SC16@Salt Lake
HPCG BoF@Room 335E

HPCG Performance Improvement on the K computer ～short introduction～

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Our previous code until SC15

Our previous tuned code marked 0.461 PFLOPS for SC15

SC15 score

Rank	Computer	Country	HPL PFLOPS	HPCG PFLOPS	Ratio to HPL %
1	Tianhe-2	China	33.86	0.580	1.7%
2	K computer	Japan	10.51	0.461	4.4%
3	Titan	USA	17.59	0.322	1.8%
4	Trinity	USA	8.10	0.183	2.3%
5	Mira	USA	8.59	0.167	1.9%

http://www.hpcg-benchmark.org/custom/index.html?lid=155&slid=282

Bandwidth on the K computer@Compute Node

	Theoretical	STREAM	SPMV	SYMGS
GB/s	64	Practical limit 46	48	44

It is impossible to improve the bandwidth.

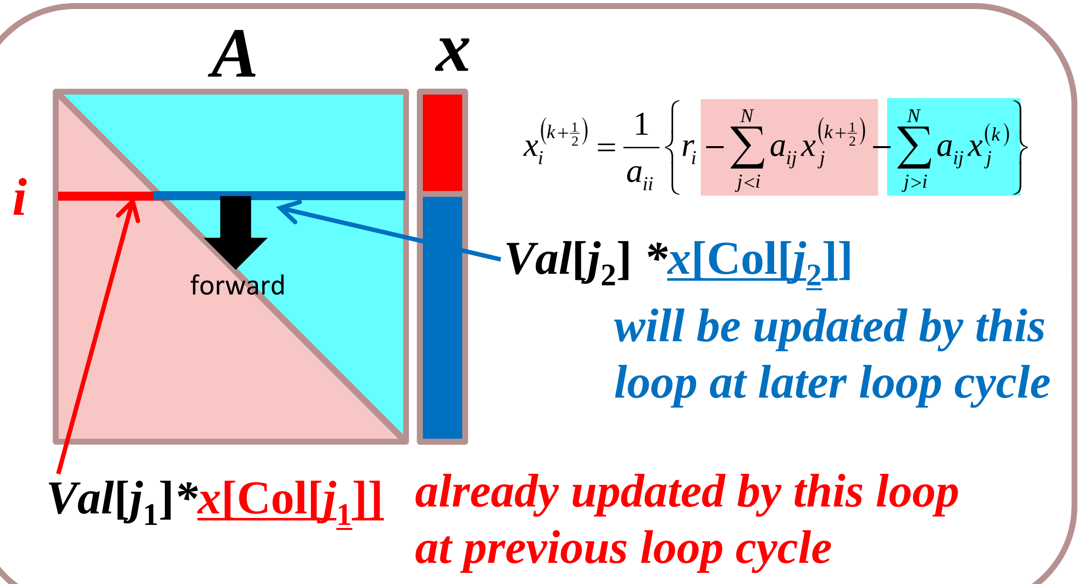
To get more score, we have to use another way, especially hot kernel SYMGS

Symmetric Gauss-Seidel

- Structure of Original Symmetric Gauss-Seidel

Forward Loop

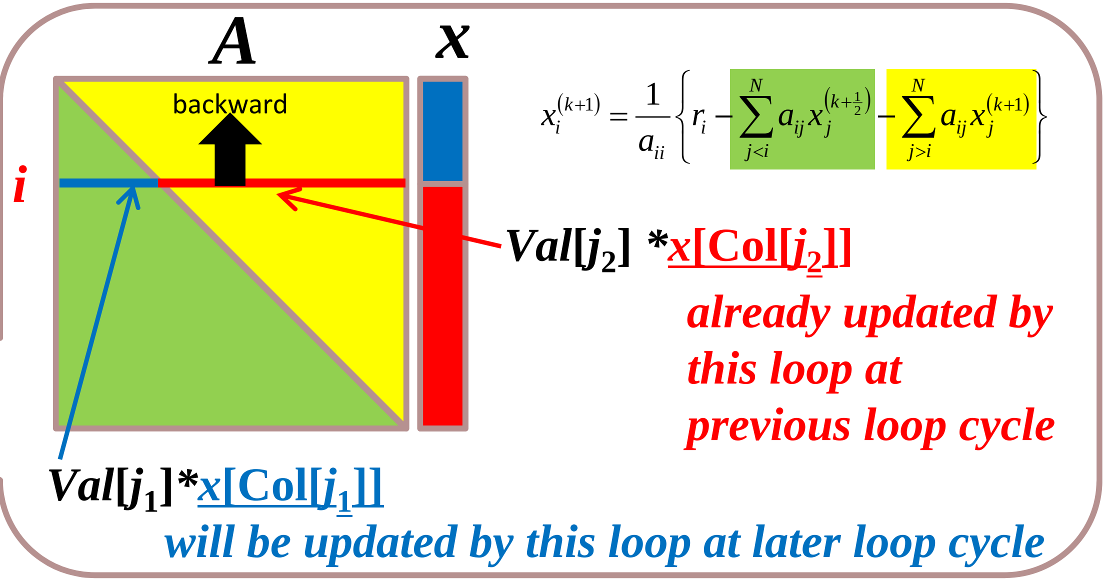
```
for (int i = 0; i < nrow; i++) {
            …
  double sum = r[i];
  for (int j = 0; j < nzInRow[i]; j++)
    sum -= Val[j]*x[Col[j]];
   sum += x[i]*Diag;
   x[i] = sum/Diag;
}
```



$$x_i^{(k+\frac{1}{2})} = \frac{1}{a_{ii}}\left\{ r_i - \sum_{j<i}^{N} a_{ij} x_j^{(k+\frac{1}{2})} - \sum_{j>i}^{N} a_{ij} x_j^{(k)} \right\}$$

Backward Loop

```
for (int i = nrow-1; i  >= 0; i--) {
            …
  double sum = r[i];
  for (int j = 0; j < nzInRow[i]; j++)
    sum -= Val[j]*x[Col[j]];
   sum += x[i]*Diag;
   x[i] = sum/Diag;
}
```



$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left\{ r_i - \sum_{j<i}^{N} a_{ij} x_j^{(k+\frac{1}{2})} - \sum_{j>i}^{N} a_{ij} x_j^{(k+1)} \right\}$$

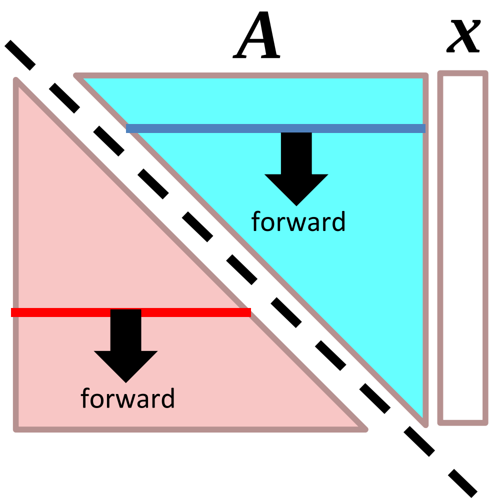
Symmetric Gauss-Seidel

- *Forward* loop can be split into two loops: *Loop1 & Loop2*

Loop2

```
for (int i = 0; i < nrow; i++) {
            …
  double sum = y[i];
  for (int j = 0; j < nzLInRow[i]; j++)
    sum -= Val[j]*x[Col[j]];
  sum += x[i]*Diag;     updated by Loop2
  x[i] = sum/Diag;      previously
}
```

$$x_i^{(k+\frac{1}{2})} = \frac{1}{a_{ii}}\left\{ y_i - \sum_{j<i}^{N} a_{ij} x_j^{(k+\frac{1}{2})} \right\}$$



Loop1

```
#omp parallel for
for (int i = 0; i < nrow; i++) {
        …
  double sum = r[i];
  for (int j = nzLInRow[i];
               j < nzInRow[i]; j++)
    sum -= Val[j]*x[Col[j]];
  y[i] = sum;        defined before Loop1
}                    and not updated
```

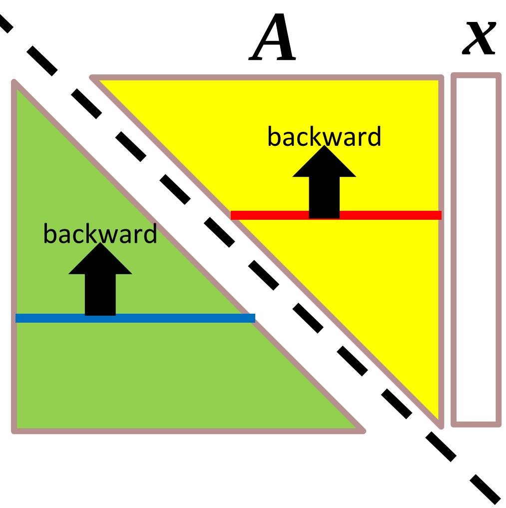
$$y_i = r_i - \sum_{j>i}^{N} a_{ij} x_j^{(k)}$$

- *Backward* loop can be split into two loops: *Loop3 & Loop4*

Loop3

```
#omp parallel for
for (int i = nrow-1; i >= 0; i--) {
            …
  double sum = r[i];
  for (int j = 0; j < nzLInRow[i]; j++)
    sum -= Val[j]*x[Col[j]];
  y[i] = sum;        updated by Loop2
}                    and not updated
```

$$y_i = r_i - \sum_{j<i}^{N} a_{ij} x_j^{(k+\frac{1}{2})}$$



Loop4

```
for (int i = nrow-1; i >= 0: i--) {
        …
  double sum = y[i];
  for (int j = nzLInRow[i];
              j < nzInRow[i];  j++)
    sum -= Val[j]*x[Col[j]];
  sum += x[i]*Diag;   updated by Loop4
  x[i] = sum/Diag;    previously
}
```

$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left\{ y_i - \sum_{j>i}^{N} a_{ij} x_j^{(k+1)} \right\}$$

- *Execution Order*: *Loop1 → Loop2 → Loop3 → Loop4*

Symmetric Gauss-Seidel

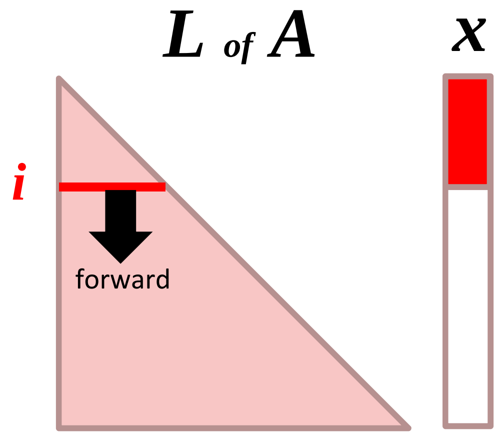
- *Loop3* can be reversed
- Row *i* of *Loop3* can be calculated *only if* from row 0 to *i* of *Loop2* are calculated → more chance to use cache effectively

Loop direction reversing does not change arithmetic order!!

Loop2

```
for (int i = 0; i < nrow; i++) {
              …
  double sum = y[i];
  for (int j = 0; j < nzLInRow[i]; j++)
     sum -= Val[j]*x[Col[j]];
   sum += x[i]*Diag;
   x[i] = sum/Diag;
}
```

defind in Loop2

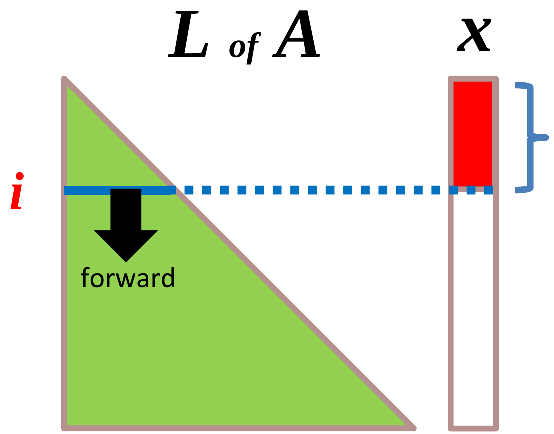


$$x_i^{(k+\frac{1}{2})} = \frac{1}{a_{ii}} \left\{ y_i - \sum_{j<i}^{N} a_{ij} x_j^{(k+\frac{1}{2})} \right\}$$

Loop3

```
for (int i = 0; i < nrow; i++) {
              …
  double sum = r[i];
  for (int j = 0; j < nzLInRow[i]; j++)
     sum -= Val[j]*x[Col[j]];
   y[i] = sum;
}
```

defined in Loop2



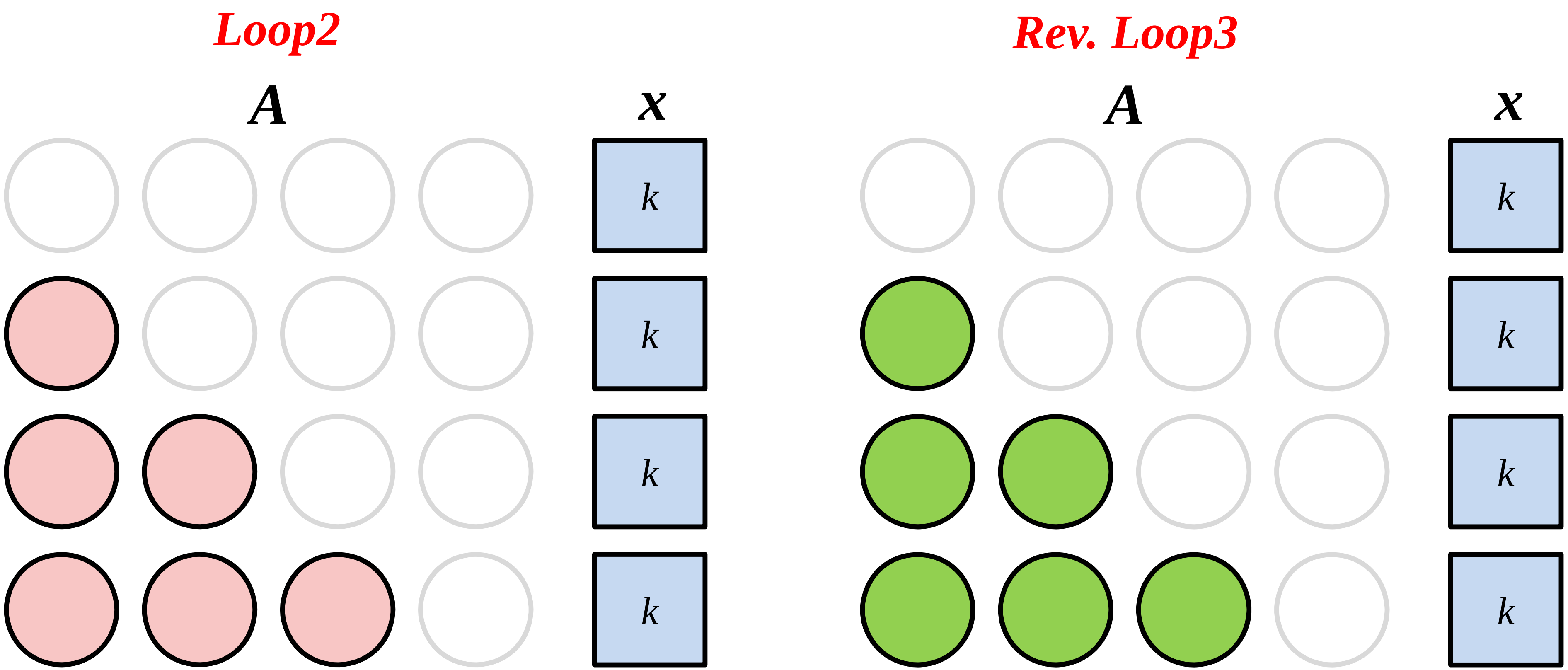
updated row 0 to i of Loop2

$$y_i = r_i - \sum_{j<i}^{N} a_{ij} x_j^{(k+\frac{1}{2})}$$

Symmetric Gauss-Seidel

Marching of updating of *Loop2* and *Loop3*
(sample by 4X4 problem)

initial



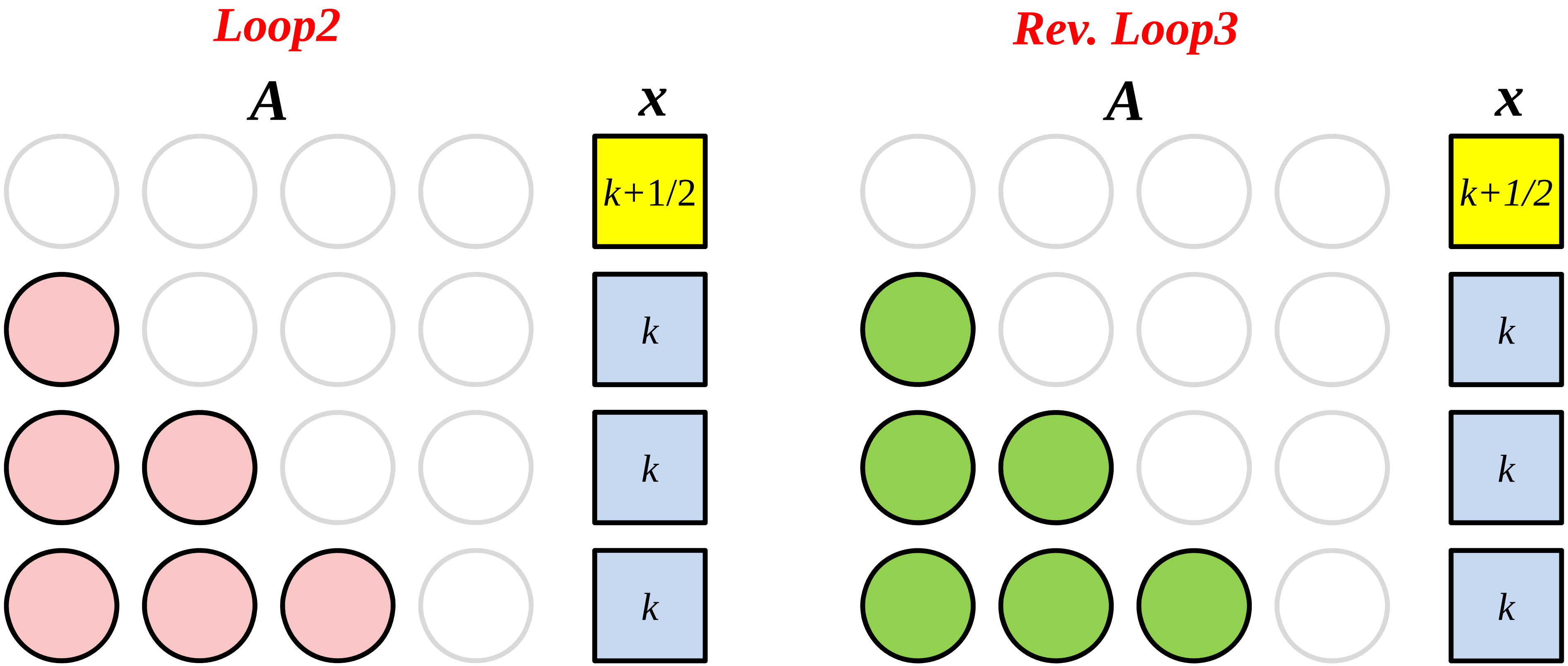
$$x_i^{\left(k+\frac{1}{2}\right)} = \frac{1}{a_{ii}}\left\{ y_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)} \right\}$$

$$y_i = r_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)}$$

Symmetric Gauss-Seidel

Marching of updating of *Loop2* and *Loop3*
(sample by 4X4 problem)

i=1



$$x_i^{\left(k+\frac{1}{2}\right)} = \frac{1}{a_{ii}}\left\{ y_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)} \right\}$$

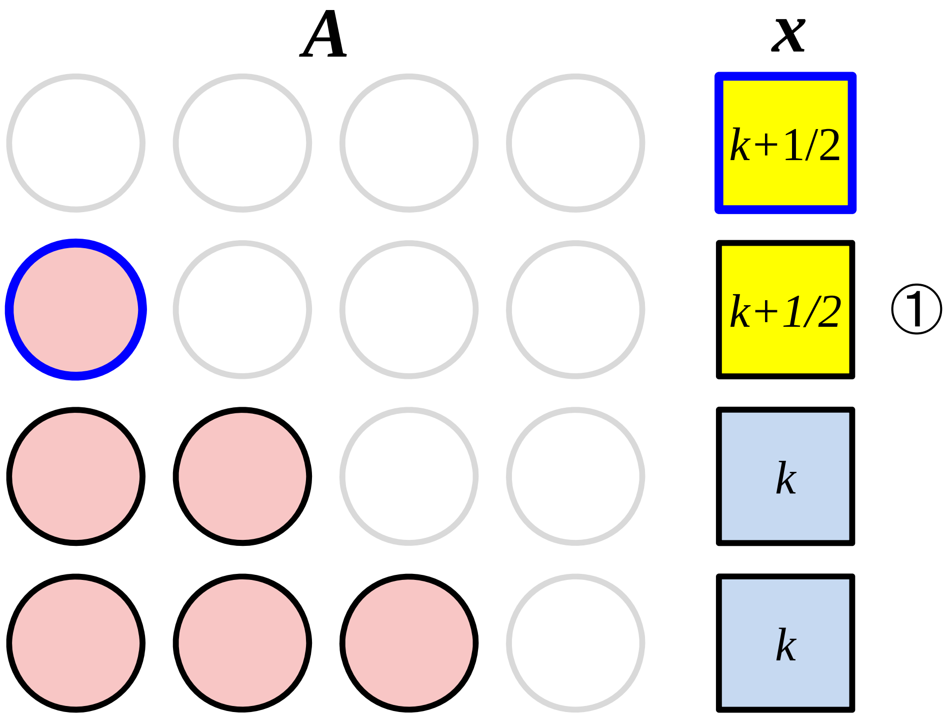
$$y_i = r_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)}$$

Symmetric Gauss-Seidel

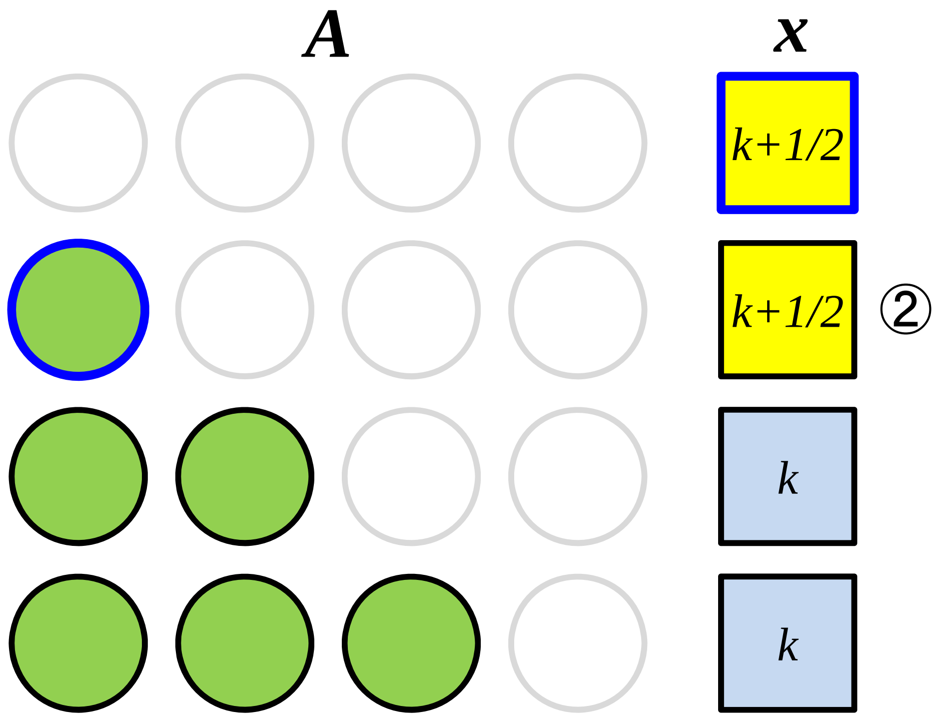
Marching of updating of *Loop2* and *Loop3*
(sample by 4X4 problem)

i=2

Loop2



Rev. Loop3



$$x_i^{\left(k+\frac{1}{2}\right)} = \frac{1}{a_{ii}} \left\{ y_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)} \right\}$$

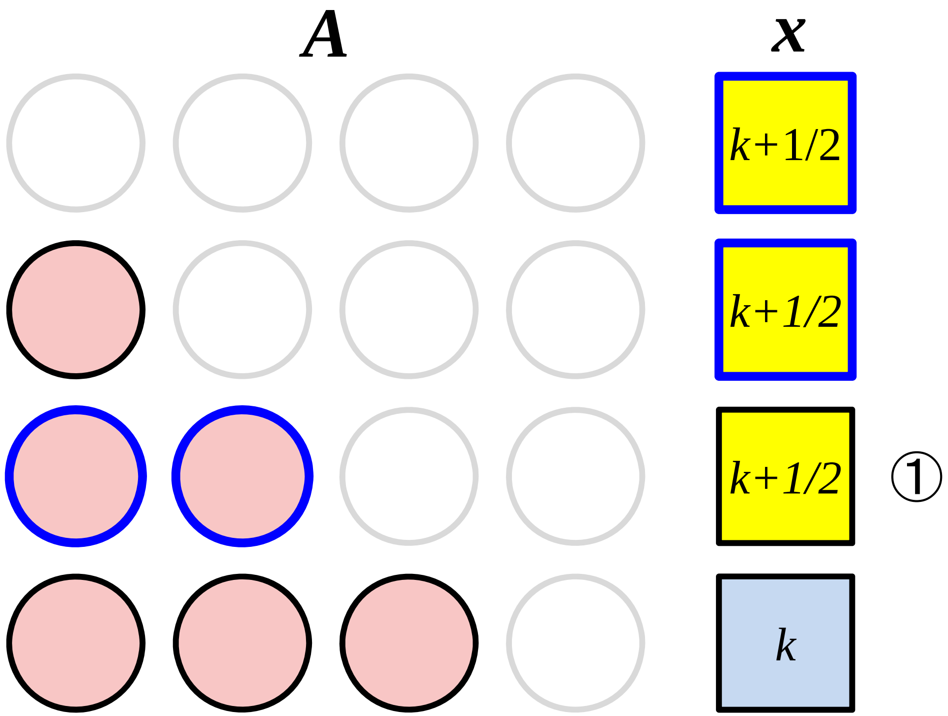
$$y_i = r_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)}$$

Symmetric Gauss-Seidel

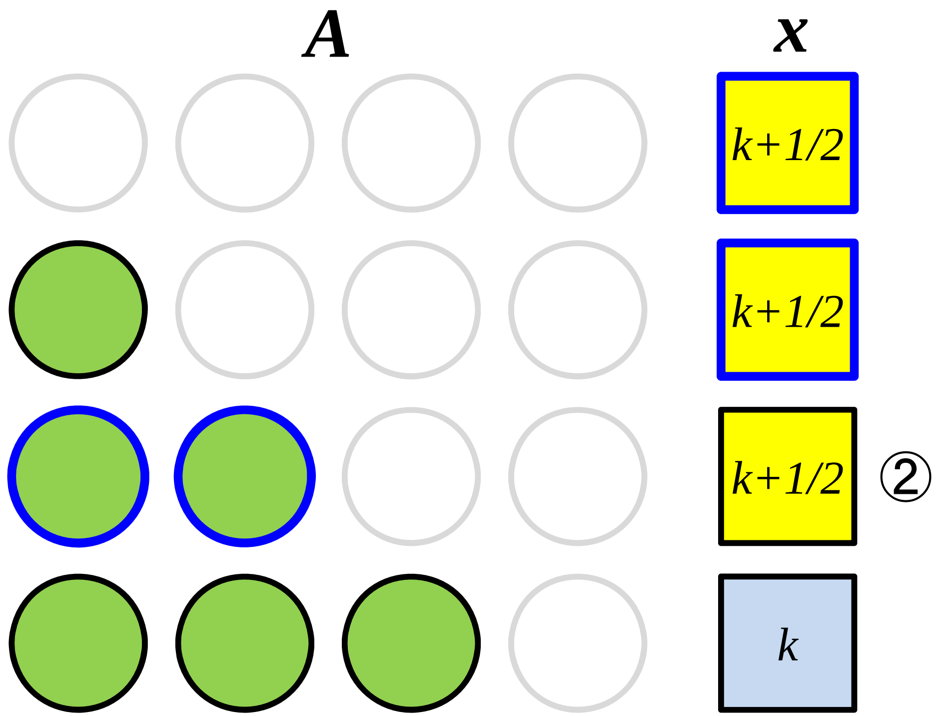
Marching of updating of *Loop2* and *Loop3*
(sample by 4X4 problem)

i=3

Loop2



Rev. Loop3



$$x_i^{\left(k+\frac{1}{2}\right)} = \frac{1}{a_{ii}}\left\{ y_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)} \right\}$$

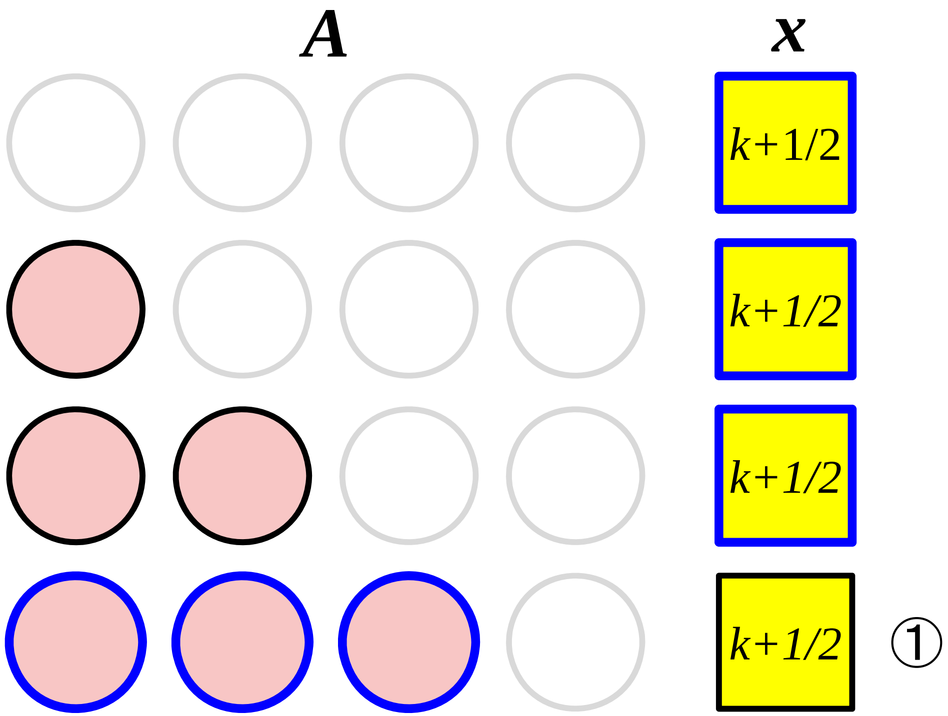
$$y_i = r_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)}$$

Symmetric Gauss-Seidel

Marching of updating of *Loop2* and *Loop3*
(sample by 4X4 problem)

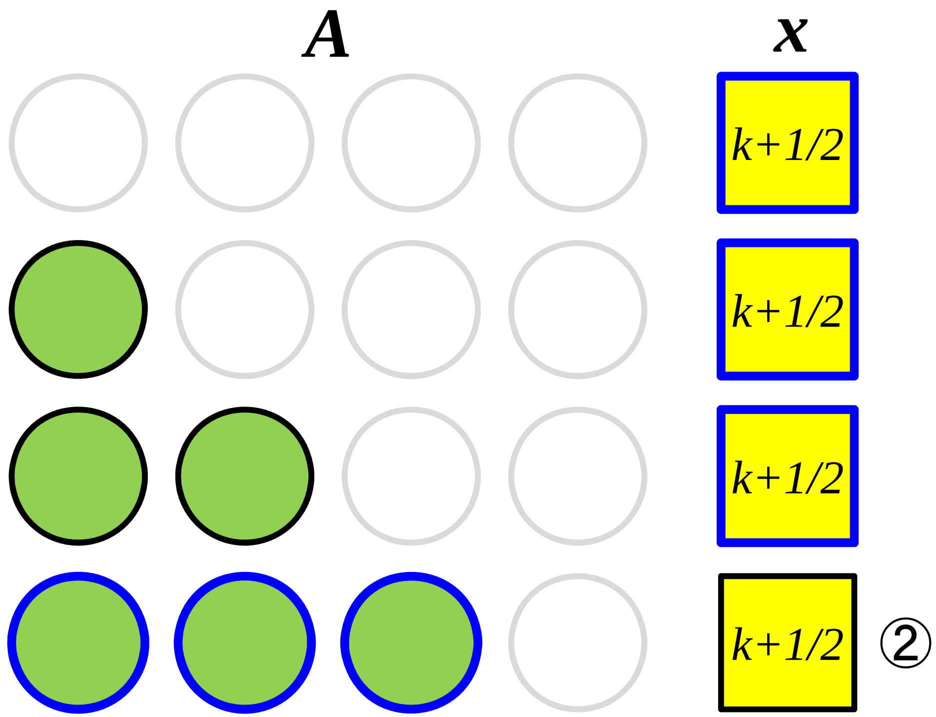
i=4

Loop2



$$x_i^{\left(k+\frac{1}{2}\right)} = \frac{1}{a_{ii}}\left\{ y_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)} \right\}$$

Rev. Loop3



$$y_i = r_i - \sum_{j<i}^{N} a_{ij} x_j^{\left(k+\frac{1}{2}\right)}$$

History of score improvement

BoF@	Tune	PFLOPS	RANK
SC15	Previous DOI: 10.1177/1094342015607950	0.461	2
ISC2016	Cache utilization by splitting SYMGS loops (just implement)	0.554	2
SC16	Cache utilization by splitting SYMGS loops (more adjustment)	0.602	1