Integral Operator Spectral Computations using PETSc/SLEPc libraries

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Outline

- The Integral Problem
- Approximation and Discretization
- Iterative Refimement
- Multipower Double Iteration
- Implementation Using PETSc and SLEPc.
- Numerical tests
- Conclusions

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Use of Parallel Libraries

- Illustrate
  - Advantages of parallel libraries
  - to support programming mathematical models
- Model
  - Integral operator on a very large interval
  - Radiative transfer in stellar atmospheres
  - Spectral computations ↔ eigenvalues of matrix discretizations

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The Integral Problem

- Radiative transfer in stellar atmospheres $Tx - x = f$,
- $T : X \rightarrow X$, where $X = L^1\left([0, t^\star]\right)$

$$(Tx)(t) = \frac{\varpi}{2}\int_0^{t^\star}\left(\int_1^{\infty}\frac{\exp(-|t-t'|\mu)}{\mu}d\mu\right)x(t')dt', \quad t \in [0, t^\star].$$

- $t^\star$ is the optical depth of the stellar atmosphere
- $\varpi \in \,]0, 1[$ is the albedo
- T has a singularity at the origin ($t = 0$).

Here we will compute the spectral elements (eigenvalues and eigenfunctions) of the operator T.

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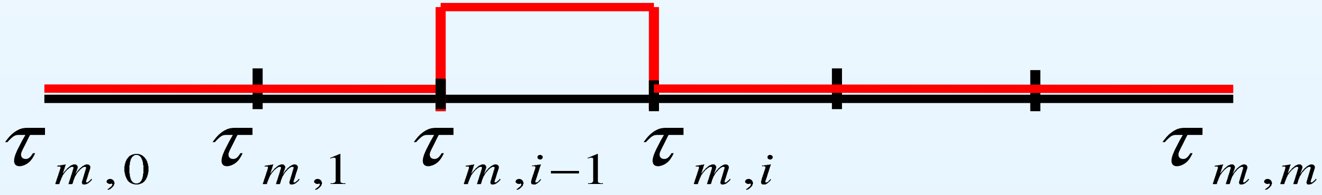
Approximation and Discretization

- Mathematical models for Scientific and Engineering problems need to be discretized for computational purposes into large dimensional matrices
- because either they do not have an analytic solution or it is too much complicated to deal with.

- The problem $T\varphi = \lambda\varphi$ defined in a infinite dimentional space X
- is approximated by $T_m\varphi_m = \lambda_m\varphi_m$ in X_m,
- m large enough.



Iterative Refimement

- To solve the approximating problem $T_m \varphi_m = \lambda_m \varphi_m$ in X_m.
- without solving $A_m x_m = \lambda_m x_m$,
- we use an iterative refinement strategy
- to improve the eigenvalues and vectors of a moderate size matrix A_n corresponding to a descretization in $X_n, n << m$.
- The refinement formula uses mainly matrix-vector multiplications with
- $A_m (m \times m)$ representing T in a very fine discretization space X_m.
- Large matrices are built and stored in a distributed manner among the processors,
- The iterative refinement provides accurate eigenpairs corresponding to a larger problem.

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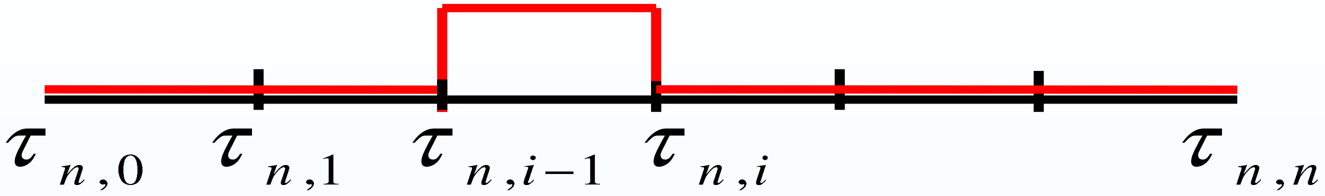

- The existence of the operator T linking the subspaces X_m and X_n allows the derivation of formulae to extend or restrict vectors from one of the finite dimensional subspaces to the other.
- The extension procedure will be denoted by E and the restriction by R

Initializations

- Given matrices A_n and A_m of dimensions n an m
- compute eigenpair of A_n (eigenvalue λ and eigenvector u) not necessarily the dominant, computed for instance Arnoldi's method
- The left eigenvector of A_n, say v, will be used as a normalization factor.

The procedure S returns y, given a vector w

- Solve the $(n+1) \times n$ linear system

$$\begin{cases} (A_n - \lambda I)t = Rw - (v^T R(w))u \\ v^T t = 0 \end{cases}$$

- compute the extension $y = E(A_n t)/\lambda$.

Multipower Double Iteration

Algorithm:

```
1. Compute the eigenpair of $A_n$ to be refined: $\lambda$, $u$
   and the left eigenvector $v$.
2. Extend eigenvalue: $x = E(u)$;
3. Compute the residual: $residual = norm(A_m x - \lambda x)$
4. While $residual$ less or equal a given tolerance
   (a) for j=1,2,...,$itpower$
         i. $\mu = v^T R(A_m x)$
        ii. $x = A_m x / \mu$
   (b) $w = A_m x - \mu x$
   (c) Update refined eigenvector: $x = x - S(w)$
   (d) compute the new residual: $residual = norm(A_m x - \lambda x)$
```

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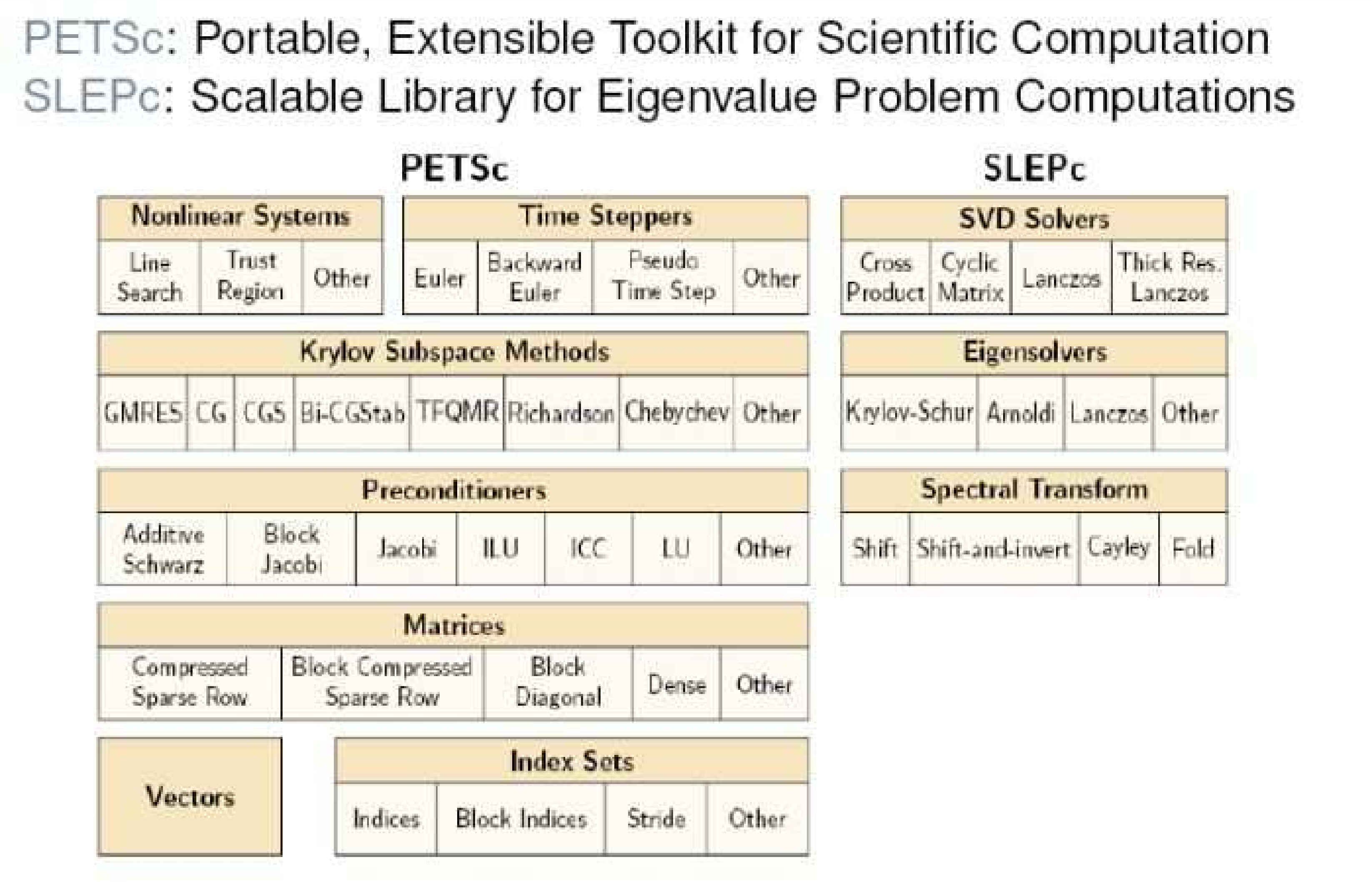
PETSc/SLEPc



PETSc: Portable, Extensible Toolkit for Scientific Computation

SLEPc: Scalable Library for Eigenvalue Problem Computations

PETSc

Nonlinear Systems		
Line Search	Trust Region	Other

Time Steppers			
Euler	Backward Euler	Pseudo Time Step	Other

Krylov Subspace Methods							
GMRES	CG	CGS	Bi-CGStab	TFQMR	Richardson	Chebychev	Other

Preconditioners						
Additive Schwarz	Block Jacobi	Jacobi	ILU	ICC	LU	Other

Matrices				
Compressed Sparse Row	Block Compressed Sparse Row	Block Diagonal	Dense	Other

Vectors

Index Sets			
Indices	Block Indices	Stride	Other

SLEPc

SVD Solvers			
Cross Product	Cyclic Matrix	Lanczos	Thick Res. Lanczos

Eigensolvers			
Krylov-Schur	Arnoldi	Lanczos	Other

Spectral Transform			
Shift	Shift-and-invert	Cayley	Fold

Libraries and the Algorithm

- Computation of initial approximations: eigenvalue and the corresponding right and left eigenvectors of matrix A_n
  - carried out only once with SLEPc, for instance with Arnoldi eigensolver
- Matrix-vector products with matrices A_n and A_m (also used in the restriction and extension from one grid to the other),
  - computed in a distributed way, are performed in PETSc with MatMult operation ; (all matrices are sparse and distributed)

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Libraries and the Algorithm (cont)

- Vector operations,
  inner product, norm, addition and scaling,
  - are performed with the VecNorm, VecAXPY and VecScale routines from PETSc.
- Solution of linear systems (involved in procedure S)
  - are also carried out in PETSc.
  - Either by an LU decomposition of dimension $(n+1) \times n$ with partial pivoting.
    (This requires a modification of the corresponding routine in PETSC).
  - or by an iterative solver.

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Libraries and the Algorithm (cont)

- Iterative solver.
  We use GMRES applied to $A_n - \lambda_n I$.
  - In order to get t satisfying $v^T t = 0$, we apply $I - uv^T$ to all Krylov vectors built by GMRES.
    (An implementation of the above scheme requires a modification of GMRES)
    - $(A_n - \lambda I)q$, the candidate vector to be added to the basis, is pre-multiplied by the projector $I - uv^T$.
    - Instead of $I - uv^T$, we consider the projector $I - vv^T$, since it can be implemented very easily in PETSc with function KSPSetNullSpace and it also guarantees $v^T t = 0$.
- PETSc provides many other iterative linear solvers and some preconditioners to improve the convergence .

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Computer System Used

Odin cluster, located at Universidad Politécnica de Valencia.

- 55 dual-processor nodes
- 2.8 GHz Pentium Xeon processors , 1 GB of memory per node.
- interconnected with a high-speed SCI network with 2-D torus topology
- only one processor per node was used in the tests.

Numerical Tests

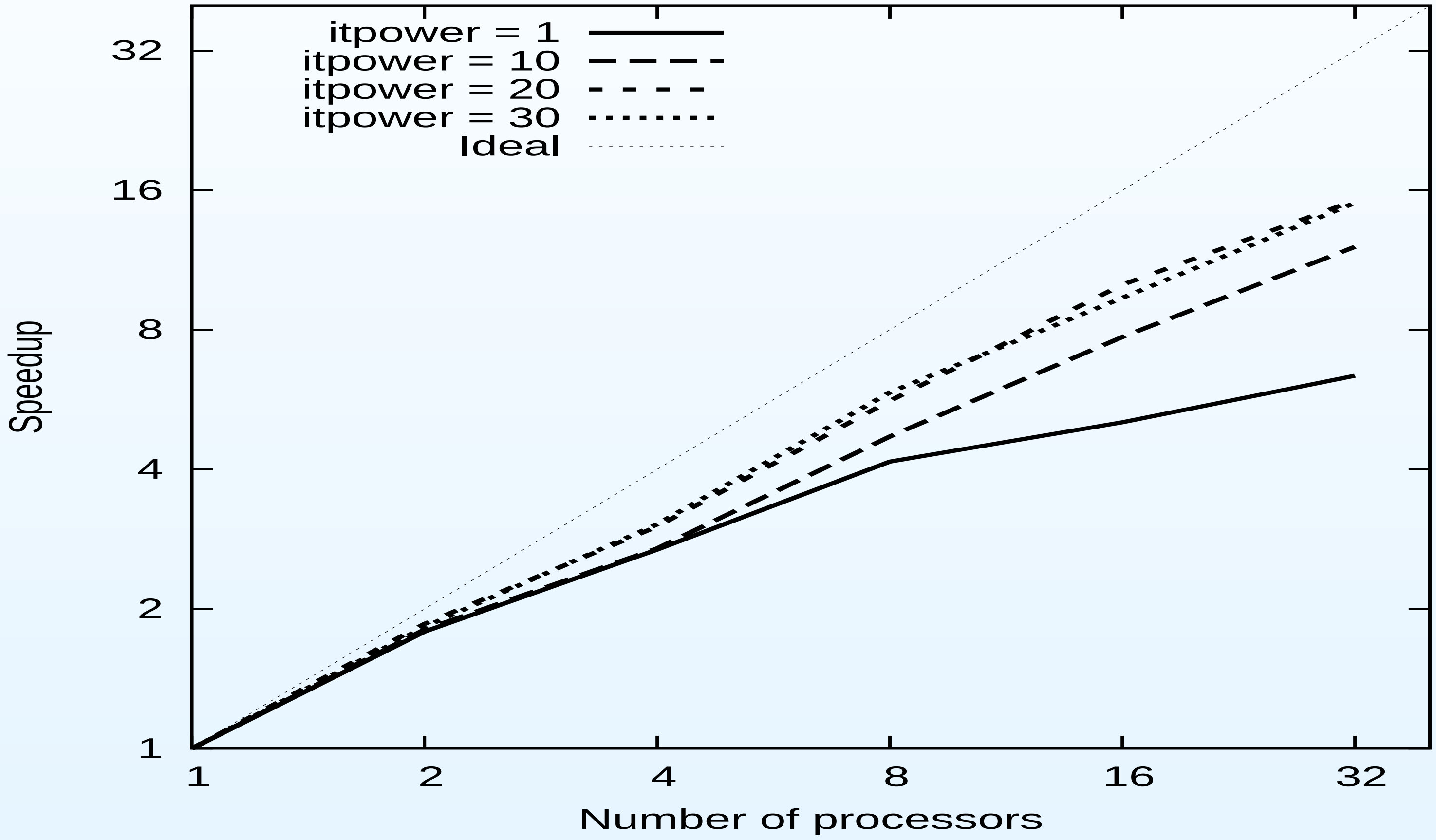
Performance analysis of the algorithm.

Several tests varying the number of processors and the algorithmic choices:

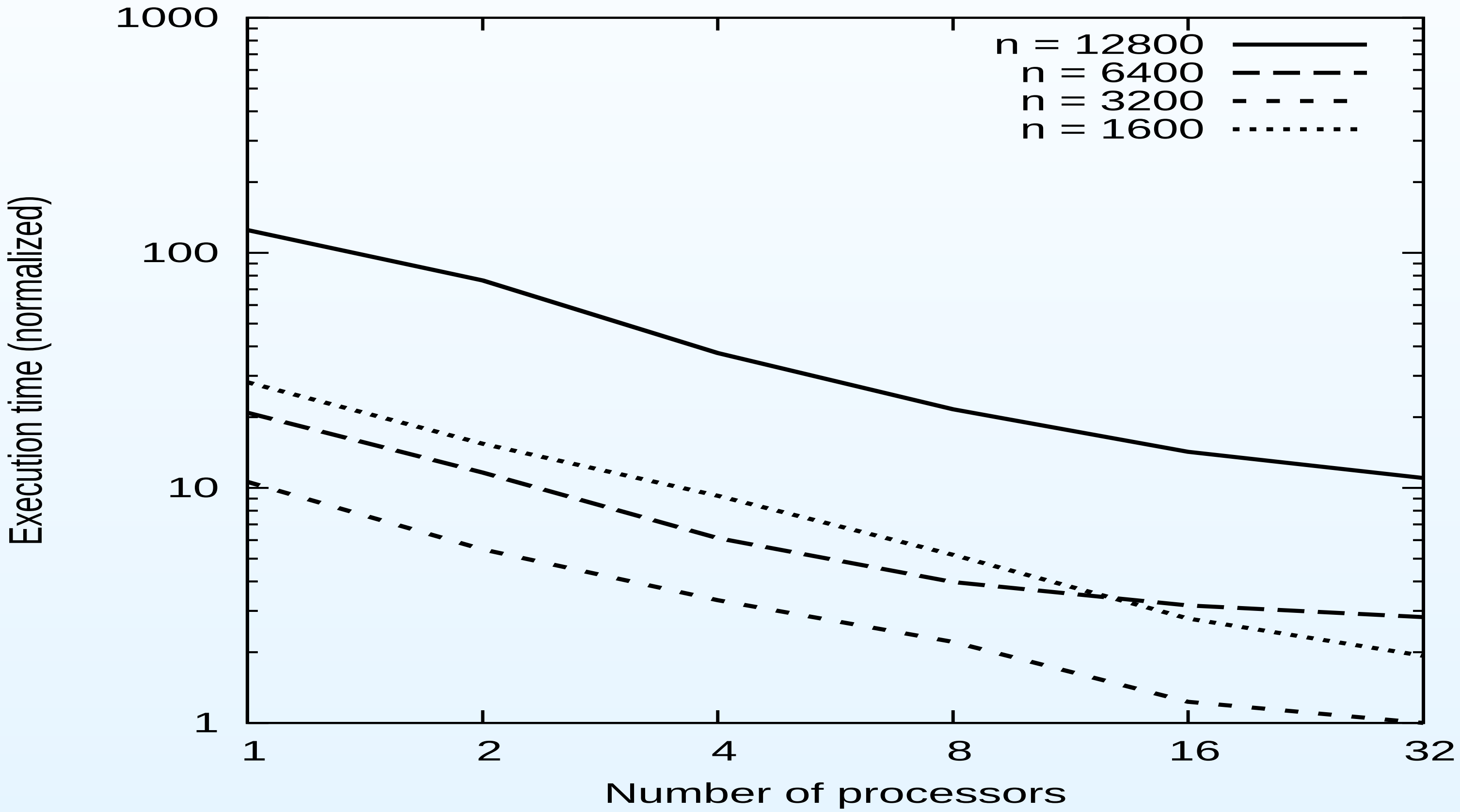
- influence of parameter $itpower$ (number of power iterations inside the refinement formula)
- influence of the dimension of initial problem
- effect of different preconditioners.

A tolerance of 10^{-12} on the residual

Speedup with different values of itpower



Times for a refined solution $m = 64000$, with several values of n



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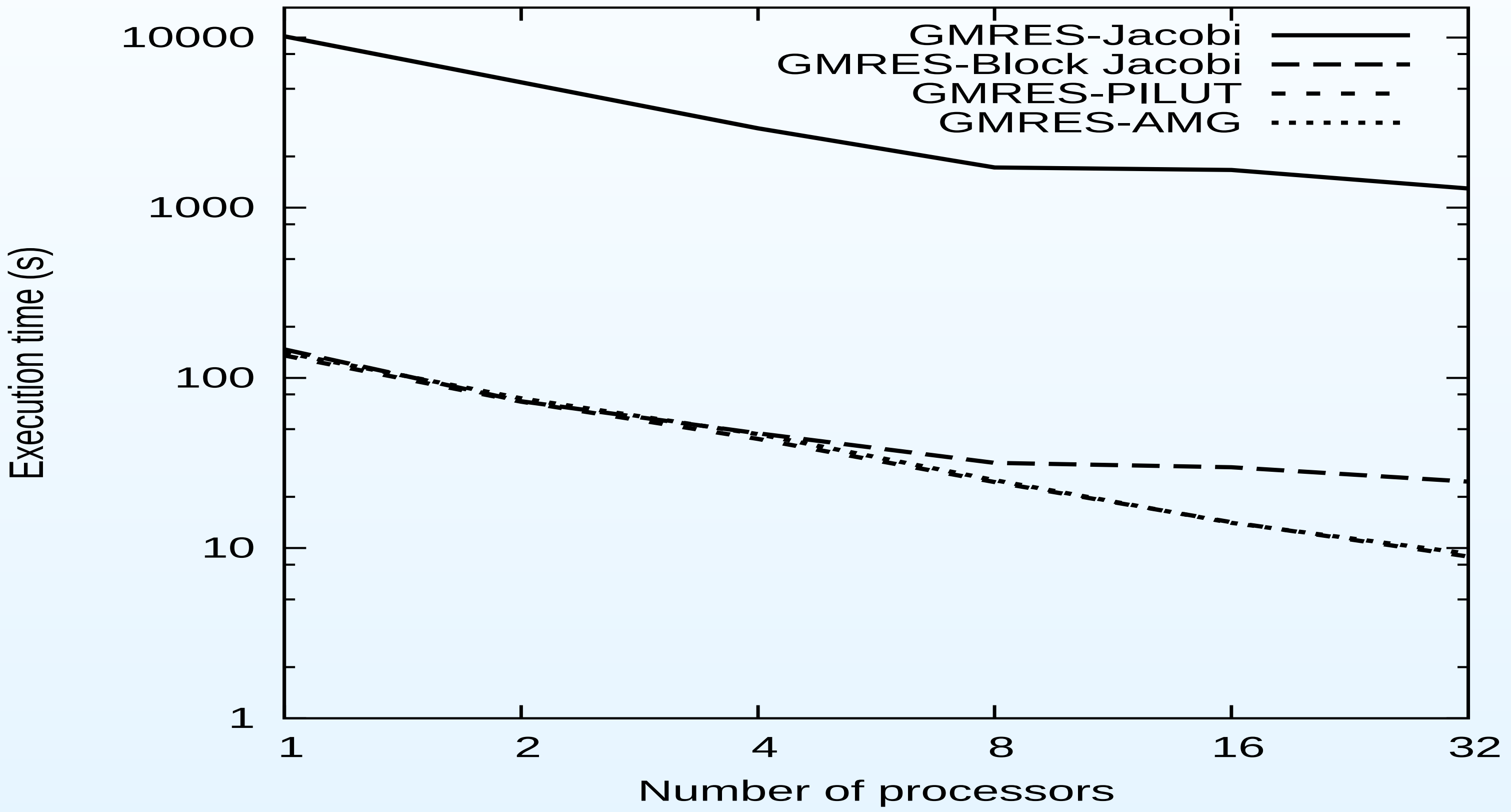
Several preconditioners to accelerate GMRES



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Conclusions

- We presented a parallel code for the Multipower Defect Correction Method
  - refines eigenvalues/eigenfunctions from rough approximations
  - is effective for the computation of specific eigenvalues
- An implementation using libraries PETSc/SLEPc
  - shows good behaviour on a distributed parallel environment

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