# A Benchmark Test for Parallel Algorithmic Differentiation

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Introduction to AD



#### Introduction to AD Zero Order Forward



#### Introduction to AD

Zero Order Forward First Order Forward



#### Introduction to AD

Zero Order Forward First Order Forward First Order Reverse



#### Introduction to AD

Zero Order Forward First Order Forward First Order Reverse Types of AD



#### Introduction to AD

Zero Order Forward First Order Forward First Order Reverse Types of AD

The Multi-Newton Benchmark



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The Multi-Newton Benchmark

Example Use of Multi-Newton Benchmark



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#### The Multi-Newton Benchmark

Example Use of Multi-Newton Benchmark Bounded Newton Method



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#### The Multi-Newton Benchmark

Example Use of Multi-Newton Benchmark Bounded Newton Method Multi-Newton Setup



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Example Use of Multi-Newton Benchmark Bounded Newton Method Multi-Newton Setup Multi-Newton Continued



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Example Use of Multi-Newton Benchmark Bounded Newton Method Multi-Newton Setup Multi-Newton Continued Threading System Interface



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#### The Multi-Newton Benchmark

Example Use of Multi-Newton Benchmark Bounded Newton Method Multi-Newton Setup Multi-Newton Continued Threading System Interface

Multi-Threaded Memory Allocation



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# Multi-Threaded Memory Allocation

Motivation

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$$z(x,y) = \log[\exp(x) + \exp(y)]$$



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1. Input: independent variable values  $(x^0, y^0)$ 



$$z(x,y) = \log[\exp(x) + \exp(y)]$$

Input: independent variable values (x<sup>0</sup>, y<sup>0</sup>)
 u<sup>0</sup> = exp(x<sup>0</sup>)



$$z(x,y) = \log[\exp(x) + \exp(y)]$$

- 1. Input: independent variable values  $(x^0, y^0)$
- 2.  $u^0 = \exp(x^0)$ 3.  $v^0 = \exp(y^0)$



$$z(x,y) = \log[\exp(x) + \exp(y)]$$

- 1. Input: independent variable values  $(x^0, y^0)$
- 2.  $u^0 = \exp(x^0)$ 3.  $v^0 = \exp(y^0)$ 4.  $s^0 = u^0 + v^0$



$$z(x, y) = \log[\exp(x) + \exp(y)]$$

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- 1. Input: independent variable values  $(x^0, y^0)$
- 2.  $u^{0} = \exp(x^{0})$ 3.  $v^{0} = \exp(y^{0})$ 4.  $s^{0} = u^{0} + v^{0}$ 5.  $z^{0} = \log(s^{0})$

$$z(x, y) = \log[\exp(x) + \exp(y)]$$

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- 1. Input: independent variable values  $(x^0, y^0)$
- 2.  $u^0 = \exp(x^0)$ 3.  $v^0 = \exp(y^0)$

4. 
$$s^0 = u^0 + v^0$$

- 5.  $z^0 = \log(s^0)$
- 6. Output: dependent variable values  $(u^0, v^0, s^0, z^0)$

$$z^{1} = \frac{\partial z}{\partial x}(x^{0}, y^{0})x^{1} + \frac{\partial z}{\partial y}(x^{0}, y^{0})y^{1}$$



$$z^{1} = \frac{\partial z}{\partial x}(x^{0}, y^{0})x^{1} + \frac{\partial z}{\partial y}(x^{0}, y^{0})y^{1}$$

1. Input:  $(x^0, y^0, u^0, v^0, s^0, z^0), (x^1, y^1)$ 



$$z^{1} = \frac{\partial z}{\partial x}(x^{0}, y^{0})x^{1} + \frac{\partial z}{\partial y}(x^{0}, y^{0})y^{1}$$

1. Input: 
$$(x^0, y^0, u^0, v^0, s^0, z^0), (x^1, y^1)$$
  
2.  $u^1 = \exp(x^0)x^1$ 



$$z^{1} = \frac{\partial z}{\partial x}(x^{0}, y^{0})x^{1} + \frac{\partial z}{\partial y}(x^{0}, y^{0})y^{1}$$

1. Input: 
$$(x^0, y^0, u^0, v^0, s^0, z^0), (x^1, y^1)$$
  
2.  $u^1 = \exp(x^0)x^1$   
3.  $v^1 = \exp(y^0)y^1$ 



$$z^{1} = \frac{\partial z}{\partial x}(x^{0}, y^{0})x^{1} + \frac{\partial z}{\partial y}(x^{0}, y^{0})y^{1}$$

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1. Input: 
$$(x^{0}, y^{0}, u^{0}, v^{0}, s^{0}, z^{0}), (x^{1}, y^{1})$$
  
2.  $u^{1} = \exp(x^{0})x^{1}$   
3.  $v^{1} = \exp(y^{0})y^{1}$   
4.  $s^{1} = u^{1} + v^{1}$ 

$$z^{1} = \frac{\partial z}{\partial x}(x^{0}, y^{0})x^{1} + \frac{\partial z}{\partial y}(x^{0}, y^{0})y^{1}$$

1. Input: 
$$(x^{0}, y^{0}, u^{0}, v^{0}, s^{0}, z^{0}), (x^{1}, y^{1})$$
  
2.  $u^{1} = \exp(x^{0})x^{1}$   
3.  $v^{1} = \exp(y^{0})y^{1}$   
4.  $s^{1} = u^{1} + v^{1}$   
5.  $z^{1} = s^{1}/s^{0}$ 



$$z^{1} = \frac{\partial z}{\partial x}(x^{0}, y^{0})x^{1} + \frac{\partial z}{\partial y}(x^{0}, y^{0})y^{1}$$

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1. Input: 
$$(x^{0}, y^{0}, u^{0}, v^{0}, s^{0}, z^{0}), (x^{1}, y^{1})$$
  
2.  $u^{1} = \exp(x^{0})x^{1}$   
3.  $v^{1} = \exp(y^{0})y^{1}$   
4.  $s^{1} = u^{1} + v^{1}$   
5.  $z^{1} = s^{1}/s^{0}$   
6. Output:  $(u^{1}, v^{1}, s^{1}, z^{1})$ 



$$(x^1, y^1) = \left[z^1 \frac{\partial z}{\partial x}(x^0, y^0), z^1 \frac{\partial z}{\partial y}(x^0, y^0)\right]$$



$$(x^1, y^1) = \left[ z^1 rac{\partial z}{\partial x} (x^0, y^0), z^1 rac{\partial z}{\partial y} (x^0, y^0) 
ight]$$

1. Input:  $(x^0, y^0, u^0, v^0, s^0, z^0), z^1$ 



$$(x^{1}, y^{1}) = \left[z^{1}\frac{\partial z}{\partial x}(x^{0}, y^{0}), z^{1}\frac{\partial z}{\partial y}(x^{0}, y^{0})\right]$$

1. Input: 
$$(x^0, y^0, u^0, v^0, s^0, z^0), z^1$$
  
2.  $s^1 = z^1/s^0$ 



$$(x^1, y^1) = \left[z^1 \frac{\partial z}{\partial x}(x^0, y^0), z^1 \frac{\partial z}{\partial y}(x^0, y^0)\right]$$

1. Input: 
$$(x^{0}, y^{0}, u^{0}, v^{0}, s^{0}, z^{0}), z^{1}$$
  
2.  $s^{1} = z^{1}/s^{0}$   
3.  $u^{1} = s^{1}, v^{1} = s^{1}$ 



$$(x^1, y^1) = \left[z^1 \frac{\partial z}{\partial x}(x^0, y^0), z^1 \frac{\partial z}{\partial y}(x^0, y^0)\right]$$

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1. Input: 
$$(x^{0}, y^{0}, u^{0}, v^{0}, s^{0}, z^{0}), z^{1}$$
  
2.  $s^{1} = z^{1}/s^{0}$   
3.  $u^{1} = s^{1}, v^{1} = s^{1}$   
4.  $y^{1} = v^{1} \exp(y^{0})$   
5.  $x^{1} = u^{1} \exp(x^{0})$
### First Order Reverse

$$(x^1, y^1) = \left[z^1 \frac{\partial z}{\partial x}(x^0, y^0), z^1 \frac{\partial z}{\partial y}(x^0, y^0)\right]$$

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1. Input: 
$$(x^{0}, y^{0}, u^{0}, v^{0}, s^{0}, z^{0}), z^{1}$$
  
2.  $s^{1} = z^{1}/s^{0}$   
3.  $u^{1} = s^{1}, v^{1} = s^{1}$   
4.  $y^{1} = v^{1} \exp(y^{0})$   
5.  $x^{1} = u^{1} \exp(x^{0})$   
6. Output:  $(x^{1}, y^{1})$ 

#### ► AD by Source Code Transformation



- AD by Source Code Transformation
- AD by Operator Overloading



- AD by Source Code Transformation
- AD by Operator Overloading
- Tapeless Forward AD



- AD by Source Code Transformation
- AD by Operator Overloading
- Tapeless Forward AD
- Recording Operations on a Tape



CppAD uses a Tape with Operator Overloading



- CppAD uses a Tape with Operator Overloading
- It comes with the the Multi-Newton benchmark test



- CppAD uses a Tape with Operator Overloading
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- Version 2011 of CppAD on 32 Core Machine



Newton: Z=1000, J=4800, N=24000

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- CppAD uses a Tape with Operator Overloading
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- Version 2011 & 2012.0 of CppAD on 32 Core Machine



Newton: Z=1000, J=4800, N=24000

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Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

1. Input: bounds [a, b], maximum iterations K, criterion  $\delta$ , function f.



Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

1. Input: bounds [a, b], maximum iterations K, criterion  $\delta$ , function f.

2. Set 
$$x_0 = (a + b)/2$$
,  $k = 0$ .



Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

- 1. Input: bounds [a, b], maximum iterations K, criterion  $\delta$ , function f.
- 2. Set  $x_0 = (a+b)/2$ , k = 0.

3. If 
$$|f(x_k)| \leq \delta$$
, output  $B = \{x_k\}$ .



Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

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- 2. Set  $x_0 = (a+b)/2$ , k = 0.
- 3. If  $|f(x_k)| \leq \delta$ , output  $B = \{x_k\}$ .

4. If 
$$k == K$$
, output  $B = \emptyset$ .

Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

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- 2. Set  $x_0 = (a+b)/2$ , k = 0.
- 3. If  $|f(x_k)| \leq \delta$ , output  $B = \{x_k\}$ .

4. If 
$$k == K$$
, output  $B = \emptyset$ .

5. If  $f(x_k)f'(x_k) \ge 0$  and  $x_k = a$ , output  $B = \emptyset$ .



Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

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, output  $B = \{x_k\}$ .

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, output  $B = \emptyset$ .

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- 6. If  $f(x_k)f'(x_k) \leq 0$  and  $x_k = b$ , output  $B = \emptyset$ .



Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

1. Input: bounds [a, b], maximum iterations K, criterion  $\delta$ , function f.

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2. Set 
$$x_0 = (a+b)/2$$
,  $k = 0$ .

3. If 
$$|f(x_k)| \le \delta$$
, output  $B = \{x_k\}$ .

4. If 
$$k == K$$
, output  $B = \emptyset$ .

5. If 
$$f(x_k)f'(x_k) \ge 0$$
 and  $x_k = a$ , output  $B = \emptyset$ .

6. If 
$$f(x_k)f'(x_k) \leq 0$$
 and  $x_k = b$ , output  $B = \emptyset$ .

7. Set 
$$y_k = x_k - f(x_k)/f'(x_k)$$
.

Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

1. Input: bounds [a, b], maximum iterations K, criterion  $\delta$ , function f.

2. Set 
$$x_0 = (a+b)/2$$
,  $k = 0$ .

3. If 
$$|f(x_k)| \le \delta$$
, output  $B = \{x_k\}$ .

4. If 
$$k == K$$
, output  $B = \emptyset$ .

5. If 
$$f(x_k)f'(x_k) \ge 0$$
 and  $x_k = a$ , output  $B = \emptyset$ .

6. If 
$$f(x_k)f'(x_k) \leq 0$$
 and  $x_k = b$ , output  $B = \emptyset$ .

7. Set 
$$y_k = x_k - f(x_k)/f'(x_k)$$
.

8. Set 
$$x_{k+1} = \min[b, \max(a, y_k)]$$
.



Set  $B(a, b, K, \delta, f)$  to one or no zeros in [a, b]:

1. Input: bounds [a, b], maximum iterations K, criterion  $\delta$ , function f.

2. Set 
$$x_0 = (a+b)/2$$
,  $k = 0$ .

3. If 
$$|f(x_k)| \le \delta$$
, output  $B = \{x_k\}$ .

4. If 
$$k == K$$
, output  $B = \emptyset$ .

5. If 
$$f(x_k)f'(x_k) \ge 0$$
 and  $x_k = a$ , output  $B = \emptyset$ .

6. If 
$$f(x_k)f'(x_k) \leq 0$$
 and  $x_k = b$ , output  $B = \emptyset$ .

7. Set 
$$y_k = x_k - f(x_k)/f'(x_k)$$
.

8. Set 
$$x_{k+1} = \min[b, \max(a, y_k)]$$
.

9. Set 
$$k = k + 1$$
. Goto step 3

Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$  :

1. Input: bounds  $[\alpha, \beta]$ , maximum iterations K, criterion  $\delta$ , number of sub-intervals J, number of threads M, function f.



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ :

- 1. Input: bounds  $[\alpha, \beta]$ , maximum iterations K, criterion  $\delta$ , number of sub-intervals J, number of threads M, function f.
- 2. Set sub-interval length  $\gamma = (\beta \alpha)/J$ , start for first thread  $s_1 = \alpha$ , end for last thread  $e_M = \beta$ .



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ :

- 1. Input: bounds  $[\alpha, \beta]$ , maximum iterations K, criterion  $\delta$ , number of sub-intervals J, number of threads M, function f.
- 2. Set sub-interval length  $\gamma = (\beta \alpha)/J$ , start for first thread  $s_1 = \alpha$ , end for last thread  $e_M = \beta$ .
- 3. For m = 1, ..., M, in sequential mode execute:



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ :

- 1. Input: bounds  $[\alpha, \beta]$ , maximum iterations K, criterion  $\delta$ , number of sub-intervals J, number of threads M, function f.
- 2. Set sub-interval length  $\gamma = (\beta \alpha)/J$ , start for first thread  $s_1 = \alpha$ , end for last thread  $e_M = \beta$ .
- 3. For m = 1, ..., M, in sequential mode execute:

3.1 Number of sub-intervals for thread m $L_m = \begin{cases} \text{floor}(J/M) + 1 & \text{if } m \leq \mod(J, M) \\ \text{floor}(J/M) & \text{otherwise} \end{cases}$ 



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ :

- 1. Input: bounds  $[\alpha, \beta]$ , maximum iterations K, criterion  $\delta$ , number of sub-intervals J, number of threads M, function f.
- 2. Set sub-interval length  $\gamma = (\beta \alpha)/J$ , start for first thread  $s_1 = \alpha$ , end for last thread  $e_M = \beta$ .
- 3. For  $m = 1, \dots, M$ , in sequential mode execute:
  - 3.1 Number of sub-intervals for thread m  $L_m = \begin{cases} floor(J/M) + 1 & \text{if } m \leq \mod(J, M) \\ floor(J/M) & \text{otherwise} \end{cases}$ 3.2 Start for thread  $m \geq 2$ ,  $s_m = s_{m-1} + \gamma L_m$ .



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ :

- 1. Input: bounds  $[\alpha, \beta]$ , maximum iterations K, criterion  $\delta$ , number of sub-intervals J, number of threads M, function f.
- 2. Set sub-interval length  $\gamma = (\beta \alpha)/J$ , start for first thread  $s_1 = \alpha$ , end for last thread  $e_M = \beta$ .

- 3. For  $m = 1, \dots, M$ , in sequential mode execute:
  - 3.1 Number of sub-intervals for thread m  $L_m = \begin{cases} \text{floor}(J/M) + 1 & \text{if } m \leq \mod(J, M) \\ \text{floor}(J/M) & \text{otherwise} \end{cases}$ 3.2 Start for thread  $m \geq 2$ ,  $s_m = s_{m-1} + \gamma L_m$ . 3.3 End for thread  $m - 1 \geq 1$ ,  $e_{m-1} = s_m$ .

Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ : 4. For m = 1, ..., M, in parallel mode execute:



Set 
$$S(\alpha, \beta, K, \delta, J, M, f)$$
 to multiple zeros in  $[\alpha, \beta]$ :  
4. For  $m = 1, ..., M$ , in parallel mode execute:  
4.1 For  $\ell = 1, ..., L_m$ , set  $a_{m,\ell} = s_m + \gamma(\ell - 1)$ , and  
 $b_{m,\ell} = a_{m,\ell} + \gamma$ .



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ : 4. For m = 1, ..., M, in parallel mode execute: 4.1 For  $\ell = 1, ..., L_m$ , set  $a_{m,\ell} = s_m + \gamma(\ell - 1)$ , and  $b_{m,\ell} = a_{m,\ell} + \gamma$ . 4.2 Set  $S_m = \bigcup_{\ell=1}^{L_m} B[a_{m,\ell}, b_{m,\ell}, K, \delta, f]$ .



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ : 4. For m = 1, ..., M, in parallel mode execute: 4.1 For  $\ell = 1, ..., L_m$ , set  $a_{m,\ell} = s_m + \gamma(\ell - 1)$ , and  $b_{m,\ell} = a_{m,\ell} + \gamma$ . 4.2 Set  $S_m = \bigcup_{\ell=1}^{L_m} B[a_{m,\ell}, b_{m,\ell}, K, \delta, f]$ . 4.3 If difference between two elements of  $S_m$  is less than  $\gamma/2$ , remove one that has larger value for |f(x)|.



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$ : 4. For m = 1, ..., M, in parallel mode execute: 4.1 For  $\ell = 1, ..., L_m$ , set  $a_{m,\ell} = s_m + \gamma(\ell - 1)$ , and  $b_{m,\ell} = a_{m,\ell} + \gamma$ . 4.2 Set  $S_m = \bigcup_{\ell=1}^{L_m} B[a_{m,\ell}, b_{m,\ell}, K, \delta, f]$ . 4.3 If difference between two elements of  $S_m$  is less than  $\gamma/2$ , remove one that has larger value for |f(x)|. 5. Set  $S = \bigcup_{m=1}^{M} S_m$ .



Set  $S(\alpha, \beta, K, \delta, J, M, f)$  to multiple zeros in  $[\alpha, \beta]$  :

4. For  $m = 1, \ldots, M$ , in parallel mode execute:

4.1 For 
$$\ell = 1, \ldots, L_m$$
, set  $a_{m,\ell} = s_m + \gamma(\ell - 1)$ , and  $b_{m,\ell} = a_{m,\ell} + \gamma$ .

4.2 Set 
$$S_m = \bigcup_{\ell=1}^{L_m} B[a_{m,\ell}, b_{m,\ell}, K, \delta, f].$$

4.3 If difference between two elements of  $S_m$  is less than  $\gamma/2$ , remove one that has larger value for |f(x)|.

5. Set 
$$S = \bigcup_{m=1}^{M} S_m$$
.

- 6. If difference between two elements of S is less than  $\gamma/2$ , remove one that has larger value for |f(x)|.
- **7**. Output *S*.

▶ m = thread\_num() identifies current thread, 0 ≤ m ≤ M − 1.



- ▶ m = thread\_num() identifies current thread, 0 ≤ m ≤ M − 1.
- ▶  $b = in_parallel()$

is true if in parallel execution mode, otherwise may be false.



- ▶ m = thread\_num() identifies current thread, 0 ≤ m ≤ M − 1.
- b = in\_parallel() is true if in parallel execution mode, otherwise may be false.
- ok = team\_create(num\_threads) creates a team of num\_threads threads.



- ▶ m = thread\_num() identifies current thread, 0 ≤ m ≤ M − 1.
- b = in\_parallel() is true if in parallel execution mode, otherwise may be false.

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- ok = team\_create(num\_threads) creates a team of num\_threads threads.
- ok = team\_work(worker)
   Each call runs num\_threads versions of worker with corresponding thread\_num() between 0 and M − 1.

- ▶ m = thread\_num() identifies current thread, 0 ≤ m ≤ M − 1.
- b = in\_parallel() is true if in parallel execution mode, otherwise may be false.

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- ok = team\_create(num\_threads) creates a team of num\_threads threads.
- ▶ ok = team\_work(worker) Each call runs num\_threads versions of worker with corresponding thread\_num() between 0 and M − 1.
- ▶ ok = team\_destroy() terminates all but the master thread; i.e., m = 0.

# Motivation

The following plot is taken from A comparison of memory allocators in multiprocessors:



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Capacity Let 
$$c_1 = 128$$
 and for  $i = 2, ..., I$ ,  
 $c_i = 3 \cdot \text{floor}[(c_{i-1} + 1)/2].$ 



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  - 2011 Uses system memory allocation with capacity modification above.
  - 2012.0 For each thread *m* and each capacity *i*, a singly linked list of available memory is retained with root  $A_{m*I+i}$ . In addition, counter vectors for the number of bytes inuse  $u_m$  and available  $a_m$  for corresponding thread.



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  - 2012.1 For each thread m, a separate structure  $S_m$  is allocated for the inuse counter, available counter, and vector of available roots for that thread.

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$$f(x) = \frac{1}{N} \sum_{n=1}^{N} \sin(x)$$



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  - J Number of bounded Newton sub-intervals J = 4800.



Sac



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900



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