Parallelization of the Nelder-Mead Simplex Algorithm

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Nelder-Mead Simplex Algorithm

- Optimization algorithm
  - Minimums, maximums
  - Fitting data
- Uses a simplex to search
- Multidimensional
- Numerical

Algorithm Outline

- Create a simplex
- Find worst vertex
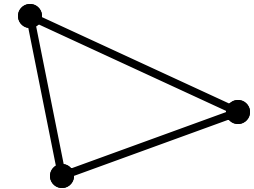- Transform vertex
- Repeat with new simplex

Algorithm Outline

- **Create a simplex**
- Find worst vertex
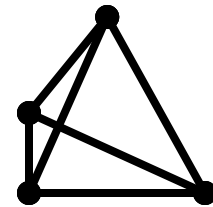- Transform vertex
- Repeat with new simplex
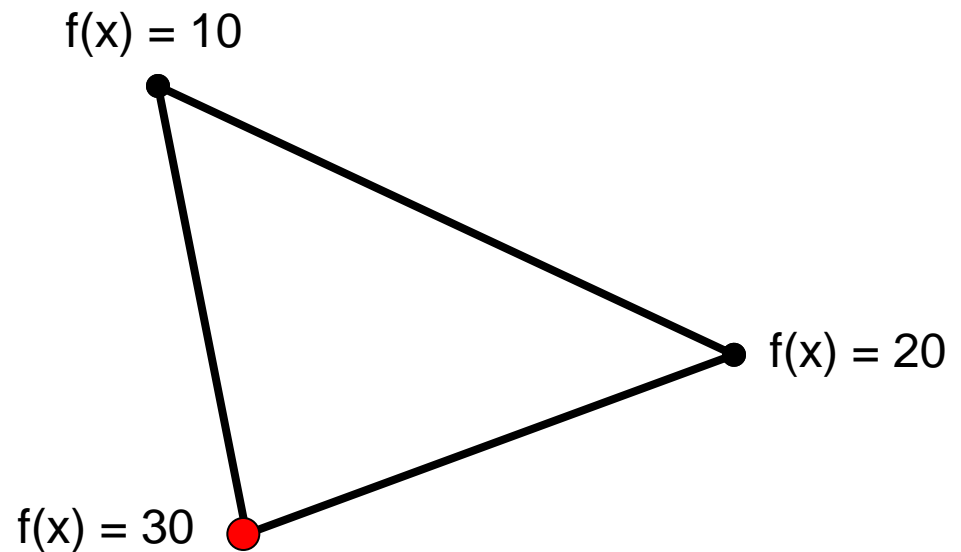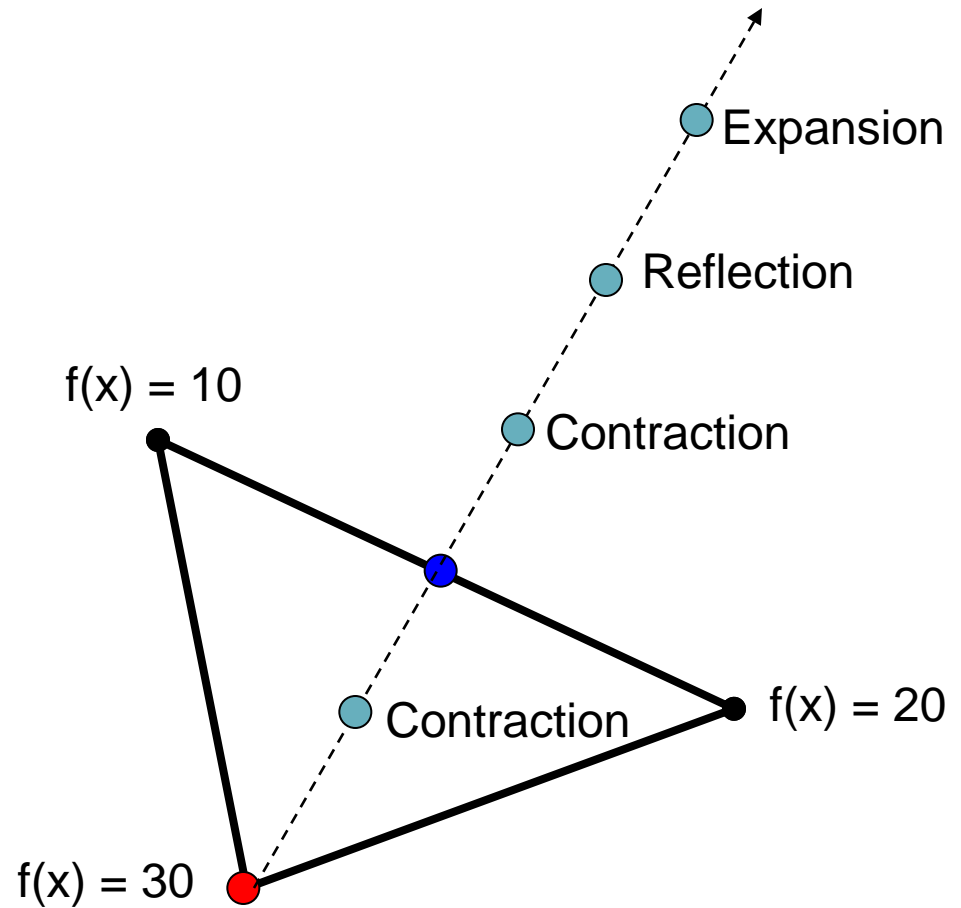
1 dimension

2 dimensions

3 dimensions

Algorithm Outline

- Create a simplex
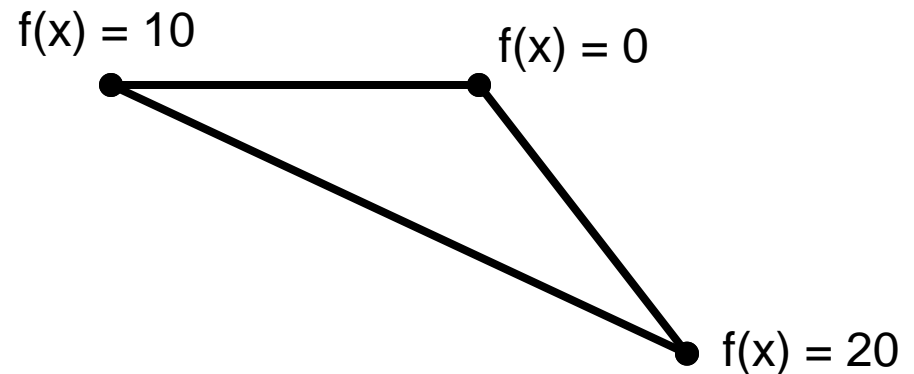- **Find worst vertex**
- Transform vertex
- Repeat with new simplex

f(x) = 10

f(x) = 20

f(x) = 30

Algorithm Outline

- Create a simplex
- Find worst vertex
- **Transform vertex**
- Repeat with new simplex

Expansion

Reflection

f(x) = 10

Contraction

Contraction

f(x) = 20

f(x) = 30

Algorithm Outline

- Create a simplex
- Find worst vertex
- Transform vertex
- **Repeat with new simplex**

f(x) = 10   f(x) = 0

f(x) = 20

Parallelization

- Function evaluations are typically the most time-consuming portion
- Transform multiple vertices
- Evaluations can be done in simultaneously
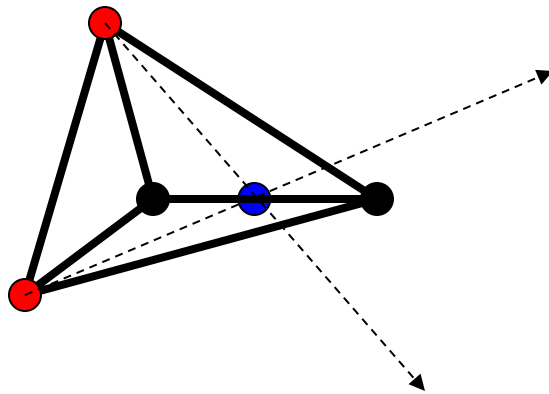
Utilization

- Multiprocessing
  Using multiple computer cores to compute simultaneously

- Cluster computing
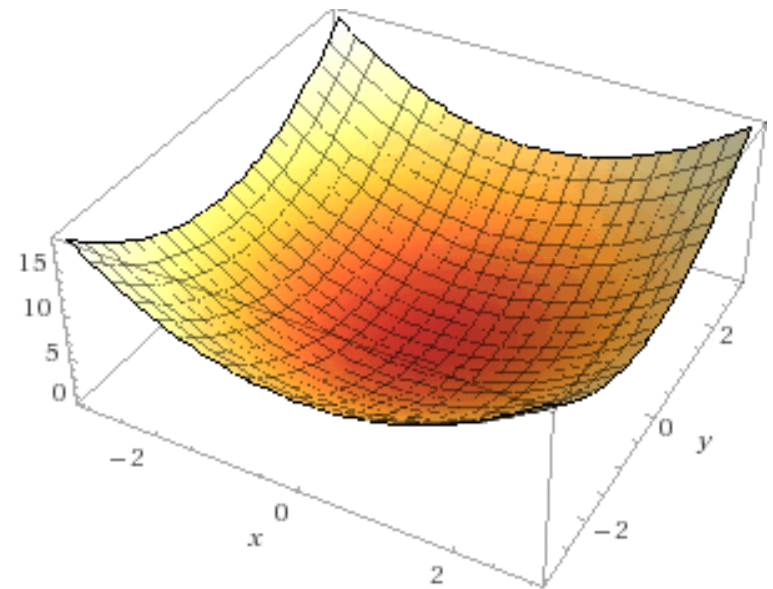 Using multiple computers to compute simultaneously

Cluster Computing

Head Node

Computing Nodes
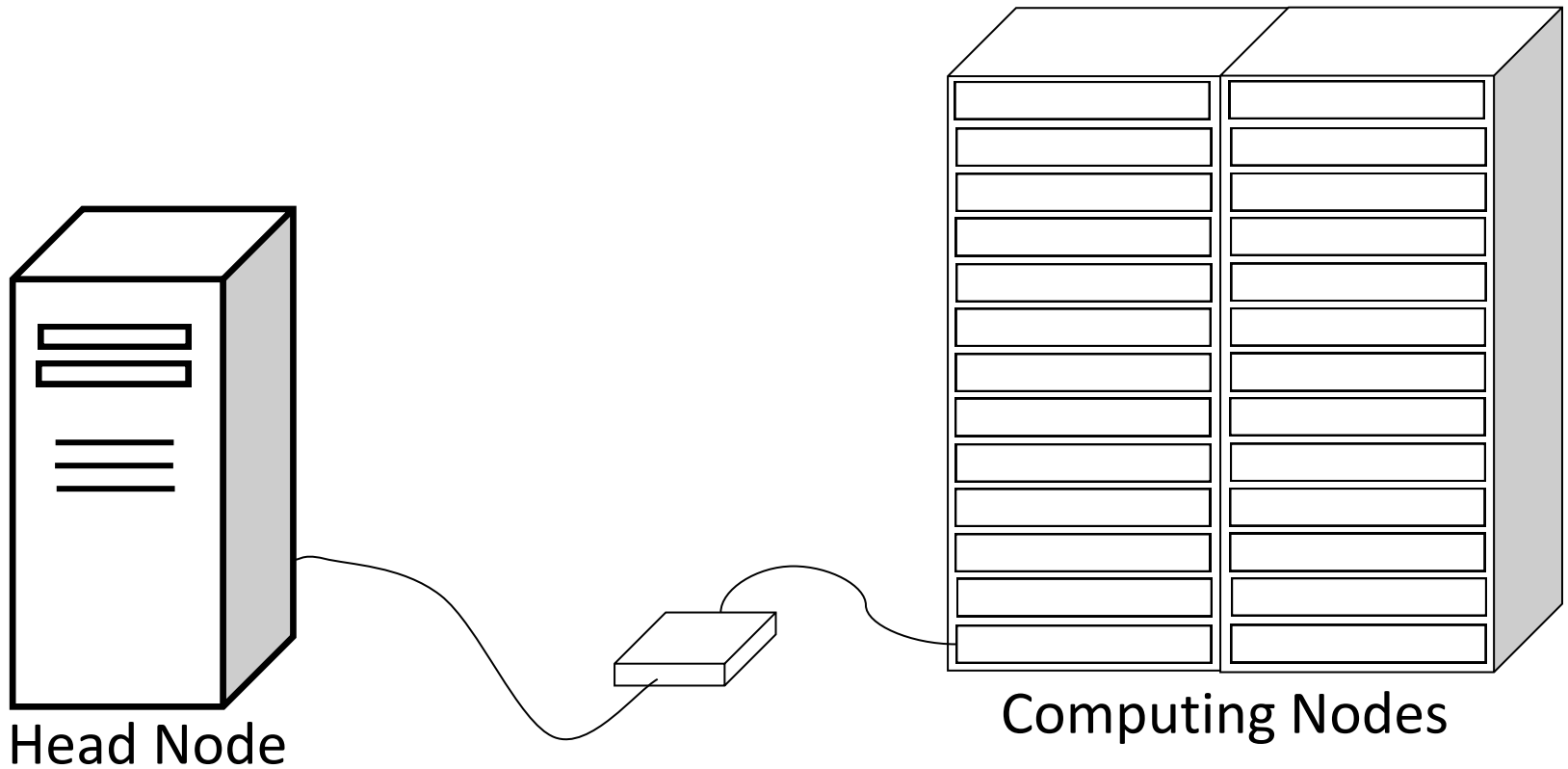
Testing Performance

- Sphere function
- Rosenbrock function
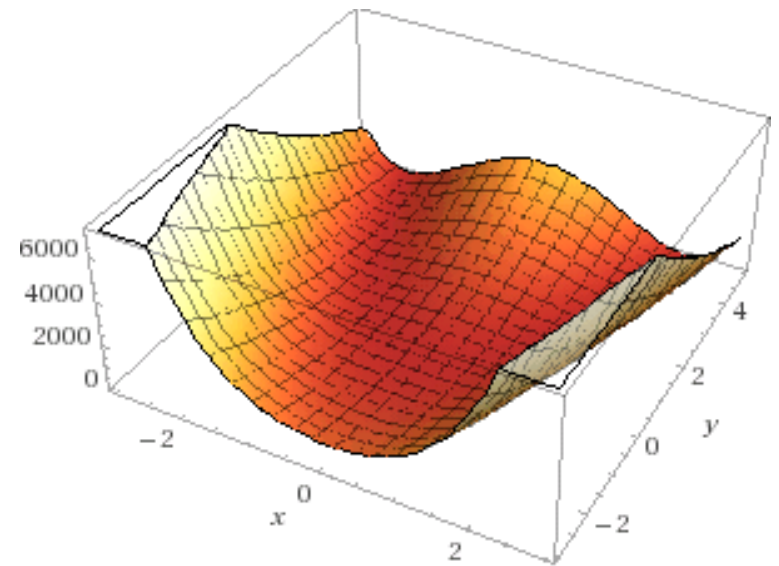- Extended simplex

Testing Performance

- **Sphere function**
- Rosenbrock function
- Extended simplex

$$f(x) = \sum_{i=0}^{N} x_i^2 / 100$$
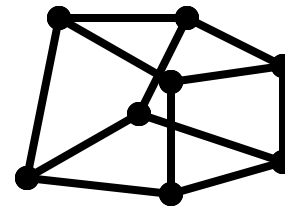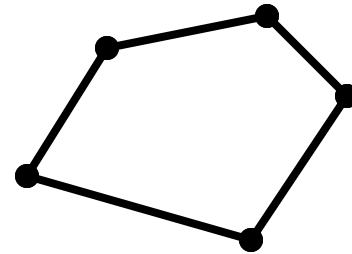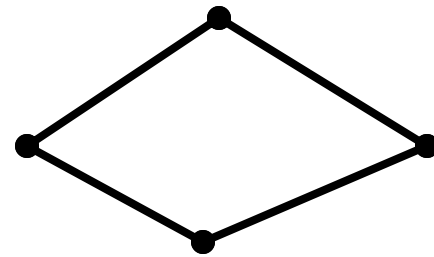
Testing Performance

- Sphere function
- **Rosenbrock function**
- Extended simplex

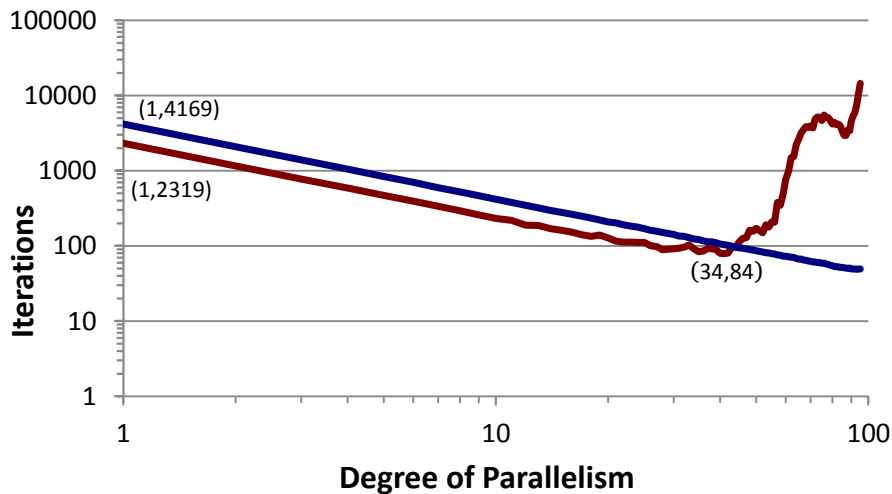$$f(x) = \sum_{i=0}^{N/2} (1 - x_i)^2 + 100(x_{i+1} - x_i^2)^2$$

Testing Performance

- Sphere function
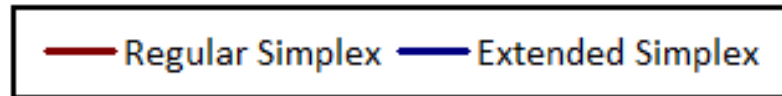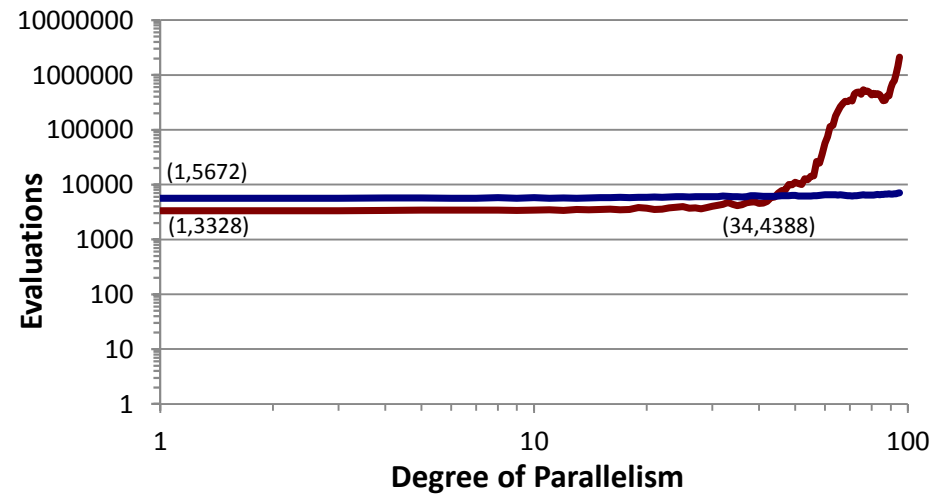- Rosenbrock function
- **Extended simplex**

Results (Sphere, 100 dimensions)
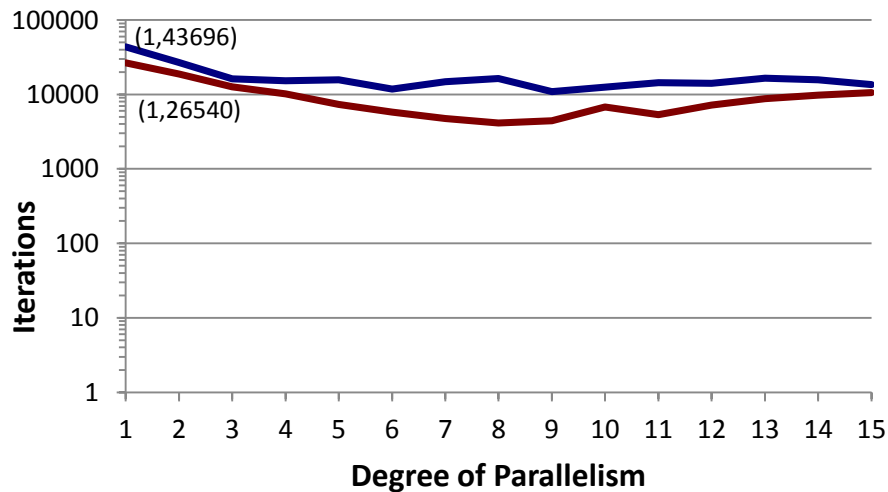

Iterations vs Degree of Parallelism

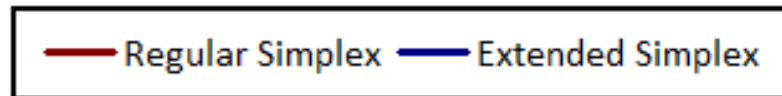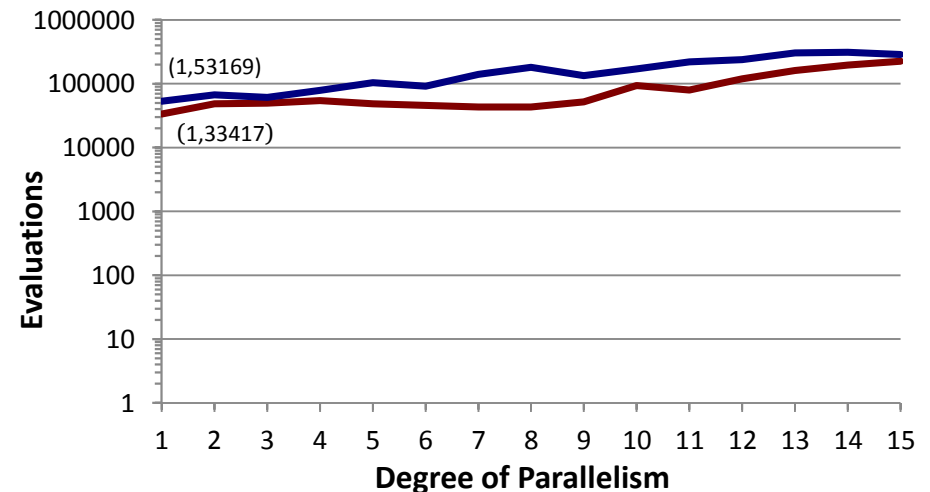**Function Evaluations vs Degree of Parallelism**

- Peak performance at approximately 30% degree of parallelism

Results (Rosenbrock, 25 dimensions)

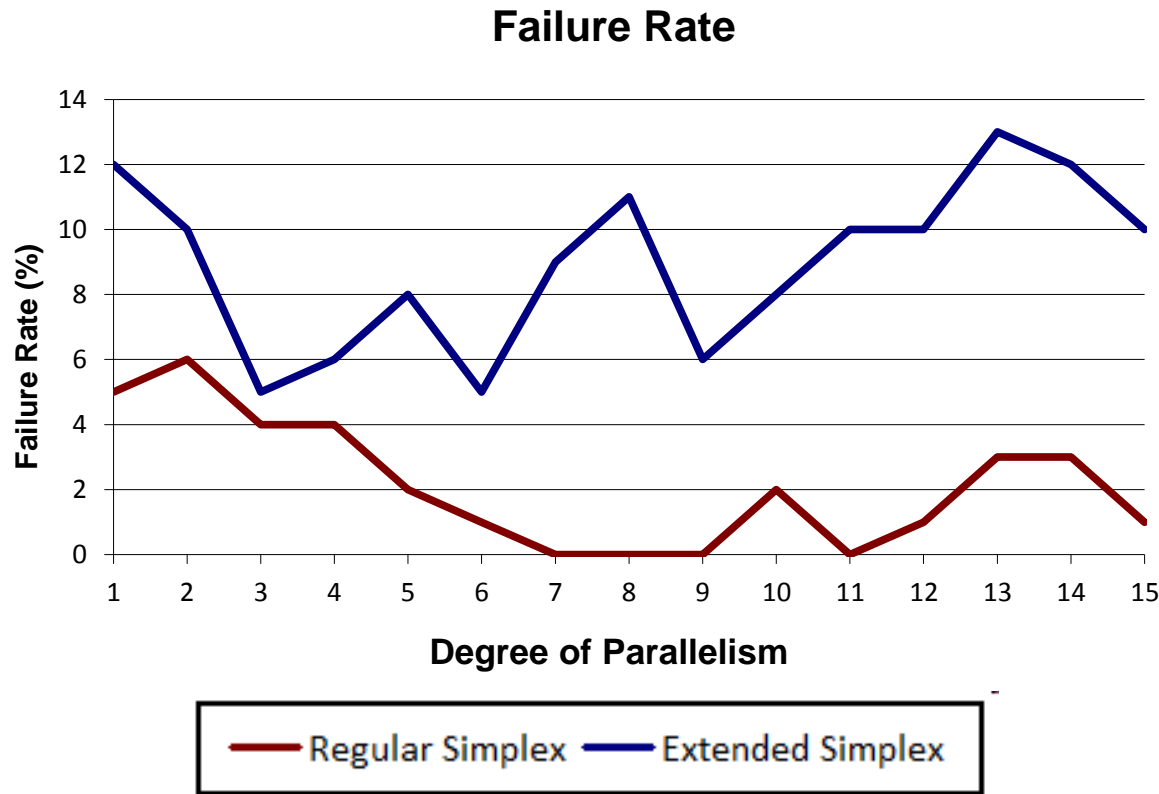**Iterations vs Degree of Parallelism**

Function Evaluations vs Degree of Parallelism

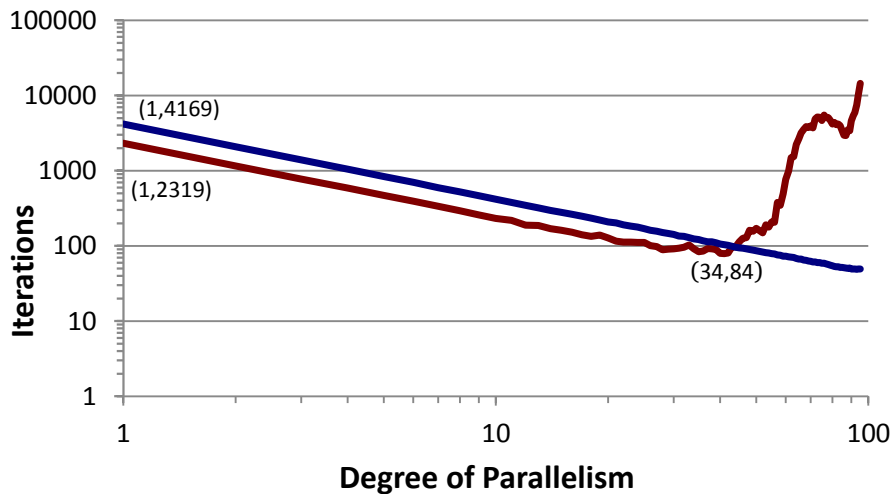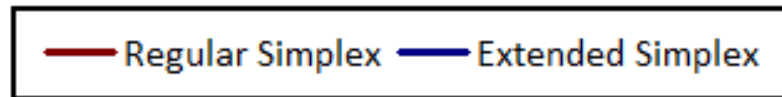- Achieves linear speedup up to the peak

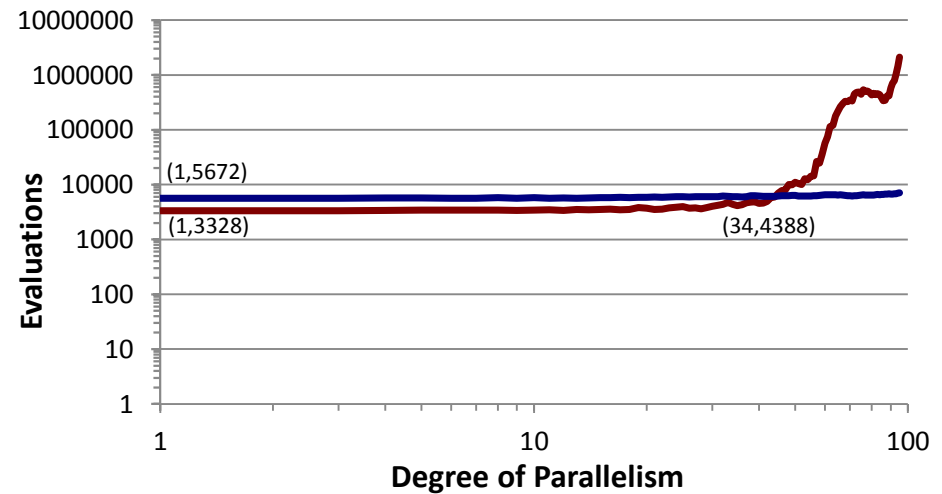# Results (Rosenbrock, 25 dimensions)

Failure Rate

- Increased robustness with minimal extra work

Results (Sphere, 100 dimensions)

Iterations vs Degree of Parallelism

Function Evaluations vs Degree of Parallelism

- Extended simplex performance peaks even further than the regular simplex

Acknowledgements

- Paul Kienzle
- NIST Center for Neutron Research

- CHRNS

~Questions

- Any?