A study of the performance of various Linear Solver Packages with ALIEN

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Introduction

- IFP New Energy
  - Technology for energy and environment
  - Reservoir and Bassin modeling
  - CO2 storage
  - Combustion, engine modeling
  - . . .

Outline

- Introduction
- Motivation
  - Industrial and research software context
  - ALIEN motivation
- Alien Framework
  - ALIEN in a nutshell
  - ALIEN : Expressions
  - ALIEN : Linear Solver Packages
  - ALIEN : Performance portability
- A linear solvers performance study with ALIEN
  - Benchmarck description
  - Hardware description
  - Single-node configuration results
  - Multi-node configuration results
  - Multi-Level Domain Decomposition benchmark results
  - Performance portability evaluation results

Outline

Industrial and research software context

Example : CO2 sequestration

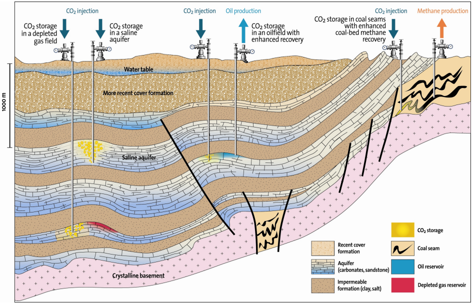


Figure: CO2 storage simulation

Various physical models :

- Bassin modeling ;
- Reservoir modeling ;
- Well modeling ;
- Reactive transport models ;
- Chemistry, Geo-mecanics

Various numerical methods :

- FV/FE methods ;
- Non linear solvers ;
- Coupling/Splitting methods ;
- Space/Time stepping. . .

- Performance is a key feature for industrial software.
- Linear Solvers are involved in many numerical schemes
- Linear Solvers contribute from 30 up to 80 % of computation time

Outline

ALIEN Motivations

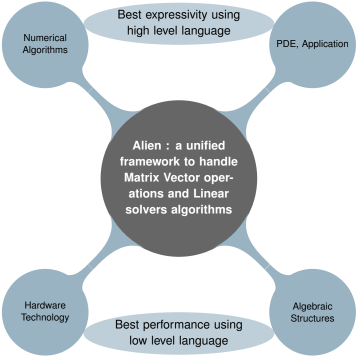
Mutiple issues to manage

Linear solvers, a key component for performance but :

Require to handle various issues :

- Variety of PDE types ;
  - Diffusion, Elasticity, Navier-Stoke, Boundary value problems
- Variety of Numerical Discretisation schemes:
  - FV, FE, DG, VEM,. . .
- Variety of the Linear Solver algorithms:
  - Direct Solvers, Krylov methods,. . .
  - Polynomial, Factorization, AMG, DD,. . .
- Variety of Hardware Architectures:
  - Processors Multi-Cores, Many-Cores,. . .
  - Accelerators GP-GPU, ARM, FGPA,. . .
  - Memory : Distributed, UMA, NUMA, remote-memory

ALIEN Motivations



ALIEN : a unified solutions for various Issues

- PDE, Applications
  - Diffusion, Elasticity, Navier-Stokes, Electromagnetim
- Numerical algorithms
  - Direct, Iterative, Krylov, Factorization, AMG, Multi-level
- Algebraic structures
  - CSR, CSC, Bande, EllPack, Dense,. . .
- Computer science
  - MPI, HPX, OpenMP, TBB, Cuda,. . .

Languages

- PDE models and Numerical algorithms complexity are better treated by a high level language
- Algebraic and computer science complexity perform often better with low level languages

ALIEN Motivations

Mutiple issues to manage

Various types of applications and PDEs

- Diffusion equation
- Linear Elasticity equations
- Navier-Stoke equations
- Boundary value equations

Various types of discretisation schemes

- FD, FV, FE, DG,. . .

Leading to various linear system types:

- Symmetric, Non symmetric;
- Definite positive, Non positive;
- Saddle point systems
- Sparse, Dense
- Structured, Unstructured

Various Numerical Algorithms

- Direct, Iterative
- Polynomial
- Factorisation
- Approximate Inverse
- Algebraic Multi Grid
- Multi-Level, Domain Decomposition

ALIEN Motivations

Mutiple issues to manage

Various types of Matrix Format

- Dense
- CSR, CSP
- Bande
- EllPack, Block Ellpack

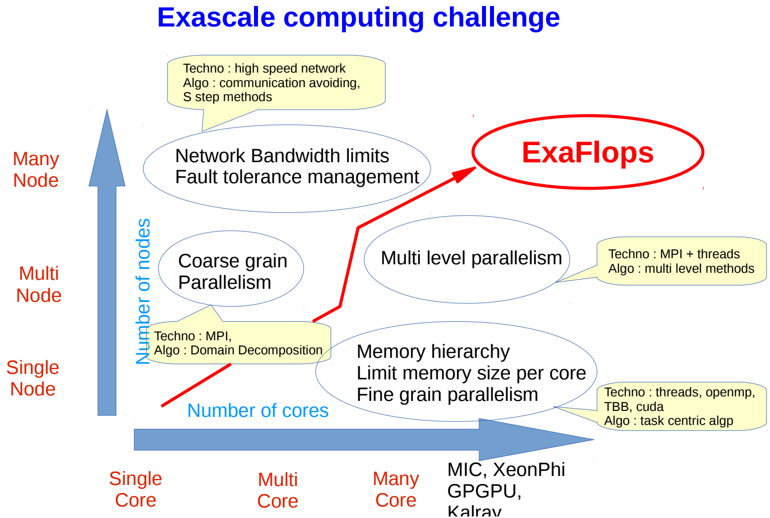
Various Hardware technology

- Memory level:
  - Distributed (MPI, HPX)
  - Shared memory (Numa, UMA)
- Execution level:
  - OpenMP, TBB, Posix threads
  - Cuda, OpenCL
  - SIMD (AVX2, AVX512)

Performance

- Adequation between:
  - Hardware features
  - Algebraic structure formats
  - Algorithms

Motivation : new challenges in the exascale road map



ALIEN a generic framework for linear solver packages

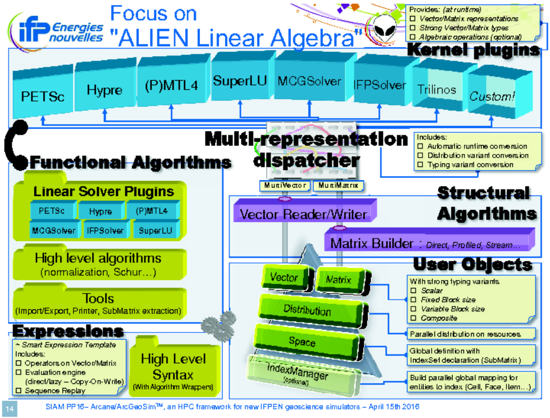


Figure: ALIEN a generic framework for linear solver package

Outline

ALIEN in a nutshell

ALIEN : Matrix Vectors handlers

Matrix Handlers

Listing 1: Matrices

```
const Alien::Space s(10,"MySpace");
Alien::MatrixDistribution
mdist(s, s, Environment::parallelMng());
Alien::Matrix A(mdist);

auto tag = Alien::DirectMatrixOptions::eResetValues;
{
  Alien::DirectMatrixBuilder builder(A, tag);
  builder.reserve(30) ;
  builder.allocate();
  for(Integer row=0;row<vdist.localSize();++i) {
    builder(row,row) = 2.;
    if(row+1<10)
      builder(row,row+1) = -1.;
    if(row-1>=0)
      builder(row,row-1) = -1.;
  }
}
```

ALIEN in a nutshell

ALIEN : Matrix Vectors handlers

Vector Handlers

Listing 2: Vectors

```
const Alien::Space s(10,"MySpace");
Alien::VectorDistribution
vdist(s, Environment::parallelMng());
Alien::Vector x(vdist);
{
  Alien::LocalVectorWriter writer(x);
  for(Integer i=0;i<10;++i)
    writer[i] = 1.;
}
```

Outline

ALIEN : Expressions

Matrix Vector expressions

Expressions

Listing 3: ALIEN expressions

```
const Alien::Space s(10,"MySpace");
Alien::MatrixDistribution mdist(s, s, Environment::parallelMng());
Alien::VectorDistribution vdist(s, Environment::parallelMng());
Alien::Matrix A(mdist);
Alien::Vector x(vdist);
Alien::Vector y(vdist);
Alien::Vector r(vdist);
Alien::Real lambda = 0.5 ;

auto solver = createSolver(/* ...*/) ;
solver->solve(A,x,y);

r = y-A*x ;
y = y+(lambda*r) ;
y = A*(lambda*x) ;
```

Outline

ALIEN : Linear Solver Packages

Linear Solver Package Descriptions

Packages	PETSc	Trilinos	HPDDM	IFPS	HTS
Language	C	C++	C++	Fortran	C++
MPI Threads AVX512 Cuda	yes OpenMP yes	yes OpenMP TBB, Posix yes yes	yes OpenMP	yes	yes OpenMP TBB, Posix yes
Direct Solver	SuperLU MUMPS	KLU2	MUMPS		SuperLU MUMPS
Krylov	CG,BiCG GEMRES	CG,BiCG GMRES	CG GMRES	BiCG	BiCG
Poly		Chebyshev			Chebyshev Neumann
Relaxation	Jacobi	GS,SymGS			
ILU	ILU(k,t)	ILU(k,t)		ILU0	ILU0,ILU0PF
AMG	BoomerAMG AMGX	MueLU AMGX		BoomerAMG	BoomerAMG
DD	HPDDM		HPDDM		DDML

Outline

Performance portability issues in Linear solver packages

High level abstractions fot Performance Portability

Unifed tools to handle parallelism, to manage memory and to write portable parallel algorithms:

Abstractions to describe Hardware

- a MemorySpace model
  - Single/Multi Node
  - LocalHost memory
  - Remote memory
- a ExecutionSpace model
  - Serial/Multi-threads
  - OpenMP, Posix, TBB,. . .
  - Cuda, OpenCL

Abstractions to write generic parallel algorirhms

- Parallel Loop concepts
- Generic Parallel Collections
- Task programming, Lambda functions
- Dispatch mechanism

Performance portability issues in Linear solver packages

Performance Portability Layer

Examples of packages managing Performance Portability issues:

Trilinos

- Kokkos:
  - MemorySpace, ExecutionSpace model
  - Array abstractions
  - parallel_for algorithms
- TPetra:
  - Structures based on Kokkos
  - generic parallel algorithms

HTS

- HARTS
  - MemorySpace, ExecutionSpace model
  - Task based algorithms
- MCKernel Algebra
  - Generic parallel Blas1,2 implementation
  - tools to write parallel algorithms

Outline

Benchmark problem

- Heterogeneous Diffusive problem:

Find $u(\mathbf{x})$ $\mathbf{x} \in \Omega$

$$\begin{cases} v = -\kappa \nabla u & \text{in } \Omega, \\ \nabla \cdot (-\kappa \nabla u) = f & \text{in } \Omega, \\ u = g & \text{on } \partial\Omega_d, \\ \partial_n u = f & \text{on } \partial\Omega_n, \end{cases}$$

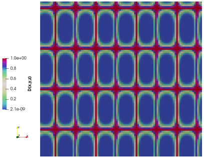


Figure: Heterogeneous Diffusive Tensor

with :

$$\kappa(x,y,z) = \kappa_0 e^{-\frac{\alpha}{2}(1+sin(2\pi\frac{x}{L_x})(1+sin(2\pi\frac{y}{L_y}))}$$

Benchmark problem

Saddle point problem

- Saddle point problem:
  Find $u, p(\mathbf{x})$ $\mathbf{x} \in \Omega$

$$\begin{cases} \alpha\nabla^2\mathbf{u} + \nabla p = f & \text{in } \Omega \\ \nabla\cdot\mathbf{u} = 0 & \text{in } \Omega \\ \mathbf{u} = \mathbf{g} & \text{on } \partial\Omega_d, \\ \partial_n\mathbf{u} = \mathbf{h} & \text{on } \partial\Omega_n, \end{cases}$$

  leading to a symmetric indefinite matrix :

$$A = \begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}. \qquad (1)$$

  with $A \in \mathbb{R}^{nxn}$ definite on the kernel of $B \in \mathbb{R}^{mxn}$ $m < n$

Outline

Benchmarcks :

- on a cluster ENER440
  - 240 dual-socket Nodes with Intel Skylake G-6140 processors at 2.3 GHz. (18 cores per socket)
  - GP-GPU NVidia P100 (16 Go)
- BiCGS : 10^{-6} tolerance parameter;
- Preconditioner :
  - ILU0
  - AMG
  - DDML
- Hardware configurations :
  - full mpi (MPI);
  - full thread (TH)
  - hybrid Mpi + OpenMP :
    - (MPIX 2p16th) with 1 MPI processus for 1 socket and 16 threads;
    - (MPIX 1p32th) with 1 MPI processus for 2 sockets and 32 threads;
  - hybrid MPI + Cuda

Outline

Benchmark MPI configuration on a single node

Performance results

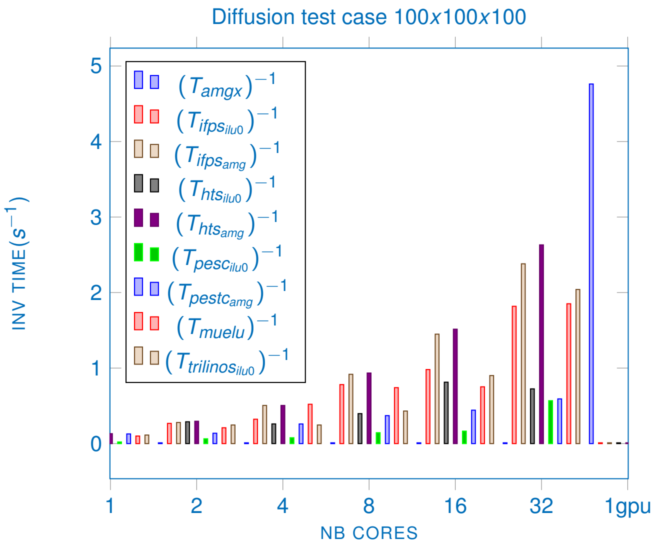


Figure: BICGS: 100x100x100 test case

Benchmark Threads/Cuda configuration on a single node

Performance results

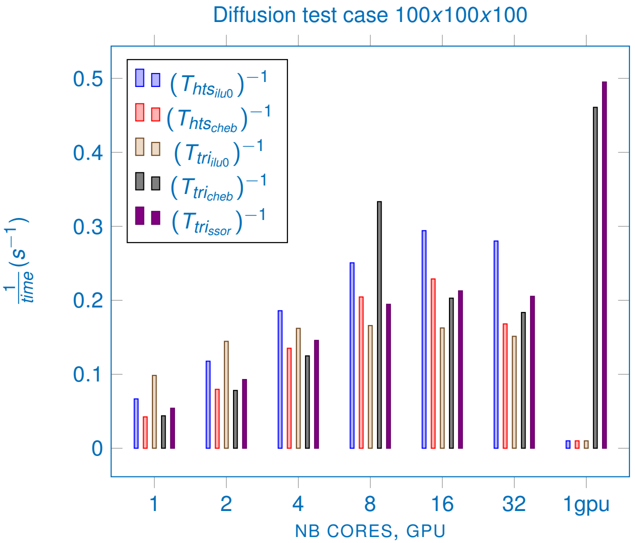


Figure: BICGS: 100x100x100 test case, OpenMP, GPU

Benchmark on a single node Node

Preconditioner results analysis

- ILU, Polynomial and Gauss-Seidel preconditioners:

Package	IFPS	HTS	HTS	PETSC	TRI	TRI	TRI
Precond	ILU0	ILU0	Cheb	ILU0	ILU0	Cheb	SSOR
Nb iter	203	203	500-600	400-700	205	400	400-700
Exec time	0.55	1.38	5.45	1.76	0.49	5.45	4.87

- Algebraic Multi Grid preconditioners :

AMG	BoomerAMG	MueLU	AMGX
Coarsening Algo	PMIS		Aggregation
Coarsening Level	25	25	24
Smoothing	GS	SymGS	Jacobi
relax factor		0.9	0.9
Cycle	V	W	W
Nb iter	3	4-6-8-10	4
Exec time	0.38	0.54	0.21

-

Outline

Benchmark results on Multi-Nodes configuration

Performance results

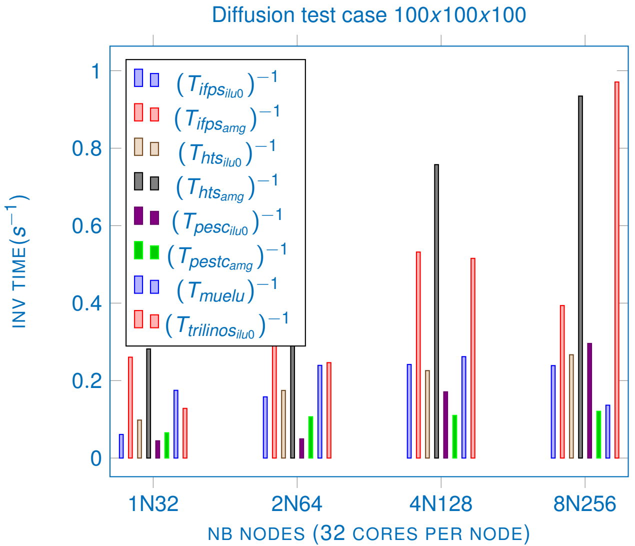


Figure: BICGS: 200x200x200 test case on 1,2,4 and 8 Nodes 32 cores per node

Outline

Benchmark Multi-Level Decomposition Domain methods

Performance results

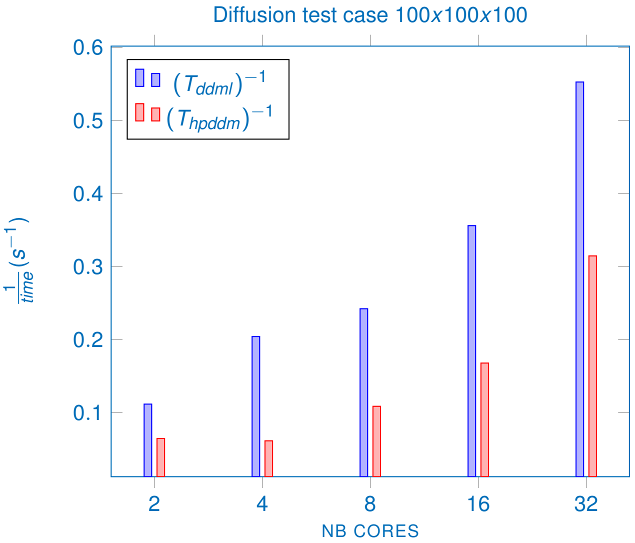


Figure: BICGS: 100x100x100 test case, DD benchmark

Multi-Level Domain Decomposition Benchmark on a single node Node

DDML results analysis

DD Algo	HTS-DDML	HPDDM
Level	2	2
EigenSolver	SpectraLib	Arpack
Nb subdomains	256	MPI_COMM_SIZE
LocalSolver	Mumps	Mumps
CoarseSolver	SuperLU	Mumps
Nb Eigenvalues	4	8
Nb iter	21	34
Exec time	1.44	3.20
SetUp Time	0.98	4.09

Outline

Performance portability evaluation

Performance portability of the Chebychev and SSOR preconditioners

A unique code addressing variours Hardware configurations:

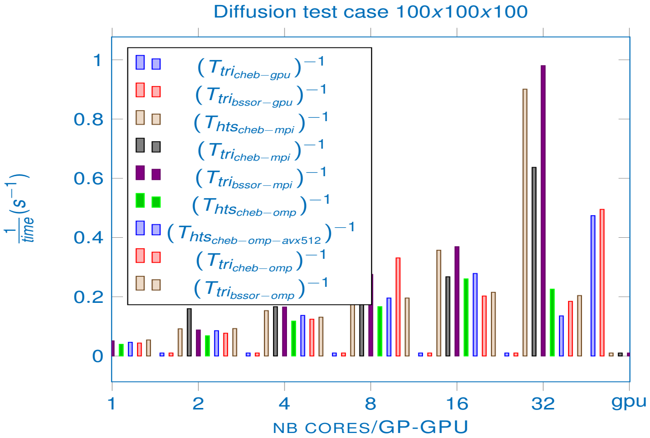


Figure: BICGS: 100x100x100 test case, Chebychev, SSOR MPI, OpenMP, AVX512 and GPU configuration

Benchmark MPI configuration within 1 Node

Performance Portability results analysis

Preconditioner	Cheb-HTS	Cheb-Trilinos	SSOR-Trilinos
ExecSpace	MPI/OpenMP/SIMD	MPI/OpenMP/Cuda	MPI/OpenMP/Cuda
Nb iter	577/584/531	649/528/581	519/523/600
Exec time	2.80/3.84/3.59	3.74/4.94/2.11	2.71/4.65/2.02

- Thank you for attention
- Questions?

References

- ALIEN : https://gitlab.ifpen.fr/Arcane/alien
- Trilinos : https://trilinos.github.io/
- Kokkos : https://github.com/kokkos/kokkos
- PETSc : https://www.mcs.anl.gov/petsc/
- HTSSolver : http://gitlab.ifpen.fr/R1140/hartssolver
- HPDDM : https://github.com/hpddm/hpddm
- HARTS : http://gitlab.ifpen.fr/R1140/harts
  Thèse d'Adrien ROUSSEL : http://www.theses.fr/2018GREAM010