A Comparison of Several Direct Sparse Linear Equation Solvers for CGWAVE on the Cray X1

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Mild Slope Equation

$$\nabla \cdot \left(CC_g \hat{h}\right) + \frac{C}{C_g} s^2 \hat{h} = 0$$

$$C = \frac{s}{k}$$

$$C_g = \frac{\partial s}{\partial k} = nC$$

$$n = \frac{1}{2}\left[1 + \frac{2kd}{\sinh\left(2kd\right)}\right]$$

$$s^2 = gk \tanh\left(kd\right)$$

$\hat{h}$ = complex surface elevation function

s = wave frequency

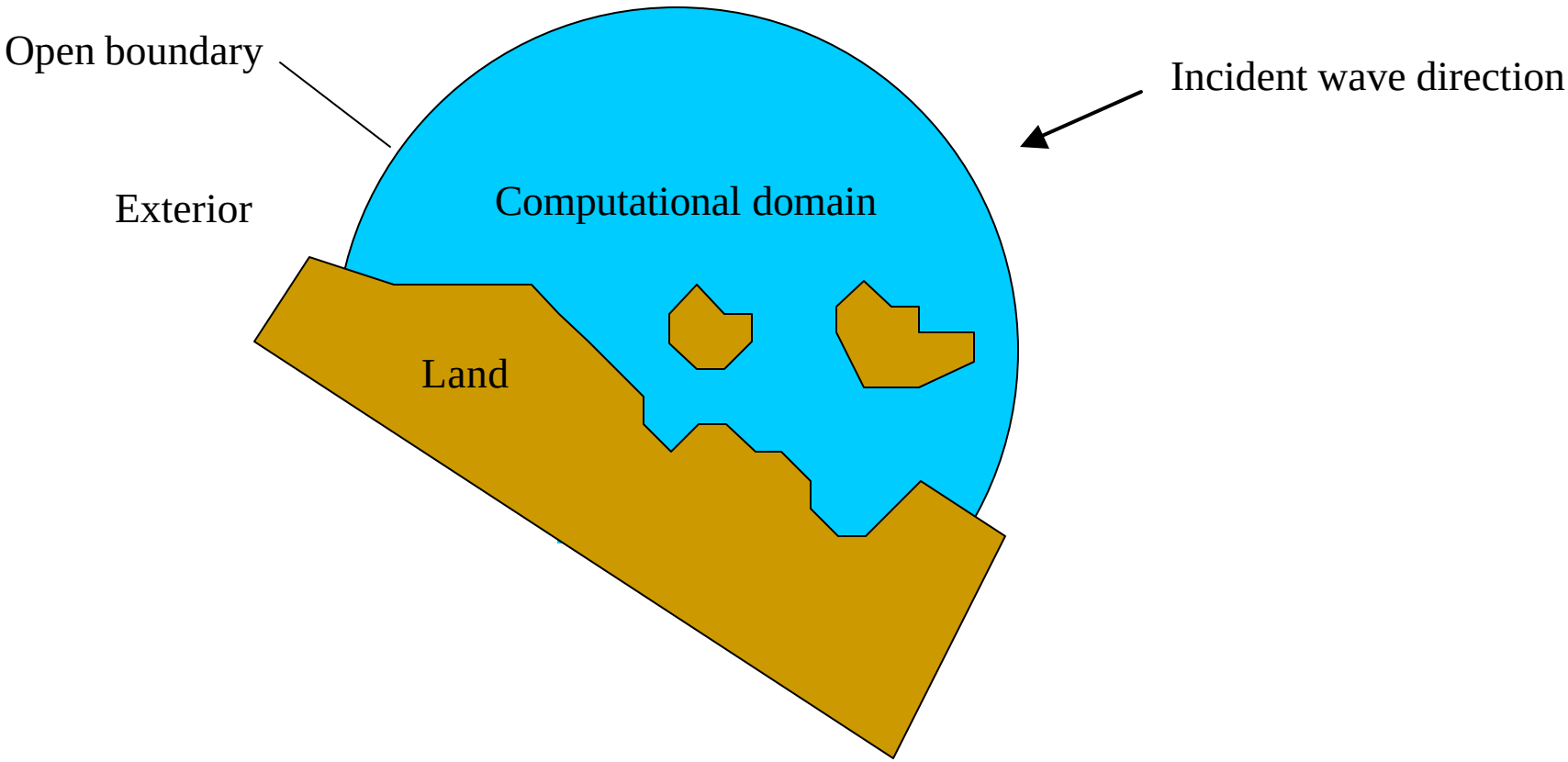
C = phase velocity

C_g = group velocity

k = wave number

d = local depth

CGWAVE


Open boundary
Incident wave direction
Exterior
Computational domain
Land

CGWAVE

- Wave prediction model
- Harbors, open coastal regions, coastal inlets, around islands, and around fixed or floating structures
- Finite element model
- Unstructured mesh
- Linear system of non-symmetric, complex equations
- Very difficult to solve by iterative methods

Direct Solvers Compared

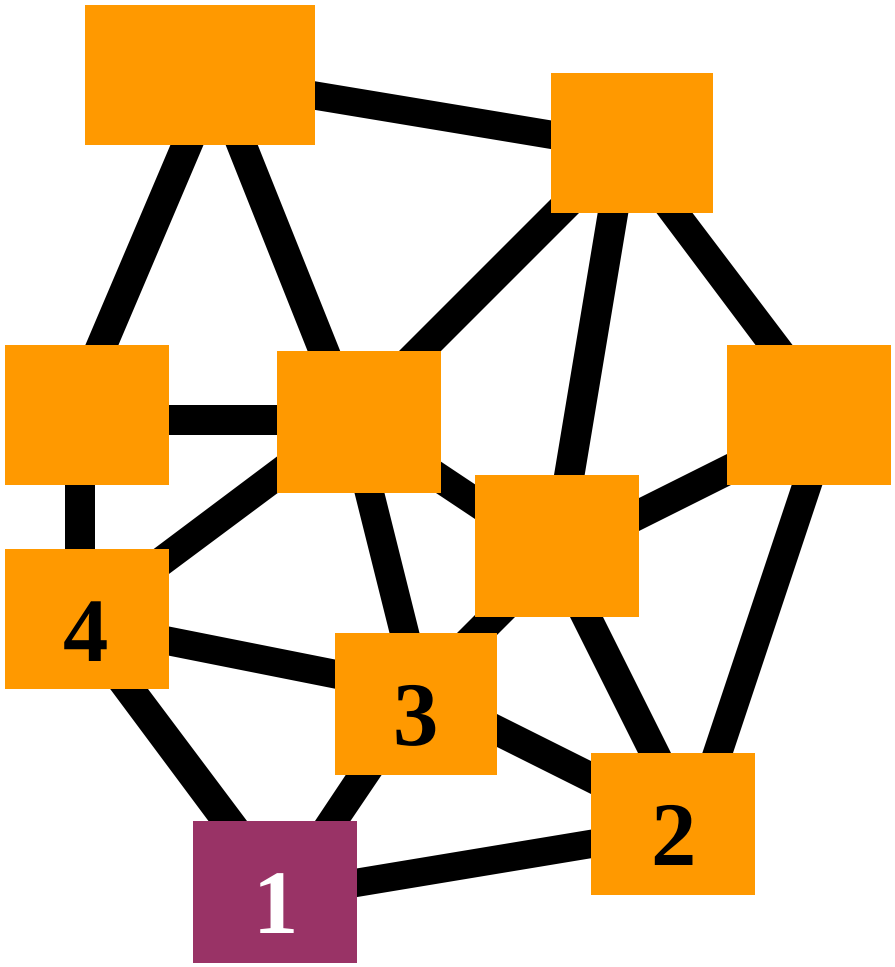
- Bansol
- SSGETRF, SSGETRS
- SSTSTRF, SSTSTRS
- SuperLU
- UMFPACK

$$\mathbf{Ax} = \mathbf{b}$$

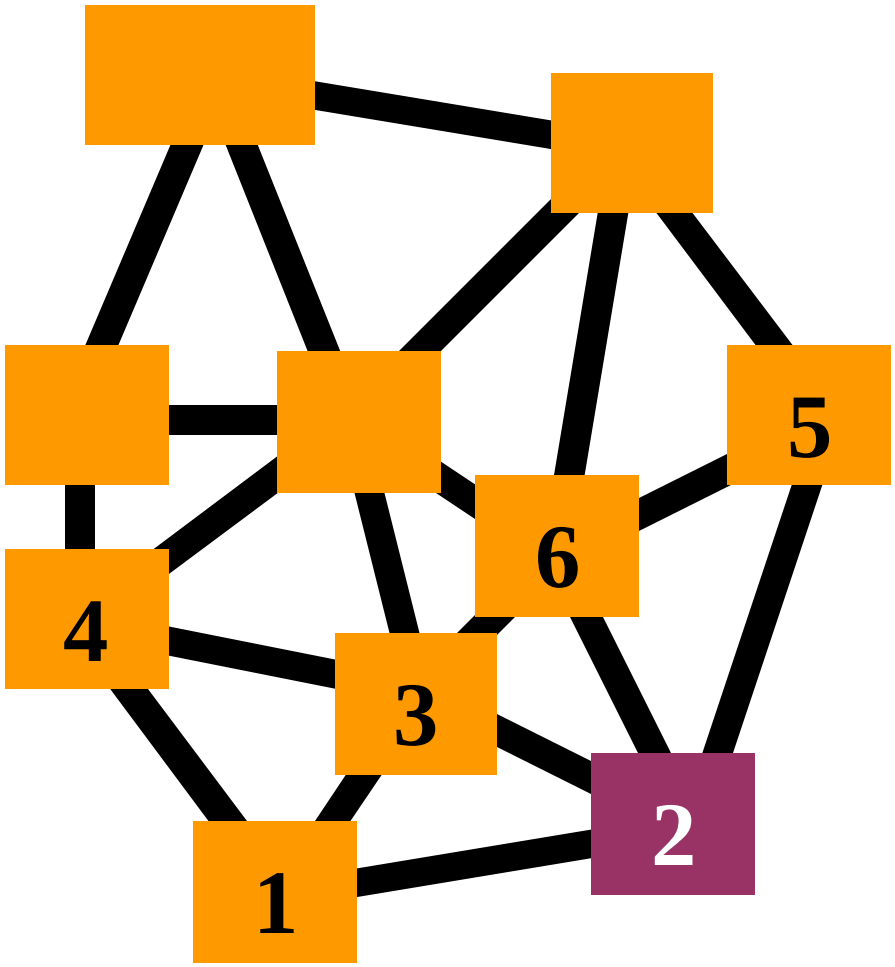
Bansol

- Out-of-core
- Banded
- FORTRAN
- Initial bandwidth reduction step
- Complex **A** and **b**
- Threshold pivoting
- Directives were used for optimization on the X1

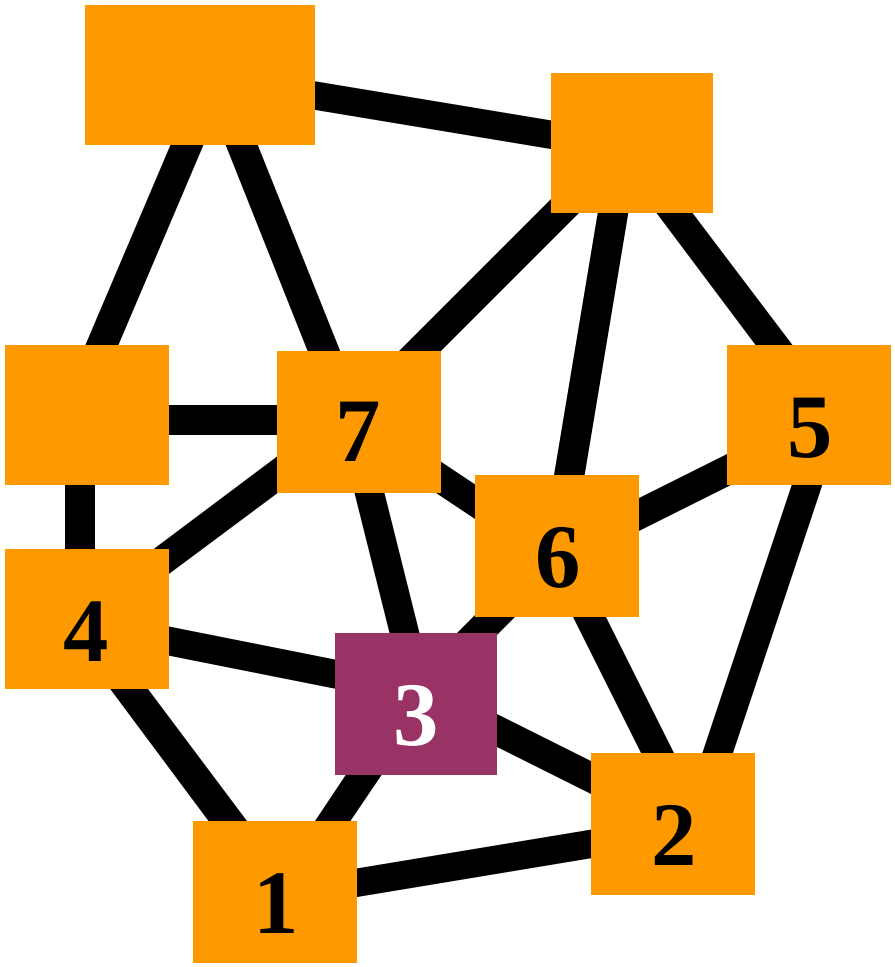
Reordering



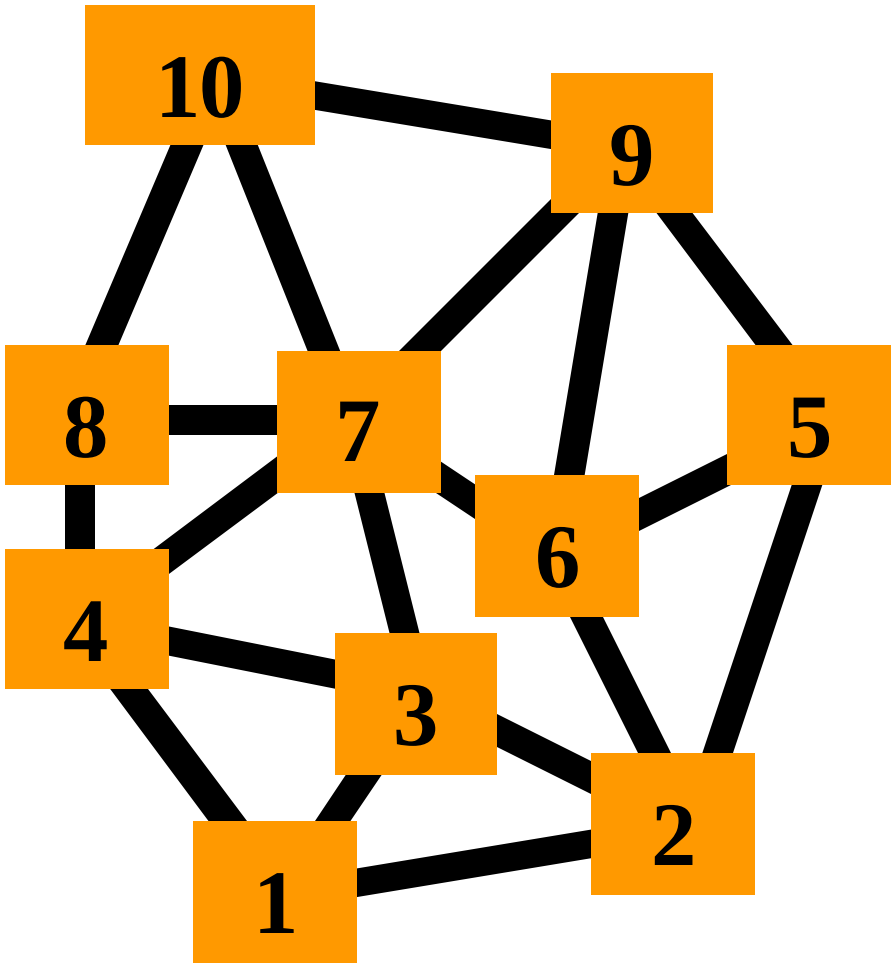
Reordering



Reordering



Reordering



Node Number Reordering

- Before directive

```
r V--<>  temp(nos(1:nn)) = phi(1:nn)
V M--<>  phi(1:nn) = temp(1:nn)
```

- After directive

```
     !dir$ concurrent
r V M--<>  temp(nos(1:nn)) = phi(1:nn)
V M----<>  phi(1:nn) = temp(1:nn)
```

Store into Blocks

```
1     !csd$ parallel do private (jj, ii,
2     !csd$& nold, jold, node, i, j)
1 M-----<  do jj = 1, nm
1 M MV--<    do ii = 1, nn
1 M MV         nold = nns(ii)
1 M MV         jold = id(nold, jj)
1 M MV         if (jold .ne. 0) then
1 M MV           node = nos(jold)
1 M MV           if ((node .ge. jst) .and.
           &        (node .le. jend)) then
1 M MV             i = ii - node + nband
1 M MV             j = node - jst + 1
1 M MV             aa(i, j) = a(nold, jj)
1 M MV           end if
1 M MV         end if
1 M MV-->    end do
1 M----->  end do
1     !csd$ end parallel do
```

SSGETRF, SSGETRS

- General unsymmetric **A**
- Sparse
- Real **A** and **b**
- Threshold pivoting
- Optimized by Cray in SciLib

SSGETRF, SSGETRS Steps

- Fill-reduction reordering
- Symbolic factorization
- Execution sequence and memory management
- Numerical factorization
- Back substitution

SSTSTRF, SSTSTRS

- Unsymmetric **A** with symmetric structure (typical FEM data)
- Sparse
- Real **A** and **b**
- No pivoting
- Optimized by Cray in SciLib

SSTSTRF, SSTSTRS Steps

- Fill-reduction reordering
- Symbolic factorization
- Execution sequence and memory management
- Numerical factorization
- Back substitution

SuperLU

- General unsymmetric **A**
- Sparse
- C
- Real **A** and **b**
- Threshold pivoting
- No optimization on the X1

SuperLU Steps

- Equilibrate
- Preorder the rows of **A**
- Order the columns of **A**
- Numerical factorization
- Back substitution

UMFPACK

- General unsymmetric **A**
- Sparse
- Multifrontal method
- Approximate Minimum Degree ordering
- C
- Real **A** and **b**
- Threshold pivoting
- No optimization on the X1

UMFPACK Steps

- Preorder and symbolic analysis
- Numerical factorization
- Back substitution

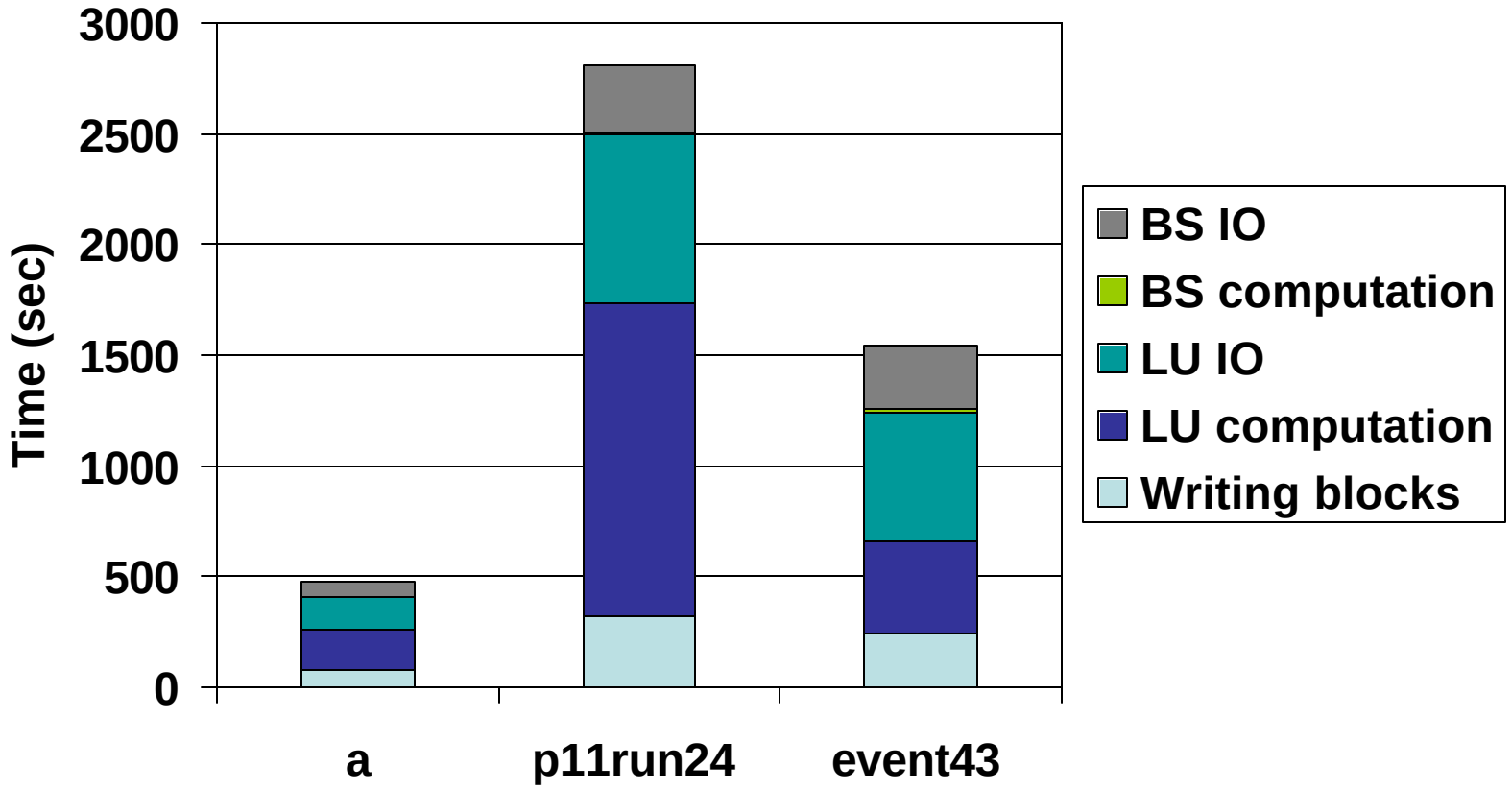
CGWAVE Data Sets

Data Set ID	a	p11run24	event43
Nodes	130,255	265,119	496,286
Old half BW	719	1,487	1,829
New half BW	719	1,487	583
$\mathrm{Max}_i \lvert(\mathbf{x}_{bm})_i\rvert$	7.58	0.000443	2.92
$\mathrm{Max}_i \lvert(\mathbf{b})_i\rvert$	596.0	0.0288	108.0

Bansol – X1

	T_h	a	p11run24	event43
Band. red.		0.7	1.6	3.2
Wr. blocks		73.7	317.6	246.1
LU comp.	0.1	189.1	1,416.1	415.8
	1.0	187.8	1,415.9	413.9
LU IO	0.1	141.7	762.9	581.5
	1.0	194.2	773.5	678.9
BS comp.	0.1	6.7	11.6	12.0
	1.0	6.7	10.9	12.2
BS IO	0.1	64.0	300.9	286.3
	1.0	79.6	311.6	316.2

Bansol – X1 (T_h = 0.1)



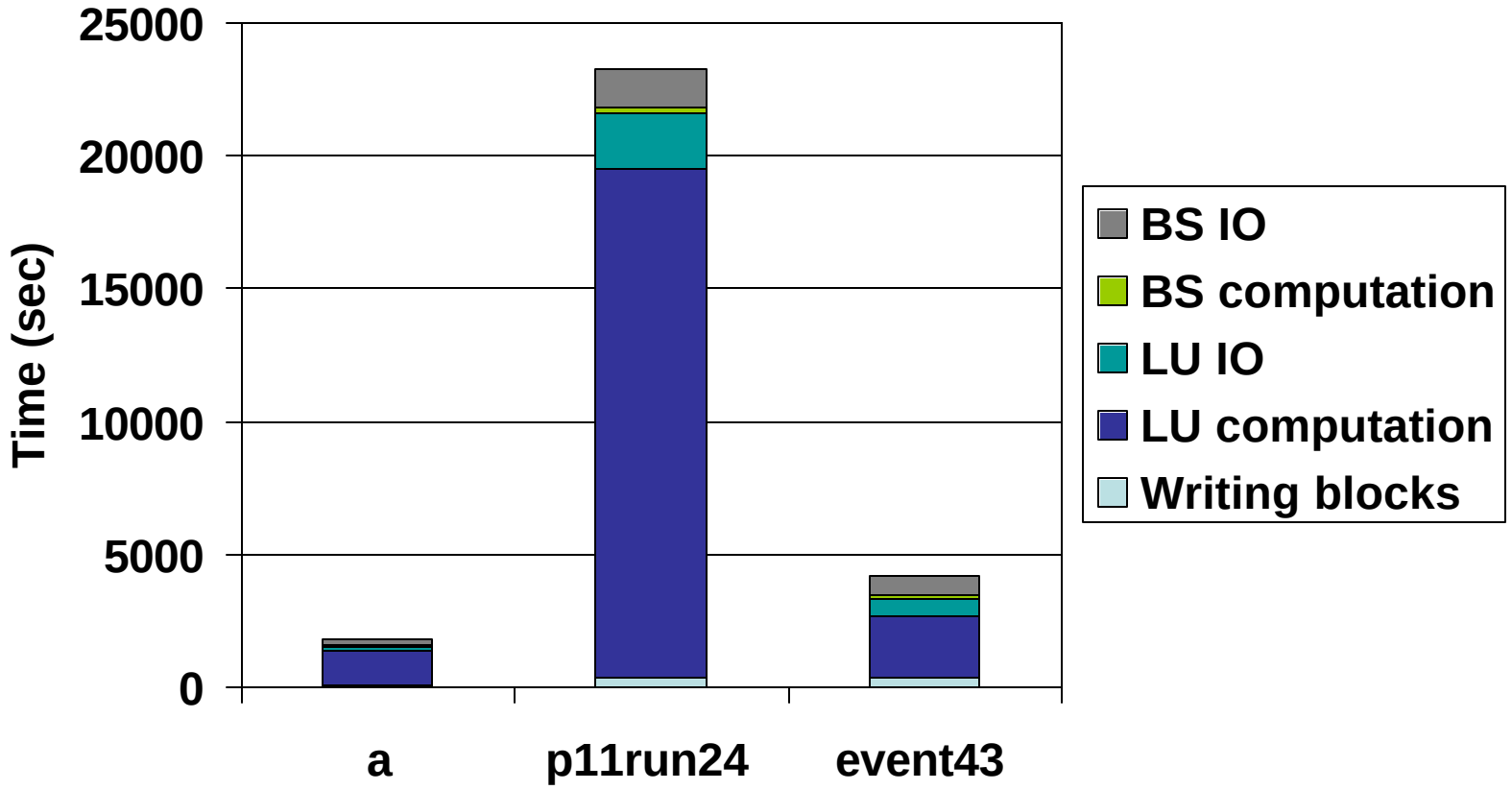
Bansol – X1

	T_h	a	p11run24	event43
Total	0.1	478.7	2,812.4	1,543.5
	1.0	538.7	2,826.9	1,665.6
$Max_i \lvert(\mathbf{x}-\mathbf{x}_{bm})_i\rvert$	0.1	5.59 (10^{-13})	1.88 (10^{-15})	5.07 (10^{-11})
	1.0	5.60 (10^{-13})	1.90 (10^{-15})	5.07 (10^{-11})
$Max_i \lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	0.1	1.41 (10^{-11})	1.25 (10^{-15})	1.13 (10^{-12})
	1.0	1.38 (10^{-11})	1.00 (10^{-15})	1.13 (10^{-12})

Bansol – O3K

	T_h	a	p11run24	event43
Band. red.		0.1	0.3	0.5
Wr. blocks		79.7	348.2	379.8
LU comp.	0.1	1,316.0	19,130.7	2,264.7
	1.0	1,313.0	19,145.3	2,256.4
LU IO	0.1	141.7	2,134.5	702.0
	1.0	240.6	2,128.1	794.0
BS comp.	0.1	49.5	216.5	139.2
	1.0	48.7	211.9	141.1
BS IO	0.1	220.6	1,443.1	680.0
	1.0	221.8	1,761.8	716.7

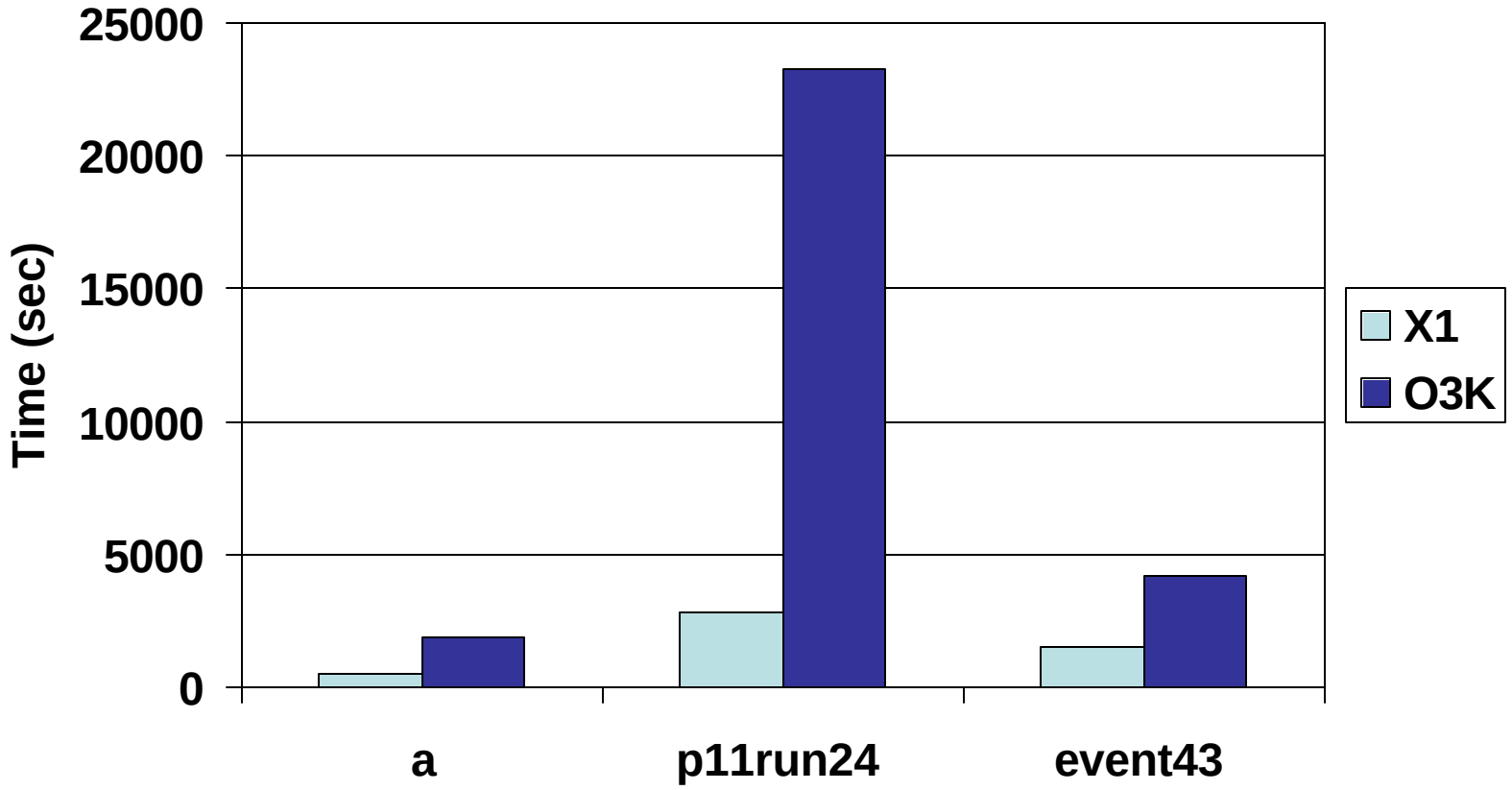
Bansol – O3K (T_h = 0.1)



Bansol – O3K

	T_h	a	p11run24	event43
Total	0.1	1,893.4	23,271.7	4,158.7
	1.0	1,909.9	23,596.6	4,295.2
$Max_i \lvert(\mathbf{x}-\mathbf{x}_{bm})_i\rvert$	0.1	5.55 (10^{-13})	1.88 (10^{-15})	5.07 (10^{-11})
	1.0	5.58 (10^{-13})	1.90 (10^{-15})	5.07 (10^{-11})
$Max_i \lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	0.1	1.80 (10^{-11})	1.52 (10^{-15})	1.20 (10^{-12})
	1.0	1.61 (10^{-11})	1.37 (10^{-15})	1.20 (10^{-12})

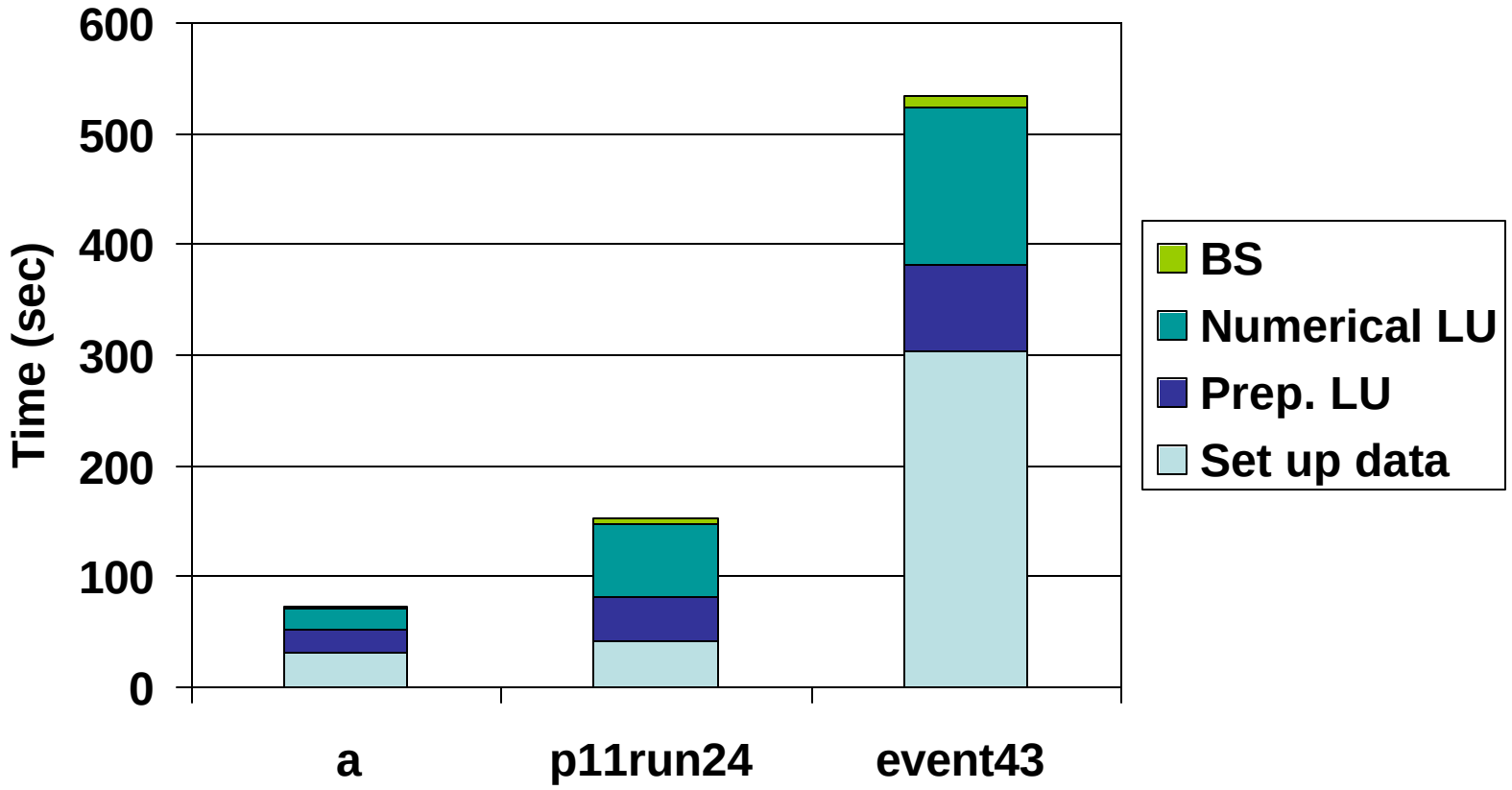
Bansol Comparison



SSGETRF/SSGETRS – X1

$T_h = 0.1$	a	p11run24	event43
Set up data	30.6	41.7	303.6
Preparation LU	21.4	39.7	77.9
Numerical LU	18.7	65.4	142.4
BS	2.9	5.8	10.9
Total	73.4	152.2	534.0
Max_i $\lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	1.09 (10^{-10})	4.37 (10^{-15})	1.26 (10^{-10})

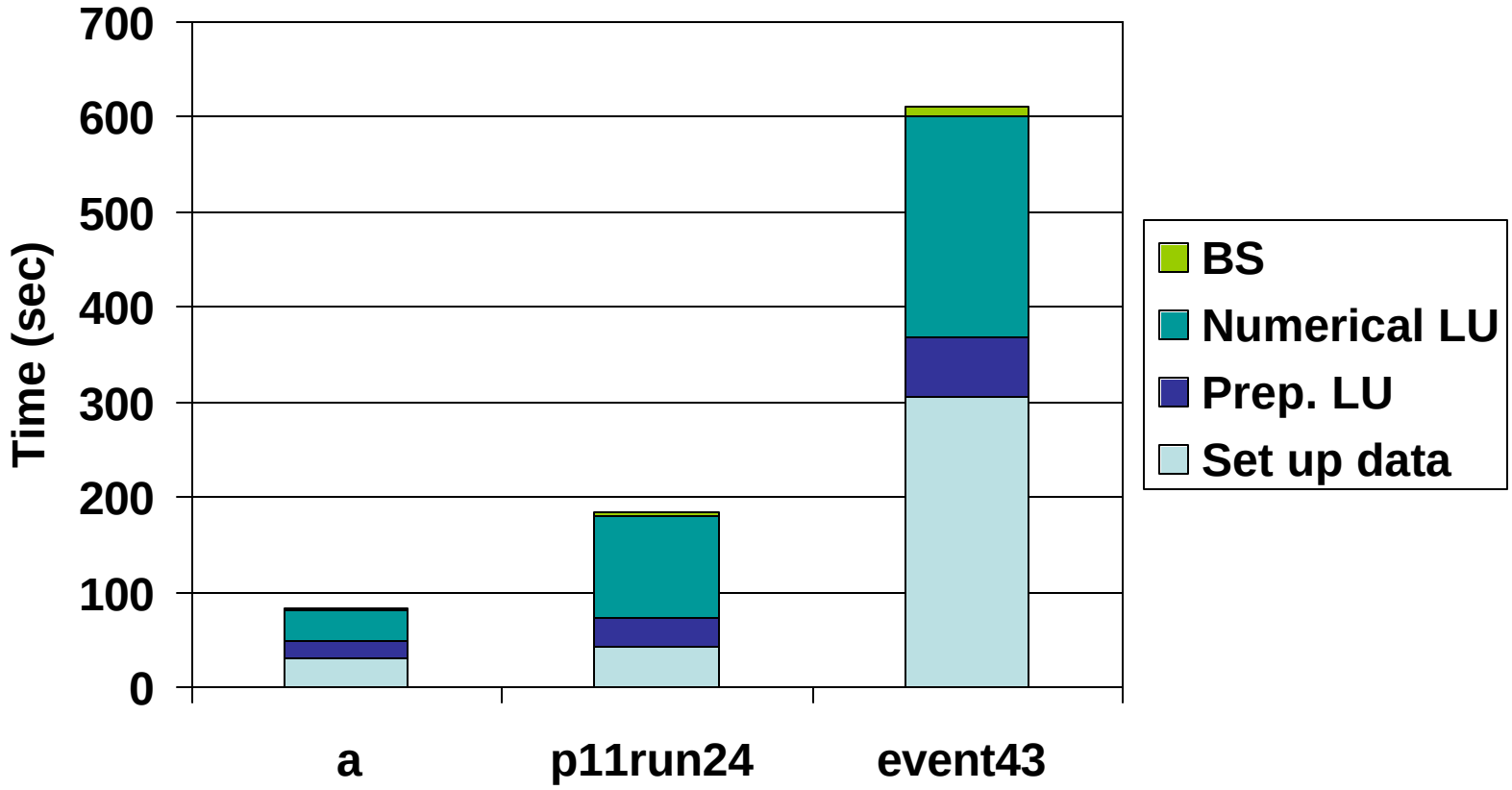
SSGETRF/SSGETRS – X1



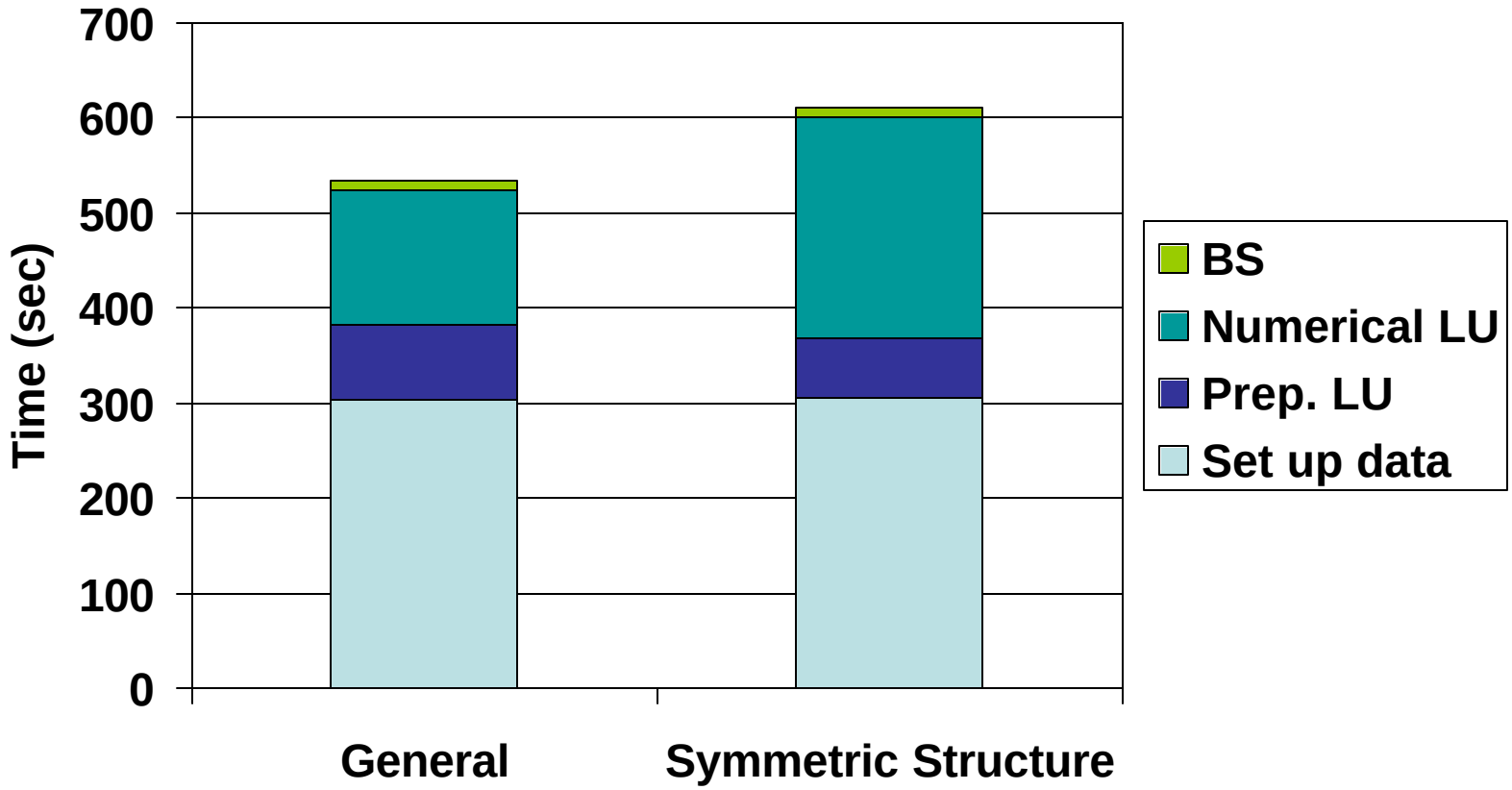
SSTSTRF/SSTSTRS – X1

	a	p11run24	event43
Set up data	30.1	41.5	305.0
Preparation LU	17.5	31.7	63.5
Numerical LU	33.1	106.4	231.9
BS	2.7	5.4	10.3
Total	83.4	185.0	610.8
Max_i $\lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	3.82 (10^{-9})	1.73 (10^{-14})	2.13 (10^{-8})

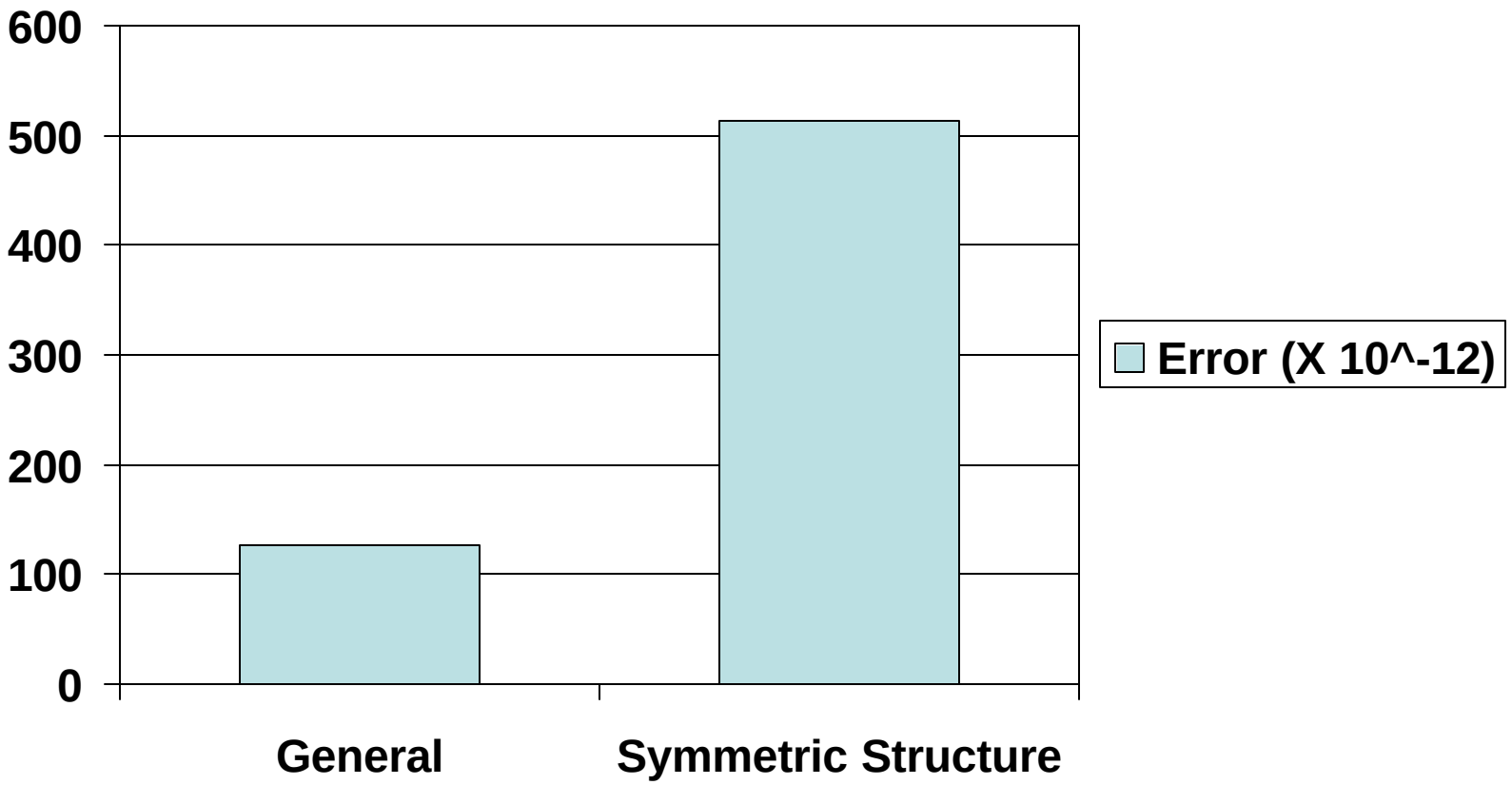
SSTSTRF/SSTSTRS – X1



General vs. Symmetric Structure Comparison



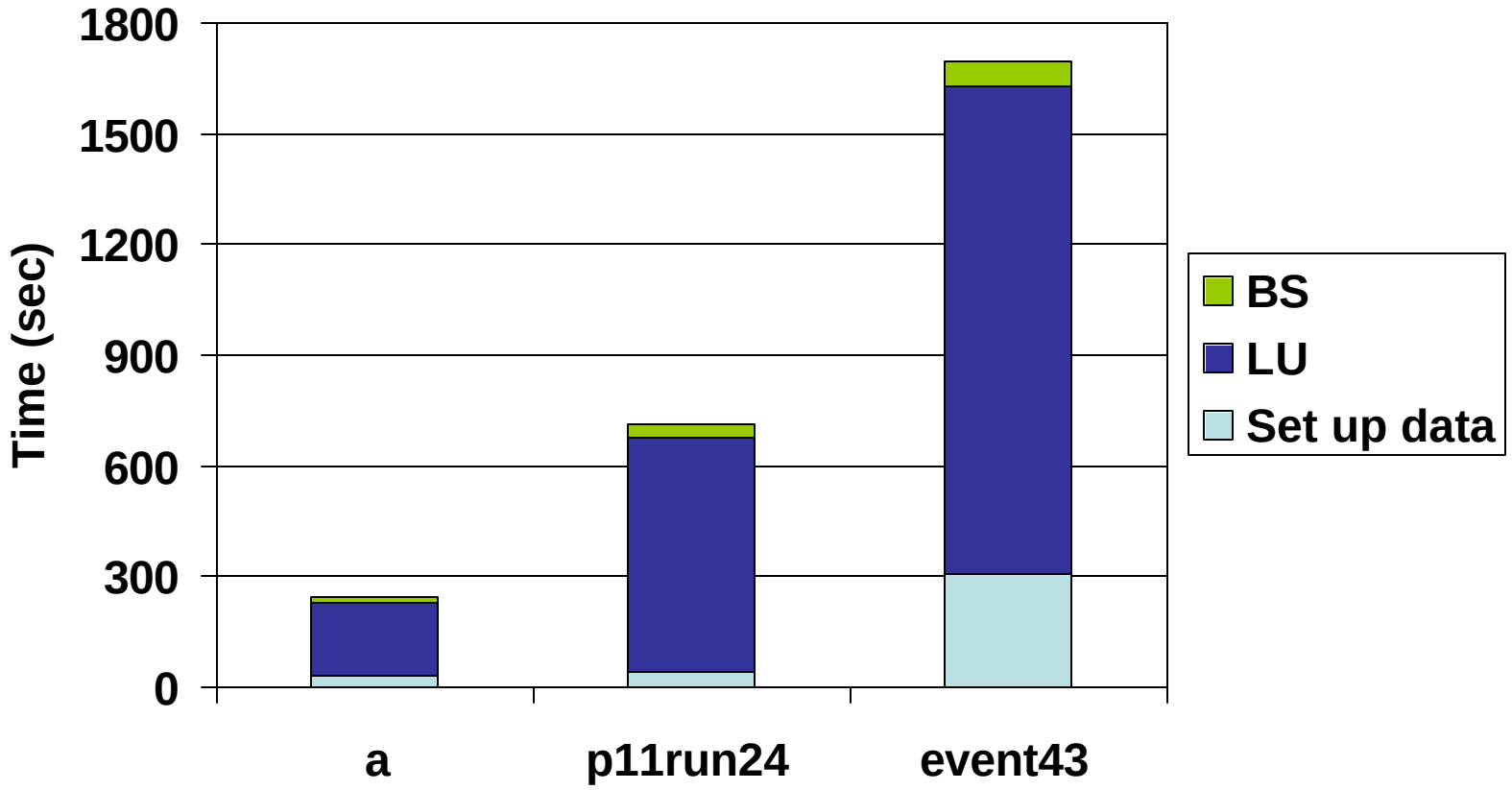
General vs. Symmetric Structure Comparison



SuperLU – X1

$T_h = 0.1$	a	p11run24	event43
Set up data	30.1	41.0	305.9
LU	199.4	633.2	1,322.4
BS	13.2	36.3	65.4
Total	242.7	710.5	1,690.8
Max_i $\lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	2.66 (10^{-10})	4.53 (10^{-15})	5.10 (10^{-10})

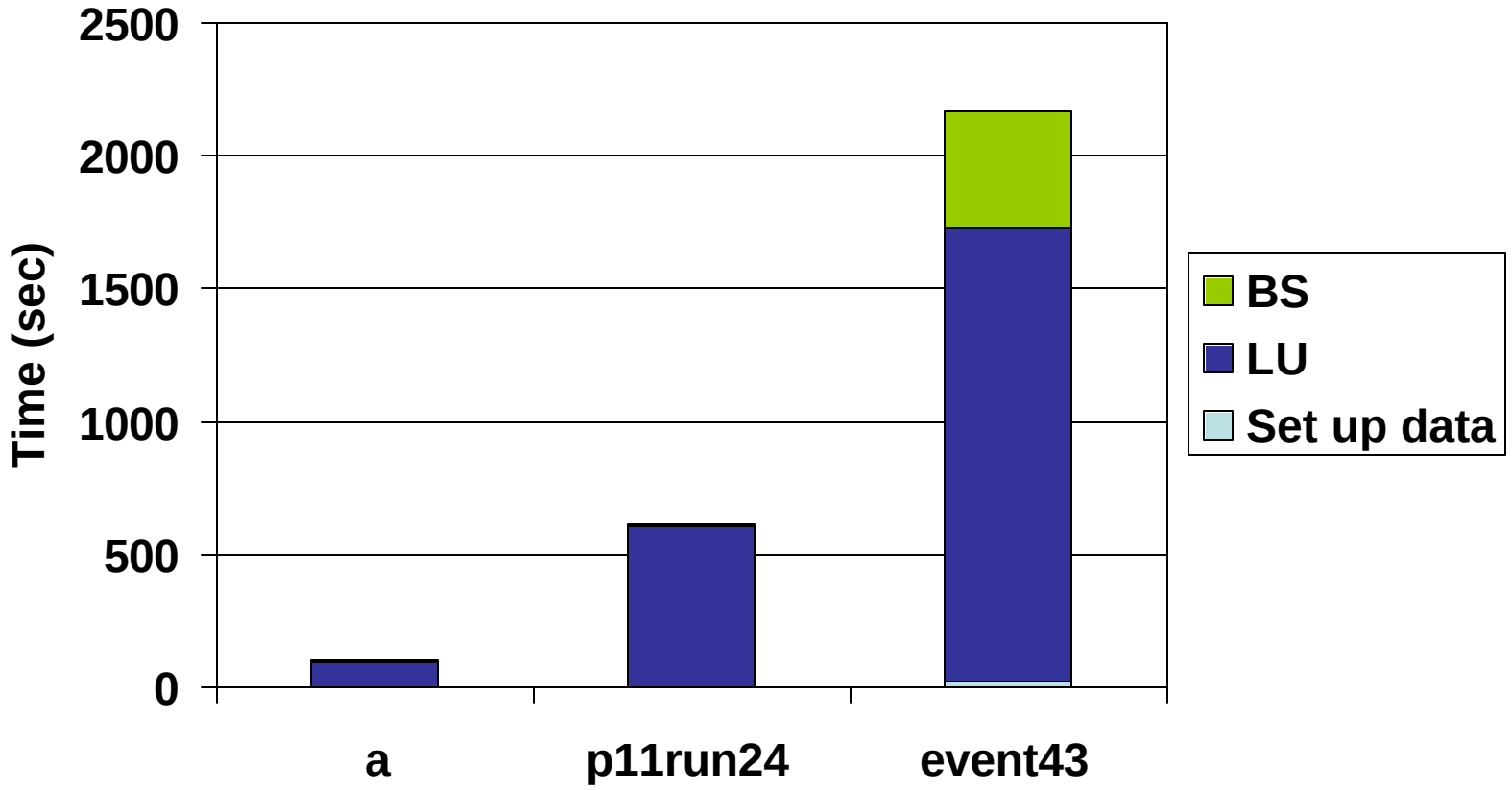
SuperLU – X1


1800
1500
1200
900
600
300
0
Time (sec)
a
p11run24
event43
BS
LU
Set up data

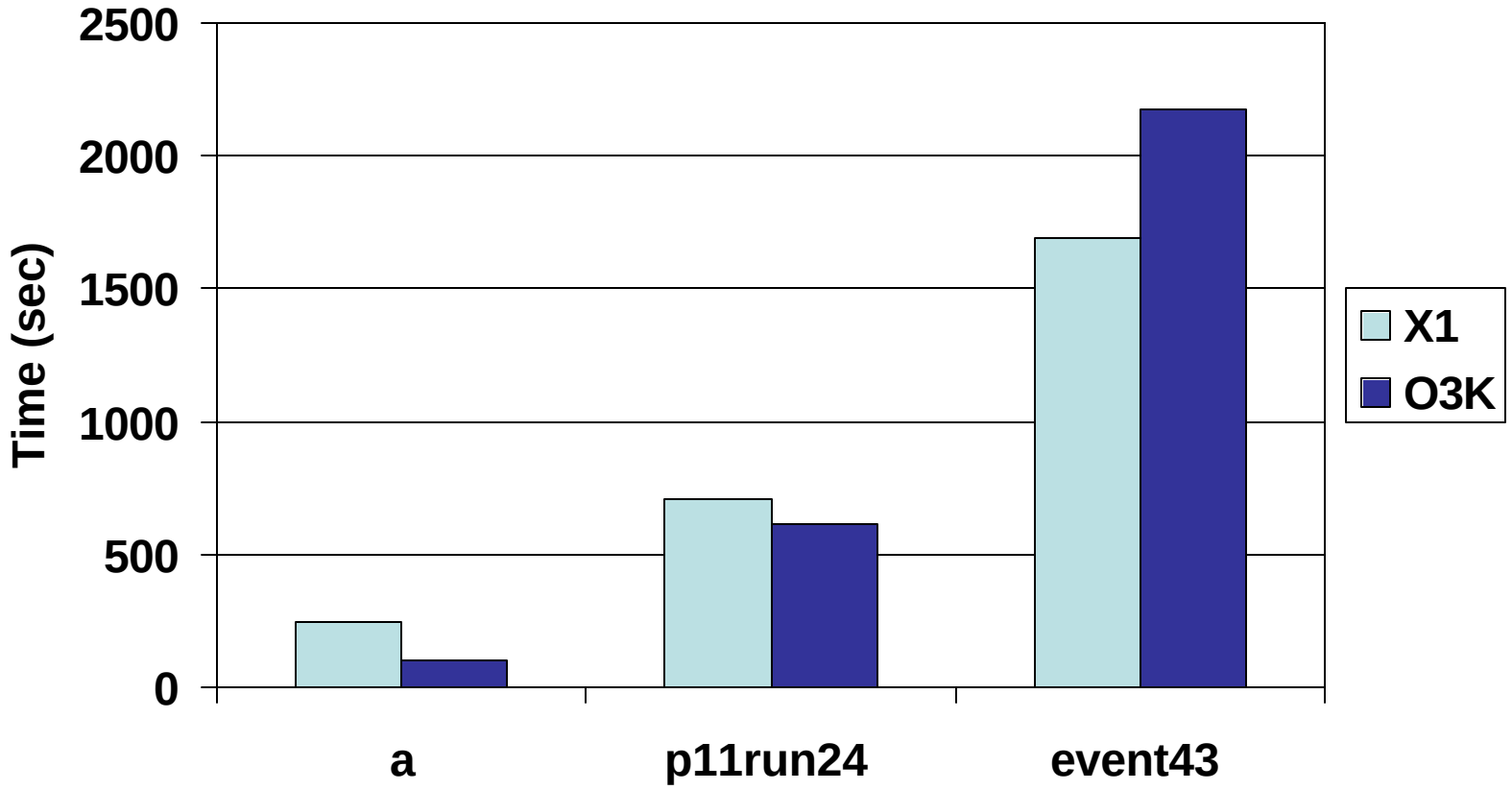
SuperLU – O3K

$T_h = 0.1$	a	p11run24	event43
Set up data	1.8	2.9	19.1
LU	93.8	603.4	1,706.7
BS	2.2	6.1	443.3
Total	97.8	612.6	2,171.5
Max_i $\lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	3.56 (10^{-10})	54.7 (10^{-16})	5.51 (10^{-11})

SuperLU – O3K


2500
2000
1500
1000
500
0
Time (sec)
a
p11run24
event43
BS
LU
Set up data

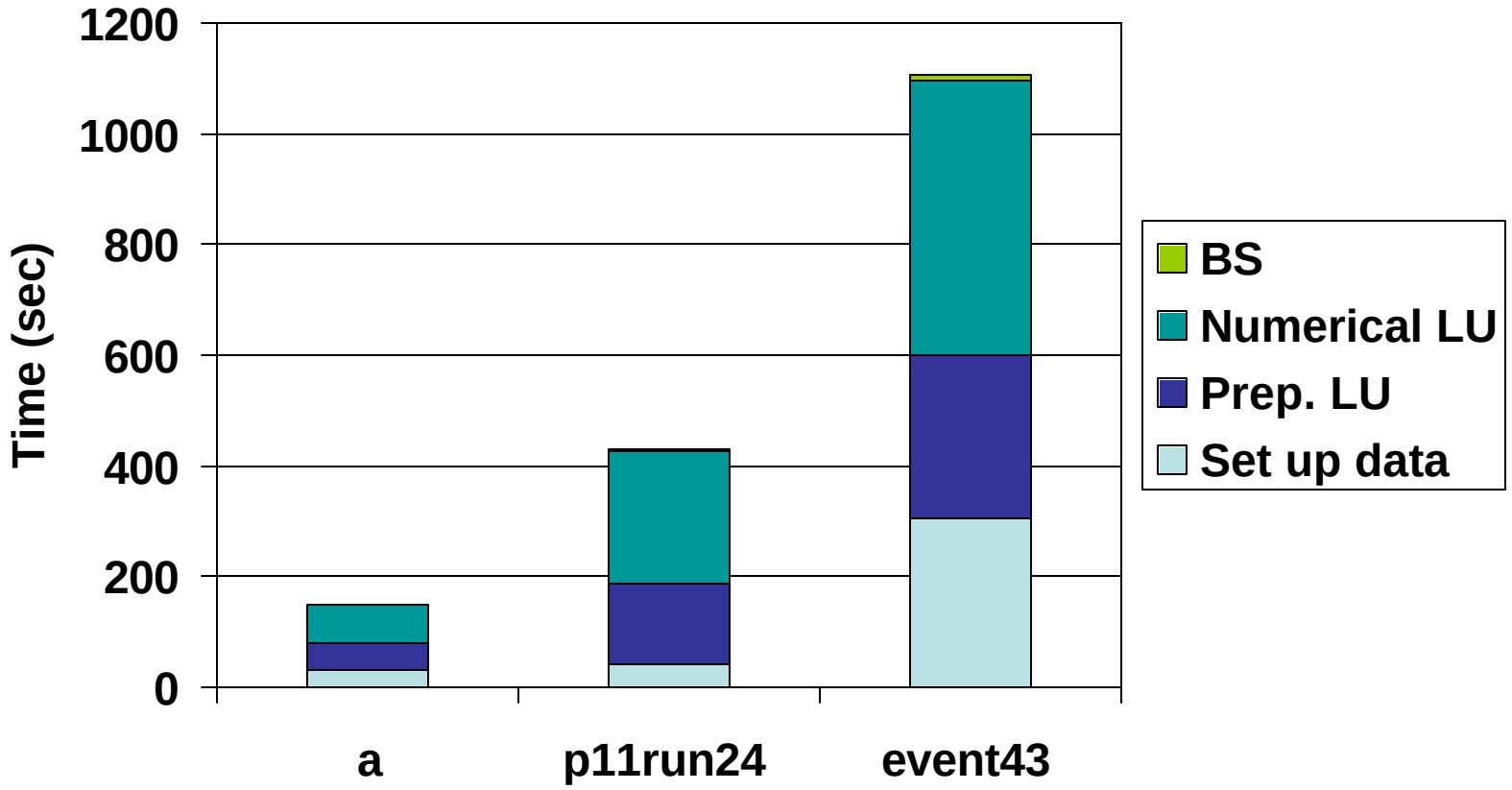
SuperLU Comparison



UMFPACK – X1

$T_h = 0.1$	a	p11run24	event43
Set up data	30.4	42.1	305.2
Preparation LU	47.7	143.9	294.6
Numerical LU	71.0	240.5	496.5
BS	1.7	4.2	9.1
Total	151.0	431.2	1,105.9
Max_i $\lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	1.85 (10^{-9})	5.06 (10^{-15})	5.43 (10^{-10})

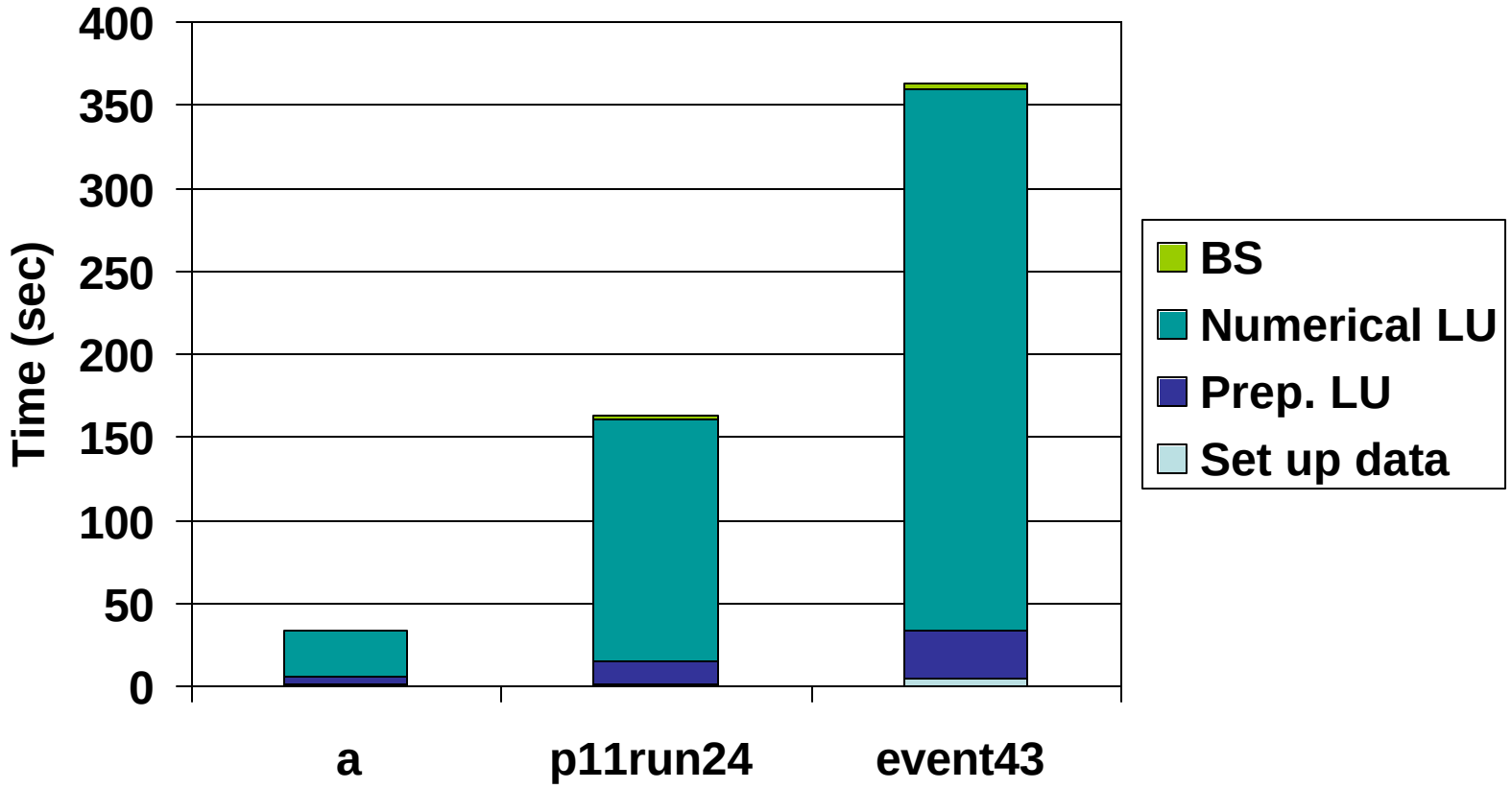
UMFPACK – X1


1200
1000
800
600
400
200
0
Time (sec)
a
p11run24
event43
BS
Numerical LU
Prep. LU
Set up data

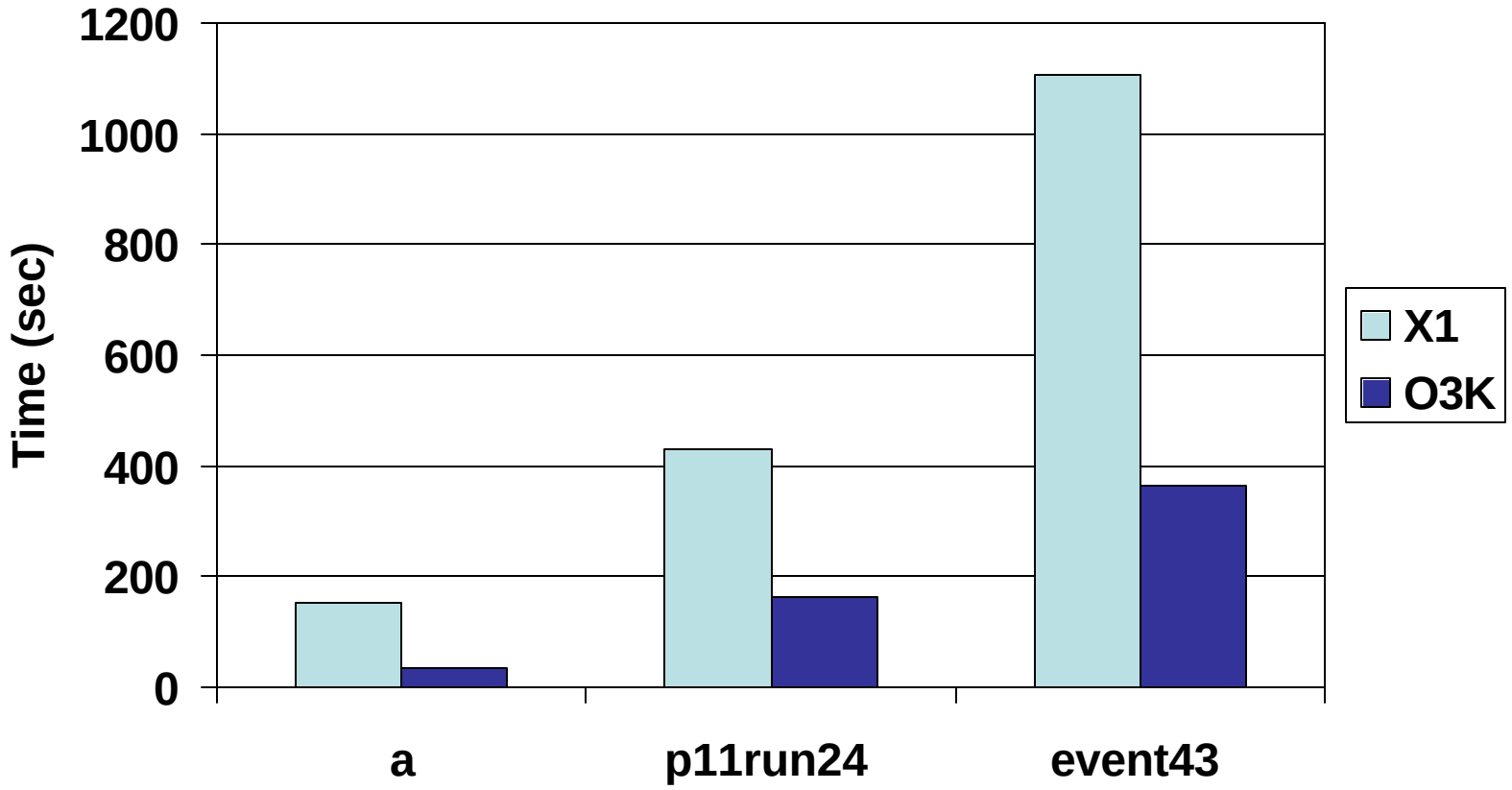
UMFPACK – O3K

$T_h = 0.1$	a	p11run24	event43
Set up data	0.7	1.2	4.7
Preparation LU	4.9	13.6	28.6
Numerical LU	27.5	146.3	325.8
BS	0.7	1.9	4.0
Total	33.8	163.0	363.1
Max_i $\lvert(\mathbf{b}-\mathbf{Ax})_i\rvert$	3.20 (10^{-9})	1.91 (10^{-14})	1.47 (10^{-9})

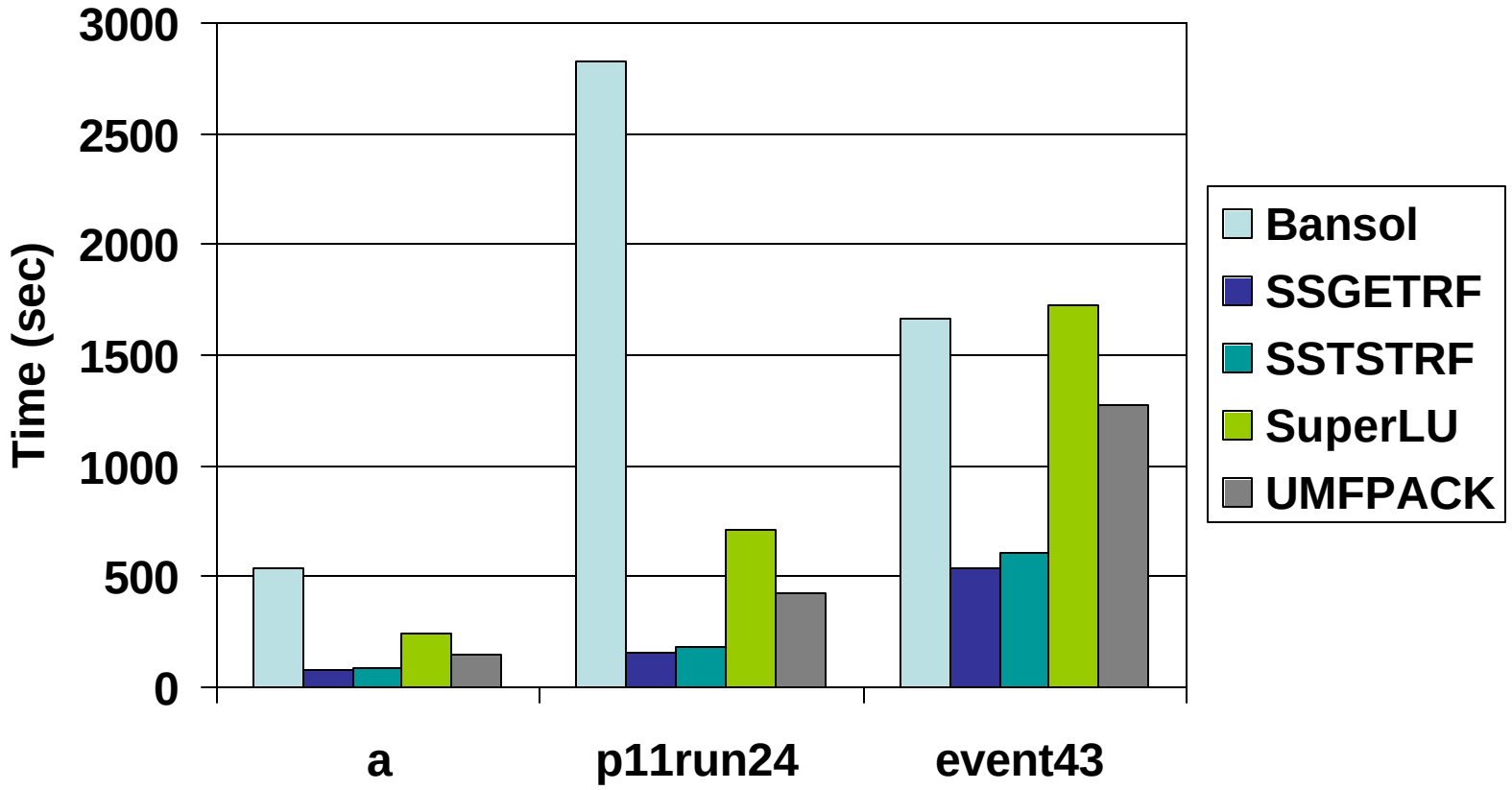
UMFPACK – O3K


400
350
300
250
200
150
100
50
0
Time (sec)
a
p11run24
event43
BS
Numerical LU
Prep. LU
Set up data

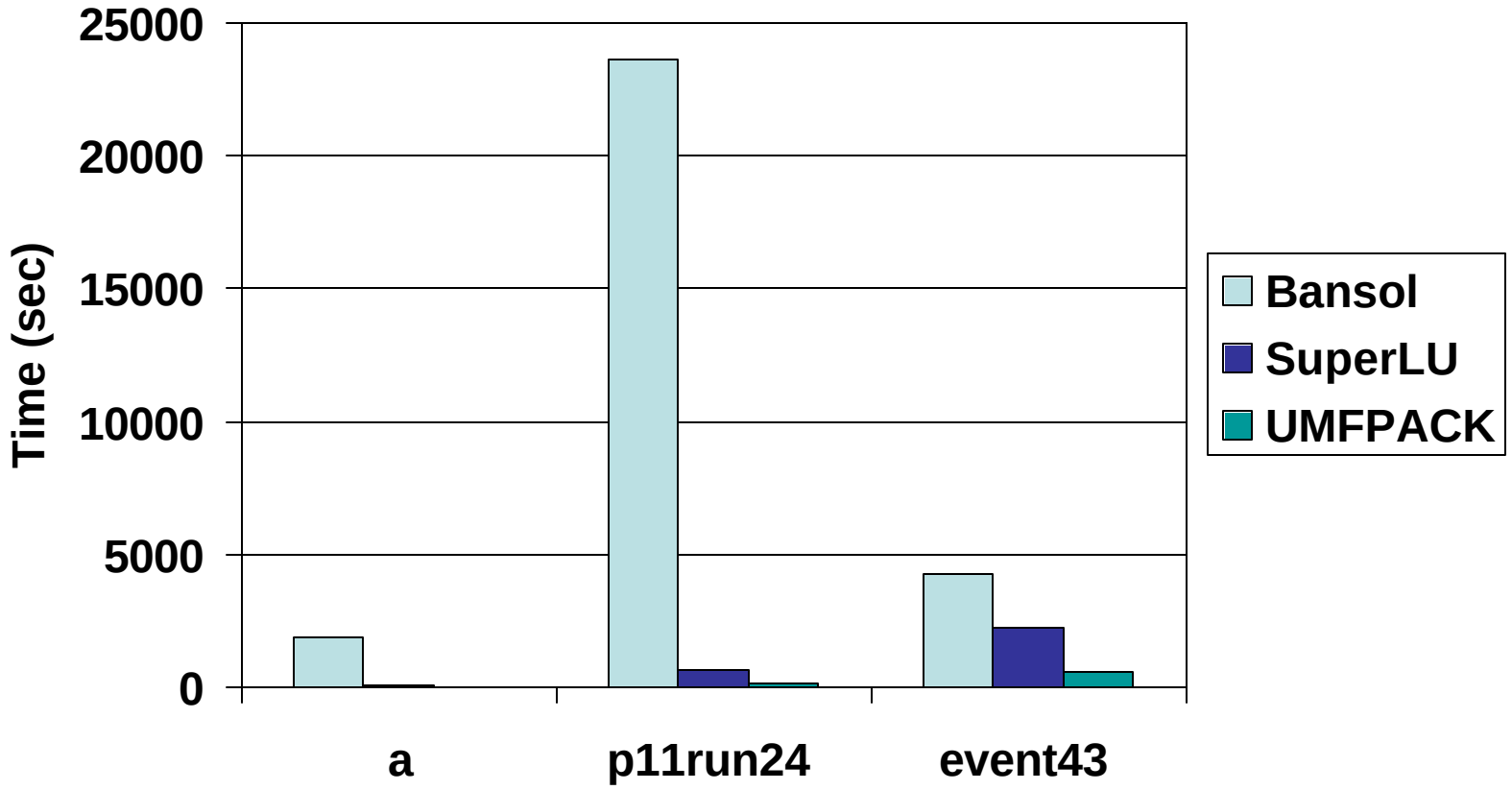
UMFPACK Comparison



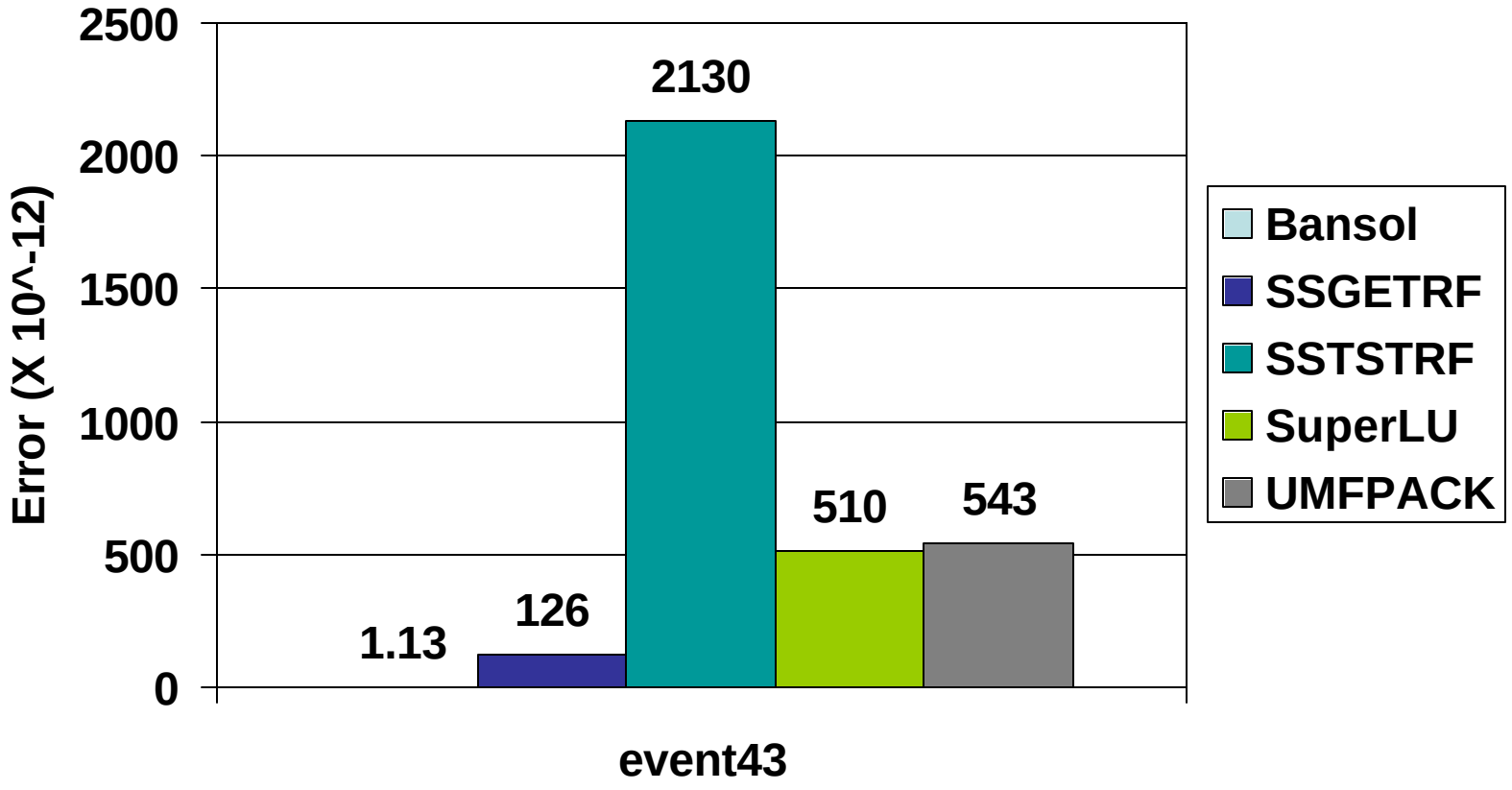
Comparison of Solvers – X1



Comparison of Solvers – O3K



Accuracy – X1 (Infinity Norm)



Questions?