



# Toward Intelligent Linear Algebra Methods and Multi-Level Programming Paradigms for Extreme Computing

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With the collaboration of several researchers

University Lille 1, Sciences and Technologies, and CNRS (CRIStAL Laboratory and Maison de la Simulation Paris-Saclay)

- Introduction
- Krylov subspace auto-tuned restarted methods
- Asynchronous Unite-and-Conquer methods
- Multilevel programming paradigm : Graph of components/PGAS
- What Intelligent Krylov methods for extreme computing?
- Conclusion

## Extreme computing (Distributed and Parallel) some correlated goals

- Minimize the global computing time,
- Accelerate the convergence (and analysis at runtime)
- Minimize the number of communications (optimized Ax, asynchronous comp, communication compiler and mapper,....)
- Minimize the number of longer size scalar products,
- Minimize memory space, cache optimization....
- Select the best sparse matrix compressed format,
- Mixed arithmetic
- Unite and Conquer methods
- Minimize energy consumption
- Resilience
- .....

These criteria are some of the requirements for future Exascale computing and beyond

Several optimizations are not possible at compile time and have to be decided at runtime: Auto-tuning, smart-tuning, ....

The goal of this talk is to illustrate that we would need **intelligent linear algebra** methods to create the next generation of High Performance numerical software, associated with adapted **programming paradigms** allowing the end-user to **give expertise** 

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  - Restart strategies
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#### GMRES example: about memory space, dot products and sparse

1 matrix vector multiplication

m, subspace size

multiplication

rt: Choose  $x_0$  and compute  $r_0 = f - Ax_0$  and  $v_1 = r_0/||r_0||$ .

2. Iterate: For  $j = 1, 2, \dots, m$  do:

$$h_{i,j} = (Av_j, v_i), i = 1, 2, ..., j,$$

$$\hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{i,j} v_i,$$

$$h_{j+1,j} = \|\hat{v}_{j+1}\|, \text{ and}$$

$$v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}.$$

3. Form the approximate solution:

$$x_m = x_0 + V_m y_m$$
, where  $y_m$  minimizes  $\|\beta e_1 - \bar{H}_m y\|$ ,  $y \in \mathbb{R}^m$ .

Subspace computation : O(m³)

4. Restart:

Compute 
$$r_m = f - Ax_m$$
; if satisfied then stop else compute  $x_0 := x_m$ ,  $v_1 := r_m / ||r_m||$  and go to 2.

Memory space :

sparse matrix: nnz elements

Krylov basis vectors : n m

Hessenberg matrix : m m

Scalar products, at j fixed:

Sparse Matrix-vector product : n of size C

Orthogonalization: j of size n

**m**, the subspace size, may be auto-tuned at runtime to minimize the space memory occupation and the number of scalar product, with better or approximately same convergence behaviors.

#### GMRES: about memory space and dot products

- 1. Start: Choose  $x_0$  and compute  $r_0 = f Ax_0$  and  $v_1 = r_0 / ||r_0||$ .
- 2. *Iterate*: For  $j = 1, 2, \dots, m$  do:

$$h_{i,j}=(Av_j,v_i), i=1,2,\cdots,j,$$
 Incomplete orthogonalization (Y. Saad): i.e. i= from  $\hat{v}_{j+1}=Av_j-\sum_{i=1}^jh_{i,j}v_i,$   $\max(1,j-q)$  to j  $q>0$ . Then, J-q+1 bands on the Hesseberg matrix.  $v_{j+1}=\hat{v}_{j+1}/h_{j+1,j}.$ 

3. Form the approximate solution:

$$x_m = x_0 + V_m y_m$$
, where  $y_m$  minimizes  $\|\beta e_1 - \bar{H}_m y\|$ ,  $y \in \mathbb{R}^m$ .

4. Restart:

Compute 
$$r_m = f - Ax_m$$
; if satisfied then stop else compute  $x_0 := x_m$ ,  $v_1 := r_m / ||r_m||$  and go to 2.

#### Memory space :

Scalar products, at j fixed:

sparse matrix : nnz (i.e. < C n) elements

Krylov basis vectors : n m

Sparse Matrix-vector product : n of size C

Orthogonalization : m of size n

Hessenberg matrix : m m

m, the subspace size, may be auto-tuned at runtime to minimize the space memory occupation and the number of scalar product, with better or approximately same convergence behaviors. The number of vectors othogonalized with the new one may be auto-tuned at runtime. The subspace size may be large!

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# Previous works, subspace auto-tuning algorithms

- Subspace size : different auto-tuning at runtime
  - Subspace size increase, until a fixed limit [Katagiri00][Sosonkina96],...
  - Subspace size decrease, until a fixed limit [Baker09],.....
  - Restart Trigger [Zhang04], restart when stagnation is detected.
- Orthogonalization : no auto-tuning at runtime
  - Prior to execution : [Jia94]

#### Remark, in general:

- Greater subspace size -> better convergence/long restart, less iterations
- Smaller subspace size -> slow convergence, stagnation, short restart, more iteration
- Choice of m is mandatory.

For difficult problems we have to use a large subspace size to reach convergence: the numerical stability and the quality of the orthogonalization are crucial.

## **Auto-Tuning Algorithms**

with Pierre-Yves Aquilenti (TOTAL)

- Subspace size
  - Evaluate convergence progression over some iterations.
  - Decrease if convergence are monotonous or if they are smoothly slowing (approximately same convergence but minimize time and space)- Cr medium
  - Increase if convergence stall (problem if we increase too much the memory space), Track memory levels : Cache, RAM, Nodes. Cr low
  - Do nothing if Cr high

 $Cr = norm2(r_i) / norm2(r_{i-1})$ 

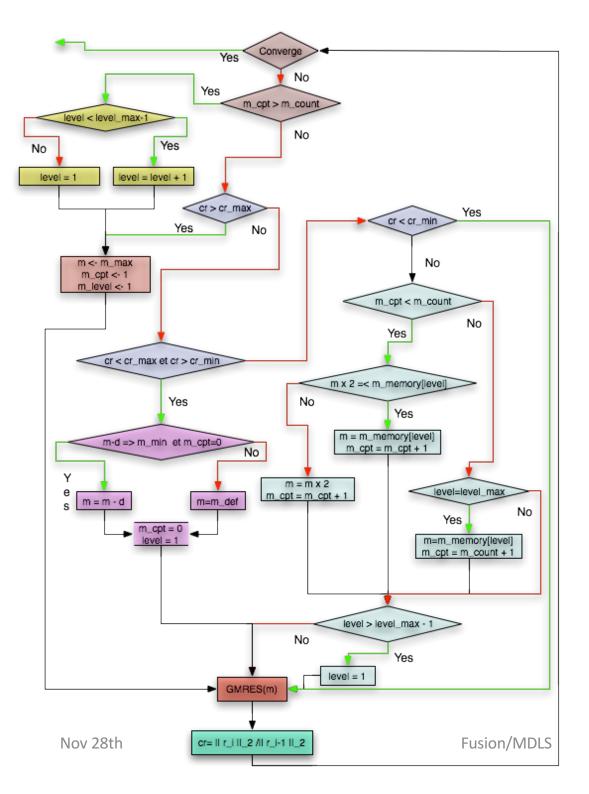
oblem if Ory oche,

Entry Point

Exit Point

Cr

Easy to implement using libraries (both for GMRES and Arnoldi method for example)



#### **Parameters**

d : number of steps between successive decreases,

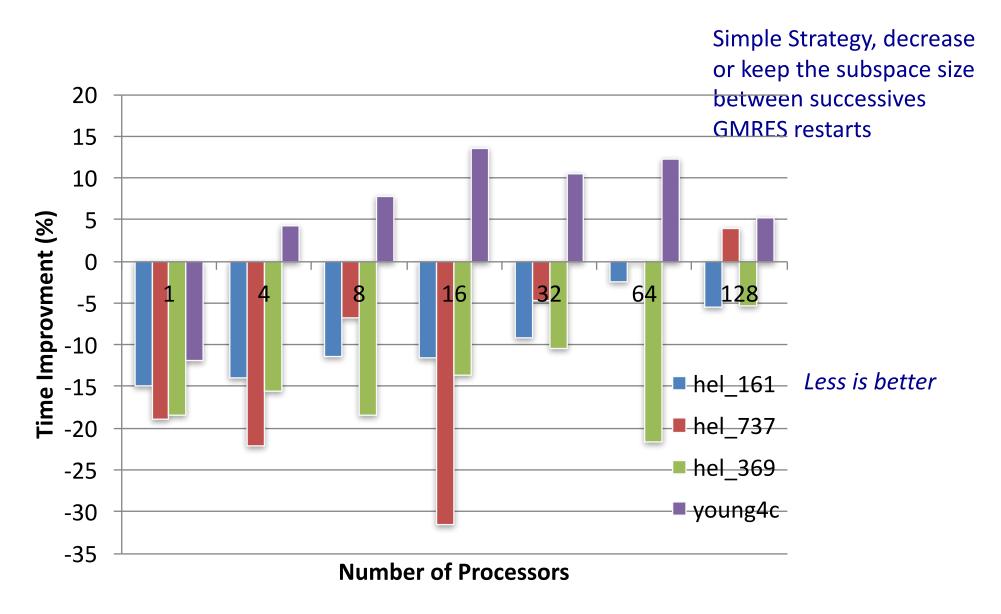
m\_min: minimum subspace size value,

m\_max : maximum subspace size value,

m\_counts: number of successive soft increase before intending "special" Increases,

m\_memory[]: array containing
subspace size values for hardware
increase

## Our algorithm compared to no auto-tuning



# Auto-Tune Restarted GMRES With Caches with Pierre-Yves Aquilenti (TOTAL)

 We define levels of GMRES restart parameter autotuning increase depending on levels of memory

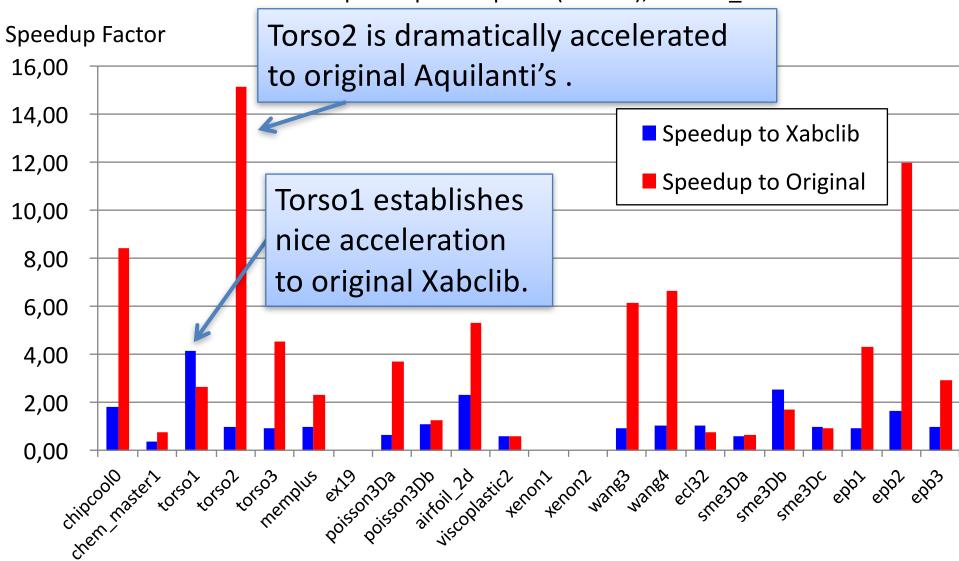
Cache L1	Cache L2	Cache L3	RAM	SWAP
4	10	20	200	1000

$$(nnz + 3n + m(m+1) + n(m+1)) \times SizeOfScalar \ge MemoryBytesLevel$$
 
$$\frac{MemoryBytesLevel}{SizeOfScalar} - nnz - 4n = m^2 + m(n+1)$$

nnz = number of non zeros of the matrix
m = subspace size / restart parameter
n = matrix size

## With Pierre-Yves Aquilenti (TOTAL) and Takahiro Katagari (U. Tokyo)

16 Threads on the T2K Open Supercomputer (1 node), Xabclib\_GMRES V1.00



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## Incomplete orthogonalization Auto-Tuning

<u>Complete orthogonalisation</u>: we orthogonalise with all the previous computed vectors of the basis, i.e. at step k, we ortogonalise with k vectors, which generates k scalar product at step k.

<u>Incomplete orthogonalisation</u>: we orthogonalize with only min(k,q) previous computed vectors of the basis, i.e. at step k, we ortogonalise only with min(k,q) vectors, q < m. DQGMRES: [Saad '94], DQGMRES: [Wu '97] IGMRES: [Brown '86][Jia '07]

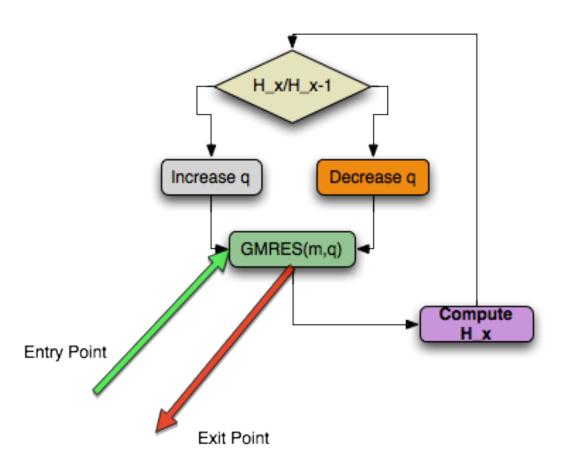
Then, we have only q scalar product at step k (for k > or equal to q).

Complete ortogonalization : k scalar product for k fixed Incomplete orthogonalization : q scalar product for k fixed, q < k

We may then save k-q scalar products, for q < k, and, then, several synchronized communications.

Even, if the number of iterations may be a little larger, we minimize a lot of long global communications generated by scalar products.

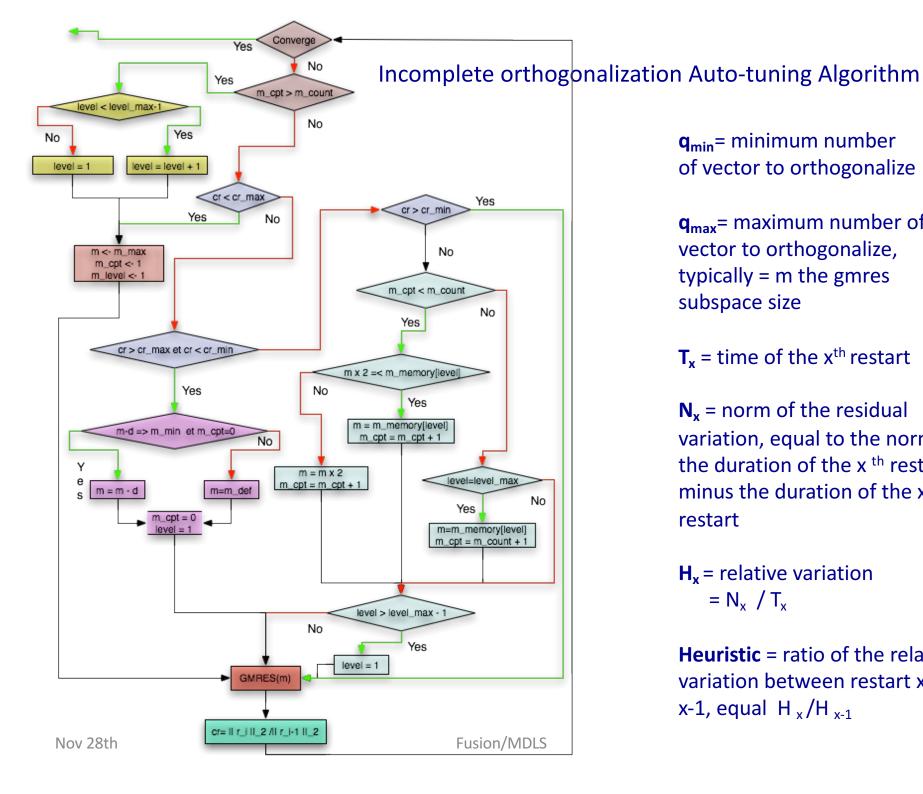
# Incomplete orthogonalization algorithm at runtime (with P.-Y. Aquilenti)



- Evaluate iteration costs in time vs. Convergence
- Decrease number of orthogonalized vectors q if ratio convergence/(time iteration) decrease

A complex heuristic-based algorithm: With respect to the variation of the residual between restarts, we change the number q of vectors concerned by the orthogonalization

Still, a lot of researches to achieve to optimize this algorithm.



**q**<sub>min</sub>= minimum number of vector to orthogonalize

 $q_{max}$ = maximum number of vector to orthogonalize, typically = m the gmres subspace size

 $T_x$  = time of the  $x^{th}$  restart

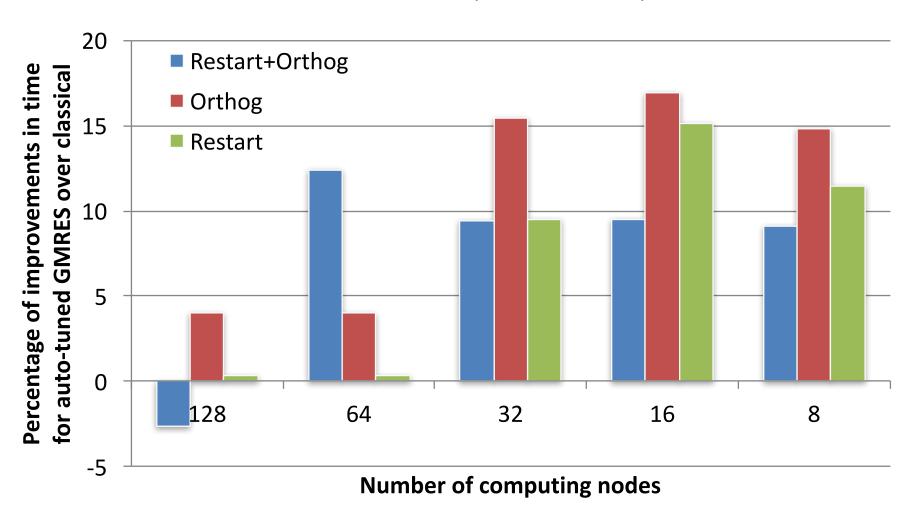
 $N_x$  = norm of the residual variation, equal to the norm of the duration of the x th restart minus the duration of the x-1<sup>th</sup> restart

$$H_x$$
 = relative variation  
=  $N_x / T_x$ 

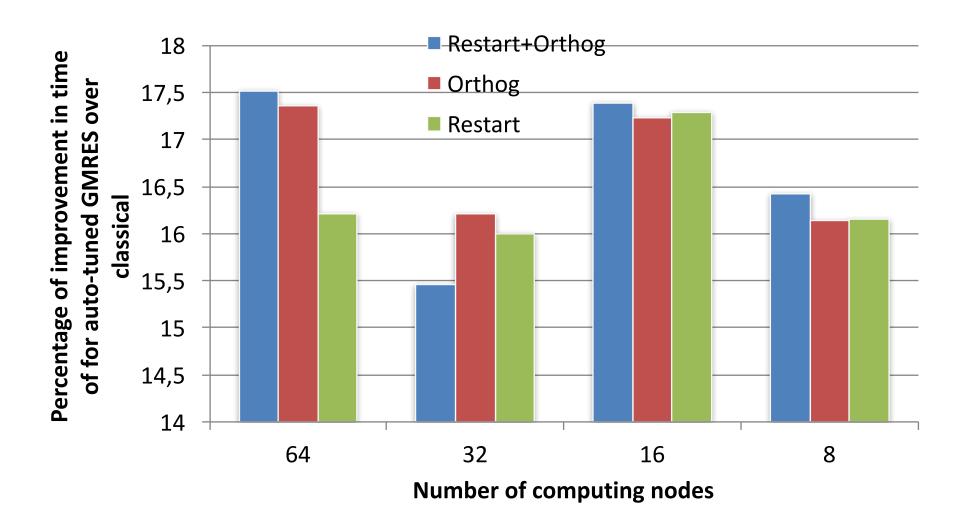
**Heuristic** = ratio of the relative variation between restart x and x-1, equal  $H_x/H_{x-1}$ 

## Results: Industrial Case (TOTAL)

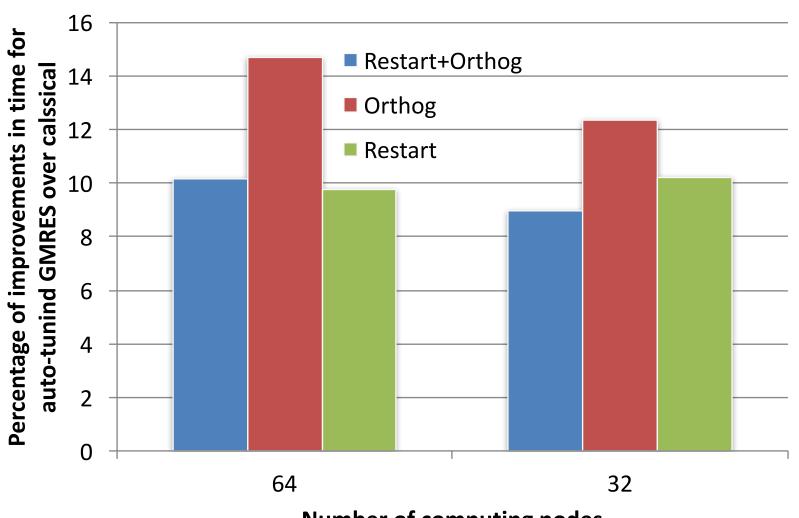
number of unknown =  $(119 \times 119 \times 115)$ , 3Hz, m=10



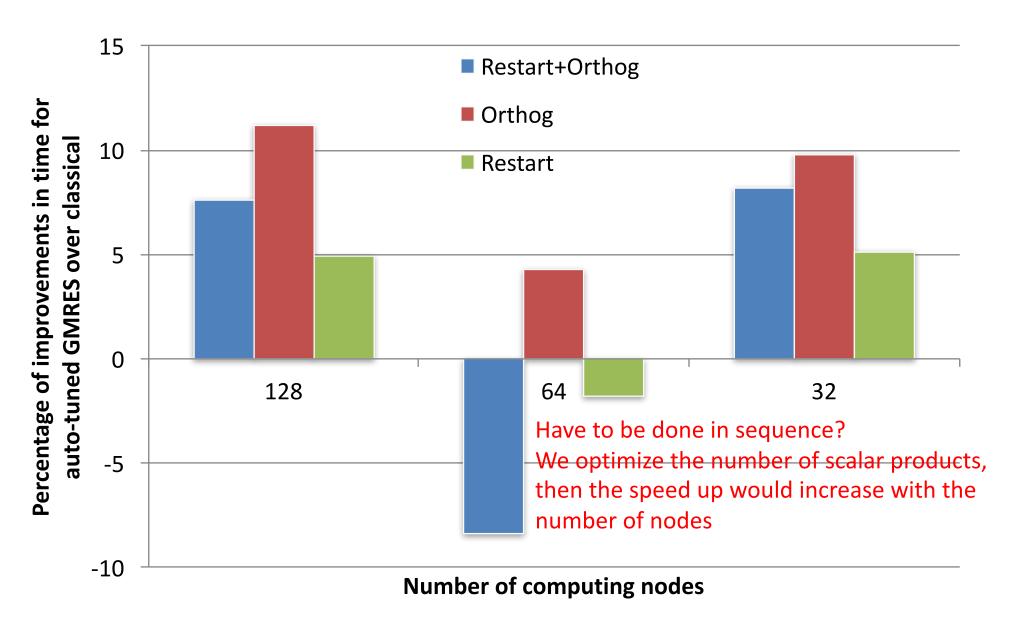
#### number of unknown = $(119 \times 119 \times 115)$ , 3 Hz, m=30



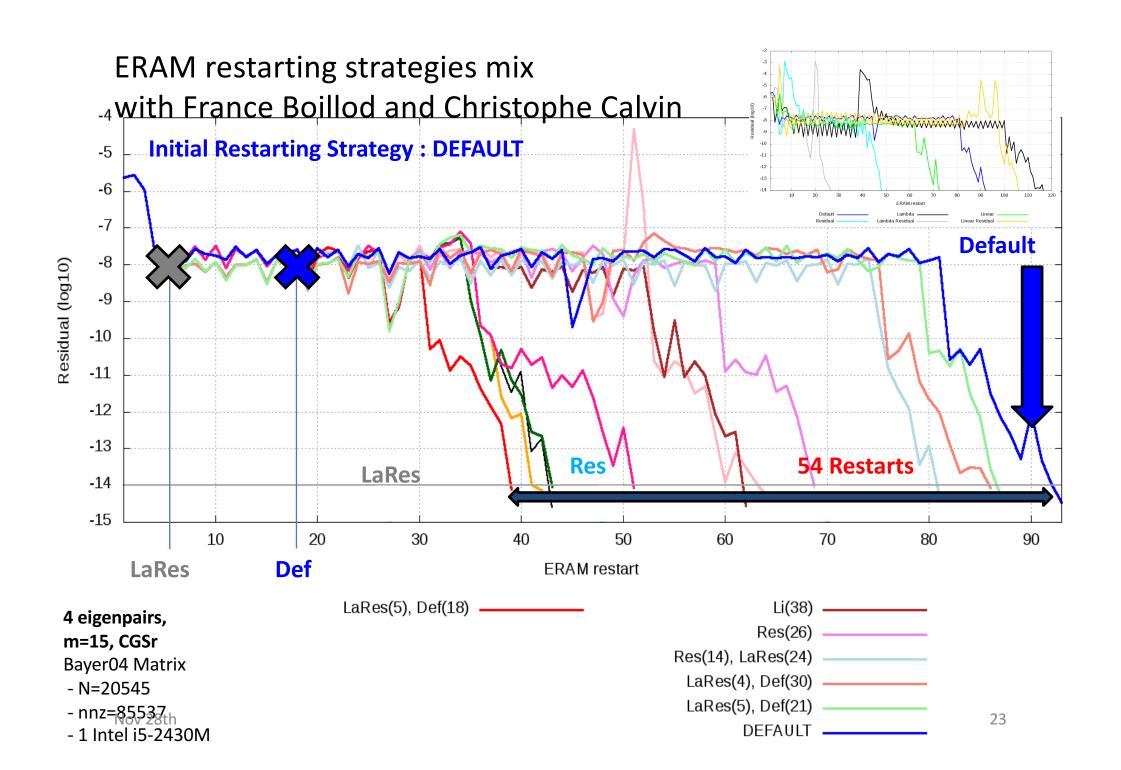
#### number of unknown = $(183 \times 183 \times 191)$ , 5 Hz, m=10



#### number of unknown = $(335 \times 327 \times 383)$ , 5Hz, m=30

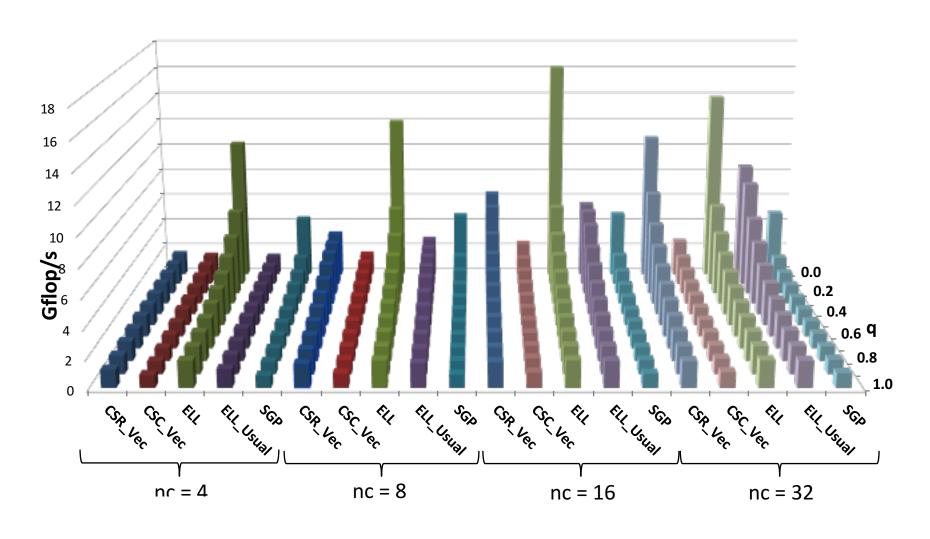


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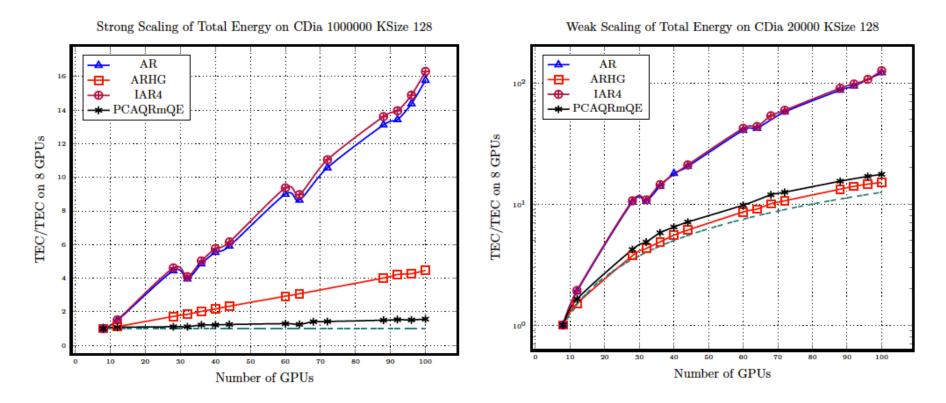


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#### Performance of SpMV



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- ArnoldiHG and PCAQRmQE have good scalability of TEC
- Communication is important to scalability of energy consumption.

#### Then, for a given method:

Several parameter have to be optimized at runtime :

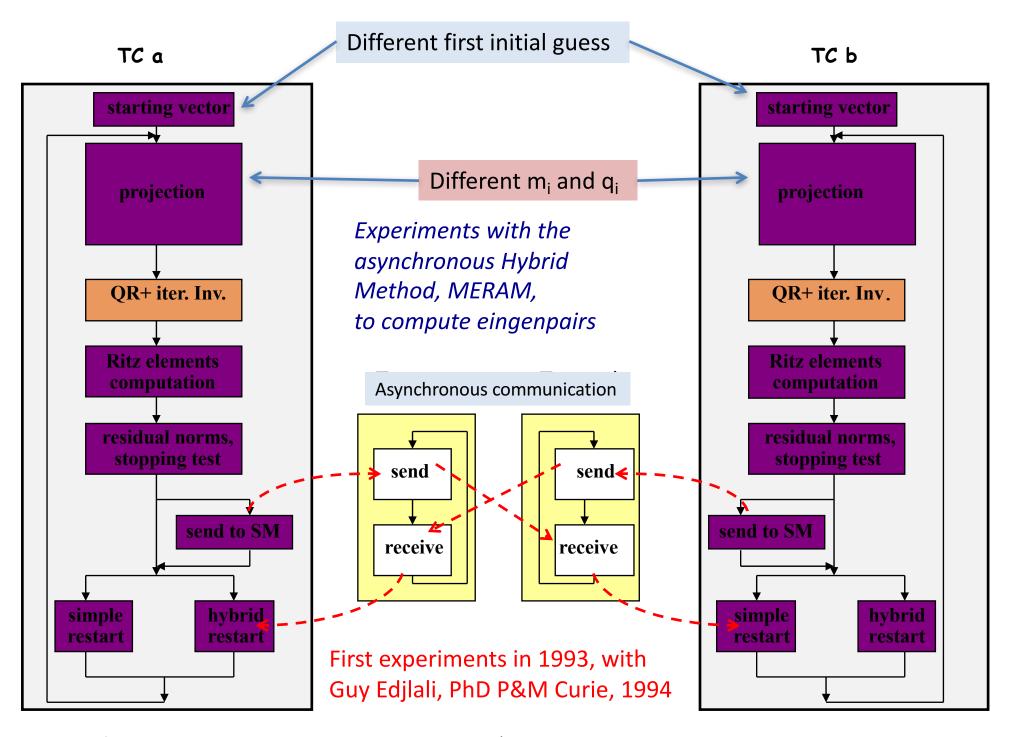
- Subspace size
- Incomplete orthogonalisation
- Restart strategies
- Energy consumption
- Sparse format compression
- Orthogonalisation algorithm
- Preconditionners
- Mixed arithmetic
- Others ....

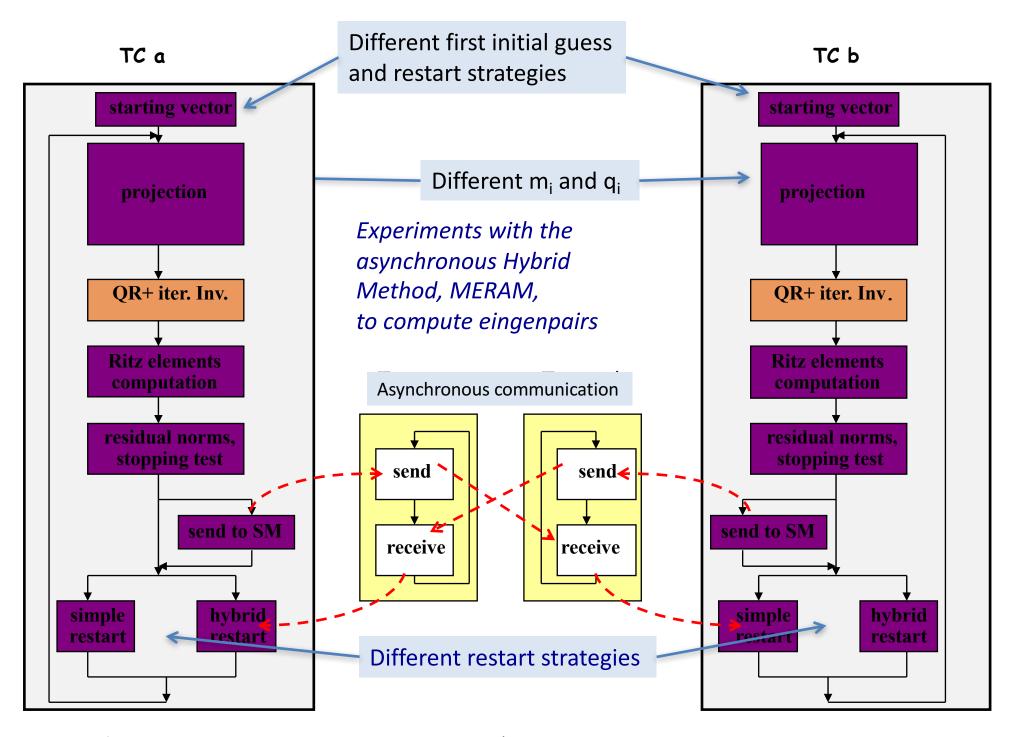
Nevertheless, we have to be able to evaluate the convergence, the stability and others importants criteria at runtime, and some learning may be introduced

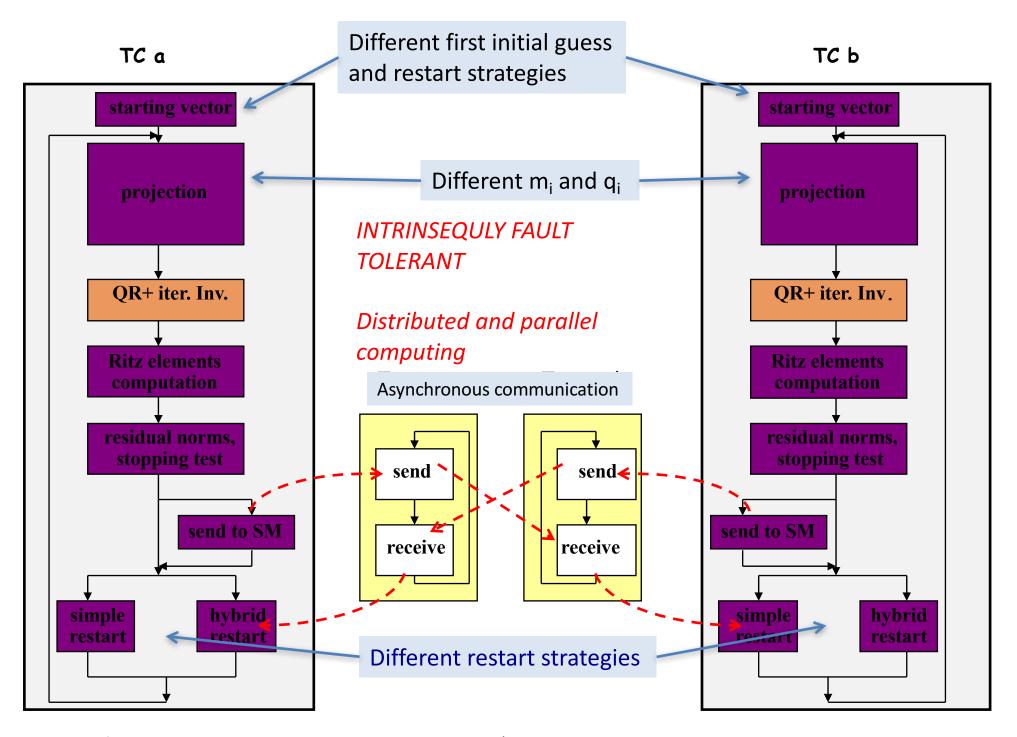
Deep learning technics may be used to learn and big analytics may help to compare with past experiments

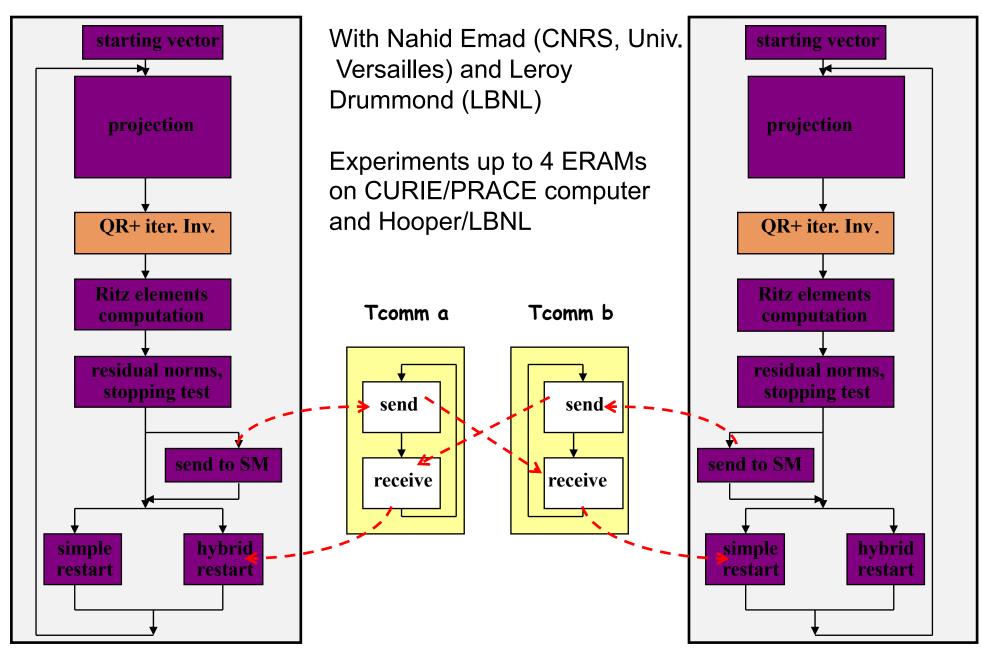
Unite-and-conquer methods would generate new potential problems, and information.

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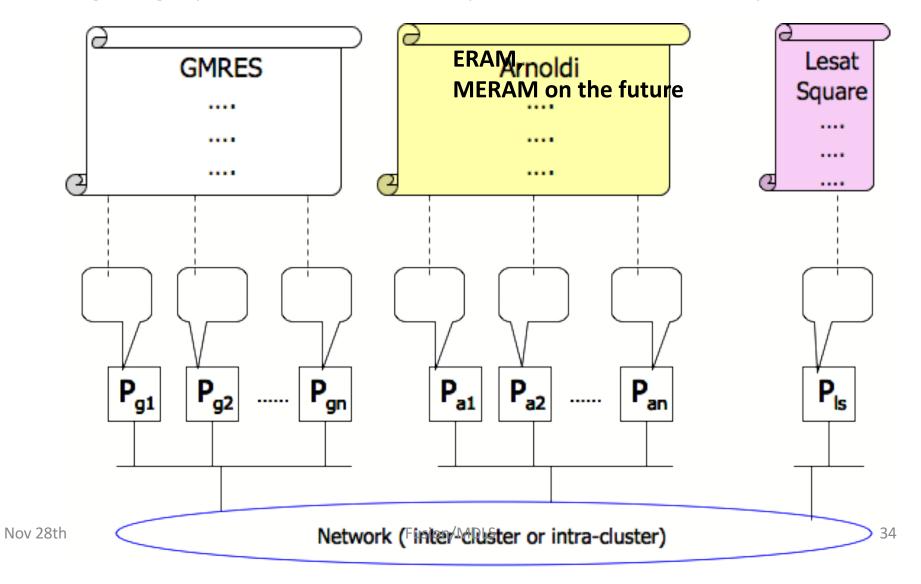




## Asynchronous Iterative Restarted Methods

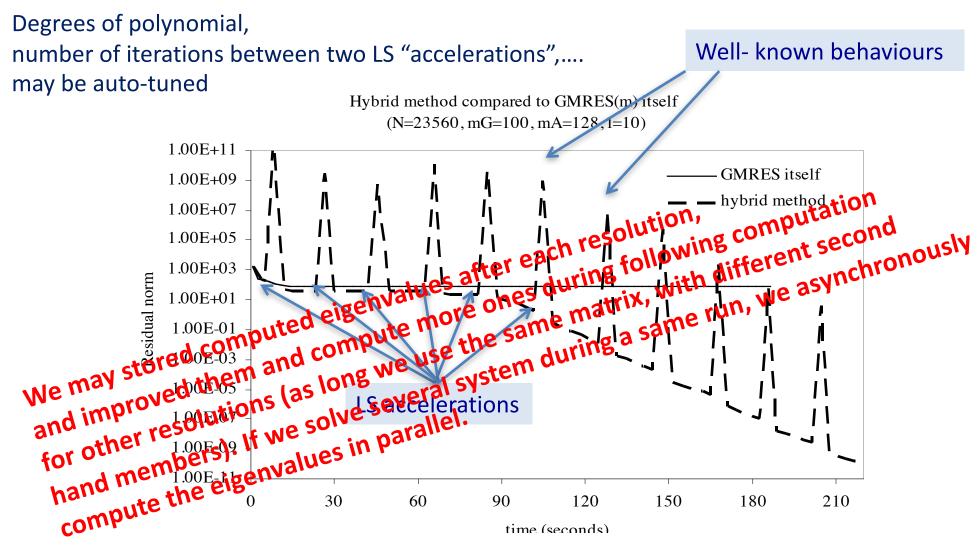
Collaboration with He Haiwu and Guy Bergère (U. Lille 1, CNRS) and Ye Zhang (Hohai Univ. Nanjing), Salim Nahi (Maison de la simulation), and Pierre-Yves Aquilenti (TOTAL), Xinzhe Wu (Lille 1 and MDLS)

Experiments on several supercomputers, or networks of clusters/supercomputers)
We are beginning experiment on Tianhe 2 and planed some on the #1 in Japan

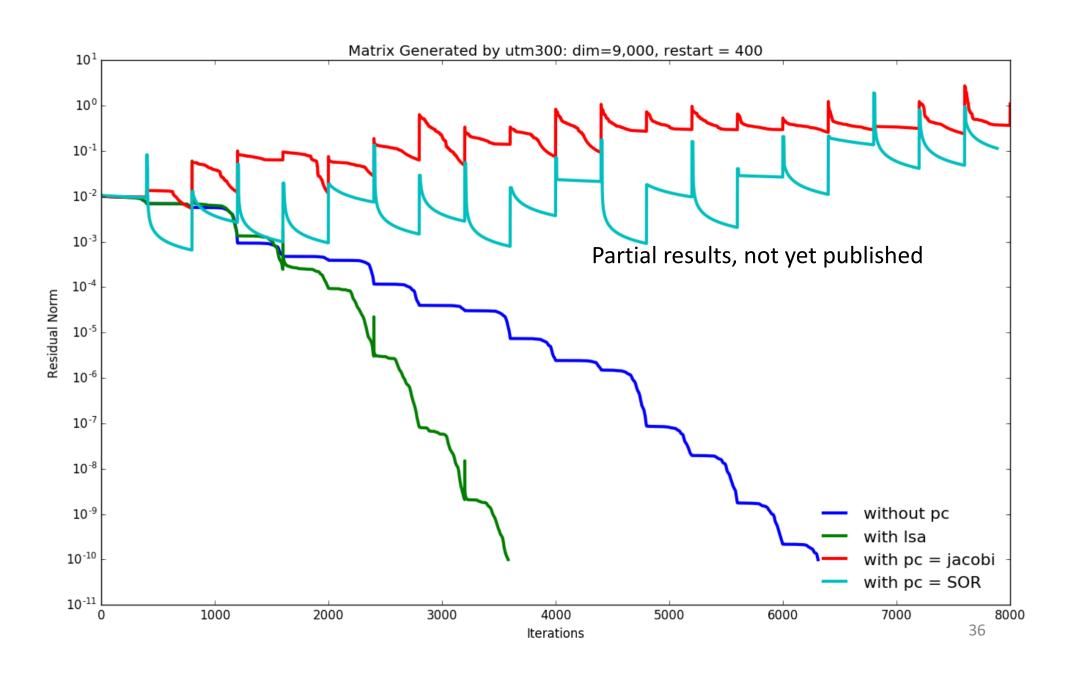


## Numeric Results and Analysis

advantage over GMRES (difficult convergence case)



Last results, last week on a Bull supercomputer in Reims (Romeo), with Xinzhe Wu We also change the number of processor to compute ERAM and GMRES at runtime



Then

Criteria of each methods have to be tuned at runtime

The information, and learning, extracted on each method have to be exchanged asynchronously with the others in order to improve all the global convergence and numerical behaviors

Each run would generate information which may be used for following computation (ex : approximated eigenvalues for GMRES-ERAM/LS, ....)

But, existing programming paradigms are not well-adapted

And end-users/scientists may help with their expertise

A new generation of numerical methods has to be invented!

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### Toward graph of parallel tasks/components

#### Supercomputers as distributed and parallel platforms

- Communications have to be minimized: but all communications have not the same costs, in term or energy and time.
- Latencies between farther cores will be very time consuming: global reduction or other synchronized global operations will be really a bottleneck.
- We have to avoid large inner products, global synchronizations, and others operations involving communications along all the cores. Large granularity parallelism is required (cf. unite-and-conquer methods).
- Graph or tasks/components programming allows to limit these communications only between the allocated cores to a given task/components.
- Communications between these tasks and the I/O may be optimized using efficient scheduling and orchestration strategies(asynchronous I/O and others)
- **Distributed computing meet parallel computing**, as the future super(hyper)computers become very hierarchical and as the communications become more and more important. Scheduling strategies would have to be developed.
- We have to allow end-user to give expertise

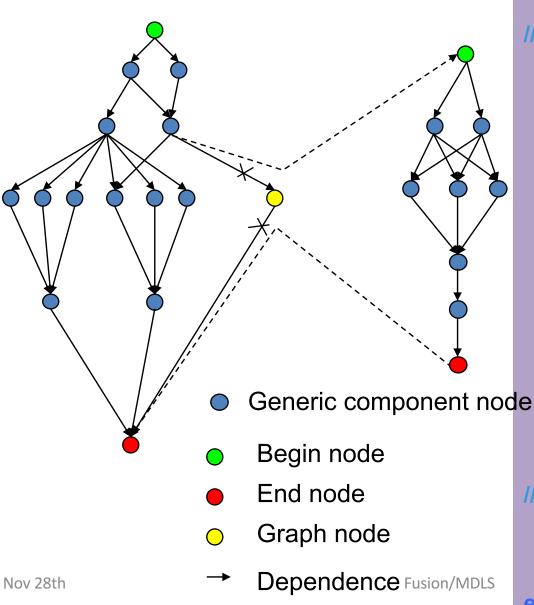
#### Some elements on YML (since 2000)

• YML¹ Framework is dedicated to develop and run parallel and distributed applications on Cluster, clusters of clusters, and **supercomputers** (schedulers and middleware would have to be optimized for more integrated computer – cf. "K" and OmnRPC for example).

#### Independent from systems and middlewares

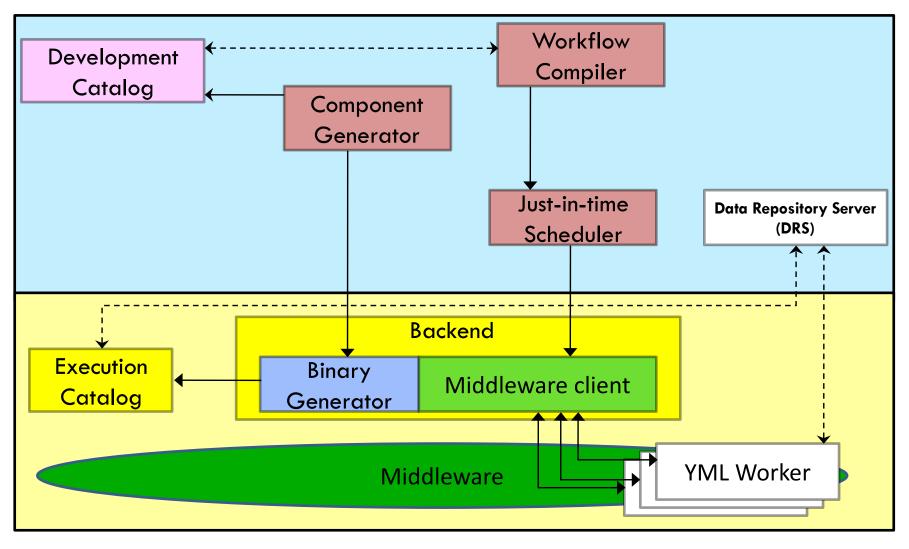
- The end users can reused their code using another middleware
- Actually the main system is OmniRPC<sup>3</sup>
- Components approach
  - Defined in XML
  - Three types: Abstract, Implementation (in FORTRAN, C or C++;XMP,..), Graph (Parallelism)
  - Reuse and Optimized
- The parallelism is expressed through a graph description language, named **Yvette** (name of the river in Gif-sur-Yvette where the ASCI lab was). **LL(1)** grammar, easy to parse.
- Deployed France, Belgium, Ireland, Japan (T2K, K, FX10), China, Tunisia, USA (LBNL, TOTAL-Houston).
- Experiment on both supercomutes, Grid (Gird5000) and P2P (100 PCs in Lille, 100 PC in Orsay, and 4 cluserts in Japon, launch from a SC INRIA boooth a few years ago)

#### **Graph (n dimensions)** of components/tasks) YML



```
par
 compute tache1(..);
 notify(e1);
 compute tache2(..); migrate matrix(..);
 notify(e2);
wait(e1 and e2);
 Par (i :=1;n) do
  par
    compute tache3(..);
  notify(e3(i));
  if(1 < n)then
    wait(e3(i+1));
    compute tache4(..);
    notify(e4);
  endif;
  compute tache5(..); control robot(..);
  notify(e5); visualize mesh(...);
  end par
end do par
wait(e3(2:n) and e4 and e5)
 compute tache6(..);
 compute tache7(..);
end par
```

#### YML Architecture



# **Abstract Component**

# Implementation Component

```
<?xml version="1.0"?>
<component type="impl" name="prodMat" abstract="prodMat" description="Implementation</pre>
    component of a Matrix Product">
                                                                    End users may add some
    <impl lang="CXX">
                                                                    expertise here (we'll see example)
     <header />
     <source>
                                     <impl lang="XMP" nodes="CPU:(5,5)" libs=" " >
     <![CDATA[
                                           <distribute>
                                                <param template=" block,block " name="A(100,100)</pre>
int i,j,k;
                                     " align="[i][i]:(i,i) " />
double ** tempMat;
                                                <param template=" block " name="Y(100);X(100)" align="[i]:(i,*)</pre>
//Allocation
 for(k = 0 ; k < blocksize ; k++)
                                           </distribute>
  for (i = 0; i < blocksize; i++)
      for (i = 0; i < blocksize; i++)
     tempMat[i][j] = tempMat[i][j] + matrixBkk.data[i][k] * matrixAki.data[k][j];
    for (i = 0; i < blocksize; i++)
           for (i = 0; i < blocksize; i++)
                                                              Several possible implementation
                 matrixAki.data[i][j] = tempMat[i][j];
                                                              components for each abstract one,
//Desallocation
                                                               using different languages
    ]]>
           </source>
     <footer />
    </impl>
                                              Fusion/MDLS
                                                                                                    44
```

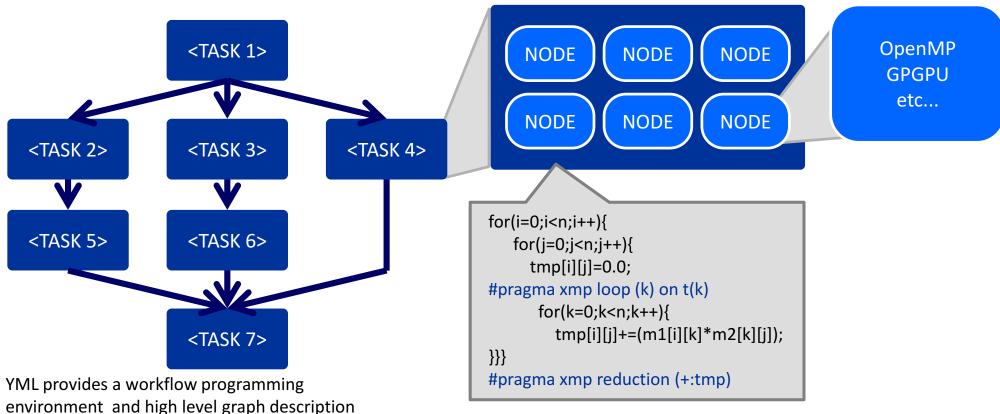
</component>

#### Graph component of Block Gauss-Jordan Method

```
<?xml version="1.0"?>
                                                                             #Step3
<application name="Gauss-Jordan">
                                                                                          par(i:= 0; blockcount - 1)
<description>produit matriciel pour deux matrice carree
</description>
                                                                                                if (i neq k) then
<graph>
                                                                                                       if (k neg blockcount - 1) then
blocksize:=4;
                                                                                                       #step 3.1
blockcount:=4;
                                                                                                             par (j:=k + 1;blockcount - 1)
     par (k:=0;blockcount - 1)
                                                                                                                    wait(prodA[k][j]);
                                                                                                                    compute
           #inversion
                                                                             prodDiff(A[i][k],A[k][j],A[i][j],blocksize);
           if (k neg 0) then
                                                                                                                    notify(prodDiffA[i][j][k]);
                 wait(prodDiffA[k][k][k - 1]);
           endif
                                                                                                       endif
           compute inversion(A[k][k],B[k][k],blocksize,blocksize);
                                                                                                       #step 3.2
           notify(bInversed[k][k]);
                                                                                                       if (k neq 0) then
                                                                                                             par(j:=0;k-1)
           #step 1
                                                                                                                    wait(prodB[k][j]);
           par (i:=k + 1; blockcount - 1)
                                                                                                                    compute
           do
                                                                             prodDiff(A[i][k],B[k][j],B[i][j],blocksize);
                 wait(bInversed[k][k]);
                                                                                                             enddo
                 compute prodMat(B[k][k],A[k][i],blocksize);
                                                                                                       endif
                 notify(prodA[k][i]);
                                                                                                endif
           enddo
                                                                                          enddo
                                                                                   enddo
           par(i:=0;blockcount - 1)
                                                                                </graph>
           do
                                                                             </application>
           #step 2.1
                 if(i neq k) then
                       wait(bInversed[k][k]);
                      compute mProdMat(A[i][k],B[k][k],B[i][k],blocksize);
                       notify(mProdB[k][i][k]);
                 endif
           #step 2.2
                 if(k qt i) then
                       wait(bInversed[k][k]);
                       compute prodMat(B[k][k],B[k][i],blocksize);
                       notify(prodB[k][i]);
                 endif
           enddo
```

# Multi-Level Parallelism Integration: YML-XMP

#### N dimension graphs available



language called YvetteML

Each task is a parallel program over several nodes.

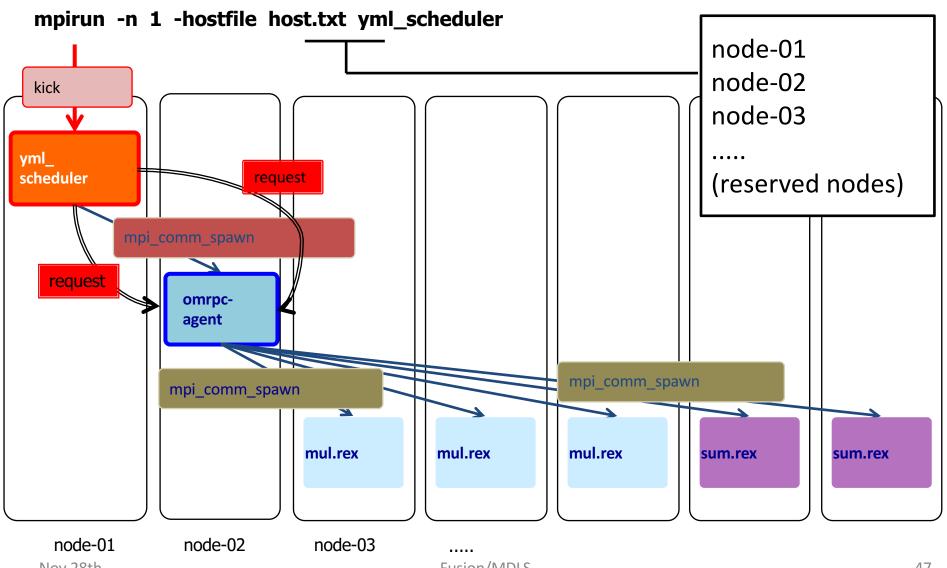
XMP language can be used to descript parallel program easily!

YML/XMP/StarPu expriments on T2K in Japan, project FP3C

#### FP2C: YML-XMP

#### on the K computer at AICS

#### Processes management: OmniRPC Extension, on MPI



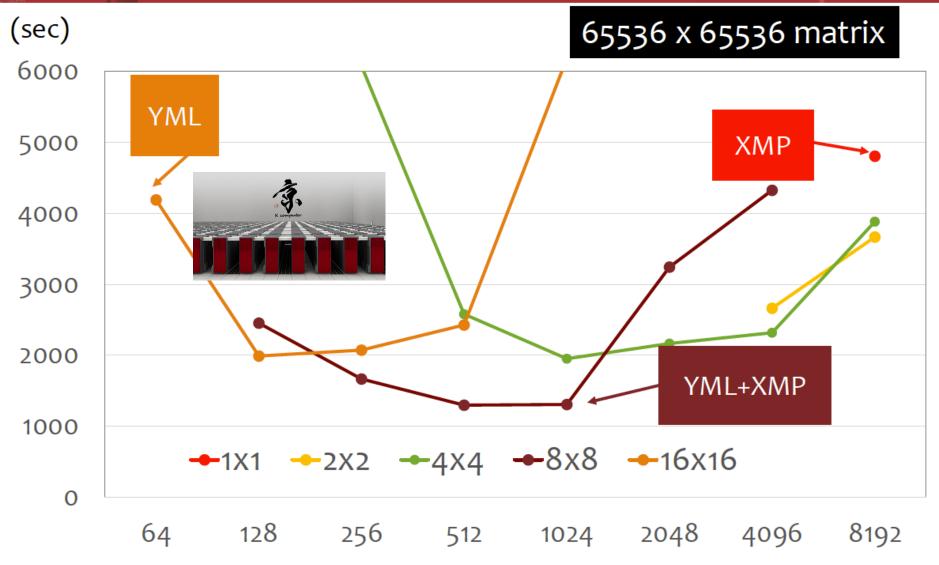
#### Implementation Component Extension

- Topology and number of processors are declared to be used at compile and run-time.
- Data distribution and mapping are declared
- Automatic generation for distributed language (XMP, CAF, ...)
- Used at run-time to distribute data over processes

```
<?xml version="1.0"?>
<component type="impl" name="Ex" abstract="Ex" description= "Example">
    <impl lang="XMP" nodes="CPU:(5,5)" libs=" " >
    <distribute>
      <param template=" block,block " name="A(100,100) " align="[i][i]:(j,i) " />
      <param template=" block " name="Y(100);X(100)" align="[i]:(i,*) "/>
    </distribute>
      <header />
      <source>
      <![CDATA[
                                                                       Information for XMP
      /* Computation Code */
      ]]>
      </source>
      <footer />
    </impl>
</component>
```

# Experiments (2) BGJ on K-Computer



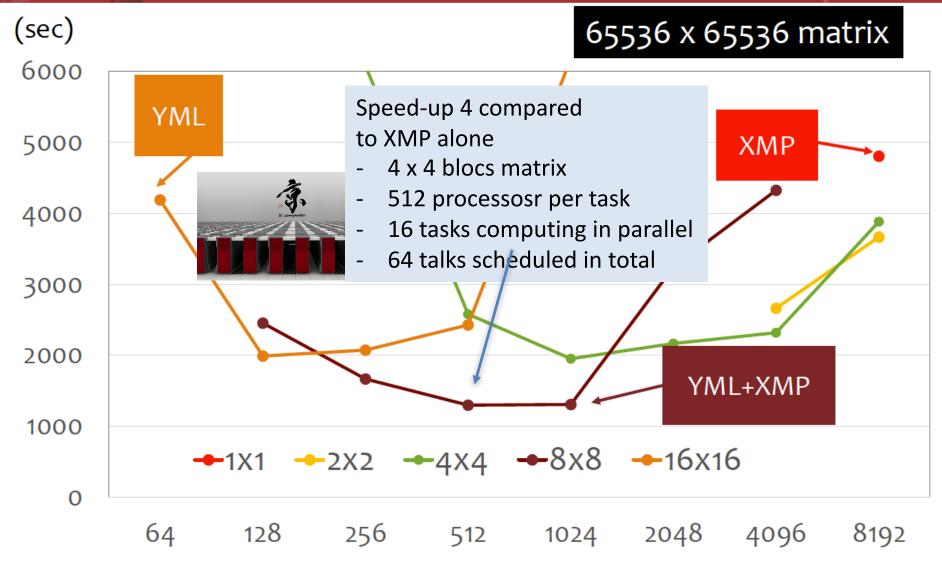


# of processors for each task

Slide written by Miwako TSUJI, RIKEN/AICS

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Then,

Such programming paradigm (with some scheduled adaptations) is well-adapted for multi-level programming and unite-and-conquer methods

We may also consider the I/O and other data movements using some software as AIDOS (and others works done with DDN and TOTAL) as we have both the data and the control flow Graphs which allow data migration anticipations

We have a fault tolerent version of YML (talk at a SC15 workshop) developed mainly at AICS

For the same "task", we have different components and the end-users may give some expertise which will may be used at any level of the software stack and at runtime by the scheduler, the middleware and others....

We may use this to allow the end-users to give expertise for future numerical methods

#### Outline

- Introduction
- Krylov subspace auto-tuned restarted methods
- Asynchronous Unite-and-Conquer methods
- Multilevel programming paradigm : Graph of components/PGAS
- What Intelligent Krylov methods for extreme computing?
- Conclusion

#### Interface between different languages

#### We already saw that:

```
<?xml version="1.0"?>
<component type="impl" name="Ex" abstract="Ex" description= "Example">
    <impl lang="XMP" nodes="CPU:(5,5)" libs=" " >
    <distribute>
            <param template=" block,block " name="A(100,100) " align="[i][j]:(j,i) " />
            <param template=" block " name="Y(100);X(100)" align="[i]:(i,*) "/>
    </distribute>
            <header />
            <source>
            <![CDATA[
      /* Computation Code */
           ]]>
      </source>
            <footer />
    </impl>
</component>
```

# Implementation Component and smart-tuning associated to a language and an implemntation

- Range of parameters to tuned
- Expertise from end-users
- Learning

```
<?xml version="1.0"?>
<component type="impl" name= "GMRES_Tuned" abstract= "GMRES_Tuned"</pre>
    description= "Example">
    < range m = {15,100} />
    <Algo tuning = is method 1 in libX if size larger than 1000, is method 2 otherwise />
    <impl lang="XMP" nodes="CPU:(5,5)" libs=" " >
    <distribute>
            <param template=" block,block " name="A(100,100) " align="[i][i]:(j,i) " />
            <param template=" block " name="Y(100);X(100)" align="[i]:(i,*) "/>
    </distribute>
            <header />
            <source>
            <![CDATA[
      /* Computation Code */
            ]]>
       </source>
            <footer />
    </impl>
</component>
```

LL(1) languages may allow end-users to give expertise

# Abstract Component associated with the method

```
<?xml version="1.0" ?>
<component type="abstract" name= »GMRES_Tuned" description="restarted
   GMRES method" >
   <Smart_tunings>
   <param name="m" type="subspace size" />
   <param name="q", type="orthogonalization parameter />
   </Smart tunings>
   <params>
    <param name="matrixA" type="Matrix" mode="in" />
    <param name="matrixV" type="Matrix" mode="out" />
    <param name="size" type="integer" mode="in" />
   </params>
</component>
Future (allowing to change the graph at runtime depending of the result):
<param name= "conv" type= " graph_param_float" mode= "inout" />
```

### **Abstract Component**

```
<?xml version="1.0" ?>
<component type="abstract" name= »GMRES_Tuned" description="restarted
   GMRES method" >
   <Smart_tunings>
   <param name="m" type="subspace size" />
   <param name="q", type="orthogonalization parameter />
   </Smart tunings>
   <params>
    <param name="matrixA" type="Matrix" mode="in" />
    <param name="matrixV" type="Matrix" mode="out" />
    <param name="size" type="integer" mode="in" />
   </params>
</component>
Future:
<param name= "conv" type= " graph_param_float" mode= "inout" />
```

#### Implementation Component and smarrt-tuning

- Range of parameters to tuned
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LL(1) languages may allow end-users to give expertise

```
<?xml version="1.0"?>
<component type="impl" name= "GMRES Tuned" abstract= "GMRES Tuned"</pre>
    description= "Example">
    < range m = {15,100} />
    <Algo tuning = is method 1 if size larger than 1000, is method_2 otherwise />
    <impl lang="XMP" nodes="CPU:(5,5)" libs=" " >
    <distribute>
            <param template=" block,block " name="A(100,100) " align="[i][i]:(j,i) " />
            <param template=" block " name="Y(100);X(100)" align="[i]:(i,*) "/>
    </distribute>
            <header />
            <source>
            <![CDATA[
      /* Computation Code */
            ]]>
      </source>
            <footer />
    </impl>
</component>
```

#### Tuning for extreme computing

- Each parameters of each method may be auto-tuned,
- Each modification of a parameter in one method have to be analyse by the others methods
- We have to analyse the convergence, the efficiency of each iteration, the energy consumed, the accuracy, the stability variation,....

We propose high level programming paradigms which allow the end-user and/or the applied mathematician to give some expertise (range of the subspace size, dominant eigenvalue clustering, condition number, ....).

YML is such a programming langage (we have a virtual machine with tutorial and documentation, send me email: serge.petiton@univ-lille1.fr)

We have to use components and high level software strategies to propose tools and language for future numerical analysis methods, who will have to take decisison at runtime: to smart-tune but also to chose methods and preconditionning, for example

Nevertheless, the important challenge is to propose new intelligent methods for such programming paradigms

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#### Conclusion

- Auto-tunning at runtime and unite-and-conquer methods are important propositions to develop methods to announced extreme computing machine; leading to "intelligent linear algebra"
- High level programming paradigms are required
- We propose both a framework based on multi-level programming and programming paradigm, and allowing end-users/scientists to give expertise
- Introducing learning into numerical methods would be an important improvements
- International collaboration are important to be able to evaluate and improve those approaches.

After HPC, High Performance Artificial Intelligence, High-Performance Data Analytics,.....

Next step, more general:
High Performance Intelligent Computing