Map/Reduce operations for scientific computing in Julia

Journée autour du langage Julia (Groupe Calcul CNRS)
Lyon

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Why considering Julia for scientific computing ?

Why considering Julia for scientific computing ?

- Julia's **mathematical syntax** makes it an ideal way to express numerical algorithms.
- **Rich ecosystem** for scientific computing with state-of-the-art packages.
- Julia is able to handle **large volume** of data efficiently.
- Julia is designed for **parallelism**, and provides built-in primitives for parallel computing at every level: **instruction level parallelism**, **multi-threading** and **distributed computing**.
- The **Celeste.jl** project [Regier et al, 2018] achieved **1.5 PetaFLOP/s** on the Cori supercomputer at NERSC using **620,000** cores.
- Julia won the **2019 James H. Wilkinson Prize for Numerical Software**.

Current challenges in high performance data analytics

Current challenges in high performance data analytics

- **Increasingly large amount of data** in current applications (web search, machine learning, social networks, genomics/proteomics data, $\cdots$).
- **State-of-the-art** deterministic methods of numerical linear algebra were designed for an environment where the matrix **fits into memory** (RAM) and the key to performance was to minimize the number of **floating point operations** (FLOP) required.
- Currently, **communication** is the real bottleneck
  - Moving data from a hard drive
  - Moving data between nodes of a parallel machine
  - Moving data between nodes of a cloud computer.
- Ideally we should target for efficient algorithms scaling **linearly** with the problem size and with **minimal data movement**.

Current challenges in high performance data analytics

Main features to analyze

- **Data distribution**.
- **Load balancing** property of the algorithm.
- **Weak and strong** scalability properties of the algorithm.
- **Resiliency** and **fault-tolerant** properties of the algorithm.

Distributed data analysis and scientific computing [Gittens et al, 2016]

- Apache **Hadoop Map/Reduce** (**RDD**: Resilient Data Distribution).
- Spark Apache **MLlib**.
- **Message Passing Interface** (MPI).
- **R and Distributed R** (Rmpi, RHadoop).

Map/Reduce algorithms

Map/Reduce algorithms

- **Framework** for processing parallelizable problems across large datasets using a large number of nodes on a cluster.
- **Methodology**:
    - **Map**: Each **worker node** applies the "**map()**" function to the local data, and writes the output to a temporary storage. A master node ensures that only one copy of redundant input data is processed.
    - **Shuffle**: **Worker nodes** redistribute data based on the output keys (produced by the "**map()**" function), such that all data belonging to one key is located on the same worker node.
    - **Reduce**: **Worker nodes** now process each group of output data, per key, in parallel.
- An efficient **distributed file system** is usely required.

Goals of the talk

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- Introduce **map/reduce strategies** available in Julia at an introductory level.
- Provide two **illustrations** with a main focus on the basic concepts.
- Discuss an **application** using map/reduce strategies in a HPC context.

My own experience in Julia

- Used for teaching in numerical analysis since 2016.
- Used for research in scientific computing (for its fast prototyping and efficiency).
- At a beginner level nevertheless !
- Julia (v 1.0.3) has been used in this talk.

Outline

1 Context

2 Map/Reduce operations in Julia
- Map, reduce and mapreduce operations
- Two simple examples
- Distributed map operation

3 A first illustration: mean computation

4 A second illustration: communication avoiding Cholesky-QR2 factorization

5 Conclusions

Map operation

```
help?> map
  search: map map! mapfoldr mapfoldl mapslices mapreduce asyncmap asyncmap!

  map(f, c...) -> collection

  Transform collection c by applying f to each element. For multiple
  collection arguments, apply f elementwise.

  See also: mapslices

  Examples
  ==========

  julia> map(x -> x * 2, [1, 2, 3])
  3-element Array{Int64,1}:
  2
  4
  6
```

Reduce operation

```
help?> reduce
  search: reduce mapreduce

  reduce(op, itr; [init])

  Reduce the given collection itr with the given binary operator op. If
  provided, the initial value init must be a neutral element for op that will
  be returned for empty collections. It is unspecified whether init is used
  for non-empty collections.

  ...

  Examples
  ==========

  julia> reduce(*, [2; 3; 4])
  24

  julia> reduce(*, [2; 3; 4]; init=-1)
  -24
```

Reduce operation

- The **reduce** operation operates on a collection (or iterable) (usually the result of map) and reduces it to a **single** object.
- **Example**: if a collection c has 4 elements, $reduce(op, c)$ successively calculates

$$op(c_1,\ c_2),$$

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$$op(\ op(\ op(c_1,\ c_2),\ c_3),\ c_4).$$

- **reduce** computes the combination of the reduce result so far and a new element in the collection returned from a map operation.
- The associativity of the reduction operation is implementation dependent.

Mapreduce operation

```
help?> mapreduce
  search: mapreduce

  mapreduce(f, op, itr; [init])

  Apply function f to each element in itr, and then reduce the result using
  the binary function op. If provided, init must be a neutral element for op
  that will be returned for empty collections. It is unspecified whether init
  is used for non-empty collections. In general, it will be necessary to
  provide init to work with empty collections.

  mapreduce is functionally equivalent to calling reduce(op, map(f, itr);
  init=init), but will in general execute faster since no intermediate
  collection needs to be created. See documentation for reduce and map.

  Examples
  ==========

  julia> mapreduce(x->x^2, +, [1:3;]) # == 1 + 4 + 9
  14
```

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Midpoint rule integration (naive implementation)

```
function my_mapper_Integration_Midpoint_Rule(x)
    return 4./(1 + x^2)
end

function my_reducer_Integration_Midpoint_Rule(s_x,s_y)
    return s_x+s_y
end

function Integration_Midpoint_Rule(a, b, n)
     h  = (b-a)/float(n)
     s  = mapreduce((x)->my_mapper_Integration_Midpoint_Rule(x),
                    (x,y)->my_reducer_Integration_Midpoint_Rule(x,y),
                    [a + (i-0.5)*h for i=1:n])
     return h*s
end
```

$\int_a^b f(x)dx \approx \frac{(b-a)}{n}\sum_{i=1}^{n} f(x_i)$ with $x_i = a + (i - \frac{1}{2})\frac{(b-a)}{n}, \quad 1 \leq i \leq n.$

Monte Carlo integration

```julia
function my_array_function(x)
    return 4 ./ (1 .+ x.^2)     # To favor array operations
end

function my_mapper_Monte_Carlo(array_sample)
    return sum(my_array_function(array_sample))
end

function my_reducer_Monte_Carlo(s_x,s_y)
    return s_x+s_y
end

function MonteCarlo(a, b, n, nsample)
    s   = mapreduce((x)->my_mapper_Monte_Carlo(x),
                    (x,y)->my_reducer_Monte_Carlo(x,y),
                    [rand(Uniform(a,b),1,n) for i=1:nsample])
    return (b-a)/float(n*nsample)*s
end
```

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Distributed map operation

- **Distributed** computing is available in Julia through the Distributed package.
- This allows to perform **map** operations in a **distributed** setting using the notion of workers and tasks available in Julia.

```
help?> pmap
  search: pmap promote_shape typemax PermutedDimsArray process_messages

  pmap(f, [::AbstractWorkerPool], c...; distributed=true, batch_size=1,
  on_error=nothing, retry_delays=[], retry_check=nothing) -> collection

  Transform collection c by applying f to each element using available
  workers and tasks.

  For multiple collection arguments, apply f elementwise.

  ...
```

Distributed map operation: example

- Performing independent linear algebra operations is then made easy and efficient.
-

```julia
using LinearAlgebra
m, n = 1000, 500
M    = [rand(m,n) for i=1:10]
pmap(svd,M)
```

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Problem statement

- **Goal**: computation of the mean of a possibly large array $v \in \mathbb{R}^m$ with the map/reduce concept.
- **Data decomposition**: partition the array v in ℓ contiguous chunks of data $v_i \in \mathbb{R}^{m_i}$ $(1 \leq i \leq \ell)$ to be able to perform **independent** computations.
- **Map**: perform local mean computation related to a local array $w \in \mathbb{R}^{m_w}$:

$$\bar{w} \quad = \quad \frac{\sum_{j=1}^{m_w} w_j}{m_w},$$

- **Reduce**: Update the mean information by combining the current result of the reducer with a result of a mapper function.

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Analysis

- **Data decomposition**: partition the array v in ℓ contiguous chunks of data $v_i \in \mathbb{R}^{m_i} (1 \leq i \leq \ell)$ to be able to perform **independent** computations.
- **Map**: the mapper function performs local mean computation and should return as output the (m_i, μ_i) information (number of elements in v_i, local mean, respectively.)
- **Reduce**: the reducer function should combine two results (one related to the reducer, the other to a result of a map) to yield an update of the mean $((m_u, \mu_u))$ as follows:

$$
\begin{aligned}
m_u &= m_r + m_j, \\
\mu_u &= \frac{m_j \mu_j + m_r \mu_r}{m_u}.
\end{aligned}
$$

Implementation of the mapper function in Julia

```julia
function my_mapper(x)
    n        = length(x)
    average  = sum(x)/float(n)
    return (n,average)
end
```

Implementation of the reducer function in Julia

```
function my_reducer(element_x,element_y)
    n_x, average_x  = element_x
    n_y, average_y  = element_y
    n               = n_x + n_y
    average         = (n_x * average_x + n_y * average_y )/float(n)
    return (n,average)
end
```

```
function compute_average(x, nsub)
    nchunks = Int64(ceil(length(x))/nsub)
    s       = mapreduce((x)->my_mapper(x), (e_x,e_y)->my_reducer(e_x,e_y),
                  [x[(i-1)*nchunks+1:min(i*nchunks, length(x))] for i=1:nsub])
    return s
end
```

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Context: dimensionality reduction

Context

- Given $A \in \mathbb{C}^{m \times n}$ with $p = (m, n)$ we seek to compute a rank-k approximation, typically with $k \ll p$ (say $m, n \sim 10^4, 10^6, 10^8, \cdots$ and $k \approx 10$ or 10^2) as

$$A \approx E\ F^H, \quad E \in \mathbb{C}^{m \times k}, \quad F \in \mathbb{C}^{n \times k}.$$

- Solving this problem usually requires algorithms for computing the **Singular Value Decomposition** (SVD), which is marginally parallel [Dongarra et al, 2018].
- **Goal**: implement in Julia a simple communication-minimizing factorization for tall and skinny matrices based on **map/reduce** strategies.

Singular Value Decomposition

SVD [Beltrami, 1873], [Jordan, 1874], [Sylvester, 1889], [Picard, 1910]

- Given $A \in \mathbb{C}^{m\times n}$ with $p = (m, n)$, the **full** singular value decomposition of A reads:

$$A = U\ \Sigma\ V^H,$$

with $U \in \mathbb{C}^{m\times m}$, $V \in \mathbb{C}^{n\times n}$ unitary ($U^H U = I_m$, $V^H V = I_n$) and $\Sigma \in \mathbb{R}^{n\times m}$.

- $\Sigma = diag(\sigma_1, \cdots, \sigma_p)$ with $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_p \geq 0$.
- $\sigma_i, (i = 1, p)$ are called **singular values** of A.

R-SVD

R-SVD [Chan, 1982]

- **Idea**: Perform an initial QR decomposition if the matrix is sufficiently tall relative to its width (i.e. $m \geq n$ with at least by a factor of 1.5): **tall and skinny** matrix.
- **First step**: QR factorization of $A \in \mathbb{C}^{m \times n}$ as $A = QR$ where $Q \in \mathbb{C}^{m \times n}$ has orthonormal columns ($Q^H Q = I_n$ and $R \in \mathbb{C}^{n \times n}$ is a triangular matrix).
- **Second step**: SVD decomposition of R as $R = U_R \Sigma_R V_R^H$.
- **Final step**: $A = U\ \Sigma_R\ V^H$ with $U = QU_R$ and $V = V_R$.
- **Complexity**: $4mn^2 + 22n^3$.
- **Parallel performance**: Tall and Skinny QR ($TSQR$) algorithm [Demmel et al, 2012] to be favored for the first step to obtain parallel performance [Benson et al, 2013]

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Problem statement: Cholesky-QR factorization

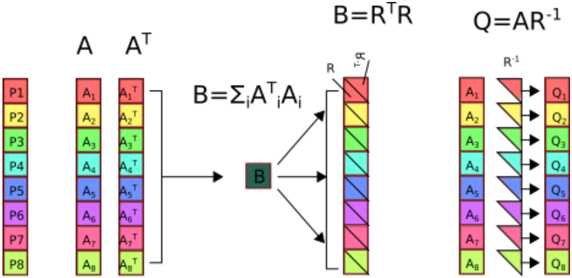
Cholesky-QR [Golub and Van Loan, 2012]

- $A \in \mathbb{R}^{m \times n}$ with $m >> n$ of full column rank.
- QR factorization of $A \in \mathbb{R}^{m \times n}$ as $A = QR$ where $Q \in \mathbb{R}^{m \times n}$ has orthonormal columns ($Q^T Q = I_n$ and $R \in \mathbb{R}^{n \times n}$ is a triangular matrix).
- **First step**: Compute the symmetric positive definite matrix $B = A^T A$.
- **Second step**: Perform the Cholesky factorization of the $n \times n$ matrix B as $B = R^T R$, where $R \in \mathbb{R}^{n \times n}$ is upper triangular. This step provides the R factor of the QR factorization.
- **Third step**: To deduce the Q factor, we simply have to solve:

$$R^T Q^T = A^T.$$

- Cholesky-QR is **not numerically stable**: deviation from orthogonality $\|Q^T\, Q - I_n\|_F$ is proportional to $\kappa_2(A)^2$.

Cholesky-QR2 factorization [Fukaya et al, 2014]



$Q, R \leftarrow$ **CholeskyQR**(A), figure from [Huetter et al, 2019]

- $\widetilde{Q}, R_1 \leftarrow$ **CholeskyQR**(A),
- $Q, R_2 \leftarrow$ **CholeskyQR**($\widetilde{Q}$),
- $R \leftarrow R_2 R_1$.
- Deviation from orthogonality $\|Q^T\, Q - I_n\|_F$ is $O(\varepsilon)$ if $\kappa_2(A) = O(\frac{1}{\sqrt{\varepsilon}})$. [Yamamoto et al, 2015]

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Analysis of Cholesky-QR

- **Data decomposition**: partition the tall and skinny matrix $A \in \mathbb{R}^{m \times n}$ into ℓ panels $A_i \in \mathbb{R}^{m_i \times n} (1 \leq i \leq \ell)$ with $\sum_{i=1}^{\ell} m_i = m$.
- **Map**: the mapper function should perform the local matrix-matrix product $A_i^T A_i$.
- **Reduce**: the reducer function should combine the current result of the reducer (B) with a result of a mapper function related to panel j to update the contribution block B i.e. $B \leftarrow B + A_j^T A_j$.
- **Cholesky factorization of** $B \in \mathbb{R}^{n \times n}$ as $B = R^T R$: this can be performed straightforwardly without any map/reduce strategy.

Implementation of the mapper/reducer function (computation of the triangular factor)

```julia
using LinearAlgebra

function my_mapper_R(M)
     return (M'*M)
end

function my_reducer_R(P,Q)
     return (P+Q)
end
```

Analysis of Cholesky-QR: computation of the orthogonal factor

- **Data decomposition**: partition the tall and skinny matrix $A \in \mathbb{R}^{m \times n}$ into ℓ panels $A_i \in \mathbb{R}^{m_i \times n} (1 \leq i \leq \ell)$ with $\sum_{i=1}^{\ell} m_i = m$.
- **Map**: the mapper function performs the solution of the triangular system of equations $R^T Q_i^T = A_i^T$ and returns $Q_i \in \mathbb{R}^{m_i \times n}$.
- **Reduce**: the reducer function should combine the current result of the reducer with a result of a mapper function (say Q_r and Q_j) i.e. concatenate vertically $[Q_r; Q_j] \in \mathbb{R}^{(m_r + m_j) \times n}$.

Implementation of the mapper/reducer function (computation of the orthogonal factor)

```
using LinearAlgebra

function my_mapper_R(M)
     return (M'*M)
end

function my_mapper_Q(M)
     return ((Tfactor')\(M'))'
end

function my_reducer_R(P,Q)
     return (P+Q)
end

function my_reducer_Q(P,Q)
     return [P;Q]
end
```

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Towards large-scale simulations with Cholesky-QR2

- Favor **BLAS** or **LAPACK** kernels for linear algebra operations: this can be performed with the BLAS package of Julia.
- Perform **inplace** operations to control allocations and memory management.
- Depending on your platform and installation of Julia, use **multithreading** in the numerical linear algebra libraries.
- Problems with $m \approx 10^6$ and $n \approx 64$ can be performed quite efficiently on a laptop [Notebook].
- Numerical results on **Olympe** (@CALMIP) to be discussed next.

Numerical experiments on Olympe

Olympe	Cholesky-QR2		
	$n = 64$		
m	$\|A - QR\|_F / \|A\|_F$	$\|Q^T Q - I_n\|_F / \sqrt{n}$	τ (seconds)
1024	$3.30\ 10^{-16}$	$1.45\ 10^{-15}$	0.002
16384	$3.11\ 10^{-16}$	$3.25\ 10^{-16}$	0.16
262144	$3.22\ 10^{-16}$	$3.21\ 10^{-16}$	2.6
1048576	$3.24\ 10^{-16}$	$8.61\ 10^{-16}$	11.6

- Experiments on **dense** rectangular random matrices performed on a single node of Olympe.
- This uses Julia 1.0.2 with **multithreaded OpenBLAS**.
- Use **distributed computing** through pmap for larger problem sizes !

Summary

Summary

- We have first discussed why **map and reduce** strategies are increasingly popular in high performance data analytics.
- We have then briefly reviewed **map and reduce operations** in Julia.
- We have provided two instructional **illustrations** in Julia.
- We have discussed numerical results related to a possible implementation of a **communication-minimizing** factorization method for dimensionality reduction.

What we have learnt about Julia

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- **Parallelism**: built-in primitives for parallel computing at multiple levels are available in Julia.

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- **Parallelism**: built-in primitives for parallel computing at multiple levels are available in Julia.

Thanks to CALMIP and Groupe Calcul @ CNRS.

Thank you for your attention !

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