Universität Stuttgart SS 2016
Institut für parallele und verteilte Systeme
Prof. Dr. rer. nat. Miriam Mehl
Dipl.-Ing. Florian Lindner

Parallel Numerics

Exercise 1: MPI & Data Dependency & BLAS

1 Setting up a MPI Environment

Setting up a MPI environment on your own linux machine for use as a personal playground should be pretty straightforward.

i) Install the necessary packages (`openmpi` on Arch, `openmpi-bin` on Debian/Ubuntu, maybe `-dev` packages as well)

ii) Compile using `mpicc`, `mpic++` or for whatever language you prefer

iii) Run your binary with `mpirun -np N ./your_app` using N processes.

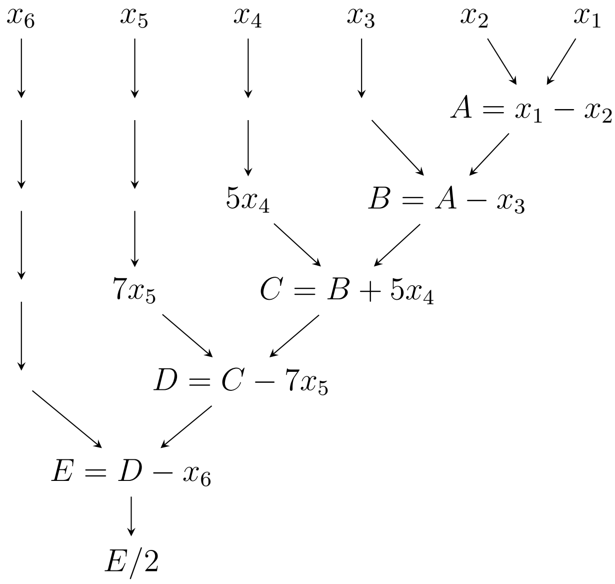
2 MPI Application Code

The MPI programs that are shown in this tutorial are available for download at Github: `https://github.com/floli/ParNum`. Download them and get your hands dirty. For questions use the forum which I will monitor.

3 Data Dependency Graphs

i) Draw the data dependency graph for the evaluation of the following expression. Follow the given parenthesis. How many parallel steps are needed to compute the result?

$$\frac{((((x_1 + x_2) - x_3) + 5x_4) - 7x_5) - x_6}{2}$$

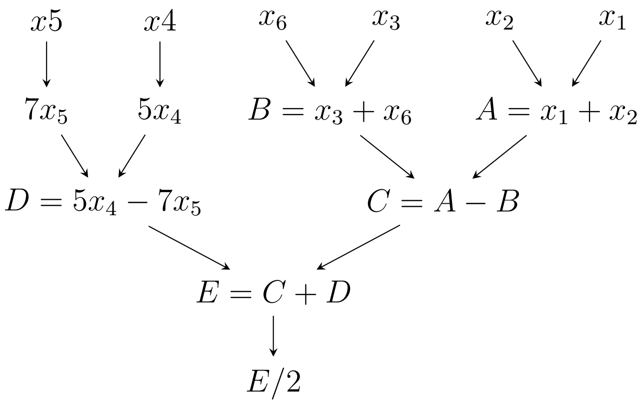


x

6 steps are needed.

ii) Design a faster algorithm that evaluates this expression by rearranging the parenthesis. How many parallel steps are needed now?

$$\frac{(x_1 + x_2) - (x_3 + x_6) + (5x_4 - 7x_5)}{2}$$

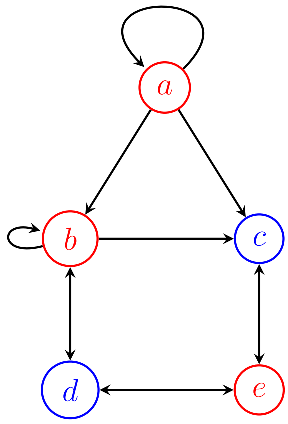


Only 4 steps are needed.

iii) Draw the data dependency graph of the following system of equations:

$$\begin{aligned} a &= f_a(a) \\ b &= f_b(a, b, d) \\ c &= f_c(a, b, e) \\ d &= f_d(b, e) \\ e &= f_e(c, d) \end{aligned}$$

Derive a suitable coloring that allows for maximal parallelism in a Gauss-Seidel type iteration over the given system.



Execution order:

$$\text{in parallel} \begin{cases} e^{k+1} = f(c^k, d^k) \\ b^{k+1} = f(a^k, c^k, d^k) \\ a^{k+1} = f(a^k) \end{cases}$$

$$\text{in parallel} \begin{cases} c^{k+1} = f(a^{k+1}, b^{k+1}, e^{k+1}) \\ d^{k+1} = f(b^{k+1}, e^{k+1}) \end{cases}$$

4 BLAS — Basic Linear Algebra Subroutines

Basic Linear Algebra Subprograms (BLAS) is a specification that prescribes a set of low-level routines for performing common linear algebra operations such as vector addition, scalar multiplication, dot products, linear combinations, and matrix multiplication. They are the de facto standard low-level routines for linear algebra libraries; the routines have bindings for both C and Fortran. Although the BLAS specification is general, BLAS implementations are often optimized for speed on a particular machine, so using them can bring substantial performance benefits. BLAS implementations will take advantage of special floating point hardware such as vector registers or SIMD instructions.

`https://en.wikipedia.org/wiki/Basic_Linear_Algebra_Subprograms`

blas level	description	complexity	example
1	Vector-vector operations Scalar-vector operations	$\mathcal{O}(n)$ $\mathcal{O}(n)$	$\alpha x + y,\ \alpha \in \mathbb{R},\ x, y \in \mathbb{R}^n$
2	Matrix-vector operations	$\mathcal{O}(n^2)$	$\alpha Ax + \beta y,\ A \in \mathbb{R}^{n\times n},\ \beta \in \mathbb{R}$
3	Matrix-matrix operations	$\mathcal{O}(n^3)$	$\alpha AB + \beta C,\ B, C \in \mathbb{R}^{n\times n}$

BLAS routines are preinstalled and, usually, not linked statically because each vendor could provide an optimized version.

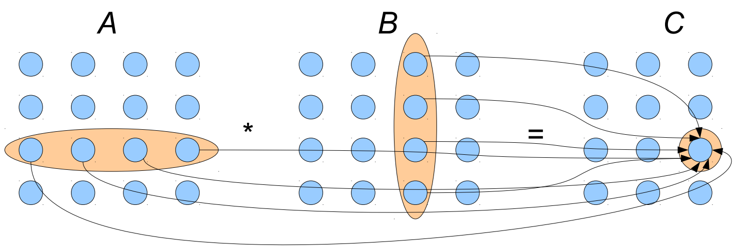
5 Matrix–Matrix Multiplication

The product $A \cdot B$ of two $N \times N$-matrices A and B is calculated as follows:

$$C = A \cdot B \qquad \text{where} \qquad c_{ij} = \sum_{k=1}^{N} a_{ik}\, b_{kj}.$$

A program that calculates this product has to use three independent loops (over i, j, k). The execution speed of the program depends on the arrangement of these loops.

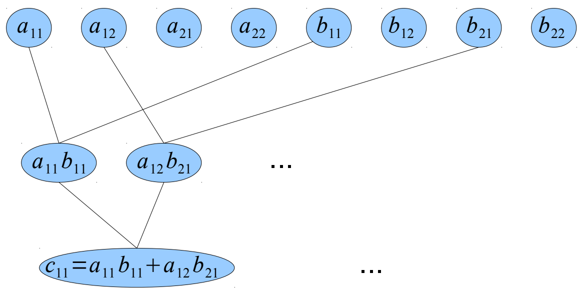
i) Give a sketch of the data dependency and the data execution graph for one c_{ij} of this problem.
A sketch of the data dependency graph is shown for one single element of C for a 4-by-4 matrix:



For a 2-by-2 matrix-matrix multiplication of the form

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \cdot \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}$$

the data execution graph has the form



ii) Assume the dimension N is a multiple of $\sqrt{p}$, with p being the number of processors. The result matrix is split up into p quadratic submatrices. Every node has to compute one complete submatrix of the result matrix C.

$A \cdot B = C$ is computed by p nodes. E.g. node #0 computes block C_{11}, node #1 computes block C_{12}, etc.:

$$\left(\begin{array}{c|c|c} A_{11} & A_{12} & A_{13} \\ \hline A_{21} & A_{22} & A_{23} \\ \hline A_{31} & A_{32} & A_{33} \end{array}\right) \cdot \left(\begin{array}{c|c|c} B_{11} & B_{12} & B_{13} \\ \hline B_{21} & B_{22} & B_{23} \\ \hline B_{31} & B_{32} & B_{33} \end{array}\right) = \left(\begin{array}{c|c|c} \#0 & \#1 & \#2 \\ \hline \#3 & \#4 & \#5 \\ \hline \#6 & \#7 & \#8 \end{array}\right)$$

What parts of A and B are required to compute the result submatrix on one node? The first few nodes have to compute the following blocks:

node #0 : $C_{11} = A_{11}B_{11} + A_{12}B_{21} + A_{13}B_{31}$
node #1 : $C_{12} = A_{11}B_{12} + A_{12}B_{22} + A_{13}B_{32}$
node #2 : $C_{13} = A_{11}B_{13} + A_{12}B_{23} + A_{13}B_{33}$
node #4 : $C_{20} = A_{21}B_{12} + A_{22}B_{22} + A_{23}B_{32}$

Interpret the multiplication formula $C_{ij} = \sum_{k=1}^{\sqrt{p}} A_{ik}\, B_{kj}$ block–wise. Let's assume every summand of the result is computed in one time step. What parts of A and B are required in which order? How many time steps are required?

The entries from the respective row and the column are required on each processor. There are $\sqrt{p}$ time steps required.

iii) Every node is allowed to communicate with the node that computes the left, right, top or bottom submatrix of C only. Assume this cartesian topology is cyclic (toroidal). Furthermore, every node is allowed to hold only one submatrix of A and B at one time. Derive a communication scheme. Implement it using MPI and a language of your choice.
Use Cannon's algorithm for matrix–matrix multiplication. A cyclic rotation scheme is used (pseudocode):

- `Determine blocks`
- `Scatter blocks on processors`
- `Loop over blocks:`
  - `Compute part of sum`
  - `Shift` A_{local} `to left`
  - `Shift` B_{local} `up`
- `Gather blocks`

See sourcecode to corresponding tutorial on webpage.