

Logo - Rallye



Texto

Séminaire Aristote
Bibliothèques
pour le calcul scientifique:
outils, enjeux et
écosystème

Gentes Dames, Gentils Seigneurs

Ce jour, une Histoire va vous être contée

C'est celle de la Compagnie du Logiciel

Gentes Dames, Gentils Seigneurs

Ce jour, une Histoire va vous être contée.

Dont les compères LEGOLAS, MAGMA et PLASMA

Ont trouvé la clé du CADNA du club OPENPALM

Dans lequel ils rencontraient le Professeur EIGEN

Consultant les News dans OPENPALM

Sous l'oeil Multiple de 2 Agences Gouvernementales

Consultant les News dans OPENPALM

Qui ostensiblement Evitaient les Communications

Tout ce beau monde se retrouvait autour d'un SOUS-TITRE

Auparavant, faisons un raccourci Philosophie-Simulation

Aristote par la voix de Philippe et Maison par celle de Michel

BIBLIOTHÈQUES POUR LE CALCUL SCIENTIFIQUE : RETOURS D'EXPÉRIENCE

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DE LA RECHERCHE À L'INDUSTRIE



ONERA

THE FRENCH AEROSPACE LAB

05/09/2013



Vos orateurs



pointe le sol
par le plat de sa main droite,
ce qui symbolise
sa croyance dans la connaissance
par le biais de l'observation empirique
et de l'expérience

pointe le doigt
vers le ciel
symbolisant sa croyance
dans les idées



info@association-aristote.fr

Qui ? Créée “informellement” en 1984 par l’INRIA, le CEA, EDF et le CNES, Aristote est depuis 1988 une association loi 1901 (34 adhérents en 2013).

Quoi ? Aristote est une société savante qui regroupe des organismes et des entreprises impliquées dans les derniers développements et les nouveaux usages des technologies de l’information.

Pourquoi ? Aristote contribue à tisser des liens entre le monde académique et celui de l’industrie et des services à travers ses activités de transfert de technologie et de veille scientifique. L’idée est de croiser regards et cultures, recherche fondamentale et retours d’expérience pour apporter des éclairages nouveaux aux problématiques abordées

Aristote organise chaque année, à l’École Polytechnique, un cycle de séminaires :

2013

- **La visualisation collaborative : un des grands défis de la science actuelle! (novembre)**
- Santé et Bien-être à l’ère numérique (juin)
- **Bibliothèques pour le calcul scientifique : outils, enjeux et écosystème (mai)**
- A la poursuite des Big Data (mars)
- Sécurité et Mobilité (février)

2012

- **CFD Workflow : Meshing, Solving, Visualizing (octobre)**
- Le bâtiment intelligent ; source de valeurs (septembre)
- Green IT & Cloud (juin)
- **Logiciel Libre et communautés : la clef du transfert ? (mai)**
- SaaS+IaaS et Tiers de confiance : Vers le Cloud de confiance (avril)



COURTESY OF :

Patrick AMESTOY - *INPT*
Marc BAADEN - *CNRS*
Marc BABOULIN - *Université Paris-Sud*
Romain BROSSIER - *Université Joseph Fourier*
Michel CAFFAREL - *CNRS - Université de Toulouse*
Christophe CALVIN - *CEA*
François COURTEILLE - *NVIDIA*
Serge van CRIKINGEN - *Maison de la Simulation*
Florian DE VUYST - *ENS-Cachan*
Florent DUCHAINE - *Cerfacs*
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Michel GAZAIX - *ONERA*
Thomas GERHOLD - *DLR*
Marc GIGET - *Institut Européen de Stratégies Créatives et d'Innovation*
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Martial MANCIP - *Maison de la Simulation*
Frédéric MILLIOT - *HPC Magazine*
Patrick MOREAU - *INRIA*
François PELLEGRINI - *Université de Bordeaux 1*
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Philippe THIERRY - *INTEL*
Julien TIERNY - *CNRS*

Les vrais amis
viennent dans les
bons moments
quand on les appelle
et dans les mauvais
moments, ils viennent
d'eux-mêmes.



Pour Quoi & Pour Qui?



Par Qui?



Travail Collaboratif

Par Vous

Travailleur Isolé



C'est Quoi Ça?

上禾一乘九斗四分斗之一
 中禾一乘四斗四分斗之一
 下禾一乘二斗四分斗之三
 方程 程課程也羣物總雜各列有數總言
 其實令每行為率二物者再程三物
 者三程皆如物數程之並列為行故謂之
 方程行之左右無所同存且為有所據而
 言耳此都術也以空言難曉故特繫
 之禾以決之又列中行如右行也
 術曰置上禾三乘中禾二乘下禾一乘實
 三十九斗於右方中左禾列如右方以右
 行上禾徧乘中行而以直除為術之意令
少行減多行
 反覆相減則頭位必先盡上無一位則此
 行亦闕一物矣然而率以相減不害餘
 數之課也若消去頭位則下去一物之實
 如是登令左右行相減審其正負則可得
 而知先令右行上禾乘中行為齊同之意
 為齊同者謂中行上禾亦乘右行也從簡
 易雖不言齊同以齊同
 之意觀之其義然矣 又乘其次亦以直
 除復去左 然以中行中禾不盡者徧乘而
左行而
 以直除亦令兩行相乘 左方下禾不盡者
 上為法下為實實即下禾之實上中禾皆
去故餘數
 是下禾實非但一乘欲約衆乘之實當以
 禾乘數為法列此下禾之乘實乘兩行以
 直除則下禾之位自決矣各以其餘一位
 之乘除其下實即斗數矣用算策而不省

算經

卷一

方程

二

二

微波附

C'est un Algo

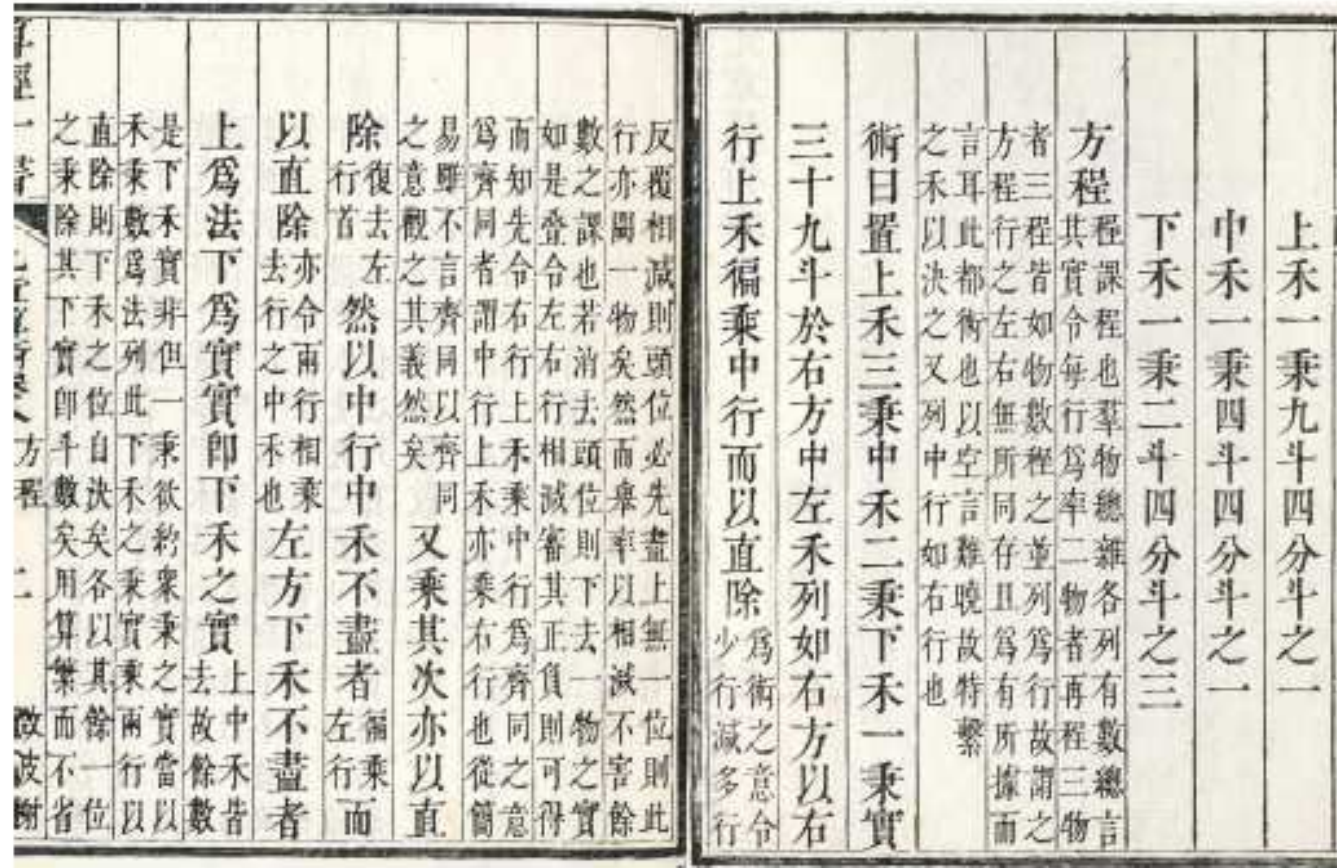
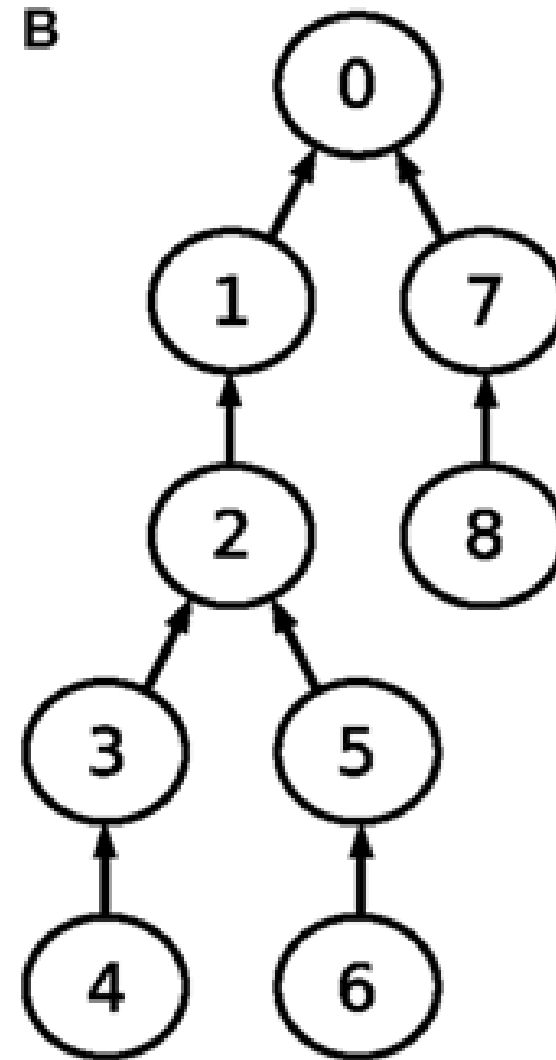
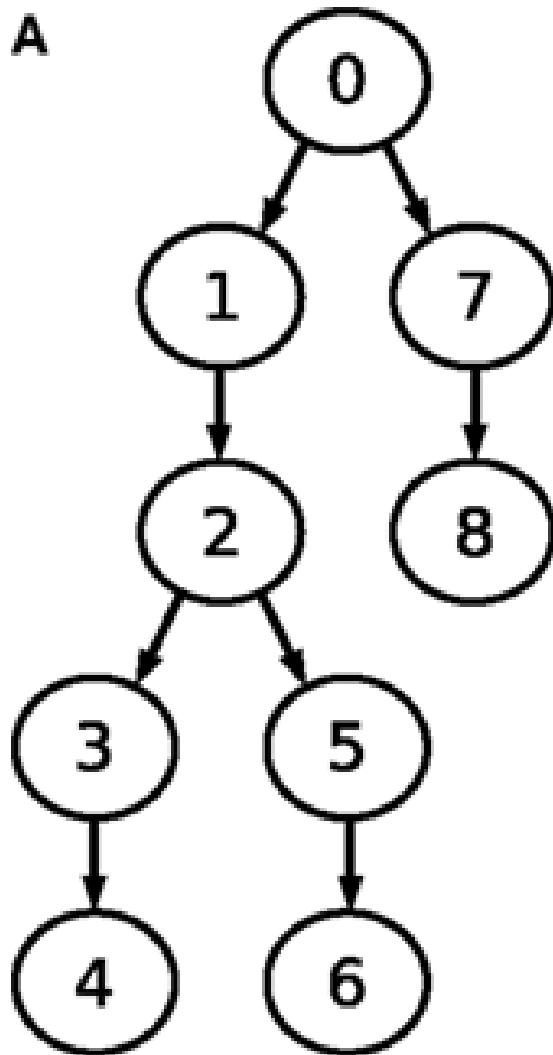


Figure 3: Algorithm descriptions, Chapter 8 of Jiu Zhang Suan Shu

La Même Chose Que Ça



Avec Quel Outil?

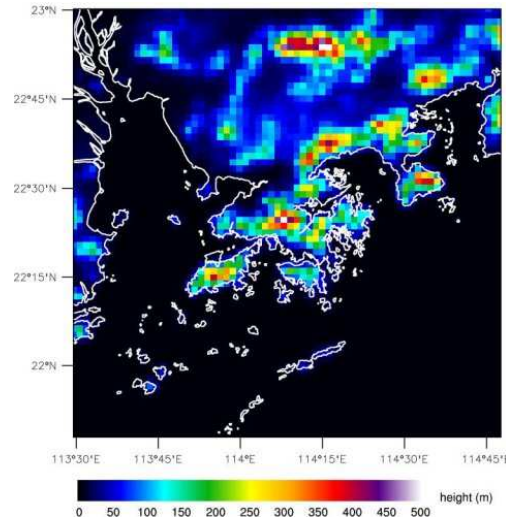
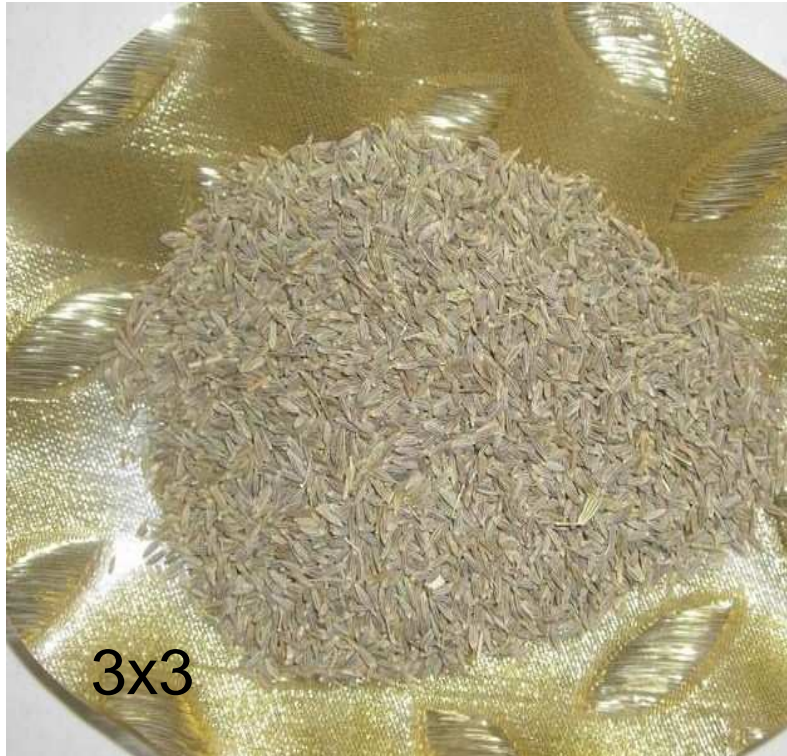


算盘, 算盤



Milky Way-2

Pour Quelles Applications?



NWP



Une Programmation

```
def rref(m, eps = 1.0/(10**10)):
    """Puts given matrix (2D array) into the Reduced Row Echelon Form. Returns True if successful, False if 'm' is
    singular.
    NOTE: make sure all the matrix items support fractions! Int matrix will NOT work!
    Written by Jarno Elonen in April 2005, released into Public Domain"""
    (h, w) = (len(m), len(m[0]))
    for y in range(0, h):
        maxrow = y
        for y2 in range(y+1, h): # Find max pivot
            if abs(m[y2][y]) > abs(m[maxrow][y]):
                maxrow = y2
        (m[y], m[maxrow]) = (m[maxrow], m[y])
        if abs(m[y][y]) <= eps: # Singular?
            return False
        for y2 in range(y+1, h): # Eliminate column y
            c = m[y2][y] / m[y][y]
            for x in range(y, w):
                m[y2][x] -= m[y][x] * c
        for y in range(h-1, 0, -1): # Backsubstitute
            c = m[y][y]
            for y2 in range(0, y):
                for x in range(w-1, y-1, -1):
                    m[y2][x] -= m[y][x] * m[y2][y] / c
            m[y][y] /= c
        for x in range(h, w): # Normalize row y
            m[y][x] /= c
    return True
```

Une Autre Programmation

Example: The system of equations
$$\begin{cases} x - y + z = 3 \\ 2x + 3y + 7z = 0 \\ x + 3y - 2z = 17 \end{cases}$$
 has augmented matrix

$$\left[\begin{array}{ccc|c} 1 & -1 & 1 & 3 \\ 2 & 3 & 7 & 0 \\ 1 & 3 & -2 & 17 \end{array} \right]$$

Row operations can be used to express the matrix in row-echelon form.

$$\left[\begin{array}{ccc|c} 1 & -1 & 1 & 3 \\ 2 & 3 & 7 & 0 \\ 1 & 3 & -2 & 17 \end{array} \right] \rightarrow \left[\begin{array}{ccc|c} 1 & -1 & 1 & 3 \\ 0 & 1 & 5 & -6 \\ 0 & 2 & -3 & 14 \end{array} \right]$$

$$\rightarrow \left[\begin{array}{ccc|c} 1 & -1 & 1 & 3 \\ 0 & 1 & 5 & -6 \\ 0 & 0 & -13 & 26 \end{array} \right]$$

$$\rightarrow \left[\begin{array}{ccc|c} 1 & -1 & 1 & 3 \\ 0 & 1 & 5 & -6 \\ 0 & 0 & 1 & -2 \end{array} \right]$$

The system has become:
$$\begin{cases} x + y + z = 3 \\ y + 5z = -6 \\ z = -2 \end{cases}$$
 By back-substitution we

find that $x = 1$, $y = 4$, and $z = -2$.

Élimination de Gauß

def gauss_jordan(m, eps = 1.0/(10**10)):



$$a_{ij}^{(p+1)} = a_{ij}^{(p)} - \frac{a_{ip}^{(p)}}{a_{pp}^{(p)}} a_{pj}^{(p)} \text{ si } p+1 \leq i \leq m \text{ et } p+1 \leq j \leq m+1$$

$$a_{ij}^{(p+1)} = a_{ij}^{(p)} \text{ si } 1 \leq i \leq p, 1 \leq j \leq m+1$$

$$a_{ij}^{(p+1)} = 0 \text{ si } p+1 \leq i \leq m \text{ et } 1 \leq j \leq m$$

Nombre fini d'opérations

$O(m^3)$

Sensibilité aux erreurs

d'arrondi

$m \sim 10^6$

La Techno : Up-to-Date

Accélérateurs



NVIDIA « Kepler »

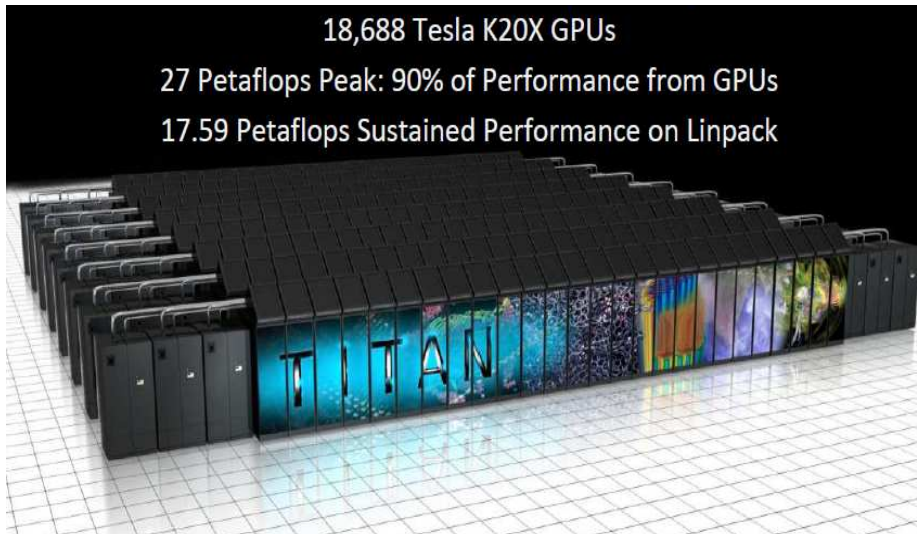
- **Caractéristiques générales**
28nm – architecture Kepler
Mémoire GDDR5
PCIe G2 16x
- **NVIDIA Kepler K10 – simple précision**
2x 1536 coeurs @ 0.745 GHz
2x 8 canaux @ 5.0 GT/s
2x 2.29 TFlop/s SP
- **NVIDIA Kepler K20 – double précision**
2496 coeurs @ 0.705 GHz
12 canaux @ 5.2 GT/s
1.17 TFlop/s DP – 3.5 TFlop/s SP

Intel Xeon Phi

- **Caractéristiques générales**
22nm – architecture MIC x86_64
PCIe G2 16x
16 c. RAM GDDR5 – 320-352 Go/s
1.02-1.22 TF/s DP; 2.02-2.44 TF/s SP
- **Intel Xeon Phi 5110P**
60 coeurs @ 1.053 GHz - 225W
RAM 5.0 GT/s
- **Intel Xeon Phi 7120P**
61 coeurs @ 1.1 GHz - 300 W
RAM 5.5 GT/s

19 Confidentiel

Research Computing Group



05/09/2013

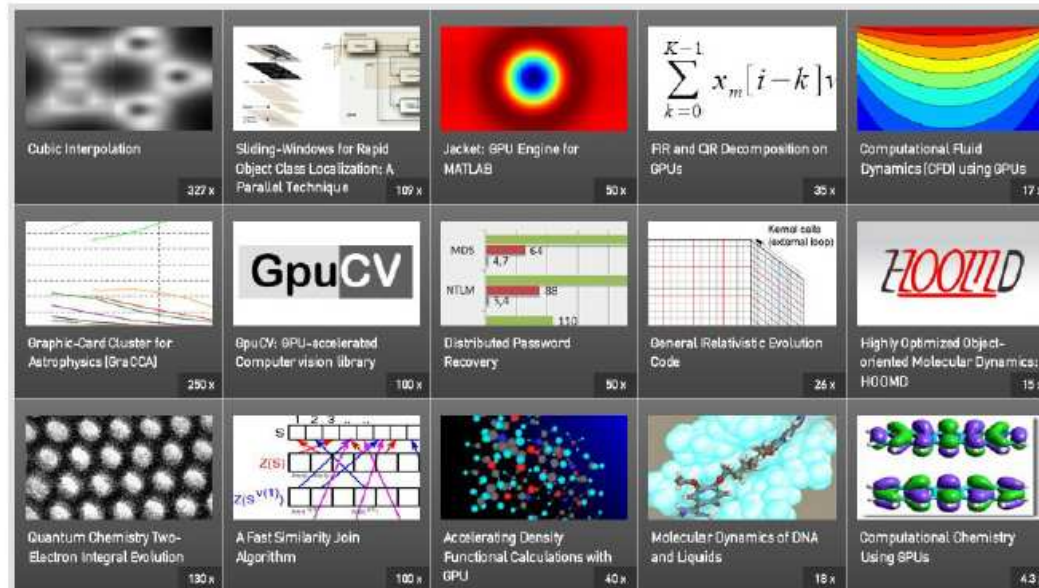


Applications

MAGMA



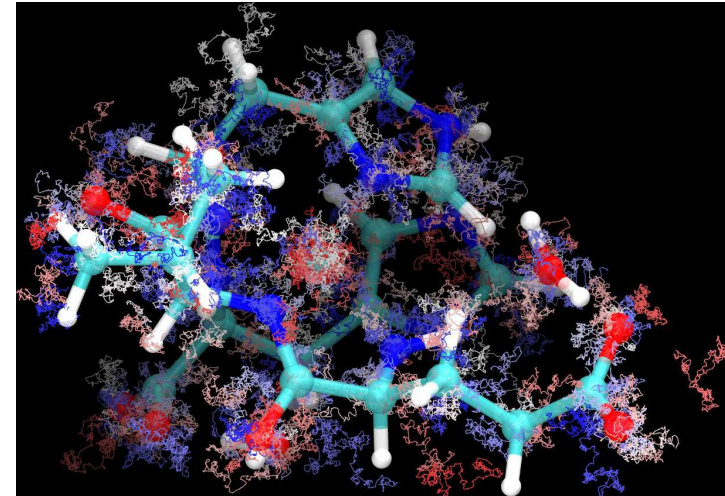
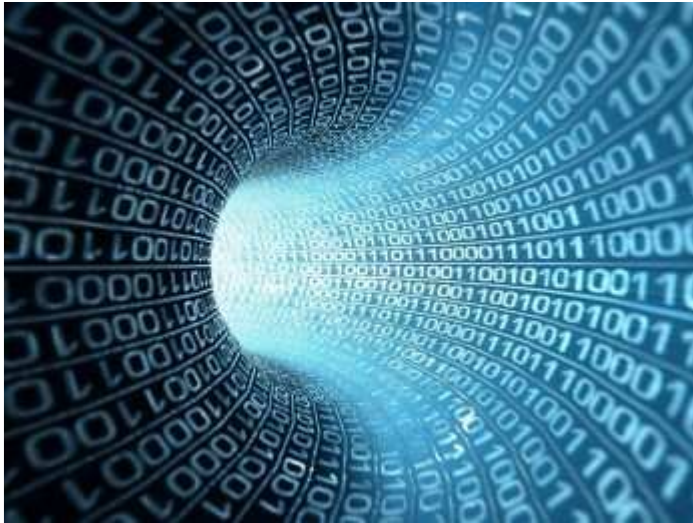
Why GPU-based computing



- Most HPC applications report high speedups with GPUs.
- **Top 500, November 2012:**
62 systems with accelerators (vs 58 in June 2012 and 39 in Dec. 2011).
#1 and #8 systems use NVIDIA GPUs.



Big Data/Scalability : Scaling Up



As the term **big data** appears more and more frequently in our daily life and research activities, it changes our knowledge of how large the scale of the data can be and challenges the application of numerical analysis for performing calculations on computers.

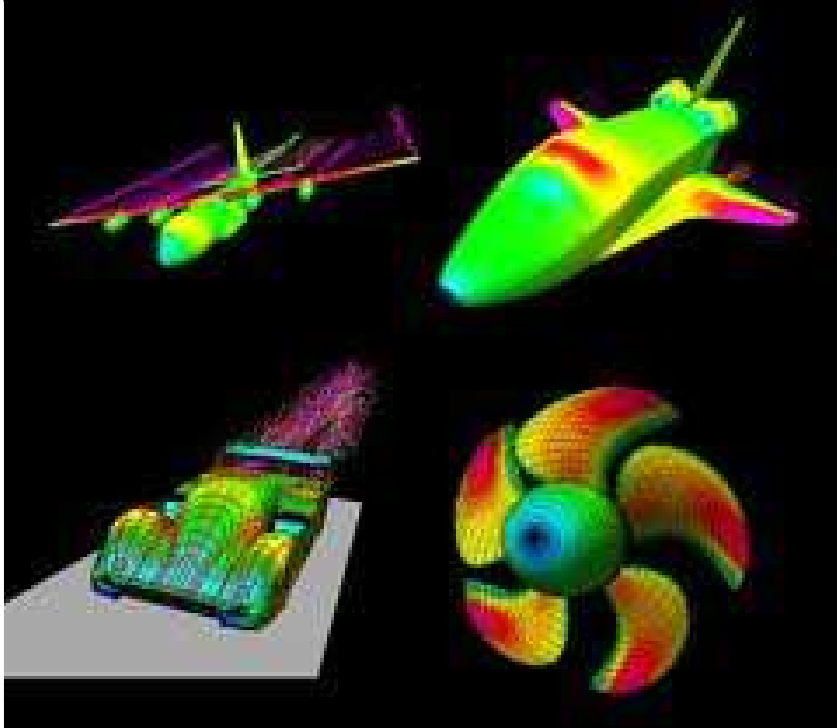
Scalability issue is what that many numerical methods are facing.

The **large-scale challenge** motivates us to develop linearly scalable numerical linear algebra techniques in the dense matrix setting, which is a common scenario in data analysis.

Reduce the quadratic cost in storage and cubic cost in computation for a general dense matrix.

Big data provides a **fresh opportunity** for numerical analysts to develop algorithms with a central goal of scalability in mind. Scalable algorithms are key **for convincing practitioners** to apply the powerful statistical theories on large-scale data that they currently feel uncomfortable to handle.

Dense Linear Systems



$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1N} & \sum_{j=1}^N B_{1j} \\ A_{21} & A_{22} & \dots & A_{2N} & \sum_{j=1}^N B_{2j} \\ & & \dots & & \\ A_{N1} & A_{N2} & \dots & A_{NN} & \sum_{j=1}^N B_{Nj} \\ K_1 & K_2 & \dots & K_N & \sum_{j=1}^N L_j \end{pmatrix} \cdot \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \dots \\ \sigma_N \\ y \end{pmatrix} = \begin{pmatrix} C_1 \\ C_2 \\ \dots \\ C_N \\ C_{N+1} \end{pmatrix} \cdot (-V_\infty)$$

+0.00	+0.14	+0.03	+0.03	+0.14	-0.08	+0.08	+0.02	+0.00	+0.00	+0.03	-0.08
-0.21	+0.00	+0.09	+0.09	+0.00	-0.20	-0.06	+0.06	+0.01	+0.01	-0.02	-0.04
-0.12	-0.28	+0.00	+0.16	-0.19	-0.12	-0.03	-0.07	+0.02	+0.00	-0.03	-0.03
+0.10	+0.16	-0.16	+0.00	+0.28	+0.11	+0.03	+0.03	-0.02	+0.02	+0.04	+0.02
+0.19	-0.00	-0.08	-0.09	+0.00	+0.21	+0.06	-0.02	-0.01	-0.01	+0.06	+0.04
+0.08	-0.13	-0.03	-0.03	-0.14	+0.00	-0.03	-0.02	-0.00	-0.00	-0.03	+0.08
+1.00	+0.00	+0.00	+0.00	+0.00	+1.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.51
+1.00	-1.00	+0.00	+0.00	+0.00	+0.00	+0.50	+0.00	+0.00	+0.00	+0.00	+0.00
+0.00	+1.00	-1.00	+0.00	+0.00	+0.00	+0.00	+0.36	+0.00	+0.00	+0.00	+0.00
+0.00	+0.00	+1.00	-1.00	+0.00	+0.00	+0.00	+0.00	+0.14	+0.00	+0.00	+0.00
+0.00	+0.00	+0.00	+1.00	-1.00	+0.00	+0.00	+0.00	+0.00	+0.15	+0.00	+0.00
+0.00	+0.00	+0.00	+0.00	+1.00	-1.00	+0.00	+0.00	+0.00	+0.00	+0.37	+0.00

Méthode des singularités

Dense Matrices

MAGMA



NUMERICAL LINEAR ALGEBRA ON EMERGING ARCHITECTURES: THE PLASMA AND MAGMA PROJECTS

Emmanuel Galassi, Jim Demmel, Javi Rodriguez, Bill Rountree, Ashish Chavhan, Albert Cohen, Helen-Joelle Flath, Luca Grigori, Paolo Bini, Timothy Scaife, Boris Fomin

The ever-growth and continuing use of multi-core architectures and graphics processing units makes it clear in the coming software era that performance will be a result of the utilization of algorithms in order to take advantage of some prevailing paradigms. Parallel Linear Algebra Software for Multi-core Architectures (PLASMA) and Matrix Algebra on GPU and Multi-core Architectures (MAGMA) are two projects that aim to achieve high performance and portability across a wide range of multi-core architectures and hybrid systems respectively.

INNOVATIVE COMPUTING LABORATORY UNIVERSITY OF TENNESSEE

<http://icl.ese.utsa.edu/>



PARALLEL LINEAR ALGEBRA SOFTWARE FOR MULTICORE ARCHITECTURES

PLASMA

<http://www.utsa.edu/~icl/plasma/>

THE PARALLEL LINEAR ALGEBRA SOFTWARE FOR MULTICORE ARCHITECTURES (PLASMA) PROJECT aims to address the critical and highly iterative situation that is facing the Linear Algebra and High Performance Computing community due to the introduction of multi-core architectures. PLASMA's ultimate goal is to create software frameworks that enable programmers to simplify the process of developing applications that can achieve both high performance and portability across a range of new architectures. PLASMA uses a programming model that allows synchronous, out-of-order scheduling of operations in order to achieve a scalable yet highly efficient software framework for Computational Linear Algebra applications.

TILE ALGORITHMS

Utilize LAPACK, which uses tiled algorithms, PLASMA releases tiled algorithms to utilize use of hierarchical parallelism.



PLASMA 2.1.0

- Enhanced Linear Algebraic
- Sparse Linear Algebra Problems
- Multiple Precision Support
- Block-Partitioned Sparse Solvers
- Sparse Scheduling
- LAPACK Interface / Backend Interface
- LAPACK Compliant Error Handling
- LAPACK-Compliant Testing Suite
- Thread Safety
- Blockwise Linear, BL, BLAS 3.0
- PLASMA User's Guide

The algorithms of Linear Algebra applications are represented as Directed Acyclic Graphs (DAG) where nodes represent the tasks in which the application can be decomposed and the edges represent the dependencies among them. As long as the task execution order does not violate the dependencies, it is considered to be correct.

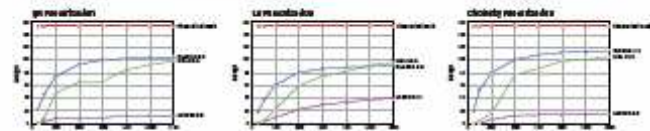


CURRENT RESEARCH

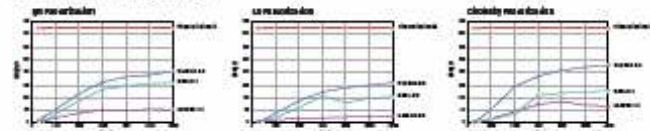
- Singular Value Decomposition
- Symmetric and Non-Symmetric Eigenvalue Problems
- Sparse Scheduling
- Communication Reducing Algorithms
- Scaling
- Hierarchical Sparse Matrices
- Bandwidth Reduction

PERFORMANCE RESULTS (8 CORES)

SPRINT (Intel Xeon X5550 quad-core processors (2x sockets))



SPRINT (Intel Xeon X5550 quad-core processors (2x sockets))



MATRIX ALGEBRA FOR GPU AND MULTICORE ARCHITECTURES

MAGMA

<http://icl.ese.utsa.edu/magma/>

THE MATRIX ALGEBRA FOR GPU AND MULTICORE ARCHITECTURES (MAGMA) PROJECT aims to create a new generation of linear algebra libraries that achieve the fastest possible time to an accurate solution on hybrid/heterogeneous architectures, starting with current multi-core/multi-GPU systems. To address the complex challenges stemming from the heterogeneity of these systems, their massive parallelism, and the gap in computational vs. CPU-GPU communication speeds, MAGMA research is based on the idea that optimal software solutions will therefore have to hybridize, combining the strengths of different algorithms within a single framework.

HYBRID ALGORITHMS

MAGMA relies on hybrid algorithms that combine algorithms optimized for the architectural strengths of the system's hybrid components.



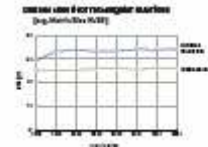
Small non-synchronous tasks, often on hierarchical paths, are scheduled on the CPU and larger synchronous tasks are offloaded to the GPU.

MAGMA 0.2

- Enhanced Linear Algebraic
- Sparse Linear Algebra Problems
- Multiple Precision Support
- Block-Partitioned Sparse Solvers
- Sparse Scheduling
- CPU / GPU Interfaces
- LAPACK Compliant Interface
- Testing Suite of Examples
- Communication Optimizations: LCGP-optimized GPU Linear

MAGMA BLAS

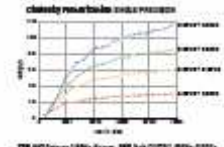
It implements the BLAS standard (S, D, E, C) and can be used for larger dimensioned matrices.



- Scalar-based kernels
- Row-major Symmetric "Eigen" for "fast" mode
- 2000x kernel for symmetric and dense
- 8700x, 8000x, and 8700x
- 170x of high parallelism performance (peak with hierarchical scaling)

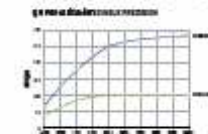
CURRENT RESEARCH

- Symmetric and Non-Symmetric Eigenvalue Problems
- Singular Value Decomposition
- Multiscale / Multiscale Algorithms

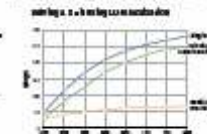


PERFORMANCE RESULTS

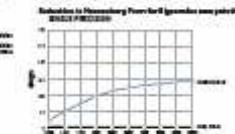
SPRINT (Intel Xeon X5550 quad-core processors (2x sockets))



SPRINT (Intel Xeon X5550 quad-core processors (2x sockets))



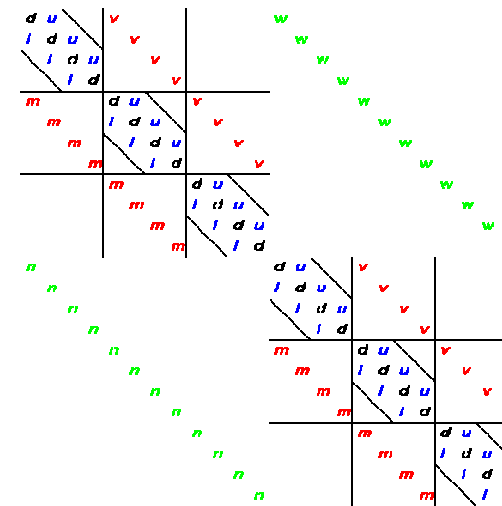
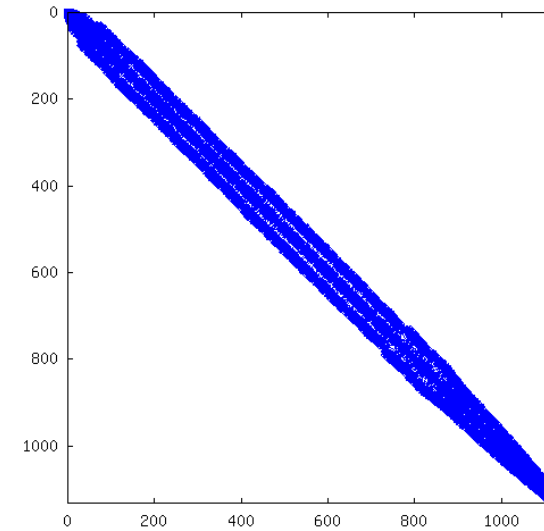
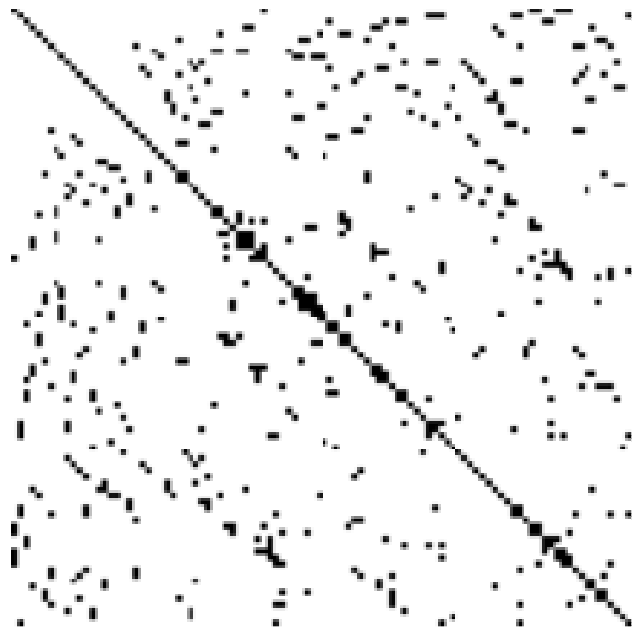
SPRINT (Intel Xeon X5550 quad-core processors (2x sockets))



Sparse - Band Matrices

```

+0.00 +0.14 +0.03 +0.03 +0.14 -0.08 +0.08 +0.02 +0.00 +0.00 +0.03 -0.08
-0.21 +0.00 +0.09 +0.09 +0.00 -0.20 -0.06 +0.06 +0.01 +0.01 -0.02 -0.04
-0.12 -0.28 +0.00 +0.16 -0.19 -0.12 -0.03 -0.07 +0.02 +0.00 -0.03 -0.03
+0.10 +0.16 -0.16 +0.00 +0.28 +0.11 +0.03 +0.03 -0.02 +0.02 +0.04 +0.02
+0.19 -0.00 -0.08 -0.09 +0.00 +0.21 +0.06 -0.02 -0.01 -0.01 +0.06 +0.04
+0.08 -0.13 -0.03 -0.03 -0.14 +0.00 -0.03 -0.02 -0.00 -0.00 -0.03 +0.08
+1.00 +0.00 +0.00 +0.00 +0.00 +1.00 +0.00 +0.00 +0.00 +0.00 +0.00 +0.51
+1.00 -1.00 +0.00 +0.00 +0.00 +0.00 +0.50 +0.00 +0.00 +0.00 +0.00 +0.00
+0.00 +1.00 -1.00 +0.00 +0.00 +0.00 +0.00 +0.36 +0.00 +0.00 +0.00 +0.00
+0.00 +0.00 +1.00 -1.00 +0.00 +0.00 +0.00 +0.00 +0.14 +0.00 +0.00 +0.00
+0.00 +0.00 +0.00 +1.00 -1.00 +0.00 +0.00 +0.00 +0.00 +0.15 +0.00 +0.00
+0.00 +0.00 +0.00 +0.00 +1.00 -1.00 +0.00 +0.00 +0.00 +0.00 +0.37 +0.00
    
```



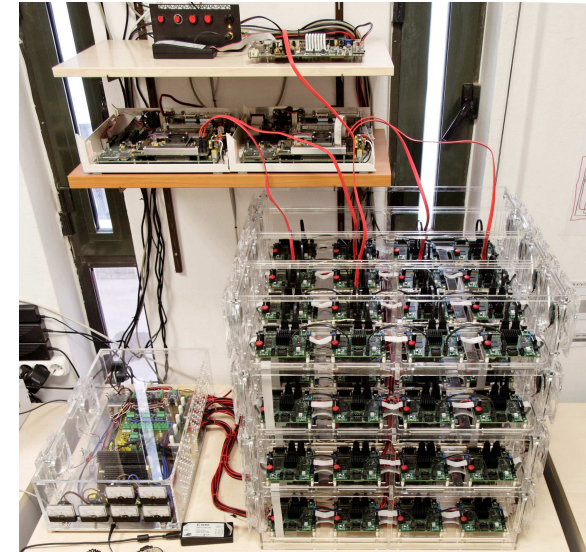
Shared - Distributed



The image at left shows the spatial distribution for multi-core computing of an engineered component that doesn't take advantage of the computer's shared-memory architecture.

The image at right represents the fine-grained spatial distribution using the researchers' new task management algorithm.

Graphic / David Holmes



Modeling emerging multicore architectures is challenging and imposes a tradeoff between **simulation speed and accuracy**.

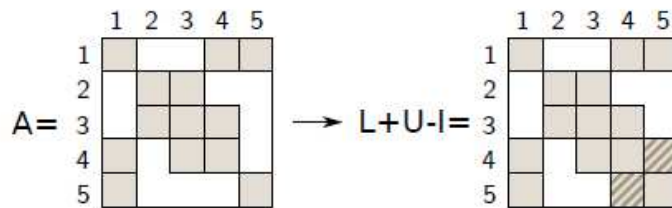
An effective practice that balances both targets well is to map the target architecture on FPGA platforms.

We find that accurate prototyping of hundreds of cores on existing FPGA boards faces at least one of the following problems:

- (i) limited fast memory resources (SRAM) to model caches,
- (ii) insufficient inter-board connectivity for scaling the design or
- (iii) the board is too expensive.

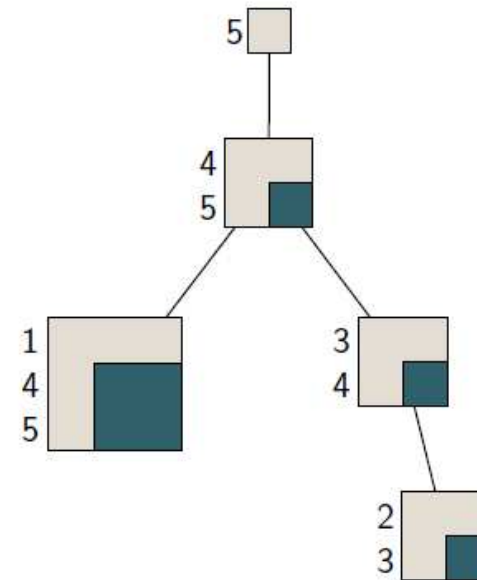
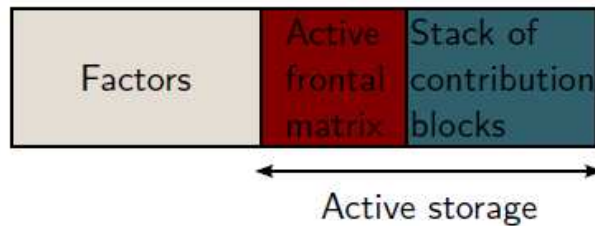
Minimise Memory

The multifrontal method [Duff & Reid '83]



Storage is divided into two parts:

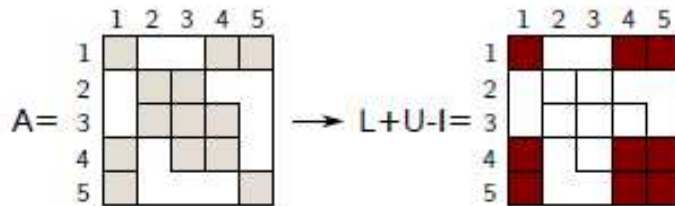
- Factors
- Active memory



Elimination tree

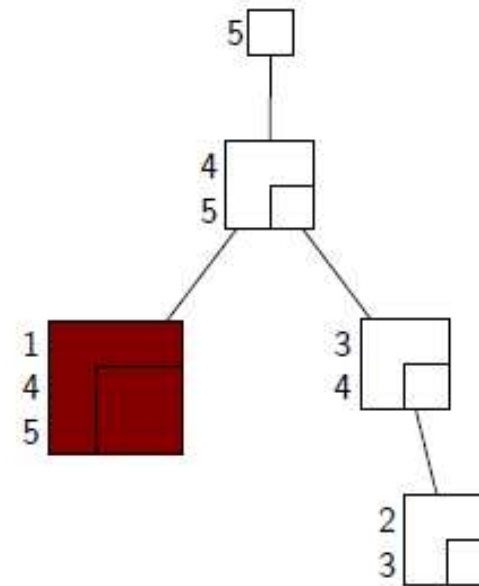
Minimise Memory

The multifrontal method [Duff & Reid '83]



Storage is divided into two parts:

- Factors
- Active memory



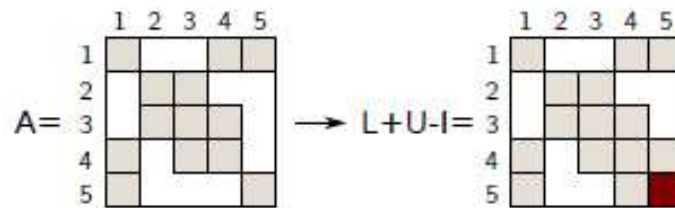
Active memory

3/21

MUMPS Users Group Meeting, May 29-30, 2013

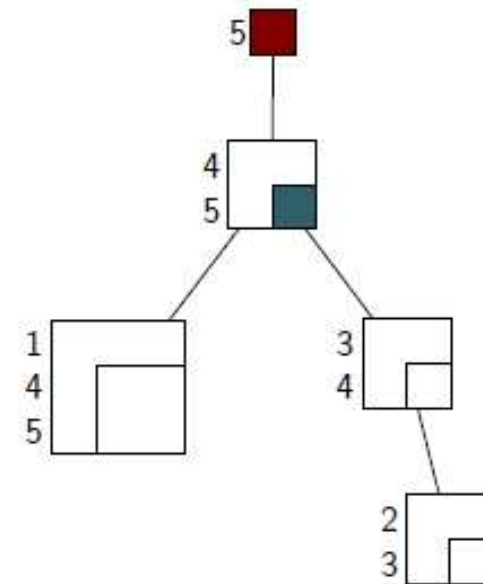
Minimise Memory

The multifrontal method [Duff & Reid '83]



Storage is divided into two parts:

- Factors
- Active memory



Active memory

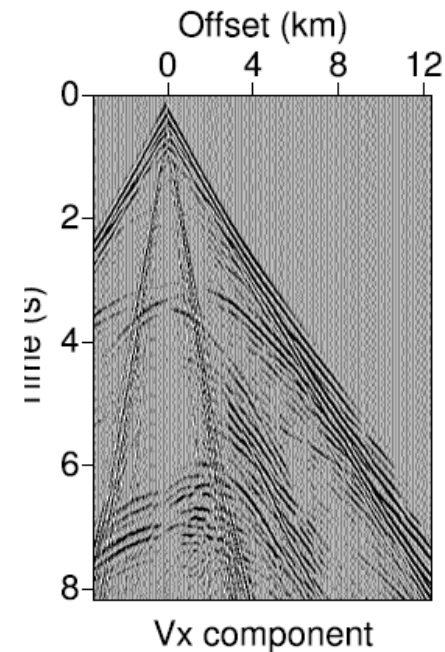
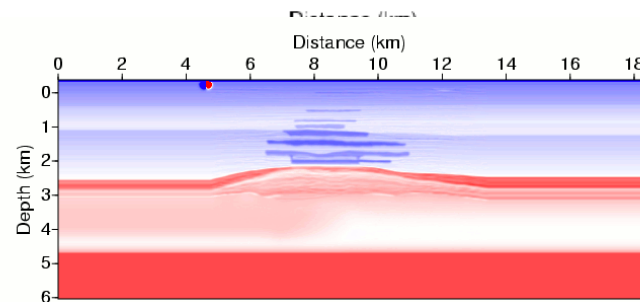
MUMPS - SEISCOPE

Seismic imaging of the Earth

- Imaging/tomography : reconstruction of Earth subsurface properties from indirect measurements of seismic waves

$$\frac{\partial U}{\partial t} + \Lambda \frac{\partial U}{\partial x_i} = F_0$$

(1)



Minimise Communications

Motivation - the communication wall

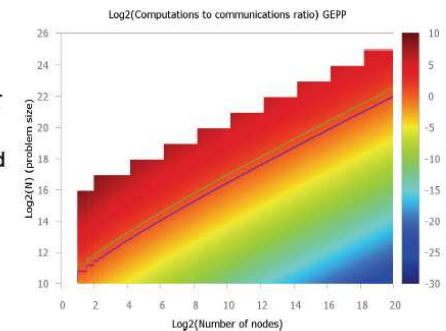
- Runtime of an algorithm is the sum of:
 - #flops x **time_per_flop**
 - #words_moved / **bandwidth**
 - #messages x **latency**
- Time to move data >> time per flop
 - Gap steadily and exponentially growing over time

Annual improvements			
Time/flop		Bandwidth	Latency
59%	Network	26%	15%
	DRAM	23%	5%

- Performance of an application is less than 5% of the peak performance

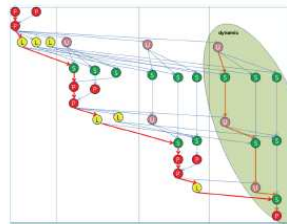
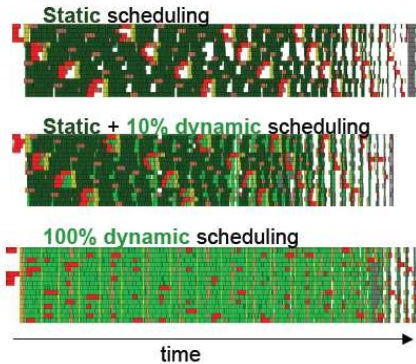
Previous work on reducing communication

- **Tuning**
 - Overlap communication and computation, at most a factor of 2 speedup
- **Ghosting**
 - Store redundantly data from neighboring processors for future computations
- **Scheduling**
 - Cache oblivious algorithms for linear algebra
 - Gustavson 97, Toledo 97, Frens and Wise 03, Ahmed and Pingali 00
 - Block algorithms for linear algebra
 - ScaLAPACK, Blackford et al 97

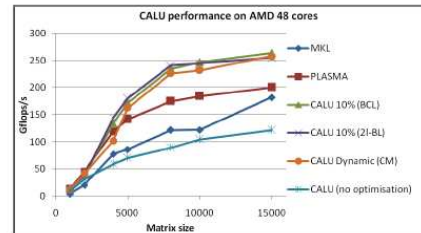


In Progress

Lightweight scheduling for CALU



Task dependency graph of CALU



Conclusions

Introduced a new class of communication avoiding algorithms that minimize communication

- Attain theoretical lower bounds on communication
- Minimize communication at the cost of redundant computation
- Are often faster than conventional algorithms in practice
- Many previous references, only a few given in the talk

Remains a lot to do for sparse linear algebra

- Communication bounds, communication optimal algorithms
- Numerical stability of s-step methods
- Preconditioners - limited by the memory size, not flops

And BEYOND

Further information:

<http://www-rocq.inria.fr/who/Laura.Grigori/>

Highlights

PASTIX

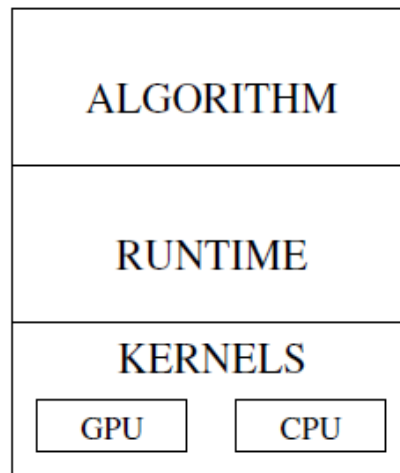
The direct solver PaStiX has been successfully used by CEA/CESTA to solve a huge symmetric complex sparse linear system arising from a 3D electromagnetism code on the TERA-10 CEA supercomputer.

- ▶ **45 millions unknowns:** required 1.4 Petaflops and was completed in half an hour on 2048 processors.
- ▶ **83 millions unknowns:** required 5 Petaflops and was completed in 5 hours on 768 processors.

To our knowledge a system of this size and this kind has never been solved by a direct solver. **Hope new runs on TERA-100 CEA supercomputer !**

GPU Runtime : DAGuE

Multiple layer approach



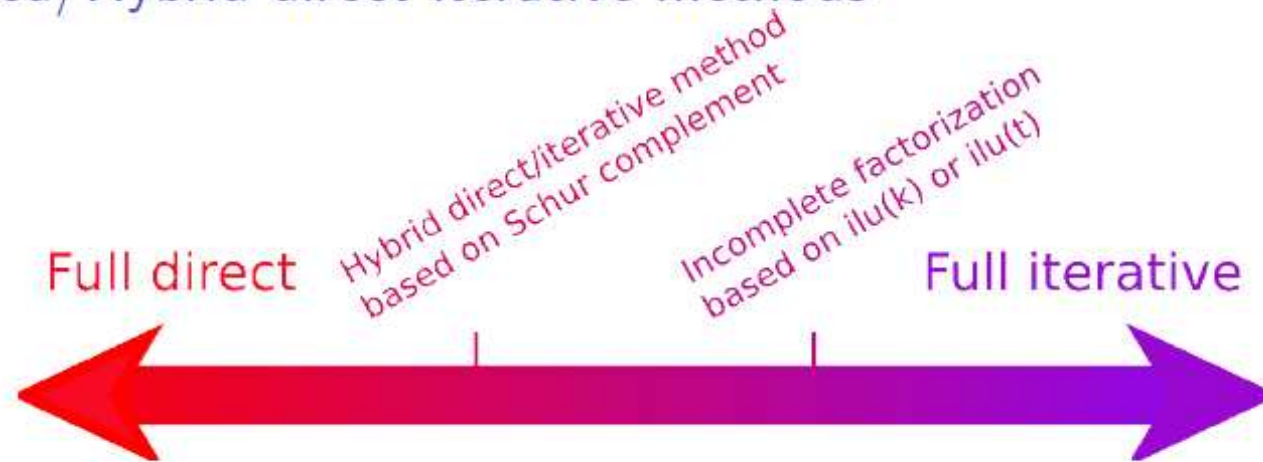
Governing ideas: Enable advanced numerical algorithms to be executed on a scalable unified runtime system for exploiting the full potential of future exascale machines.

Basics:

- ▶ Graph of tasks
- ▶ Out-of-order scheduling
- ▶ Fine granularity

Large Spectre

Mixed/Hybrid direct-iterative methods



The "spectrum" of linear algebra solvers

- ▶ Robust/accurate for general problems
- ▶ BLAS-3 based implementation
- ▶ Memory/CPU prohibitive for large 3D problems
- ▶ Limited parallel scalability
- ▶ Problem dependent efficiency/controlled accuracy
- ▶ Only mat-vec required, fine grain computation
- ▶ Less memory consumption, possible trade-off with CPU
- ▶ Attractive "build-in" parallel features

Features



- ▶ LLt, LDLt, LU : supernodal implementation (BLAS3)
- ▶ ILUCT, ICT : scalar column left-looking factorization
- ▶ Full iterative or hybrid direct/iterative methods
- ▶ Krylov method : CG/GMRES
- ▶ Can be used as a preconditioner inside another method
- ▶ Simple/Double precision and Float/Complex operations
- ▶ Can use a domain decomposition given by the user

Hybrid direct-iterative solver

Based on a domain decomposition : interface one node-wide (no overlap in DD lingo)

$$\begin{pmatrix} A_B & F \\ E & A_C \end{pmatrix}$$



- B : Interior nodes of subdomains (direct factorization).
- C : Interface nodes.

Special decomposition and ordering of the subset C :

Goal : Building a **global** Schur complement preconditioner (ILU) from the **local** domain matrices only.

Schur / Schwarz

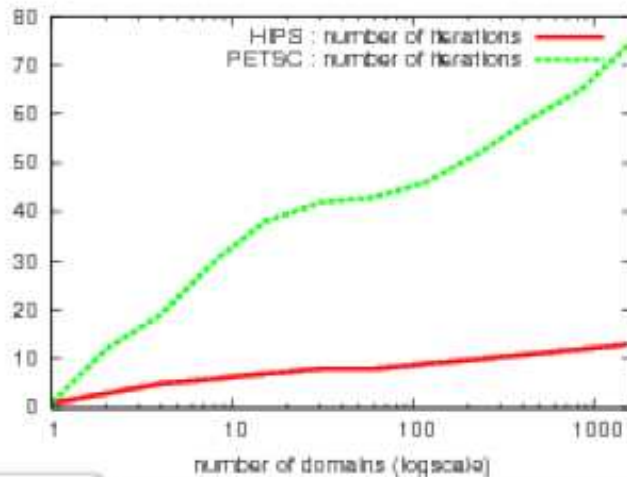


Experimental conditions

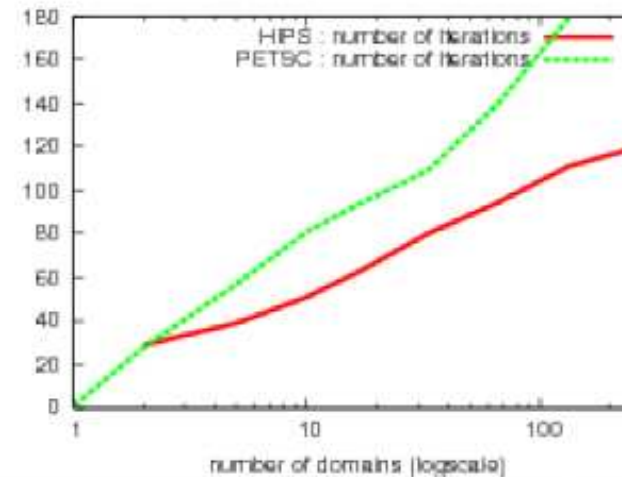
These curves compare HIPS (Hybrid) with Additive Schwarz from PETSc.

Parameters were tuned to compare the result with a very similar fill-in

Haltere



MHD



P. Ramet - ETSN13

July 2, 2013 - 90

Create & Set Matrix

PETSc

```
KSPCreate(MPI_Comm comm, KSP *ksp);
```

```
KSPSetOperators(KSP ksp, Mat A, Mat preconditioner,  
               MatStructure flag);
```

A = system matrix

preconditioner = base matrix to derive the preconditioner
(typically A itself)

flag = SAME_PRECONDITIONER, SAME_NONZERO_PATTERN,
DIFFERENT_NONZERO_PATTERN
(ignored if only one solve)

Note : A can be a shell matrix \Rightarrow matrix-free methods.



Set Solution Method

PETSc

```
KSPSetType(KSP ksp, KSPTType kspType);  
KSPSetTolerances(KSP ksp,  
                 real rtol, real atol, real dtol, int maxits);
```

kspType = KSPCG, KSPGMRES, KSPBCGS, KSPMINRES, ...
rtol, atol, dtol = relative, absolute, divergence tolerance

or for run-time specification :

```
KSPSetFromOptions(KSP ksp);
```

and program launched using :

```
mpirun ... -ksp_type <method> -ksp_rtol <rtol>
```


Solve & After

PETSc

```
KSPSetUp(KSP ksp);
```

To solve $A x = b$:

```
KSPSolve(KSP ksp, Vec b, Vec x);
```

- x overwritten with answer.
- initial guess $x=0$ unless `KSPSetInitialGuessNonzero` before solve.

After solve :

```
KSPGetConvergedReason (e.g., rtol achieved)  
KSPGetIterationNumber  
KSPGetResidualNorm  
KSPDestroy
```



Encore Lui

Gauss Invents an Iterative Method in a Letter

Gauss (1823), in a letter to Gerling: in order to compute a least squares solution based on angle measurements between the locations Berger Warte, Johannisberg, Taufstein and Milseburg:

Die Bedingungsgleichungen sind also:

$$\begin{aligned}0 &= + 6 + 67a - 13b - 28c - 26d \\0 &= - 7558 - 13a + 69b - 50c - 6d \\0 &= - 14604 - 28a - 50b + 156c - 78d \\0 &= + 22156 - 26a - 6b - 78c + 110d; \\&\text{Summe} = 0.\end{aligned}$$

Um nun indirect zu eliminiren, bemerke ich, dass, wenn 3 der Grössen a, b, c, d gleich 0 gesetzt werden, die vierte den grössten Werth bekommt, wenn d dafür gewählt wird. Natürlich muss jede Grösse aus ihrer eigenen Gleichung, also d aus der vierten, bestimmt werden. Ich setze also $d = -201$ und substituire diesen Werth. Die absoluten Theile werden dann: $+5232, -6352, +1074, +46$; das Übrige bleibt dasselbe.



Invention of Iterative Methods

Martin J. Gander

Gauss

Least Squares
Iteration

Jacobi

Least Squares
Preconditioning

Seidel

Gauss Method
Parallelization

Richardson

PDEs
Time Stepping
Extrapolation
Laplace Equation
CPU Times
Iteration
Chebyshev ?

Krylov Methods

Conjugate Gradients
Relaxation
Steepest Descent
Remedies
Krylov

Conclusion

Bibliothèque Générique : Legolas++

Sans bibliothèques : logiciels spécifiques

Sans outils disponibles, l'approche classique est de développer des **solveurs spécifiques** avec des langages procéduraux (F77/C).

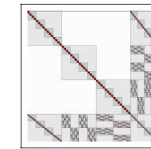
Deux inconvénients :

- ▶ Pas de mutualisation.
- ▶ Pas de séparation des champs sémantiques
solveNeutronicScatteringProblemWithGaussSeidelMethod().
- ▶ Pas d'équipe pluri-disciplinaire
→ développeurs pluri-disciplinaires.

Machines parallèles multi-niveaux...

Pour des objets exotiques

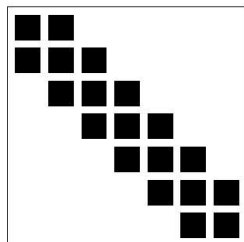
Pourquoi n'y a-t-il pas d'outils ?



- ▶ Le problème est-il d'intérêt général ?
 - ▶ Est-il possible de concevoir ces outils avec les langages du HPC (C/F77) ?
 - ▶ Bibliothèque classique ? Framework ? mini-langage ?
- Contraintes : **intensité arithmétique** et **granularité** des opérations envisagées → **polymorphisme statique** en C++.

Opérateurs polymorphiques : $Y=A*X$

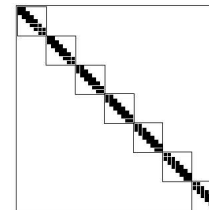
7/66



Produit Matrix-Vecteur **Banded** :

```
Mat A; Vec X,Y;  
  
int linf=A.linf();  
int lsup=A.lsup();  
for (int i=0; i< A.nrows(); i++){  
    Vec::Elt s=0.0;  
    int jmin=max(i-linf,0);  
    int jmax=min(i+lsup+1,size);  
    for (int j=jmin; j< jmax; j++){  
        s+=A.bandGetElt(i,j)*X[j];  
    }  
    Y[i]=s;  
}
```

Écrit par un développeur (de Legolas++)



Produit Matrix-Vecteur **Diagonal<Banded>** :

```
for (int i=0; i < A.nrows(); i++){  
    Mat::Elt & Ai = A.diagGetElt(i);  
    Vec::Elt & Xi = X[i];  
    Vec::Elt & Yi = Y[i];  
    // Yi=Ai*Xi  
    int linf=Ai.linf();  
    int lsup=Ai.lsup();  
    for (int j=0; j< Ai.nrows(); j++){  
        s=0.0;  
        int kmin=max(j-linf,0);  
        int kmax=min(j+lsup+1,size);  
        for (int k=kmin; k< kmax; k++){  
            s+=Ai.bandGetElt(j,k)*Xi[k];  
        }  
        Yi[j]=s;  
    }  
}
```

PAS écrit par un développeur!

40

ONERA
THE FRENCH AEROSPACE LAB

Outils de Bibliothèques



- ▶ Legolas++ s'appuie sur d'autres bibliothèques génériques TBB (multithread), Eigen (SIMD).

Context

- Matrix computation everywhere
 - Various applications:
 - simulators/simulations, video games, audio/image processing, design, robotic, computer vision, augmented reality, etc.
 - Need various tools:
 - numerical data manipulation, space transformations
 - inverse problems, PDE, spectral analysis
 - Need performance:
 - on standard PC, smartphone, embedded systems, etc.
 - real-time performance

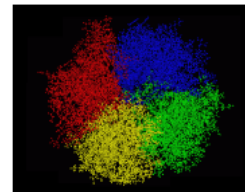
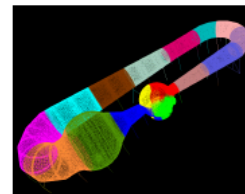
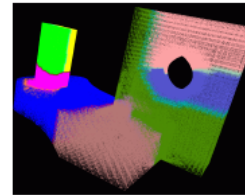
Developer Community

- Jan 2008: start of Eigen2
 - part of KDE
 - packaged by all Linux distributions
 - open repository
 - open discussions on mailing/IRC
 - 300 members, 300 messages/month
 - high quality API
- Today
 - most development @ Inria (Gaël + full-time engineer)
- Future
 - consortium... ??

<http://eigen.tuxfamily.org>

Graph partitioning (2)

- Two main problems for our team, in relation to sparse linear system solving ($Ax = b$) :
 - Sparse matrix ordering for direct methods
 - Domain decomposition for iterative methods
- These problems can be modeled as graph partitioning problems on the adjacency graph of symmetric positive-definite matrices
 - Edge separator problem for domain decomposition
 - Vertex separator problem for sparse matrix ordering by nested dissection



Used by



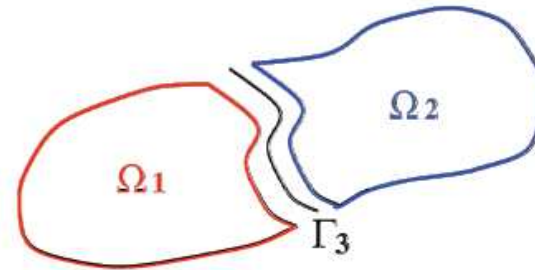
Multi- Domaines : Principes



Conditions de raccord de Fourier : méthode FETI-2LM

- Système linéaire global

$$\begin{pmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$



- Systèmes linéaires locaux

$$\begin{pmatrix} K_{11} & K_{13} \\ K_{31} & K_{33} + k_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_3^{(1)} + \lambda_1 \end{pmatrix}$$

$$\begin{pmatrix} K_{22} & K_{23} \\ K_{32} & K_{33} + k_2 \end{pmatrix} \begin{pmatrix} x_2 \\ x_3^{(2)} \end{pmatrix} = \begin{pmatrix} b_2 \\ b_3^{(2)} + \lambda_2 \end{pmatrix}$$

- Equations de raccord aux interfaces

$$\begin{cases} x_3^{(1)} = x_3^{(2)} \\ k_1 x_3^{(1)} + k_2 x_3^{(2)} = \lambda_1 + \lambda_2 \end{cases} \Leftrightarrow$$

$$\begin{cases} \lambda_1 + \lambda_2 - (k_1 + k_2) x_3^{(2)} = 0 \\ \lambda_1 + \lambda_2 - (k_2 + k_1) x_3^{(1)} = 0 \end{cases}$$

Ariéle 15 mai 2013

17

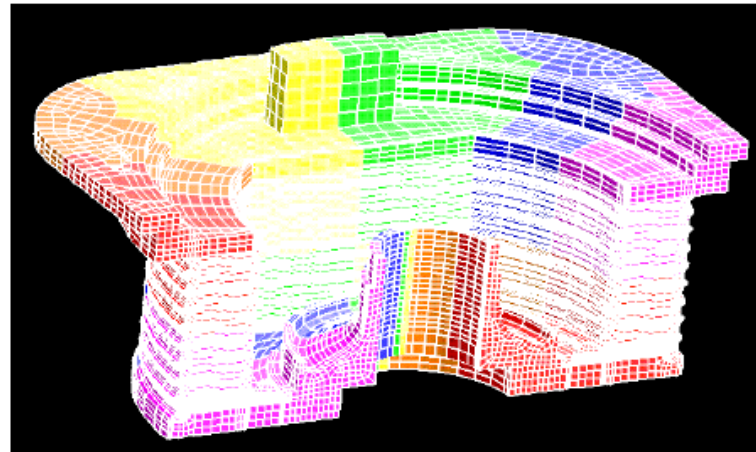


Intégration



Intégration dans un code existant

- Nécessité d'un partitionnement du maillage par éléments
- « Coloriage »
- Par l'utilisateur en fonction de critères géométriques ou physiques
- Automatique à l'aide d'un partitionneur de graphe, SCOTCH, METIS



15 mai 2013

Open Source Code :



Co-development CERFACS – ONERA
http://www.cerfacs.fr/globc/PALM_WEB/

WHY?

To treat a global system

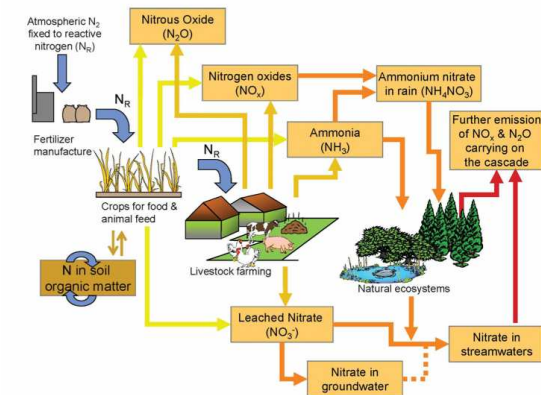
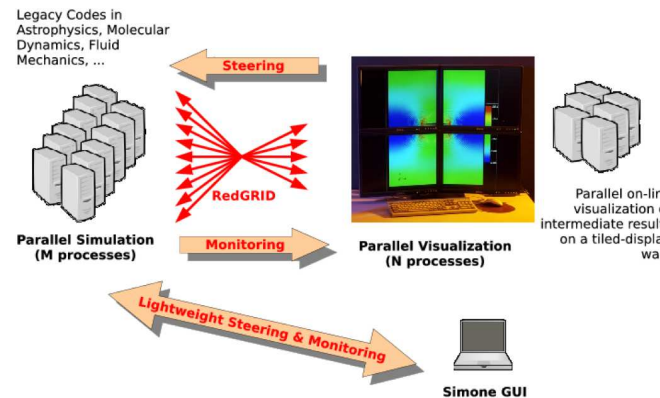
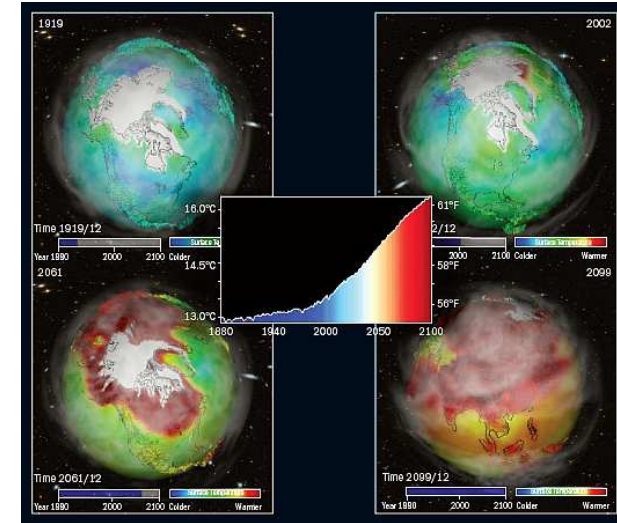
- The earth system: coupling between ocean-atmosphere-sea ice ...
- Fluid structure interaction
- Multi-components simulations

To construct applications around existing codes

- On the fly post-processing,
- Optimization loop around a code
- Ensemble simulations

To construct modular applications by assembling elementary components

- data assimilation
- model coupling



Training



A software to manage complex applications in a modular way while respecting the performances of the codes,

An easy to use GUI to integrate, present and supervise applications,

Multiples interests :

- Facilitate evolution and maintenance of complex applications and of its components,
- Easy integration of new codes replacement, in existing applications (multi-physic coupling, collaborative development ...)
- Maximize the use of intrinsic parallelism of applications and algorithms
- A constant evolution of the code in direct link with user needs
 - Parasol
 - Python interface
- Connection to commercial codes or heterogeneous coupling via IP
- ...
- New uses as people are aware of the soft
- Tested over 12,000 cores for conjugate heat transfer applications



Current Version
OpenPALM 4.1.4
PrePALM 4.1.4
CWIPT 0.5.5

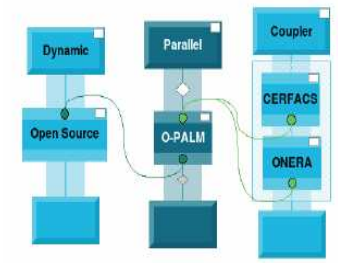
IMPORTANT NEWS

- * Starting on January 2011 OpenPALM has become Open Source under the LGPL v3 license
- * Efficient parallel grid to grid mapping and interpolation for multiphysics applications.
- * OpenPALM supports coupling industrial codes thanks to TCP/IP connections.

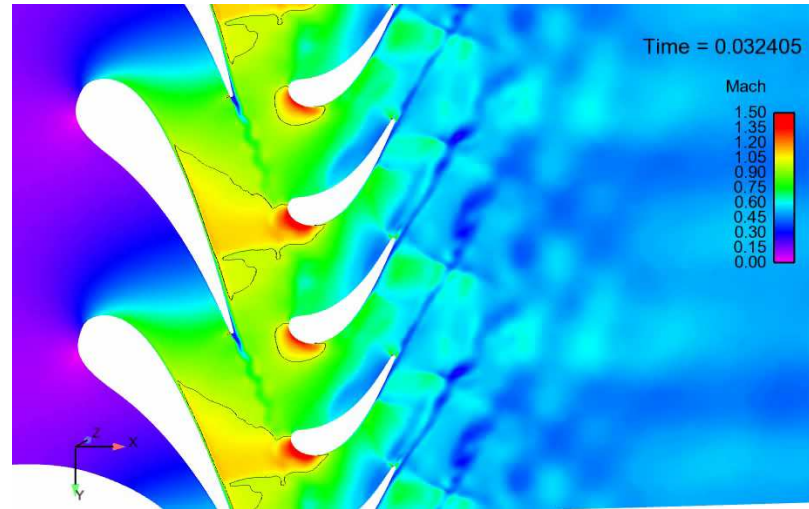
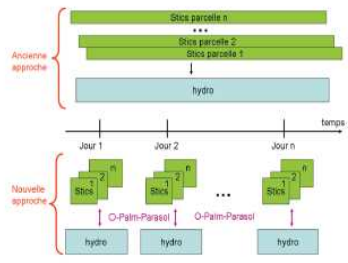
[How to obtain OpenPALM](#)

In order to efficiently represent complex systems, numerical modelling has to rely on many physical models at a time: an ocean model coupled with an atmospheric model is at the basis of climate modelling. A combustion model coupled with a radiation model allows the computation of a combustion chamber temperature. The continuity of the solution is granted only if these models can constantly exchange information.

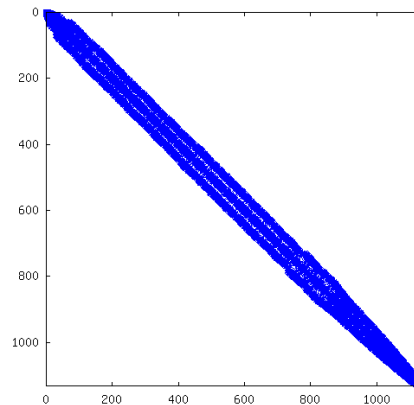
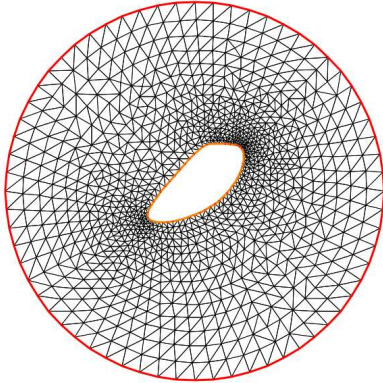
Training session



OpenPALM is a software allowing the concurrent execution and the intercommunication of programs based on in-house as well as commercial codes.



Bibliothèque++ : FreeFem++



Stokes equation

The Stokes equation is find a velocity field $\mathbf{u} = (u_1, \dots, u_d)$ and the pressure p on domain Ω of \mathbb{R}^d , such that

$$\begin{aligned} -\Delta \mathbf{u} + \nabla p &= 0 & \text{in } \Omega \\ \nabla \cdot \mathbf{u} &= 0 & \text{in } \Omega \\ \mathbf{u} &= \mathbf{u}_\Gamma & \text{on } \Gamma \end{aligned}$$

where \mathbf{u}_Γ is a given velocity on boundary Γ .

The classical variational formulation is : Find $\mathbf{u} \in H^1(\Omega)^d$ with $\mathbf{u}|_\Gamma = \mathbf{u}_\Gamma$, and $p \in L^2(\Omega)/\mathbb{R}$ such that

$$\forall \mathbf{v} \in H_0^1(\Omega)^d, \forall q \in L^2(\Omega)/\mathbb{R}, \quad \int_{\Omega} \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} - q \nabla \cdot \mathbf{u} = 0$$

or now find $p \in L^2(\Omega)$ such than (with $\varepsilon = 10^{-10}$)

$$\forall \mathbf{v} \in H_0^1(\Omega)^d, \forall q \in L^2(\Omega), \quad \int_{\Omega} \nabla \mathbf{u} : \nabla \mathbf{v} - p \nabla \cdot \mathbf{v} - q \nabla \cdot \mathbf{u} + \varepsilon pq = 0$$

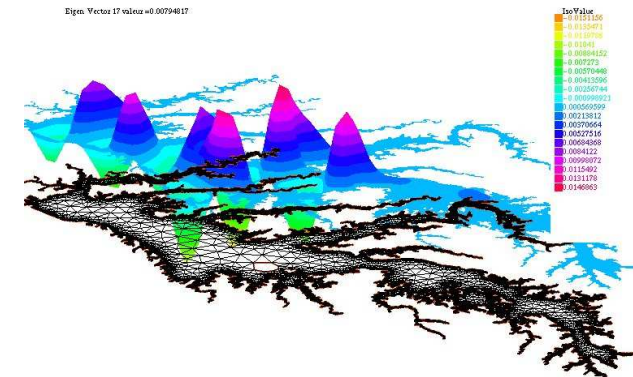
Séminaire Aristote: Bibliothèques pour le calcul scientifique: outils, enjeux et écosystème.

14

Stokes equation in FreeFem++

```
... build mesh .... Th (3d) T2d ( 2d)
fespace VVh(Th, [P2,P2,P2,P1]); // Taylor Hood FE.
macro Grad(u) [dx(u), dy(u), dz(u)] // EOM
macro div(u1,u2,u3) (dx(u1)+dy(u2)+dz(u3)) // EOM
VVh [u1,u2,u3,p], [v1,v2,v3,q];
solve vStokes([u1,u2,u3,p],[v1,v2,v3,q]) =
  int3d(Th) (
    ( D(u1,u2,u3):D(v1,v2,v3) )
    - div(u1,u2,u3)*q - div(v1,v2,v3)*p
    - 1e-10*q*p )
+ on(1,u1=0,u2=0,u3=0) + on(2,u1=1,u2=0,u3=0);
```

Run:Stokes3d.edp



FreeFem++ pass 10^9 unknowns

For who, for what !

For what

1. R&D
2. Academic Research ,
3. Teaching of FEM, PDE, Weak form and variational form
4. Algorithmes prototyping
5. Numerical experimentation
6. Scientific computing and Parallel computing

For who : the researcher, engineer, professor, student...

The mailing list <mailto:Freefempp@ljl11.math.upmc.fr> with 410 members with a flux of 5-20 messages per day.

More than 2000 true Users (more than 1000 download / month)



FreeFem++, un logiciel pour résoudre numériquement des équations aux dérivées partielles.

F. Hecht
Laboratoire Jacques-Louis Lions
Université Pierre et Marie Curie
Paris, France

with , O. Pironneau, I. Danaila, S. Auliac, P. Jolivet

<http://www.freefem.org> <mailto:hecht@ann.jussieu.fr>

Freefem++ v3.20 is

- ▶ very good tool to solve non standard PDE in 2D/3D
- ▶ to try new domain decomposition domain algorithm

The the future we try to do :

- ▶ Build more graphic with VTK, paraview , ... (in progress)
- ▶ Add Finite volume facility for hyperbolic PDE (just begin C.F. FreeVol Projet)
- ▶ 3d anisotrope mesh adaptation
- ▶ automate the parallel tool

The message from Pierre Jolivet

```
Machine: Curie Thin Node@CEA
Financement: PRACE project HPC-PDE (number 2011050840)
Nombre de coeurs: 6144      Mémoire par coeurs: 4 Go
Eléments finis: P3 Dimension: 2D
Précision: 1e-08
Nombres d'inconnues: 1 224 387 085
Méthode de résolution: GMRES préconditionné par une méthode de
décomposition de domaine à deux niveaux
Nombre d'itérations: 18
Temps de résolution: 2 minutes
Type de problème: équation de diffusion avec coefficients très
hétérogènes (5 ordres de grandeur de variation)
```

The FreeFem++ days, Begin of the December, 2013, UPMC, Jussieu, Paris, France

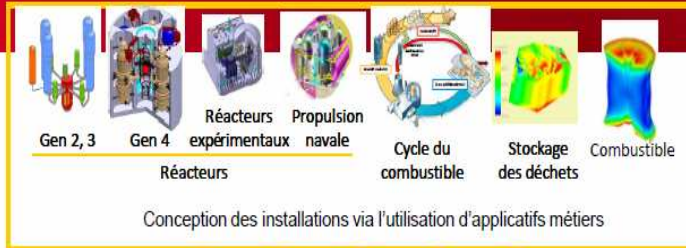
05/09/2013

Dans les Grands Codes



Les Grands Outils pour le Développement du Nucléaire

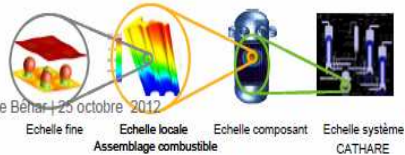
Le programme Simulation



- Explorer des domaines difficilement accessibles par l'expérimentation
- Réduire les durées d'étude
- Limiter les investissements

Nécessité d'amplifier cette activité

Exemple: Couplage Multi-échelle en thermo-hydraulique



Christophe Béhar | 25 octobre 2012 CEA | MAI 2013 | PAGE 4



SYSTÈMES ET SOLVEURS LINÉAIRES DANS TRIO_U

- Grande diversité de méthodes et schémas numériques entraînant une grande variété de systèmes linéaires à résoudre

		Sparse	Symmetric	Constant
Pressure solvers	Pressure linear systems for incompressible flow	X	X	X
	Pressure linear systems for quasi compressible flow	X	X	
	Pressure linear systems for diphasic flow	X	X	
Implicit Scheme		X		

- Solveurs linéaires
 - Native solvers : GCP, GMRES, Precond : diag, ssor

- PETSC

PETSc

CEA | MAI 2013 | PAGE 17

49



État des Lieux



UTILISATION DE BIBLIOTHÈQUES DANS LES APPLICATIONS SCIENTIFIQUES DE LA DEN

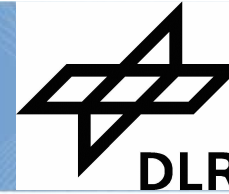
- Les situations sont assez contrastées :
 - Des applications utilisent, généralement avec succès, des bibliothèques externes et pas uniquement des bib. numériques parallèles
 - Des applications n'en utilisent pas du tout
 - La DEN est fournisseur d'outils pour la communauté :
 - Outil à utiliser
 - Plateforme d'intégration
 - Plateforme générique

- Quelques raisons principales à la non utilisation d'outils externes :
 - Nécessaire adaptation de l'application à l'outil : à prendre en termes de contrainte de conception
 - Intégration de développements non maîtrisés
 - Très (trop) grande optimisation de certaines parties des applications qui rend très délicat voire quasi impossible l'utilisation de bib. externes :
 - Stockage de matrices
 - Problème à résoudre couplant plusieurs équations
 - Langage/env. de programmation non standard

- Mais l'utilisation de bibliothèques externes va devenir de plus en plus nécessaire



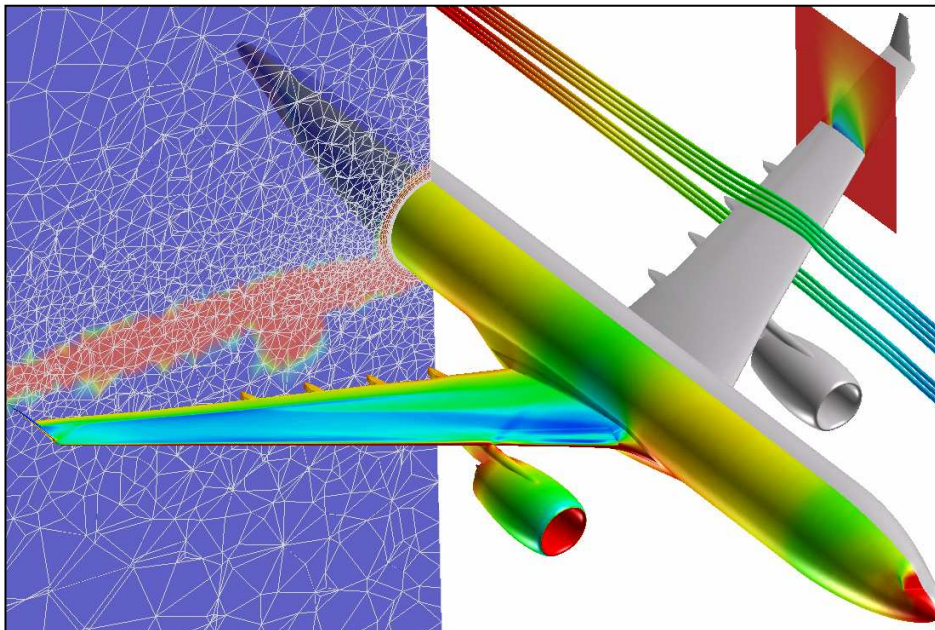
LES FRÈRES ENNEMIS



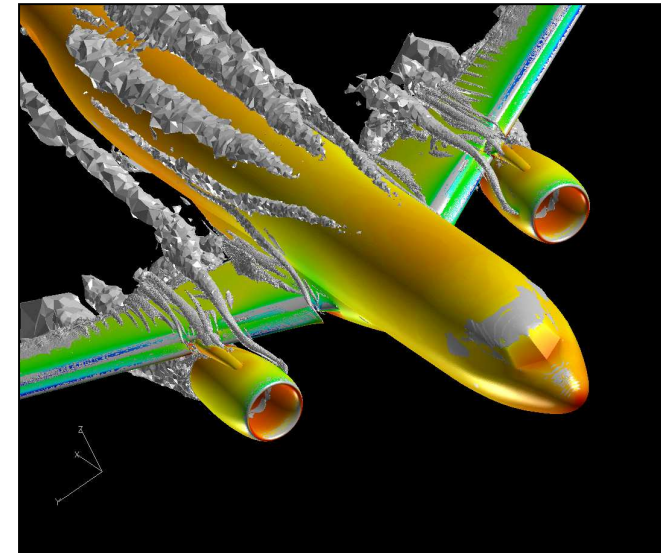
ONERA
THE FRENCH AEROSPACE LAB

Tool for complex configurations

- steady & unsteady compressible flows
- **hybrid unstructured meshes**
- high-level turbulence & transition models
- **state-of-the-art** algorithms (multigrid, ...)
- local mesh adaptation (re- & derefinement)
- deforming mesh capability, chimera technique
- fluid / structure coupling
- continuous/discrete adjoint
- extensions to incompressible & hypersonic flows



DLR RANS Solver TAU



Code structure

- edge-based data structure
- C-code, Python
- portable code, optimized for cache hardware
- **high performance on parallel computers**
parallel solver, adaptation, deformation, grid partitioning, data-extraction

LES FRÈRES ENNEMIS

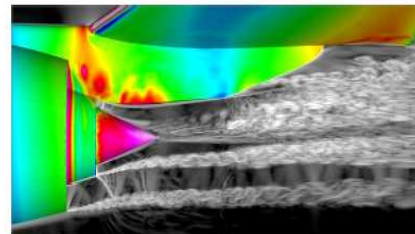
Many unknowns, both in hardware and software

Selection of LES for first GPU computation with *elsA*

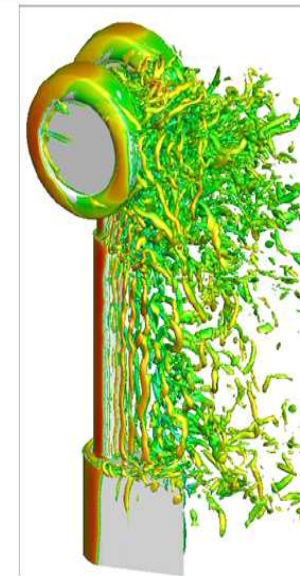
- "Conventional" many-core nodes (AMD, Intel) – how many cores?
 - MPI only?
 - MPI + OpenMP? MPI+Pthreads?
- GPU
 - CUDA?
 - OpenCL?
 - can we expect an easier programming interface?
- Intel MIC
- ARM processor: low power, low cost (used in most mobile phone)

- We must improve loop computational intensity
 - better usage of memory bandwidth – valid for GPU AND conventional computing nodes
 - We have to reduce the number of numerical options
- We must anticipate hardware major changes
 - Use abstraction to hide (some) hardware details
- Explore the potential of Domain Specific Language (DSL)

- High comput. cost of LES/DES cheaper hardware always welcome!
- Increased usage of LES/DES
- Relatively easy to port to GPU
no chimera, no sliding mesh interface...



ONERA/DAAP



ONERA/DAAP

9/22

M. Gazaix, J.F. Boussuge, M. Montagnac

Xtrem CFD 2011 ONERA

Précision



$$0.3 * x^2 + 2.1 * x + 3.675 = 0$$

- **Rounding to nearest**

d = -3.81470E-06

There are two conjugate complex roots.

z1 = -.3500000E+01 + i * 0.9765625E-03

z2 = -.3500000E+01 + i * -.9765625E-03

- **Rounding to zero**

d = 0.

The discriminant is null.

The double real root is -.3500000E+01

Round-off error analysis

Several approaches

- **Inverse analysis**

based on the "Wilkinson principle": the computed solution is assumed to be the exact solution of a nearby problem

- provides error bounds for the computed results

- **Interval arithmetic**

The result of an operation between two intervals contains all values that can be obtained by performing this operation on elements from each interval.

- guaranteed bounds for each computed result
- the error may be overestimated
- specific algorithms

- **Probabilistic approach**

- uses a random rounding mode
- estimates the number of exact significant digits of any computed result

The IEEE 754 standard

The IEEE 754 standard specifies the **single precision** format and **double precision** format, both using the radix 2.

1	2 ...	9	10	32
s	$E + 2^7 - 1$	a_1	a_{23}

IEEE 754 single precision

1	2 ...	12	13	64
s	$E + 2^{10} - 1$	a_1	a_{52}

IEEE 754 double precision



About



How to implement CADNA

The use of the CADNA library involves six steps:

- declaration of the CADNA library for the compiler,
- initialization of the CADNA library,
- substitution of the type REAL or DOUBLE PRECISION by stochastic types in variable declarations,
- possible changes in the input data if perturbation is desired, to take into account uncertainty in initial values,
- change of output statements to print stochastic results with their accuracy,
- termination of the CADNA library.

In direct methods - Example

$$0.3x^2 - 2.1x + 3.675 = 0$$

Without CADNA, in single precision with rounding to the nearest:

d = -3.8146972E-06

Two complex roots

z1 = 0.3499999E+01 + i * 0.9765625E-03

z2 = 0.3499999E+01 + i * -.9765625E-03

With CADNA:

d = @.0

The discriminant is null

The double real root is 0.3500000E+01

The run with CADNA

CADNA software — University P. et M. Curie — LIP6

Self-validation detection: ON

Mathematical instabilities detection: ON

Branching instabilities detection: ON

Intrinsic instabilities detection: ON

Cancellation instabilities detection: ON

P(10864,18817) = @.0

P(1/3,2/3) = 0.802469135802469E+000

CADNA software — University P. et M. Curie — LIP6

There are 2 numerical instabilities

0 UNSTABLE DIVISION(S)

0 UNSTABLE POWER FUNCTION(S)

0 UNSTABLE MULTIPLICATION(S)

0 UNSTABLE BRANCHING(S)

0 UNSTABLE MATHEMATICAL FUNCTION(S)

0 UNSTABLE INTRINSIC FUNCTION(S)

2 UNSTABLE CANCELLATION(S)

Conclusion

- ☹ can be used on real life applications
- ☹ difficult to understand the numerical instabilities in large codes
- ☹ time and memory consuming
- ☹ solution for parallel programs (MPI and GPU)
- ☹ difficult to use with the libraries (BLAS, LAPACK ...)

Solve $Ax = b$ where matrix A: small perturbation around discretisation of 1D Laplace equation

```

#define N 16          // matrix size
#define epsilon 0.00001
float A[N][N]; float b[N], xi[N], ....;

void evalA(float *x, float *y);          // y = Ax
float scalarproduct(fl *x, fl *y);      // return <x,y>
void multadd(fl *x, fl *y, fl a, fl b, fl *z); // z = a*x+b*y

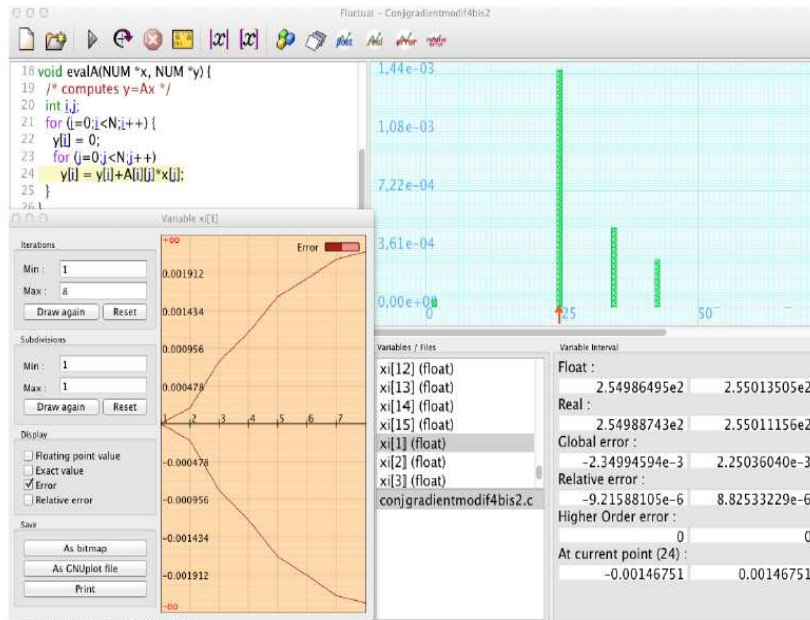
[...]
for (i=0;i<N;i++) { // init A - discretisation Laplacien 1D
  A[i][i] = FBETWEEN(2.0/(N+1)-0.0000001,2.0/(N+1)+0.0000001);
  if (i < N-1) {
    A[i][i+1] = -1.0/(N+1);
    A[i+1][i] = -1.0/(N+1);
  }
}
for (i=0;i<N;i++) b[i] = 1;
for (i=0;i<N;i++) xi[i] = FBETWEEN(0,0.0000001);

evalA(xi,temp);          /* temp = Ax */
multadd(b,temp,1,-1,gi); /* residue gi = b-Ax */
for (j=0;j<N;j++) hi[j] = gi[j]; /* descent direction hi = gi */
norm = scalarproduct(gi,gi); /* residue norm = <gi,gi> */

```


Around

FLUCTUAT



- First extension to the analysis of hybrid systems by interaction with the ODE guaranteed solver GrkLib (HybridFluctuat, CAV 2009, with O. Bouissou, E. Goubault, K. Tekkal, F. Védrine)
- First interface with Esterel's SCADe (with library version of Fluctuat)
- (Present/Future) Interaction with constraint solvers
 - first demonstration of refinement of Fluctuat's result (Ponsini, Michel, Rueher 2011-2012)
 - natural for us because increasing use of constraints on noise symbols (and we could provide more for non linear operations)
- (Present/Future) Floating-point to fixed point automatic conversion (ANR DEFIS project 2012-2015, first steps in 2005 with intern J. Mascunan)
- (Future) Interaction with provers, Frama-C platform
 - ACSL language to exchange information on real, float and errors
 - provide provers with loop invariants
 - use locally refined results and properties
 - towards formally proved abstract domain implementations ? (cf D. Pichardie)





Challenges for Software/Libraries

- 1. Synchronization**
 - Break Fork-Join model
- 2. Communication**
 - Use methods which have lower bound on communication
- 3. Mixed precision methods**
 - SP:DP; 2x speed of ops and 2x speed for data movement
- 4. Autotuning**
 - Today's machines are too complicated, build "smarts" into software to adapt to the hardware
- 5. Fault resilient algorithms**
 - Implement algorithms that can recover from failures/bit flips

3

Destruction Créative



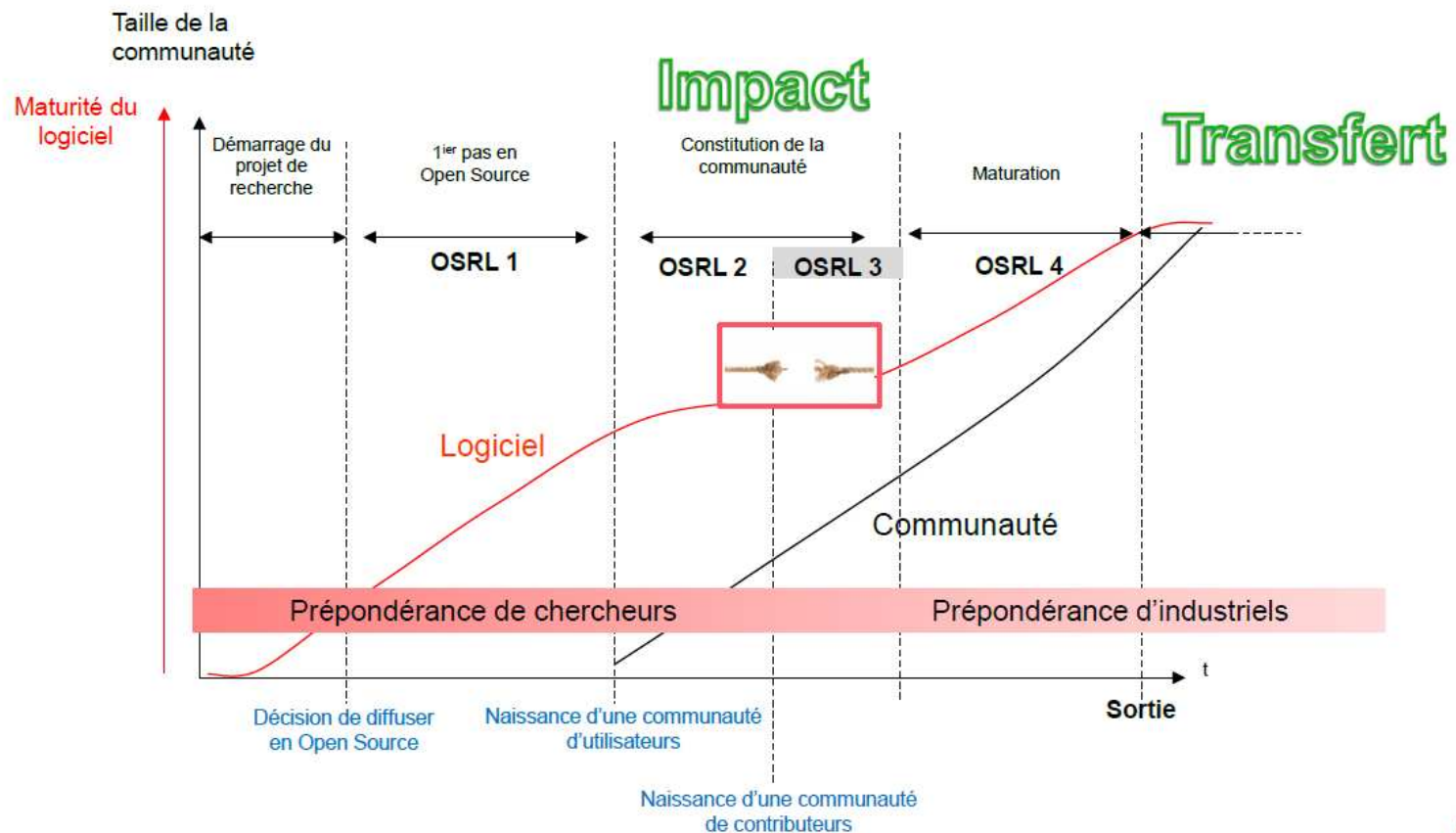
Major Changes to Algorithms/Software

- **Must rethink the design of our algorithms and software**
 - **Manycore and Hybrid architectures are disruptive technology**
 - Similar to what happened with cluster computing and message passing
 - **Rethink and rewrite the applications, algorithms, and software**
 - **Data movement is expensive**
 - **Flops are cheap**

2

OSRL

Cycle de vie



Le Logiciel

Grande généralité

- Les membres, bien que concurrents, peuvent être partenaires dans le consortium



L'analyse


- Décrire pourquoi il y a une forte mutualisation sur le logiciel



Benefits of going free software

- Inclusion of software on the form of packages within the main free software distributions
 - Increased visibility : Linux (Debian, Ubuntu), FreeBSD, ...
 - Packaging done by autonomous maintainers (Debian Science, ...)
- Exclusive use within academic and/or industrial free software
 - E.g. OpenFOAM
- No contribution to the software itself
 - Expertise is scarce, mostly owned by competitors
 - Build a testbed environment that they can join !

Choosing the proper license (2)

- Within a given class, choose the license according to its own merits and to environmental constraints
- In the case of , for weak copyleft licenses :
 - LGPL allows “legal forking” towards GPL
 - Inria was my employer
 - So... CeCILL-C
 - But it is incompatible with GPL...
- Define a licensing policy from the inception of your project
 - Using a free software license reduces the impact of external contributors as long as the software is kept within the same license perimeter

Pérennisation

Montage du consortium

Un consortium se caractérise en général par un **contrat d'adhésion** unique hormis les clauses financières qui peuvent être adaptées.

- Quel est le financement probable des membres?
 - Possibilité d'une segmentation de l'offre aux membres (Gold, Silver, ...)?
 - Cotisation selon la taille de l'entreprise?
- Durée de l'engagement initial
- Choix de la gouvernance (Comité de pilotage, comité scientifique, ...)
- Choix du montage juridique (par ordre croissant de complexité de mise en œuvre et d'indépendance vis à vis de l'Institut)
 - Sans structure dédiée (hébergé par Inria)
 - GIS
 - Association loi 1901
 - Fondation(s)
- Définition des protections (marque, logo, ...) si pas déjà fait

L'EQUATION DU MILLENAIRE

11 - 5
Click to read

PARTOUT



05/09/2013



1821 – 1822 : Now



Millennium Prize:
the Navier–Stokes existence and
uniqueness problem



Navier–Stokes Equations 3 – dimensional – unsteady

Glenn
Research
Center

Coordinates: (x,y,z) Time: t Pressure: p Heat Flux: q
Density: ρ Stress: τ Reynolds Number: Re
Velocity Components: (u,v,w) Total Energy: Et Prandtl Number: Pr

Continuity:
$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

X – Momentum:
$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right]$$

Y – Momentum:
$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right]$$

Z – Momentum:
$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right]$$

Energy:
$$\frac{\partial(E_T)}{\partial t} + \frac{\partial(uE_T)}{\partial x} + \frac{\partial(vE_T)}{\partial y} + \frac{\partial(wE_T)}{\partial z} = -\frac{\partial(u p)}{\partial x} - \frac{\partial(v p)}{\partial y} - \frac{\partial(w p)}{\partial z} - \frac{1}{Re_r Pr_r} \left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right] + \frac{1}{Re_r} \left[\frac{\partial}{\partial x} (u \tau_{xx} + v \tau_{xy} + w \tau_{xz}) + \frac{\partial}{\partial y} (u \tau_{xy} + v \tau_{yy} + w \tau_{yz}) + \frac{\partial}{\partial z} (u \tau_{xz} + v \tau_{yz} + w \tau_{zz}) \right]$$





Contexte et Evolution des Moyens de calcul

Echelle Nationale :

□ **Création du GENCI**

→ Financement pérenne des centres nationaux



Echelle Européenne : le Projet **PRACE**

Partnership for Advanced Computing in Europe

→ Développement d'une infrastructure de Européenne de classe mondiale pour le calcul haute performance



2011 : Installation de la machine Curie au TGCC





MAISON DE LA SIMULATION



11/05/2013

Open Space



Conclusions



Formation et animation scientifique

Formation initiale :

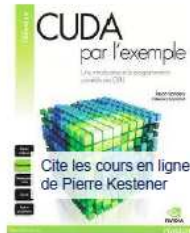
Contribuer, en collaboration avec les partenaires, à assurer une implication forte de la MdS dans les masters "HPC" du plateau de Saclay.

□ M2S :

- Etablissement partenaire
- Mise en place et hébergement du site web
- Accueil des certains cours et participations à 3 modules

□ MIHPS

□ Utilisation de la plateforme par deux autres Masters



Formation continue : (6 semaines de formation, ~150 personnes formées)

Former les chercheurs et ingénieurs à l'utilisation des grands moyens de calculs.

□ Labélisation PRACE Advanced Training Center (PATC) :

- Candidature française portée par la Maison de la Simulation et regroupant les trois centres de calcul nationaux et Inria
- Dix formations/an

□ Sessions de formation

□ Organisation d'ateliers, de conférences et d'écoles. Soutien au CECAM Ile-de-France



- Outil scientifique : **Ordinateur + Applications**
- Développer en France une communauté des *Sciences pour et par la Simulation* (Computational sciences)
- La Maison de la Simulation est un lieu d'expertise et d'accueil que les chercheurs et les laboratoires doivent s'approprier



HPC Magazine



•Actualités

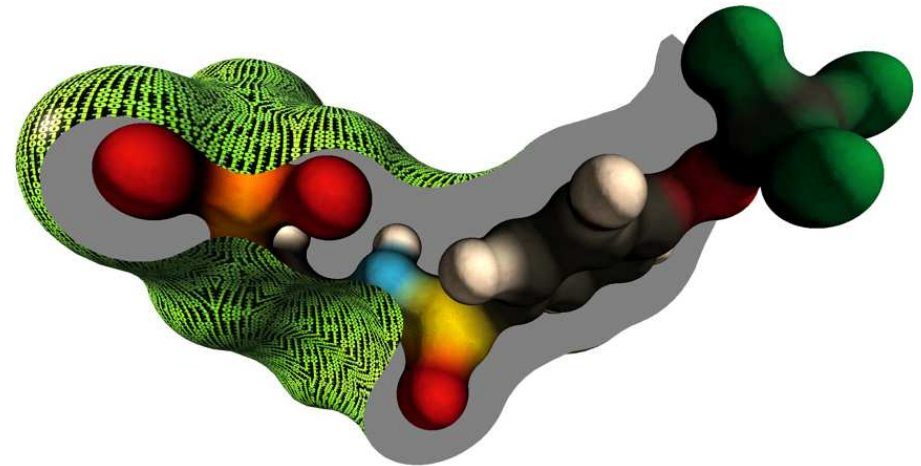
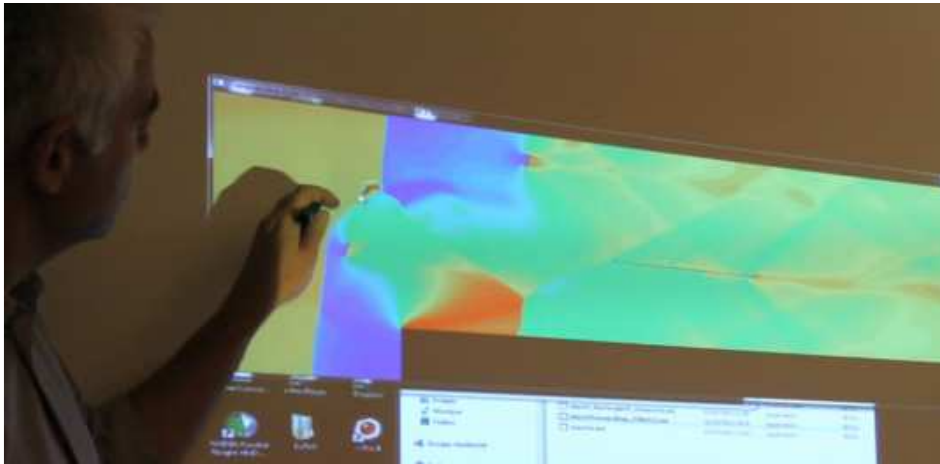
JDEV2013 - A vos agendas !

- La deuxième édition des Journées nationales du Développement Logiciel aura lieu les [...]



Article à paraître dans le numéro d'octobre

ANNONCES



**La visualisation collaborative:
un des grands défis
de la science actuelle!**

7 novembre

Maison de la Simulation
Gif-sur-Yvette

Visu 2013

En novembre

Institut de Biologie Physico-
Chimique

Paris

Les 3 Piliers

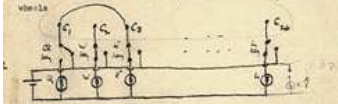
erschleckt und hat so alles
 Satz von der Äquivalenz von
 an) durch die Formel ausgedr

$$E_0 = mc^2$$
 Lichtgeschwindigkeit ($3 \cdot 10^{10}$
 cines mechanische (ruhendens,
 die zu der Masse m gehört, ist gleich
 at die ...

Handwritten mathematical notes and diagrams, including the equation $E = mc^2$ and various derivations.

The particular order we have chosen is known as **HEATON** order.

The diagram shows the connections when the key **Q** is depressed and suggests that **C**₁ is connected to **C**₂ through the wheels.




The only outlet for the positive of the battery is through the **Q** key to **C**₁ hence to **C**₂ and then through the **W** bulb. The result is that the **W** bulb lights. More generally we can say

If two contacts **C**₁, **C**₂ of the **Electrified** are connected through the wheels to the result of enciphering the letter associated with **C** is the letter associated with **C**₂.

Notice that if **P** is the result of enciphering **Q**, then **Q** is the result of enciphering **P** at the same place, also that the result of enciphering **Q** can never be **Q**.

On the wheels are rings or tyres carrying 'alphabets', and rotatable with respect to the rest of the wheel; more about this under 'mechanism'. When the machine is being used three of the wheels are put in between the **C.W.** and the **R.W.** in some prescribed order. The way that the current might flow from the **R.W.** through the wheels and back is shown below:

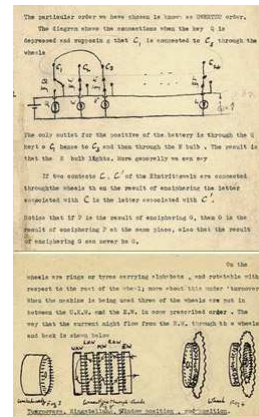
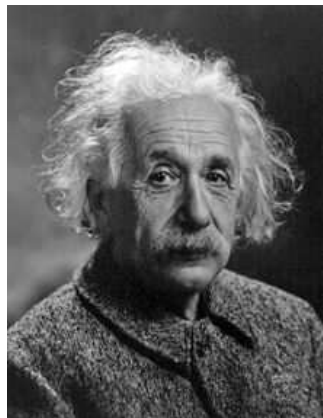


Enciphering 'P' through wheels. Deciphering 'P' through wheels. Enciphering 'Q' through wheels. Deciphering 'Q' through wheels.

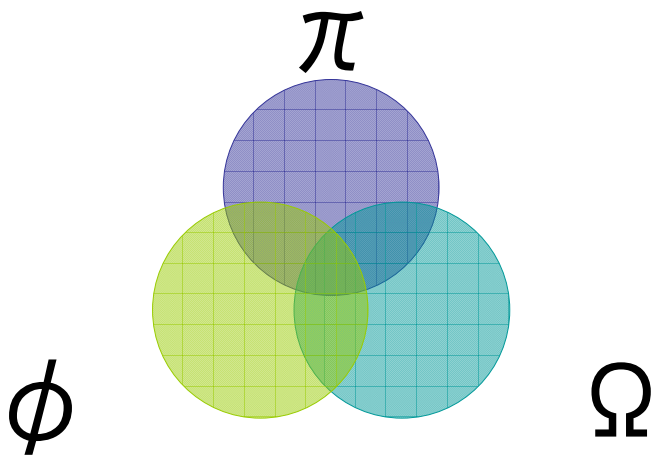
C'est Eux

erschleuchtet und hat so alles
 Satz von der Äquivalenz von
 an) durch die Formel ausgedr

$$E_0 = mc^2,$$
 Lichtgeschwindigkeit ($3 \cdot 10^{10}$
 einer mechanischen (ruhenden,
 die zu der Masse m gehört, ist gleich
 at der ...

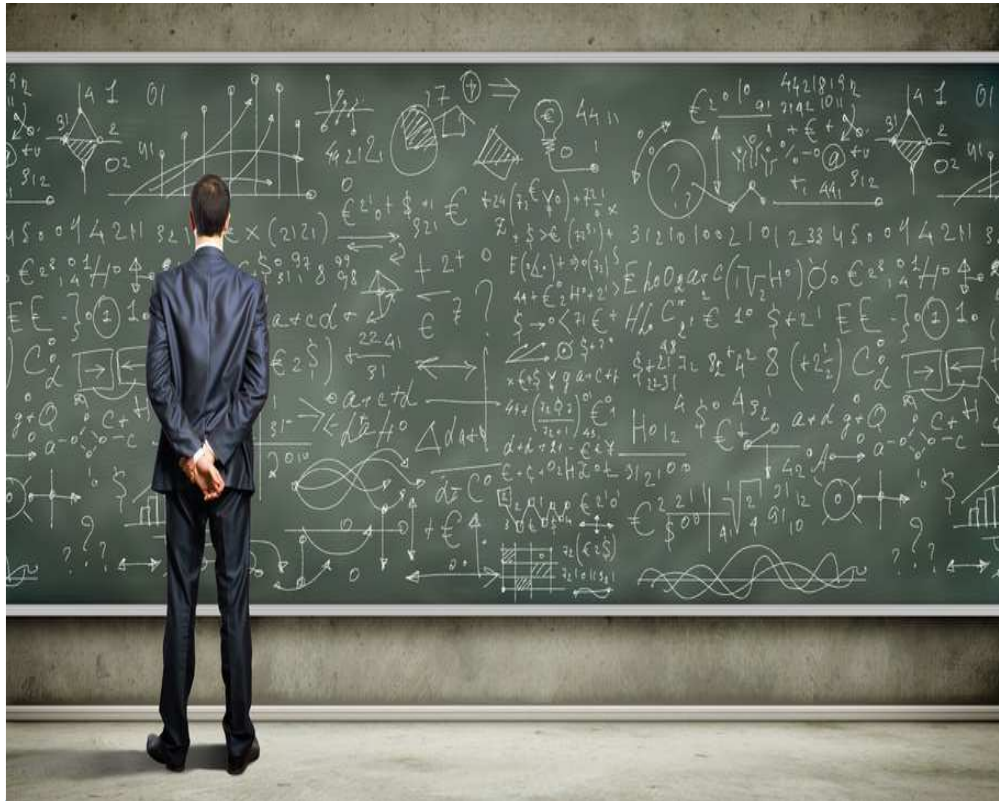


C'est Vous, Ensemble



To Bib or Not To Bib

Your Opinion
is requested



See You Soon

05/09/2013