^t}$$

Velocity Components
- Inertial component
- Cognitive component
- Social component

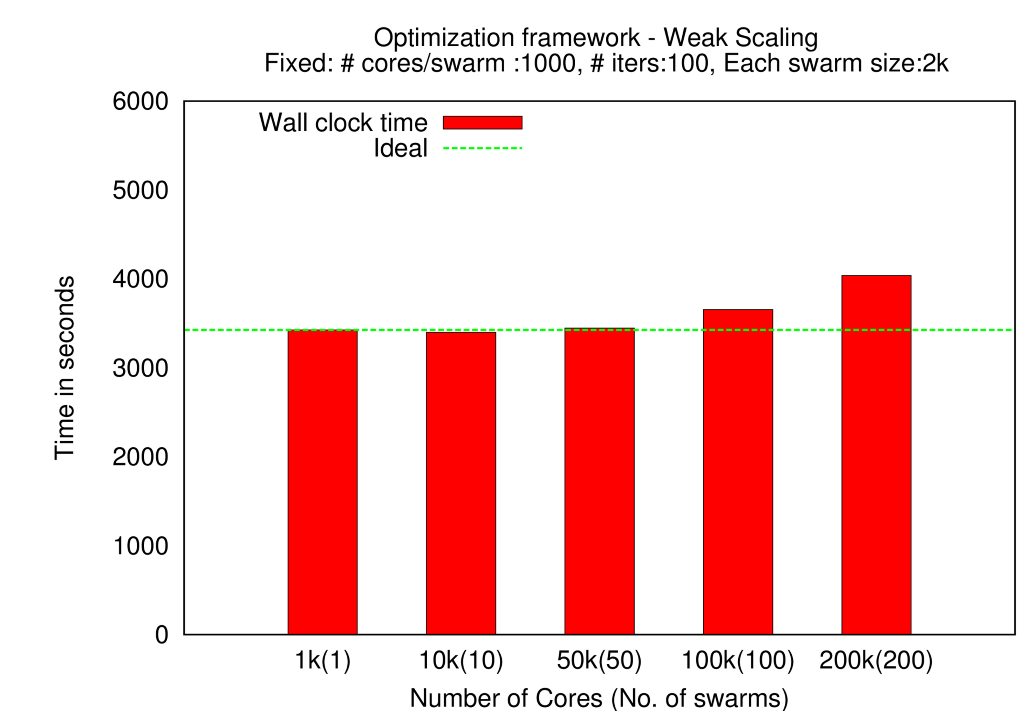
Cooperative Multi-Swarm Optimization (CoMSO)



Communication Patterns

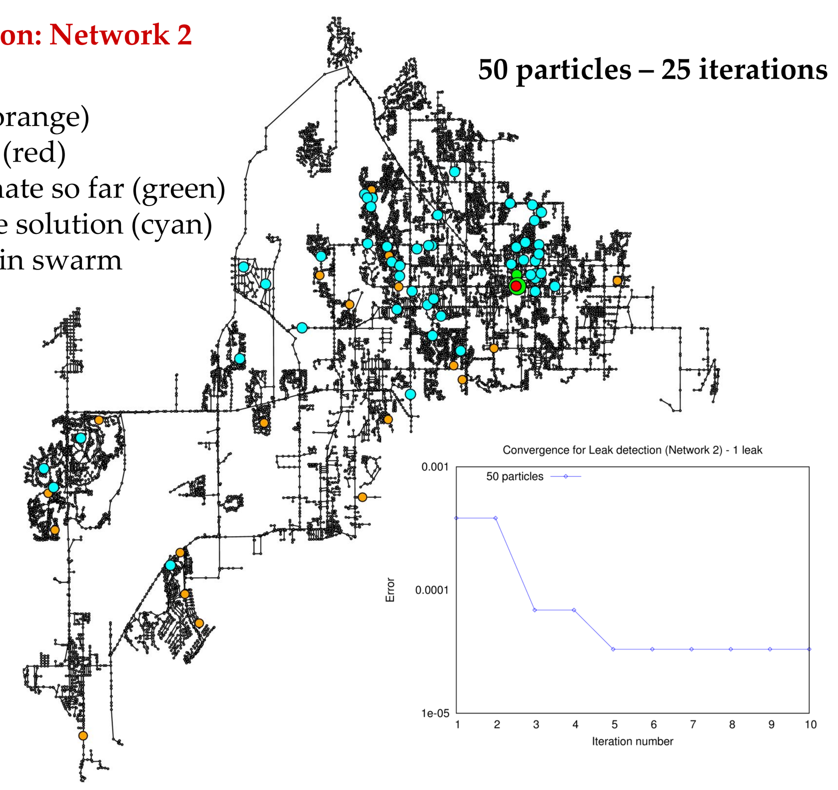


Optimization Framework: Weak Scaling



Single computer (40 million simulations) : 18.66 years

Water Distribution Systems (WDS)



- Simulator: EPANET
- Two optimization problems
  - Contaminant source characterization
  - Leak detection
- Match sensor observations to simulations
- Compare 'Estimated Leak' to 'True Leak' scenario
- Minimize error between concentration, flow and pressure measurements at sensors at various timesteps

WDS problems: Objectives

Contaminant Source Characterization

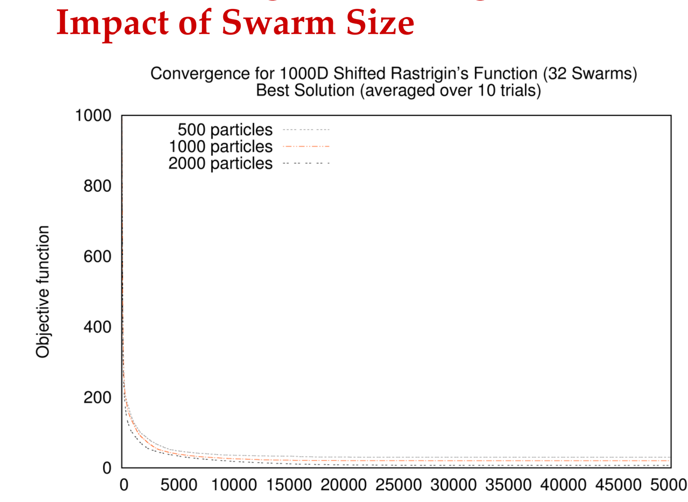
Minimize $\left\{ \|\mathbf{C}_{obs} - C(\vec{\mathbf{m}})\|^2 \right\}$

Leak Detection

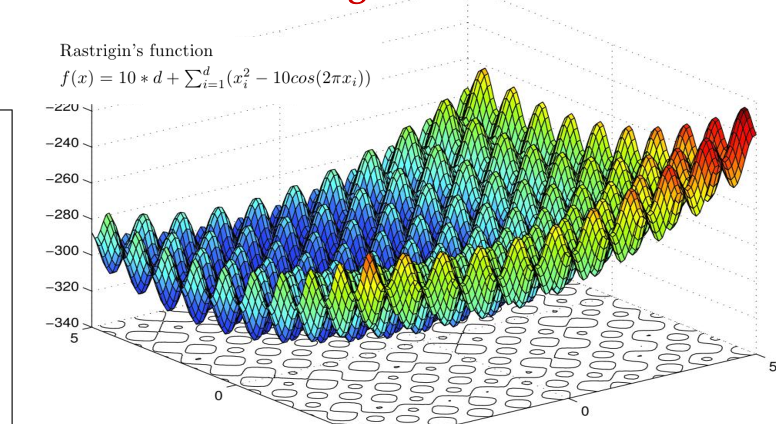
Minimize $\left\{ w_1\|\mathbf{C}_{obs} - C(\vec{\mathbf{m}})\|^2 + w_2\|\mathbf{q}_{obs} - q(\vec{\mathbf{m}})\|^2 + w_3\|\mathbf{p}_{obs} - p(\vec{\mathbf{m}})\|^2 \right\}$

- $\mathbf{C}_{obs}$, $\mathbf{q}_{obs}$, $\mathbf{p}_{obs}$ concentration, flow and pressure measurements at sensors at various sampling times
- **m** – parameter vector
- *C*, *q*, *p* – functions operating on parameter vector

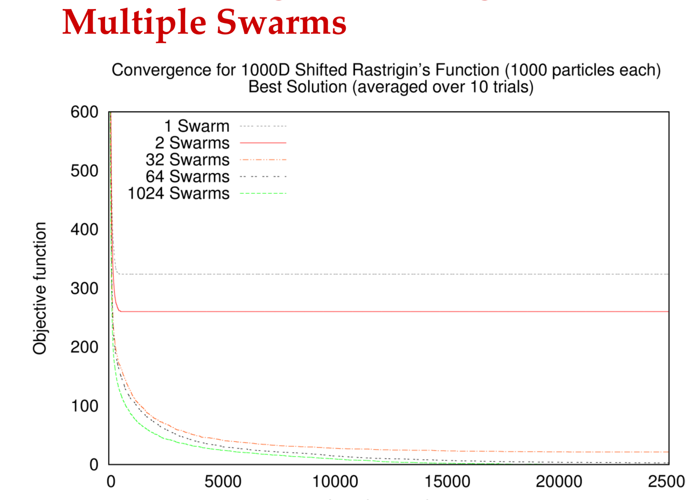
1000D Rastrigin's Convergence Impact of Swarm Size



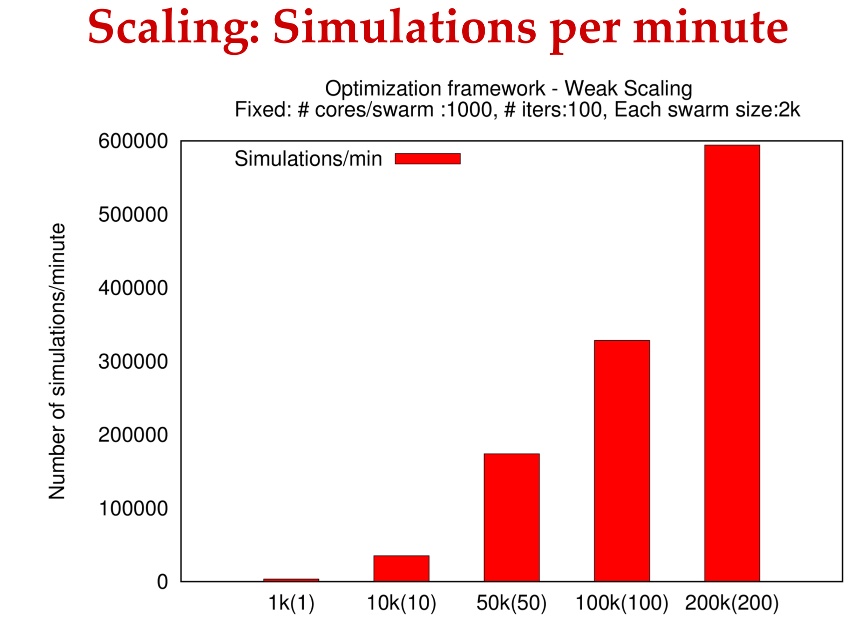
Shifted Rastrigin's function



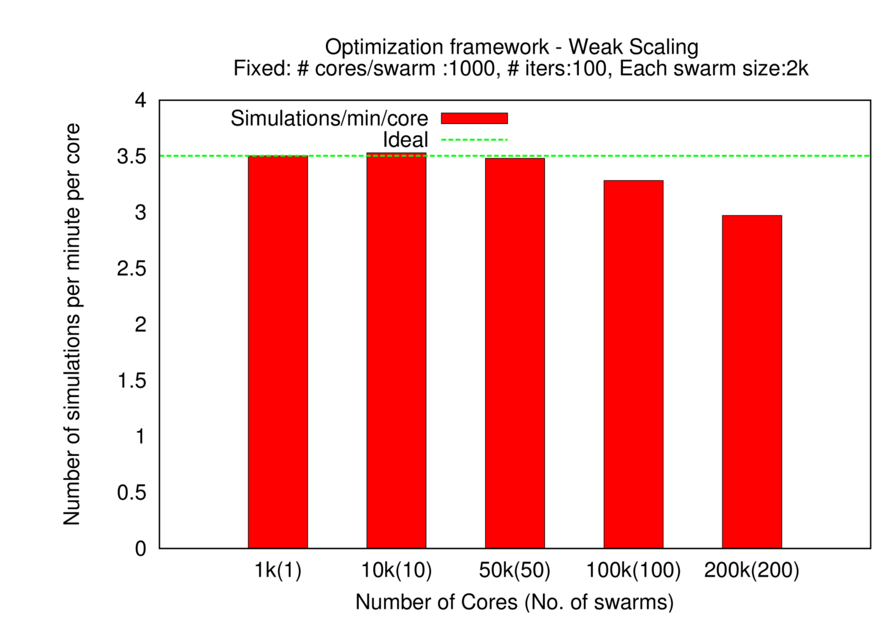
1000D Rastrigin's Convergence Multiple Swarms



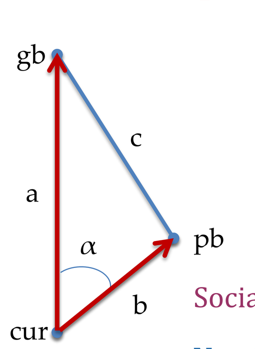
Scaling: Simulations per minute



Scaling: Simulations per minute per core



TAPSO: Topology Aware Particle Swarm Optimization



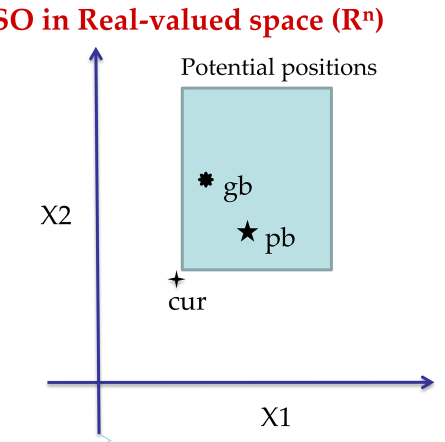
$Eff.Social = a + b\cos(\alpha)$

$Eff.Cognitive = b\sin(\alpha)$

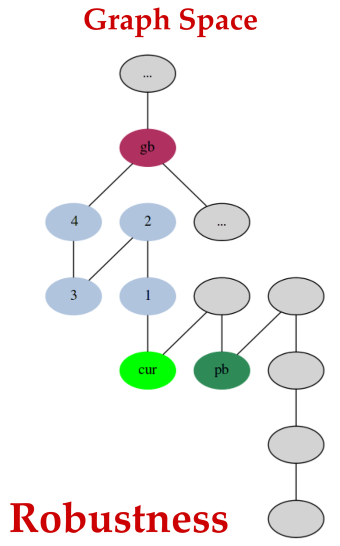
SocialHops $= Eff.Social * U(0,1) *$ tapsoSocialCoeff

NewPosition $= JumpTowardsGlobalBest$ (SocialHops)

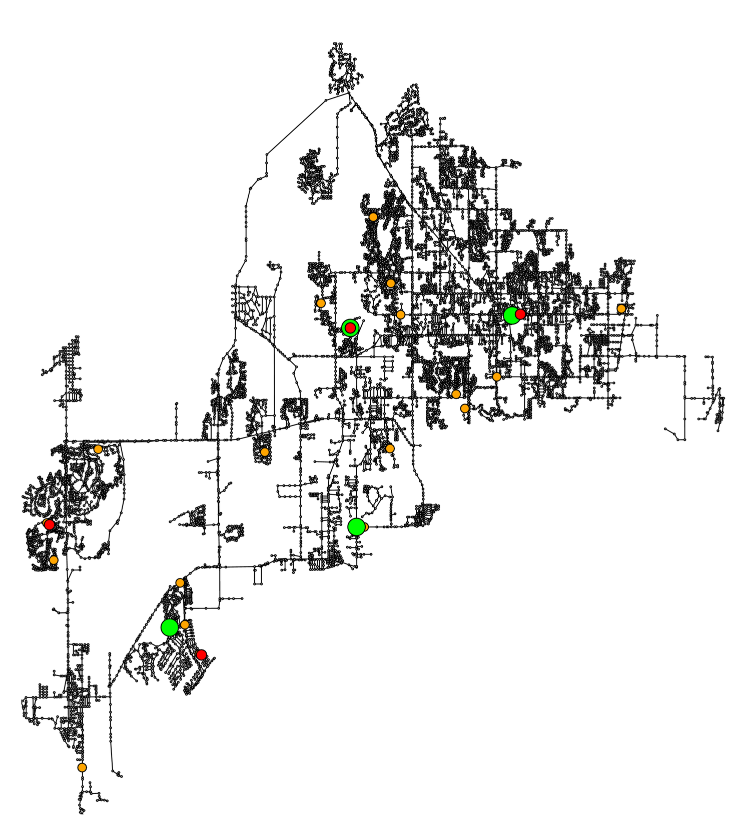
PSO in Real-valued space (R^n)



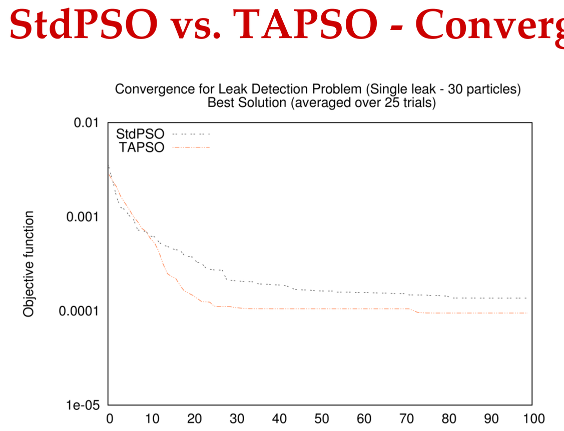
Graph Space



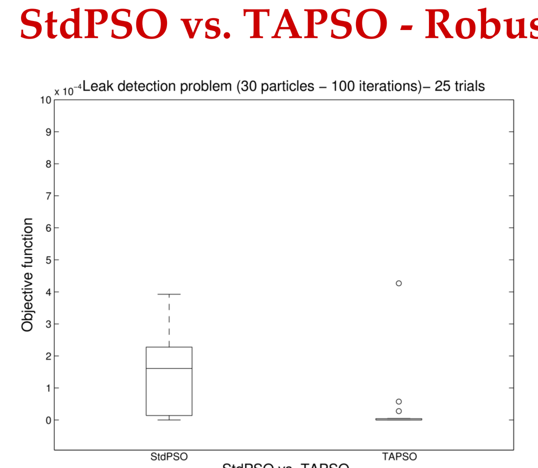
TAPSO Multi-Leak – 4 leaks 10 Swarms (1k particles) - 100 iterations



StdPSO vs. TAPSO - Convergence

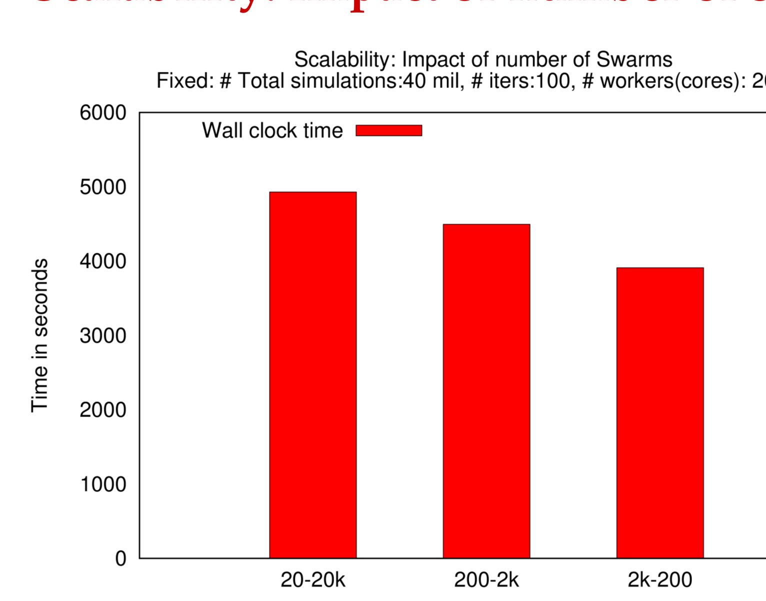


StdPSO vs. TAPSO - Robustness

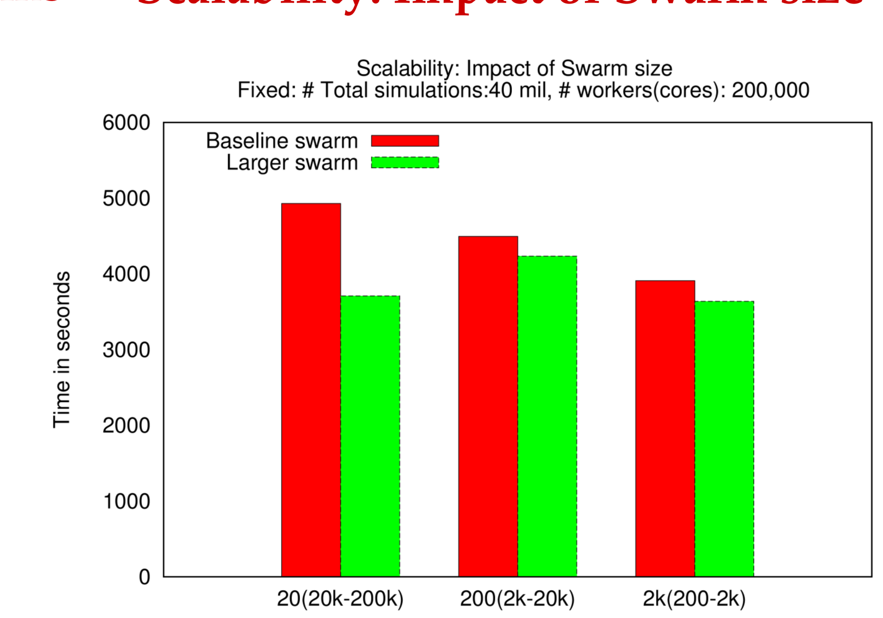


Multi –Swarm Configurations

Scalability: Impact of number of swarms



Scalability: Impact of Swarm size



Conclusions

- The parallel optimization framework (Optimus) demonstrated extreme scalability on leadership class supercomputers (primarily due to asynchronous communication protocol and ring topology)
- The parallel cooperative multi-swarm approach (CoMSO) achieved better solutions & faster convergence for difficult multi-modal problems than single swarm methods
- The graph-based optimization technique (TAPSO) outperformed standard PSO for Water Distribution Systems applications
- PSO and its derivatives integrated with EPANET simulator proved effective in solving leak detection problem in Water Distribution Systems

Acknowledgments

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