Scalable Domain Decomposition Preconditioners in FreeFem++

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http://www.freefem.org/ff++

Outline

1. Introduction
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   - Optimisation : Bose Einstein Condensate
3. A first way to break complexity
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   - Poisson equation with Schwarz method
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Main characteristics I/II (2D)(3D)

- Wide range of finite elements : continuous P1,P2 elements, discontinuous P0, P1, RT0,RT1,BDM1, elements ,Edge element, vectorial element, mini-element, ...
- Automatic interpolation of data from a mesh to an other one (with matrix construction if need), so a finite element function is view as a function of (x, y, z) or as an array.
- LU, Cholesky, Crout, CG, GMRES, UMFPack, SuperLU, MUMPS, HIPS , SUPERLU_DIST, PASTIX. ... sparse linear solver ; eigenvalue and eigenvector computation with ARPACK.

Main characteristics II/II (2D)(3D)

- Automatic mesh generator, based on the Delaunay-Voronoï algorithm. (2d,3d (tetgen))
- Mesh adaptation based on metric, possibly anisotropic (only in 2d), with optional automatic computation of the metric from the Hessian of a solution. (2d,3d).
- Dynamic linking to add plugin.
- Full MPI interface
- Nonlinear Optimisation tools : CG, Ipopt, NLOpt, stochastic
- Wide range of examples : Navier-Stokes 3d, elasticity 3d, fluid structure, eigenvalue problem, Schwarz' domain decomposition algorithm, residual error indicator ...

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Poisson equation, weak form

Let a domain Ω with a partition of $\partial\Omega$ in Γ_2, Γ_e.
Find u a solution in such that :

$$-\Delta u = 1 \text{ in } \Omega, \quad u = 2 \text{ on } \Gamma_2, \quad \frac{\partial u}{\partial \vec{n}} = 0 \text{ on } \Gamma_e \qquad (1)$$

Denote $V_g = \{v \in H^1(\Omega) / v_{|\Gamma_2} = g\}$.
The Basic variational formulation with is : find $u \in V_2(\Omega)$, such that

$$\int_\Omega \nabla u . \nabla v = \int_\Omega 1 v + \int_\Gamma \frac{\partial u}{\partial n} v, \quad \forall v \in V_0(\Omega) \qquad (2)$$

The finite element method is just : replace V_g with a finite element space, and the `FreeFem++` code :

Poission equation in FreeFem++

The finite element method is just : replace V_g with a finite element space, and the FreeFem++ code :

```
mesh3 Th("fish3d.msh");                       //    read a mesh 3d
fespace Vh(Th,P1);                        //    define the P1 EF space

 Vh u,v;        //    set test and unknow FE function in Vh.
macro Grad(u) [dx(u),dy(u),dz(u)]          //   EOM Grad def
solve laplace(u,v,solver=CG) =
   int3d(Th)(  Grad(u)'*Grad(v)   )
   - int3d(Th) ( 1*v)
   + on(2,u=2);                                //     int on γ2
plot(u,fill=1,wait=1,value=0,wait=1);
```

Run:fish.edp   Run:fish3d.edp

Bose Einstein Condensate

Just a direct use of `Ipopt` interface (2day of works)
The problem is find a complex field u on domain $\mathcal{D}$ such that :

$$u = \underset{||u||=1}{\operatorname{argmin}} \int_{\mathcal{D}} \frac{1}{2}|\nabla u|^2 + V_{trap}|u|^2 + \frac{g}{2}|u|^4 - \Omega i \overline{u}\left(\left(\begin{smallmatrix} -y \\ x \end{smallmatrix}\right).\nabla\right)u$$

to code that in FreeFem++
use

- Ipopt interface (`https://projects.coin-or.org/Ipopt`)
- Adaptation de maillage
- Analyse of the result

Run:BEC.edp

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A first way to break complexity

Idea :

$$a(u, v) = \int_{\Omega} \nabla u . \nabla v$$

take an equi-partition of Ω in Ω_i for $i = 0$ to $N_p - 1$ the number of processor.
then

$$a(u, v) = \sum_{i=0}^{N_p - 1} \int_{\Omega_i} \nabla u . \nabla v$$

A first way to break complexity

1. Build matrix in parallel by assembling par region, remark the change function you modify the region numbering, to defined Ω_i.

```
real c = mpisize/real(Th.nt) ;
Th=change(Th,fregion= min(mpisize-1,int(nuTriangle*c)));
```

2. Assemble the full matrix

```
varf vlaplace(uh,vh) =          //    definition de problem
     int3d(Th,mpirank)( uh*vh+ dt*Grad(uh)'*grad(vh) )
   + int3d(Th,mpirank)( dt*vh*f) + on(1,uh=g) ;
matrix A = vlaplace(Vh,Vh) ;
real[int] b =  vlaplace(0,Vh) ;
```

3. Solve the linear using a good parallel solver (MUMPS)

```
load "MUMPS"
set(A,solver=sparsesolver,master=-1);   //   Distributed A.
uh[] = A^-1*b ;                             //    resolution
```

Run:Heat3d.edp   Run:NSCaraCyl-100-mpi2.edp

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To solve the following Poisson problem on domain Ω with boundary Γ in $L^2(\Omega)$:

$$-\Delta u = f, \text{ in } \Omega, \text{ and } u = g \text{ on } \Gamma,$$

where $f \in L^2(\Omega)$ and $g \in H^{\frac{1}{2}}(\Gamma)$ are two given functions.
Let introduce $(\pi_i)_{i=1,..,N_p}$ a positive regular partition of the unity of Ω, q-e-d :

$$\pi_i \in \mathcal{C}^0(\Omega) : \quad \pi_i \ge 0 \text{ and } \sum_{i=1}^{N_p} \pi_i = 1.$$

Denote Ω_i the sub domain which is the support of π_i function and also denote Γ_i the boundary of Ω_i, and $\Omega_i^\circ = \{x / 0 < \pi_i < 1\}$
The parallel Schwarz method is Let $\ell = 0$ the iterator and a initial guest u^0 respecting the boundary condition (i.e. $u^0_{|\Gamma} = g$).

$$\forall i = 1.., N_p : \quad -\Delta u_i^\ell = f, \text{ in } \Omega_i, \quad \text{and } u_i^\ell = u^\ell \text{ on } \Gamma_i \qquad (3)$$

$$u^{\ell+1} = \sum_{i=1}^{N_p} \pi_i u_i^\ell \qquad (4)$$

Some Remark

We never use finite element space associated to the full domain Ω because it to expensive.

We have to defined to operator to build the previous algorithm :
We denote $u^\ell_{h|i}$ the restriction of u^ℓ_h on V_{hi}, so the discrete problem on Ω_i of problem (3) is find $u^\ell_{hi} \in V_{hi}$ such that :

$$\forall v_{hi} \in V_{0i} : \int_{\Omega_i} \nabla v_{hi}.\nabla u^\ell_{hi} = \int_{\Omega_i} f v_{hi},$$

$$\forall k \in \mathcal{N}^{\Gamma_i}_{hi} \; : \; \sigma^k_i(u^\ell_{hi}) = \sigma^k_i(u^\ell_{h|i})$$

where g^k_i is the value of g associated to the degree of freedom $k \in \mathcal{N}^{\Gamma_i}_{hi}$.

To compute $v_i = \pi_i u_i + \sum_{j\in J_i} \pi_j u_j$ and can be write the freefem++ function Update with asynchronous send/recv.

```
func bool Update(real[int] &ui, real[int] &vi)
{ int n= jpart.n;
  for(int j=0;j<njpart;++j)  Usend[j][]=sMj[j]*ui;
  mpiRequest[int] rq(n*2);
  for (int j=0;j<n;++j)
        Irecv(processor(jpart[j],comm,rq[j  ]), Ri[j][]);
  for (int j=0;j<n;++j)
        Isend(processor(jpart[j],comm,rq[j+n]), Si[j][]);
  for (int j=0;j<n*2;++j)   int k= mpiWaitAny(rq);
  vi = Pii*ui;                                  //    set to πi ui
  //    apply the unity local partition .
   for(int j=0;j<njpart;++j)
     vi += rMj[j]*Vrecv[j][];                     //    add πj uj
 return true; }
```

parallel GMRES

Finally you can easily accelerate the fixe point algorithm by using a parallel GMRES algorithm after the introduction the following affine $\mathcal{S}_i$ operator sub domain Ω_i.

```
func real[int] Si(real[int]& U) {
 real[int] V(U.n)   ;   b= onG .* U;
  b  = onG ? b : Bi ;
  V = Ai^-1*b;                                        //     (3)
  Update(V,U);                                        //     (4)
  V -= U;   return V; }
```

Where the parallel MPIGMRES or MPICG algorithm is to solve $A_i x_i = b_i, i = 1, .., N_p$ by just changing the dot product by reduce the local dot product of all process with the following MPI code :

```
template<class R> R ReduceSum1(R s,MPI_Comm * comm)
{   R r=0;
    MPI_Allreduce( &s, &r, 1 ,MPI_TYPE<R>::TYPE(),
                            MPI_SUM,  *comm );
    return r; }
```

A simple coarse grid is we solve the problem on the coarse grid :

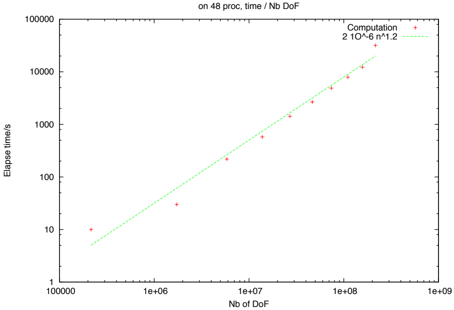
```
func bool  CoarseSolve(real[int]& V,real[int]& U,
               mpiComm& comm)
{
    if(AC.n==0 && mpiRank(comm)==0) //    first time build
      AC = vPbC(VhC,VhC,solver=sparsesolver);
   real[int] Uc(Rci.n),Bc(Uc.n);
   Uc= Rci*U;                             //    Fine to Coarse
   mpiReduce(Uc,Bc,processor(0,comm),mpiSUM);
   if(mpiRank(comm)==0)
      Uc = AC^-1*Bc;                     //    solve of proc 0
    broadcast(processor(0,comm),Uc);
   V = Pci*Uc;                            //    Coarse to Fine
}
```

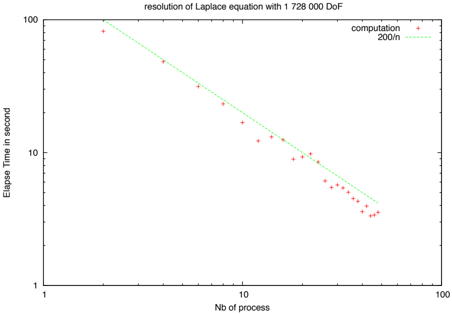
Limitation : if the initial problem, data have oscillation, you must an other on coarse problem : The GENO algorithm for example form the Nataf and co., See section 5.

So we finally we get 4 algorithms

1. The basic schwarz algorithm $u^{\ell+1} = \mathcal{S}(u^\ell)$, where $\mathcal{S}$ is one iteration of schwarz process.
2. Use the GMRES to find u solution of the linear system $\mathcal{S}u - u = 0$.
3. Use the GMRES to solve parallel problem $\mathcal{A}_i u_i = b_i$, $i = 1, \ldots, N_p$, with RAS precondicionneur
4. Use the method with two level precondicionneur RAS and Coarse.

On the SGI UV 100 of the lab :





A Parallel Numerical experiment on laptop

We consider first example in an academic situation to solve Poisson Problem on the cube $\Omega =]0,1[^3$

$$-\Delta u = 1, \text{in } \Omega; \qquad u = 0, \text{ on } \partial\Omega. \tag{5}$$

With a cartesian meshes $\mathcal{T}_{hn}$ of Ω with $6n^3$ tetrahedron, the coarse mesh is $\mathcal{T}^*_{hm}$, and m is a divisor of n.
We do the validation of the algorithm on a Laptop Intel Core i7 with 4 core at 1.8 Ghz with $4Go$ of RAM DDR3 at 1067 Mhz,

Run:DDM-Schwarz-Lap-2dd.edp Run:DDM-Schwarz-Lame-2d.edp
Run:DDM-Schwarz-Lame-3d.edp

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Motivation

Large discretized system of PDEs
strongly heterogeneous coefficients
(high contrast, nonlinear, multiscale)

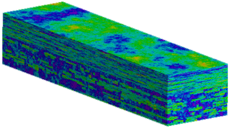
E.g. Darcy pressure equation,
P_1-finite elements :

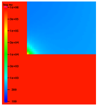
$$A\mathbf{U} = \mathbf{F}$$

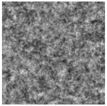
$$\text{cond}(A) \sim \frac{\alpha_{\max}}{\alpha_{\min}} h^{-2}$$

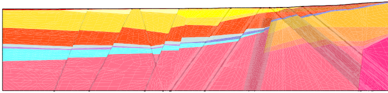
Goal :
iterative solvers
robust in size and heterogeneities

Applications :
flow in heterogeneous / stochastic / layered media
structural mechanics
electromagnetics
etc.









Adding a coarse space

We add a coarse space correction (*aka* second level)
Let V_H be the coarse space and Z be a basis, $V_H = \mathrm{span}\, Z$, writing $R_0 = Z^T$ we define the two level preconditioner as :

$$M^{-1}_{ASM,2} := R_0^T \left(R_0 A R_0^T\right)^{-1} R_0 + \sum_{i=1}^{N} R_i^T A_i^{-1} R_i.$$

The Nicolaides approach is to use the kernel of the operator as a coarse space, this is the constant vectors, in local form this writes :

$$Z := (R_i^T D_i R_i \mathbf{1})_{1 \le i \le N}$$

where D_i are chosen so that we have a partition of unity :

$$\sum_{i=1}^{N} R_i^T D_i R_i = Id.$$

Theoretical convergence result

Theorem (Widlund, Dryija)

Let $M_{ASM,2}^{-1}$ *be the two-level additive Schwarz method :*

$$\kappa(M_{ASM,2}^{-1}A) \leq C\left(1 + \frac{H}{\delta}\right)$$

where δ *is the size of the overlap between the subdomains and* H *the subdomain size.*

This does indeed work very well

Number of subdomains	8	16	32	64
ASM	18	35	66	128
ASM + Nicolaides	20	27	28	27

Failure for Darcy equation with heterogeneities

$$
\begin{aligned}
-\nabla \cdot (\alpha(x,y)\nabla u) &= 0 \quad \text{in} \quad \Omega \subset \mathbb{R}^2, \\
u &= 0 \quad \text{on} \quad \partial\Omega_D, \\
\frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \partial\Omega_N.
\end{aligned}
$$

Decomposition

$\alpha(x,y)$

Jump	1	10	10^2	10^3	10^4
ASM	39	45	60	72	73
ASM + Nicolaides	30	36	50	61	65

Our approach

Fix the problem by an optimal and proven choice of a coarse space Z.

Objectives

Strategy

Define an appropriate coarse space $V_{H2} = \text{span}(Z_2)$ and use the framework previously introduced, writing $R_0 = Z_2^T$ the two level preconditioner is :

$$P_{ASM2}^{-1} := R_0^T (R_0 A R_0^T)^{-1} R_0 + \sum_{i=1}^{N} R_i^T A_i^{-1} R_i.$$

The coarse space must be

- Local (calculated on each subdomain) $\rightarrow$ parallel
- Adaptive (calculated automatically)
- Easy and cheap to compute
- Robust (must lead to an algorithm whose convergence is proven not to depend on the partition nor the jumps in coefficients)

Abstract eigenvalue problem

Gen.EVP per subdomain :

Find $p_{j,k} \in V_{h|\Omega_j}$ and $\lambda_{j,k} \geq 0$:

$$a_{\Omega_j}(p_{j,k},\, v) \;=\; \lambda_{j,k}\, a_{\Omega_j^\circ}(\Xi_j p_{j,k},\, \Xi_j v) \qquad \forall v \in V_{h|\Omega_j}$$

$$A_j \mathbf{p}_{j,k} \;=\; \lambda_{j,k}\, \mathbf{X}_j A_j^\circ \mathbf{X}_j\, \mathbf{p}_{j,k} \qquad (\mathbf{X}_j \text{ ...diagonal})$$

Ξ_j is the partition unity

$a_D \ldots$ restriction of a to D

In the two-level ASM :

Choose first m_j eigenvectors per subdomain :

$$V_0 \;=\; \text{span}\{\Xi_j p_{j,k}\}_{k=1,\ldots,m_j}^{j=1,\ldots,N}$$

This automatically includes Zero Energy Modes.

Galvis & Efendiev (SIAM 2010) :

$$\int_{\Omega_j} \boldsymbol{\kappa}\, \nabla p_{j,k} \cdot \nabla v \, dx \;=\; \lambda_{j,k} \int_{\Omega_j} \boldsymbol{\kappa}\, p_{j,k}\, v\, dx \qquad \forall v \in V_{h|\Omega_j}$$

Efendiev, Galvis, Lazarov & Willems (submitted) :

$$a_{\Omega_j}(p_{j,k},\, v) \;=\; \lambda_{j,k} \sum_{i \in \text{neighb}(j)} a_{\Omega_j}(\xi_j\, \xi_i\, p_{j,k},\, \xi_j\, \xi_i\, v) \qquad \forall v \in V_{|\Omega_j}$$

ξ_j ... partition of unity, calculated adaptively (MS)

Our gen.EVP :

$$a_{\Omega_j}(p_{j,k},\, v) \;=\; \lambda_{j,k}\, a_{\Omega_j^\circ}(\Xi_j p_{j,k},\, \Xi_j v) \qquad \forall v \in V_{h|\Omega_j}$$

both matrices typically singular $\Longrightarrow$ $\lambda_{j,k} \in [0,\, \infty]$

Theory

Two technical assumptions.

Theorem (Spillane, Dolean, Hauret, N., Pechstein, Scheichl)

If for all j : $\quad 0 < \lambda_{j,m_{j+1}} < \infty$ *:*

$$\kappa(M^{-1}_{ASM,2}A) \;\leq\; (1+k_0)\Big[2 + k_0\,(2k_0+1)\,\max_{j=1}^{N}\Big(1 + \frac{1}{\lambda_{j,m_j+1}}\Big)\Big]$$

Possible criterion for picking m_j : (used in our Numerics)

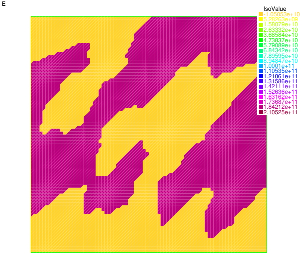
$$\lambda_{j,m_j+1} \;<\; \frac{\delta_j}{H_j}$$

$H_j \ldots$ subdomain diameter, $\delta_j \ldots$ overlap

Numerical results via a Domain Specific Language

`FreeFem++` (`http://www.freefem.org/ff++`), with :

- Metis Karypis and Kumar 1998
- SCOTCH Chevalier and Pellegrini 2008
- UMFPACK Davis 2004
- ARPACK Lehoucq et al. 1998
- MPI Snir et al. 1995
- Intel MKL
- PARDISO Schenk et al. 2004
- MUMPS Amestoy et al. 1998
- PaStiX Hénon et al. 2005



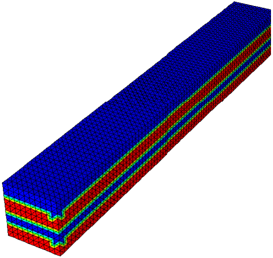
$$E_1 = 2 \cdot 10^{11}$$
$$\nu_1 = 0.3$$

$$E_2 = 2 \cdot 10^{7}$$
$$\nu_2 = 0.45$$

METIS partitions with 2 layers added

subd.	dofs	AS-1	AS-ZEM	(V_H)	GENEO	(V_H)
4	13122	93	134	*(12)*	42	*(42)*
16	13122	164	165	*(48)*	45	*(159)*
25	13122	211	229	*(75)*	47	*(238)*
64	13122	279	167	*(192)*	45	*(519)*

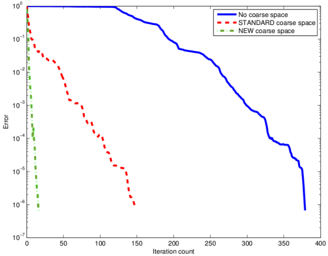
Iterations (CG) vs. number of subdomains



$$E_1 = 2 \cdot 10^{11}$$
$$\nu_1 = 0.3$$

$$E_2 = 2 \cdot 10^{7}$$
$$\nu_2 = 0.45$$

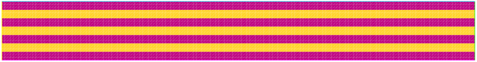
Relative error vs. iterations
16 regular subdomains



subd.	dofs	AS-1	AS-ZEM	(V_H)	GENEO	(V_H)
4	1452	79	54	*(24)*	16	*(46)*
8	29040	177	87	*(48)*	16	*(102)*
16	58080	378	145	*(96)*	16	*(214)*

AS-ZEM (Rigid body motions) : $m_j = 6$

Numerical results – Optimality



Layers of hard and soft elastic materials

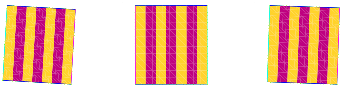
m_i is given automatically by the strategy.

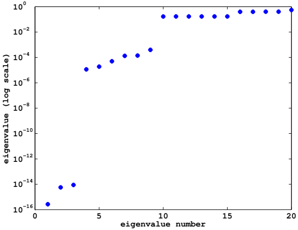
$\#Z$ per subd.	one level	ZEM	GenEO
$\max(m_i - 1, 3)$			2600 (93)
m_i	$5.1\,e5$ (184)	$1.4\,e4$ (208)	53 (35)
$m_i + 1$			45 (25)

condition number (iteration count) for one and two level ASMs

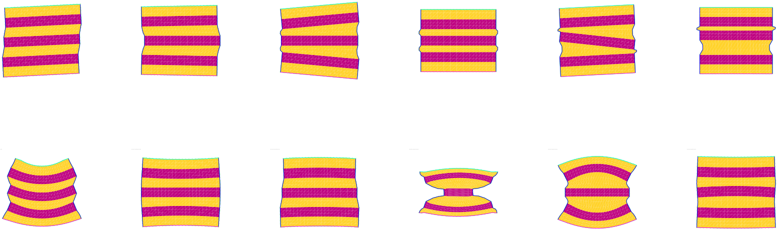
- Taking one fewer eigenvalue has a huge influence on the iteration count
- Taking one more has only a small influence

Eigenvalues and eigenvectors





Logarithmic scale



Darcy pressure equation

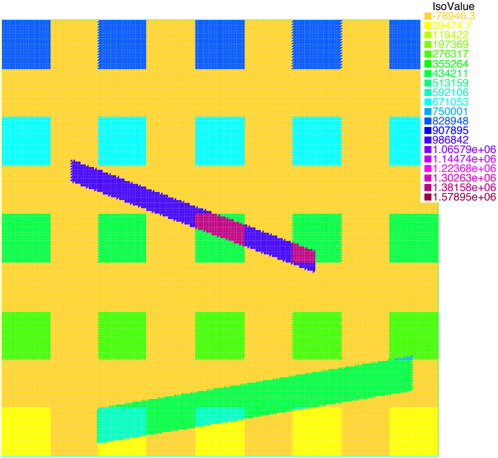
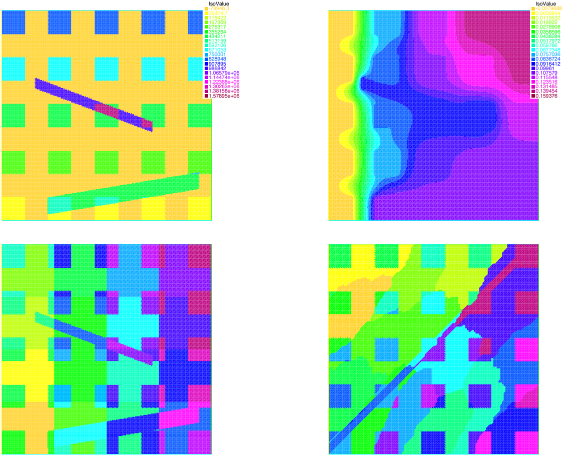


Figure : Two dimensional diffusivity κ



Channels and inclusions : $1 \leq \alpha \leq 1.5 \times 10^6$, the solution and partitionings (Metis or not)

Parallel implementation

PhD of Pierre Jolivet.

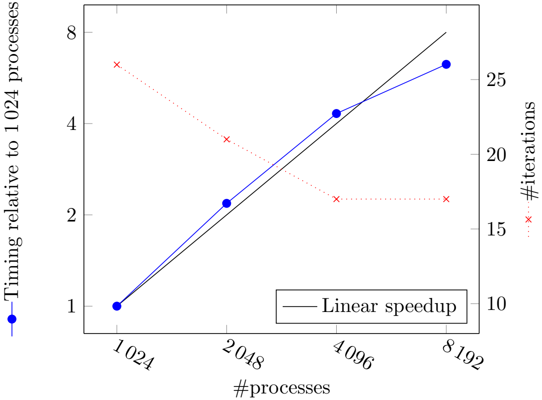
Since version 1.16, bundled with the `Message Passing Interface`. `FreeFem++` is working on the following parallel architectures (among others) :

	N° of cores	Memory	Peak perf
hpc1@LJLL	160@2.00 Ghz	640 Go	$\sim$ 10 TFLOP/s
titane@CEA	12192@2.93 Ghz	37 To	140 TFLOP/s
babel@IDRIS	40960@850 Mhz	20 To	139 TFLOP/s
curie@CEA	92000@2.93 Ghz	315 To	1.6 PFLOP/s

`http://www-hpc.cea.fr`, Bruyères-le-Châtel, France.
`http://www.idris.fr`, Orsay, France.

`http://www.prace-project.eu`.

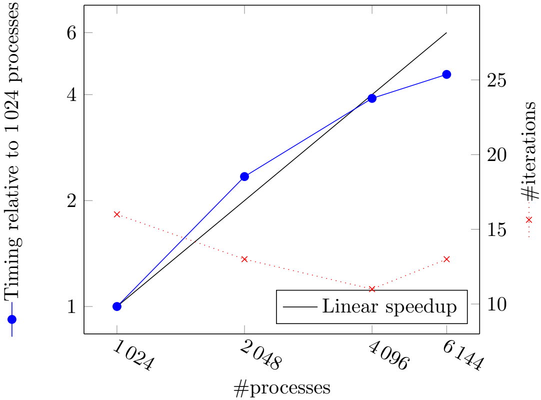
Elasticity problem with heterogeneous coefficients



Speed-up for a 1.2 billion unknowns 2D problem. Direct solvers in the subdomains. Peak performance wall-clock time : 26s.

Strong scalability in three dimensions heterogeneous elasticity

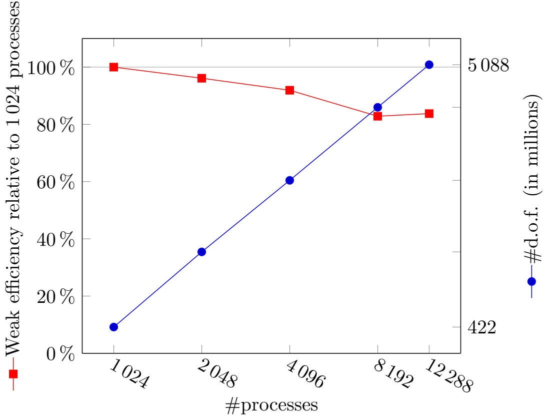
Elasticity problem with heterogeneous coefficients



Speed-up for a 160 million unknowns 3D problem. Direct solvers in subdomains. Peak performance wall-clock time : 36s.

Weak scalability in two dimensions

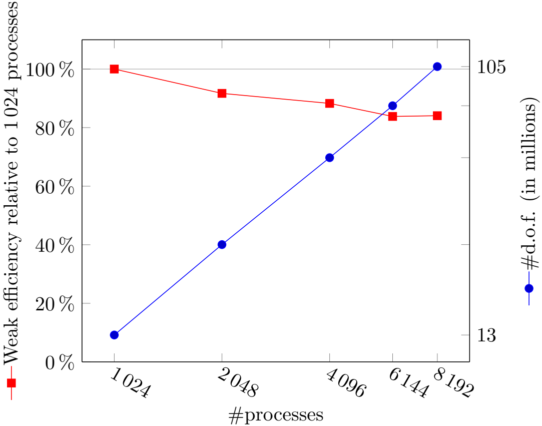
Darcy problems with heterogeneous coefficients



Efficiency for a 2D problem. Direct solvers in the subdomains. Final size : 22 billion unknowns. Wall-clock time : $\simeq$ 200s.

Weak scalability in three dimensions

Darcy problems with heterogeneous coefficients



Efficiency for a 3D problem. Direct solvers in the subdomains. Final size : 2 billion unknowns. Wall-clock time : $\simeq$ 200s.

Outline

1. Introduction
2. Academic Examples
3. A first way to break complexity
4. Schwarz method with overlap
5. An other way to build a 2-level Schwarz with oscilation
6. Future/Conclusion

Conclusion/Future

Freefem++ v3 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

Thank for you attention.

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