Lessons from Implementing the BiCGStab Method with SkeTo Library

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Agenda

Examine programmability and performance of skeletal parallelism with a real application

- BiCGStab method and target application
- SkeTo: parallel skeleton library
- Two approaches to development
- Experiment results
- Conclusion

BiCGStab Method

- Bi-Conjugate Gradient Stabilized method
  [van der Vorst, 1992]
  - Solve systems of linear equations: Ax = b
  - An iterative method
    - ✓ 2 matrix-vector multiplication (probmv function)
    - ✓ 4 inner-products
    - ✓ Other basic linear algebraic computations

$$
\begin{array}{l}
\textbf{function } \mathrm{bicgstab}(\boldsymbol{A}, \boldsymbol{x}, \boldsymbol{b}, err, itrmax) \\
\textbf{begin} \\
\quad \boldsymbol{c} := \mathrm{probmv}(\boldsymbol{A}, \boldsymbol{x}) \\
\quad \boldsymbol{p} := \boldsymbol{s} := \boldsymbol{r} := \boldsymbol{b} - \boldsymbol{c} \\
\quad \alpha := \boldsymbol{r} \cdot \boldsymbol{r} \\
\quad \textbf{if } (\boldsymbol{r} \cdot \boldsymbol{r} < err) \textbf{ then return } \boldsymbol{x} \\
\quad \textbf{for } it = 1 \textbf{ upto } itrmax \\
\quad \textbf{begin} \\
\qquad \boldsymbol{y} := \mathrm{probmv}(\boldsymbol{A}, \boldsymbol{p}) \\
\qquad \beta := \boldsymbol{s} \cdot \boldsymbol{y} \\
\qquad \boldsymbol{e} := \boldsymbol{r} - (\alpha/\beta)\boldsymbol{y} \\
\qquad \boldsymbol{v} := \mathrm{probmv}(\boldsymbol{A}, \boldsymbol{e}) \\
\qquad \gamma := (\boldsymbol{e} \cdot \boldsymbol{v})/(\boldsymbol{v} \cdot \boldsymbol{v}) \\
\qquad \boldsymbol{x} := \boldsymbol{x} + (\alpha/\beta)\boldsymbol{p} + \gamma\boldsymbol{e} \\
\qquad \boldsymbol{r} := \boldsymbol{e} - \gamma\boldsymbol{v} \\
\qquad \textbf{if } (\boldsymbol{r} \cdot \boldsymbol{r} < err) \textbf{ then return } \boldsymbol{x} \\
\qquad \alpha := \boldsymbol{s} \cdot \boldsymbol{r} \\
\qquad \boldsymbol{p} := \boldsymbol{r} + (\alpha/(\beta\gamma))\boldsymbol{p} - (\alpha/\beta)\boldsymbol{y} \\
\quad \textbf{end} \\
\quad \textbf{return } \boldsymbol{x} \\
\textbf{end}
\end{array}
$$

Target Application

- Original program is given by a researcher
- BiCGStab is used in a 3D-space situation
  - The matrix-vector multiplication is actually a 3D-stencil computation
  - A set of data is
    - ✓ a vector (in linear algebra)
    - ✓ a 3D-array (in stencil comp.)

for $i = 0$ **upto** $I - 1$
for $j = 0$ **upto** $J - 1$
for $k = 0$ **upto** $K - 1$

$$
\begin{aligned}
\boldsymbol{c}[i][j][k] = {} & \\
& a_p * \boldsymbol{b}[i][j][k] \\
& + a_e * \boldsymbol{b}[i+1][j][k] + a_w * \boldsymbol{b}[i-1][j][k] \\
& + a_n * \boldsymbol{b}[i][j+1][k] + a_s * \boldsymbol{b}[i][j-1][k] \\
& + a_t * \boldsymbol{b}[i][j][k+1] + a_b * \boldsymbol{b}[i][j][k-1]
\end{aligned}
$$

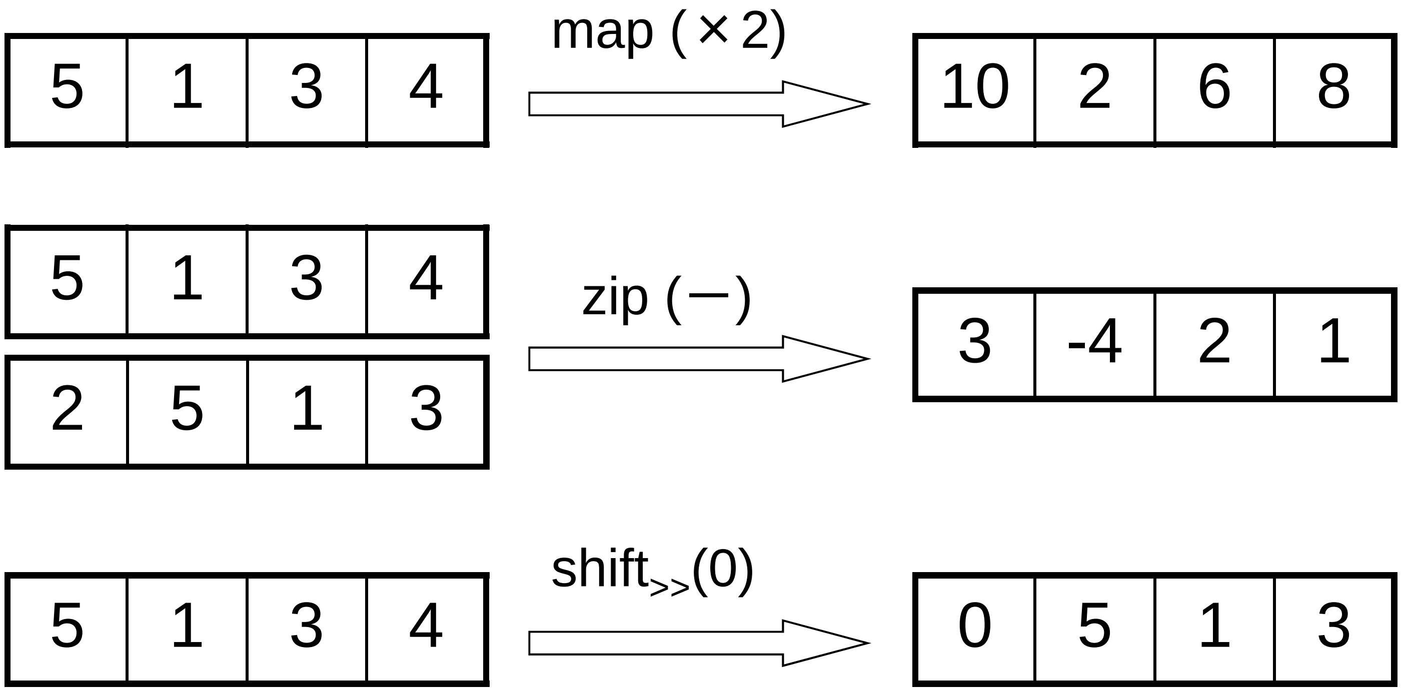
end
end
end

SkeTo: Parallel Skeleton Library

- A library with data-parallel skeletons
  - Data-parallel skeletons
    = collective operations on distributed data
  - Data structures: 1D-arrays (lists), 2D-arrays, trees
- Implemented in C++ and MPI
  - Originally for PC cluster computing
    - ✓ Also available for recent multicore CPUs
  - SPMD model: but, parallelism is only in skeletons
- Optimization by fusion transformation

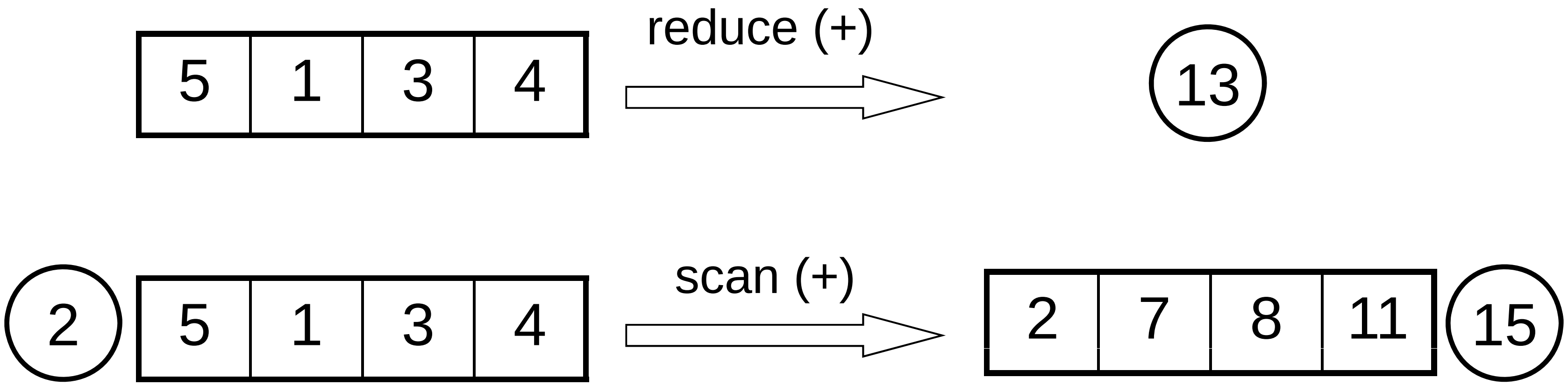
Parallel List Skeletons (1)

- (Almost) Element-wise computations
  - For N elements, $O(N/P)$ time with P processors.



Parallel List Skeletons (2)

- Reduction and scans (prefix-sums)
  - For *N* elements, O(*N*/*P* + log *P*) time with *P* procs.
  - Operators should be associative.



Fusion Optimization

- One overhead of skeletal programs
  ➔ Intermediate data between skeletons
  - E.g. reduce(+, map(^2, map(-ave, as)))
    (2 intermediate arrays among 3 loops)
- Fuse skeletons and remove intermediate data
  [IFL 2009]
  - By C++ template technique
  - Not only map and reduce, we can (partially) optimize scan or shift skeletons.
  - For simple programs like above, compiled code is as efficient as hand-written code.

Two Approaches

The first step to programming with SkeTo

Deciding how to map data in problems
to distributed structures in SkeTo

- Target application involves:
  - Linear algebraic computations (for 1D vectors)
  - 3D-stencil computations
- Two approaches to implementation
  - The whole vector → distributed list
  - 1D of 3D-space → distributed list

1st approach: mapping the whole vector to list

- 3D-stencil computation
  - First, we flatten the nested loop.
  - We need to access originally neighbor (in 3D) but far-away elements (e.g. b[i][j+1][k])
  - Implement an extended shift skeleton: gshift
    - ✓ As a user-defined skeleton

$$
\begin{array}{l}
\textbf{function}\ \mathsf{gshift}(e, +d, [a_0, a_1, \ldots, a_d]) \\
\textbf{begin} \\
\quad \textbf{return}\ [\underbrace{e, \ldots, e}_{d}, a_0, a_1, \ldots, a_{n-1-d}] \\
\textbf{end}
\end{array}
$$

$$
\begin{array}{l}
\textbf{for}\ i = 0\ \textbf{upto}\ I - 1 \\
\textbf{for}\ j = 0\ \textbf{upto}\ J - 1 \\
\textbf{for}\ k = 0\ \textbf{upto}\ K - 1 \\
\quad \boldsymbol{c}[i][j][k] = \\
\qquad a_p * \boldsymbol{b}[i][j][k] \\
\qquad + a_e * \boldsymbol{b}[i+1][j][k] + a_w \\
\qquad + a_n * \boldsymbol{b}[i][j+1][k] + a_s \\
\qquad + a_t * \boldsymbol{b}[i][j][k+1] + a_b \\
\textbf{end} \\
\textbf{end} \\
\textbf{end}
\end{array}
$$

- Linear algebraic computation
  - Easy to implement

Code for Stencil Computation

```
*c = sl::zipwith(timesd, f,
       sl::zipwith(plusd, sl::map(std::bind1st(timesd, ap), b),
       sl::zipwith(plusd, sl::map(std::bind1st(timesd, aw), sl::shiftr(0.0, b)),
       sl::zipwith(plusd, sl::map(std::bind1st(timesd, ae), sl::shiftl(0.0, b)),
       sl::zipwith(plusd, sl::map(std::bind1st(timesd, as), gshift(+dy, 0.0, b)),
       sl::zipwith(plusd, sl::map(std::bind1st(timesd, an), gshift(-dy, 0.0, b)),
       sl::zipwith(plusd, sl::map(std::bind1st(timesd, ab), gshift(+dz, 0.0, b)),
                          sl::map(std::bind1st(timesd, at), gshift(-dz, 0.0, b))))))));
```

addition   ‘$a_?$ *’   shifted access

- Skeletal code corresponds to algebraic definition

- Skeletons except for gshift can be optimized by fusion

2nd Approach:
Mapping 1D of 3D-spcae to list

- Slice 3D-space and define a list of planes

```
struct array2D {
  double data[jmax+2][imax+2];
}
```

- 3D stencil computation
  - We can implement with map, zip, and shift
- Linear algebraic computation
  - We need to define element-wise +, *, etc.
    - ✓ Function objects with a 2-nested loop
  - ➔ additional 70 lines of code

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Manual Fusion Transformation

- But, the 2nd one ran slow after fusion
  - E.g. For computing $\boldsymbol{e} := \boldsymbol{r} - (\alpha/\beta)\boldsymbol{y}$

```
for (i = 0; i < local_size; i++) {
  array2D tmp;
  for (int j = 1; j <= jmax; j++) {
    for (int i = 1; i <= imax; i++) {
       tmp[j][i] = alp * y[i][j][i];
    }
  }
  for (int j = 1; j <= jmax; j++) {
    for (int i = 1; i <= imax; i++) {
       e[i][j][i] = r[i][j][i] - tmp[j][i];
    }
  }
}
```

Inner loops are not fused

- Solutions: nested optimization, 3D-array skeletons, manual fusion (+50 lines)

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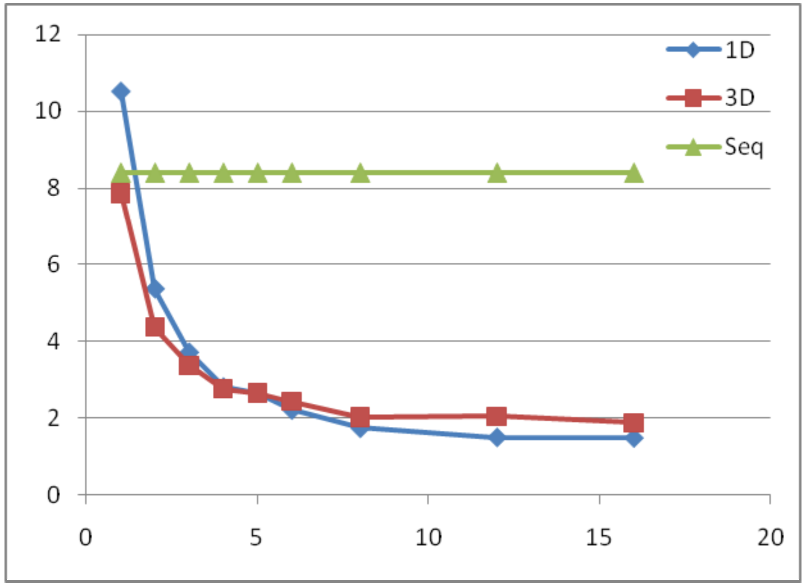
Further Optimization

- The program still had large overhead.
- Reason: Elements are copied in skeletons
  - Design for simplicity (and fast for simple elements)
  - Type of function objects: `B operator()(const A&);`
- Our solution:
  - Use smart pointers to avoid data copies; and a special implementation of skeletons with serialization
  - Serialization will be imported in SkeTo ver1.10

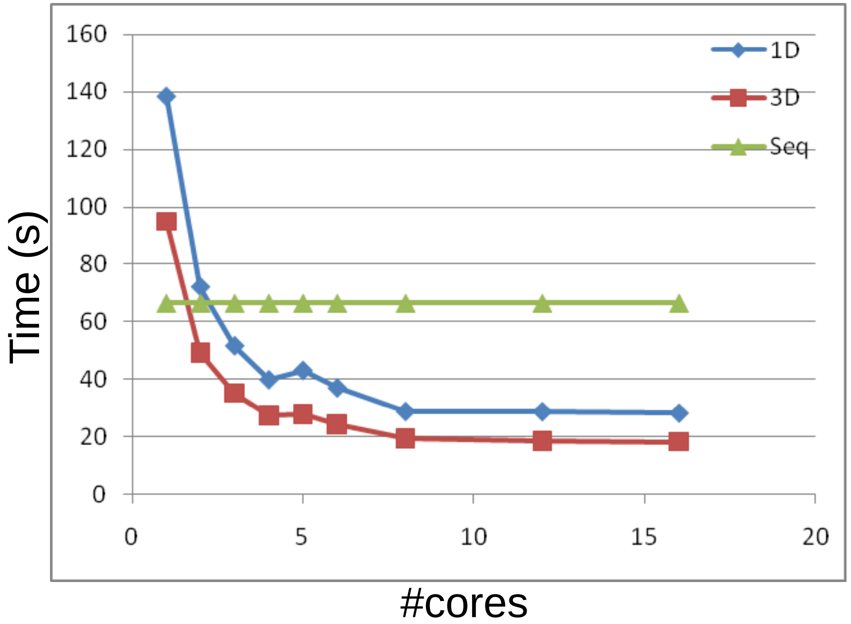
Experiment 1:
On PC Cluster with Multicore-CPUs

- Relative speedup: 1D (1st) > 3D (2nd)
- Performance: Depend on size, #cores

Smaller (N=100^3)



Larger (N=200^3)



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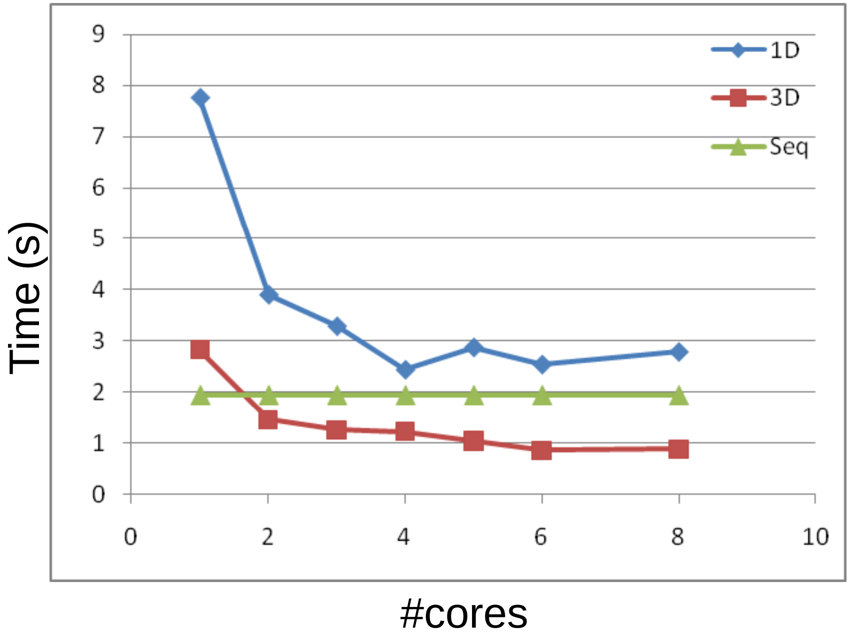
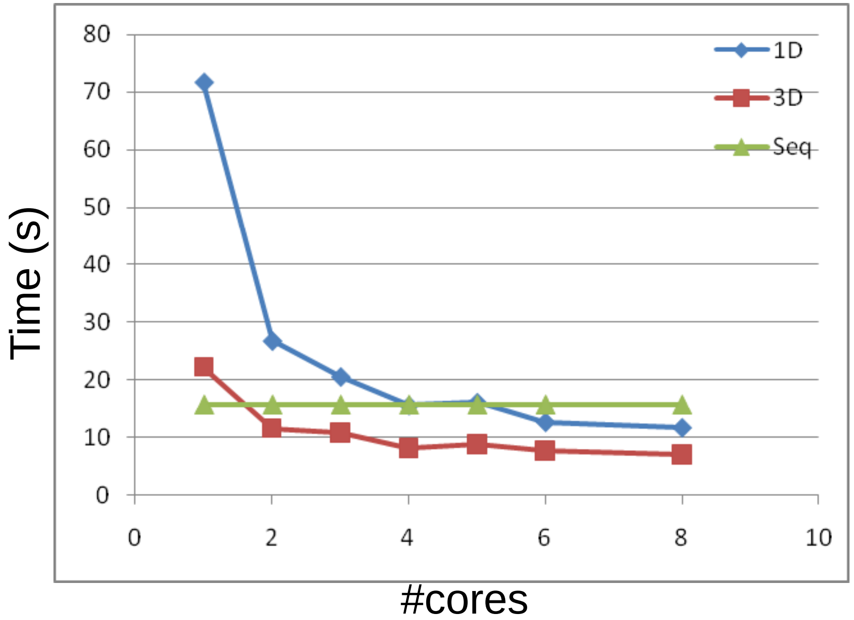
Experiment 2:
On Dual-quadcore Server

- Performance: 3D (2nd) > 1D (1st)
- Overhead w.r.t. sequential programs (1D)

Smaller (N=100^3)

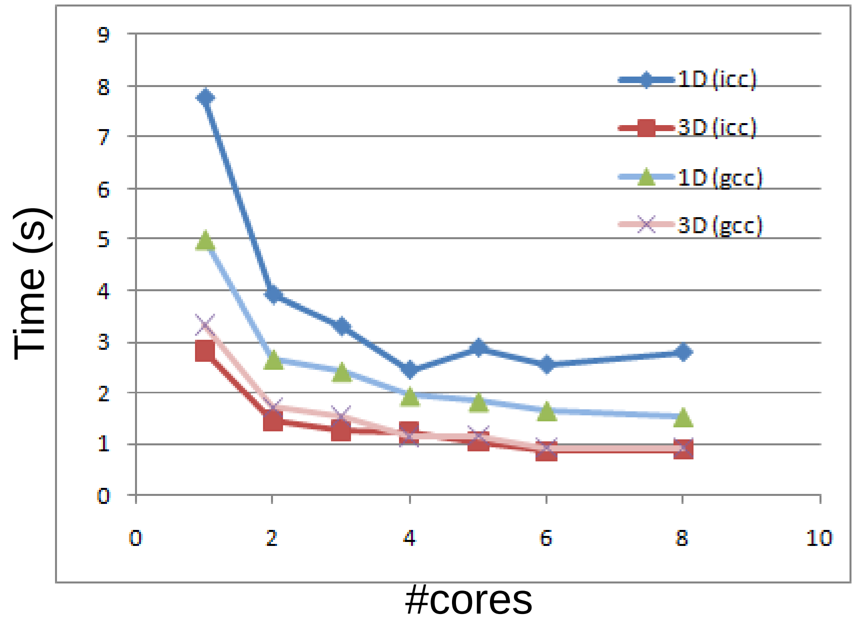


Larger (N=200^3)



Experiment 3:
Comparing Two Compilers

- Performance depends on approaches and compilers
  - Faster 1D code by GCC
  - Faster 3D code by Intel Compiler



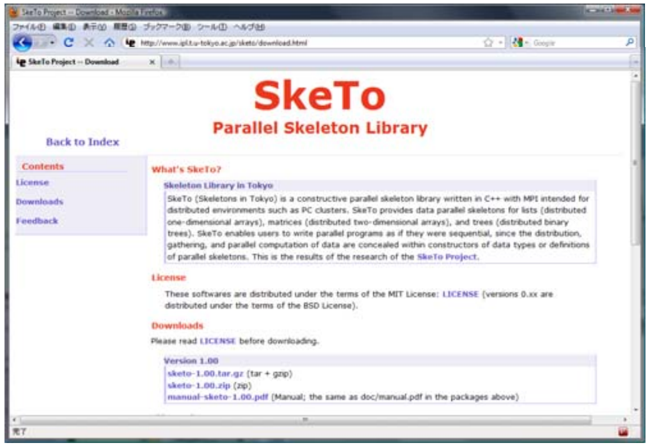
Conclusion

- We have obtained 7 lessons (in the paper) in implementing the BiCGStab with SkeTo
  - Two implementation with list skeletons
    - ✓ By mapping the whole vector to list
    - ✓ By mapping 1D of 3D-space to list
  - Performed optimization with fusion transformation automatically/manually
  - Several experiment results are shown
    - ✓ Performance depends on problem-size, architecture, and compiler

Future Work

- Implement other real applications and examine what we need more
  - Application: Machine Learning, etc.
  - Skeletons: permute, groupByKey

- SkeTo ver. 1.10 coming soon
  http://www.ipl.t.u-tokyo.ac.jp/sketo/
  - Re-implementation of matrix skeletons
  - Support for serialization of user-defined data
  - (Experimental) C++0x support



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