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Toward Automatic Performance Tuning for Numerical Simulations in the SILC Matrix Computation Framework

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Outline

- The SILC matrix computation framework
  - Easy-to-use interface for matrix computation libraries
- Automatic performance tuning in SILC
  - Performance modeling
  - Related work
- Experimental results
- Concluding remarks

Numerical simulations

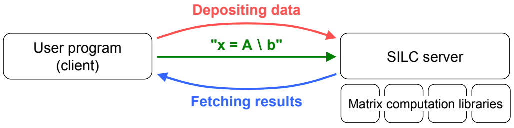
- A common feature: Appearance of PDEs
  - Discretization of PDEs results in linear systems, which are solved by linear solvers
- Some simulations require only one linear system to be solved
  - E.g. Steady-state simulations in linear problems
- Others require many linear systems to be solved repeatedly
  - E.g. Steady-state simulations in nonlinear problems, time-dependent simulations

Matrix computation libraries

- Key components of numerical simulations
- Problem: Using libraries is not easy
  - Many libraries having different APIs
  - Diversity of computing environments
  - Interoperability issues of various programming languages
- Solution: The SILC framework

Simple **I**nterface for **L**ibrary **C**ollections

- Benefits
  - Independent of libraries, environments & languages
  - Easy to use
- Three steps to use libraries
  - **Depositing data** (matrices, vectors, etc.) to a server
  - **Making requests for computation** by means of mathematical expressions
  - **Fetching the results of computation** if necessary



Example: Using SILC in C

```
silc_envelope_t A, C, u;

/* create matrices A, C and vector u0 */

SILC_PUT("A", &A);
SILC_PUT("C", &C);
SILC_PUT("u", &u); /* u0 */
for (k = 1; k <= n_steps; k++)
{
   SILC_EXEC("b = C * u");
   SILC_EXEC(“u = A \\ b");
   SILC_GET(&u, "u"); /* uk */

   /* output solution uk at time tk */

}
```

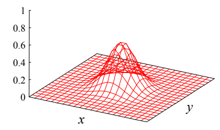
Solve the initial value problem of 2D diffusion equation below using the Crank-Nicolson method:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}, \quad x, y \in (0, 1),$$

$$u(x, y, t) = 0, \quad t > 0,$$

$$u(x, y, 0) = \begin{cases} 1 & \text{if } x, y \in (0.4, 0.6) \\ 0 & \text{otherwise} \end{cases}$$

$u(x, y, 0.004)$



Functionalities of SILC

- Data structures for matrix computations
  - Matrices (dense, band, sparse), vectors, etc.
- Math operators, functions, and subscript
  - 2-norm of vector ***x***: `sqrt(x' * x)`
  - 5×5 submatrix of *A*: `A[1:5, k:k+4]`
- No loops and conditional branching
  - These are realized with the languages used to write user programs for SILC

Main characteristics of SILC

- Independence from programming languages
  - User programs for SILC in your favorite languages
- Independence from libraries and environments
  - Using alternative libraries and environments requires no modification in user programs
  - Flexible combinations of client & server environments

User program (client)	SILC server
Sequential	Sequential
Sequential	Shared-memory parallel (OpenMP)
Sequential	Distributed parallel (MPI)
Distributed parallel (MPI)	Distributed parallel (MPI)

Cost in SILC: Communication time

- Likely to be smaller than computation time

Matrix (Solver)	Time for solving a linear system $Ax = b$	Time for depositing A and b and fetching x
Dense (LU decomposition)	$O(N^3)$	$O(N^2)$
Sparse (CG method)	$O(CZ)$	$O(Z)$

(N: dimension, C: iteration count, Z: number of non-zero elements)

- Possible speedups by parallel computation even at the cost of data communications

Automatic performance tuning (APT)

- SILC needs APT
  - To achieve as much speedup as possible in order to relatively minimize the cost of data communications
  - Using all available processors (or threads) is not always optimal
- SILC is an ideal framework in which APT is implemented
  - SILC servers can carry out various types of APT independently of user programs

Purposes of the present research

- Performance modeling of time-dependent simulations in SILC
- Outline of an APT mechanism for SILC

- Assumptions
  - A sequential user program, running with
  - A shared-memory parallel SILC server

Performance modeling

- The execution time (in seconds) of a user program is modeled as a function of p (the number of threads) as follows:

$$f(p) = a/p + bp + c$$

a/p : time for parallelized computations

bp : parallelization overhead

c : time for sequential computations

$(a, b, c > 0)$

The least squares method

- Suppose we have measured the execution time of the user program with n different numbers of threads (e.g., $p_i = 2^{i-1}$, $i = 1, \ldots, n$)

Number of threads	p_1	p_2	…	p_n
Execution time [sec.]	f_1	f_2	…	f_n

- By using the least squares method, we can find a, b, and c that minimize

$$q = \sum_{i=1}^{n} \{f_i - f(p_i)\}^2$$

The optimal number of threads p_{opt}

- With a performance model $f(p)$, we can predict the optimal number of threads p_{opt} that leads to the minimum execution time
- Since $f > 0$, p_{opt} satisfies

$$\frac{df}{dp} = -\frac{a}{p^2} + b = 0$$

- By solving the equation for p, we have $p = \sqrt{a/b}$ and thus

$$p_{\mathrm{opt}} = \begin{cases} \lfloor p \rfloor & \text{if } f(\lfloor p \rfloor) < f(\lceil p \rceil) \\ \lceil p \rceil & \text{otherwise} \end{cases}$$

Proposed performance modeling

1. Measure the execution time of a user program with different numbers of threads
2. Learn a performance model

   $$f(p) = a/p + bp + c$$

   with the 3 parameters a, b, and c determined by the least squares method
3. Predict the optimal number of threads p_{opt}

Related work

- Various approaches to detailed performance modeling
- E.g. Performance Analysis and Characterization Environment (PACE) by Kerbyson *et al.*
  - Semi-automated code analysis of user programs
  - Predefined hardware models

- Our performance modeling is much simpler
  - Due to the primary objective of SILC: Independence from libraries, environments, and languages

Numerical experiments

- Purpose: Validation of the performance modeling
- Example applications
  1. Cloth simulation based on the implicit Euler method
  2. CFD simulation based on the Moving Particle Semi-implicit (MPS) method
  3. An initial value problem of the 2-dimensional diffusion equation

Test environments

User programs (clients)	Parallel SILC server
Dell Dimension 8400 Intel Pentium 4 3.4 GHz, 1 GB RAM, Microsoft Windows XP SP2	SGI Altix 3700 32 Intel Itanium 2 1.3 GHz, 32 GB RAM (cc-NUMA), Red Hat Linux AS 2.1
MinGW (GCC 3.2.3) `-O3` option enabled	Intel C Compiler 9.1 `-O3` option enabled

- Both machines in the same Gigabit Ethernet LAN

Validation criterion

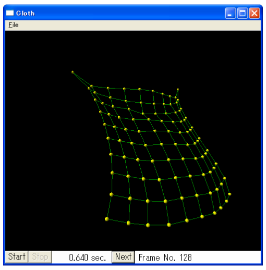
- Relative error $\varepsilon_{\mathrm{rel}}$ in the execution time t measured with p_{opt}

$$\varepsilon_{\mathrm{rel}} = \frac{|t_{\mathrm{true}} - t|}{t_{\mathrm{true}}}$$

where t_{true} is the execution time measured with the true optimal number of threads ($\varepsilon_{\mathrm{rel}} = 0$ if p_{opt} is truly optimal)

Example #1

- Time-dependent simulation of cloth motion
  - A mass-spring model for representing cloth
  - The implicit Euler method for computing cloth motion
  - A sparse linear system is solved for each time step
  - Solver: CG method in the Lis iterative solvers library
  - Visualization via OpenGL



Outline of the simulation #1

Do some initialization (defining cloth geometry, etc.)
For each time step:

1. Calculate force $\boldsymbol{f}$ and its derivatives $\partial \boldsymbol{f} / \partial \boldsymbol{x}$ and $\partial \boldsymbol{f} / \partial \boldsymbol{v}$ (Jacobian matrices).

2. Solve a linear system $A \Delta \boldsymbol{v} = \boldsymbol{b}$, where

$$A = \left\{ M - \Delta t^2 \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} - \Delta t \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{v}} \right\}$$

$$\boldsymbol{b} = \left\{ \boldsymbol{f} + \Delta t \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} \boldsymbol{v} \right\} \Delta t$$

3. Update particle motion.

$$\boldsymbol{v} \leftarrow \boldsymbol{v} + \Delta \boldsymbol{v}$$

$$\boldsymbol{x} \leftarrow \boldsymbol{x} + \Delta t\, \boldsymbol{v}$$

Force and its derivatives

- Force

$$\boldsymbol{f}_i = \sum_{j \in P_i} (\boldsymbol{f}_{ij} + \boldsymbol{d}_{ij})$$

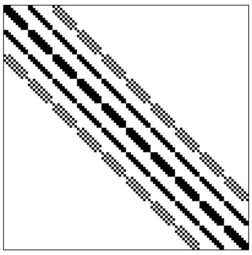
$$\boldsymbol{f}_{ij} = b_k \left(|\boldsymbol{x}_j - \boldsymbol{x}_i| - l_k \right) \frac{\boldsymbol{x}_j - \boldsymbol{x}_i}{|\boldsymbol{x}_j - \boldsymbol{x}_i|} \qquad \text{(spring force)}$$

$$\boldsymbol{d}_{ij} = -h_k (\boldsymbol{v}_i - \boldsymbol{v}_j) \qquad \text{(damping)}$$

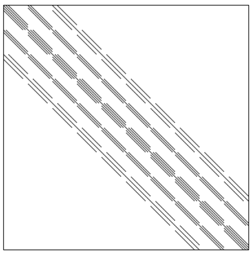
- Derivatives (Jacobian matrices)

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{pmatrix} \frac{\partial \boldsymbol{f}_1}{\partial \boldsymbol{x}_1} & \cdots & \frac{\partial \boldsymbol{f}_1}{\partial \boldsymbol{x}_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial \boldsymbol{f}_n}{\partial \boldsymbol{x}_1} & \cdots & \frac{\partial \boldsymbol{f}_n}{\partial \boldsymbol{x}_n} \end{pmatrix}, \quad \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{v}} = \begin{pmatrix} \frac{\partial \boldsymbol{f}_1}{\partial \boldsymbol{v}_1} & \cdots & \frac{\partial \boldsymbol{f}_1}{\partial \boldsymbol{v}_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial \boldsymbol{f}_n}{\partial \boldsymbol{v}_1} & \cdots & \frac{\partial \boldsymbol{f}_n}{\partial \boldsymbol{v}_n} \end{pmatrix}$$

Non-zero patterns of the derivatives



$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}$$



$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{v}}$$

Elements of the derivatives

- Off-diagonal blocks (3×3 submatrices)

$$\frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_j} = b_k I - \frac{b_k l_k}{|\boldsymbol{x}_j - \boldsymbol{x}_i|} \left(I - \frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)(\boldsymbol{x}_j - \boldsymbol{x}_i)^T}{|\boldsymbol{x}_j - \boldsymbol{x}_i|^2} \right), \quad \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{v}_j} = h_k I$$

- Diagonal blocks (3×3 submatrices)

$$\frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_i} = \sum_{j \in P_i} \left(-\frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_j} \right), \quad \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{v}_i} = \sum_{j \in P_i} \left(-\frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{v}_j} \right)$$

- All computations can be implemented by means of SILC's mathematical expressions

The body of the loop over time steps

```
/* 1. Calculate f, ∂f / ∂x and ∂f / ∂v */
SILC_EXEC("p = Y_L * x - Y_R * x");
SILC_EXEC("P = sparse(P_row, P_col, p, 3*s, s)");
SILC_EXEC("z = sqrt(diagvec(P' * P))");
SILC_EXEC("fij = P * (K_stiff *@ (z - L) /@ z)");
SILC_EXEC("q = Y_L * v - Y_R * v");
SILC_EXEC("Q = sparse(P_row, P_col, q, 3*s, s)");
SILC_EXEC("dij = Q * K_damp");
SILC_EXEC("f = Sum_f * (fij + dij) - M * g");

SILC_EXEC("zhat = ones(s, 1) /@ z; Pzhat = P * zhat");
SILC_EXEC("U_L = sparse(U_L_row, U_col, Pzhat, 3*n, s)");
SILC_EXEC("U_R = sparse(U_R_row, U_col, Pzhat, 3*n, s)");
SILC_EXEC("tmp = sqrt(zhat *@ K_stiff *@ L)");
SILC_EXEC("C1 = diag(X * sqrt(K_stiff))");
SILC_EXEC("C2 = diag(X * tmp); D = diag(tmp)");
SILC_EXEC("A1 = Y_LT * C1 - Y_RT * C1; T1 = -A1 * A1'");
SILC_EXEC("A2 = Y_LT * C2 - Y_RT * C2; T2 = -A2 * A2'");
SILC_EXEC("A3 = U_L * D - U_R * D; T3 = -A3 * A3'");
SILC_EXEC("DfDx = T1 - T2 + T3");

/* 2. Solve AΔv = b */
SILC_EXEC("A = M - (dt * dt) * DfDx - dt * DfDv");
SILC_EXEC("b = dt * (f + dt * (DfDx * v))");
SILC_EXEC("dv = A \\ b");

/* 3. Update particle motion */
SILC_EXEC("v += dv *@ fixed");
SILC_EXEC("x += dt * v");
```

Example #1: Results

- The execution time of the first 20 time steps
  - Problem size: 1,024 particles (3,096 unknowns)

Number of threads	1	2	4	8	16
Execution time [sec.]	13.5	7.23	4.41	3.28	3.24

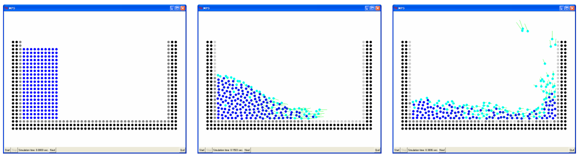
- Performance model

$$f(p) = 12.540/p + 0.103p + 0.838 \quad (q = 1.12\times10^{-2})$$

- The optimal number of threads $p_{\mathrm{opt}} = 11$
  - The true optimal number of threads was equal to p_{opt}
  - Relative error $\varepsilon_{\mathrm{rel}} = 0$

Example #2

- Simulation of incompressible flow based on the Moving Particle Semi-implicit (MPS) method
  - A sparse linear system is solved for each time step
  - Linear solver: ICCG method in Lis



t = 0 [sec.] t = 0.15 t = 0.3

Outline of the simulation #2

Do some initialization (generating particles, etc.)
For each time step ($k = 1, 2, 3, \ldots$):

Explicitly calculated

Implicitly calculated

1. Calculate source terms and particle motion

$$\boldsymbol{u}^* = \boldsymbol{u}^k + \Delta t \left[\nu\nabla^2\boldsymbol{u} + \boldsymbol{g}\right]^k$$
$$\boldsymbol{r}^* = \boldsymbol{r}^k + \Delta t\, \boldsymbol{u}^*$$

2. Solve pressure Poisson equation

$$\nabla^2 P^{k+1} = \frac{\rho}{\Delta t^2}\frac{n^* - n'}{n^0}$$

Discretizing the equation results in a sparse linear system, which is solved by the ICCG method

3. Calculate pressure gradient terms

$$\boldsymbol{u}' = -\frac{\Delta t}{\rho}\nabla P^{k+1}$$

4. Correct particle motion

$$\boldsymbol{u}^{k+1} = \boldsymbol{u}^* + \boldsymbol{u}'$$
$$\boldsymbol{r}^{k+1} = \boldsymbol{r}^* + \Delta t\, \boldsymbol{u}'$$

All computations can be implemented by means of SILC's mathematical expressions

Example #2: Results

- The execution time of the first 200 time steps
  - Problem size: 470 particles (470 unknowns)

Number of threads	1	2	4	8	16	32
Execution time [sec.]	29.4	19.6	14.4	12.1	12.2	20.5

- Performance model

$$f(p) = 23.467/p + 0.402p + 6.103 \quad (q = 5.97\times10^{0})$$

- The optimal number of threads $p_{\mathrm{opt}} = 8$
  - The true optimal number of threads was equal to p_{opt}
  - Relative error $\varepsilon_{\mathrm{rel}} = 0$

Example #3

- Solve the following initial value problem using the Crank-Nicolson method

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad (t \ge 0,\ x,\ y \in (0, 1))$$

$$u(x, y, 0) = \begin{cases} 1 & \text{if } x, y \in (0.4, 0.6) \\ 0 & \text{otherwise} \end{cases}$$

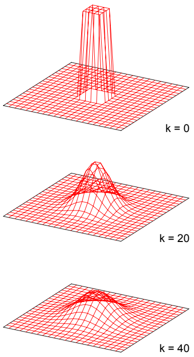
$$u(0, y, t) = u(1, y, t) = u(x, 0, t) = u(x, 1, t) = 0$$

- Let $t_0 = 0$ be the initial time and $\Delta t > 0$ be a time interval, and find $\boldsymbol{u}_k$ at $t_k = t_{k-1} + \Delta t$ by solving

$$A\boldsymbol{u}_k = C\boldsymbol{u}_{k-1}$$

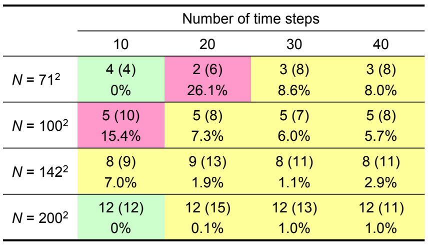
Outline of the simulation #3

```
silc_envelope_t A, C, u;

/* create matrices A, C and vector u0 */

SILC_PUT("A", &A);
SILC_PUT("C", &C);
SILC_PUT("u", &u); /* u0 */
for (k = 1; k <= n_steps; k++)
{
   SILC_EXEC("b = C * u");
   SILC_EXEC("u = A \\ b");
   SILC_GET(&u, "u"); /* uk */

   /* output solution uk at time tk */

}
```



Example #3: Results

- p_{opt} is accurate or $\varepsilon_{\mathrm{rel}}$ is small (< 10%) : OK
- $\varepsilon_{\mathrm{rel}}$ is large : NG (2 of 16)



	Number of time steps			
	10	20	30	40
$N = 71^2$	4 (4) 0%	2 (6) 26.1%	3 (8) 8.6%	3 (8) 8.0%
$N = 100^2$	5 (10) 15.4%	5 (8) 7.3%	5 (7) 6.0%	5 (8) 5.7%
$N = 142^2$	8 (9) 7.0%	9 (13) 1.9%	8 (11) 1.1%	8 (11) 2.9%
$N = 200^2$	12 (12) 0%	12 (15) 0.1%	12 (13) 1.0%	12 (11) 1.0%

Upper: p_{opt} (the true optimal number of threads in parentheses)
Lower: Relative error $\varepsilon_{\mathrm{rel}}$ in the execution time measured with p_{opt}

APT mechanism for SILC

- Outline
  1. A server collects n samples of execution time with different numbers of threads. For each number of threads, timing is done m times and the shortest is picked
  2. The server learns a performance model using the least squares method and predicts p_{opt}
  3. The server continues the simulation with the optimal number of threads
- Open issue
  - How to determine n and m

Summary

- Proposal of simple performance modeling for time-dependent simulations in SILC
  - Use of the least squares method
  - Accurate prediction of p_{opt}
- Outline of an APT mechanism for SILC
- Future work
  - Implementation of the APT mechanism
  - How to determine the two parameters n and m

Advertisement

- SILC v1.2 is freely available at

  http://ssi.is.s.u-tokyo.ac.jp/silc/

  - Source (Unix/Linux, Windows, Mac OS X)
  - Precompiled binary package for Windows
  - Documentation, sample programs