## Scientific Computing - Exercise Sheet 1

Jonathan Hellwig, Jule Schütt, Mika Tode, Giuliano Taccogna

May 7, 2021

## 1 Exercise

```
(a) Input: \mathbf{A} \in \mathbb{R}^{n \times n} b, x_0 \in \mathbb{R}^n

1: h_0 = \mathbf{A}x_0 (matrix multiplication)

2: r_0 = b - h_0 (1.1 loop)

3: p_0 = r_0

4: for k = 1, 2, \dots do

5: h_{k-1} = \mathbf{A}p_{k-1} (matrix multiplication)

6: \gamma_{k-1} = p_{k-1}^T \cdot h_{k-1} (2.1 loop)

7: \beta_{k-1} = r_{k-1}^T \cdot r_{k-1} (2.2 loop)

8: \delta_{k-1} = r_{k-1}^T \cdot h_{k-1} (2.3 loop)

9: \zeta_{k-1} = h_{k-1}^T \cdot h_{k-1} (2.4 loop)

10: \alpha_{k-1} = \frac{\beta^{k-1}}{\gamma^{k-1}}

11: \beta_k = \beta_{k-1} - 2\alpha_{k-1}\delta_{k-1} + \alpha_{k-1}^2\zeta_{k-1}

12: x_k = x_{k-1} + \alpha_{k-1}p_{k-1} (2.5 loop)

13: r_k = r_{k-1} - \alpha_{k-1}h_{k-1} (2.6 loop)

14: p_k = r_k + \frac{\beta_k}{\beta_{k-1}}p_{k-1} (2.7 loop)

15: end for
```

All sections which are marked to be a loop can be parallelized. The minimal number of loops within the iteration loop is 2, since the loops 2.1, 2.2, 2.3, 2.4 and the loops 2.5, 2.6, 2.7 can be summarized to one loop respectively.

(b) The idea is to split the vectors such that the first coordinates were computed by one processor and the last coordinates were computed by the second processor. Therefore i denotes the counter, which is needed for the loop operation. Notice that for the Vectormultiplications in the loops 2.1, 2.2, 2.3 and 2.4 normally also a reduce operation should be included.

```
Input: \mathbf{A} \in \mathbb{R}^{n \times n} b, x_0 \in \mathbb{R}^n

1: h_0 = \mathbf{A}x_0 (matrix multiplication)

2: begin parallel private(i, r_0) shared(b, h_0)

3: r_0 = b - h_0 (1.1 loop)

4: end parallel
```

```
5: p_0 = r_0
 6: for k = 1, 2, \dots do
            h_{k-1} = \mathbf{A} p_{k-1} (matrix multiplication)
            begin parallel private(i, \gamma_{(k-1)}, \beta_{(k-1)}, \delta_{(k-1)}, \zeta_{(k-1)}) shared(r_{k-1}, p_{k-1}, h_{k-1})
 9:
            \gamma_{k-1} = p_{k-1}^T \cdot h_{k-1} \ (2.1 \text{ loop})
            \beta_{k-1} = r_{k-1}^T \cdot r_{k-1} \ (2.2 \text{ loop})
\delta_{k-1} = r_{k-1}^T \cdot h_{k-1} \ (2.3 \text{ loop})
10:
11:
            \zeta_{k-1} = h_{k-1}^T \cdot h_{k-1} \ (2.4 \text{ loop})
12:
            end parallel
13:
            \alpha_{k-1} = \frac{\beta^{k-1}}{\gamma^{k-1}}
14:
            \beta_k = \beta_{k-1} - 2\alpha_{k-1}\delta_{k-1} + \alpha_{k-1}^2\zeta_{k-1}
15:
            begin parallel private(i, x_k, r_k, p_k) shared(x_{k-1}, \alpha_{k-1}, p_{k-1}, r_{k-1}, h_{k-1}, r_k, \beta_k, \beta_{k-1})
16:
            x_k = x_{k-1} + \alpha_{k-1} p_{k-1}  (2.5 loop)
17:
            r_k = r_{k-1} - \alpha_{k-1} h_{k-1} (2.6 loop)

p_k = r_k + \frac{\beta_k}{\beta_{k-1}} p_{k-1} (2.7 loop)
18:
19:
            end parallel
20:
21: end for
```

(c) We determine that for all parallelizable parts Processor 0 works on the for-loop for i=1,...,n/2 and Processor 1 works on the for-loop for i=n/2+1,...,n, with n/2 possibly rounded.

Accordingly  $v^{(j)}$  denotes a scalar product or a vector which is calculated by processor j=0,1. If  $v^{(j)}$  denotes a Vector we mean  $v^{(0)}=(v(1),v(2),...,v(n/2))^T$  and  $v^{(1)}=(v(n/2+1),v(n/2+2),...,v(n))^T$ . If  $v^{(j)}$  denotes a scalar product, we mean  $v^{(j)}=H^{T(j)}\cdot K^{(j)}$  for  $H,K\in\mathbb{R}^n$ .

If a processor recives data through the **recv** command, we implicitly include in **recv** that the recieved data is combined with the data that was calculated on the processor itself in the right way.

That means if one half of a vector  $v^{(i)}$  is recieved **recv** creates the whole vector  $v = v^{(0)} + v^{(1)}$ . If "one half" of a scalar product is recived **recv** adds the corresponding scalar products to the final scalar product. If the processor is not specified in a calculation, the calculation is executed on both processors.

For the first processor (index 0):

```
Input: \mathbf{A} \in \mathbb{R}^{n \times n} b, x_0 \in \mathbb{R}^n

1: h_0 = \mathbf{A}x_0 (matrix multiplication)

2: r_0^{(0)} = b^{(0)} - h_0^{(0)} (1.1 loop)

3: barrier

4: send(r_0^{(0)})

5: recv(r_0^{(1)})

6: p_0 = r_0

7: for k = 1, 2, \dots do

8: h_{k-1} = \mathbf{A}p_{k-1} (matrix multiplication)

9: \gamma_{k-1}^{(0)} = p_{k-1}^{T(0)} \cdot h_{k-1}^{(0)} (2.1 loop)
```

```
\beta_{k-1}^{(0)} = r_{k-1}^{T(0)} \cdot r_{k-1}^{(0)} \ (2.2 \text{ loop})
\delta_{k-1}^{(0)} = r_{k-1}^{T(0)} \cdot h_{k-1}^{(0)} \ (2.3 \text{ loop})
\zeta_{k-1}^{(0)} = h_{k-1}^{T(0)} \cdot h_{k-1}^{(0)} \ (2.4 \text{ loop})
barrier
\operatorname{send}(\gamma_{k-1}^{(0)}, \beta_{k-1}^{(0)}, \delta_{k-1}^{(0)}, \zeta_{k-1}^{(0)})
\operatorname{recv}(\gamma_{k-1}^{(1)}, \beta_{k-1}^{(1)}, \delta_{k-1}^{(1)}, \zeta_{k-1}^{(1)})
\alpha_{k-1} = \frac{\beta^{k-1}}{\gamma^{k-1}}
\beta_{k-1}^{(1)} = \beta_{k-1}^{(1)} = \beta_{k-1}^{(1)} + \beta_{k-1}^{(1)} + \beta_{k-1}^{(1)} + \beta_{k-1}^{(1)}
    10:
    11:
    12:
    13:
    15:
    16:
                                       \begin{aligned} &\alpha_{k-1} - \frac{\gamma^{k-1}}{\gamma^{k-1}} \\ &\beta_k = \beta_{k-1} - 2\alpha_{k-1}\delta_{k-1} + \alpha_{k-1}^2 \zeta_{k-1} \\ &x_k^{(0)} = x_{k-1}^{(0)} + \alpha_{k-1} p_{k-1}^{(0)} \text{ (2.5 loop)} \\ &r_k^{(0)} = r_{k-1}^{(0)} - \alpha_{k-1} h_{k-1}^{(0)} \text{ (2.6 loop)} \\ &p_k^{(0)} = r_k^{(0)} + \frac{\beta_k}{\beta_{k-1}} p_{k-1}^{(0)} \text{ (2.7 loop)} \end{aligned}
    17:
    18:
    19:
    20:
    21:
22: \operatorname{send}(p_k^{(0)})

23: \operatorname{recv}(p_k^{(1)})

24: \operatorname{end} for
   For the second processor (index 1):
   Input: \mathbf{A} \in \mathbb{R}^{n \times n} b, x_0 \in \mathbb{R}^n
        1: h_0 = \mathbf{A}x_0 (matrix multiplication)
        2: r_0^{(1)} = b^{(1)} - h_0^{(1)} (1.1 loop)
        3: barrier
        4: \mathbf{send}(r_0^{(1)})
5: \mathbf{recv}(r_0^{(0)})
        6: p_0 = r_0
        7: for k = 1, 2, \dots do
                                         h_{k-1} = \mathbf{A}p_{k-1} (matrix multiplication)
                                      h_{k-1} = \mathbf{A}p_{k-1} \text{ (matrix multip } \\ \gamma_{k-1}^{(1)} = p_{k-1}^{T(1)} \cdot h_{k-1}^{(1)} \text{ (2.1 loop)} \\ \beta_{k-1}^{(1)} = r_{k-1}^{T(1)} \cdot r_{k-1}^{(1)} \text{ (2.2 loop)} \\ \delta_{k-1}^{(1)} = r_{k-1}^{T(1)} \cdot h_{k-1}^{(1)} \text{ (2.3 loop)} \\ \zeta_{k-1}^{(1)} = h_{k-1}^{T(1)} \cdot h_{k-1}^{(1)} \text{ (2.4 loop)} \\ \mathbf{barrier} \\ \mathbf{1} \begin{pmatrix} 1 & g(1) & g(1) & g(1) \end{pmatrix}
    10:
    11:
    12:
    13:
                                      barrier \operatorname{send}(\gamma_{k-1}^{(1)}, \beta_{k-1}^{(1)}, \delta_{k-1}^{(1)}, \zeta_{k-1}^{(1)}) \operatorname{recv}(\gamma_{k-1}^{(0)}, \beta_{k-1}^{(0)}, \delta_{k-1}^{(0)}, \zeta_{k-1}^{(0)}) \alpha_{k-1} = \frac{\beta^{k-1}}{\gamma^{k-1}}
    14:
    15:
    16:
                                       \alpha_{k-1} - \frac{1}{\gamma^{k-1}}
\beta_k = \beta_{k-1} - 2\alpha_{k-1}\delta_{k-1} + \alpha_{k-1}^2\zeta_{k-1}
x_k^{(1)} = x_{k-1}^{(1)} + \alpha_{k-1}p_{k-1}^{(1)} (2.5 \text{ loop})
r_k^{(1)} = r_{k-1}^{(1)} - \alpha_{k-1}h_{k-1}^{(1)} (2.6 \text{ loop})
p_k^{(1)} = r_k^{(1)} + \frac{\beta_k}{\beta_{k-1}}p_{k-1}^{(1)} (2.7 \text{ loop})
    17:
    18:
    19:
    20:
    21:
                                         barrier
                                        \operatorname{send}(p_k^{(1)})
    22:
```

23:  $\mathbf{recv}(p_k^{(0)})$ 24: **end for**